



## Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 08:56 AM UTC

PDB ID : 7O7Y / pdb\_00007o7y  
EMDB ID : EMD-12756  
Title : Rabbit 80S ribosome stalled close to the mutated SARS-CoV-2 slippery site  
by a pseudoknot (high resolution)  
Authors : Bhatt, P.R.; Scaiola, A.; Leibundgut, M.A.; Atkins, J.F.; Ban, N.  
Deposited on : 2021-04-14  
Resolution : 2.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

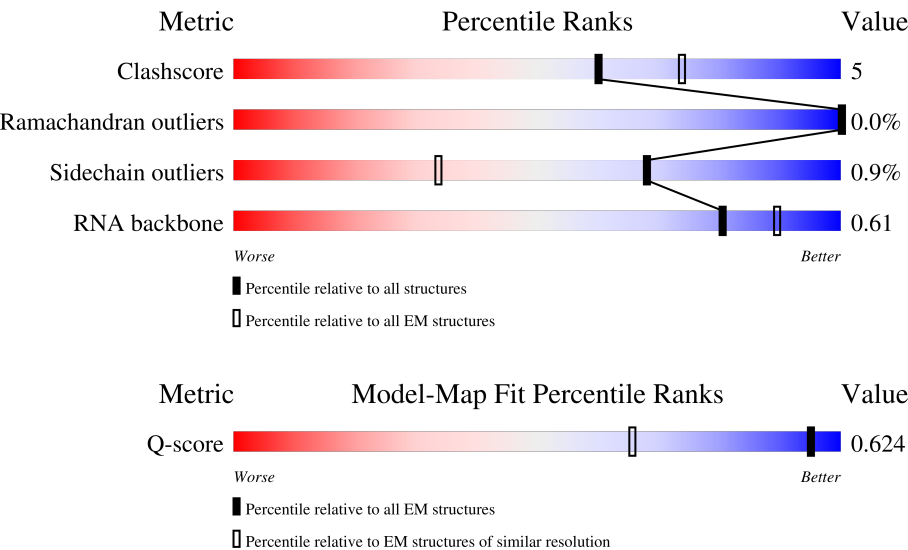
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3184 ( 1.71 - 2.70 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A2	1870	
2	AA	84	
3	AB	69	

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Mol	Chain	Length	Quality of chain
4	AC	156	
5	AD	133	
6	AE	115	
7	AF	317	
8	AG	56	
9	AH	217	
10	AI	76	
11	AT	76	
12	AZ	295	
13	Aa	264	
14	Ab	293	
15	Ac	281	
16	Ad	263	
17	Ae	204	
18	Af	249	
19	Ag	432	
20	Ah	208	
21	Ai	194	
22	Aj	165	
23	Ak	158	
24	Al	132	
25	Am	151	
26	An	151	
27	Ao	145	
28	Ap	172	





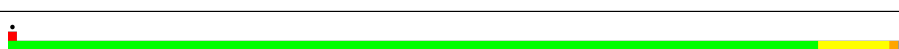
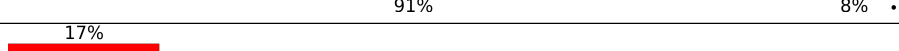

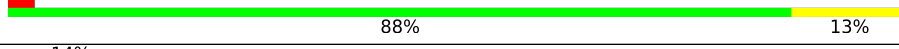



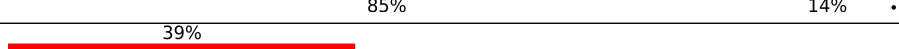



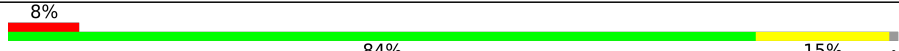

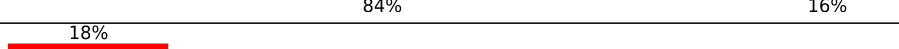
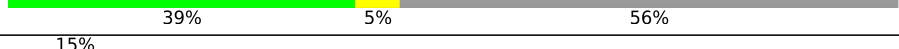


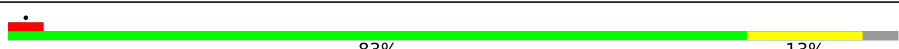

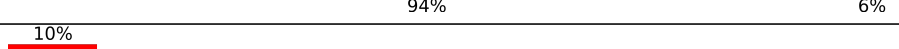
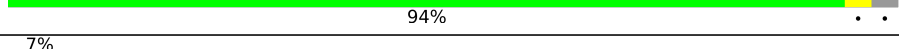
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Mol	Chain	Length	Quality of chain
29	Aq	135	
30	Ar	152	
31	As	145	
32	At	119	
33	Au	83	
34	Av	130	
35	Aw	143	
36	Ax	130	
37	Ay	124	
38	Az	25	
39	B5	4808	
40	B7	120	
41	B8	158	
42	BA	257	
43	BB	403	
44	BC	413	
45	BD	297	
46	BE	291	
47	BF	247	
48	BG	266	
49	BH	192	
50	BI	214	
51	BJ	178	
52	BK	1071	
53	BL	211	

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Mol	Chain	Length	Quality of chain
54	BM	218	
55	BN	204	
56	BO	203	
57	BP	184	
58	BQ	188	
59	BR	196	
60	BS	176	
61	BT	160	
62	BU	128	
63	BV	140	
64	BW	157	
65	BX	156	
66	BY	145	
67	BZ	136	
68	Ba	148	
69	Bb	245	
70	Bc	115	
71	Bd	125	
72	Be	135	
73	Bf	110	
74	Bg	117	
75	Bh	123	
76	Bi	105	
77	Bj	97	
78	Bk	70	

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Mol	Chain	Length	Quality of chain
79	Bl	51	
80	Bm	128	
81	Bo	106	
82	Bp	92	
83	Br	137	
84	Bs	318	
85	Bt	165	
86	Bv	217	

## 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 237077 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A2	1770	Total	C	N	O	P	0	0
			37833	16911	6781	12371	1770		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A2	1249	B8N	C	conflict	GB GBCT01000564.1
A2	1338	4AC	C	conflict	GB GBCT01000564.1
A2	1843	4AC	C	conflict	GB GBCT01000564.1

- Molecule 2 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AA	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 3 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	63	Total	C	N	O	S	0	0
			495	302	98	93	2		

- Molecule 4 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	74	Total	C	N	O	S	0	0
			610	385	117	101	7		

- Molecule 5 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 6 is a protein called Ribosomal protein eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 7 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 8 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 9 is a RNA chain called mRNA containing SARS-CoV-2 sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	8	Total	C	N	O	P	0	1
			128	55	16	50	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AH	3466	U	A	conflict	GB NC_045512.2
AH	3468	A	C	conflict	GB NC_045512.2

- Molecule 10 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AI	76	Total	C	N	O	P	0	0
			939	393	11	459	76		

- Molecule 11 is a RNA chain called P-site Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AT	76	Total	C	N	O	P	0	0
			1652	746	294	536	76		

- Molecule 12 is a protein called 40S ribosomal protein SA.



Mol	Chain	Residues	Atoms					AltConf	Trace
12	AZ	221	Total	C	N	O	S	0	0
			1743	1107	305	323	8		

- Molecule 13 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Aa	224	Total	C	N	O	S	0	0
			1815	1152	328	321	14		

- Molecule 14 is a protein called Ribosomal protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Ab	220	Total	C	N	O	S	0	0
			1706	1105	292	300	9		

- Molecule 15 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ac	225	Total	C	N	O	S	0	0
			1751	1116	315	313	7		

- Molecule 16 is a protein called Ribosomal protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ad	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

- Molecule 17 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Ae	191	Total	C	N	O	S	0	0
			1509	943	286	273	7		

- Molecule 18 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Af	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 19 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Ag	190	Total	C	N	O	S	0	0
			1529	975	281	272	1		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Ah	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ah	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 21 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Ai	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 22 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Aj	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 23 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Ak	154	Total	C	N	O	S	0	0
			1262	804	236	216	6		

- Molecule 24 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Al	124	Total	C	N	O	S	0	0
			958	600	170	179	9		

- Molecule 25 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Am	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 26 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	An	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 27 is a protein called 40S ribosomal protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Ao	128	Total	C	N	O	S	0	0
			1048	665	197	179	7		

- Molecule 28 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ap	141	Total	C	N	O	S	0	0
			1124	715	212	194	3		

- Molecule 29 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Aq	134	Total	C	N	O	S	0	0
			1080	678	201	197	4		

- Molecule 30 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ar	148	Total	C	N	O	S	0	0
			1217	763	245	208	1		

- Molecule 31 is a protein called Ribosomal protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	As	143	Total	C	N	O	S	0	0
			1113	698	214	198	3		

- Molecule 32 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	At	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 33 is a protein called Ribosomal protein eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Au	83	Total	C	N	O	S	0	0
			640	394	117	124	5		

- Molecule 34 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Av	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 35 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Aw	141	Total	C	N	O	S	0	0
			1099	693	219	184	3		

- Molecule 36 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Ax	125	Total	C	N	O	S	0	0
			1015	642	199	169	5		

- Molecule 37 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ay	85	Total	C	N	O	S	0	0
			683	439	128	115	1		

- Molecule 38 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Az	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 39 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B5	3764	Total	C	N	O	P	0	0
			80772	36003	14762	26243	3764		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	3550	UY1	U	conflict	GB GBCN01009604.1

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B7	120	Total	C	N	O	P	0	0
			2570	1141	456	851	122		

- Molecule 41 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	B8	156	Total	C	N	O	P	0	0
			3319	1481	585	1097	156		

- Molecule 42 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BA	253	Total	C	N	O	S	0	0
			1940	1214	396	324	6		

- Molecule 43 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BB	398	Total	C	N	O	S	0	0
			3206	2042	605	546	13		

- Molecule 44 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BC	362	Total	C	N	O	S	0	0
			2886	1814	577	481	14		

- Molecule 45 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BD	294	Total	C	N	O	S	0	0
			2398	1516	439	429	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BD	2	AAC	GLY	conflict	UNP G1SYJ6

- Molecule 46 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BE	243	Total	C	N	O	S	0	0
			1960	1258	378	321	3		

- Molecule 47 is a protein called Ribosomal Protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BF	226	Total	C	N	O	S	0	0
			1886	1211	362	304	9		

- Molecule 48 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BG	233	Total	C	N	O	S	0	0
			1877	1197	361	315	4		

- Molecule 49 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BH	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 50 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BI	213	Total	C	N	O	S	0	0
			1717	1086	332	285	14		

- Molecule 51 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 52 is a protein called Replicase polyprotein 1ab.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BK	35	Total	C	N	O	S	0	0
			265	163	45	51	6		

- Molecule 53 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BL	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 54 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BM	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 55 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 56 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BO	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 57 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BP	159	Total	C	N	O	S	0	0
			1289	809	249	222	9		

- Molecule 58 is a protein called Ribosomal Protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BQ	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 59 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BR	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 60 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	BS	176	Total	C	N	O	S	0	0
			1457	924	288	234	11		

- Molecule 61 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	BT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 62 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	BU	99	Total	C	N	O	S	0	0
			806	516	141	147	2		

- Molecule 63 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	BV	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 64 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	BW	121	Total	C	N	O	S	0	0
			991	619	202	166	4		

- Molecule 65 is a protein called uL23.



Mol	Chain	Residues	Atoms					AltConf	Trace
65	BX	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 66 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	BY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 67 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	BZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 68 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Ba	147	Total	C	N	O	S	0	0
			1163	734	239	186	4		

- Molecule 69 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Bb	108	Total	C	N	O	S	0	0
			881	548	196	134	3		

- Molecule 70 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Bc	108	Total	C	N	O	S	0	0
			836	530	148	151	7		

- Molecule 71 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Bd	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 72 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Be	130	Total	C	N	O	S	0	0
			1070	676	221	168	5		

- Molecule 73 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	Bf	110	Total	C	N	O	S	0	0
			884	560	175	144	5		

- Molecule 74 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Bg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 75 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Bh	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 76 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	Bi	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 77 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Bj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 78 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Bk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Bk	24	LYS	ASN	conflict	UNP G1U001

- Molecule 79 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	Bl	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 80 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	Bm	52	Total	C	N	O	S	0	0
			432	269	90	67	6		

- Molecule 81 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	Bo	105	Total	C	N	O	S	0	0
			863	543	175	139	6		

- Molecule 82 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	Bp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 83 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	Br	126	Total	C	N	O	S	0	0
			1014	629	209	170	6		

- Molecule 84 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	Bs	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

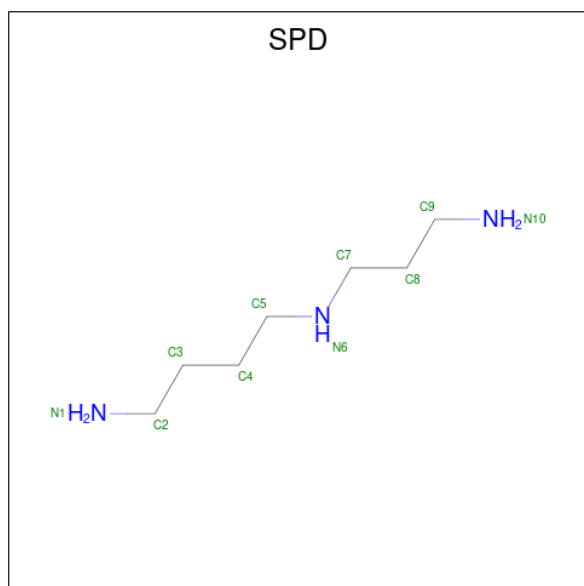
- Molecule 85 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	Bt	156	Total	C	N	O	S	0	0
			1178	733	221	220	4		

- Molecule 86 is a protein called Ribosomal protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	Bv	212	Total	C	N	O	S	0	0
			1707	1092	308	299	8		

- Molecule 87 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



Mol	Chain	Residues	Atoms			AltConf
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	
87	A2	1	Total	C	N	0
			10	7	3	

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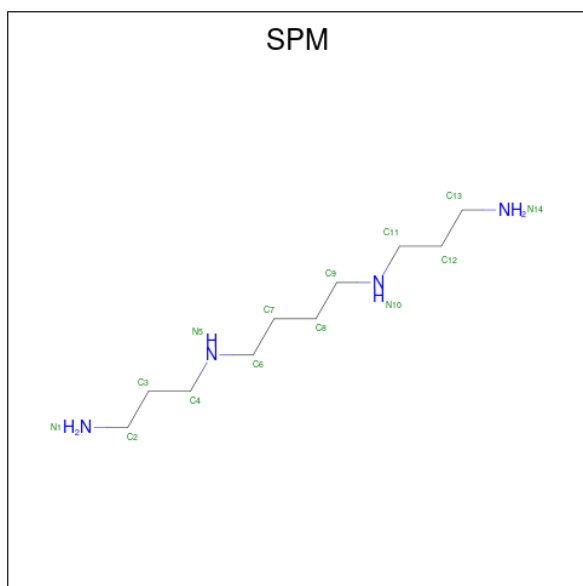
[illegible]

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Mol	Chain	Residues	Atoms			AltConf
87	BN	1	Total	C	N	0
			10	7	3	

- Molecule 88 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
88	A2	1	Total	C	N	0
			14	10	4	
88	B5	1	Total	C	N	0
			14	10	4	
88	B5	1	Total	C	N	0
			14	10	4	

- Molecule 89 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
89	A2	110	Total	Mg	0
			110	110	
89	AT	3	Total	Mg	0
			3	3	
89	Af	1	Total	Mg	0
			1	1	
89	B5	284	Total	Mg	0
			284	284	
89	B7	9	Total	Mg	0
			9	9	

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Mol	Chain	Residues	Atoms		AltConf
89	B8	9	Total 9	Mg 9	0
89	BP	1	Total 1	Mg 1	0
89	BR	1	Total 1	Mg 1	0
89	BV	1	Total 1	Mg 1	0
89	Ba	1	Total 1	Mg 1	0

- Molecule 90 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
90	A2	61	Total 61	X 61	0
90	AT	4	Total 4	X 4	0
90	Ad	1	Total 1	X 1	0
90	An	1	Total 1	X 1	0
90	Ar	1	Total 1	X 1	0
90	B5	225	Total 225	X 225	0
90	B7	6	Total 6	X 6	0
90	B8	7	Total 7	X 7	0
90	BA	4	Total 4	X 4	0
90	BB	3	Total 3	X 3	0
90	BC	1	Total 1	X 1	0
90	BH	1	Total 1	X 1	0
90	BI	1	Total 1	X 1	0
90	BL	1	Total 1	X 1	0

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Mol	Chain	Residues	Atoms		AltConf
90	BN	1	Total 1	X 1	0
90	BQ	2	Total 2	X 2	0
90	BT	2	Total 2	X 2	0
90	Bb	1	Total 1	X 1	0
90	Be	2	Total 2	X 2	0
90	Bf	1	Total 1	X 1	0
90	Bg	1	Total 1	X 1	0
90	Bj	1	Total 1	X 1	0
90	Bl	1	Total 1	X 1	0
90	Bo	1	Total 1	X 1	0

- Molecule 91 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
91	AC	1	Total 1	Zn 1	0
91	AE	1	Total 1	Zn 1	0
91	AG	1	Total 1	Zn 1	0
91	Bg	1	Total 1	Zn 1	0
91	Bj	1	Total 1	Zn 1	0
91	Bm	1	Total 1	Zn 1	0
91	Bo	1	Total 1	Zn 1	0
91	Bp	1	Total 1	Zn 1	0

- Molecule 92 is water.



Mol	Chain	Residues	Atoms		AltConf
92	A2	1579	Total 1579	O 1579	0
92	AA	6	Total 6	O 6	0
92	AD	2	Total 2	O 2	0
92	AE	19	Total 19	O 19	0
92	AG	1	Total 1	O 1	0
92	AH	14	Total 14	O 14	0
92	AI	12	Total 12	O 12	0
92	AT	35	Total 35	O 35	0
92	AZ	1	Total 1	O 1	0
92	Aa	16	Total 16	O 16	0
92	Ab	10	Total 10	O 10	0
92	Ad	9	Total 9	O 9	0
92	Ae	4	Total 4	O 4	0
92	Af	6	Total 6	O 6	0
92	Ag	4	Total 4	O 4	0
92	Ah	22	Total 22	O 22	0
92	Ai	4	Total 4	O 4	0
92	Ak	31	Total 31	O 31	0
92	Am	22	Total 22	O 22	0
92	An	20	Total 20	O 20	0
92	Ap	10	Total 10	O 10	0
92	Ar	2	Total 2	O 2	0

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Mol	Chain	Residues	Atoms		AltConf
92	As	4	Total 4	O 4	0
92	At	4	Total 4	O 4	0
92	Au	1	Total 1	O 1	0
92	Av	16	Total 16	O 16	0
92	Aw	23	Total 23	O 23	0
92	Ax	1	Total 1	O 1	0
92	Ay	1	Total 1	O 1	0
92	Az	9	Total 9	O 9	0
92	B5	7033	Total 7033	O 7033	0
92	B7	199	Total 199	O 199	0
92	B8	250	Total 250	O 250	0
92	BA	114	Total 114	O 114	0
92	BB	131	Total 131	O 131	0
92	BC	148	Total 148	O 148	0
92	BD	45	Total 45	O 45	0
92	BE	34	Total 34	O 34	0
92	BF	88	Total 88	O 88	0
92	BG	34	Total 34	O 34	0
92	BH	34	Total 34	O 34	0
92	BI	64	Total 64	O 64	0
92	BJ	13	Total 13	O 13	0

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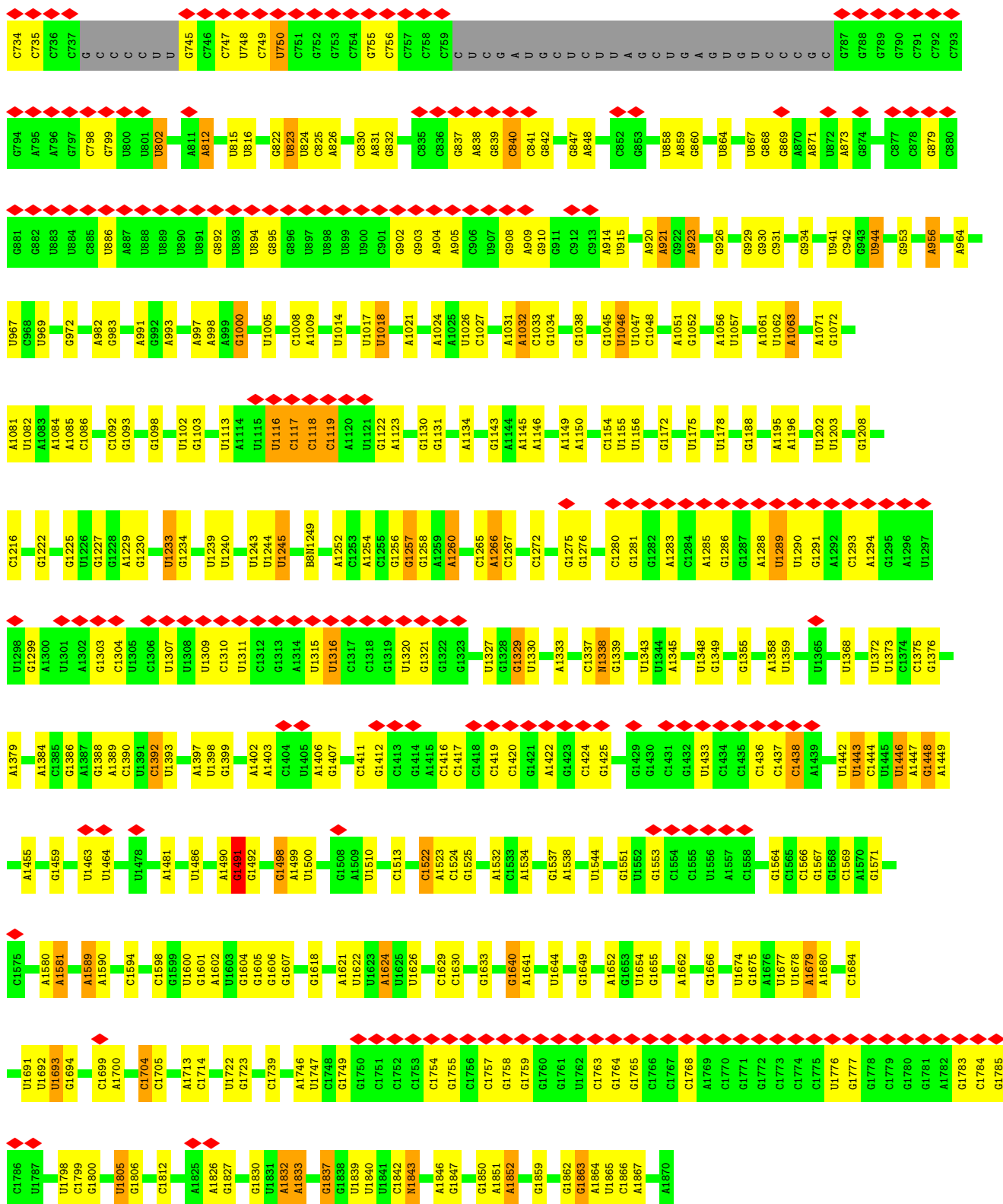
Mol	Chain	Residues	Atoms		AltConf
92	BK	5	Total 5	O 5	0
92	BL	79	Total 79	O 79	0
92	BM	20	Total 20	O 20	0
92	BN	139	Total 139	O 139	0
92	BO	69	Total 69	O 69	0
92	BP	51	Total 51	O 51	0
92	BQ	84	Total 84	O 84	0
92	BR	44	Total 44	O 44	0
92	BS	58	Total 58	O 58	0
92	BT	55	Total 55	O 55	0
92	BU	5	Total 5	O 5	0
92	BV	36	Total 36	O 36	0
92	BW	15	Total 15	O 15	0
92	BX	22	Total 22	O 22	0
92	BY	21	Total 21	O 21	0
92	BZ	12	Total 12	O 12	0
92	Ba	87	Total 87	O 87	0
92	Bb	24	Total 24	O 24	0
92	Bc	13	Total 13	O 13	0
92	Bd	31	Total 31	O 31	0
92	Be	77	Total 77	O 77	0

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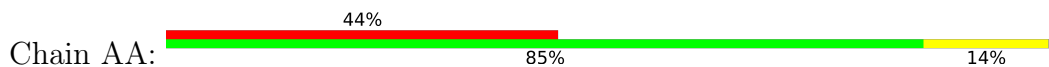
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Mol	Chain	Residues	Atoms		AltConf
92	Bf	36	Total 36	O 36	0
92	Bg	45	Total 45	O 45	0
92	Bh	17	Total 17	O 17	0
92	Bi	19	Total 19	O 19	0
92	Bj	52	Total 52	O 52	0
92	Bk	1	Total 1	O 1	0
92	Bl	16	Total 16	O 16	0
92	Bm	14	Total 14	O 14	0
92	Bo	46	Total 46	O 46	0
92	Bp	32	Total 32	O 32	0
92	Br	41	Total 41	O 41	0

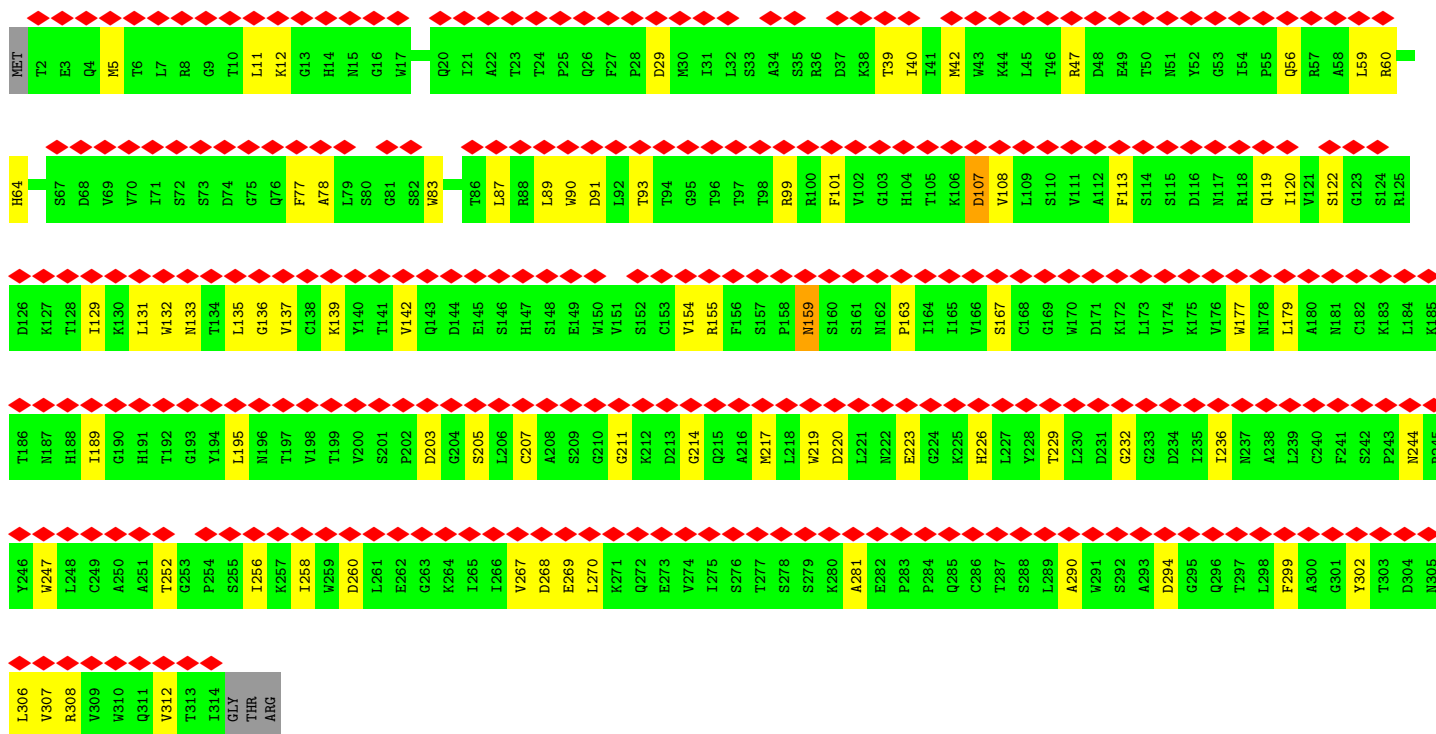




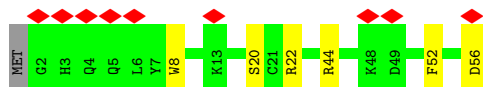
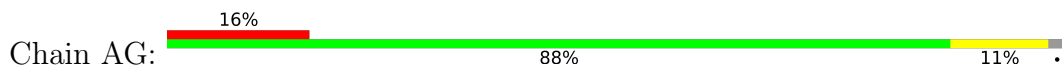
• Molecule 2: 40S ribosomal protein S27







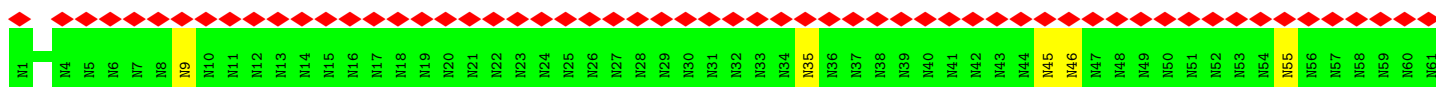
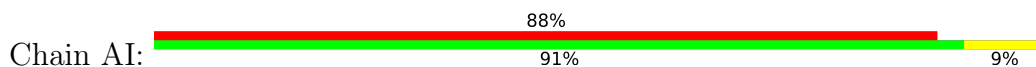
• Molecule 8: uS14



• Molecule 9: mRNA containing SARS-CoV-2 sequence

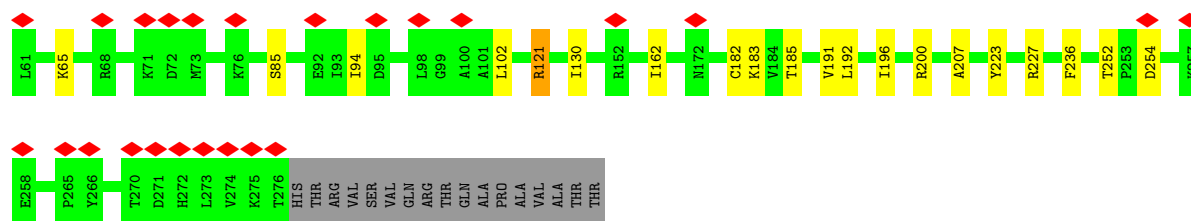


• Molecule 10: E-site tRNA

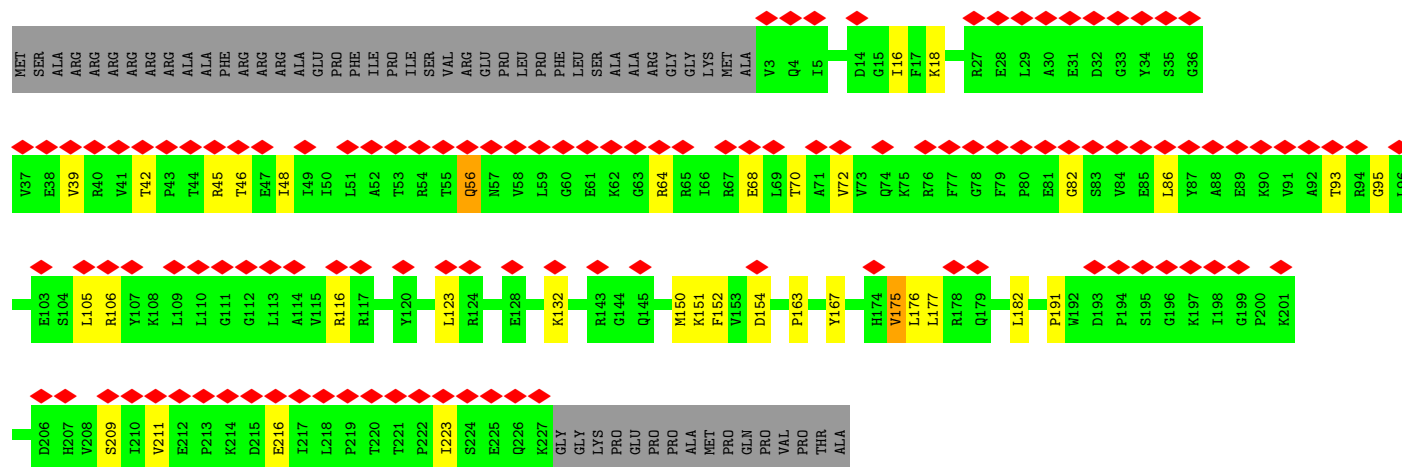
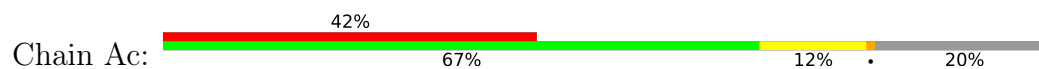




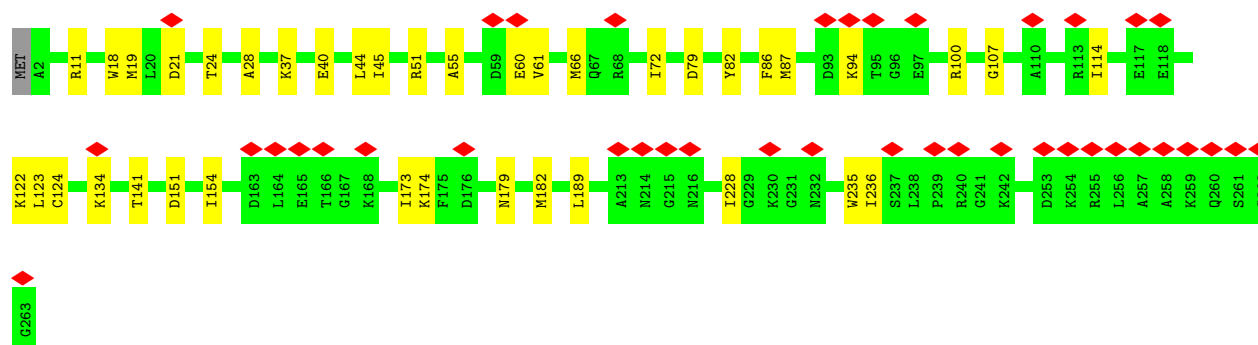
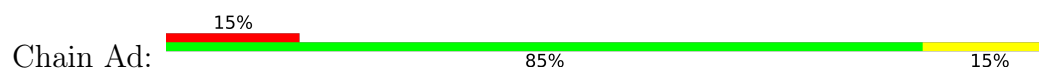




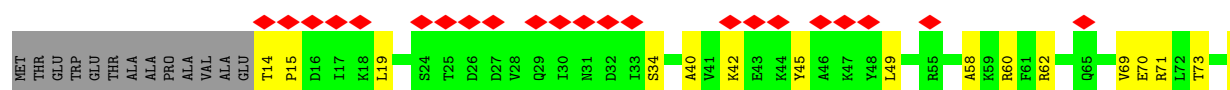
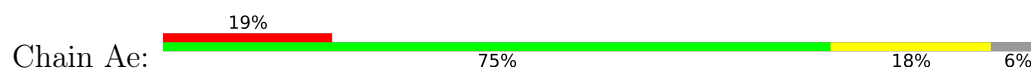
• Molecule 15: 40S ribosomal protein S3



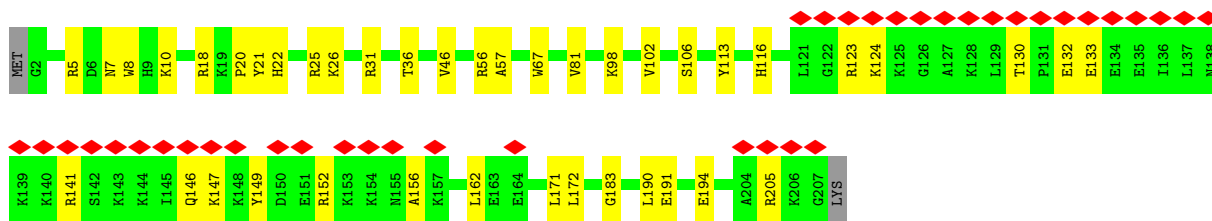
• Molecule 16: Ribosomal protein eS4



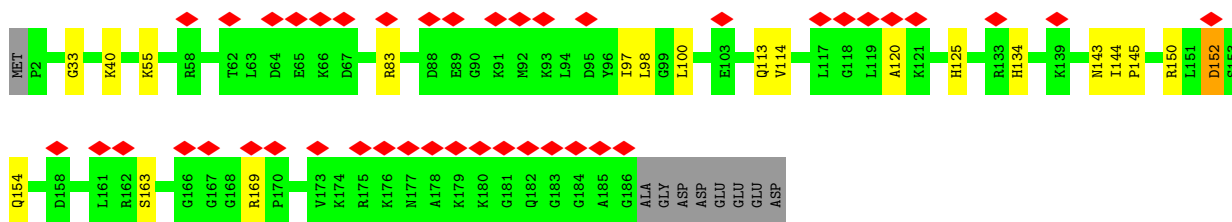
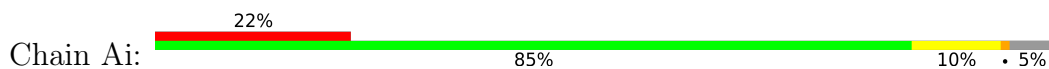
• Molecule 17: Ribosomal protein S5



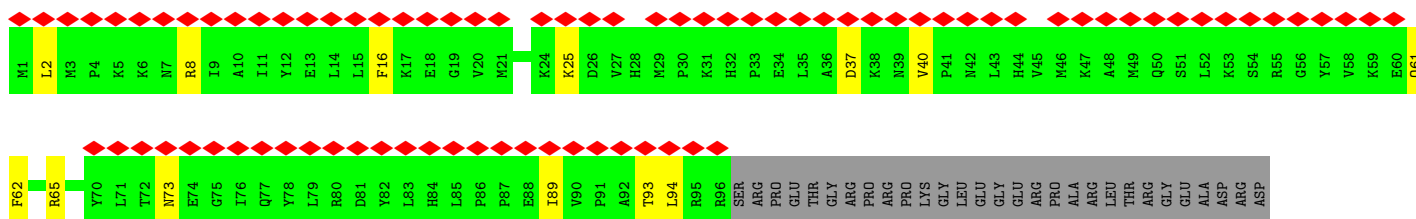




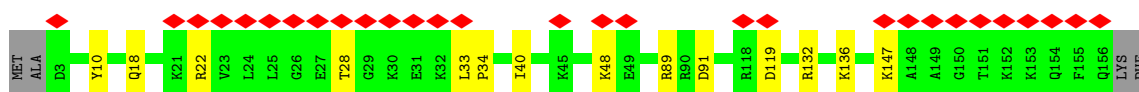
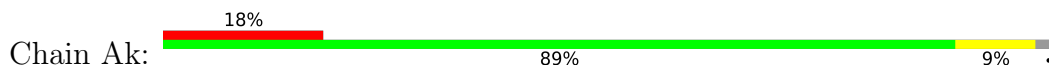
• Molecule 21: Ribosomal protein S9 (Predicted)



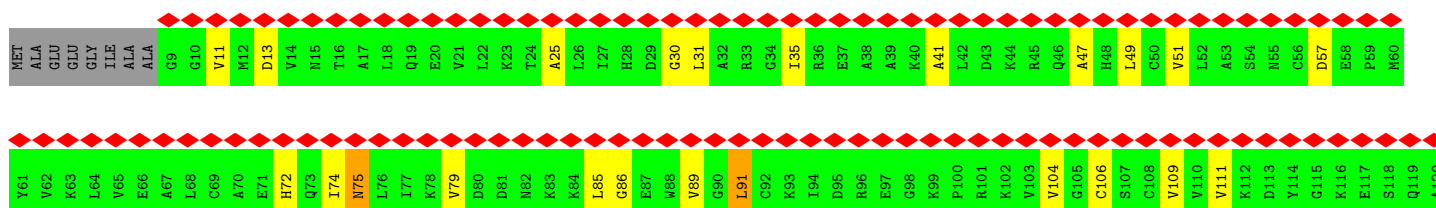
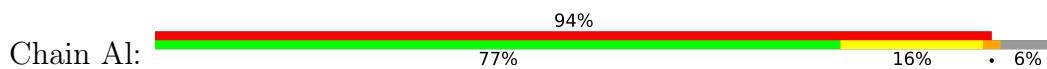
• Molecule 22: eS10

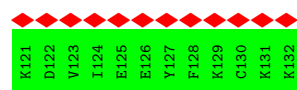


• Molecule 23: 40S ribosomal protein S11

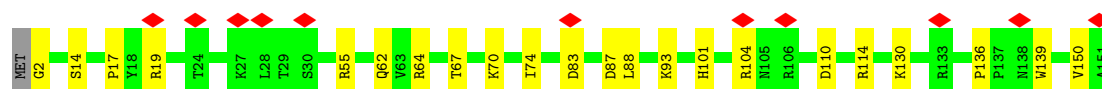
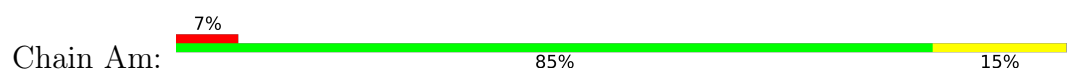


• Molecule 24: 40S ribosomal protein S12

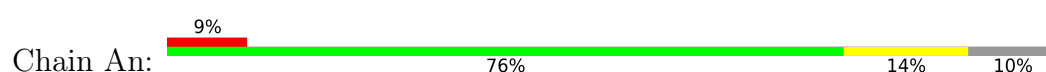




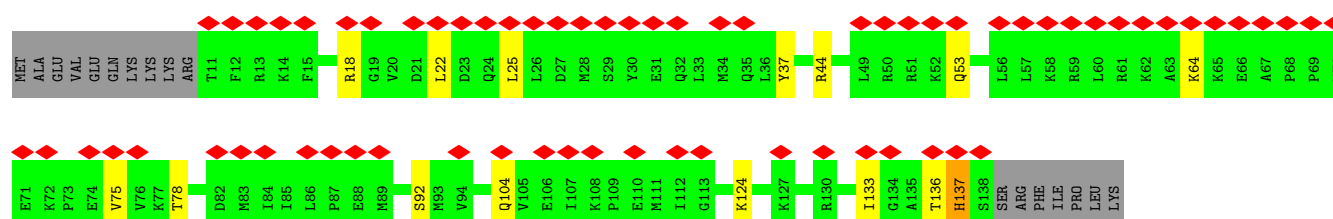
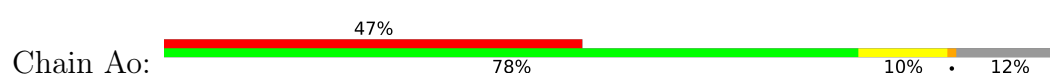
• Molecule 25: uS15



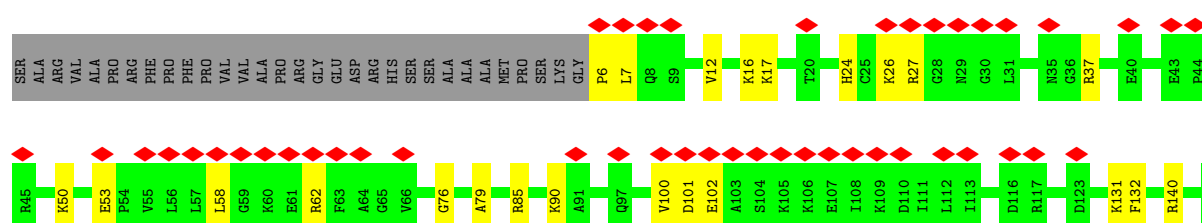
• Molecule 26: 40S ribosomal protein uS11



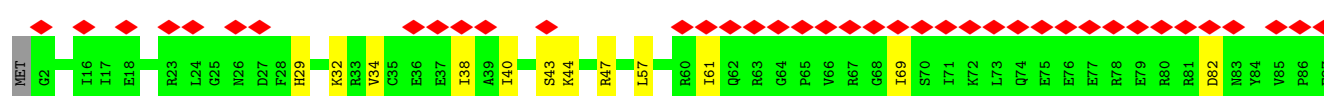
• Molecule 27: 40S ribosomal protein uS19

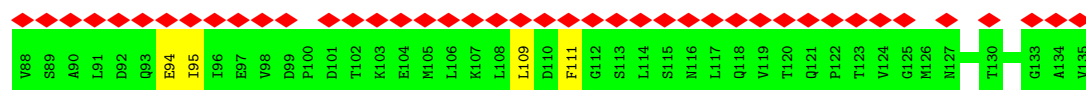


• Molecule 28: uS9

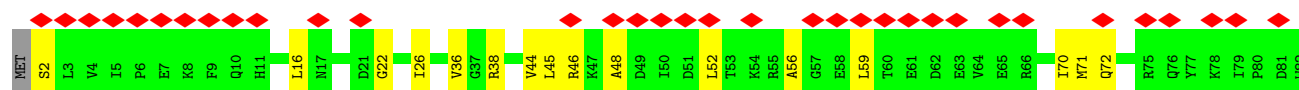
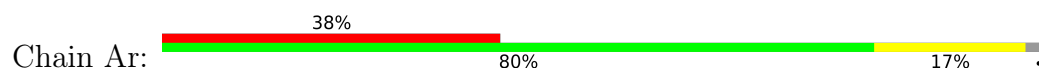


• Molecule 29: 40S ribosomal protein eS17

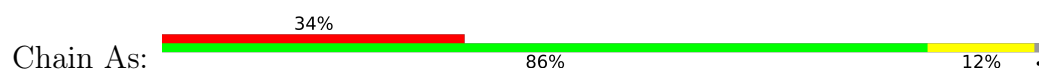




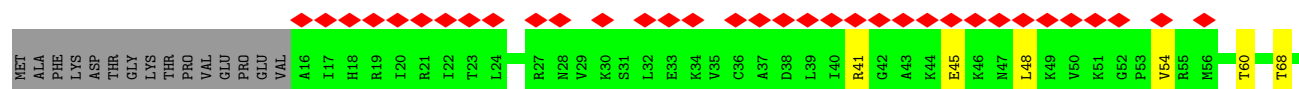
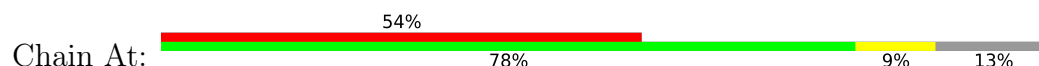
• Molecule 30: 40S ribosomal protein S18



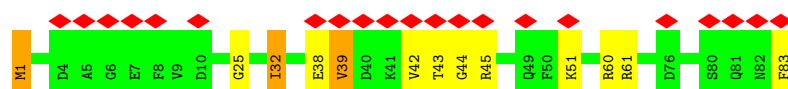
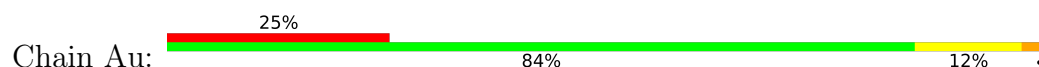
• Molecule 31: Ribosomal protein eS19



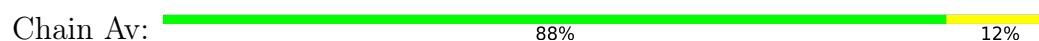
• Molecule 32: 40S ribosomal protein uS10



• Molecule 33: Ribosomal protein eS21



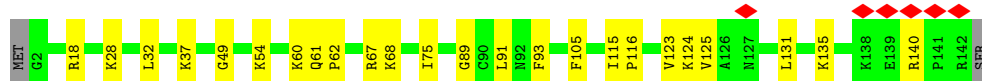
• Molecule 34: Ribosomal protein S15a





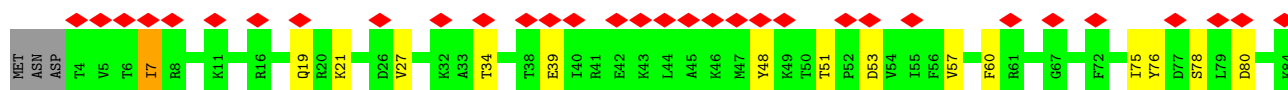
- Molecule 35: 40S ribosomal protein S23

Chain Aw: 82% 17%



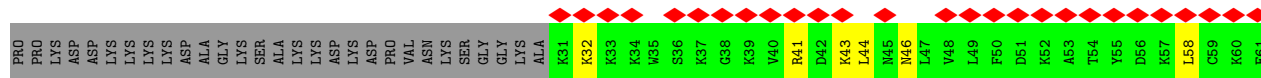
- Molecule 36: 40S ribosomal protein S24

Chain Ax: 42% 79% 16%



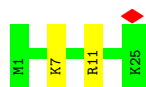
- Molecule 37: 40S ribosomal protein S25

Chain Ay: 43% 52% 16% 31%



- Molecule 38: 60s ribosomal protein l41

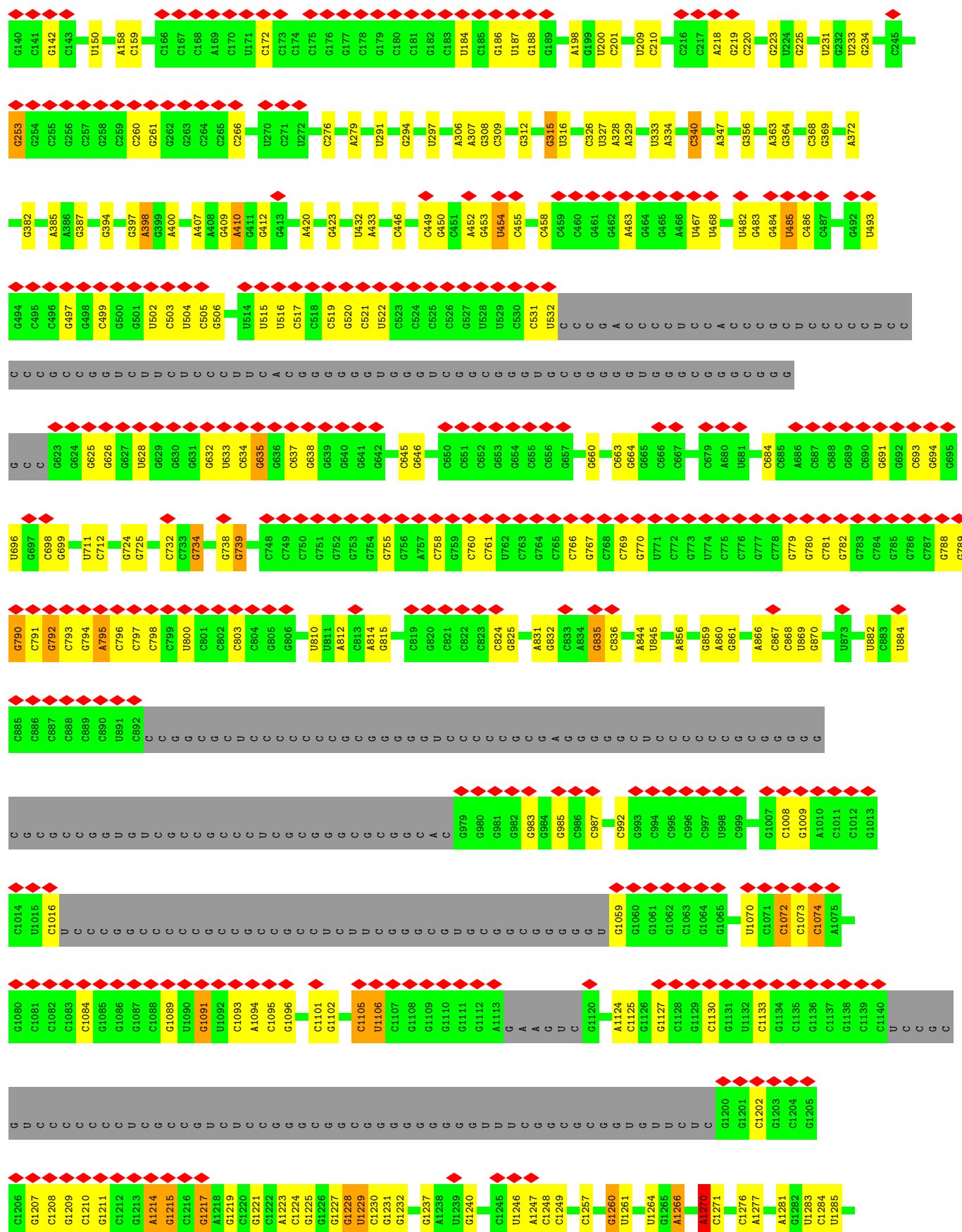
Chain Az: 92% 8%



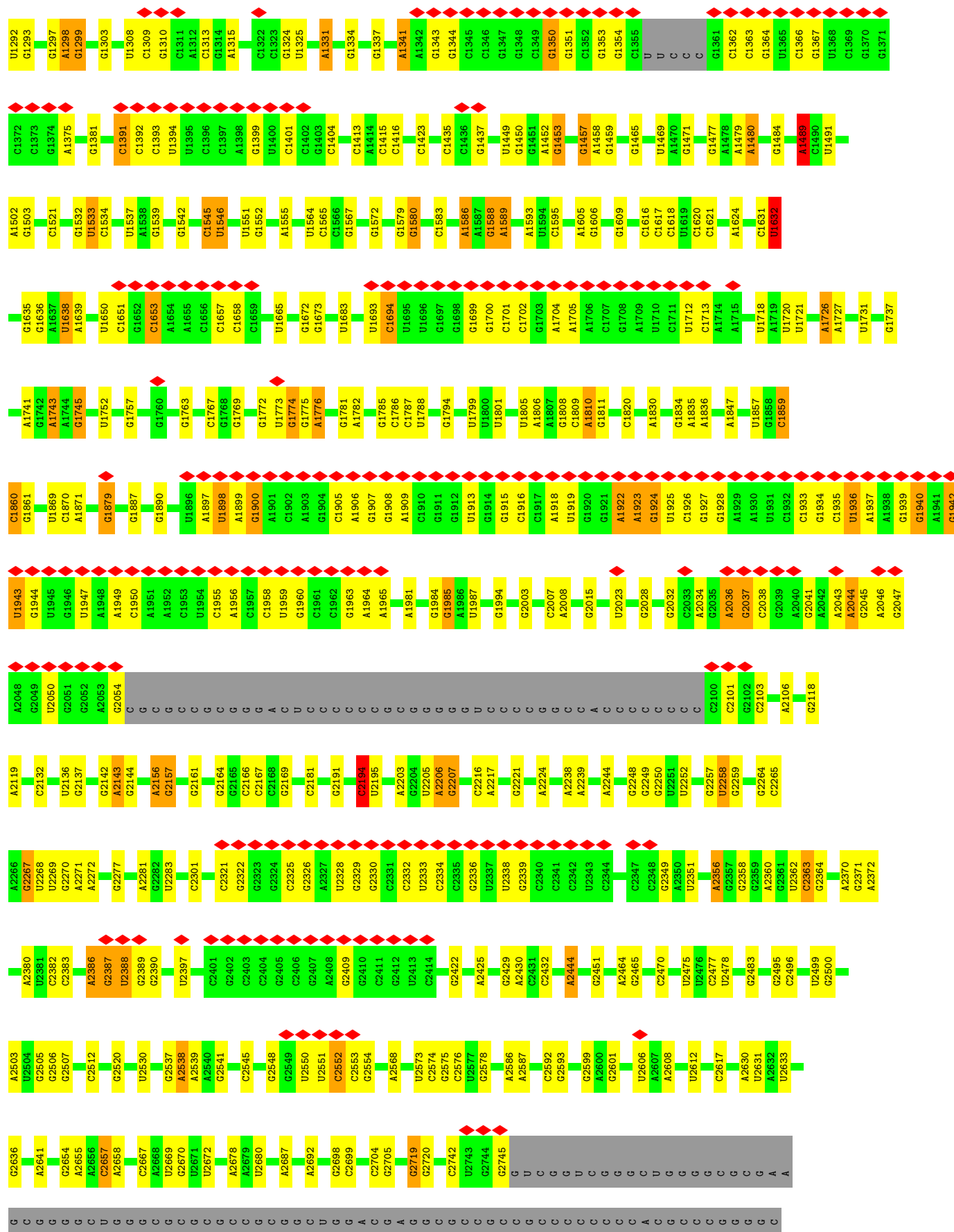
- Molecule 39: 28S rRNA

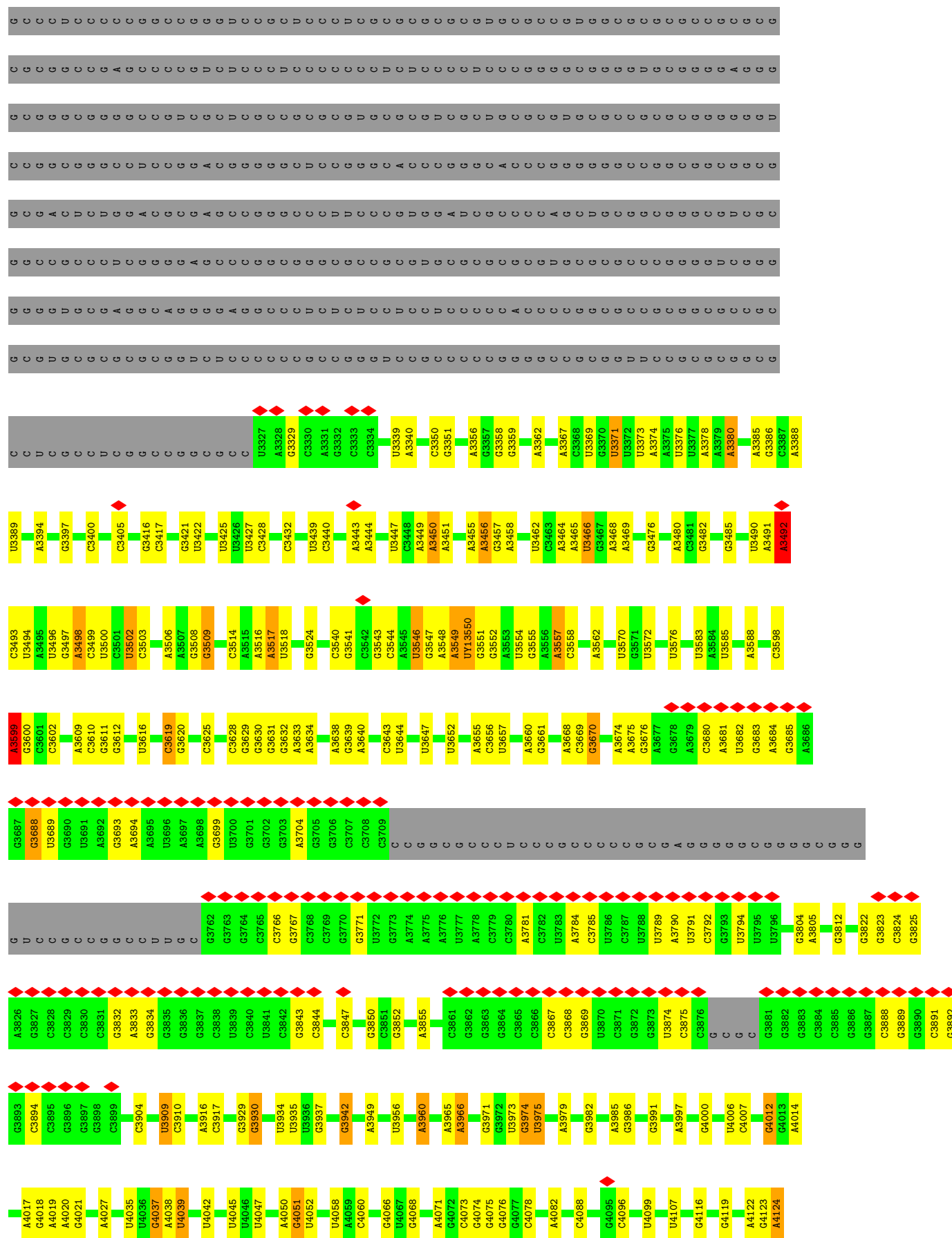
Chain B5: 16% 55% 20% 22%

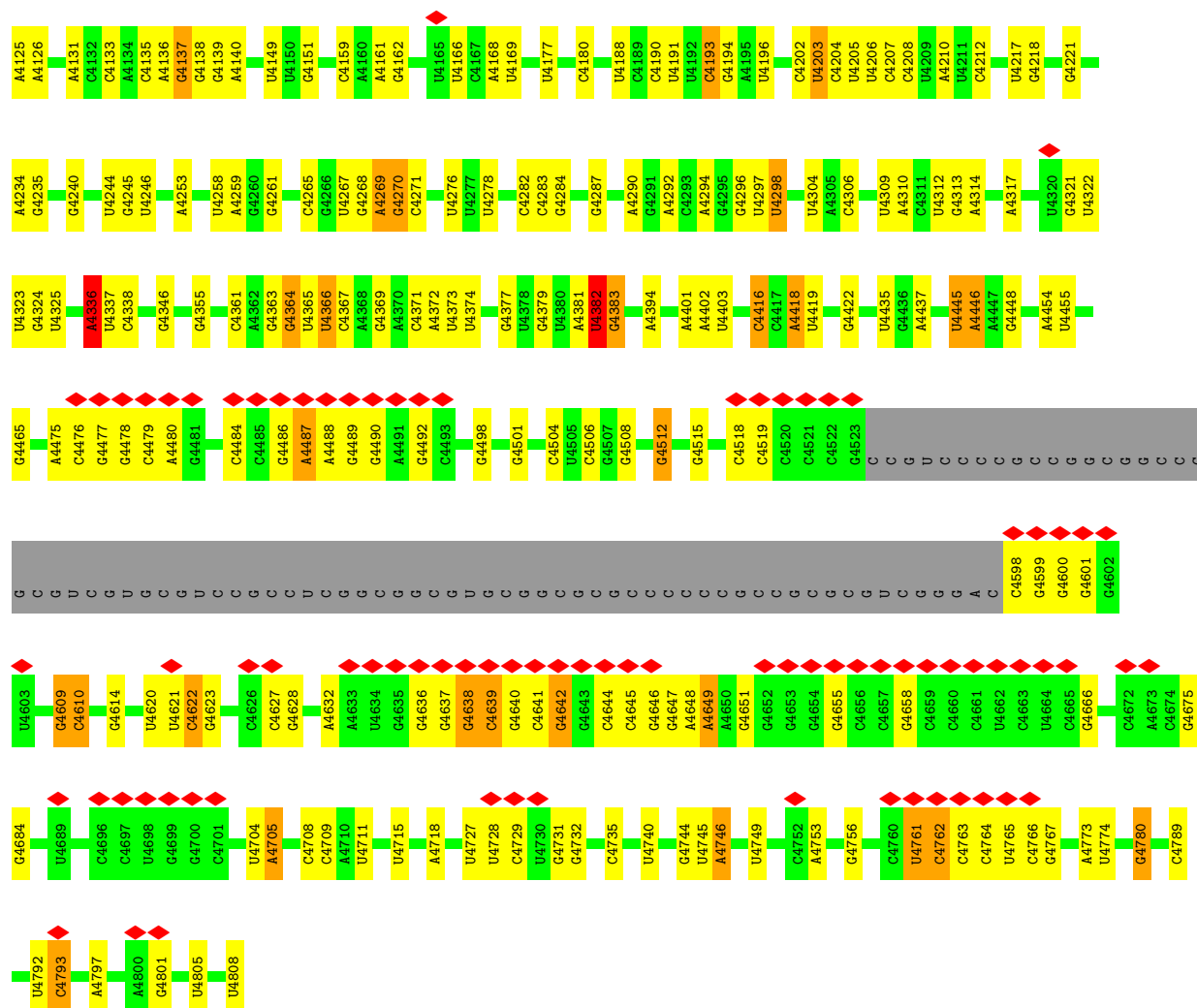




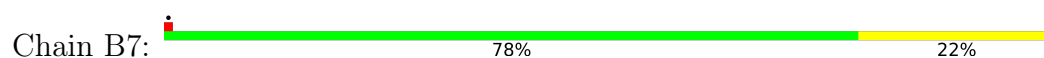




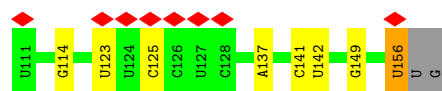
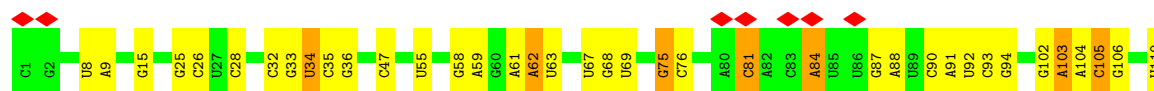
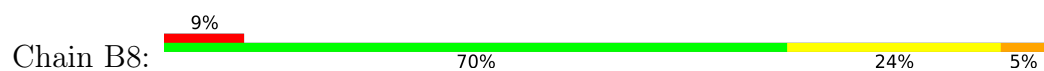





• Molecule 40: 5S rRNA



• Molecule 41: 5.8S rRNA




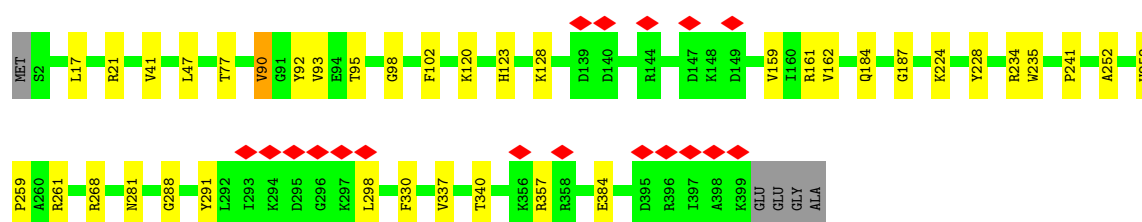
• Molecule 42: Ribosomal protein uL2

Chain BA: 




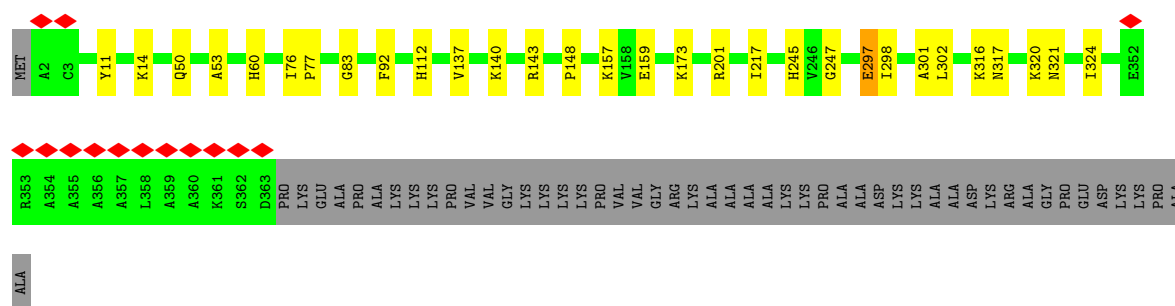
- Molecule 43: Ribosomal protein L3

Chain BB: 




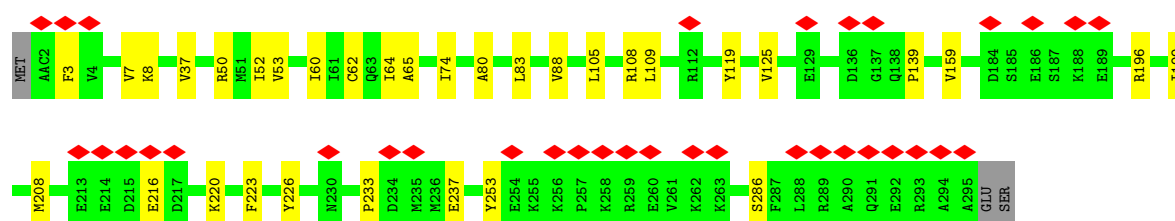
- Molecule 44: 60S ribosomal protein L4

Chain BC: 



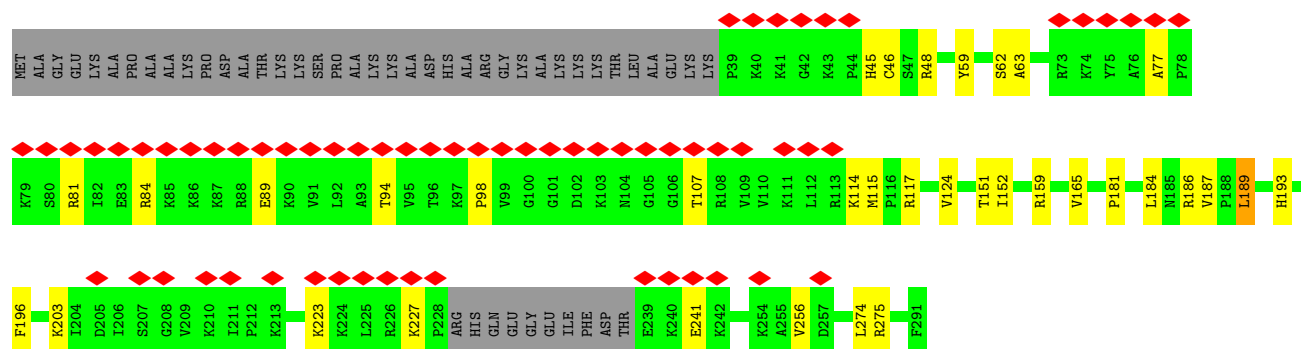
- Molecule 45: Ribosomal\_L18\_c domain-containing protein

Chain BD: 



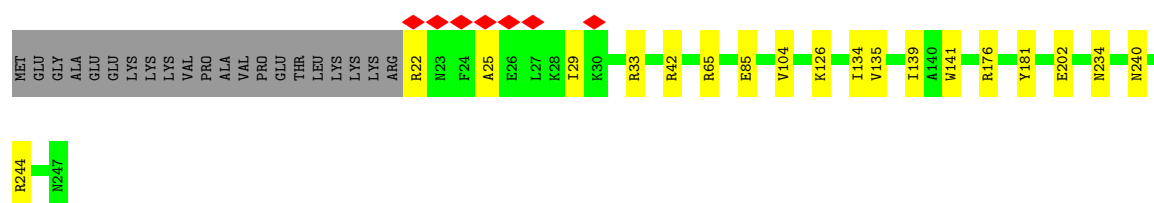
- Molecule 46: 60S ribosomal protein L6

Chain BE: 



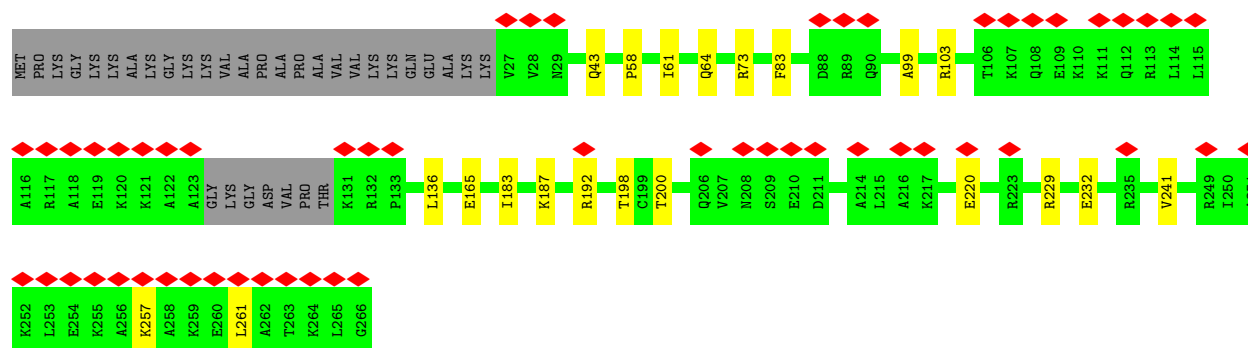
• Molecule 47: Ribosomal Protein uL30

Chain BF: 84% 8% 9%



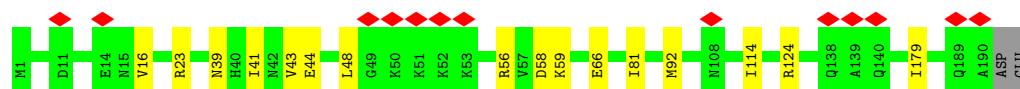
• Molecule 48: Ribosomal protein eL8

Chain BG: 21% 80% 8% 12%



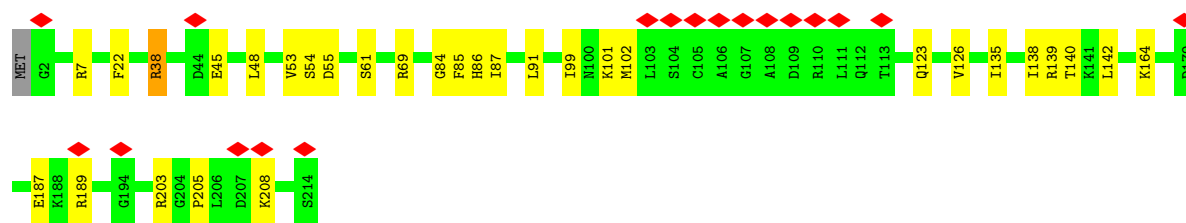
• Molecule 49: 60S ribosomal protein L9

Chain BH: 7% 91% 8%

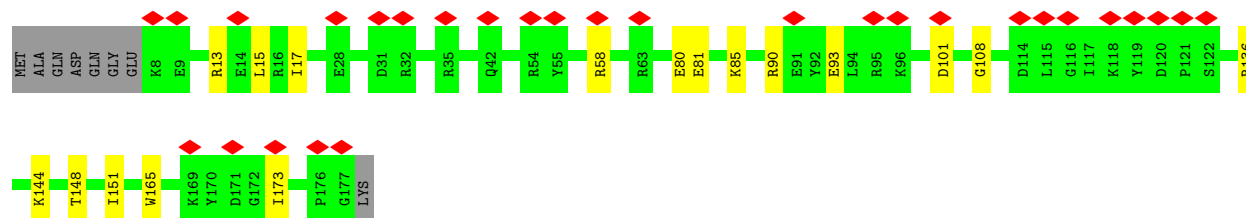
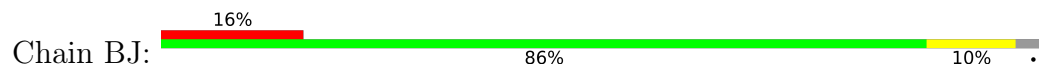


• Molecule 50: 60S ribosomal protein L10

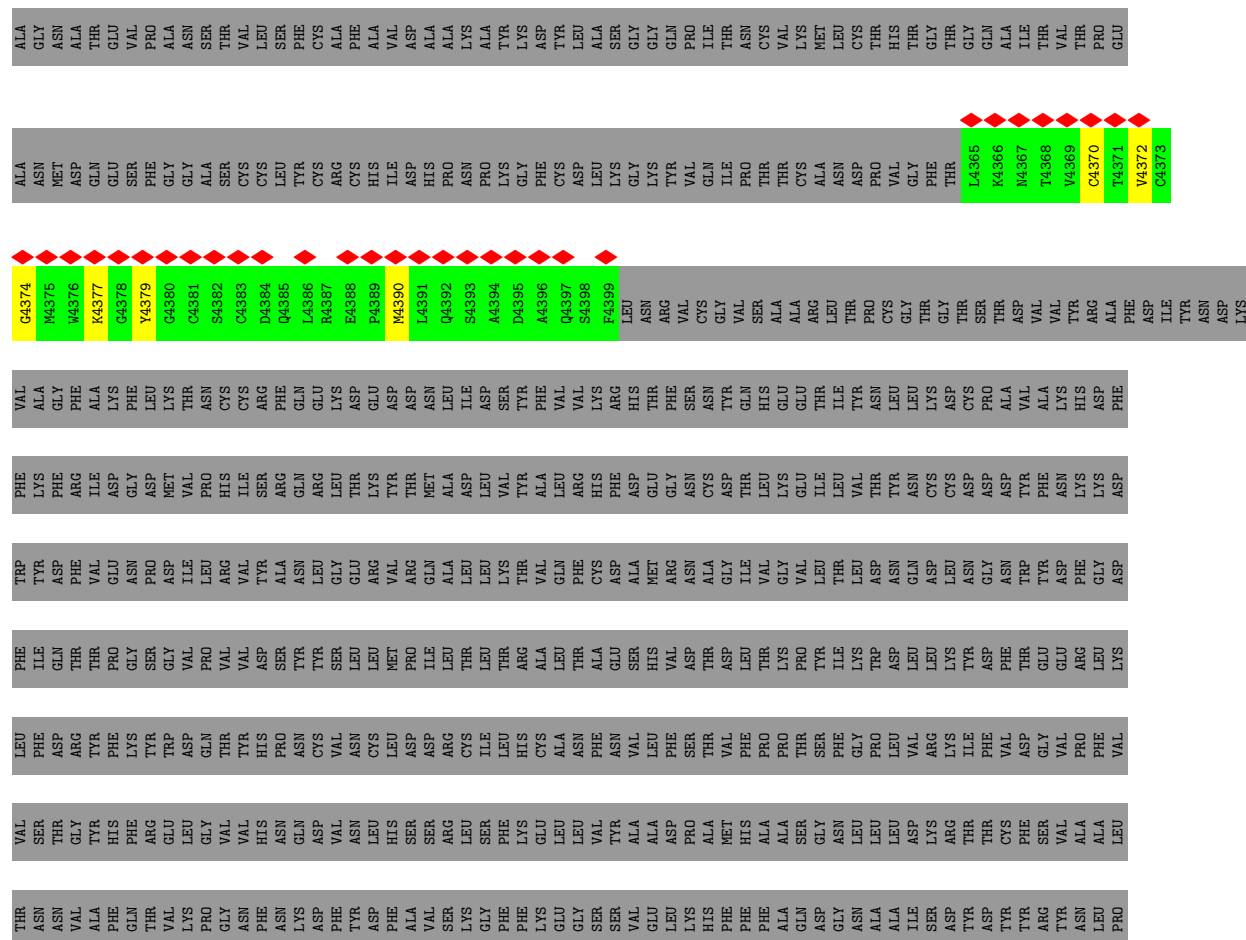
Chain BI: 8% 85% 14%



• Molecule 51: Ribosomal protein L11

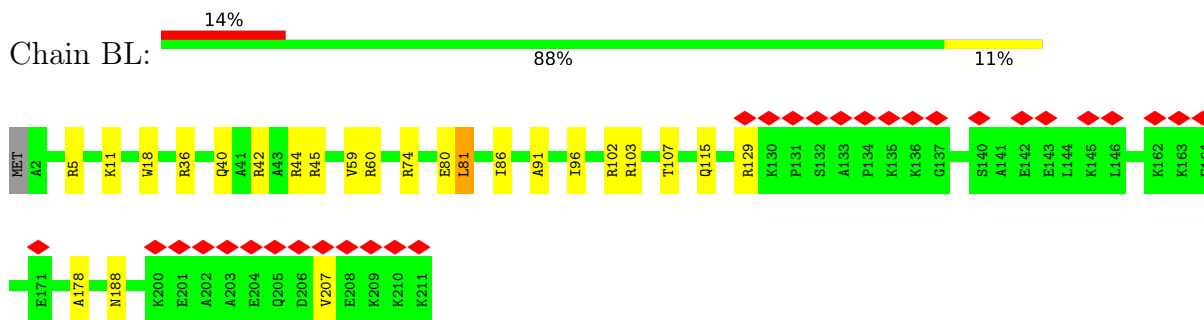


• Molecule 52: Replicase polypeptide 1ab

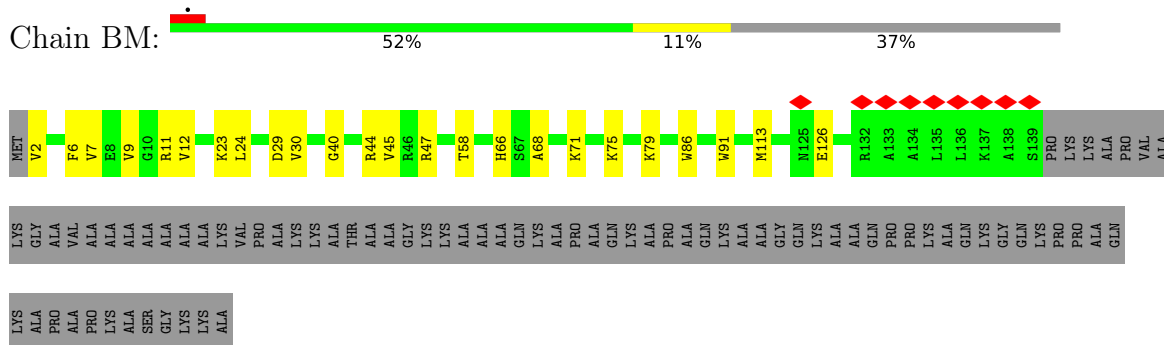


[illegible]

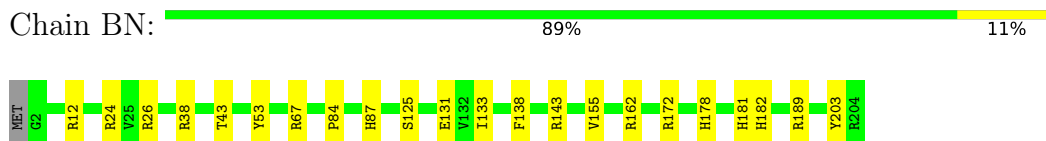
- Molecule 53: Ribosomal protein eL13



- Molecule 54: Ribosomal protein L14



- Molecule 55: Ribosomal protein L15




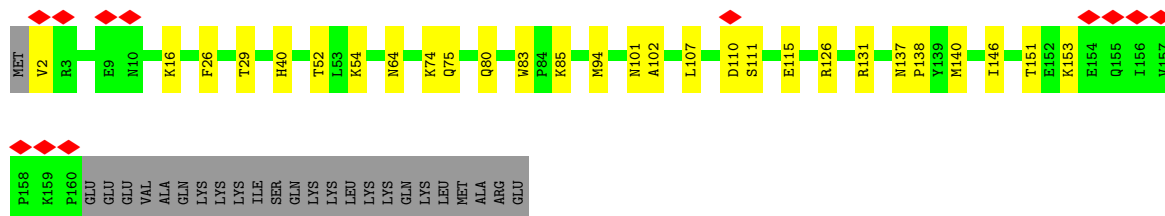
- Molecule 56: Ribosomal protein uL13

Chain BO:  90% 8%



- Molecule 57: uL22

Chain BP:  7% 71% 15% 14%




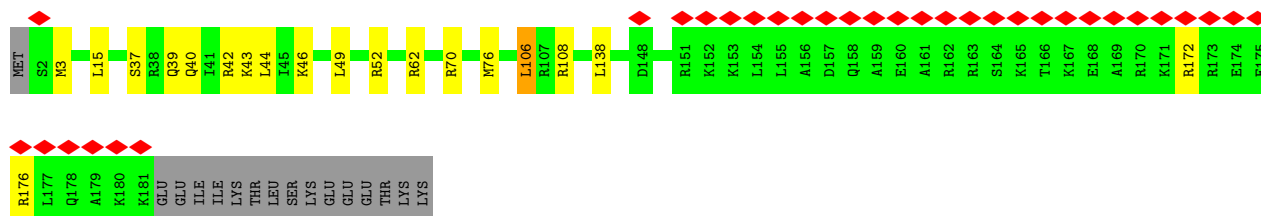
- Molecule 58: Ribosomal Protein eL18

Chain BQ:  91% 8%




- Molecule 59: 60S ribosomal protein L19

Chain BR:  17% 82% 9% 8%




- Molecule 60: Ribosomal protein eL20

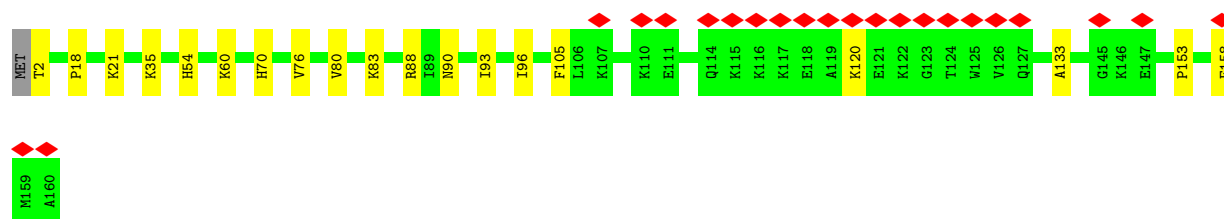
Chain BS:  88% 13%



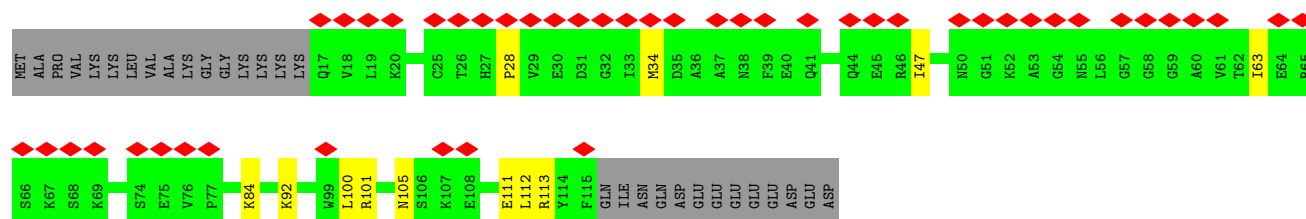
- Molecule 61: eL21

Chain BT:  14% 88% 12%

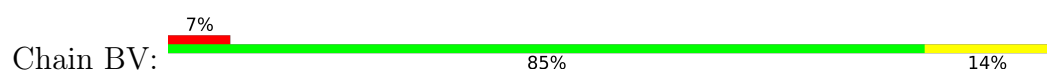




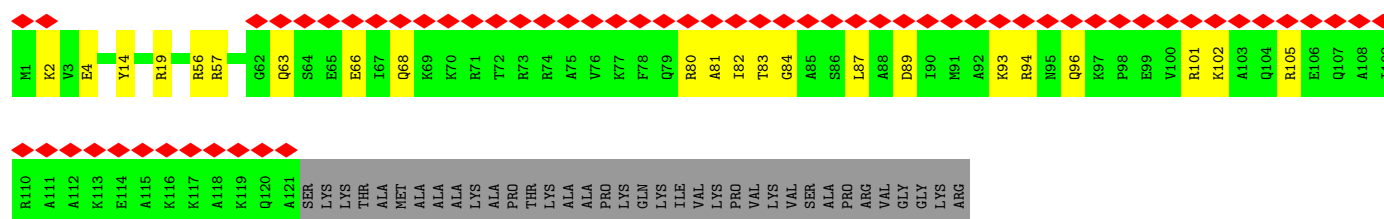
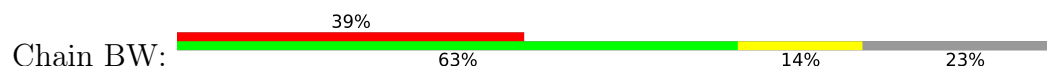
- Molecule 62: Ribosomal protein eL22



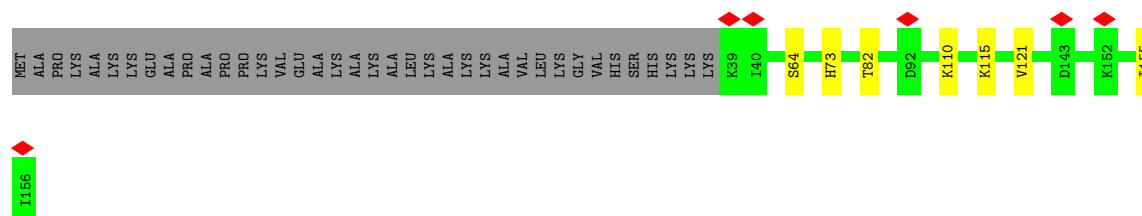
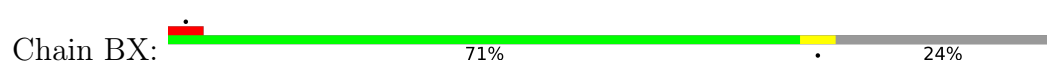
- Molecule 63: Ribosomal protein L23



- Molecule 64: eL24




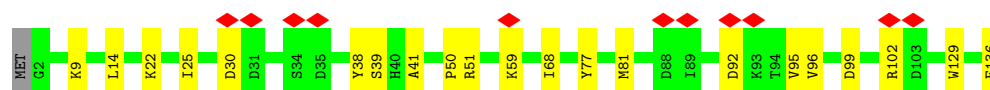
- Molecule 65: uL23




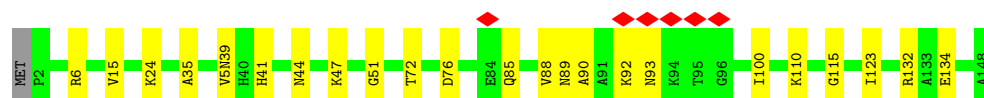
- Molecule 66: Ribosomal protein L26

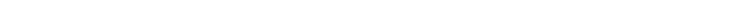
Sequence logo for the 1000bp upstream region of the H100 promoter. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows positions from -1000 to +100. The logo shows a strong consensus for the TATA box (TATATA) around position -25. Other notable features include a GC-rich region around position -100 and a T-rich region around position +50. The sequence TATATA is highlighted in red.

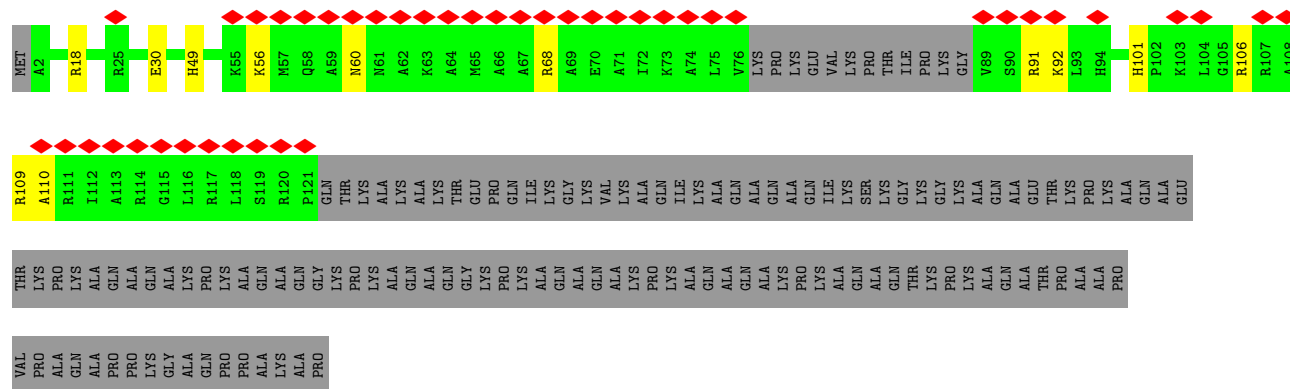
- Chain BZ: 

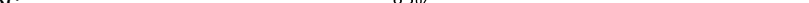


- Chain Ba:  84% 16%

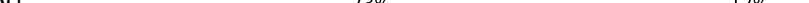


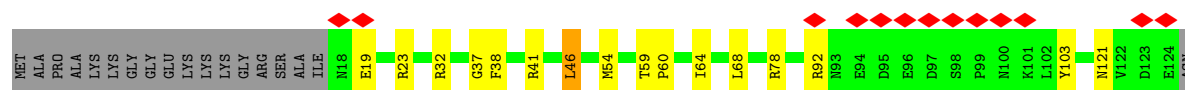
- Chain Bb: 



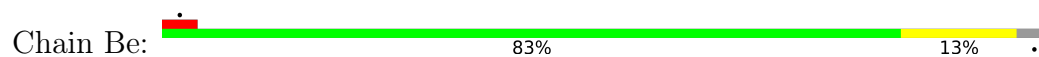
- Chain Bc: 



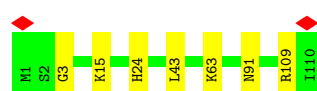
- Chain Bd: 



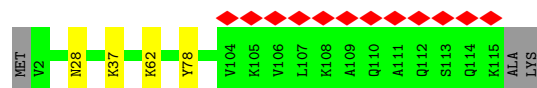
- Molecule 72: eL32



- Molecule 73: eL33



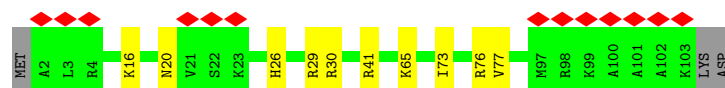
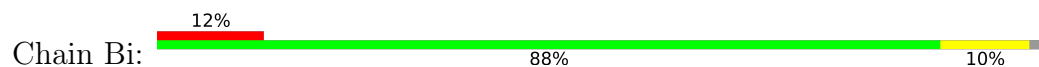
- Molecule 74: 60S ribosomal protein L34



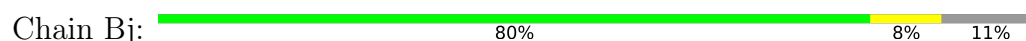
- Molecule 75: uL29



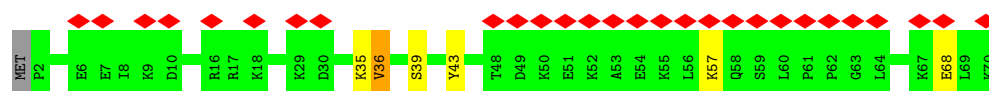
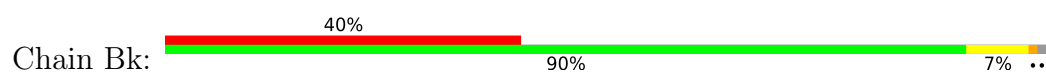
- Molecule 76: 60S ribosomal protein L36



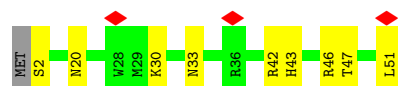
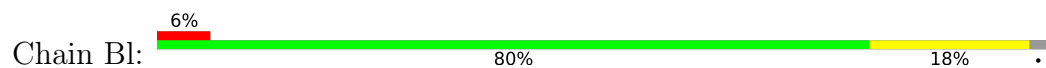
- Molecule 77: Ribosomal protein L37



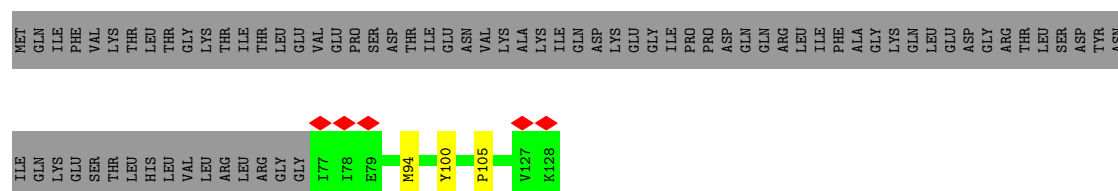
- Molecule 78: eL38



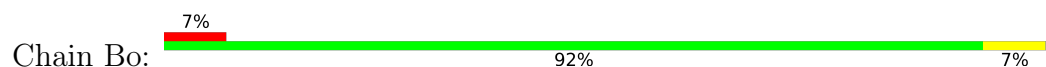
- Molecule 79: eL39



- Molecule 80: 60S ribosomal protein L40



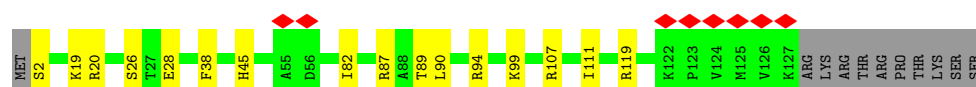
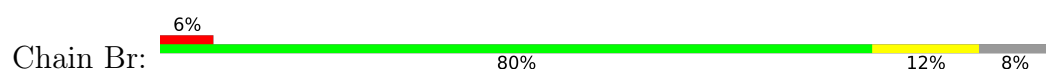
- Molecule 81: eL42



- Molecule 82: eL43

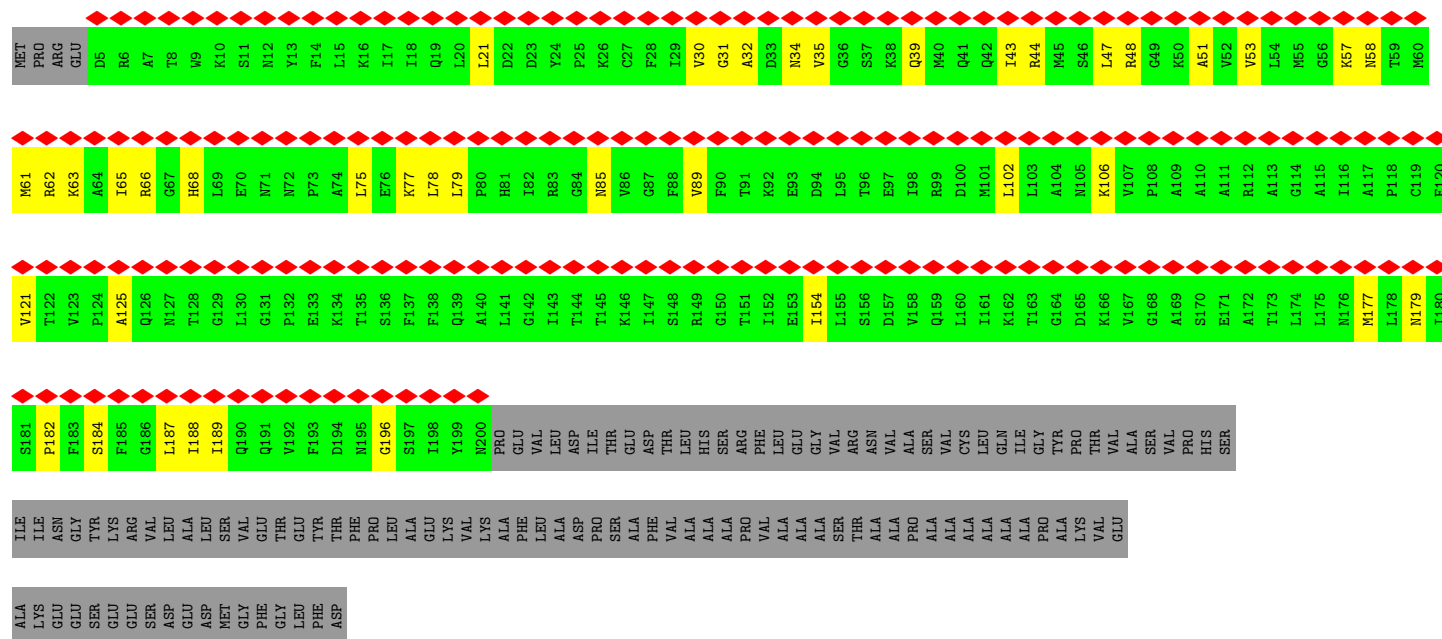


- Molecule 83: Ribosomal protein eL28

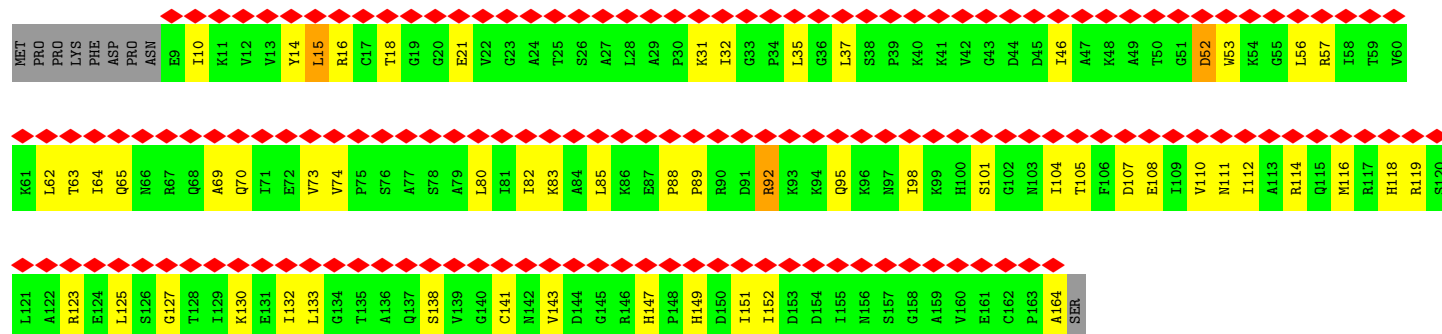


- Molecule 84: 60S acidic ribosomal protein P0





• Molecule 85: Ribosomal protein L12



• Molecule 86: Ribosomal protein uL1



Y181	N182	I183	H184	L185	A186	V187	N188	F189	L190	V191	S192	L193	L194	K195	K196	N197	W198	Q199	N200	V201	R202	A203	L204	Y205	I206	K207	S208	T209	M210	G211	K212	P213	Q214	R215	L216	Y217
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	695501	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	56604	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	16.275	Depositor
Minimum map value	-6.791	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.307	Depositor
Recommended contour level	1.5	Depositor
Map size ( $\text{\AA}$ )	593.6, 593.6, 593.6	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, UY1, GTP, NMM, 1MA, M2G, YYG, 2MG, AME, OMC, SPM, AYA, H2U, MLZ, PSU, MA6, M3L, SPD, UNX, A2M, AAC, MG, HY3, UR3, 5MC, 4AC, ZN, B8N, 6MZ, OMG, HIC, OMU, 7MG, SAC, V5N

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A2	0.14	0/40342	0.18	0/62877
2	AA	0.08	0/665	0.25	0/891
3	AB	0.09	0/497	0.23	0/666
4	AC	0.08	0/622	0.25	0/822
5	AD	0.08	0/462	0.26	0/607
6	AE	0.10	0/828	0.26	0/1109
7	AF	0.09	0/2493	0.26	0/3394
8	AG	0.09	0/470	0.26	0/623
9	AH	0.08	0/140	0.15	0/217
10	AI	0.19	0/68	0.35	0/103
11	AT	0.09	0/1440	0.15	0/2242
12	AZ	0.09	0/1771	0.23	0/2406
13	Aa	0.10	0/1841	0.23	0/2459
14	Ab	0.10	0/1742	0.26	0/2354
15	Ac	0.09	0/1779	0.25	0/2395
16	Ad	0.10	0/2118	0.27	0/2849
17	Ae	0.09	0/1531	0.26	0/2059
18	Af	0.09	0/1946	0.24	0/2590
19	Ag	0.09	0/1552	0.26	0/2079
20	Ah	0.09	0/1715	0.25	0/2287
21	Ai	0.08	0/1550	0.21	0/2069
22	Aj	0.09	0/834	0.27	0/1125
23	Ak	0.10	0/1284	0.26	0/1717
24	Al	0.08	0/968	0.26	0/1296
25	Am	0.10	0/1232	0.25	0/1656
26	An	0.10	0/1029	0.31	0/1380
27	Ao	0.10	0/1069	0.27	0/1429
28	Ap	0.10	0/1142	0.29	0/1528
29	Aq	0.09	0/1094	0.23	0/1469
30	Ar	0.08	0/1226	0.23	0/1643



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
31	As	0.09	0/1119	0.23	0/1498
32	At	0.09	0/831	0.25	0/1115
33	Au	0.09	0/636	0.25	0/852
34	Av	0.10	0/1051	0.25	0/1406
35	Aw	0.09	0/1107	0.25	0/1475
36	Ax	0.09	0/1032	0.23	0/1371
37	Ay	0.08	0/691	0.23	0/922
38	Az	0.10	0/240	0.24	0/305
39	B5	0.13	5/87403 (0.0%)	0.20	0/136359
40	B7	0.09	0/2835	0.17	0/4418
41	B8	0.09	0/3635	0.18	0/5661
42	BA	0.11	0/1965	0.30	0/2633
43	BB	0.10	0/3261	0.28	0/4364
44	BC	0.10	0/2932	0.26	0/3939
45	BD	0.09	0/2437	0.26	0/3264
46	BE	0.09	0/1998	0.24	0/2673
47	BF	0.10	0/1922	0.27	0/2563
48	BG	0.09	0/1908	0.25	0/2566
49	BH	0.10	0/1535	0.25	0/2063
50	BI	0.10	0/1756	0.25	0/2346
51	BJ	0.09	0/1385	0.24	0/1852
52	BK	0.09	0/269	0.27	0/361
53	BL	0.10	0/1733	0.25	0/2316
54	BM	0.09	0/1158	0.23	0/1547
55	BN	0.10	0/1746	0.27	0/2338
56	BO	0.11	0/1662	0.24	0/2222
57	BP	0.10	0/1317	0.26	0/1768
58	BQ	0.10	0/1539	0.28	0/2054
59	BR	0.08	0/1524	0.23	0/2013
60	BS	0.11	0/1497	0.24	0/2008
61	BT	0.09	0/1326	0.26	0/1770
62	BU	0.08	0/820	0.24	0/1100
63	BV	0.11	0/1048	0.30	0/1402
64	BW	0.09	0/1006	0.25	0/1334
65	BX	0.09	0/984	0.24	0/1323
66	BY	0.08	0/1132	0.23	0/1504
67	BZ	0.08	0/1130	0.23	0/1507
68	Ba	0.10	0/1179	0.28	0/1572
69	Bb	0.09	0/884	0.28	0/1169
70	Bc	0.09	0/847	0.23	0/1134
71	Bd	0.11	0/903	0.24	0/1216
72	Be	0.09	0/1088	0.27	0/1451
73	Bf	0.11	0/903	0.28	0/1208

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
74	Bg	0.09	0/916	0.26	0/1220
75	Bh	0.07	0/1021	0.21	0/1348
76	Bi	0.08	0/841	0.26	0/1112
77	Bj	0.11	0/720	0.30	0/952
78	Bk	0.08	0/575	0.22	0/761
79	Bl	0.10	0/459	0.26	0/608
80	Bm	0.09	0/426	0.25	0/564
81	Bo	0.11	0/866	0.26	0/1141
82	Bp	0.10	0/718	0.27	0/953
83	Br	0.10	0/1020	0.27	0/1366
84	Bs	0.09	0/1530	0.25	0/2064
85	Bt	0.09	0/1193	0.25	0/1609
86	Bv	0.09	0/1735	0.30	0/2328
All	All	0.12	5/234844 (0.0%)	0.22	0/344329

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
81	Bo	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4269	A2M	O3'-P	5.15	1.61	1.56
39	B5	4761	U	C4-O4	5.15	1.33	1.23
39	B5	2258	OMU	O3'-P	5.08	1.61	1.56
39	B5	3562	A2M	O3'-P	5.04	1.61	1.56
39	B5	1810	A2M	O3'-P	5.03	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
81	Bo	53	MLZ	Mainchain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A2	37833	0	19168	306	0
2	AA	651	0	672	8	0
3	AB	495	0	523	7	0
4	AC	610	0	634	7	0
5	AD	457	0	502	10	0
6	AE	814	0	863	11	0
7	AF	2436	0	2393	45	0
8	AG	459	0	448	7	0
9	AH	128	0	62	0	0
10	AI	939	0	618	5	0
11	AT	1652	0	860	11	0
12	AZ	1743	0	1748	24	0
13	Aa	1815	0	1908	24	0
14	Ab	1706	0	1796	15	0
15	Ac	1751	0	1846	24	0
16	Ad	2076	0	2177	24	0
17	Ae	1509	0	1563	24	0
18	Af	1923	0	2089	44	0
19	Ag	1529	0	1627	23	0
20	Ah	1686	0	1772	31	0
21	Ai	1525	0	1640	14	0
22	Aj	810	0	836	10	0
23	Ak	1262	0	1335	11	0
24	Al	958	0	993	15	0
25	Am	1208	0	1293	15	0
26	An	1016	0	1039	16	0
27	Ao	1048	0	1093	10	0
28	Ap	1124	0	1193	15	0
29	Aq	1080	0	1135	13	0
30	Ar	1217	0	1279	18	0
31	As	1113	0	1145	16	0
32	At	821	0	883	7	0
33	Au	640	0	633	10	0
34	Av	1034	0	1080	12	0
35	Aw	1099	0	1162	16	0
36	Ax	1015	0	1086	15	0
37	Ay	683	0	761	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Az	239	0	289	1	0
39	B5	80772	0	40880	553	0
40	B7	2570	0	1295	12	0
41	B8	3319	0	1684	30	0
42	BA	1940	0	2028	20	0
43	BB	3206	0	3352	29	0
44	BC	2886	0	3057	20	0
45	BD	2398	0	2430	19	0
46	BE	1960	0	2153	24	0
47	BF	1886	0	2008	14	0
48	BG	1877	0	2023	13	0
49	BH	1516	0	1596	10	0
50	BI	1717	0	1764	21	0
51	BJ	1362	0	1399	10	0
52	BK	265	0	254	5	0
53	BL	1702	0	1820	19	0
54	BM	1137	0	1211	16	0
55	BN	1701	0	1749	15	0
56	BO	1630	0	1778	13	0
57	BP	1289	0	1329	18	0
58	BQ	1515	0	1634	14	0
59	BR	1508	0	1664	12	0
60	BS	1457	0	1492	12	0
61	BT	1298	0	1366	17	0
62	BU	806	0	827	8	0
63	BV	1034	0	1097	17	0
64	BW	991	0	1048	16	0
65	BX	967	0	1040	5	0
66	BY	1115	0	1205	5	0
67	BZ	1107	0	1182	13	0
68	Ba	1163	0	1202	15	0
69	Bb	881	0	957	10	0
70	Bc	836	0	888	8	0
71	Bd	888	0	930	10	0
72	Be	1070	0	1165	12	0
73	Bf	884	0	924	5	0
74	Bg	906	0	998	4	0
75	Bh	1013	0	1147	14	0
76	Bi	830	0	916	8	0
77	Bj	705	0	737	7	0
78	Bk	569	0	637	4	0
79	Bl	447	0	480	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	Bm	432	0	471	2	0
81	Bo	863	0	929	4	0
82	Bp	708	0	756	3	0
83	Br	1014	0	1083	11	0
84	Bs	1507	0	1564	32	0
85	Bt	1178	0	1235	38	0
86	Bv	1707	0	1815	41	0
87	A2	80	0	152	6	0
87	B5	210	0	399	18	0
87	BN	10	0	19	0	0
88	A2	14	0	26	2	0
88	B5	28	0	52	4	0
89	A2	110	0	0	0	0
89	AT	3	0	0	0	0
89	Af	1	0	0	0	0
89	B5	284	0	0	0	0
89	B7	9	0	0	0	0
89	B8	9	0	0	0	0
89	BP	1	0	0	0	0
89	BR	1	0	0	0	0
89	BV	1	0	0	0	0
89	Ba	1	0	0	0	0
90	A2	61	0	0	0	0
90	AT	4	0	0	0	0
90	Ad	1	0	0	0	0
90	An	1	0	0	0	0
90	Ar	1	0	0	0	0
90	B5	225	0	0	0	0
90	B7	6	0	0	0	0
90	B8	7	0	0	0	0
90	BA	4	0	0	0	0
90	BB	3	0	0	0	0
90	BC	1	0	0	0	0
90	BH	1	0	0	0	0
90	BI	1	0	0	0	0
90	BL	1	0	0	0	0
90	BN	1	0	0	0	0
90	BQ	2	0	0	0	0
90	BT	2	0	0	0	0
90	Bb	1	0	0	0	0
90	Be	2	0	0	0	0
90	Bf	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
90	Bg	1	0	0	0	0
90	Bj	1	0	0	0	0
90	Bl	1	0	0	0	0
90	Bo	1	0	0	0	0
91	AC	1	0	0	0	0
91	AE	1	0	0	0	0
91	AG	1	0	0	0	0
91	Bg	1	0	0	0	0
91	Bj	1	0	0	0	0
91	Bm	1	0	0	0	0
91	Bo	1	0	0	0	0
91	Bp	1	0	0	0	0
92	A2	1579	0	0	12	0
92	AA	6	0	0	0	0
92	AD	2	0	0	1	0
92	AE	19	0	0	2	0
92	AG	1	0	0	0	0
92	AH	14	0	0	0	0
92	AI	12	0	0	0	0
92	AT	35	0	0	1	0
92	AZ	1	0	0	0	0
92	Aa	16	0	0	0	0
92	Ab	10	0	0	1	0
92	Ad	9	0	0	0	0
92	Ae	4	0	0	0	0
92	Af	6	0	0	0	0
92	Ag	4	0	0	1	0
92	Ah	22	0	0	1	0
92	Ai	4	0	0	0	0
92	Ak	31	0	0	2	0
92	Am	22	0	0	0	0
92	An	20	0	0	1	0
92	Ap	10	0	0	0	0
92	Ar	2	0	0	0	0
92	As	4	0	0	0	0
92	At	4	0	0	0	0
92	Au	1	0	0	0	0
92	Av	16	0	0	0	0
92	Aw	23	0	0	1	0
92	Ax	1	0	0	0	0
92	Ay	1	0	0	0	0
92	Az	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	B5	7033	0	0	38	0
92	B7	199	0	0	4	0
92	B8	250	0	0	1	0
92	BA	114	0	0	2	0
92	BB	131	0	0	1	0
92	BC	148	0	0	2	0
92	BD	45	0	0	0	0
92	BE	34	0	0	0	0
92	BF	88	0	0	1	0
92	BG	34	0	0	0	0
92	BH	34	0	0	0	0
92	BI	64	0	0	1	0
92	BJ	13	0	0	0	0
92	BK	5	0	0	0	0
92	BL	79	0	0	0	0
92	BM	20	0	0	0	0
92	BN	139	0	0	0	0
92	BO	69	0	0	0	0
92	BP	51	0	0	0	0
92	BQ	84	0	0	1	0
92	BR	44	0	0	0	0
92	BS	58	0	0	0	0
92	BT	55	0	0	2	0
92	BU	5	0	0	0	0
92	BV	36	0	0	1	0
92	BW	15	0	0	1	0
92	BX	22	0	0	0	0
92	BY	21	0	0	0	0
92	BZ	12	0	0	0	0
92	Ba	87	0	0	1	0
92	Bb	24	0	0	0	0
92	Bc	13	0	0	0	0
92	Bd	31	0	0	0	0
92	Be	77	0	0	0	0
92	Bf	36	0	0	0	0
92	Bg	45	0	0	0	0
92	Bh	17	0	0	0	0
92	Bi	19	0	0	1	0
92	Bj	52	0	0	1	0
92	Bk	1	0	0	0	0
92	Bl	16	0	0	0	0
92	Bm	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
92	Bo	46	0	0	0	0
92	Bp	32	0	0	0	0
92	Br	41	0	0	1	0
All	All	237077	0	167991	1692	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1092:C:HO2'	34:Av:2:VAL:N	1.65	0.94
41:B8:81:C:HO2'	75:Bh:2:ALA:N	1.75	0.84
1:A2:926:G:H1	1:A2:1018:U:H3	1.26	0.81
39:B5:1:C:H42	41:B8:156:U:H3	1.31	0.79
39:B5:2194:OMC:HM22	39:B5:2195:U:H5'	1.68	0.74
57:BP:126:ARG:HG3	57:BP:140:MET:HE1	1.68	0.73
1:A2:46:A:OP2	92:A2:2101:HOH:O	2.08	0.71
28:Ap:132:PHE:O	28:Ap:140:ARG:NH2	2.23	0.71
1:A2:929:G:H1	1:A2:1014:U:H3	1.37	0.71
39:B5:1415:C:H5''	58:BQ:144:LYS:HG2	1.71	0.71
39:B5:3456:A2M:HM'2	39:B5:3457:G:H5'	1.73	0.71
39:B5:2444:A:N6	39:B5:2587:A:OP2	2.24	0.70
39:B5:1480:A:N7	92:B5:5560:HOH:O	2.25	0.70
39:B5:3555:G:N2	39:B5:3555:G:OP2	2.25	0.70
39:B5:3852:G:N2	48:BG:43:GLN:O	2.24	0.70
1:A2:1397:A:O2'	1:A2:1399:G:N7	2.24	0.69
39:B5:432:U:O2	87:B5:4924:SPD:N6	2.24	0.69
84:Bs:65:ILE:HG23	84:Bs:75:LEU:HB3	1.73	0.69
1:A2:1675:G:N7	28:Ap:17:LYS:NZ	2.41	0.69
13:Aa:44:ILE:HD12	13:Aa:69:VAL:HG21	1.75	0.69
84:Bs:48:ARG:HD3	85:Bt:123:ARG:HG2	1.73	0.69
86:Bv:74:CYS:SG	86:Bv:78:LYS:NZ	2.66	0.69
1:A2:577:A2M:HM'2	1:A2:578:U:H5'	1.75	0.69
7:AF:120:ILE:HB	7:AF:132:TRP:HB2	1.74	0.69
7:AF:256:ILE:HB	7:AF:270:LEU:HB2	1.75	0.69
39:B5:1299:G:OP1	58:BQ:108:ARG:NH2	2.24	0.69
39:B5:1763:G:H5''	61:BT:35:LYS:HE3	1.74	0.68
40:B7:105:C:OP2	50:BI:203:ARG:NH1	2.25	0.68
64:BW:2:LYS:NZ	64:BW:4:GLU:OE2	2.27	0.68
39:B5:198:A:OP2	66:BY:126:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:484:G:H3'	39:B5:485:U:H2'	1.76	0.68
60:BS:1:MET:HE3	60:BS:35:PRO:HD3	1.75	0.68
1:A2:953:G:H21	26:An:52:THR:HG21	1.58	0.67
86:Bv:63:PHE:O	86:Bv:152:LYS:NZ	2.27	0.67
39:B5:1605:A:H5''	87:B5:4920:SPD:H22	1.77	0.67
1:A2:1392:OMC:HM22	1:A2:1393:U:H5'	1.76	0.67
84:Bs:47:LEU:HB3	84:Bs:51:ALA:HB3	1.75	0.67
21:Ai:120:ALA:O	21:Ai:125:HIS:ND1	2.25	0.67
85:Bt:63:THR:HB	85:Bt:70:GLN:HB2	1.75	0.67
1:A2:1052:G:N7	92:A2:2142:HOH:O	2.28	0.67
7:AF:87:LEU:HB2	7:AF:101:PHE:HB2	1.77	0.67
39:B5:3600:G:H22	39:B5:3632:G:H1'	1.59	0.67
48:BG:58:PRO:HD2	48:BG:61:ILE:HD12	1.76	0.67
71:Bd:64:ILE:HG23	71:Bd:68:LEU:HD23	1.75	0.66
29:Aq:94:GLU:HG2	29:Aq:95:ILE:HG13	1.77	0.66
46:BE:227:LYS:HE2	46:BE:241:GLU:H	1.59	0.66
1:A2:1000:G:OP2	92:A2:2102:HOH:O	2.13	0.66
11:AT:32:OMC:HM22	11:AT:33:U:H5'	1.77	0.66
14:Ab:121:ARG:NH1	92:Ab:301:HOH:O	2.29	0.66
86:Bv:52:THR:HG22	86:Bv:156:LYS:HG2	1.78	0.66
63:BV:13:LYS:HD2	63:BV:128:LEU:HD21	1.77	0.66
1:A2:1522:C:OP2	30:Ar:136:THR:OG1	2.13	0.66
39:B5:2103:C:O2	83:Br:99:LYS:NZ	2.29	0.66
24:Al:91:LEU:HD22	24:Al:106:CYS:HB2	1.77	0.66
30:Ar:46:ARG:HG2	31:As:35:ASP:HB2	1.78	0.66
39:B5:4764:C:O2'	39:B5:4767:G:N3	2.28	0.66
3:AB:47:LYS:NZ	17:Ae:125:SER:O	2.29	0.65
39:B5:1879:G:N2	39:B5:4180:C:OP1	2.30	0.65
39:B5:4336:A2M:HM'2	39:B5:4337:U:H5'	1.77	0.65
19:Ag:106:ARG:NH1	92:Ag:201:HOH:O	2.29	0.65
24:Al:79:VAL:HG11	24:Al:85:LEU:HB2	1.78	0.65
41:B8:102:G:OP1	77:Bj:20:ARG:NH1	2.29	0.65
62:BU:100:LEU:HD13	62:BU:112:LEU:HD23	1.77	0.65
23:Ak:119:ASP:O	23:Ak:147:LYS:NZ	2.26	0.65
39:B5:1919:U:O4	85:Bt:57:ARG:NH2	2.29	0.65
7:AF:247:TRP:HB3	7:AF:258:ILE:HD11	1.79	0.65
39:B5:4373:U:OP2	92:B5:5503:HOH:O	2.14	0.65
1:A2:1056:A:N7	92:A2:2149:HOH:O	2.29	0.65
39:B5:3468:A:OP2	92:B5:5504:HOH:O	2.14	0.65
1:A2:1018:U:OP1	25:Am:62:GLN:NE2	2.29	0.65
50:BI:48:LEU:HB2	50:BI:142:LEU:HD23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:An:34:PHE:HB3	26:An:41:PHE:HB2	1.78	0.64
1:A2:1337:C:N4	1:A2:1338:4AC:O7	2.30	0.64
1:A2:64:A:H2	1:A2:83:A:H62	1.45	0.64
39:B5:2207:OMG:N7	92:B5:5718:HOH:O	2.30	0.64
39:B5:3397:G:N7	92:B5:5708:HOH:O	2.30	0.64
10:AI:9:N:H1'2	10:AI:45:N:H2'	1.79	0.64
39:B5:632:G:H5''	39:B5:633:U:H5'	1.79	0.64
39:B5:1694:C:O2	45:BD:3:PHE:N	2.30	0.64
39:B5:3843:G:H4'	39:B5:3844:C:H5'	1.79	0.64
5:AD:105:ARG:NH1	92:AD:201:HOH:O	2.31	0.64
39:B5:3373:U:OP2	39:B5:3378:A:N6	2.29	0.64
1:A2:612:G:N7	92:A2:2152:HOH:O	2.29	0.64
1:A2:672:A:N7	92:A2:2158:HOH:O	2.30	0.64
39:B5:4679:C:OP1	46:BE:159:ARG:NH1	2.31	0.64
36:Ax:57:VAL:HB	36:Ax:60:PHE:HE2	1.63	0.63
68:Ba:72:THR:HG22	68:Ba:110:LYS:HB3	1.79	0.63
30:Ar:98:VAL:HG11	30:Ar:106:LYS:HG3	1.80	0.63
86:Bv:89:ALA:HA	86:Bv:92:LYS:HD3	1.80	0.63
39:B5:2541:G:H21	74:Bg:28:ASN:HD21	1.46	0.63
28:Ap:58:LEU:HB3	28:Ap:62:ARG:HD2	1.80	0.63
39:B5:4364:OMG:H5''	63:BV:15:ARG:HB2	1.80	0.63
39:B5:1546:U:OP2	39:B5:2699:C:O2'	2.14	0.63
1:A2:165:G:N2	1:A2:165:G:OP2	2.32	0.62
36:Ax:117:VAL:HG11	36:Ax:125:VAL:HG21	1.81	0.62
39:B5:74:G:H5''	53:BL:59:VAL:HB	1.79	0.62
39:B5:3844:C:O2'	48:BG:43:GLN:NE2	2.32	0.62
86:Bv:117:ILE:HD13	86:Bv:137:LEU:HD21	1.80	0.62
1:A2:142:C:N4	1:A2:330:G:OP1	2.32	0.62
39:B5:1606:G:OP2	87:B5:4920:SPD:N1	2.31	0.62
39:B5:1919:U:OP2	85:Bt:92:ARG:NH1	2.33	0.62
39:B5:2143:A:N7	44:BC:143:ARG:NH1	2.46	0.62
39:B5:4379:G:OP2	87:B5:4917:SPD:N1	2.31	0.62
45:BD:83:LEU:HB3	45:BD:88:VAL:HB	1.79	0.62
15:Ac:177:LEU:HD13	15:Ac:182:LEU:HD13	1.82	0.62
13:Aa:71:LEU:HD11	13:Aa:189:ILE:HG23	1.82	0.62
85:Bt:10:ILE:HG12	85:Bt:65:GLN:HG2	1.81	0.62
1:A2:513:A2M:HM'2	1:A2:514:G:H5'	1.80	0.62
33:Au:38:GLU:OE2	33:Au:51:LYS:NZ	2.32	0.62
39:B5:1940:G:N2	39:B5:1955:C:O2	2.25	0.62
39:B5:2328:U:H3	39:B5:2336:G:H1	1.48	0.62
40:B7:55:A:O2'	51:BJ:151:ILE:O	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:1284:OMC:OP1	68:Ba:6:ARG:NH2	2.32	0.62
39:B5:4218:G:O2'	80:Bm:100:TYR:O	2.16	0.62
39:B5:1737:G:O2'	61:BT:60:LYS:NZ	2.32	0.62
39:B5:3991:G:N7	92:B5:5768:HOH:O	2.31	0.62
39:B5:291:U:OP1	88:B5:4915:SPM:N1	2.32	0.62
85:Bt:101:SER:HA	85:Bt:141:CYS:HA	1.82	0.62
26:An:101:GLY:HA3	26:An:134:PRO:HG2	1.82	0.62
39:B5:4666:G:OP2	39:B5:4666:G:N2	2.33	0.62
63:BV:13:LYS:HB3	63:BV:128:LEU:HD11	1.82	0.62
1:A2:1240:U:H5''	27:Ao:124:LYS:HD3	1.82	0.61
54:BM:40:GLY:HA3	54:BM:45:VAL:HB	1.82	0.61
68:Ba:89:ASN:OD1	68:Ba:92:LYS:NZ	2.31	0.61
20:Ah:205:ARG:NH2	92:Ah:301:HOH:O	2.31	0.61
1:A2:678:G:O6	88:A2:1909:SPM:N1	2.33	0.61
18:Af:161:PRO:HD3	64:BW:84:GLY:HA2	1.81	0.61
46:BE:115:MET:O	83:Br:87:ARG:NH1	2.32	0.61
39:B5:329:A:OP2	87:B5:4907:SPD:N10	2.32	0.61
39:B5:1394:U:O2'	47:BF:33:ARG:NE	2.32	0.61
39:B5:1639:A:OP1	68:Ba:47:LYS:NZ	2.32	0.61
86:Bv:183:ILE:HD13	86:Bv:206:ILE:HD13	1.82	0.61
39:B5:2003:G:N7	92:B5:5758:HOH:O	2.31	0.61
63:BV:69:LYS:NZ	63:BV:71:GLU:OE2	2.33	0.61
1:A2:1285:A:H2'	24:Al:91:LEU:HD21	1.82	0.61
39:B5:4366:OMU:OP2	39:B5:4416:C:N4	2.31	0.61
39:B5:1936:U:OP2	85:Bt:123:ARG:NH1	2.34	0.61
86:Bv:65:VAL:HG22	86:Bv:109:ALA:HB3	1.83	0.61
1:A2:382:C:OP2	20:Ah:31:ARG:NH2	2.34	0.61
19:Ag:57:ARG:NH2	19:Ag:89:GLY:O	2.31	0.61
39:B5:104:G:N7	92:B5:5779:HOH:O	2.31	0.61
39:B5:136:U:O4	75:Bh:79:LYS:NZ	2.28	0.61
39:B5:3518:U:OP1	39:B5:4296:G:O2'	2.14	0.61
39:B5:2106:A:OP1	83:Br:107:ARG:NH2	2.29	0.61
1:A2:1569:C:OP1	31:As:96:SER:OG	2.19	0.60
71:Bd:19:GLU:OE1	71:Bd:92:ARG:NH1	2.34	0.60
1:A2:430:C:O2'	1:A2:812:A:N1	2.34	0.60
15:Ac:64:ARG:NH1	22:Aj:73:ASN:OD1	2.30	0.60
39:B5:3450:A2M:HM'2	39:B5:3451:A:H5'	1.82	0.60
1:A2:1624:A:OP2	87:A2:1903:SPD:N1	2.34	0.60
49:BH:44:GLU:HB3	49:BH:58:ASP:HB2	1.82	0.60
60:BS:15:ARG:HB3	60:BS:27:LEU:HD23	1.83	0.60
1:A2:75:G:O2'	1:A2:77:A:OP1	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:AG:44:ARG:NH1	32:At:78:ASP:OD2	2.34	0.60
24:Al:89:VAL:HG11	24:Al:109:VAL:HG11	1.82	0.60
27:Ao:18:ARG:NH1	30:Ar:88:LYS:O	2.35	0.60
39:B5:2169:G:OP1	72:Be:108:ARG:NH2	2.34	0.60
86:Bv:114:GLU:HA	86:Bv:137:LEU:HD22	1.84	0.60
1:A2:1021:A:N1	87:A2:1906:SPD:N1	2.49	0.60
39:B5:3455:A:H2'	39:B5:3456:A2M:H8	1.83	0.60
44:BC:14:LYS:HA	44:BC:173:LYS:HD3	1.82	0.60
44:BC:201:ARG:NH2	92:BC:605:HOH:O	2.33	0.60
20:Ah:57:ALA:HB2	20:Ah:183:GLY:HA2	1.83	0.60
39:B5:1237:G:OP2	39:B5:1237:G:N2	2.26	0.60
1:A2:1684:C:H5'	17:Ae:130:ARG:HD2	1.84	0.60
39:B5:1458:A:H4'	39:B5:1459:G:H5'	1.81	0.60
39:B5:2470:C:OP1	62:BU:92:LYS:NZ	2.31	0.59
39:B5:4403:U:H3	87:B5:4917:SPD:H82	1.67	0.59
15:Ac:106:ARG:HG3	15:Ac:175:VAL:HB	1.83	0.59
49:BH:59:LYS:HE2	49:BH:66:GLU:HB3	1.84	0.59
1:A2:944:U:O2'	26:An:135:ILE:O	2.20	0.59
14:Ab:196:ILE:HB	14:Ab:223:TYR:HB2	1.83	0.59
30:Ar:26:ILE:HG13	30:Ar:45:LEU:HD21	1.84	0.59
39:B5:340:C:OP2	92:B5:5506:HOH:O	2.17	0.59
39:B5:2545:C:OP1	62:BU:101:ARG:NH2	2.33	0.59
59:BR:39:GLN:OE1	59:BR:42:ARG:NH1	2.35	0.59
61:BT:90:ASN:ND2	92:BT:301:HOH:O	2.30	0.59
7:AF:78:ALA:HB3	7:AF:90:TRP:HB2	1.84	0.59
22:Aj:61:GLN:HE21	22:Aj:62:PHE:H	1.50	0.59
39:B5:1260:OMG:HM22	39:B5:1261:U:H5'	1.83	0.59
50:BI:87:ILE:HG12	50:BI:138:ILE:HG12	1.85	0.59
67:BZ:92:ASP:HB3	67:BZ:95:VAL:HG12	1.84	0.59
84:Bs:30:VAL:HG12	84:Bs:189:ILE:HG12	1.83	0.59
1:A2:166:A2M:HM'2	1:A2:167:G:H5'	1.84	0.59
1:A2:1355:G:N2	1:A2:1358:A:OP2	2.33	0.59
3:AB:29:GLN:NE2	3:AB:66:ARG:O	2.36	0.59
39:B5:1806:A:N6	92:B5:5946:HOH:O	2.35	0.59
39:B5:186:G:N2	39:B5:186:G:OP2	2.32	0.59
19:Ag:162:GLN:OE1	19:Ag:165:ASN:ND2	2.34	0.59
1:A2:1594:C:H1'	31:As:12:GLN:HE22	1.65	0.59
39:B5:1741:A:O2'	39:B5:1776:A:OP1	2.20	0.59
41:B8:149:G:H21	48:BG:64:GLN:HE22	1.50	0.59
39:B5:3432:C:O2'	39:B5:3506:A:N3	2.33	0.58
1:A2:380:C:O2	20:Ah:5:ARG:NE	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BD:62:CYS:HB3	45:BD:105:LEU:HD22	1.84	0.58
53:BL:80:GLU:OE2	53:BL:102:ARG:NH2	2.36	0.58
12:AZ:177:MET:SD	12:AZ:180:ARG:NH2	2.76	0.58
39:B5:992:C:OP1	39:B5:1106:U:O2'	2.21	0.58
64:BW:81:ALA:HB2	64:BW:87:LEU:HB2	1.86	0.58
1:A2:1704:OMC:HM22	1:A2:1705:C:H5'	1.86	0.58
39:B5:1620:C:O2'	88:B5:4912:SPM:N1	2.37	0.58
58:BQ:65:ARG:NH2	92:BQ:306:HOH:O	2.37	0.58
85:Bt:80:LEU:HD13	85:Bt:112:ILE:HG23	1.85	0.58
7:AF:217:MET:HG2	7:AF:229:THR:HG22	1.84	0.58
18:Af:98:ARG:NH2	18:Af:103:ASP:OD1	2.37	0.58
1:A2:1311:U:H5''	4:AC:130:VAL:HG13	1.86	0.58
1:A2:1402:A:N6	1:A2:1442:U:O2'	2.37	0.58
35:Aw:93:PHE:O	35:Aw:140:ARG:NH1	2.36	0.58
39:B5:3930:G:H5'	42:BA:233:ARG:HB2	1.85	0.58
33:Au:32:ILE:HG12	33:Au:60:ARG:HD2	1.86	0.58
7:AF:87:LEU:HD21	7:AF:108:VAL:HG11	1.86	0.58
39:B5:3812:G:O6	42:BA:72:ARG:NH2	2.34	0.58
62:BU:28:PRO:HB2	62:BU:34:MET:HG2	1.85	0.58
12:AZ:17:LYS:HB3	12:AZ:173:LEU:HD11	1.86	0.58
20:Ah:10:LYS:O	20:Ah:18:ARG:NH1	2.37	0.58
1:A2:1299:G:H4'	27:Ao:78:THR:HA	1.86	0.57
12:AZ:108:PHE:HB2	12:AZ:136:GLU:HG2	1.84	0.57
39:B5:407:A:O2'	39:B5:410:A:OP1	2.20	0.57
39:B5:1915:G:N3	85:Bt:138:SER:OG	2.36	0.57
1:A2:485:A2M:O5'	1:A2:485:A2M:H8	2.05	0.57
1:A2:1131:G:OP2	1:A2:1131:G:N2	2.34	0.57
43:BB:41:VAL:HA	43:BB:187:GLY:HA3	1.85	0.57
57:BP:138:PRO:HB3	57:BP:140:MET:HE3	1.86	0.57
4:AC:102:VAL:HG21	24:Al:35:ILE:HG21	1.87	0.57
7:AF:167:SER:HG	7:AF:177:TRP:HE1	1.52	0.57
19:Ag:143:ARG:HB2	19:Ag:155:LYS:HB2	1.85	0.57
39:B5:1503:G:OP1	87:B5:4916:SPD:N10	2.36	0.57
1:A2:25:A:HO2'	1:A2:26:U:H6	1.53	0.57
1:A2:920:A:OP2	25:Am:64:ARG:NH2	2.37	0.57
2:AA:23:ARG:HH22	2:AA:29:ASN:HD21	1.50	0.57
6:AE:3:LYS:NZ	6:AE:8:ASN:OD1	2.38	0.57
39:B5:4268:G:O2'	39:B5:4271:C:OP2	2.20	0.57
27:Ao:37:TYR:O	30:Ar:88:LYS:NZ	2.38	0.57
55:BN:53:TYR:HB2	55:BN:133:ILE:HD13	1.85	0.57
16:Ad:11:ARG:HA	16:Ad:28:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Ar:22:GLY:HA2	30:Ar:56:ALA:HB3	1.86	0.57
67:BZ:50:PRO:HD3	67:BZ:68:ILE:HG12	1.86	0.57
83:Br:90:LEU:HD22	83:Br:111:ILE:HG23	1.85	0.57
15:Ac:70:THR:HG22	15:Ac:86:LEU:HD13	1.87	0.57
50:BI:101:LYS:NZ	50:BI:102:MET:O	2.35	0.57
1:A2:665:A:O2'	1:A2:671:A:N1	2.38	0.56
16:Ad:45:ILE:HA	16:Ad:61:VAL:HG11	1.85	0.56
18:Af:58:LYS:HA	18:Af:107:SER:HB2	1.86	0.56
26:An:151:LEU:O	92:An:301:HOH:O	2.18	0.56
39:B5:4394:A:OP1	59:BR:62:ARG:NH2	2.38	0.56
59:BR:70:ARG:HB3	59:BR:76:MET:HE2	1.86	0.56
1:A2:1172:G:O2'	1:A2:1188:G:O6	2.21	0.56
13:Aa:28:LYS:HB3	13:Aa:48:LEU:HD11	1.87	0.56
24:Al:49:LEU:HB3	24:Al:111:VAL:HB	1.87	0.56
39:B5:4416:C:O2'	63:BV:15:ARG:NH2	2.37	0.56
1:A2:920:A:O2'	87:A2:1906:SPD:N1	2.38	0.56
1:A2:1031:A:H2'	1:A2:1032:A2M:H8	1.86	0.56
1:A2:1598:C:H4'	1:A2:1604:G:C6	2.41	0.56
10:AI:55:N:H5'	86:Bv:48:ARG:HH21	1.70	0.56
19:Ag:144:ILE:HB	34:Av:52:ILE:HB	1.87	0.56
39:B5:1665:U:H5'	47:BF:134:ILE:HD11	1.86	0.56
39:B5:2538:A:OP1	78:Bk:35:LYS:NZ	2.32	0.56
64:BW:56:ARG:NH2	92:BW:201:HOH:O	2.36	0.56
86:Bv:36:ILE:HD11	86:Bv:165:LEU:HD12	1.87	0.56
86:Bv:204:LEU:HD22	86:Bv:216:LEU:HD23	1.88	0.56
24:Al:51:VAL:HB	24:Al:109:VAL:HG22	1.87	0.56
7:AF:5:MET:HG2	7:AF:312:VAL:HG22	1.86	0.56
39:B5:1399:G:OP2	39:B5:1399:G:N2	2.28	0.56
52:BK:4379:TYR:HB3	79:Bl:46:ARG:HH12	1.71	0.56
62:BU:105:ASN:OD1	62:BU:113:ARG:NH2	2.38	0.56
1:A2:381:G:OP1	20:Ah:31:ARG:NE	2.34	0.56
2:AA:84:HIS:OXT	25:Am:19:ARG:NH1	2.39	0.56
18:Af:129:VAL:O	64:BW:80:ARG:NH2	2.35	0.56
20:Ah:113:TYR:OH	20:Ah:156:ALA:O	2.23	0.56
1:A2:156:G:OP1	18:Af:2:LYS:NZ	2.36	0.56
10:AI:75:C:O2'	81:Bo:54:PRO:O	2.19	0.56
28:Ap:131:LYS:HB2	28:Ap:140:ARG:HH12	1.70	0.56
39:B5:1334:G:N2	39:B5:1337:G:OP2	2.39	0.56
39:B5:1788:U:H3'	53:BL:5:ARG:HH22	1.70	0.56
39:B5:2301:C:H5''	55:BN:67:ARG:HD2	1.88	0.56
84:Bs:102:LEU:HD11	84:Bs:187:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:4649:A:H4'	43:BB:95:THR:HG22	1.88	0.56
1:A2:1600:U:OP2	37:Ay:46:ASN:ND2	2.38	0.56
2:AA:11:SER:OG	2:AA:14:GLU:OE1	2.24	0.56
32:At:48:LEU:HD22	32:At:93:SER:HB3	1.88	0.56
34:Av:80:ASP:OD1	34:Av:124:LYS:NZ	2.31	0.56
39:B5:1924:G:H1'	39:B5:1942:G:H2'	1.88	0.56
43:BB:261:ARG:HB2	56:BO:64:THR:HG21	1.88	0.56
51:BJ:101:ASP:OD1	51:BJ:101:ASP:N	2.39	0.56
62:BU:111:GLU:OE2	62:BU:113:ARG:NE	2.32	0.56
1:A2:1598:C:OP2	37:Ay:85:ARG:NH2	2.33	0.56
16:Ad:87:MET:HE1	16:Ad:236:ILE:HG21	1.88	0.56
39:B5:3540:OMC:HM22	39:B5:3541:G:H5'	1.88	0.56
39:B5:4379:G:O6	92:B5:5505:HOH:O	2.16	0.56
87:B5:4924:SPD:H101	56:BO:91:LYS:HD3	1.68	0.56
1:A2:1245:PSU:H5''	4:AC:78:LYS:HD2	1.87	0.55
39:B5:793:C:N3	39:B5:794:G:N1	2.54	0.55
48:BG:229:ARG:NE	48:BG:232:GLU:OE2	2.38	0.55
1:A2:953:G:OP1	13:Aa:56:LYS:NZ	2.39	0.55
1:A2:1230:G:OP1	37:Ay:32:LYS:NZ	2.39	0.55
42:BA:137:ILE:HD11	42:BA:149:LYS:HB2	1.87	0.55
43:BB:291:TYR:HB3	43:BB:298:LEU:HD11	1.87	0.55
81:Bo:59:LYS:NZ	81:Bo:61:LYS:O	2.39	0.55
1:A2:434:A:H5''	20:Ah:22:HIS:HB3	1.88	0.55
1:A2:1448:OMG:HM22	1:A2:1449:A:H5'	1.87	0.55
7:AF:40:ILE:HB	7:AF:59:LEU:HB2	1.88	0.55
12:AZ:8:LEU:HD11	33:Au:39:VAL:HG11	1.89	0.55
19:Ag:34:SER:HA	19:Ag:37:LYS:HB2	1.87	0.55
42:BA:117:GLU:HG2	42:BA:124:GLY:H	1.71	0.55
85:Bt:64:ILE:HA	85:Bt:69:ALA:HA	1.88	0.55
1:A2:99:A2M:HM'2	1:A2:100:U:H5'	1.88	0.55
2:AA:67:THR:OG1	2:AA:70:LYS:O	2.25	0.55
39:B5:1653:C:O2'	47:BF:176:ARG:NH2	2.40	0.55
41:B8:58:G:N7	77:Bj:63:ARG:NH2	2.43	0.55
51:BJ:17:ILE:HD12	51:BJ:80:GLU:HG2	1.89	0.55
63:BV:46:LYS:NZ	92:BV:304:HOH:O	2.38	0.55
1:A2:930:G:OP1	70:Bc:5:LYS:NZ	2.36	0.55
5:AD:83:VAL:HG22	35:Aw:68:LYS:HE2	1.89	0.55
12:AZ:79:SER:HA	12:AZ:101:GLY:HA2	1.88	0.55
13:Aa:189:ILE:HB	13:Aa:190:PRO:HD3	1.87	0.55
39:B5:4512:G:OP1	49:BH:23:ARG:NH1	2.40	0.55
86:Bv:49:PHE:HB2	86:Bv:159:MET:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:642:A:OP1	21:Ai:40:LYS:NZ	2.39	0.55
1:A2:1085:A:OP1	1:A2:1859:G:O2'	2.25	0.55
39:B5:1423:C:OP1	68:Ba:132:ARG:NH2	2.38	0.55
39:B5:1918:A:N1	85:Bt:57:ARG:NH1	2.54	0.55
84:Bs:53:VAL:HG22	84:Bs:89:VAL:HG13	1.89	0.55
86:Bv:35:GLN:HB2	86:Bv:205:TYR:HB2	1.88	0.55
7:AF:214:GLY:HA2	7:AF:236:ILE:HG13	1.88	0.55
18:Af:22:ARG:HG2	18:Af:25:ARG:HH22	1.71	0.55
39:B5:3619:OMC:HM22	39:B5:3620:G:H5'	1.88	0.55
39:B5:4381:A:OP1	39:B5:4382:PSU:O2'	2.25	0.55
49:BH:44:GLU:OE2	54:BM:2:VAL:N	2.40	0.55
53:BL:91:ALA:HB1	53:BL:96:ILE:HB	1.89	0.55
27:Ao:44:ARG:HH21	27:Ao:53:GLN:HE21	1.54	0.55
39:B5:3620:G:H4'	87:B5:4924:SPD:H21	1.89	0.55
46:BE:151:THR:OG1	46:BE:203:LYS:NZ	2.39	0.55
48:BG:83:PHE:HA	48:BG:183:ILE:HD13	1.88	0.55
66:BY:30:MET:HB3	66:BY:101:PRO:HG2	1.88	0.55
85:Bt:53:TRP:HD1	85:Bt:56:LEU:HB2	1.72	0.55
1:A2:910:G:H5'	59:BR:176:ARG:HH12	1.72	0.55
20:Ah:106:SER:HB3	20:Ah:171:LEU:HG	1.88	0.55
25:Am:101:HIS:HA	25:Am:104:ARG:HH21	1.72	0.55
49:BH:23:ARG:HE	49:BH:39:ASN:HA	1.72	0.55
86:Bv:138:LEU:HD21	86:Bv:147:LYS:HG2	1.89	0.55
25:Am:130:LYS:NZ	25:Am:139:TRP:O	2.30	0.55
1:A2:679:U:OP2	1:A2:1027:C:N4	2.33	0.54
1:A2:1329:OMG:HM22	1:A2:1330:U:H5'	1.89	0.54
4:AC:116:ARG:NH1	4:AC:120:GLU:OE2	2.40	0.54
27:Ao:75:VAL:HB	27:Ao:104:GLN:HE21	1.71	0.54
39:B5:3374:A:C4	77:Bj:3:LYS:HB3	2.42	0.54
61:BT:88:ARG:NH2	69:Bb:30:GLU:OE2	2.35	0.54
1:A2:1832:A:H2'	1:A2:1833:6MZ:H8	1.88	0.54
7:AF:77:PHE:HB3	7:AF:89:LEU:HD11	1.89	0.54
8:AG:52:PHE:HB3	32:At:80:PHE:HB3	1.89	0.54
11:AT:29:A:H4'	30:Ar:148:VAL:HG11	1.88	0.54
39:B5:3682:U:H2'	39:B5:3683:G:C8	2.42	0.54
85:Bt:80:LEU:HD23	85:Bt:83:LYS:HD2	1.89	0.54
7:AF:133:ASN:HD21	7:AF:137:VAL:HB	1.71	0.54
7:AF:232:GLY:HA3	7:AF:252:THR:HG21	1.88	0.54
14:Ab:191:VAL:HG11	14:Ab:236:PHE:HA	1.89	0.54
39:B5:734:G:OP2	54:BM:71:LYS:NZ	2.37	0.54
39:B5:1341:A:N1	39:B5:1453:G:O2'	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:2257:G:H2'	39:B5:2258:OMU:H6	1.88	0.54
39:B5:2451:G:N7	92:B5:5856:HOH:O	2.33	0.54
39:B5:4735:C:OP1	71:Bd:32:ARG:NH1	2.41	0.54
41:B8:102:G:OP2	41:B8:104:A:O2'	2.25	0.54
1:A2:168:C:OP1	18:Af:131:ARG:NH2	2.40	0.54
15:Ac:45:ARG:NH2	15:Ac:82:GLY:O	2.41	0.54
39:B5:2330:G:H1'	41:B8:125:C:H1'	1.89	0.54
1:A2:292:G:N2	23:Ak:40:ILE:O	2.40	0.54
18:Af:2:LYS:HB3	18:Af:15:LEU:HD11	1.89	0.54
39:B5:4151:G:OP2	50:BI:7:ARG:NH2	2.37	0.54
41:B8:81:C:O2'	75:Bh:2:ALA:N	2.38	0.54
12:AZ:63:ARG:HH21	33:Au:38:GLU:HA	1.73	0.54
33:Au:43:THR:OG1	33:Au:45:ARG:NH1	2.41	0.54
39:B5:2568:A:N1	92:B5:5839:HOH:O	2.33	0.54
39:B5:3781:A:H5''	86:Bv:213:PRO:HD3	1.90	0.54
47:BF:104:VAL:HG13	47:BF:135:VAL:HG12	1.89	0.54
1:A2:421:G:O2'	1:A2:661:C:N3	2.37	0.54
1:A2:1513:C:H5''	8:AG:8:TRP:HZ3	1.72	0.54
18:Af:148:SER:N	18:Af:151:ASP:OD2	2.41	0.54
39:B5:1458:A:H62	58:BQ:87:THR:HG21	1.71	0.54
39:B5:2007:C:N4	92:B5:5844:HOH:O	2.33	0.54
50:BI:55:ASP:OD2	50:BI:164:LYS:NZ	2.41	0.54
51:BJ:90:ARG:NH2	51:BJ:108:GLY:O	2.39	0.54
85:Bt:14:TYR:O	85:Bt:31:LYS:NZ	2.40	0.54
14:Ab:85:SER:OG	33:Au:25:GLY:O	2.25	0.54
24:Al:11:VAL:HG13	24:Al:13:ASP:H	1.72	0.54
39:B5:1937:A:N3	39:B5:1958:C:O2'	2.34	0.54
39:B5:4082:A:N7	92:B5:5849:HOH:O	2.33	0.54
7:AF:29:ASP:OD1	7:AF:47:ARG:NH1	2.37	0.54
84:Bs:125:ALA:HA	84:Bs:154:ILE:HB	1.90	0.54
1:A2:642:A:O2'	1:A2:646:C:OP1	2.25	0.54
3:AB:32:VAL:HG11	3:AB:56:LEU:HD12	1.90	0.54
79:BI:20:ASN:ND2	79:BI:42:ARG:O	2.39	0.54
1:A2:840:C:H42	36:Ax:48:TYR:HA	1.74	0.53
11:AT:46:7MG:O2'	11:AT:48:C:OP2	2.26	0.53
24:Al:75:ASN:OD1	24:Al:75:ASN:N	2.41	0.53
26:An:16:SER:OG	26:An:17:LEU:N	2.41	0.53
37:Ay:73:VAL:HG21	37:Ay:88:LEU:HD21	1.89	0.53
39:B5:1217:G:H4'	46:BE:77:ALA:HB2	1.89	0.53
84:Bs:30:VAL:HG21	84:Bs:187:LEU:HD13	1.90	0.53
86:Bv:94:ASN:O	86:Bv:97:LYS:NZ	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1846:A:H2'	1:A2:1847:G:C8	2.43	0.53
6:AE:10:ARG:NH1	92:AE:303:HOH:O	2.40	0.53
37:Ay:74:SER:OG	37:Ay:79:ILE:O	2.21	0.53
39:B5:1070:U:O2	45:BD:286:SER:OG	2.24	0.53
39:B5:3628:C:O2'	43:BB:268:ARG:NH1	2.40	0.53
51:BJ:13:ARG:O	51:BJ:136:ARG:NH1	2.42	0.53
52:BK:4370:CYS:HB2	52:BK:4377:LYS:HG2	1.91	0.53
72:Be:117:GLN:O	83:Br:119:ARG:NH2	2.37	0.53
78:Bk:57:LYS:NZ	78:Bk:68:GLU:OE2	2.36	0.53
84:Bs:68:HIS:HB3	84:Bs:75:LEU:HD22	1.90	0.53
28:Ap:53:GLU:OE1	28:Ap:85:ARG:NH2	2.39	0.53
39:B5:2325:C:H2'	39:B5:2326:G:H8	1.73	0.53
50:BI:69:ARG:NH1	92:BI:408:HOH:O	2.38	0.53
39:B5:1297:G:N7	58:BQ:104:ARG:NH2	2.56	0.53
39:B5:2259:G:N2	39:B5:2270:G:N7	2.54	0.53
39:B5:4020:A:H2'	39:B5:4021:G:C8	2.44	0.53
39:B5:755:G:H1	39:B5:800:U:H3	1.57	0.53
39:B5:4445:U:H1'	39:B5:4446:A:H5''	1.90	0.53
39:B5:4480:A:H61	39:B5:4704:U:H3	1.56	0.53
92:B5:5771:HOH:O	56:BO:82:ARG:NH1	2.41	0.53
43:BB:384:GLU:OE2	64:BW:14:TYR:OH	2.26	0.53
1:A2:1009:A:OP2	70:Bc:8:LYS:NZ	2.36	0.53
39:B5:1394:U:HO2'	47:BF:33:ARG:HE	1.51	0.53
39:B5:4636:G:O2'	39:B5:4666:G:N7	2.40	0.53
1:A2:1286:G:H1	24:Al:57:ASP:HB2	1.73	0.53
7:AF:42:MET:O	7:AF:56:GLN:N	2.40	0.53
14:Ab:102:LEU:HD22	14:Ab:130:ILE:HG12	1.90	0.53
20:Ah:162:LEU:HD11	20:Ah:191:GLU:HG2	1.89	0.53
39:B5:4708:C:O2'	57:BP:75:GLN:NE2	2.41	0.53
69:Bb:101:HIS:O	69:Bb:109:ARG:NH1	2.37	0.53
7:AF:99:ARG:NH2	7:AF:135:LEU:O	2.41	0.53
30:Ar:44:VAL:HG11	30:Ar:71:MET:HG3	1.91	0.53
39:B5:184:U:H3	39:B5:253:G:H1	1.57	0.53
39:B5:1215:G:H5''	69:Bb:110:ALA:HB1	1.90	0.53
49:BH:92:MET:HE2	49:BH:179:ILE:HG22	1.91	0.53
62:BU:47:ILE:HD12	62:BU:63:ILE:HD11	1.90	0.53
75:Bh:13:LYS:NZ	75:Bh:16:GLU:OE2	2.41	0.53
81:Bo:26:TYR:HB3	81:Bo:67:VAL:HB	1.91	0.53
86:Bv:32:VAL:HA	86:Bv:208:SER:HA	1.91	0.53
1:A2:445:G:O6	20:Ah:26:LYS:HE3	2.09	0.53
7:AF:12:LYS:HG2	7:AF:306:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Ae:19:LEU:HD21	17:Ae:69:VAL:HG11	1.90	0.53
24:Al:25:ALA:O	24:Al:30:GLY:N	2.39	0.53
63:BV:87:SER:HB3	64:BW:19:ARG:HH21	1.74	0.53
64:BW:96:GLN:O	64:BW:101:ARG:NH2	2.41	0.53
1:A2:1551:G:H3'	1:A2:1580:A:H61	1.73	0.53
12:AZ:94:THR:HG23	12:AZ:186:ARG:HH12	1.73	0.53
39:B5:1757:G:OP2	39:B5:1757:G:N2	2.32	0.53
39:B5:4190:C:OP1	92:B5:5507:HOH:O	2.18	0.53
85:Bt:116:MET:HG3	85:Bt:132:ILE:HD11	1.91	0.53
16:Ad:124:CYS:HB3	16:Ad:141:THR:HB	1.91	0.52
20:Ah:123:ARG:NH1	20:Ah:133:GLU:OE1	2.42	0.52
39:B5:328:A:OP2	92:B5:5509:HOH:O	2.19	0.52
39:B5:4283:C:H2'	39:B5:4284:G:C8	2.43	0.52
68:Ba:100:ILE:HG13	68:Ba:123:ILE:HB	1.91	0.52
85:Bt:82:ILE:HA	85:Bt:85:LEU:HD12	1.90	0.52
1:A2:1316:U:H4'	22:Aj:2:LEU:HG	1.91	0.52
16:Ad:87:MET:HE2	16:Ad:123:LEU:HB2	1.92	0.52
18:Af:144:LEU:O	64:BW:94:ARG:NH1	2.42	0.52
39:B5:1820:OMC:OP1	92:B5:5508:HOH:O	2.19	0.52
47:BF:42:ARG:NH1	92:BF:305:HOH:O	2.37	0.52
85:Bt:105:THR:HG22	85:Bt:107:ASP:H	1.73	0.52
65:BX:73:HIS:CD2	65:BX:115:LYS:HD3	2.44	0.52
1:A2:521:A:O2'	1:A2:826:A:N3	2.34	0.52
1:A2:1118:C:O2'	1:A2:1119:C:O4'	2.28	0.52
1:A2:1827:G:HO2'	39:B5:3491:A:HO2'	1.55	0.52
7:AF:133:ASN:HB3	7:AF:139:LYS:HE3	1.92	0.52
1:A2:378:G:H5'	20:Ah:98:LYS:HB3	1.91	0.52
17:Ae:129:GLY:HA3	17:Ae:135:ARG:HH22	1.73	0.52
57:BP:115:GLU:OE1	57:BP:151:THR:OG1	2.27	0.52
15:Ac:39:VAL:HG22	15:Ac:48:ILE:HG22	1.90	0.52
25:Am:136:PRO:HG2	25:Am:139:TRP:HB2	1.92	0.52
39:B5:1934:G:O6	39:B5:1939:G:N2	2.42	0.52
1:A2:518:OMC:HM22	1:A2:519:G:H5'	1.91	0.52
20:Ah:67:TRP:NE1	20:Ah:191:GLU:OE2	2.43	0.52
21:Ai:113:GLN:OE1	21:Ai:154:GLN:NE2	2.39	0.52
39:B5:1672:G:N3	39:B5:3960:A:H2'	2.25	0.52
85:Bt:18:THR:OG1	85:Bt:21:GLU:O	2.26	0.52
85:Bt:95:GLN:HG3	85:Bt:98:ILE:HG12	1.92	0.52
1:A2:1486:U:OP1	15:Ac:151:LYS:NZ	2.42	0.52
37:Ay:91:LEU:HD22	37:Ay:96:LEU:HD12	1.92	0.52
39:B5:1809:C:H2'	39:B5:1810:A2M:H8	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:3894:C:OP1	67:BZ:59:LYS:NZ	2.34	0.52
39:B5:4639:C:O2'	39:B5:4641:C:OP2	2.24	0.52
20:Ah:141:ARG:HB2	20:Ah:146:GLN:HG2	1.91	0.52
21:Ai:114:VAL:HG12	21:Ai:120:ALA:HB2	1.92	0.52
29:Aq:29:HIS:HA	29:Aq:32:LYS:HE2	1.92	0.52
39:B5:1879:G:H22	39:B5:4180:C:H5''	1.75	0.52
39:B5:4367:C:OP1	63:BV:48:ARG:HD2	2.09	0.52
51:BJ:15:LEU:HD12	51:BJ:165:TRP:HB2	1.92	0.52
57:BP:40:HIS:NE2	57:BP:110:ASP:O	2.38	0.52
39:B5:1283:U:H2'	39:B5:1284:OMC:C6	2.45	0.52
39:B5:1391:C:O2'	69:Bb:106:ARG:NH2	2.43	0.52
39:B5:1572:G:H1'	39:B5:2356:A:N6	2.25	0.52
39:B5:3620:G:H1'	87:B5:4924:SPD:H42	1.91	0.52
19:Ag:146:VAL:HG12	34:Av:42:MET:HE1	1.92	0.51
75:Bh:4:ILE:HD12	75:Bh:53:SER:HB3	1.92	0.51
83:Br:26:SER:OG	83:Br:28:GLU:OE1	2.18	0.51
7:AF:203:ASP:OD1	7:AF:205:SER:OG	2.26	0.51
39:B5:3643:C:H2'	39:B5:3644:U:C6	2.45	0.51
39:B5:4037:G:H5'	39:B5:4039:PSU:C6	2.44	0.51
7:AF:120:ILE:O	7:AF:132:TRP:N	2.39	0.51
26:An:92:ALA:HA	26:An:125:LYS:HB2	1.92	0.51
39:B5:1276:C:H2'	39:B5:1277:A:C8	2.45	0.51
39:B5:1788:U:H3'	53:BL:5:ARG:NH2	2.25	0.51
39:B5:4124:A:O2'	39:B5:4125:A:H2'	2.09	0.51
40:B7:6:C:H4'	45:BD:52:ILE:HD13	1.92	0.51
44:BC:301:ALA:HB1	58:BQ:132:LYS:HE3	1.92	0.51
55:BN:155:VAL:O	55:BN:162:ARG:NH2	2.36	0.51
84:Bs:53:VAL:HG13	84:Bs:89:VAL:HG22	1.93	0.51
5:AD:122:THR:HG21	5:AD:126:LYS:HG2	1.92	0.51
39:B5:4381:A:H3'	39:B5:4382:PSU:H4'	1.93	0.51
45:BD:37:VAL:HG12	45:BD:50:ARG:HD3	1.93	0.51
59:BR:44:LEU:HD22	59:BR:49:LEU:HD12	1.92	0.51
7:AF:154:VAL:O	7:AF:155:ARG:NH1	2.39	0.51
16:Ad:182:MET:HB2	16:Ad:228:ILE:HD13	1.91	0.51
18:Af:138:ALA:HA	18:Af:176:ILE:HD11	1.92	0.51
39:B5:184:U:H3	39:B5:253:G:H22	1.59	0.51
39:B5:1693:U:H4'	39:B5:1694:C:H5'	1.92	0.51
43:BB:161:ARG:HG2	43:BB:184:GLN:HA	1.91	0.51
53:BL:81:LEU:HD12	53:BL:86:ILE:HB	1.92	0.51
1:A2:17:C:O2'	1:A2:1195:A:N1	2.37	0.51
1:A2:1315:U:O2'	22:Aj:8:ARG:NH2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:1491:OMG:HM22	1:A2:1492:G:H5'	1.93	0.51
39:B5:2363:C:O2	39:B5:2483:G:N2	2.44	0.51
85:Bt:127:GLY:HA2	85:Bt:130:LYS:HD3	1.93	0.51
86:Bv:35:GLN:HG3	86:Bv:166:ALA:HB2	1.93	0.51
86:Bv:73:HIS:ND1	86:Bv:144:MET:SD	2.79	0.51
1:A2:602:OMG:HM22	1:A2:603:G:H5'	1.92	0.51
18:Af:78:SER:HB3	18:Af:92:ARG:HG2	1.93	0.51
39:B5:788:G:H2'	39:B5:789:G:H8	1.75	0.51
39:B5:1726:A:N3	39:B5:3956:U:O2'	2.43	0.51
15:Ac:18:LYS:HE2	15:Ac:39:VAL:HB	1.93	0.51
39:B5:172:C:O2	75:Bh:112:ARG:NH1	2.43	0.51
39:B5:364:G:O6	77:Bj:55:ARG:NH2	2.41	0.51
39:B5:1897:A:O2'	39:B5:1964:A:N1	2.43	0.51
1:A2:657:G:H5'	1:A2:663:G:N2	2.25	0.51
1:A2:1256:G:OP1	1:A2:1257:G:O2'	2.16	0.51
1:A2:1446:PSU:O2	1:A2:1447:A:N6	2.43	0.51
7:AF:11:LEU:HB2	7:AF:307:VAL:HB	1.93	0.51
18:Af:131:ARG:O	64:BW:83:THR:N	2.41	0.51
20:Ah:116:HIS:O	20:Ah:152:ARG:NH2	2.36	0.51
39:B5:62:A:OP1	55:BN:172:ARG:NH1	2.42	0.51
39:B5:398:A2M:O5'	39:B5:398:A2M:H8	2.11	0.51
39:B5:788:G:H2'	39:B5:789:G:C8	2.46	0.51
39:B5:4487:A:H2'	39:B5:4639:C:H5	1.76	0.51
42:BA:30:ARG:NH1	42:BA:36:GLU:OE2	2.37	0.51
64:BW:57:ARG:HA	64:BW:63:GLN:HE22	1.75	0.51
1:A2:1500:U:H4'	15:Ac:176:LEU:HD13	1.93	0.51
39:B5:1224:C:O2'	44:BC:321:ASN:OD1	2.22	0.51
39:B5:1539:G:N7	87:B5:4909:SPD:N10	2.58	0.51
39:B5:1955:C:H2'	39:B5:1956:A:H8	1.76	0.51
57:BP:54:LYS:HA	57:BP:83:TRP:CD1	2.46	0.51
72:Be:89:LEU:HD13	72:Be:118:LEU:HD22	1.93	0.51
79:Bl:42:ARG:HG3	79:Bl:47:THR:HG23	1.93	0.51
84:Bs:32:ALA:HB1	84:Bs:35:VAL:HG21	1.93	0.51
1:A2:64:A:OP1	18:Af:177:GLN:NE2	2.44	0.50
1:A2:477:A:N3	1:A2:489:U:O2'	2.38	0.50
10:AI:9:N:H4'	10:AI:46:N:H5'	1.93	0.50
12:AZ:176:TRP:HE1	12:AZ:197:VAL:HG23	1.76	0.50
39:B5:3625:C:O2'	39:B5:4718:A:N1	2.42	0.50
39:B5:4745:U:H4'	39:B5:4746:A:H5'	1.93	0.50
1:A2:921:A:O2'	1:A2:923:A:OP1	2.26	0.50
14:Ab:182:CYS:HB2	34:Av:95:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:1532:G:O2'	39:B5:1567:G:H4'	2.12	0.50
86:Bv:94:ASN:HB2	86:Bv:123:ILE:HB	1.93	0.50
1:A2:1390:C:OP1	29:Aq:43:SER:OG	2.20	0.50
27:Ao:22:LEU:HA	27:Ao:25:LEU:HD12	1.93	0.50
39:B5:1105:C:O2	69:Bb:91:ARG:NE	2.35	0.50
71:Bd:37:GLY:O	71:Bd:41:ARG:HG3	2.10	0.50
85:Bt:32:ILE:HB	85:Bt:35:LEU:HD11	1.92	0.50
39:B5:1016:C:O2'	39:B5:1059:G:O4'	2.30	0.50
39:B5:1542:G:OP1	92:B5:5511:HOH:O	2.20	0.50
39:B5:2601:G:O2'	39:B5:2608:A:N3	2.41	0.50
1:A2:127:C:O2	16:Ad:134:LYS:NZ	2.37	0.50
14:Ab:254:ASP:HB2	33:Au:1:AME:HT22	1.94	0.50
39:B5:308:G:OP2	39:B5:308:G:N2	2.37	0.50
61:BT:93:ILE:HA	61:BT:96:ILE:HG12	1.93	0.50
73:Bf:43:LEU:O	73:Bf:109:ARG:NH1	2.40	0.50
1:A2:1227:G:N1	1:A2:1640:7MG:OP2	2.34	0.50
11:AT:20:G:OP2	51:BJ:58:ARG:NH2	2.35	0.50
12:AZ:206:ASP:OD1	12:AZ:206:ASP:N	2.38	0.50
17:Ae:40:ALA:HB1	17:Ae:45:TYR:CG	2.46	0.50
39:B5:369:G:N2	39:B5:372:A:OP2	2.37	0.50
39:B5:1933:C:H2'	39:B5:1934:G:H8	1.77	0.50
39:B5:3699:G:N2	86:Bv:164:CYS:SG	2.84	0.50
12:AZ:33:GLN:HB3	12:AZ:154:LEU:HD12	1.94	0.50
23:Ak:18:GLN:HG2	23:Ak:33:LEU:HD21	1.94	0.50
39:B5:347:A:O2'	44:BC:50:GLN:NE2	2.42	0.50
39:B5:1907:G:H2'	39:B5:1908:G:H8	1.77	0.50
39:B5:2252:U:H4'	39:B5:2271:A:H4'	1.94	0.50
39:B5:2422:G:N2	39:B5:2425:A:OP2	2.35	0.50
39:B5:3386:G:O2'	39:B5:3425:U:OP1	2.26	0.50
39:B5:4018:G:OP2	39:B5:4018:G:N2	2.35	0.50
56:BO:130:LYS:HB2	56:BO:133:ARG:HG2	1.93	0.50
86:Bv:111:LEU:HD21	86:Bv:151:VAL:HG21	1.92	0.50
1:A2:463:OMC:HM22	1:A2:464:C:H5'	1.94	0.50
1:A2:647:G:N7	92:A2:2196:HOH:O	2.34	0.50
1:A2:1093:G:OP1	25:Am:2:GLY:N	2.45	0.50
1:A2:1532:A:H4'	1:A2:1606:G:H4'	1.92	0.50
39:B5:1859:C:H3'	39:B5:1860:C:H5''	1.92	0.50
39:B5:3497:G:O2'	39:B5:3499:C:N4	2.45	0.50
39:B5:3655:A:H2'	39:B5:3656:C:C6	2.47	0.50
43:BB:90:VAL:HG13	43:BB:161:ARG:HB2	1.92	0.50
1:A2:30:C:O2'	1:A2:597:U:OP1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Ag:130:LEU:HD21	19:Ag:156:VAL:HG21	1.93	0.50
39:B5:1935:C:H42	39:B5:1939:G:H22	1.59	0.50
46:BE:181:PRO:HD2	46:BE:184:LEU:HD12	1.94	0.50
39:B5:2250:G:O6	79:Bl:2:SER:N	2.44	0.49
46:BE:193:HIS:HB3	46:BE:196:PHE:HD2	1.77	0.49
65:BX:82:THR:HG22	65:BX:155:ILE:HG23	1.94	0.49
83:Br:38:PHE:O	83:Br:45:HIS:NE2	2.30	0.49
86:Bv:128:LEU:HD13	86:Bv:135:PRO:HD3	1.93	0.49
1:A2:65:C:C6	18:Af:174:PRO:HB3	2.47	0.49
30:Ar:46:ARG:HH12	30:Ar:52:LEU:HD11	1.77	0.49
36:Ax:39:GLU:N	36:Ax:39:GLU:OE1	2.45	0.49
39:B5:779:G:H2'	39:B5:780:G:H8	1.76	0.49
39:B5:2142:G:H3'	39:B5:2143:A:H5''	1.94	0.49
57:BP:64:ASN:ND2	57:BP:80:GLN:OE1	2.45	0.49
1:A2:485:A2M:HM'2	1:A2:486:A:C4	2.47	0.49
12:AZ:52:LYS:HB2	29:Aq:109:LEU:HD13	1.95	0.49
18:Af:102:VAL:HG13	18:Af:106:LEU:HD12	1.94	0.49
39:B5:1214:A:H61	39:B5:2054:G:H21	1.58	0.49
39:B5:1959:U:H5''	84:Bs:57:LYS:HG3	1.94	0.49
39:B5:4202:OMC:HM22	39:B5:4203:PSU:H5''	1.94	0.49
39:B5:4641:C:H2'	39:B5:4642:G:C8	2.47	0.49
1:A2:437:OMG:HM22	1:A2:438:G:H5'	1.95	0.49
1:A2:1764:G:H2'	1:A2:1765:G:C8	2.48	0.49
39:B5:4073:C:OP1	61:BT:70:HIS:NE2	2.44	0.49
39:B5:4403:U:N3	87:B5:4917:SPD:H82	2.26	0.49
84:Bs:31:GLY:N	84:Bs:188:ILE:O	2.33	0.49
18:Af:137:ARG:HB3	18:Af:140:ARG:HG3	1.94	0.49
21:Ai:152:ASP:OD1	21:Ai:152:ASP:N	2.37	0.49
39:B5:3351:G:N7	87:B5:4913:SPD:H72	2.28	0.49
86:Bv:85:MET:HE2	86:Bv:93:LEU:HD21	1.93	0.49
1:A2:57:U:OP1	1:A2:505:G:O2'	2.31	0.49
1:A2:1092:C:O2'	34:Av:2:VAL:N	2.39	0.49
1:A2:1564:G:OP1	31:As:121:ARG:NH1	2.45	0.49
7:AF:244:ASN:ND2	7:AF:294:ASP:O	2.46	0.49
16:Ad:107:GLY:HA2	16:Ad:189:LEU:HG	1.95	0.49
18:Af:5:ILE:HG12	18:Af:111:LEU:HB2	1.94	0.49
39:B5:1095:C:H2'	39:B5:1096:G:H8	1.78	0.49
39:B5:1276:C:H2'	39:B5:1277:A:H8	1.78	0.49
39:B5:4006:U:H2'	39:B5:4007:C:C6	2.47	0.49
39:B5:4448:G:N7	92:B5:5931:HOH:O	2.35	0.49
1:A2:228:C:H42	1:A2:902:G:H1'	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:1701:C:H2'	39:B5:1702:C:C6	2.47	0.49
39:B5:2101:C:O2	46:BE:94:THR:OG1	2.28	0.49
39:B5:2499:U:H5''	67:BZ:38:TYR:HB3	1.94	0.49
39:B5:3351:G:H22	39:B5:3356:A:H1'	1.78	0.49
50:BI:53:VAL:HG11	61:BT:158:PHE:HZ	1.78	0.49
64:BW:63:GLN:N	64:BW:63:GLN:OE1	2.44	0.49
67:BZ:95:VAL:HG13	67:BZ:96:VAL:HG23	1.93	0.49
72:Be:78:LEU:O	83:Br:20:ARG:NH1	2.40	0.49
14:Ab:94:ILE:HG21	14:Ab:162:ILE:HD12	1.94	0.49
39:B5:109:G:OP2	53:BL:74:ARG:NH2	2.40	0.49
39:B5:1093:C:H2'	39:B5:1094:A:C8	2.48	0.49
40:B7:26:C:OP2	92:B7:301:HOH:O	2.18	0.49
50:BI:187:GLU:HG3	50:BI:189:ARG:HG3	1.95	0.49
57:BP:131:ARG:HG3	57:BP:137:ASN:ND2	2.28	0.49
1:A2:956:A:N1	1:A2:969:U:O2'	2.44	0.49
31:As:60:THR:HG23	31:As:75:MET:HE2	1.94	0.49
39:B5:4287:G:N2	39:B5:4290:A:OP2	2.42	0.49
71:Bd:59:THR:HG21	71:Bd:103:TYR:HA	1.95	0.49
85:Bt:133:LEU:HD11	85:Bt:151:ILE:HG13	1.95	0.49
23:Ak:132:ARG:NH2	92:Ak:208:HOH:O	2.42	0.49
36:Ax:78:SER:OG	36:Ax:80:ASP:OD1	2.24	0.49
39:B5:67:C:OP2	39:B5:312:G:N2	2.46	0.49
1:A2:563:U:H2'	1:A2:564:G:C8	2.48	0.48
1:A2:1293:C:N3	4:AC:138:ARG:NH2	2.55	0.48
5:AD:83:VAL:HG11	35:Aw:91:LEU:HB3	1.95	0.48
25:Am:67:THR:HG21	25:Am:74:ILE:HD11	1.95	0.48
39:B5:4727:U:OP2	43:BB:123:HIS:ND1	2.40	0.48
83:Br:82:ILE:HG22	83:Br:89:THR:HG22	1.95	0.48
17:Ae:167:LYS:NZ	17:Ae:175:ASP:OD2	2.33	0.48
23:Ak:89:ARG:NH1	23:Ak:91:ASP:OD1	2.47	0.48
39:B5:1489:A2M:N3	77:Bj:11:ARG:HB2	2.29	0.48
39:B5:2205:U:H2'	39:B5:2206:A2M:H8	1.95	0.48
39:B5:3934:U:H2'	39:B5:3935:U:C6	2.48	0.48
85:Bt:125:LEU:HD12	85:Bt:164:ALA:HB3	1.96	0.48
1:A2:1566:C:OP2	31:As:101:ARG:NH1	2.46	0.48
6:AE:44:ILE:HD12	6:AE:65:PRO:HG2	1.95	0.48
19:Ag:43:LEU:HB3	19:Ag:72:PHE:CE1	2.48	0.48
29:Aq:109:LEU:HG	29:Aq:111:PHE:HD2	1.77	0.48
39:B5:1924:G:OP1	39:B5:1924:G:N2	2.46	0.48
42:BA:101:VAL:HG22	42:BA:165:VAL:HG22	1.95	0.48
86:Bv:15:ARG:HH21	86:Bv:18:LEU:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AF:195:LEU:HA	7:AF:211:GLY:HA3	1.94	0.48
16:Ad:151:ASP:HB3	16:Ad:154:ILE:HG13	1.96	0.48
39:B5:1898:U:H1'	39:B5:1900:G:C2	2.48	0.48
39:B5:3670:G:OP1	55:BN:24:ARG:NE	2.46	0.48
39:B5:3791:U:H2'	39:B5:3792:C:C6	2.49	0.48
45:BD:208:MET:HE3	45:BD:233:PRO:HG3	1.96	0.48
84:Bs:30:VAL:HA	84:Bs:189:ILE:HA	1.95	0.48
24:Al:72:HIS:CD2	24:Al:74:ILE:HD11	2.47	0.48
27:Ao:64:LYS:HZ1	27:Ao:92:SER:HG	1.54	0.48
39:B5:1869:U:OP2	56:BO:49:ARG:NH1	2.34	0.48
1:A2:1222:G:O2'	1:A2:1677:U:O2	2.27	0.48
1:A2:1746:A:O3'	18:Af:31:ARG:NH1	2.45	0.48
8:AG:20:SER:OG	22:Aj:65:ARG:NH1	2.46	0.48
15:Ac:209:SER:HB3	29:Aq:40:ILE:HB	1.95	0.48
24:Al:41:ALA:HB1	24:Al:47:ALA:HB2	1.96	0.48
39:B5:1621:C:H4'	88:B5:4912:SPM:H31	1.95	0.48
43:BB:93:VAL:HG23	43:BB:102:PHE:HB2	1.96	0.48
46:BE:81:ARG:HA	46:BE:84:ARG:HD2	1.96	0.48
68:Ba:24:LYS:NZ	92:Ba:405:HOH:O	2.38	0.48
72:Be:35:TRP:CZ2	72:Be:56:PRO:HD2	2.49	0.48
1:A2:908:G:H2'	1:A2:909:A:C8	2.49	0.48
12:AZ:85:ARG:NH2	29:Aq:82:ASP:O	2.44	0.48
15:Ac:132:LYS:HE3	15:Ac:191:PRO:HA	1.94	0.48
39:B5:4361:C:H5''	43:BB:357:ARG:NE	2.29	0.48
60:BS:99:ASP:OD1	60:BS:100:LEU:N	2.47	0.48
84:Bs:58:ASN:O	84:Bs:62:ARG:HG3	2.14	0.48
1:A2:381:G:N1	1:A2:384:G:OP2	2.32	0.48
18:Af:162:LEU:HD11	18:Af:172:LYS:HB2	1.95	0.48
39:B5:1264:U:O2'	39:B5:1830:A:N1	2.47	0.48
39:B5:1847:A:N7	92:B5:5947:HOH:O	2.35	0.48
39:B5:3552:G:N7	92:B5:5930:HOH:O	2.35	0.48
39:B5:3634:A:OP1	92:B5:5512:HOH:O	2.20	0.48
68:Ba:85:GLN:HA	68:Ba:88:VAL:HG22	1.96	0.48
77:Bj:27:TYR:HA	77:Bj:34:CYS:HA	1.96	0.48
1:A2:191:A:H3'	1:A2:192:C:H5''	1.96	0.48
1:A2:381:G:OP1	20:Ah:56:ARG:NH2	2.42	0.48
1:A2:523:A:H5''	21:Ai:145:PRO:HD2	1.95	0.48
1:A2:571:C:O2'	36:Ax:34:THR:O	2.28	0.48
1:A2:1320:U:H2'	1:A2:1321:G:C8	2.49	0.48
13:Aa:103:MET:HE1	13:Aa:212:VAL:O	2.13	0.48
29:Aq:57:LEU:HD13	29:Aq:69:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Ar:16:LEU:HD21	30:Ar:72:GLN:HE21	1.78	0.48
36:Ax:7:ILE:HG22	36:Ax:27:VAL:HG22	1.96	0.48
39:B5:1922:A:H4'	39:B5:1923:A:C8	2.48	0.48
39:B5:2007:C:OP1	73:Bf:15:LYS:NZ	2.47	0.48
39:B5:2161:G:N2	39:B5:2164:G:OP2	2.38	0.48
39:B5:3588:A:H5''	57:BP:83:TRP:O	2.13	0.48
39:B5:4282:OMC:HM22	39:B5:4283:C:O4'	2.14	0.48
47:BF:126:LYS:HB2	61:BT:133:ALA:HB3	1.95	0.48
1:A2:1051:A:OP1	87:A2:1905:SPD:H92	2.14	0.48
39:B5:1435:C:O2'	39:B5:1437:G:OP2	2.23	0.48
39:B5:1712:U:H2'	39:B5:1713:C:C6	2.48	0.48
40:B7:24:C:H2'	40:B7:25:G:O4'	2.14	0.48
41:B8:105:C:OP2	92:B8:301:HOH:O	2.20	0.48
41:B8:106:G:H4'	41:B8:137:A:H5'	1.96	0.48
63:BV:21:PRO:HA	63:BV:54:ALA:HA	1.96	0.48
1:A2:1063:A:OP1	87:A2:1905:SPD:H52	2.13	0.47
13:Aa:179:ASN:HB3	13:Aa:183:GLU:HB2	1.96	0.47
58:BQ:119:LYS:HE3	58:BQ:121:LEU:HD21	1.96	0.47
3:AB:27:CYS:SG	17:Ae:126:THR:HG21	2.54	0.47
19:Ag:73:GLN:HA	19:Ag:76:GLN:HB2	1.97	0.47
21:Ai:97:ILE:HA	21:Ai:100:LEU:HD13	1.96	0.47
33:Au:39:VAL:HG13	33:Au:44:GLY:HA2	1.96	0.47
39:B5:790:G:O2'	39:B5:792:G:O4'	2.29	0.47
39:B5:2250:G:OP2	39:B5:2250:G:N2	2.46	0.47
39:B5:4269:A2M:H5''	39:B5:4270:G:H5'	1.96	0.47
39:B5:4422:G:OP1	43:BB:281:ASN:ND2	2.40	0.47
39:B5:4773:A:H2'	39:B5:4774:U:O4'	2.14	0.47
45:BD:108:ARG:CZ	45:BD:253:TYR:HB2	2.43	0.47
54:BM:47:ARG:NH1	54:BM:68:ALA:O	2.47	0.47
1:A2:167:G:O3'	64:BW:80:ARG:NH1	2.48	0.47
1:A2:869:G:OP2	1:A2:869:G:N2	2.34	0.47
1:A2:1567:G:N7	31:As:101:ARG:NH2	2.61	0.47
1:A2:1649:G:O2'	1:A2:1675:G:O6	2.32	0.47
5:AD:86:VAL:HA	5:AD:89:GLN:HE21	1.78	0.47
13:Aa:92:GLN:NE2	13:Aa:229:MET:SD	2.73	0.47
13:Aa:99:ASN:OD1	13:Aa:100:PHE:N	2.47	0.47
39:B5:2167:C:O2'	72:Be:98:GLU:OE2	2.25	0.47
39:B5:2272:A:OP1	79:Bl:43:HIS:NE2	2.40	0.47
39:B5:2692:A:OP2	87:B5:4903:SPD:H52	2.15	0.47
39:B5:4270:G:C2	43:BB:252:ALA:HB1	2.49	0.47
43:BB:17:LEU:HD21	43:BB:235:TRP:HH2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:BC:140:LYS:HE3	44:BC:245:HIS:HB2	1.97	0.47
50:BI:91:LEU:HD12	50:BI:135:ILE:HG23	1.96	0.47
63:BV:48:ARG:HH21	63:BV:49:LEU:HB3	1.79	0.47
84:Bs:65:ILE:HA	84:Bs:75:LEU:HD23	1.96	0.47
1:A2:191:A:H62	1:A2:208:G:H21	1.61	0.47
1:A2:1034:G:N1	1:A2:1081:A:O2'	2.37	0.47
1:A2:1229:A:H2'	1:A2:1230:G:C8	2.49	0.47
5:AD:83:VAL:HG12	35:Aw:89:GLY:HA2	1.97	0.47
39:B5:1503:G:O2'	39:B5:2655:A:N3	2.43	0.47
39:B5:3681:A:H5'	76:Bi:65:LYS:HE2	1.96	0.47
60:BS:173:ASN:ND2	60:BS:175:PHE:O	2.34	0.47
86:Bv:114:GLU:N	86:Bv:138:LEU:O	2.44	0.47
1:A2:74:G:H2'	1:A2:75:G:H8	1.78	0.47
1:A2:204:G:OP2	20:Ah:147:LYS:NZ	2.46	0.47
1:A2:496:U:H4'	16:Ad:24:THR:HG22	1.96	0.47
7:AF:290:ALA:HB3	7:AF:299:PHE:HB2	1.96	0.47
11:AT:33:U:H4'	11:AT:37:YYG:H243	1.96	0.47
12:AZ:77:ILE:HD11	12:AZ:99:ILE:HD12	1.95	0.47
17:Ae:102:LEU:HD21	37:Ay:100:VAL:HG21	1.95	0.47
39:B5:1350:G:H1	39:B5:1366:C:H42	1.61	0.47
39:B5:2363:C:H2'	39:B5:2364:G:C8	2.49	0.47
39:B5:3464:A:H2'	39:B5:3465:A:C8	2.49	0.47
61:BT:18:PRO:HG2	61:BT:21:LYS:HB2	1.95	0.47
86:Bv:104:ALA:O	86:Bv:133:LYS:NZ	2.38	0.47
1:A2:909:A:H5''	59:BR:172:ARG:HH12	1.79	0.47
1:A2:1234:G:OP1	92:A2:2103:HOH:O	2.20	0.47
1:A2:1498:G:N7	22:Aj:25:LYS:NZ	2.40	0.47
1:A2:1525:G:O2'	11:AT:30:G:OP1	2.31	0.47
7:AF:101:PHE:CD2	7:AF:136:GLY:HA2	2.49	0.47
11:AT:62:C:H2'	11:AT:63:G:H8	1.80	0.47
39:B5:18:C:H4'	55:BN:138:PHE:CD2	2.50	0.47
39:B5:1922:A:H1'	39:B5:1949:A:H4'	1.95	0.47
39:B5:2216:C:H5'	71:Bd:46:LEU:HD22	1.95	0.47
39:B5:2678:A:O2'	43:BB:228:TYR:O	2.27	0.47
39:B5:4292:A:N7	42:BA:215:ASN:ND2	2.60	0.47
45:BD:223:PHE:HB3	45:BD:226:TYR:HB2	1.96	0.47
70:Bc:99:PRO:HG3	70:Bc:105:ILE:HG13	1.96	0.47
1:A2:1038:G:H4'	1:A2:1846:A:H4'	1.97	0.47
6:AE:2:THR:N	92:AE:304:HOH:O	2.48	0.47
7:AF:129:ILE:HB	7:AF:142:VAL:HB	1.95	0.47
8:AG:56:ASP:OXT	32:At:79:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ac:68:GLU:HG3	22:Aj:93:THR:HG21	1.95	0.47
39:B5:58:G:H4'	39:B5:59:A:H4'	1.97	0.47
39:B5:95:G:N7	53:BL:11:LYS:NZ	2.61	0.47
39:B5:1313:C:N4	87:B5:4922:SPD:H31	2.30	0.47
39:B5:1811:G:O2'	39:B5:3965:A:N3	2.43	0.47
39:B5:2548:G:O6	59:BR:46:LYS:NZ	2.28	0.47
39:B5:3669:C:H1'	55:BN:125:SER:HB3	1.96	0.47
42:BA:206:PRO:HG3	42:BA:213:GLY:HA3	1.97	0.47
43:BB:95:THR:OG1	43:BB:98:GLY:O	2.27	0.47
48:BG:257:LYS:O	48:BG:261:LEU:N	2.46	0.47
79:Bl:30:LYS:HB2	79:Bl:33:ASN:HB2	1.96	0.47
84:Bs:106:LYS:HB3	84:Bs:184:SER:HB3	1.96	0.47
1:A2:745:G:N3	19:Ag:109:ARG:NH2	2.63	0.47
17:Ae:71:ARG:NH2	17:Ae:148:ASN:OD1	2.48	0.47
37:Ay:68:ILE:HB	37:Ay:109:TYR:HB2	1.96	0.47
39:B5:1907:G:H2'	39:B5:1908:G:C8	2.50	0.47
42:BA:2:GLY:N	92:BA:416:HOH:O	2.48	0.47
58:BQ:122:THR:OG1	58:BQ:124:ASP:OD1	2.27	0.47
72:Be:23:HIS:HD2	72:Be:43:ASN:HD21	1.63	0.47
1:A2:1443:OMU:HM22	1:A2:1444:C:H5'	1.97	0.47
3:AB:37:ASP:OD2	3:AB:39:SER:OG	2.31	0.47
32:At:60:THR:HG23	32:At:81:GLN:HG3	1.96	0.47
39:B5:1404:C:HO2'	39:B5:2044:A:HO2'	1.60	0.47
39:B5:2249:G:N7	79:Bl:2:SER:N	2.63	0.47
39:B5:2338:U:H2'	39:B5:2339:G:H8	1.80	0.47
84:Bs:85:ASN:OD1	84:Bs:85:ASN:N	2.45	0.47
1:A2:17:C:H2'	1:A2:18:C:C6	2.49	0.47
6:AE:37:LYS:HD2	6:AE:70:LYS:HZ1	1.79	0.47
55:BN:178:HIS:HA	55:BN:181:HIS:NE2	2.30	0.47
59:BR:37:SER:H	59:BR:40:GLN:HE21	1.61	0.47
71:Bd:54:MET:HE3	71:Bd:60:PRO:HA	1.97	0.47
15:Ac:123:LEU:HD22	15:Ac:152:PHE:HB3	1.96	0.46
25:Am:83:ASP:OD1	25:Am:83:ASP:N	2.47	0.46
39:B5:835:G:OP1	54:BM:44:ARG:NH1	2.47	0.46
39:B5:1270:A2M:OP2	39:B5:4191:U:O2'	2.30	0.46
39:B5:2386:A:H2'	39:B5:2387:G:C8	2.50	0.46
39:B5:3439:U:H2'	39:B5:3440:C:C6	2.51	0.46
39:B5:4638:G:H5'	39:B5:4639:C:OP2	2.15	0.46
67:BZ:22:LYS:NZ	67:BZ:129:TRP:O	2.44	0.46
69:Bb:56:LYS:O	69:Bb:60:ASN:ND2	2.34	0.46
85:Bt:15:LEU:HD22	85:Bt:16:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:77:A:H4'	18:Af:157:VAL:HG11	1.96	0.46
39:B5:1125:C:H5	46:BE:62:SER:HB2	1.80	0.46
39:B5:1394:U:HO2'	47:BF:33:ARG:NE	2.12	0.46
39:B5:1545:C:H5''	39:B5:1546:U:O5'	2.15	0.46
39:B5:2687:A:O2'	39:B5:4377:G:H4'	2.14	0.46
39:B5:3668:A:OP1	87:B5:4923:SPD:N10	2.48	0.46
39:B5:4203:PSU:H1'	43:BB:252:ALA:HB3	1.97	0.46
41:B8:47:C:H1'	41:B8:61:A:H2'	1.96	0.46
45:BD:65:ALA:HB2	45:BD:74:ILE:HD13	1.97	0.46
45:BD:119:TYR:OH	45:BD:139:PRO:O	2.34	0.46
85:Bt:105:THR:HB	85:Bt:108:GLU:HG3	1.95	0.46
1:A2:1416:C:O2'	31:As:132:ASP:OD2	2.27	0.46
1:A2:1680:A:H2'	17:Ae:60:ARG:HD2	1.96	0.46
1:A2:1739:C:OP1	18:Af:92:ARG:NH1	2.32	0.46
1:A2:1805:OMU:HM22	1:A2:1806:G:H5'	1.97	0.46
13:Aa:129:THR:OG1	13:Aa:131:ASP:OD1	2.31	0.46
31:As:40:ALA:HB3	31:As:43:LYS:HG2	1.97	0.46
39:B5:1416:C:OP1	58:BQ:144:LYS:NZ	2.46	0.46
39:B5:4620:U:C4	54:BM:113:MET:HG3	2.50	0.46
40:B7:61:G:N7	92:B7:311:HOH:O	2.36	0.46
43:BB:224:LYS:HE3	43:BB:340:THR:HG22	1.98	0.46
70:Bc:4:ALA:O	70:Bc:7:THR:OG1	2.32	0.46
71:Bd:38:PHE:HB3	71:Bd:78:ARG:HG2	1.98	0.46
84:Bs:121:VAL:HG22	84:Bs:182:PRO:HB3	1.97	0.46
86:Bv:48:ARG:HH22	86:Bv:161:LYS:HD2	1.79	0.46
17:Ae:76:MET:HE1	17:Ae:169:ILE:HD11	1.97	0.46
18:Af:213:LEU:HG	18:Af:217:MET:HE2	1.97	0.46
19:Ag:25:GLN:O	19:Ag:29:GLU:HG2	2.15	0.46
26:An:136:PRO:HB3	26:An:139:SER:HB3	1.97	0.46
39:B5:308:G:O6	55:BN:12:ARG:NH1	2.48	0.46
42:BA:30:ARG:HG3	42:BA:76:PHE:HZ	1.81	0.46
52:BK:4370:CYS:SG	52:BK:4372:VAL:HG12	2.56	0.46
55:BN:43:THR:OG1	55:BN:131:GLU:OE2	2.27	0.46
59:BR:15:LEU:HD13	59:BR:52:ARG:HB2	1.98	0.46
1:A2:65:C:N4	18:Af:134:GLY:O	2.41	0.46
1:A2:1233:PSU:H2'	1:A2:1234:G:C8	2.51	0.46
1:A2:1607:G:N2	1:A2:1633:G:H1'	2.31	0.46
4:AC:107:LYS:HB3	4:AC:117:LEU:HD11	1.97	0.46
12:AZ:80:ARG:O	12:AZ:84:GLN:HG3	2.16	0.46
39:B5:394:G:N2	39:B5:397:G:OP2	2.38	0.46
39:B5:1130:C:H42	39:B5:1209:G:H1	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:4627:C:H2'	39:B5:4628:G:H8	1.81	0.46
39:B5:4792:U:H3'	39:B5:4793:C:C6	2.51	0.46
48:BG:99:ALA:HB1	48:BG:136:LEU:HD11	1.96	0.46
56:BO:61:ARG:HA	56:BO:70:PRO:HD2	1.97	0.46
1:A2:28:U:H2'	1:A2:29:G:H8	1.81	0.46
13:Aa:190:PRO:O	13:Aa:192:SER:N	2.47	0.46
39:B5:1936:U:H4'	84:Bs:44:ARG:CZ	2.45	0.46
39:B5:4068:G:N2	39:B5:4071:A:OP2	2.41	0.46
39:B5:4159:C:OP2	87:B5:4921:SPD:H92	2.16	0.46
40:B7:12:U:OP2	40:B7:67:C:O2'	2.34	0.46
44:BC:201:ARG:NH2	92:BC:620:HOH:O	2.47	0.46
57:BP:111:SER:HB2	57:BP:153:LYS:O	2.16	0.46
1:A2:1537:G:H2'	1:A2:1538:A:C8	2.51	0.46
12:AZ:76:VAL:HG23	12:AZ:87:VAL:HG13	1.98	0.46
35:Aw:131:LEU:HD11	35:Aw:135:LYS:HE3	1.97	0.46
39:B5:2136:U:H2'	39:B5:2137:G:C8	2.51	0.46
39:B5:4204:C:H2'	39:B5:4205:U:C6	2.51	0.46
39:B5:4684:G:N1	73:Bf:3:GLY:O	2.41	0.46
50:BI:84:GLY:O	50:BI:140:THR:OG1	2.29	0.46
76:Bi:26:HIS:O	76:Bi:29:ARG:HG3	2.16	0.46
1:A2:387:C:H5'	20:Ah:7:ASN:HD22	1.81	0.46
1:A2:495:C:N4	1:A2:510:OMG:HN22	2.14	0.46
1:A2:1143:G:N2	1:A2:1146:A:OP2	2.37	0.46
16:Ad:44:LEU:HD21	16:Ad:72:ILE:HD11	1.98	0.46
20:Ah:130:THR:OG1	20:Ah:132:GLU:OE1	2.26	0.46
20:Ah:130:THR:HG23	20:Ah:133:GLU:H	1.81	0.46
39:B5:519:C:H2'	39:B5:520:G:C8	2.50	0.46
39:B5:1266:1MA:OP1	92:B5:5513:HOH:O	2.20	0.46
39:B5:1785:G:H2'	39:B5:1786:C:C6	2.51	0.46
39:B5:3380:A:H1'	39:B5:3517:A2M:N6	2.30	0.46
71:Bd:23:ARG:HG2	71:Bd:121:ASN:HA	1.96	0.46
1:A2:454:C:O2'	18:Af:92:ARG:O	2.23	0.46
1:A2:1102:U:H2'	1:A2:1103:G:C8	2.51	0.46
1:A2:1544:U:OP1	28:Ap:37:ARG:NH1	2.45	0.46
1:A2:1763:C:H2'	1:A2:1764:G:C8	2.51	0.46
1:A2:1812:C:OP1	35:Aw:37:LYS:NZ	2.47	0.46
29:Aq:109:LEU:HG	29:Aq:111:PHE:CD2	2.50	0.46
39:B5:1772:G:N2	39:B5:1774:G:O4'	2.48	0.46
39:B5:1960:G:OP1	84:Bs:58:ASN:ND2	2.47	0.46
39:B5:3450:A2M:H8	39:B5:3450:A2M:O5'	2.16	0.46
48:BG:73:ARG:NH1	48:BG:241:VAL:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:BW:89:ASP:O	64:BW:93:LYS:HG2	2.16	0.46
1:A2:1294:A:H61	1:A2:1307:U:H3	1.63	0.46
12:AZ:52:LYS:NZ	33:Au:83:PHE:O	2.49	0.46
12:AZ:125:THR:HG22	12:AZ:175:TRP:CZ2	2.50	0.46
28:Ap:101:ASP:OD1	28:Ap:102:GLU:N	2.49	0.46
35:Aw:18:ARG:NH1	92:Aw:202:HOH:O	2.49	0.46
39:B5:1955:C:H2'	39:B5:1956:A:C8	2.51	0.46
39:B5:2267:OMG:HM22	39:B5:2269:U:C6	2.51	0.46
39:B5:4135:C:H2'	39:B5:4136:A:C8	2.51	0.46
1:A2:585:A:P	21:Ai:169:ARG:HH12	2.39	0.45
1:A2:903:G:H2'	1:A2:904:A:H8	1.81	0.45
1:A2:1098:G:H4'	12:AZ:32:PHE:CD1	2.52	0.45
1:A2:1641:A:H5''	10:AI:35:N:H4'	1.97	0.45
1:A2:1757:C:H2'	1:A2:1758:G:C8	2.51	0.45
39:B5:423:G:H5'	57:BP:26:PHE:HZ	1.81	0.45
50:BI:85:PHE:CD2	50:BI:87:ILE:HG13	2.52	0.45
60:BS:93:MET:HE1	60:BS:117:HIS:CE1	2.50	0.45
60:BS:147:ASP:HB3	60:BS:150:ILE:HB	1.98	0.45
1:A2:675:C:H2'	1:A2:676:U:C6	2.52	0.45
1:A2:1747:U:P	18:Af:31:ARG:HH12	2.39	0.45
17:Ae:73:THR:O	17:Ae:89:THR:HG21	2.16	0.45
39:B5:1095:C:H2'	39:B5:1096:G:C8	2.52	0.45
39:B5:1588:G:H5'	39:B5:1589:A:OP1	2.17	0.45
39:B5:1772:G:OP1	61:BT:120:LYS:NZ	2.49	0.45
39:B5:2719:OMG:HM22	39:B5:2720:G:O5'	2.16	0.45
39:B5:3451:A:N6	92:B5:6635:HOH:O	2.47	0.45
42:BA:118:GLU:OE2	42:BA:156:LYS:NZ	2.50	0.45
45:BD:60:ILE:HB	45:BD:80:ALA:HB2	1.98	0.45
76:Bi:73:ILE:O	76:Bi:77:VAL:HG22	2.16	0.45
1:A2:1014:U:OP1	1:A2:1130:G:O2'	2.33	0.45
13:Aa:86:LEU:HB3	13:Aa:98:THR:HB	1.98	0.45
19:Ag:65:PRO:HD2	19:Ag:68:GLN:HE21	1.82	0.45
39:B5:382:G:N1	39:B5:385:A:OP2	2.48	0.45
39:B5:693:C:H2'	39:B5:694:G:H8	1.81	0.45
39:B5:1210:C:H2'	39:B5:1211:G:H8	1.81	0.45
39:B5:1308:U:OP2	53:BL:36:ARG:NH2	2.39	0.45
66:BY:134:LYS:HE3	66:BY:134:LYS:HB3	1.83	0.45
80:Bm:94:MET:HG2	80:Bm:105:PRO:HA	1.97	0.45
1:A2:1691:U:H2'	1:A2:1692:U:C6	2.51	0.45
12:AZ:77:ILE:HG13	12:AZ:99:ILE:HB	1.99	0.45
19:Ag:27:LEU:HD21	19:Ag:83:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Ax:76:TYR:OH	36:Ax:86:GLU:OE1	2.23	0.45
39:B5:1905:C:H2'	39:B5:1906:A:H8	1.82	0.45
44:BC:159:GLU:HA	44:BC:217:ILE:HB	1.98	0.45
63:BV:87:SER:HA	63:BV:97:TYR:HB3	1.97	0.45
78:Bk:36:VAL:HG13	78:Bk:43:TYR:HB2	1.99	0.45
85:Bt:108:GLU:HA	85:Bt:111:ASN:HD21	1.81	0.45
1:A2:71:G:O6	18:Af:170:ARG:NH1	2.49	0.45
1:A2:658:U:O2	92:A2:2105:HOH:O	2.21	0.45
19:Ag:134:VAL:O	19:Ag:137:SER:OG	2.25	0.45
39:B5:684:C:OP2	46:BE:114:LYS:NZ	2.39	0.45
39:B5:4088:C:O3'	81:Bo:37:GLY:HA3	2.16	0.45
39:B5:4314:A:O3'	43:BB:21:ARG:NH2	2.49	0.45
39:B5:4648:A:OP1	56:BO:163:LYS:NZ	2.44	0.45
44:BC:112:HIS:HB3	55:BN:203:TYR:CE1	2.51	0.45
1:A2:240:G:H2'	1:A2:241:G:C8	2.51	0.45
1:A2:858:U:H2'	1:A2:859:A:C8	2.52	0.45
15:Ac:175:VAL:HG13	15:Ac:182:LEU:HB2	1.99	0.45
20:Ah:124:LYS:HE2	39:B5:4762:C:H5'	1.99	0.45
39:B5:1909:A:N6	39:B5:1955:C:OP2	2.49	0.45
39:B5:2599:G:O6	67:BZ:51:ARG:NH2	2.34	0.45
39:B5:3465:A:H2'	39:B5:3466:PSU:O4'	2.16	0.45
39:B5:4202:OMC:HM21	43:BB:241:PRO:HD3	1.98	0.45
40:B7:11:A:N1	40:B7:66:G:O2'	2.41	0.45
50:BI:61:SER:HA	50:BI:126:VAL:HG12	1.98	0.45
84:Bs:65:ILE:HG21	84:Bs:79:LEU:HB2	1.97	0.45
1:A2:1649:G:N7	28:Ap:17:LYS:HE2	2.31	0.45
13:Aa:136:ARG:HB2	13:Aa:218:LEU:HD11	1.99	0.45
15:Ac:163:PRO:O	15:Ac:167:TYR:HB2	2.17	0.45
16:Ad:79:ASP:HB3	16:Ad:82:TYR:HB2	1.99	0.45
21:Ai:83:ARG:HH21	21:Ai:150:ARG:NH1	2.14	0.45
39:B5:637:C:H2'	39:B5:638:G:C8	2.52	0.45
39:B5:1632:PSU:H4'	39:B5:1635:G:N1	2.32	0.45
39:B5:1942:G:N2	39:B5:1943:U:O4	2.46	0.45
39:B5:1984:G:O6	39:B5:3602:C:O2'	2.35	0.45
39:B5:3966:6MZ:O5'	39:B5:3966:6MZ:H8	2.17	0.45
39:B5:4234:A:H4'	39:B5:4235:G:C8	2.52	0.45
42:BA:23:ARG:O	92:BA:401:HOH:O	2.21	0.45
43:BB:120:LYS:NZ	92:BB:612:HOH:O	2.46	0.45
53:BL:178:ALA:N	68:Ba:134:GLU:OE2	2.40	0.45
55:BN:84:PRO:HA	55:BN:87:HIS:CG	2.52	0.45
57:BP:16:LYS:O	57:BP:101:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:BZ:9:LYS:HB3	67:BZ:25:ILE:HD12	1.97	0.45
87:A2:1903:SPD:N1	30:Ar:133:GLY:O	2.49	0.45
39:B5:260:C:H2'	39:B5:261:G:H8	1.81	0.45
39:B5:4709:C:OP1	57:BP:74:LYS:NZ	2.43	0.45
44:BC:76:ILE:HD12	44:BC:77:PRO:HD2	1.98	0.45
51:BJ:144:LYS:O	51:BJ:148:THR:OG1	2.25	0.45
15:Ac:116:ARG:HG2	15:Ac:150:MET:HE1	1.98	0.45
19:Ag:8:ILE:HD13	19:Ag:16:PRO:HB3	1.98	0.45
37:Ay:102:LYS:HD2	37:Ay:107:VAL:HG12	1.99	0.45
39:B5:1465:G:N7	92:B5:5982:HOH:O	2.36	0.45
39:B5:1727:A:H2'	50:BI:22:PHE:CZ	2.52	0.45
39:B5:1947:U:H1'	39:B5:1950:C:H5	1.82	0.45
39:B5:4705:A:H5'	43:BB:128:LYS:HG3	1.98	0.45
45:BD:208:MET:HG2	45:BD:223:PHE:CE2	2.51	0.45
46:BE:89:GLU:CD	46:BE:89:GLU:H	2.25	0.45
86:Bv:204:LEU:N	86:Bv:216:LEU:O	2.49	0.45
1:A2:51:U:H2'	1:A2:52:G:C8	2.52	0.45
7:AF:119:GLN:HB3	7:AF:131:LEU:HD11	1.99	0.45
7:AF:207:CYS:SG	7:AF:219:TRP:HB2	2.57	0.45
15:Ac:93:THR:HG22	15:Ac:95:GLY:H	1.80	0.45
18:Af:164:LYS:HG2	18:Af:165:GLU:H	1.81	0.45
25:Am:93:LYS:HA	25:Am:150:VAL:HG21	1.98	0.45
31:As:39:LEU:HD21	31:As:52:TRP:CZ3	2.52	0.45
34:Av:30:CYS:SG	34:Av:31:SER:N	2.89	0.45
39:B5:1101:C:H42	47:BF:65:ARG:CZ	2.30	0.45
39:B5:1227:G:N1	39:B5:2015:G:OP1	2.34	0.45
39:B5:3468:A:H2'	39:B5:3469:A:C8	2.52	0.45
39:B5:4131:A:O2'	92:B5:5502:HOH:O	2.13	0.45
41:B8:26:C:O2'	44:BC:53:ALA:O	2.31	0.45
45:BD:216:GLU:O	45:BD:220:LYS:HG2	2.17	0.45
47:BF:141:TRP:CZ2	47:BF:234:ASN:HB2	2.52	0.45
84:Bs:21:LEU:HD13	84:Bs:75:LEU:HD21	1.99	0.45
1:A2:1149:A:H4'	1:A2:1150:A:O4'	2.17	0.44
7:AF:220:ASP:HB3	7:AF:223:GLU:HG2	1.98	0.44
14:Ab:192:LEU:HB3	14:Ab:227:ARG:HG2	1.99	0.44
28:Ap:7:LEU:HD23	28:Ap:7:LEU:H	1.82	0.44
35:Aw:54:LYS:HE3	35:Aw:91:LEU:HG	1.99	0.44
39:B5:38:A:H5''	68:Ba:35:ALA:HB2	1.98	0.44
39:B5:1943:U:H2'	39:B5:1944:G:C8	2.52	0.44
39:B5:1943:U:C2	39:B5:1955:C:H1'	2.53	0.44
39:B5:4051:G:O5'	61:BT:83:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:BL:107:THR:HG22	76:Bi:20:ASN:HB3	1.99	0.44
55:BN:143:ARG:NH1	75:Bh:95:LEU:HD23	2.32	0.44
86:Bv:54:ARG:NH1	86:Bv:153:SER:OG	2.48	0.44
1:A2:1032:A2M:HM'2	1:A2:1033:C:H5'	1.98	0.44
1:A2:1338:4AC:H2'	1:A2:1339:G:C8	2.53	0.44
2:AA:12:PRO:HB3	19:Ag:192:PHE:CG	2.53	0.44
19:Ag:135:PHE:CG	19:Ag:136:PRO:HA	2.52	0.44
39:B5:231:U:H4'	66:BY:100:HIS:CD2	2.52	0.44
39:B5:3974:OMG:H5''	39:B5:3975:U:O4'	2.17	0.44
45:BD:7:VAL:HG23	45:BD:8:LYS:HG3	1.99	0.44
1:A2:192:C:H4'	1:A2:192:C:OP1	2.18	0.44
1:A2:1280:C:H2'	1:A2:1281:G:C8	2.53	0.44
30:Ar:36:VAL:HG21	30:Ar:71:MET:HE3	1.98	0.44
34:Av:26:LEU:HD11	34:Av:60:LYS:HB3	2.00	0.44
39:B5:1093:C:H2'	39:B5:1094:A:H8	1.82	0.44
39:B5:1315:A:N1	41:B8:28:C:O2'	2.50	0.44
39:B5:2742:C:P	59:BR:108:ARG:HH22	2.41	0.44
39:B5:3339:U:H2'	39:B5:3340:A:C8	2.52	0.44
75:Bh:6:ALA:O	75:Bh:10:ARG:HG3	2.17	0.44
84:Bs:65:ILE:HG12	84:Bs:75:LEU:HD23	1.99	0.44
1:A2:63:U:O2'	1:A2:170:A:N3	2.44	0.44
1:A2:1233:PSU:H2'	1:A2:1234:G:H8	1.82	0.44
1:A2:1417:C:OP1	31:As:129:ARG:NH1	2.50	0.44
1:A2:1589:A:H2'	1:A2:1590:A:C8	2.53	0.44
7:AF:64:HIS:HB3	7:AF:83:TRP:HB2	1.99	0.44
39:B5:327:U:O2'	76:Bi:30:ARG:NH1	2.48	0.44
39:B5:1292:U:H2'	39:B5:1293:G:H8	1.81	0.44
39:B5:2465:G:OP2	62:BU:84:LYS:NZ	2.49	0.44
39:B5:3693:G:O2'	39:B5:3771:G:N2	2.51	0.44
39:B5:4270:G:N3	43:BB:252:ALA:HB1	2.32	0.44
39:B5:4337:U:H2'	39:B5:4338:C:C6	2.52	0.44
39:B5:4731:G:H2'	39:B5:4732:G:C8	2.52	0.44
54:BM:24:LEU:HD11	54:BM:86:TRP:CG	2.53	0.44
65:BX:110:LYS:HG3	65:BX:121:VAL:HB	2.00	0.44
72:Be:67:LYS:HG2	72:Be:68:HIS:CD2	2.52	0.44
76:Bi:16:LYS:HA	76:Bi:16:LYS:HD3	1.77	0.44
1:A2:99:A2M:O5'	1:A2:99:A2M:H8	2.18	0.44
1:A2:449:A:H5''	20:Ah:25:ARG:HA	1.99	0.44
1:A2:941:U:H2'	1:A2:942:C:C6	2.52	0.44
1:A2:1693:PSU:H2'	1:A2:1694:G:C8	2.52	0.44
39:B5:368:C:O4'	44:BC:83:GLY:HA3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:693:C:H2'	39:B5:694:G:C8	2.53	0.44
39:B5:3789:U:H2'	39:B5:3790:A:C8	2.52	0.44
60:BS:154:LEU:HB3	60:BS:157:ARG:HD3	1.99	0.44
85:Bt:147:HIS:CD2	85:Bt:149:HIS:HB2	2.52	0.44
1:A2:190:G:OP1	20:Ah:149:TYR:OH	2.28	0.44
1:A2:982:A:H2'	1:A2:983:G:C8	2.53	0.44
1:A2:1113:U:H1'	13:Aa:146:ARG:HH22	1.82	0.44
11:AT:51:U:H2'	11:AT:52:G:C8	2.53	0.44
13:Aa:87:ILE:HG22	13:Aa:101:HIS:HB2	2.00	0.44
22:Aj:37:ASP:N	22:Aj:37:ASP:OD1	2.49	0.44
39:B5:3497:G:H21	39:B5:3498:A:N6	2.16	0.44
39:B5:3557:A2M:HM'2	39:B5:3558:C:H5'	1.99	0.44
43:BB:288:GLY:HA3	43:BB:330:PHE:CZ	2.53	0.44
44:BC:60:HIS:HA	44:BC:92:PHE:HE1	1.83	0.44
1:A2:539:U:H3	1:A2:546:A:H61	1.66	0.44
7:AF:189:ILE:HB	15:Ac:223:ILE:HB	2.00	0.44
7:AF:226:HIS:NE2	7:AF:229:THR:HG23	2.33	0.44
20:Ah:8:TRP:CE3	20:Ah:20:PRO:HB3	2.53	0.44
39:B5:1834:G:H2'	39:B5:1835:A:O4'	2.18	0.44
39:B5:2028:G:H1	39:B5:2038:C:H41	1.65	0.44
41:B8:141:C:H2'	41:B8:142:U:C6	2.53	0.44
59:BR:106:LEU:HD13	59:BR:138:LEU:HD21	1.99	0.44
67:BZ:136:PHE:O	74:Bg:78:TYR:OH	2.28	0.44
72:Be:82:VAL:HG13	72:Be:114:ARG:HG2	1.99	0.44
1:A2:613:U:H4'	5:AD:89:GLN:NE2	2.33	0.44
1:A2:1244:U:OP1	92:A2:2104:HOH:O	2.20	0.44
1:A2:1713:A:H2'	1:A2:1714:C:C6	2.52	0.44
23:Ak:89:ARG:NH2	92:Ak:211:HOH:O	2.51	0.44
32:At:41:ARG:O	32:At:45:GLU:HG2	2.17	0.44
36:Ax:21:LYS:HB2	36:Ax:75:ILE:HB	2.00	0.44
39:B5:696:U:H5'	46:BE:124:VAL:HG21	2.00	0.44
44:BC:137:VAL:HA	44:BC:247:GLY:O	2.18	0.44
45:BD:53:VAL:HG11	45:BD:159:VAL:HA	1.99	0.44
63:BV:89:ARG:HB2	63:BV:95:PHE:CE2	2.52	0.44
84:Bs:39:GLN:HE21	84:Bs:43:ILE:HD11	1.83	0.44
1:A2:78:C:OP1	18:Af:159:ARG:NH2	2.50	0.44
1:A2:1459:G:OP1	7:AF:281:ALA:HB2	2.18	0.44
5:AD:112:TYR:CG	21:Ai:33:GLY:HA3	2.53	0.44
6:AE:46:GLU:O	6:AE:50:VAL:HG23	2.18	0.44
11:AT:70:G:N7	92:AT:203:HOH:O	2.37	0.44
14:Ab:183:LYS:NZ	34:Av:91:ASN:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Ap:12:VAL:HG11	28:Ap:90:LYS:HB3	2.00	0.44
39:B5:2371:G:N2	92:B5:6799:HOH:O	2.50	0.44
47:BF:181:TYR:CZ	47:BF:202:GLU:HG2	2.53	0.44
47:BF:240:ASN:O	47:BF:244:ARG:HG2	2.17	0.44
48:BG:103:ARG:NH2	48:BG:192:ARG:O	2.50	0.44
52:BK:4374:GLY:HA3	57:BP:126:ARG:O	2.18	0.44
60:BS:83:ARG:HG3	60:BS:125:GLN:HB2	2.00	0.44
66:BY:2:LYS:HE3	66:BY:2:LYS:HB3	1.84	0.44
67:BZ:41:ALA:HB2	67:BZ:77:TYR:HE1	1.83	0.44
85:Bt:52:ASP:OD1	85:Bt:52:ASP:N	2.40	0.44
1:A2:589:G:OP2	1:A2:589:G:N2	2.39	0.43
1:A2:997:A:H2'	1:A2:998:A:C8	2.53	0.43
17:Ae:80:GLY:HA2	17:Ae:83:ASN:ND2	2.32	0.43
36:Ax:51:THR:OG1	36:Ax:53:ASP:OD1	2.31	0.43
39:B5:1363:C:H2'	39:B5:1364:G:C8	2.53	0.43
39:B5:1769:G:H4'	69:Bb:68:ARG:CZ	2.47	0.43
39:B5:1907:G:H4'	84:Bs:34:ASN:HD22	1.83	0.43
39:B5:2507:G:H4'	39:B5:2520:G:H4'	2.00	0.43
42:BA:80:GLU:HB2	42:BA:170:ALA:HA	1.99	0.43
42:BA:83:HIS:CE1	42:BA:86:GLN:HB2	2.53	0.43
54:BM:29:ASP:OD1	54:BM:30:VAL:N	2.46	0.43
63:BV:13:LYS:HE3	63:BV:13:LYS:HB2	1.88	0.43
70:Bc:37:MET:HE3	70:Bc:42:LYS:HB2	2.00	0.43
85:Bt:46:ILE:HD11	85:Bt:62:LEU:HD21	1.99	0.43
86:Bv:204:LEU:HB3	86:Bv:216:LEU:HB3	2.00	0.43
1:A2:1260:A:H1'	1:A2:1265:C:N4	2.33	0.43
1:A2:1842:C:H2'	1:A2:1843:4AC:H6	1.99	0.43
3:AB:55:VAL:HB	17:Ae:34:SER:HA	2.00	0.43
13:Aa:44:ILE:HD11	13:Aa:74:LEU:HD21	2.00	0.43
21:Ai:134:HIS:ND1	21:Ai:163:SER:OG	2.46	0.43
28:Ap:16:LYS:HG3	28:Ap:17:LYS:H	1.83	0.43
31:As:39:LEU:HD23	31:As:39:LEU:HA	1.81	0.43
39:B5:356:G:O2'	41:B8:25:G:N3	2.51	0.43
39:B5:663:C:H2'	39:B5:664:G:H8	1.82	0.43
39:B5:711:U:H2'	39:B5:712:C:C6	2.54	0.43
39:B5:1343:G:H2'	39:B5:1344:G:C8	2.54	0.43
39:B5:4744:G:N2	39:B5:4780:G:O2'	2.49	0.43
47:BF:135:VAL:O	47:BF:139:ILE:HG12	2.18	0.43
57:BP:94:MET:HE1	57:BP:146:ILE:HB	2.00	0.43
84:Bs:77:LYS:HE2	84:Bs:196:GLY:HA2	2.00	0.43
85:Bt:104:ILE:HB	85:Bt:143:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AF:302:TYR:HE1	7:AF:308:ARG:HB2	1.83	0.43
14:Ab:252:THR:OG1	14:Ab:254:ASP:OD1	2.25	0.43
16:Ad:18:TRP:C	16:Ad:51:ARG:HH22	2.26	0.43
19:Ag:98:ARG:NH1	19:Ag:132:ASP:OD2	2.42	0.43
39:B5:74:G:O6	53:BL:103:ARG:NH2	2.49	0.43
39:B5:835:G:OP1	54:BM:23:LYS:NZ	2.38	0.43
39:B5:1907:G:H4'	84:Bs:34:ASN:ND2	2.33	0.43
39:B5:3888:C:H2'	39:B5:3889:G:C8	2.53	0.43
50:BI:99:ILE:HG22	50:BI:123:GLN:HB2	2.01	0.43
53:BL:42:ARG:HG3	53:BL:45:ARG:HH21	1.83	0.43
61:BT:2:THR:N	92:BT:310:HOH:O	2.51	0.43
1:A2:360:U:OP2	35:Aw:18:ARG:HD2	2.19	0.43
1:A2:1375:C:H2'	1:A2:1376:G:O4'	2.18	0.43
1:A2:1524:C:H4'	30:Ar:148:VAL:HA	2.00	0.43
6:AE:23:CYS:O	26:An:142:ARG:NH1	2.51	0.43
7:AF:87:LEU:HD11	7:AF:122:SER:HB3	2.01	0.43
39:B5:1933:C:H2'	39:B5:1934:G:C8	2.52	0.43
41:B8:36:G:C5	75:Bh:89:ARG:HD3	2.54	0.43
41:B8:84:A:C5	41:B8:88:A:H4'	2.53	0.43
1:A2:469:A2M:HM'2	1:A2:470:A:H5'	2.00	0.43
1:A2:905:A:O2'	23:Ak:48:LYS:NZ	2.48	0.43
3:AB:21:THR:HB	3:AB:68:LEU:HD21	2.01	0.43
13:Aa:48:LEU:O	26:An:51:GLU:HG3	2.19	0.43
39:B5:1810:A2M:HM'2	39:B5:1811:G:H5'	1.99	0.43
39:B5:1933:C:H4'	85:Bt:152:ILE:HD11	2.00	0.43
39:B5:3400:C:H5'	42:BA:8:GLN:O	2.18	0.43
39:B5:4205:U:H2'	39:B5:4206:U:C6	2.53	0.43
39:B5:4253:A:O2'	63:BV:41:SER:OG	2.34	0.43
43:BB:258:HIS:HA	43:BB:259:PRO:C	2.42	0.43
44:BC:317:ASN:HD22	44:BC:320:LYS:HD3	1.84	0.43
48:BG:165:GLU:OE2	55:BN:26:ARG:NH1	2.51	0.43
68:Ba:90:ALA:HA	68:Ba:93:ASN:ND2	2.34	0.43
1:A2:1202:U:H2'	1:A2:1203:U:C6	2.53	0.43
13:Aa:30:TRP:CE2	13:Aa:48:LEU:HD13	2.53	0.43
24:Al:86:GLY:HA2	24:Al:89:VAL:HG22	2.00	0.43
39:B5:1936:U:N3	39:B5:1939:G:OP2	2.29	0.43
39:B5:2156:A:H5'	39:B5:2157:G:OP2	2.18	0.43
39:B5:2206:A2M:HM'2	39:B5:2207:OMG:H5'	1.99	0.43
39:B5:3643:C:H4'	39:B5:3942:OMG:HM22	1.99	0.43
39:B5:3694:A:N6	39:B5:3767:G:OP1	2.51	0.43
39:B5:4035:U:H4'	39:B5:4066:G:O3'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:BO:54:TYR:OH	56:BO:73:PHE:O	2.37	0.43
63:BV:45:ILE:HG21	63:BV:53:PRO:HB3	2.00	0.43
65:BX:64:SER:OG	75:Bh:82:ASP:OD2	2.31	0.43
67:BZ:30:ASP:O	67:BZ:39:SER:OG	2.29	0.43
84:Bs:177:MET:O	84:Bs:179:ASN:ND2	2.51	0.43
39:B5:19:G:P	75:Bh:93:ARG:HE	2.42	0.43
39:B5:1743:A:H5'	39:B5:1745:G:O4'	2.19	0.43
39:B5:2036:A:H3'	39:B5:2037:G:H5'	2.00	0.43
39:B5:3388:A:H2'	39:B5:3389:U:C6	2.54	0.43
39:B5:3985:A:H2'	39:B5:3986:G:C8	2.54	0.43
39:B5:4365:U:H2'	39:B5:4366:OMU:H6	2.00	0.43
43:BB:77:THR:HG21	43:BB:337:VAL:HG22	2.00	0.43
49:BH:48:LEU:HD11	49:BH:56:ARG:HH11	1.83	0.43
1:A2:324:C:H42	1:A2:328:G:N2	2.17	0.43
1:A2:1447:A:O2'	1:A2:1448:OMG:H8	2.00	0.43
11:AT:34:OMG:HM22	11:AT:35:A:H5'	2.01	0.43
16:Ad:174:LYS:O	16:Ad:179:ASN:ND2	2.52	0.43
28:Ap:6:PRO:O	28:Ap:27:ARG:NH2	2.52	0.43
39:B5:21:G:H1'	41:B8:103:A:N3	2.34	0.43
39:B5:279:A:N1	39:B5:306:A:H5''	2.34	0.43
39:B5:307:A:N6	92:B5:6834:HOH:O	2.50	0.43
39:B5:4047:U:H4'	61:BT:54:HIS:CD2	2.54	0.43
49:BH:41:ILE:HG22	49:BH:43:VAL:HG13	2.00	0.43
61:BT:80:VAL:O	61:BT:83:LYS:HG2	2.19	0.43
86:Bv:21:ASN:HB2	86:Bv:26:ARG:HD3	2.01	0.43
20:Ah:81:VAL:HG22	20:Ah:102:VAL:HG12	2.01	0.43
25:Am:110:ASP:O	25:Am:114:ARG:HG2	2.19	0.43
39:B5:52:G:H4'	39:B5:1484:G:H4'	2.01	0.43
39:B5:625:G:H2'	39:B5:626:G:C8	2.54	0.43
39:B5:2028:G:H22	39:B5:2038:C:H5	1.67	0.43
39:B5:2221:G:N2	39:B5:2224:A:OP2	2.49	0.43
39:B5:4135:C:H2'	39:B5:4136:A:H8	1.84	0.43
41:B8:67:U:H2'	41:B8:68:G:C8	2.54	0.43
53:BL:40:GLN:O	53:BL:44:ARG:HG3	2.19	0.43
86:Bv:67:VAL:HG12	86:Bv:84:HIS:HD2	1.82	0.43
86:Bv:93:LEU:HB3	86:Bv:124:LEU:HD21	2.01	0.43
1:A2:528:C:H2'	1:A2:529:A:C8	2.54	0.43
1:A2:1799:C:H2'	1:A2:1800:G:O4'	2.18	0.43
7:AF:268:ASP:OD1	7:AF:269:GLU:N	2.52	0.43
16:Ad:100:ARG:HB2	16:Ad:114:ILE:HD13	2.00	0.43
18:Af:201:LYS:HB3	18:Af:201:LYS:HE3	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Ag:101:LEU:HB2	19:Ag:116:ARG:HD2	2.01	0.43
39:B5:108:A:N1	39:B5:333:U:O2'	2.52	0.43
39:B5:1230:C:O2'	39:B5:1232:G:O5'	2.31	0.43
39:B5:1489:A2M:H2	92:Bj:237:HOH:O	2.19	0.43
39:B5:2575:G:H2'	39:B5:2576:C:C6	2.54	0.43
39:B5:2654:G:N2	39:B5:2657:C:OP2	2.47	0.43
39:B5:3371:PSU:OP2	92:B5:5516:HOH:O	2.22	0.43
39:B5:4416:C:O2'	39:B5:4418:A:OP2	2.29	0.43
1:A2:115:U:H2'	1:A2:116:OMU:C6	2.49	0.42
1:A2:126:G:OP2	18:Af:195:LYS:NZ	2.51	0.42
1:A2:847:G:C4	16:Ad:19:MET:HG2	2.54	0.42
1:A2:1590:A:N3	1:A2:1654:U:O2'	2.39	0.42
1:A2:1606:G:OP1	31:As:84:ARG:NH2	2.52	0.42
22:Aj:94:LEU:HD23	22:Aj:94:LEU:HA	1.83	0.42
39:B5:28:C:H4'	39:B5:61:A:H4'	2.01	0.42
39:B5:106:A:H2'	39:B5:107:G:O4'	2.19	0.42
39:B5:3790:A:H2'	39:B5:3791:U:C6	2.54	0.42
39:B5:4371:C:O2'	39:B5:4372:A:H5'	2.19	0.42
39:B5:4515:G:OP1	56:BO:168:TYR:OH	2.30	0.42
39:B5:4627:C:H2'	39:B5:4628:G:C8	2.54	0.42
44:BC:316:LYS:HB2	44:BC:324:ILE:HG13	2.01	0.42
72:Be:88:LEU:HB2	72:Be:120:ILE:HD13	2.00	0.42
83:Br:94:ARG:NH1	92:Br:205:HOH:O	2.40	0.42
85:Bt:107:ASP:HA	85:Bt:110:VAL:HG12	2.01	0.42
1:A2:1309:U:O2'	1:A2:1310:C:O4'	2.37	0.42
6:AE:65:PRO:HG3	26:An:129:ILE:O	2.20	0.42
13:Aa:30:TRP:CE2	26:An:19:PRO:HD3	2.54	0.42
17:Ae:78:MET:HB2	17:Ae:159:ARG:CZ	2.49	0.42
31:As:65:TYR:HE2	31:As:128:GLN:HG3	1.83	0.42
39:B5:766:C:H2'	39:B5:767:G:C8	2.54	0.42
39:B5:1105:C:O2'	39:B5:1106:U:OP1	2.35	0.42
39:B5:4012:G:H2'	39:B5:4012:G:N3	2.34	0.42
47:BF:25:ALA:O	47:BF:29:ILE:HG12	2.19	0.42
1:A2:68:A:OP2	18:Af:164:LYS:NZ	2.40	0.42
1:A2:503:C:O4'	16:Ad:66:MET:HG3	2.19	0.42
1:A2:830:C:OP1	16:Ad:21:ASP:HB2	2.19	0.42
7:AF:159:ASN:HD22	7:AF:159:ASN:H	1.66	0.42
18:Af:67:VAL:HG12	18:Af:69:THR:HG22	2.01	0.42
34:Av:90:GLN:HE22	34:Av:117:ARG:HE	1.68	0.42
39:B5:1786:C:H2'	39:B5:1787:C:C6	2.54	0.42
39:B5:2166:C:H2'	39:B5:2167:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:B8:33:G:H4'	41:B8:34:U:C5	2.54	0.42
41:B8:67:U:H2'	41:B8:68:G:H8	1.84	0.42
45:BD:64:ILE:HG13	45:BD:109:LEU:HD22	2.02	0.42
48:BG:187:LYS:HB2	48:BG:198:THR:HG23	2.02	0.42
50:BI:205:PRO:HD2	50:BI:208:LYS:NZ	2.34	0.42
1:A2:116:OMU:HM22	1:A2:117:C:H5'	2.01	0.42
1:A2:824:U:N3	21:AI:143:ASN:OD1	2.45	0.42
1:A2:1498:G:H4'	1:A2:1499:A:H5'	2.01	0.42
17:Ae:49:LEU:HD12	28:Ap:50:LYS:HG2	2.01	0.42
17:Ae:126:THR:HG23	17:Ae:128:ILE:HG13	2.01	0.42
23:Ak:22:ARG:HD3	23:Ak:28:THR:HB	2.01	0.42
39:B5:420:A:H61	41:B8:15:G:H1'	1.84	0.42
53:BL:207:VAL:HG12	86:Bv:7:ARG:HH12	1.84	0.42
1:A2:62:G:H1'	1:A2:172:OMU:HM23	2.00	0.42
1:A2:507:G:OP1	36:Ax:108:LYS:NZ	2.35	0.42
1:A2:558:U:H2'	1:A2:559:G:C8	2.55	0.42
1:A2:1017:U:H5''	25:Am:14:SER:HB3	2.02	0.42
1:A2:1618:G:N1	1:A2:1621:A:OP2	2.52	0.42
1:A2:1629:C:H2'	1:A2:1630:C:C6	2.54	0.42
1:A2:1758:G:H2'	1:A2:1759:G:H8	1.84	0.42
2:AA:23:ARG:O	34:Av:60:LYS:NZ	2.53	0.42
8:AG:22:ARG:NH1	15:Ac:16:ILE:HG21	2.34	0.42
15:Ac:42:THR:OG1	15:Ac:45:ARG:O	2.22	0.42
29:Aq:44:LYS:HG3	29:Aq:47:ARG:HH21	1.84	0.42
37:Ay:58:LEU:HD12	37:Ay:62:VAL:HG21	2.01	0.42
39:B5:1449:U:H2'	39:B5:1450:G:H8	1.84	0.42
39:B5:1555:A:H1'	52:BK:4390:MET:HE1	2.01	0.42
39:B5:2387:G:H4'	39:B5:2389:G:C8	2.54	0.42
39:B5:3619:OMC:H5''	56:BO:71:TYR:CE2	2.55	0.42
39:B5:4346:G:O2'	39:B5:4355:G:O6	2.32	0.42
70:Bc:20:LEU:HD23	70:Bc:102:SER:HA	2.02	0.42
1:A2:1008:C:H2'	1:A2:1009:A:C8	2.55	0.42
1:A2:1048:C:H5''	26:An:143:LYS:HB2	2.02	0.42
1:A2:1116:U:H1'	1:A2:1117:C:H2'	2.01	0.42
1:A2:1290:U:H2'	1:A2:1291:G:C8	2.55	0.42
1:A2:1674:U:O2'	17:Ae:84:GLY:O	2.25	0.42
1:A2:1678:U:H2'	1:A2:1679:A2M:H8	2.02	0.42
92:A2:2320:HOH:O	26:An:139:SER:HB2	2.19	0.42
5:AD:111:GLN:O	5:AD:115:ARG:HG2	2.20	0.42
7:AF:39:THR:HG22	7:AF:60:ARG:HG2	2.02	0.42
11:AT:58:1MA:O2'	11:AT:60:C:OP2	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Aw:67:ARG:HG3	35:Aw:115:ILE:HG12	2.01	0.42
35:Aw:123:VAL:HG12	35:Aw:124:LYS:HG3	2.01	0.42
39:B5:769:C:H2'	39:B5:770:G:H8	1.84	0.42
39:B5:1617:C:H2'	39:B5:1618:C:C6	2.55	0.42
39:B5:1805:U:H2'	39:B5:1806:A:O4'	2.19	0.42
39:B5:2500:G:O6	70:Bc:32:LYS:NZ	2.53	0.42
39:B5:3805:A:N1	39:B5:3917:C:N4	2.65	0.42
39:B5:4037:G:H4'	39:B5:4038:A:H5''	2.01	0.42
39:B5:4622:C:N4	46:BE:184:LEU:O	2.47	0.42
41:B8:90:C:H2'	41:B8:91:A:C8	2.55	0.42
73:Bf:63:LYS:HD3	73:Bf:63:LYS:HA	1.81	0.42
1:A2:220:U:H2'	1:A2:221:A:C8	2.54	0.42
1:A2:1345:A:N1	1:A2:1386:G:O2'	2.50	0.42
1:A2:1544:U:OP2	31:As:62:ARG:NH2	2.44	0.42
18:Af:41:LEU:HD23	18:Af:45:TRP:CD2	2.55	0.42
22:Aj:16:PHE:HE1	22:Aj:89:ILE:HG22	1.84	0.42
39:B5:645:C:H2'	39:B5:646:G:C8	2.55	0.42
39:B5:1752:U:H4'	69:Bb:49:HIS:O	2.20	0.42
39:B5:4020:A:H2'	39:B5:4021:G:H8	1.85	0.42
43:BB:92:TYR:HB2	43:BB:159:VAL:HB	2.00	0.42
49:BH:16:VAL:HG21	49:BH:81:ILE:HG23	2.00	0.42
85:Bt:35:LEU:HD12	85:Bt:37:LEU:H	1.85	0.42
1:A2:31:U:O2'	1:A2:644:A:N1	2.51	0.42
1:A2:126:G:H8	18:Af:199:THR:HG21	1.85	0.42
7:AF:91:ASP:OD2	7:AF:93:THR:OG1	2.30	0.42
7:AF:107:ASP:OD1	7:AF:107:ASP:N	2.53	0.42
17:Ae:164:ARG:HH21	37:Ay:41:ARG:HD3	1.85	0.42
18:Af:142:ARG:HA	18:Af:147:LEU:HB2	2.01	0.42
30:Ar:48:ALA:HB2	30:Ar:70:ILE:HD12	2.02	0.42
39:B5:1552:G:O2'	92:B5:5514:HOH:O	2.21	0.42
39:B5:2552:C:H5''	59:BR:43:LYS:HD2	2.02	0.42
39:B5:3599:A2M:HM'3	39:B5:3612:G:N2	2.35	0.42
43:BB:161:ARG:HE	43:BB:184:GLN:HE21	1.68	0.42
67:BZ:99:ASP:HB3	67:BZ:102:ARG:HH21	1.84	0.42
76:Bi:76:ARG:HD3	76:Bi:76:ARG:HA	1.81	0.42
85:Bt:111:ASN:HA	85:Bt:114:ARG:HD2	2.02	0.42
1:A2:371:G:O2'	20:Ah:10:LYS:NZ	2.53	0.42
1:A2:1266:A:H5''	1:A2:1267:C:OP2	2.20	0.42
7:AF:260:ASP:HB2	7:AF:267:VAL:HG23	2.01	0.42
14:Ab:200:ARG:O	21:Ai:98:LEU:HB3	2.20	0.42
17:Ae:58:ALA:HB3	17:Ae:62:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Aw:49:GLY:HA2	35:Aw:75:ILE:HG13	2.00	0.42
39:B5:223:G:H4'	39:B5:225:G:N7	2.35	0.42
39:B5:433:A:C2	39:B5:3599:A2M:H4'	2.54	0.42
39:B5:458:C:OP2	46:BE:117:ARG:NH1	2.53	0.42
41:B8:8:U:H2'	41:B8:9:A:C8	2.55	0.42
54:BM:75:LYS:O	54:BM:79:LYS:HG2	2.20	0.42
1:A2:673:A:OP2	88:A2:1909:SPM:H132	2.20	0.42
1:A2:1437:C:H2'	1:A2:1438:C:C5	2.54	0.42
2:AA:33:MET:HE2	2:AA:48:SER:HA	2.02	0.42
29:Aq:34:VAL:O	29:Aq:38:ILE:HG13	2.19	0.42
30:Ar:104:ASP:OD1	30:Ar:104:ASP:N	2.52	0.42
39:B5:1223:A:O2'	39:B5:1225:G:N7	2.44	0.42
39:B5:2358:G:OP1	74:Bg:37:LYS:NZ	2.41	0.42
39:B5:2382:C:H2'	39:B5:2383:C:C6	2.54	0.42
39:B5:3458:A:OP1	86:Bv:199:GLN:NE2	2.52	0.42
39:B5:3684:A:H2'	39:B5:3685:G:H8	1.83	0.42
41:B8:75:OMG:HM22	41:B8:76:C:O4'	2.19	0.42
50:BI:86:HIS:HB3	50:BI:139:ARG:HG2	2.02	0.42
84:Bs:32:ALA:O	84:Bs:85:ASN:ND2	2.52	0.42
1:A2:239:C:H2'	1:A2:240:G:C8	2.55	0.41
1:A2:583:U:H2'	1:A2:584:A:H5''	2.02	0.41
1:A2:1123:A:N3	13:Aa:146:ARG:NH1	2.68	0.41
1:A2:1754:C:H2'	1:A2:1755:G:C8	2.54	0.41
15:Ac:56:GLN:H	15:Ac:56:GLN:HG3	1.57	0.41
18:Af:131:ARG:HB2	64:BW:82:ILE:HA	2.02	0.41
39:B5:74:G:H5'	53:BL:60:ARG:O	2.20	0.41
39:B5:1008:C:H2'	39:B5:1009:G:C8	2.55	0.41
39:B5:1353:G:H2'	39:B5:1354:G:C8	2.55	0.41
39:B5:2169:G:H5''	72:Be:127:ALA:HB2	2.01	0.41
39:B5:2321:C:H2'	39:B5:2322:G:O4'	2.20	0.41
39:B5:2362:U:H1'	39:B5:2363:C:C6	2.55	0.41
39:B5:2636:G:N7	92:B5:6048:HOH:O	2.37	0.41
39:B5:3909:U:H5'	39:B5:3910:C:H5''	2.01	0.41
39:B5:4623:G:N7	46:BE:275:ARG:NH2	2.68	0.41
39:B5:4675:G:C5	46:BE:186:ARG:HD3	2.55	0.41
87:B5:4919:SPD:H51	92:B5:6575:HOH:O	2.20	0.41
44:BC:11:TYR:CZ	44:BC:148:PRO:HB2	2.54	0.41
50:BI:38:ARG:NH1	50:BI:45:GLU:OE1	2.52	0.41
54:BM:126:GLU:HG3	56:BO:185:VAL:HG13	2.01	0.41
64:BW:102:LYS:HG2	64:BW:105:ARG:NH2	2.35	0.41
86:Bv:64:SER:HB3	86:Bv:107:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:568:C:H2'	1:A2:569:C:H5''	2.02	0.41
1:A2:894:U:H2'	1:A2:895:G:C8	2.56	0.41
1:A2:1018:U:H5'	25:Am:55:ARG:HE	1.84	0.41
1:A2:1826:A:H3'	39:B5:3492:A2M:N1	2.34	0.41
12:AZ:125:THR:HG22	12:AZ:175:TRP:HZ2	1.85	0.41
19:Ag:69:LEU:HD13	19:Ag:96:ALA:HB2	2.02	0.41
27:Ao:136:THR:O	27:Ao:137:HIS:HB2	2.20	0.41
33:Au:1:AME:HA	33:Au:1:AME:HT23	1.67	0.41
37:Ay:79:ILE:HB	37:Ay:83:LEU:HD23	2.02	0.41
39:B5:150:U:OP2	48:BG:200:THR:OG1	2.33	0.41
39:B5:1105:C:C5	69:Bb:92:LYS:HD2	2.55	0.41
39:B5:3421:G:O2'	39:B5:3550:UY1:OP2	2.31	0.41
39:B5:3867:C:H2'	39:B5:3868:C:C6	2.55	0.41
39:B5:4312:U:O2'	43:BB:234:ARG:NH1	2.52	0.41
39:B5:4598:C:H2'	39:B5:4599:G:H8	1.83	0.41
39:B5:4632:A:OP1	56:BO:188:LYS:NZ	2.45	0.41
40:B7:97:G:N7	92:B7:314:HOH:O	2.37	0.41
1:A2:386:G:H3'	23:Ak:136:LYS:HB2	2.02	0.41
1:A2:619:C:H41	35:Aw:67:ARG:NH2	2.18	0.41
1:A2:1289:OMU:HM22	1:A2:1290:U:H5'	2.02	0.41
1:A2:1411:C:H2'	1:A2:1412:G:C8	2.56	0.41
1:A2:1513:C:H5''	8:AG:8:TRP:CZ3	2.54	0.41
1:A2:1867:A:N6	6:AE:84:VAL:HB	2.35	0.41
13:Aa:123:ALA:HB2	13:Aa:165:ARG:HG3	2.02	0.41
15:Ac:18:LYS:HG2	15:Ac:39:VAL:HG21	2.03	0.41
23:Ak:33:LEU:HG	23:Ak:34:PRO:HD2	2.02	0.41
29:Aq:57:LEU:O	29:Aq:61:ILE:HG12	2.20	0.41
34:Av:115:GLU:OE2	34:Av:119:LYS:NZ	2.48	0.41
39:B5:1636:G:O2'	68:Ba:41:HIS:NE2	2.51	0.41
39:B5:1638:PSU:OP1	68:Ba:44:ASN:ND2	2.47	0.41
39:B5:4161:A:H2'	39:B5:4162:G:O4'	2.21	0.41
39:B5:4309:U:H2'	39:B5:4310:A:C8	2.55	0.41
39:B5:4610:C:N4	60:BS:171:ARG:O	2.50	0.41
42:BA:245:ARG:NH1	42:BA:247:ARG:HH21	2.18	0.41
1:A2:1045:G:O2'	1:A2:1046:PSU:N1	2.48	0.41
1:A2:1156:U:OP1	14:Ab:185:THR:OG1	2.36	0.41
1:A2:1416:C:H2'	1:A2:1417:C:C6	2.56	0.41
7:AF:163:PRO:HB2	7:AF:179:LEU:HB3	2.02	0.41
16:Ad:86:PHE:CD2	16:Ad:87:MET:HG2	2.55	0.41
17:Ae:14:THR:HB	17:Ae:15:PRO:HD3	2.02	0.41
19:Ag:36:LEU:HD13	19:Ag:75:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Ah:172:LEU:HB3	20:Ah:190:LEU:HD12	2.02	0.41
39:B5:1927:G:H2'	39:B5:1928:G:H8	1.85	0.41
39:B5:2118:G:H2'	39:B5:2119:A:C8	2.55	0.41
39:B5:2281:A:O2'	39:B5:2283:U:OP2	2.26	0.41
39:B5:3660:A:H2'	39:B5:3661:G:O4'	2.20	0.41
39:B5:4297:U:H2'	39:B5:4298:PSU:C6	2.55	0.41
42:BA:173:GLY:O	82:Bp:69:TRP:NE1	2.51	0.41
46:BE:45:HIS:ND1	46:BE:46:CYS:O	2.43	0.41
46:BE:165:VAL:HG11	46:BE:187:VAL:HG11	2.02	0.41
85:Bt:53:TRP:O	85:Bt:56:LEU:HG	2.20	0.41
1:A2:25:A:O2'	1:A2:26:U:H5''	2.20	0.41
1:A2:617:A:H1'	5:AD:86:VAL:HG23	2.03	0.41
1:A2:1601:G:H4'	37:Ay:43:LYS:HE3	2.03	0.41
1:A2:1863:G:N7	6:AE:34:LYS:NZ	2.59	0.41
19:Ag:75:ILE:HA	19:Ag:78:ARG:HE	1.85	0.41
39:B5:1564:U:H2'	39:B5:1565:C:O4'	2.21	0.41
39:B5:1923:A:N7	39:B5:1949:A:O2'	2.40	0.41
39:B5:3502:PSU:H2'	39:B5:3503:C:C6	2.55	0.41
88:B5:4915:SPM:H22	92:B5:7207:HOH:O	2.20	0.41
41:B8:92:U:H2'	41:B8:93:C:O4'	2.21	0.41
65:BX:82:THR:HG21	75:Bh:37:THR:HG22	2.03	0.41
84:Bs:63:LYS:HA	84:Bs:66:ARG:HB2	2.01	0.41
85:Bt:118:HIS:CD2	85:Bt:119:ARG:HG2	2.55	0.41
85:Bt:133:LEU:HD22	85:Bt:152:ILE:HD12	2.02	0.41
1:A2:28:U:H2'	1:A2:29:G:C8	2.56	0.41
1:A2:220:U:H2'	1:A2:221:A:H8	1.86	0.41
1:A2:1026:U:H2'	1:A2:1027:C:O4'	2.20	0.41
1:A2:1601:G:OP1	37:Ay:44:LEU:HG	2.21	0.41
1:A2:1605:G:OP2	30:Ar:38:ARG:NH2	2.48	0.41
2:AA:28:PRO:HG3	25:Am:17:PRO:HG3	2.01	0.41
7:AF:59:LEU:HD23	7:AF:90:TRP:CD2	2.56	0.41
12:AZ:77:ILE:HG21	12:AZ:133:PRO:HG3	2.02	0.41
18:Af:162:LEU:HD12	18:Af:170:ARG:HD2	2.01	0.41
28:Ap:24:HIS:HE1	28:Ap:26:LYS:HD3	1.86	0.41
39:B5:632:G:C2	39:B5:635:G:H1'	2.56	0.41
39:B5:781:C:H2'	39:B5:782:G:C8	2.56	0.41
39:B5:1248:C:H2'	39:B5:1249:C:C6	2.56	0.41
39:B5:1270:A2M:HM'2	39:B5:1271:C:O4'	2.20	0.41
39:B5:2325:C:H2'	39:B5:2326:G:C8	2.54	0.41
39:B5:3643:C:H2'	39:B5:3644:U:H6	1.83	0.41
39:B5:4600:G:H2'	39:B5:4601:G:H8	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:BJ:81:GLU:OE2	51:BJ:85:LYS:NZ	2.53	0.41
57:BP:29:THR:HG21	57:BP:146:ILE:HD11	2.02	0.41
58:BQ:43:PHE:CD2	58:BQ:133:GLY:HA3	2.56	0.41
1:A2:77:A:N3	18:Af:176:ILE:HG22	2.36	0.41
1:A2:158:A:H2'	1:A2:159:A2M:O4'	2.20	0.41
1:A2:508:G:OP2	36:Ax:104:ARG:NH2	2.54	0.41
1:A2:1071:A:H2'	1:A2:1072:G:O4'	2.20	0.41
1:A2:1776:U:H2'	1:A2:1777:G:C8	2.56	0.41
17:Ae:110:GLN:HE21	17:Ae:114:ASN:ND2	2.18	0.41
28:Ap:76:GLY:H	28:Ap:79:ALA:HB3	1.84	0.41
31:As:71:GLY:O	31:As:75:MET:HG2	2.21	0.41
35:Aw:60:LYS:HG3	35:Aw:116:PRO:HG3	2.03	0.41
39:B5:521:C:H2'	39:B5:522:U:C6	2.55	0.41
39:B5:531:C:H2'	39:B5:532:U:C6	2.56	0.41
39:B5:769:C:H2'	39:B5:770:G:C8	2.56	0.41
39:B5:1331:A:OP2	92:B5:5515:HOH:O	2.21	0.41
39:B5:1457:G:H1	58:BQ:89:ASP:HA	1.85	0.41
39:B5:1471:G:O2'	53:BL:18:TRP:NE1	2.51	0.41
39:B5:2217:A:H5'	71:Bd:64:ILE:O	2.20	0.41
39:B5:2477:C:H2'	39:B5:2478:U:C6	2.56	0.41
39:B5:2495:G:N1	82:Bp:58:GLY:O	2.47	0.41
39:B5:4323:U:H2'	39:B5:4324:G:C8	2.56	0.41
39:B5:4379:G:O2'	39:B5:4381:A:OP2	2.34	0.41
39:B5:4609:G:H5''	54:BM:91:TRP:CE2	2.56	0.41
54:BM:7:VAL:O	60:BS:151:ARG:HA	2.20	0.41
60:BS:70:LYS:HA	60:BS:70:LYS:HD3	1.85	0.41
68:Ba:76:ASP:HB3	68:Ba:115:GLY:HA3	2.01	0.41
84:Bs:61:MET:HE2	84:Bs:61:MET:HB3	1.90	0.41
86:Bv:26:ARG:HG3	86:Bv:30:GLU:HG3	2.02	0.41
1:A2:351:C:O2'	1:A2:384:G:N1	2.38	0.41
1:A2:749:C:H2'	1:A2:750:U:H5''	2.02	0.41
1:A2:1330:U:O2'	1:A2:1333:A:OP2	2.30	0.41
12:AZ:59:LEU:O	12:AZ:63:ARG:HG3	2.20	0.41
18:Af:57:ASP:OD1	18:Af:61:PHE:N	2.54	0.41
27:Ao:53:GLN:OE1	27:Ao:53:GLN:N	2.51	0.41
39:B5:294:G:O6	39:B5:315:G:H1'	2.20	0.41
39:B5:1089:G:H2'	39:B5:1091:G:H8	1.86	0.41
39:B5:1583:C:OP2	42:BA:9:ARG:HD2	2.21	0.41
39:B5:2248:G:H5'	77:Bj:12:ARG:O	2.21	0.41
39:B5:2573:U:H2'	39:B5:2574:C:C6	2.56	0.41
39:B5:3982:G:H4'	39:B5:4074:G:O2'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:BE:59:TYR:HB3	46:BE:63:ALA:HB3	2.03	0.41
56:BO:61:ARG:HD2	56:BO:66:PRO:HB3	2.03	0.41
57:BP:102:ALA:HB1	57:BP:107:LEU:HB2	2.02	0.41
1:A2:65:C:C4	18:Af:133:LEU:HB3	2.56	0.41
1:A2:92:A:C6	1:A2:447:G:C6	3.09	0.41
1:A2:154:U:O2'	18:Af:4:ASN:OD1	2.31	0.41
1:A2:494:A:H1'	1:A2:575:A:H5'	2.03	0.41
1:A2:825:C:H1'	21:Ai:144:ILE:HG21	2.03	0.41
1:A2:1604:G:H4'	30:Ar:38:ARG:NH2	2.36	0.41
1:A2:1652:A:OP2	92:A2:2106:HOH:O	2.22	0.41
6:AE:94:ASP:OD1	6:AE:96:THR:HG22	2.21	0.41
16:Ad:37:LYS:HB2	16:Ad:40:GLU:HG2	2.03	0.41
20:Ah:21:TYR:CZ	20:Ah:22:HIS:HD2	2.39	0.41
20:Ah:36:THR:OG1	20:Ah:57:ALA:O	2.38	0.41
20:Ah:194:GLU:HG2	23:Ak:10:TYR:CE2	2.55	0.41
39:B5:114:G:N2	39:B5:158:A:H61	2.19	0.41
39:B5:158:A:N1	39:B5:276:C:O2'	2.41	0.41
39:B5:1072:C:H1'	39:B5:1074:C:C2	2.55	0.41
39:B5:1228:G:O2'	39:B5:1229:U:H5''	2.21	0.41
39:B5:1284:OMC:HM22	39:B5:1285:U:O4'	2.21	0.41
39:B5:1298:A:H5'	58:BQ:108:ARG:HH21	1.86	0.41
39:B5:1324:G:H4'	39:B5:1325:U:H6	1.86	0.41
39:B5:1437:G:N7	53:BL:188:ASN:ND2	2.69	0.41
39:B5:1453:G:OP1	58:BQ:150:ARG:NH1	2.53	0.41
39:B5:2360:A:H5'	74:Bg:62:LYS:HD3	2.03	0.41
39:B5:2617:C:OP2	78:Bk:39:SER:OG	2.34	0.41
39:B5:2704:OMC:HM22	39:B5:2705:G:H5'	2.02	0.41
39:B5:3548:A:OP1	39:B5:3550:UY1:N1	2.54	0.41
39:B5:3766:C:H2'	39:B5:3767:G:O4'	2.21	0.41
39:B5:3784:A:OP1	86:Bv:202:ARG:NH2	2.50	0.41
39:B5:4206:U:H2'	39:B5:4207:C:C6	2.55	0.41
41:B8:62:A:OP1	75:Bh:52:LYS:NZ	2.48	0.41
45:BD:125:VAL:HG11	45:BD:199:ILE:HG21	2.01	0.41
46:BE:98:PRO:HA	46:BE:107:THR:HA	2.03	0.41
46:BE:189:LEU:HD21	46:BE:256:VAL:HG21	2.02	0.41
49:BH:114:ILE:HB	49:BH:124:ARG:HB2	2.03	0.41
50:BI:54:SER:HB2	50:BI:135:ILE:HD11	2.02	0.41
57:BP:52:THR:HG23	57:BP:85:LYS:HG3	2.03	0.41
58:BQ:178:ARG:N	68:Ba:51:GLY:HA2	2.36	0.41
60:BS:127:MET:HG2	61:BT:153:PRO:HB2	2.03	0.41
67:BZ:14:LEU:HD21	67:BZ:81:MET:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:Bf:24:HIS:HA	73:Bf:91:ASN:OD1	2.21	0.41
76:Bi:41:ARG:NH1	92:Bi:203:HOH:O	2.47	0.41
1:A2:1288:A:C5	1:A2:1289:OMU:H1'	2.56	0.41
1:A2:1598:C:H4'	1:A2:1604:G:O6	2.20	0.41
15:Ac:211:VAL:HG22	29:Aq:38:ILE:O	2.21	0.41
39:B5:645:C:H2'	39:B5:646:G:H8	1.86	0.41
39:B5:2388:U:OP2	41:B8:125:C:N4	2.53	0.41
39:B5:3449:A:H2'	39:B5:3450:A2M:C8	2.51	0.41
39:B5:3480:A:O2'	42:BA:223:SER:OG	2.38	0.41
39:B5:3598:C:H2'	39:B5:3599:A2M:O4'	2.21	0.41
39:B5:3634:A:OP1	39:B5:4196:U:H4'	2.21	0.41
39:B5:4139:G:O4'	39:B5:4193:5MC:HM52	2.20	0.41
46:BE:152:ILE:HD12	46:BE:274:LEU:HD21	2.03	0.41
53:BL:129:ARG:HH11	75:Bh:117:ARG:HD2	1.86	0.41
54:BM:12:VAL:O	54:BM:58:THR:OG1	2.35	0.41
1:A2:107:A:H2'	1:A2:108:G:C8	2.56	0.40
1:A2:588:A:H5'	1:A2:593:C:H41	1.87	0.40
1:A2:1446:PSU:H1'	1:A2:1581:A:N6	2.36	0.40
1:A2:1798:U:H2'	1:A2:1799:C:C6	2.56	0.40
1:A2:1837:G:OP1	1:A2:1840:U:H4'	2.21	0.40
17:Ae:70:GLU:OE2	17:Ae:86:LYS:NZ	2.48	0.40
39:B5:882:U:P	46:BE:48:ARG:HH12	2.44	0.40
39:B5:1381:G:N1	39:B5:1413:C:OP2	2.43	0.40
39:B5:4234:A:H4'	39:B5:4235:G:H8	1.85	0.40
54:BM:6:PHE:H	54:BM:11:ARG:NH2	2.19	0.40
63:BV:107:ASN:OD1	63:BV:111:GLU:HG2	2.20	0.40
1:A2:152:U:H1'	18:Af:132:ARG:HD2	2.02	0.40
1:A2:294:C:O2	1:A2:294:C:H2'	2.20	0.40
1:A2:1338:4AC:O2'	32:At:68:THR:HB	2.22	0.40
1:A2:1388:G:H2'	1:A2:1389:A:O4'	2.21	0.40
1:A2:1433:U:H4'	1:A2:1438:C:C4	2.56	0.40
4:AC:123:SER:HB2	4:AC:126:CYS:SG	2.61	0.40
13:Aa:168:MET:HG2	13:Aa:197:ILE:HG21	2.03	0.40
24:Al:31:LEU:HD21	24:Al:89:VAL:HG12	2.02	0.40
25:Am:87:ASP:OD1	25:Am:88:LEU:N	2.53	0.40
26:An:63:LYS:HE2	26:An:63:LYS:HB3	1.93	0.40
39:B5:738:G:H2'	39:B5:739:G:O4'	2.21	0.40
39:B5:1624:A:OP1	69:Bb:18:ARG:NH1	2.46	0.40
39:B5:1984:G:O2'	39:B5:1985:G:H5''	2.21	0.40
39:B5:2277:G:O2'	39:B5:2370:A:N1	2.46	0.40
39:B5:2592:C:H2'	39:B5:2593:G:H8	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:3680:C:H2'	39:B5:3681:A:C8	2.56	0.40
39:B5:4363:G:N7	92:B5:6062:HOH:O	2.37	0.40
39:B5:4401:A:OP2	92:B5:5519:HOH:O	2.22	0.40
40:B7:88:A:OP2	92:B7:302:HOH:O	2.22	0.40
41:B8:141:C:OP1	55:BN:38:ARG:NH1	2.54	0.40
44:BC:298:ILE:O	44:BC:302:LEU:HG	2.21	0.40
45:BD:196:ARG:NH2	45:BD:237:GLU:OE2	2.50	0.40
50:BI:53:VAL:HG11	61:BT:158:PHE:CZ	2.57	0.40
51:BJ:93:GLU:HG2	51:BJ:173:ILE:HB	2.02	0.40
82:Bp:8:VAL:O	82:Bp:11:VAL:HG22	2.21	0.40
86:Bv:205:TYR:HD2	86:Bv:213:PRO:HB2	1.85	0.40
16:Ad:55:ALA:HB1	16:Ad:60:GLU:HB2	2.02	0.40
16:Ad:94:LYS:NZ	36:Ax:19:GLN:HE21	2.19	0.40
35:Aw:115:ILE:HA	35:Aw:116:PRO:HD3	1.92	0.40
36:Ax:100:LYS:HE2	36:Ax:100:LYS:HB3	1.97	0.40
39:B5:795:A:H3'	39:B5:796:C:C6	2.56	0.40
39:B5:1699:G:H2'	39:B5:1700:G:H8	1.85	0.40
39:B5:2464:A:H2'	39:B5:2465:G:C8	2.57	0.40
39:B5:3416:G:H2'	39:B5:3417:C:C6	2.57	0.40
39:B5:3422:U:O2'	39:B5:3549:A:N3	2.45	0.40
39:B5:3518:U:O2	39:B5:3546:U:H4'	2.21	0.40
39:B5:4136:A:H2'	39:B5:4137:G:O4'	2.22	0.40
39:B5:4269:A2M:H1'	39:B5:4304:U:C4	2.57	0.40
44:BC:297:GLU:H	44:BC:297:GLU:CD	2.28	0.40
63:BV:42:VAL:HB	63:BV:45:ILE:HG13	2.03	0.40
86:Bv:37:SER:HB2	86:Bv:202:ARG:HB2	2.03	0.40
1:A2:543:U:C5	1:A2:544:C:H1'	2.57	0.40
12:AZ:118:GLU:HG3	14:Ab:65:LYS:HD2	2.02	0.40
13:Aa:92:GLN:HE21	13:Aa:225:LEU:HD11	1.87	0.40
15:Ac:154:ASP:OD1	15:Ac:154:ASP:N	2.55	0.40
16:Ad:100:ARG:HH12	16:Ad:122:LYS:HA	1.86	0.40
16:Ad:173:ILE:HD11	16:Ad:235:TRP:CD2	2.57	0.40
36:Ax:99:LYS:HE2	36:Ax:99:LYS:HB3	1.95	0.40
38:Az:7:LYS:HE2	38:Az:11:ARG:NH2	2.36	0.40
39:B5:454:U:H1'	72:Be:5:ARG:NE	2.37	0.40
39:B5:1586:A:N7	42:BA:199:VAL:HG21	2.37	0.40
39:B5:1741:A:H4'	61:BT:105:PHE:CD1	2.56	0.40
39:B5:1905:C:H2'	39:B5:1906:A:C8	2.57	0.40
39:B5:1981:A:O4'	39:B5:4208:C:O2'	2.39	0.40
39:B5:2181:C:OP1	83:Br:19:LYS:NZ	2.43	0.40
39:B5:2239:A:C8	39:B5:2657:C:H2'	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:B5:2505:G:H2'	39:B5:2506:G:C8	2.56	0.40
39:B5:3509:G:N2	39:B5:3547:G:H2'	2.36	0.40
41:B8:32:C:H2'	41:B8:33:G:O4'	2.22	0.40
50:BI:85:PHE:HD2	50:BI:87:ILE:HG13	1.85	0.40
54:BM:9:VAL:HG21	54:BM:66:HIS:HB3	2.03	0.40
70:Bc:47:ILE:HB	70:Bc:94:LEU:HG	2.04	0.40
1:A2:4:C:H4'	14:Ab:207:ALA:HB2	2.03	0.40
1:A2:165:G:H2'	1:A2:166:A2M:H8	2.04	0.40
1:A2:443:C:O2'	18:Af:90:GLY:O	2.30	0.40
1:A2:894:U:H2'	1:A2:895:G:H8	1.86	0.40
12:AZ:184:ARG:HD3	12:AZ:191:ARG:HG2	2.01	0.40
13:Aa:2:ALA:HB2	26:An:68:GLU:OE2	2.22	0.40
17:Ae:42:LYS:HA	17:Ae:42:LYS:HD3	1.78	0.40
35:Aw:28:LYS:HE2	35:Aw:32:LEU:HD22	2.03	0.40
39:B5:1208:C:H2'	39:B5:1209:G:C8	2.56	0.40
39:B5:1533:U:H2'	39:B5:1534:C:C6	2.57	0.40
39:B5:1650:U:H2'	39:B5:1651:C:O4'	2.20	0.40
39:B5:3674:A:H2'	39:B5:3675:A:C8	2.56	0.40
39:B5:3688:G:N2	39:B5:3785:C:O2	2.54	0.40
40:B7:3:C:H2'	40:B7:4:U:C6	2.56	0.40
40:B7:74:A:N1	40:B7:100:A:H5''	2.37	0.40
85:Bt:88:PRO:HA	85:Bt:89:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AA	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
3	AB	61/69 (88%)	61 (100%)	0	0	100	100
4	AC	72/156 (46%)	69 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AD	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
6	AE	99/115 (86%)	98 (99%)	1 (1%)	0	100	100
7	AF	311/317 (98%)	303 (97%)	8 (3%)	0	100	100
8	AG	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
12	AZ	219/295 (74%)	213 (97%)	6 (3%)	0	100	100
13	Aa	220/264 (83%)	217 (99%)	3 (1%)	0	100	100
14	Ab	218/293 (74%)	217 (100%)	1 (0%)	0	100	100
15	Ac	223/281 (79%)	221 (99%)	2 (1%)	0	100	100
16	Ad	260/263 (99%)	258 (99%)	2 (1%)	0	100	100
17	Ae	189/204 (93%)	186 (98%)	3 (2%)	0	100	100
18	Af	235/249 (94%)	235 (100%)	0	0	100	100
19	Ag	188/432 (44%)	185 (98%)	3 (2%)	0	100	100
20	Ah	204/208 (98%)	200 (98%)	4 (2%)	0	100	100
21	Ai	183/194 (94%)	180 (98%)	3 (2%)	0	100	100
22	Aj	94/165 (57%)	91 (97%)	3 (3%)	0	100	100
23	Ak	152/158 (96%)	148 (97%)	4 (3%)	0	100	100
24	Al	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
25	Am	148/151 (98%)	148 (100%)	0	0	100	100
26	An	134/151 (89%)	130 (97%)	4 (3%)	0	100	100
27	Ao	126/145 (87%)	123 (98%)	2 (2%)	1 (1%)	16	16
28	Ap	139/172 (81%)	135 (97%)	3 (2%)	1 (1%)	18	19
29	Aq	132/135 (98%)	132 (100%)	0	0	100	100
30	Ar	146/152 (96%)	142 (97%)	4 (3%)	0	100	100
31	As	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
32	At	102/119 (86%)	101 (99%)	1 (1%)	0	100	100
33	Au	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
34	Av	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
35	Aw	138/143 (96%)	136 (99%)	2 (1%)	0	100	100
36	Ax	123/130 (95%)	123 (100%)	0	0	100	100
37	Ay	83/124 (67%)	82 (99%)	1 (1%)	0	100	100
38	Az	23/25 (92%)	23 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BA	250/257 (97%)	243 (97%)	7 (3%)	0	100	100
43	BB	395/403 (98%)	389 (98%)	6 (2%)	0	100	100
44	BC	360/413 (87%)	358 (99%)	2 (1%)	0	100	100
45	BD	291/297 (98%)	289 (99%)	2 (1%)	0	100	100
46	BE	239/291 (82%)	235 (98%)	4 (2%)	0	100	100
47	BF	224/247 (91%)	219 (98%)	5 (2%)	0	100	100
48	BG	229/266 (86%)	229 (100%)	0	0	100	100
49	BH	188/192 (98%)	187 (100%)	1 (0%)	0	100	100
50	BI	211/214 (99%)	208 (99%)	3 (1%)	0	100	100
51	BJ	168/178 (94%)	167 (99%)	1 (1%)	0	100	100
52	BK	33/1071 (3%)	33 (100%)	0	0	100	100
53	BL	208/211 (99%)	205 (99%)	3 (1%)	0	100	100
54	BM	136/218 (62%)	135 (99%)	1 (1%)	0	100	100
55	BN	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
56	BO	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
57	BP	157/184 (85%)	155 (99%)	2 (1%)	0	100	100
58	BQ	185/188 (98%)	184 (100%)	1 (0%)	0	100	100
59	BR	178/196 (91%)	178 (100%)	0	0	100	100
60	BS	174/176 (99%)	174 (100%)	0	0	100	100
61	BT	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
62	BU	97/128 (76%)	96 (99%)	1 (1%)	0	100	100
63	BV	137/140 (98%)	137 (100%)	0	0	100	100
64	BW	119/157 (76%)	118 (99%)	1 (1%)	0	100	100
65	BX	116/156 (74%)	115 (99%)	1 (1%)	0	100	100
66	BY	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
67	BZ	133/136 (98%)	133 (100%)	0	0	100	100
68	Ba	144/148 (97%)	139 (96%)	4 (3%)	1 (1%)	18	19
69	Bb	103/245 (42%)	97 (94%)	6 (6%)	0	100	100
70	Bc	106/115 (92%)	106 (100%)	0	0	100	100
71	Bd	105/125 (84%)	105 (100%)	0	0	100	100
72	Be	128/135 (95%)	128 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
73	Bf	108/110 (98%)	108 (100%)	0	0	100	100
74	Bg	112/117 (96%)	111 (99%)	1 (1%)	0	100	100
75	Bh	120/123 (98%)	119 (99%)	1 (1%)	0	100	100
76	Bi	100/105 (95%)	99 (99%)	1 (1%)	0	100	100
77	Bj	84/97 (87%)	84 (100%)	0	0	100	100
78	Bk	67/70 (96%)	67 (100%)	0	0	100	100
79	Bl	48/51 (94%)	48 (100%)	0	0	100	100
80	Bm	49/128 (38%)	49 (100%)	0	0	100	100
81	Bo	102/106 (96%)	101 (99%)	1 (1%)	0	100	100
82	Bp	89/92 (97%)	86 (97%)	3 (3%)	0	100	100
83	Br	124/137 (90%)	121 (98%)	3 (2%)	0	100	100
84	Bs	194/318 (61%)	188 (97%)	6 (3%)	0	100	100
85	Bt	154/165 (93%)	153 (99%)	1 (1%)	0	100	100
86	Bv	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
All	All	11943/14908 (80%)	11781 (99%)	159 (1%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	Ao	137	HIS
28	Ap	100	VAL
68	Ba	15	VAL

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AA	75/76 (99%)	74 (99%)	1 (1%)	61	76
3	AB	56/62 (90%)	55 (98%)	1 (2%)	51	68
4	AC	67/140 (48%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AD	47/106 (44%)	46 (98%)	1 (2%)	47	63
6	AE	88/98 (90%)	85 (97%)	3 (3%)	32	44
7	AF	272/275 (99%)	269 (99%)	3 (1%)	65	79
8	AG	48/49 (98%)	48 (100%)	0	100	100
12	AZ	182/243 (75%)	176 (97%)	6 (3%)	33	45
13	Aa	203/231 (88%)	202 (100%)	1 (0%)	81	90
14	Ab	185/223 (83%)	184 (100%)	1 (0%)	81	90
15	Ac	189/232 (82%)	183 (97%)	6 (3%)	34	47
16	Ad	224/225 (100%)	224 (100%)	0	100	100
17	Ae	161/170 (95%)	161 (100%)	0	100	100
18	Af	207/218 (95%)	206 (100%)	1 (0%)	81	90
19	Ag	170/360 (47%)	169 (99%)	1 (1%)	78	89
20	Ah	178/180 (99%)	177 (99%)	1 (1%)	78	89
21	Ai	161/168 (96%)	159 (99%)	2 (1%)	63	78
22	Aj	87/136 (64%)	86 (99%)	1 (1%)	65	79
23	Ak	139/142 (98%)	139 (100%)	0	100	100
24	Al	104/108 (96%)	101 (97%)	3 (3%)	37	51
25	Am	130/131 (99%)	129 (99%)	1 (1%)	73	85
26	An	106/119 (89%)	105 (99%)	1 (1%)	70	84
27	Ao	114/130 (88%)	113 (99%)	1 (1%)	70	84
28	Ap	117/140 (84%)	117 (100%)	0	100	100
29	Aq	120/121 (99%)	120 (100%)	0	100	100
30	Ar	127/131 (97%)	123 (97%)	4 (3%)	35	48
31	As	112/114 (98%)	112 (100%)	0	100	100
32	At	94/107 (88%)	93 (99%)	1 (1%)	65	79
33	Au	67/67 (100%)	63 (94%)	4 (6%)	17	21
34	Av	112/113 (99%)	112 (100%)	0	100	100
35	Aw	112/114 (98%)	109 (97%)	3 (3%)	39	53
36	Ax	107/112 (96%)	106 (99%)	1 (1%)	70	84
37	Ay	75/102 (74%)	75 (100%)	0	100	100
38	Az	24/24 (100%)	24 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BA	194/198 (98%)	193 (100%)	1 (0%)	81	90
43	BB	344/347 (99%)	341 (99%)	3 (1%)	70	84
44	BC	302/337 (90%)	300 (99%)	2 (1%)	76	87
45	BD	247/250 (99%)	247 (100%)	0	100	100
46	BE	216/251 (86%)	214 (99%)	2 (1%)	70	84
47	BF	197/215 (92%)	195 (99%)	2 (1%)	68	81
48	BG	199/223 (89%)	198 (100%)	1 (0%)	81	90
49	BH	169/171 (99%)	169 (100%)	0	100	100
50	BI	180/181 (99%)	179 (99%)	1 (1%)	78	89
51	BJ	143/149 (96%)	143 (100%)	0	100	100
52	BK	30/936 (3%)	30 (100%)	0	100	100
53	BL	175/176 (99%)	173 (99%)	2 (1%)	65	79
54	BM	117/161 (73%)	117 (100%)	0	100	100
55	BN	171/172 (99%)	169 (99%)	2 (1%)	63	78
56	BO	171/173 (99%)	170 (99%)	1 (1%)	78	89
57	BP	140/163 (86%)	139 (99%)	1 (1%)	76	87
58	BQ	164/165 (99%)	162 (99%)	2 (1%)	63	78
59	BR	159/175 (91%)	157 (99%)	2 (1%)	61	76
60	BS	154/154 (100%)	152 (99%)	2 (1%)	61	76
61	BT	139/140 (99%)	138 (99%)	1 (1%)	76	87
62	BU	88/113 (78%)	88 (100%)	0	100	100
63	BV	106/107 (99%)	106 (100%)	0	100	100
64	BW	100/126 (79%)	98 (98%)	2 (2%)	48	64
65	BX	106/134 (79%)	106 (100%)	0	100	100
66	BY	124/135 (92%)	124 (100%)	0	100	100
67	BZ	117/118 (99%)	117 (100%)	0	100	100
68	Ba	118/119 (99%)	118 (100%)	0	100	100
69	Bb	87/183 (48%)	87 (100%)	0	100	100
70	Bc	92/98 (94%)	92 (100%)	0	100	100
71	Bd	98/110 (89%)	97 (99%)	1 (1%)	68	81
72	Be	116/121 (96%)	116 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
73	Bf	89/89 (100%)	89 (100%)	0	100	100
74	Bg	98/100 (98%)	98 (100%)	0	100	100
75	Bh	109/110 (99%)	109 (100%)	0	100	100
76	Bi	86/89 (97%)	86 (100%)	0	100	100
77	Bj	73/80 (91%)	73 (100%)	0	100	100
78	Bk	64/65 (98%)	63 (98%)	1 (2%)	55	71
79	Bl	47/48 (98%)	46 (98%)	1 (2%)	47	63
80	Bm	47/115 (41%)	47 (100%)	0	100	100
81	Bo	92/93 (99%)	92 (100%)	0	100	100
82	Bp	74/75 (99%)	74 (100%)	0	100	100
83	Br	109/120 (91%)	109 (100%)	0	100	100
84	Bs	164/258 (64%)	163 (99%)	1 (1%)	78	89
85	Bt	128/137 (93%)	123 (96%)	5 (4%)	28	39
86	Bv	191/195 (98%)	186 (97%)	5 (3%)	40	55
All	All	10394/12642 (82%)	10305 (99%)	89 (1%)	68	84

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	AA	74	THR
3	AB	14	VAL
5	AD	91	LEU
6	AE	30	VAL
6	AE	40	VAL
6	AE	75	VAL
7	AF	107	ASP
7	AF	113	PHE
7	AF	159	ASN
12	AZ	77	ILE
12	AZ	87	VAL
12	AZ	121	LEU
12	AZ	125	THR
12	AZ	192	GLU
12	AZ	206	ASP
13	Aa	178	THR
14	Ab	121	ARG
15	Ac	46	THR

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Mol	Chain	Res	Type
15	Ac	56	GLN
15	Ac	72	VAL
15	Ac	105	LEU
15	Ac	175	VAL
15	Ac	216	GLU
18	Af	44	GLU
19	Ag	53	VAL
20	Ah	46	VAL
21	Ai	55	LYS
21	Ai	152	ASP
22	Aj	40	VAL
24	Al	75	ASN
24	Al	91	LEU
24	Al	104	VAL
25	Am	70	LYS
26	An	138	ASP
27	Ao	133	ILE
30	Ar	59	LEU
30	Ar	83	PHE
30	Ar	94	LYS
30	Ar	103	LEU
32	At	54	VAL
33	Au	32	ILE
33	Au	39	VAL
33	Au	42	VAL
33	Au	61	ARG
35	Aw	61	GLN
35	Aw	105	PHE
35	Aw	125	VAL
36	Ax	7	ILE
42	BA	208	GLU
43	BB	47	LEU
43	BB	90	VAL
43	BB	162	VAL
44	BC	157	LYS
44	BC	297	GLU
46	BE	189	LEU
46	BE	223	LYS
47	BF	22	ARG
47	BF	85	GLU
48	BG	220	GLU
50	BI	38	ARG

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Mol	Chain	Res	Type
53	BL	81	LEU
53	BL	115	GLN
55	BN	182	HIS
55	BN	189	ARG
56	BO	174	LEU
57	BP	2	VAL
58	BQ	14	ARG
58	BQ	87	THR
59	BR	3	MET
59	BR	106	LEU
60	BS	82	LEU
60	BS	102	THR
61	BT	76	VAL
64	BW	66	GLU
64	BW	68	GLN
71	Bd	46	LEU
78	Bk	36	VAL
79	Bl	51	LEU
84	Bs	78	LEU
85	Bt	15	LEU
85	Bt	52	ASP
85	Bt	73	VAL
85	Bt	74	VAL
85	Bt	92	ARG
86	Bv	58	THR
86	Bv	60	ARG
86	Bv	96	ASN
86	Bv	99	LEU
86	Bv	167	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
2	AA	9	HIS
2	AA	19	HIS
2	AA	29	ASN
2	AA	51	GLN
5	AD	89	GLN
6	AE	72	HIS
7	AF	147	HIS
7	AF	196	ASN
7	AF	305	ASN

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Mol	Chain	Res	Type
12	AZ	193	HIS
13	Aa	76	ASN
13	Aa	158	HIS
13	Aa	159	GLN
14	Ab	115	GLN
15	Ac	145	GLN
15	Ac	159	HIS
15	Ac	174	HIS
16	Ad	142	HIS
16	Ad	157	ASN
17	Ae	65	GLN
17	Ae	114	ASN
17	Ae	118	ASN
18	Af	81	HIS
19	Ag	68	GLN
19	Ag	97	GLN
20	Ah	7	ASN
20	Ah	167	GLN
22	Aj	7	ASN
22	Aj	28	HIS
22	Aj	32	HIS
22	Aj	61	GLN
22	Aj	66	HIS
22	Aj	77	GLN
22	Aj	84	HIS
23	Ak	11	GLN
23	Ak	39	ASN
24	Al	72	HIS
25	Am	13	GLN
25	Am	36	GLN
25	Am	58	HIS
26	An	113	GLN
27	Ao	104	GLN
27	Ao	137	HIS
28	Ap	11	GLN
28	Ap	97	GLN
28	Ap	114	GLN
29	Aq	121	GLN
30	Ar	72	GLN
31	As	12	GLN
31	As	51	ASN
33	Au	35	ASN

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Mol	Chain	Res	Type
34	Av	82	GLN
34	Av	90	GLN
34	Av	91	ASN
35	Aw	23	HIS
35	Aw	26	GLN
35	Aw	73	GLN
35	Aw	92	ASN
36	Ax	19	GLN
36	Ax	85	ASN
37	Ay	112	ASN
38	Az	22	GLN
42	BA	140	ASN
42	BA	205	ASN
43	BB	11	HIS
43	BB	184	GLN
43	BB	289	GLN
44	BC	41	HIS
44	BC	48	ASN
44	BC	61	GLN
44	BC	85	HIS
44	BC	212	ASN
44	BC	329	ASN
45	BD	81	HIS
47	BF	118	ASN
48	BG	38	ASN
48	BG	43	GLN
48	BG	64	GLN
48	BG	81	ASN
49	BH	42	ASN
49	BH	98	HIS
50	BI	59	GLN
50	BI	73	ASN
50	BI	163	GLN
50	BI	166	HIS
52	BK	4397	GLN
54	BM	33	GLN
56	BO	63	ASN
56	BO	180	GLN
57	BP	28	ASN
57	BP	34	GLN
57	BP	137	ASN
58	BQ	160	HIS

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Mol	Chain	Res	Type
59	BR	36	ASN
59	BR	40	GLN
59	BR	75	HIS
59	BR	118	HIS
59	BR	143	HIS
61	BT	77	ASN
61	BT	131	GLN
64	BW	120	GLN
65	BX	107	HIS
65	BX	111	GLN
67	BZ	78	ASN
68	Ba	28	HIS
69	Bb	12	GLN
71	Bd	116	ASN
72	Be	23	HIS
74	Bg	28	ASN
76	Bi	36	HIS
76	Bi	80	HIS
77	Bj	13	ASN
77	Bj	66	HIS
78	Bk	58	GLN
79	Bl	4	HIS
81	Bo	102	GLN
84	Bs	34	ASN
84	Bs	68	HIS
85	Bt	70	GLN
85	Bt	103	ASN
86	Bv	35	GLN
86	Bv	199	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A2	1764/1870 (94%)	226 (12%)	0
10	AI	2/76 (2%)	1 (50%)	0
11	AT	75/76 (98%)	10 (13%)	0
39	B5	3752/4808 (78%)	471 (12%)	3 (0%)
40	B7	118/120 (98%)	9 (7%)	0
41	B8	155/158 (98%)	15 (9%)	0
9	AH	5/217 (2%)	0	0
All	All	5871/7325 (80%)	732 (12%)	3 (0%)

All (732) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A2	2	A
1	A2	3	C
1	A2	33	G
1	A2	41	G
1	A2	46	A
1	A2	56	G
1	A2	58	C
1	A2	67	C
1	A2	68	A
1	A2	73	C
1	A2	74	G
1	A2	75	G
1	A2	76	U
1	A2	77	A
1	A2	79	A
1	A2	103	A
1	A2	113	G
1	A2	115	U
1	A2	126	G
1	A2	130	G
1	A2	143	U
1	A2	147	A
1	A2	155	G
1	A2	162	C
1	A2	163	U
1	A2	168	C
1	A2	178	C
1	A2	184	G
1	A2	188	C
1	A2	192	C
1	A2	226	A
1	A2	282	C
1	A2	303	A
1	A2	306	U
1	A2	308	G
1	A2	310	G
1	A2	313	G
1	A2	320	C
1	A2	324	C
1	A2	325	U
1	A2	327	C
1	A2	328	G

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Mol	Chain	Res	Type
1	A2	336	G
1	A2	348	G
1	A2	363	C
1	A2	365	A
1	A2	369	U
1	A2	370	C
1	A2	386	G
1	A2	387	C
1	A2	401	C
1	A2	410	C
1	A2	422	G
1	A2	439	G
1	A2	449	A
1	A2	450	A
1	A2	451	C
1	A2	465	A
1	A2	466	A
1	A2	472	G
1	A2	473	C
1	A2	474	A
1	A2	475	G
1	A2	483	G
1	A2	488	U
1	A2	493	C
1	A2	497	C
1	A2	526	A
1	A2	557	U
1	A2	565	A
1	A2	569	C
1	A2	577	A2M
1	A2	584	A
1	A2	590	G
1	A2	592	U
1	A2	607	G
1	A2	608	U
1	A2	609	C
1	A2	615	C
1	A2	629	A
1	A2	630	A
1	A2	632	U
1	A2	633	C
1	A2	644	A

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Mol	Chain	Res	Type
1	A2	645	OMG
1	A2	656	A
1	A2	661	C
1	A2	669	A2M
1	A2	670	A
1	A2	672	A
1	A2	673	A
1	A2	674	G
1	A2	698	G
1	A2	734	C
1	A2	735	C
1	A2	747	C
1	A2	748	U
1	A2	750	U
1	A2	755	G
1	A2	756	C
1	A2	798	C
1	A2	799	G
1	A2	802	PSU
1	A2	812	A
1	A2	822	G
1	A2	823	PSU
1	A2	831	A
1	A2	832	G
1	A2	837	G
1	A2	838	A
1	A2	839	G
1	A2	840	C
1	A2	841	C
1	A2	842	G
1	A2	848	A
1	A2	860	G
1	A2	871	A
1	A2	873	A
1	A2	879	G
1	A2	886	U
1	A2	892	G
1	A2	914	A
1	A2	915	U
1	A2	921	A
1	A2	923	A
1	A2	931	C

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Mol	Chain	Res	Type
1	A2	934	G
1	A2	944	U
1	A2	956	A
1	A2	964	A
1	A2	972	G
1	A2	991	A
1	A2	993	A
1	A2	1000	G
1	A2	1018	U
1	A2	1024	A
1	A2	1061	A
1	A2	1062	U
1	A2	1063	A
1	A2	1084	A
1	A2	1086	C
1	A2	1116	U
1	A2	1117	C
1	A2	1118	C
1	A2	1119	C
1	A2	1122	G
1	A2	1134	A
1	A2	1145	A
1	A2	1154	C
1	A2	1155	U
1	A2	1196	A
1	A2	1208	G
1	A2	1216	C
1	A2	1225	G
1	A2	1243	U
1	A2	1252	A
1	A2	1254	A
1	A2	1257	G
1	A2	1258	G
1	A2	1260	A
1	A2	1266	A
1	A2	1272	C
1	A2	1275	G
1	A2	1276	G
1	A2	1283	A
1	A2	1303	G
1	A2	1304	C
1	A2	1316	U

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Mol	Chain	Res	Type
1	A2	1343	U
1	A2	1349	G
1	A2	1359	U
1	A2	1372	U
1	A2	1373	U
1	A2	1379	A
1	A2	1398	U
1	A2	1403	A
1	A2	1406	A
1	A2	1407	G
1	A2	1419	C
1	A2	1420	C
1	A2	1422	A
1	A2	1424	C
1	A2	1425	G
1	A2	1436	C
1	A2	1438	C
1	A2	1455	A
1	A2	1463	U
1	A2	1464	U
1	A2	1481	A
1	A2	1490	A
1	A2	1491	OMG
1	A2	1498	G
1	A2	1510	U
1	A2	1522	C
1	A2	1523	A
1	A2	1534	A
1	A2	1553	G
1	A2	1571	G
1	A2	1581	A
1	A2	1589	A
1	A2	1602	A
1	A2	1622	U
1	A2	1624	A
1	A2	1655	G
1	A2	1662	A
1	A2	1666	G
1	A2	1699	C
1	A2	1700	A
1	A2	1722	U
1	A2	1723	G

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Mol	Chain	Res	Type
1	A2	1749	G
1	A2	1768	C
1	A2	1783	G
1	A2	1784	C
1	A2	1785	G
1	A2	1830	G
1	A2	1832	A
1	A2	1837	G
1	A2	1839	U
1	A2	1850	G
1	A2	1852	MA6
1	A2	1862	G
1	A2	1863	G
1	A2	1864	A
1	A2	1865	U
1	A2	1866	C
10	AI	76	A
11	AT	16	H2U
11	AT	17	H2U
11	AT	18	G
11	AT	19	G
11	AT	20	G
11	AT	21	A
11	AT	22	G
11	AT	23	A
11	AT	48	C
11	AT	76	A
39	B5	39	A
39	B5	42	A
39	B5	58	G
39	B5	59	A
39	B5	64	A
39	B5	65	A
39	B5	85	G
39	B5	91	G
39	B5	98	A
39	B5	109	G
39	B5	110	C
39	B5	119	G
39	B5	127	G
39	B5	135	G
39	B5	136	U

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Mol	Chain	Res	Type
39	B5	142	G
39	B5	159	C
39	B5	187	U
39	B5	188	G
39	B5	200	U
39	B5	201	C
39	B5	209	U
39	B5	210	C
39	B5	218	A
39	B5	219	G
39	B5	220	C
39	B5	233	U
39	B5	234	G
39	B5	253	G
39	B5	266	C
39	B5	297	U
39	B5	309	C
39	B5	315	G
39	B5	316	U
39	B5	326	C
39	B5	334	A
39	B5	340	C
39	B5	363	A
39	B5	387	G
39	B5	409	G
39	B5	410	A
39	B5	412	G
39	B5	446	C
39	B5	449	C
39	B5	450	G
39	B5	452	A
39	B5	453	G
39	B5	454	U
39	B5	455	C
39	B5	463	A
39	B5	467	U
39	B5	468	U
39	B5	482	U
39	B5	483	G
39	B5	485	U
39	B5	486	C
39	B5	493	U

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Mol	Chain	Res	Type
39	B5	497	G
39	B5	499	C
39	B5	502	U
39	B5	503	C
39	B5	504	U
39	B5	505	C
39	B5	506	G
39	B5	515	U
39	B5	516	U
39	B5	517	C
39	B5	628	U
39	B5	634	C
39	B5	635	G
39	B5	660	G
39	B5	691	G
39	B5	698	C
39	B5	699	G
39	B5	724	G
39	B5	725	G
39	B5	732	C
39	B5	734	G
39	B5	739	G
39	B5	758	C
39	B5	760	C
39	B5	761	C
39	B5	790	G
39	B5	791	C
39	B5	792	G
39	B5	795	A
39	B5	797	C
39	B5	798	C
39	B5	803	C
39	B5	810	U
39	B5	812	A
39	B5	814	A
39	B5	815	G
39	B5	824	C
39	B5	825	G
39	B5	831	A
39	B5	832	G
39	B5	835	G
39	B5	836	C

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Mol	Chain	Res	Type
39	B5	844	A
39	B5	845	U
39	B5	856	A
39	B5	859	G
39	B5	860	A
39	B5	861	G
39	B5	866	A
39	B5	867	C
39	B5	868	C
39	B5	869	U
39	B5	870	G
39	B5	884	U
39	B5	983	G
39	B5	985	G
39	B5	987	C
39	B5	1072	C
39	B5	1073	C
39	B5	1074	C
39	B5	1084	C
39	B5	1091	G
39	B5	1102	G
39	B5	1105	C
39	B5	1106	U
39	B5	1124	A
39	B5	1127	G
39	B5	1133	C
39	B5	1202	C
39	B5	1207	G
39	B5	1214	A
39	B5	1215	G
39	B5	1217	G
39	B5	1219	G
39	B5	1221	G
39	B5	1228	G
39	B5	1229	U
39	B5	1231	G
39	B5	1240	G
39	B5	1246	U
39	B5	1247	A
39	B5	1257	C
39	B5	1270	A2M
39	B5	1281	A

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Mol	Chain	Res	Type
39	B5	1298	A
39	B5	1299	G
39	B5	1303	G
39	B5	1309	C
39	B5	1310	G
39	B5	1331	A
39	B5	1341	A
39	B5	1350	G
39	B5	1351	G
39	B5	1362	C
39	B5	1367	G
39	B5	1375	A
39	B5	1391	C
39	B5	1392	C
39	B5	1393	C
39	B5	1401	C
39	B5	1452	A
39	B5	1453	G
39	B5	1457	G
39	B5	1469	U
39	B5	1480	A
39	B5	1489	A2M
39	B5	1502	A
39	B5	1521	C
39	B5	1533	U
39	B5	1546	U
39	B5	1551	U
39	B5	1579	G
39	B5	1580	OMG
39	B5	1586	A
39	B5	1588	G
39	B5	1589	A
39	B5	1593	A
39	B5	1595	C
39	B5	1609	G
39	B5	1616	C
39	B5	1631	C
39	B5	1632	PSU
39	B5	1653	C
39	B5	1657	C
39	B5	1658	C
39	B5	1673	G

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Mol	Chain	Res	Type
39	B5	1694	C
39	B5	1704	A
39	B5	1705	A
39	B5	1726	A
39	B5	1743	A
39	B5	1745	G
39	B5	1767	C
39	B5	1773	U
39	B5	1774	G
39	B5	1775	G
39	B5	1776	A
39	B5	1781	G
39	B5	1782	A
39	B5	1794	G
39	B5	1808	G
39	B5	1836	A
39	B5	1857	U
39	B5	1859	C
39	B5	1860	C
39	B5	1861	G
39	B5	1870	C
39	B5	1871	A
39	B5	1879	G
39	B5	1887	G
39	B5	1890	G
39	B5	1898	U
39	B5	1899	A
39	B5	1900	G
39	B5	1913	U
39	B5	1916	C
39	B5	1922	A
39	B5	1923	A
39	B5	1924	G
39	B5	1925	U
39	B5	1926	C
39	B5	1936	U
39	B5	1940	G
39	B5	1942	G
39	B5	1943	U
39	B5	1963	G
39	B5	1965	A
39	B5	1985	G

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Mol	Chain	Res	Type
39	B5	1987	U
39	B5	1994	G
39	B5	2008	A
39	B5	2023	U
39	B5	2032	G
39	B5	2034	A
39	B5	2036	A
39	B5	2037	G
39	B5	2041	G
39	B5	2043	A
39	B5	2044	A
39	B5	2045	G
39	B5	2046	A
39	B5	2047	G
39	B5	2050	U
39	B5	2132	C
39	B5	2143	A
39	B5	2144	G
39	B5	2156	A
39	B5	2157	G
39	B5	2191	G
39	B5	2194	OMC
39	B5	2203	A
39	B5	2238	A
39	B5	2264	G
39	B5	2268	U
39	B5	2329	G
39	B5	2332	C
39	B5	2333	U
39	B5	2334	C
39	B5	2349	G
39	B5	2356	A
39	B5	2363	C
39	B5	2372	A
39	B5	2380	A
39	B5	2386	A
39	B5	2387	G
39	B5	2388	U
39	B5	2390	G
39	B5	2397	U
39	B5	2409	G
39	B5	2429	G

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Mol	Chain	Res	Type
39	B5	2430	A
39	B5	2432	C
39	B5	2444	A
39	B5	2496	C
39	B5	2503	A
39	B5	2512	C
39	B5	2530	U
39	B5	2537	G
39	B5	2538	A
39	B5	2539	A
39	B5	2550	U
39	B5	2551	U
39	B5	2552	C
39	B5	2553	C
39	B5	2554	G
39	B5	2578	G
39	B5	2586	A
39	B5	2606	U
39	B5	2612	U
39	B5	2631	U
39	B5	2633	U
39	B5	2641	A
39	B5	2657	C
39	B5	2669	U
39	B5	2670	G
39	B5	2672	U
39	B5	2698	G
39	B5	2745	G
39	B5	3329	G
39	B5	3350	C
39	B5	3358	G
39	B5	3362	A
39	B5	3367	A
39	B5	3376	U
39	B5	3380	A
39	B5	3385	A
39	B5	3394	A
39	B5	3405	C
39	B5	3428	C
39	B5	3443	A
39	B5	3444	A
39	B5	3482	G

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Mol	Chain	Res	Type
39	B5	3485	G
39	B5	3492	A2M
39	B5	3493	C
39	B5	3498	A
39	B5	3508	G
39	B5	3509	G
39	B5	3516	A
39	B5	3543	G
39	B5	3544	C
39	B5	3546	U
39	B5	3549	A
39	B5	3551	G
39	B5	3570	U
39	B5	3572	U
39	B5	3599	A2M
39	B5	3609	A
39	B5	3610	C
39	B5	3611	G
39	B5	3629	G
39	B5	3630	G
39	B5	3633	A
39	B5	3638	A
39	B5	3639	G
39	B5	3640	A
39	B5	3647	U
39	B5	3670	G
39	B5	3688	G
39	B5	3689	U
39	B5	3704	A
39	B5	3794	U
39	B5	3804	G
39	B5	3822	G
39	B5	3823	G
39	B5	3824	C
39	B5	3825	G
39	B5	3832	G
39	B5	3833	A
39	B5	3834	G
39	B5	3847	C
39	B5	3850	G
39	B5	3855	A
39	B5	3869	G

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Mol	Chain	Res	Type
39	B5	3874	U
39	B5	3875	C
39	B5	3891	C
39	B5	3892	G
39	B5	3904	C
39	B5	3909	U
39	B5	3916	A
39	B5	3929	G
39	B5	3930	G
39	B5	3937	G
39	B5	3949	A
39	B5	3960	A
39	B5	3971	G
39	B5	3975	U
39	B5	3979	A
39	B5	3997	A
39	B5	4000	G
39	B5	4012	G
39	B5	4014	A
39	B5	4017	A
39	B5	4019	A
39	B5	4027	A
39	B5	4037	G
39	B5	4050	A
39	B5	4051	G
39	B5	4060	C
39	B5	4075	G
39	B5	4076	G
39	B5	4078	C
39	B5	4096	C
39	B5	4119	G
39	B5	4122	A
39	B5	4123	G
39	B5	4124	A
39	B5	4126	A
39	B5	4133	C
39	B5	4137	G
39	B5	4140	A
39	B5	4168	A
39	B5	4194	G
39	B5	4210	A
39	B5	4212	C

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Mol	Chain	Res	Type
39	B5	4221	G
39	B5	4258	U
39	B5	4259	A
39	B5	4261	G
39	B5	4265	C
39	B5	4270	G
39	B5	4294	A
39	B5	4306	C
39	B5	4313	G
39	B5	4321	G
39	B5	4336	A2M
39	B5	4382	PSU
39	B5	4383	OMG
39	B5	4402	A
39	B5	4416	C
39	B5	4418	A
39	B5	4437	A
39	B5	4446	A
39	B5	4454	A
39	B5	4455	U
39	B5	4465	G
39	B5	4475	A
39	B5	4476	C
39	B5	4477	G
39	B5	4478	G
39	B5	4479	C
39	B5	4484	C
39	B5	4486	G
39	B5	4487	A
39	B5	4488	A
39	B5	4489	G
39	B5	4490	G
39	B5	4492	G
39	B5	4498	G
39	B5	4501	G
39	B5	4504	C
39	B5	4506	C
39	B5	4508	G
39	B5	4512	G
39	B5	4518	C
39	B5	4519	C
39	B5	4609	G

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Mol	Chain	Res	Type
39	B5	4610	C
39	B5	4614	G
39	B5	4621	U
39	B5	4622	C
39	B5	4637	G
39	B5	4638	G
39	B5	4639	C
39	B5	4640	G
39	B5	4642	G
39	B5	4644	C
39	B5	4645	C
39	B5	4646	G
39	B5	4647	G
39	B5	4649	A
39	B5	4651	G
39	B5	4655	G
39	B5	4658	G
39	B5	4705	A
39	B5	4715	U
39	B5	4728	U
39	B5	4729	C
39	B5	4746	A
39	B5	4753	A
39	B5	4756	G
39	B5	4761	U
39	B5	4762	C
39	B5	4763	C
39	B5	4765	U
39	B5	4766	C
39	B5	4780	G
39	B5	4789	C
39	B5	4793	C
39	B5	4797	A
39	B5	4801	G
39	B5	4805	U
39	B5	4808	U
40	B7	7	G
40	B7	33	U
40	B7	42	A
40	B7	50	A
40	B7	53	U
40	B7	54	A

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Mol	Chain	Res	Type
40	B7	64	G
40	B7	110	G
40	B7	120	U
41	B8	34	U
41	B8	35	C
41	B8	59	A
41	B8	62	A
41	B8	63	U
41	B8	81	C
41	B8	84	A
41	B8	87	G
41	B8	94	G
41	B8	103	A
41	B8	105	C
41	B8	110	U
41	B8	114	G
41	B8	123	U
41	B8	156	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
39	B5	1545	C
39	B5	1588	G
39	B5	4445	U

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

239 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
39	OMC	B5	4282	39,89	19,22,23	0.78	0	25,31,34	0.81	0
39	OMC	B5	2667	39	19,22,23	0.78	0	25,31,34	0.81	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	A2M	A2	577	1	22,25,26	1.50	4 (18%)	30,36,39	2.15	10 (33%)
39	OMG	B5	3631	39	23,26,27	1.18	3 (13%)	32,38,41	2.04	7 (21%)
1	PSU	A2	210	1	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
39	PSU	B5	4217	39	18,21,22	1.39	2 (11%)	21,30,33	2.03	3 (14%)
39	A2M	B5	4269	39,89	22,25,26	1.50	5 (22%)	30,36,39	2.16	8 (26%)
42	V5N	BA	216	42	8,11,12	2.11	2 (25%)	8,14,16	1.73	2 (25%)
39	PSU	B5	2351	39	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
1	PSU	A2	93	1	18,21,22	1.39	2 (11%)	21,30,33	2.06	4 (19%)
11	H2U	AT	16	11	18,21,22	1.00	2 (11%)	19,30,33	0.95	1 (5%)
39	PSU	B5	4107	39	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
39	OMG	B5	4245	39	23,26,27	1.18	3 (13%)	32,38,41	1.98	6 (18%)
39	A2M	B5	400	39	22,25,26	1.50	4 (18%)	30,36,39	2.05	10 (33%)
1	OMU	A2	1443	1,89	19,22,23	1.24	4 (21%)	25,31,34	1.79	4 (16%)
39	OMG	B5	3942	39,11	23,26,27	1.20	3 (13%)	32,38,41	2.02	6 (18%)
1	OMU	A2	1289	1	19,22,23	1.25	4 (21%)	25,31,34	1.78	5 (20%)
39	OMC	B5	3601	39	19,22,23	0.76	0	25,31,34	0.79	0
39	OMG	B5	4240	39	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
39	OMC	B5	3540	39	19,22,23	0.77	0	25,31,34	0.80	0
39	PSU	B5	3554	39	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	A2	1644	1,89	18,21,22	1.38	2 (11%)	21,30,33	2.02	4 (19%)
1	PSU	A2	218	1	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
39	PSU	B5	1683	39	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	A2	1368	1	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
39	OMC	B5	2704	39	19,22,23	0.78	0	25,31,34	0.81	0
39	OMG	B5	2719	39	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
1	A2M	A2	469	1	22,25,26	1.51	4 (18%)	30,36,39	2.12	10 (33%)
1	PSU	A2	1178	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
39	OMG	B5	4383	39	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
11	H2U	AT	17	11	18,21,22	1.01	2 (11%)	19,30,33	0.82	1 (5%)
1	PSU	A2	1245	1	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
1	OMG	A2	1329	1	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)
39	PSU	B5	4246	39	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
1	PSU	A2	1057	1	18,21,22	1.38	2 (11%)	21,30,33	2.11	4 (19%)
39	PSU	B5	1801	39	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
41	PSU	B8	69	41	18,21,22	1.38	2 (11%)	21,30,33	2.08	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	1MA	B5	1266	39,89	21,25,26	1.36	4 (19%)	30,37,40	1.67	6 (20%)
39	OMG	B5	1580	39	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
39	PSU	B5	3427	39	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
39	PSU	B5	3585	39,89	18,21,22	1.37	2 (11%)	21,30,33	2.08	3 (14%)
39	PSU	B5	3616	39	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
11	PSU	AT	39	11	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
33	AME	Au	1	33	9,10,11	0.50	0	9,11,13	0.90	1 (11%)
1	A2M	A2	1032	1	22,25,26	1.49	5 (22%)	30,36,39	2.15	11 (36%)
39	OMU	B5	4366	39	19,22,23	1.24	3 (15%)	25,31,34	1.80	4 (16%)
39	PSU	B5	3494	39	18,21,22	1.39	2 (11%)	21,30,33	2.01	3 (14%)
1	PSU	A2	864	1	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)
11	PSU	AT	55	11	18,21,22	1.34	2 (11%)	21,30,33	2.07	4 (19%)
39	PSU	B5	4298	39	18,21,22	1.36	2 (11%)	21,30,33	2.07	4 (19%)
39	A2M	B5	4317	39	22,25,26	1.50	4 (18%)	30,36,39	2.06	9 (30%)
11	OMC	AT	32	11	19,22,23	0.77	0	25,31,34	0.78	0
1	A2M	A2	27	1,89	22,25,26	1.49	4 (18%)	30,36,39	2.09	9 (30%)
44	AYA	BC	2	44	6,7,8	0.72	0	6,8,10	0.62	0
39	A2M	B5	2244	39,89	22,25,26	1.49	4 (18%)	30,36,39	2.09	9 (30%)
39	PSU	B5	4278	39	18,21,22	1.39	2 (11%)	21,30,33	2.04	3 (14%)
1	MA6	A2	1852	1	23,26,27	1.57	5 (21%)	33,38,41	2.06	10 (30%)
39	A2M	B5	4336	39	22,25,26	1.51	4 (18%)	30,36,39	2.13	9 (30%)
39	A2M	B5	3517	39	22,25,26	1.44	5 (22%)	30,36,39	2.27	11 (36%)
39	OMG	B5	3974	39	23,26,27	1.16	2 (8%)	32,38,41	1.97	6 (18%)
39	OMC	B5	2647	39	19,22,23	0.77	0	25,31,34	0.79	0
1	PSU	A2	967	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
1	A2M	A2	1384	1	22,25,26	1.51	4 (18%)	30,36,39	2.09	9 (30%)
39	PSU	B5	4099	39	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
39	5MC	B5	3514	39,89	19,22,23	1.66	3 (15%)	26,32,35	1.11	3 (11%)
1	OMG	A2	684	1	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
39	A2M	B5	3456	39	22,25,26	1.50	4 (18%)	30,36,39	2.09	9 (30%)
39	PSU	B5	2475	39	18,21,22	1.39	2 (11%)	21,30,33	2.00	4 (19%)
39	PSU	B5	4149	39	18,21,22	1.36	2 (11%)	21,30,33	2.08	4 (19%)
11	PSU	AT	28	11	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
1	A2M	A2	669	1,89	22,25,26	1.50	5 (22%)	30,36,39	2.04	9 (30%)
11	YYG	AT	37	11	38,42,43	1.95	8 (21%)	45,62,65	2.43	11 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	GTP	B7	1	40	33,34,34	0.58	0	50,54,54	0.59	0
39	PSU	B5	1491	39	18,21,22	1.38	2 (11%)	21,30,33	2.09	4 (19%)
39	PSU	B5	1638	39	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
1	PSU	A2	573	1	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
1	OMG	A2	645	1	23,26,27	1.17	3 (13%)	32,38,41	2.01	6 (18%)
1	PSU	A2	1626	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
39	A2M	B5	398	39	22,25,26	1.52	4 (18%)	30,36,39	2.12	8 (26%)
39	A2M	B5	3562	39	22,25,26	1.49	4 (18%)	30,36,39	2.19	10 (33%)
39	OMG	B5	4369	39	23,26,27	1.17	3 (13%)	32,38,41	2.01	6 (18%)
41	PSU	B8	55	41	18,21,22	1.35	2 (11%)	21,30,33	2.04	4 (19%)
39	A2M	B5	3557	39	22,25,26	1.47	4 (18%)	30,36,39	2.17	9 (30%)
39	PSU	B5	4169	39	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	OMU	A2	628	1	19,22,23	1.18	2 (10%)	25,31,34	1.81	5 (20%)
11	5MC	AT	49	11	19,22,23	1.64	3 (15%)	26,32,35	1.15	3 (11%)
1	PSU	A2	867	1	18,21,22	1.37	2 (11%)	21,30,33	2.05	4 (19%)
39	6MZ	B5	3966	39	22,25,26	1.48	4 (18%)	29,36,39	2.15	9 (31%)
1	PSU	A2	34	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
1	4AC	A2	1843	1	21,24,25	0.97	1 (4%)	28,34,37	1.12	3 (10%)
1	OMU	A2	1327	1,89	19,22,23	1.23	3 (15%)	25,31,34	1.80	5 (20%)
1	PSU	A2	36	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
39	PSU	B5	3490	39	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
1	OMG	A2	868	1	23,26,27	1.18	3 (13%)	32,38,41	1.98	6 (18%)
39	PSU	B5	3369	39	18,21,22	1.39	3 (16%)	21,30,33	2.08	4 (19%)
81	MLZ	Bo	53	81	8,9,10	0.50	0	4,9,11	0.15	0
39	PSU	B5	3462	39	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
1	OMG	A2	510	1,89	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
39	A2M	B5	3492	39,1	22,25,26	1.49	4 (18%)	30,36,39	2.13	10 (33%)
80	M3L	Bm	98	80	10,11,12	0.84	0	9,14,16	0.45	0
1	PSU	A2	1233	1	18,21,22	1.37	2 (11%)	21,30,33	2.10	4 (19%)
11	1MA	AT	14	11	21,25,26	1.38	4 (19%)	30,37,40	1.71	5 (16%)
39	PSU	B5	4039	39	18,21,22	1.38	2 (11%)	21,30,33	2.11	4 (19%)
1	PSU	A2	1446	1	18,21,22	1.36	2 (11%)	21,30,33	2.04	4 (19%)
39	OMU	B5	4052	39	19,22,23	1.26	4 (21%)	25,31,34	1.78	4 (16%)
39	PSU	B5	3652	39,89	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
11	M2G	AT	26	11	24,27,28	1.29	4 (16%)	33,40,43	1.89	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	OMG	B5	4138	39	23,26,27	1.17	3 (13%)	32,38,41	1.95	6 (18%)
39	PSU	B5	1720	39	18,21,22	1.37	2 (11%)	21,30,33	2.01	4 (19%)
11	2MG	AT	10	11	23,26,27	1.24	4 (17%)	33,38,41	2.19	7 (21%)
83	SAC	Br	2	83	7,8,9	0.57	0	7,9,11	0.93	1 (14%)
1	A2M	A2	1679	1	22,25,26	1.50	4 (18%)	30,36,39	2.12	10 (33%)
1	PSU	A2	816	1	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
1	PSU	A2	1693	1	18,21,22	1.36	2 (11%)	21,30,33	2.02	4 (19%)
1	OMG	A2	437	1	23,26,27	1.18	3 (13%)	32,38,41	1.99	6 (18%)
39	A2M	B5	3450	39	22,25,26	1.49	4 (18%)	30,36,39	2.10	9 (30%)
1	6MZ	A2	1833	1,89	22,25,26	1.53	4 (18%)	29,36,39	2.13	9 (31%)
39	OMG	B5	1260	39	23,26,27	1.19	3 (13%)	32,38,41	2.04	6 (18%)
39	OMC	B5	2208	39,89	19,22,23	0.76	0	25,31,34	0.79	0
39	OMC	B5	2194	39,89	19,22,23	0.78	0	25,31,34	0.98	1 (4%)
1	PSU	A2	687	1	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
39	OMU	B5	2258	39	19,22,23	1.23	4 (21%)	25,31,34	1.78	4 (16%)
39	PSU	B5	3447	39	18,21,22	1.36	2 (11%)	21,30,33	2.07	5 (23%)
1	PSU	A2	1082	1	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)
1	OMU	A2	121	1	19,22,23	1.24	4 (21%)	25,31,34	1.77	4 (16%)
11	OMG	AT	34	9,11	23,26,27	1.18	3 (13%)	32,38,41	2.00	6 (18%)
39	PSU	B5	4166	39	18,21,22	1.40	2 (11%)	21,30,33	1.99	4 (19%)
35	HY3	Aw	62	35	7,8,9	1.81	1 (14%)	7,10,12	2.44	2 (28%)
1	OMG	A2	602	1	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)
1	PSU	A2	802	1	18,21,22	1.37	2 (11%)	21,30,33	2.02	4 (19%)
39	A2M	B5	1479	39	22,25,26	1.48	4 (18%)	30,36,39	2.07	8 (26%)
39	PSU	B5	4382	39	18,21,22	1.40	2 (11%)	21,30,33	2.05	4 (19%)
39	PSU	B5	3576	39	18,21,22	1.41	2 (11%)	21,30,33	2.00	3 (14%)
39	PSU	B5	4740	39	18,21,22	1.37	2 (11%)	21,30,33	2.03	4 (19%)
39	PSU	B5	4749	39	18,21,22	1.35	2 (11%)	21,30,33	2.07	4 (19%)
11	5MU	AT	54	11	19,22,23	1.38	6 (31%)	27,32,35	2.07	7 (25%)
30	SAC	Ar	2	30	7,8,9	0.57	0	7,9,11	0.96	1 (14%)
39	OMG	B5	4364	39	23,26,27	1.17	3 (13%)	32,38,41	2.01	6 (18%)
1	PSU	A2	650	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
1	OMC	A2	463	1	19,22,23	0.79	0	25,31,34	0.81	0
11	1MA	AT	58	11	21,25,26	1.40	4 (19%)	30,37,40	1.73	5 (16%)
39	PSU	B5	4203	39	18,21,22	1.37	2 (11%)	21,30,33	2.02	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	PSU	B5	4374	39	18,21,22	1.38	2 (11%)	21,30,33	2.14	4 (19%)
39	OMG	B5	3476	39	23,26,27	1.19	3 (13%)	32,38,41	1.98	6 (18%)
1	OMU	A2	116	1	19,22,23	1.21	3 (15%)	25,31,34	1.79	5 (20%)
11	7MG	AT	46	11	23,26,27	1.30	3 (13%)	27,39,42	2.65	7 (25%)
39	UY1	B5	3550	39	19,22,23	1.39	3 (15%)	21,31,34	2.19	5 (23%)
39	PSU	B5	4325	39	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
39	OMG	B5	1477	39	23,26,27	1.18	3 (13%)	32,38,41	1.96	6 (18%)
1	OMC	A2	518	1	19,22,23	0.78	0	25,31,34	0.82	0
39	PSU	B5	4322	39	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
1	4AC	A2	1338	1	21,24,25	1.06	1 (4%)	28,34,37	1.16	2 (7%)
39	OMC	B5	3619	39	19,22,23	0.78	0	25,31,34	0.85	1 (4%)
39	OMC	B5	1284	39	19,22,23	0.77	0	25,31,34	0.74	0
1	OMU	A2	429	1	19,22,23	1.20	2 (10%)	25,31,34	1.81	5 (20%)
1	OMU	A2	355	1	19,22,23	1.24	3 (15%)	25,31,34	1.80	4 (16%)
1	A2M	A2	166	1	22,25,26	1.52	4 (18%)	30,36,39	2.15	9 (30%)
1	MA6	A2	1851	1	23,26,27	1.58	6 (26%)	33,38,41	2.14	11 (33%)
1	PSU	A2	1348	1	18,21,22	1.34	2 (11%)	21,30,33	2.06	4 (19%)
39	OMC	B5	1820	39,89	19,22,23	0.76	0	25,31,34	0.86	0
39	PSU	B5	1632	39	18,21,22	1.41	3 (16%)	21,30,33	2.07	4 (19%)
39	PSU	B5	4058	39	18,21,22	1.35	2 (11%)	21,30,33	2.03	4 (19%)
1	PSU	A2	105	1	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
39	PSU	B5	3583	39	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
39	PSU	B5	3371	39	18,21,22	1.39	2 (11%)	21,30,33	2.02	4 (19%)
39	PSU	B5	4188	39	18,21,22	1.38	2 (11%)	21,30,33	2.06	5 (23%)
39	OMU	B5	3657	39	19,22,23	1.24	2 (10%)	25,31,34	1.84	5 (20%)
39	OMG	B5	2207	39	23,26,27	1.19	3 (13%)	32,38,41	1.99	6 (18%)
39	PSU	B5	3502	39	18,21,22	1.35	2 (11%)	21,30,33	2.08	4 (19%)
39	OMG	B5	4116	39	23,26,27	1.17	3 (13%)	32,38,41	2.00	6 (18%)
43	HIC	BB	245	43	10,11,12	0.58	0	9,14,16	0.82	0
1	OMC	A2	1392	1	19,22,23	0.80	0	25,31,34	0.96	2 (8%)
39	A2M	B5	2630	39,89	22,25,26	1.51	4 (18%)	30,36,39	2.04	7 (23%)
1	A2M	A2	485	1	22,25,26	1.50	4 (18%)	30,36,39	2.06	8 (26%)
39	PSU	B5	4045	39	18,21,22	1.37	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	A2	610	1	18,21,22	1.36	2 (11%)	21,30,33	2.05	4 (19%)
39	OMC	B5	3433	39	19,22,23	0.76	0	25,31,34	0.80	0
1	OMC	A2	174	1,89	19,22,23	0.79	0	25,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	A2M	B5	1270	39	22,25,26	1.50	4 (18%)	30,36,39	2.08	8 (26%)
39	PSU	B5	4711	39	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)
1	OMU	A2	172	1	19,22,23	1.22	2 (10%)	25,31,34	1.81	5 (20%)
41	OMG	B8	75	41	23,26,27	1.17	3 (13%)	32,38,41	1.99	6 (18%)
11	PSU	AT	27	11	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
39	PSU	B5	3466	39	18,21,22	1.39	2 (11%)	21,30,33	2.03	5 (23%)
39	OMG	B5	3524	39	23,26,27	1.20	3 (13%)	32,38,41	1.99	6 (18%)
1	OMG	A2	1448	1	23,26,27	1.20	3 (13%)	32,38,41	2.01	6 (18%)
39	OMC	B5	2265	39,89	19,22,23	0.78	0	25,31,34	0.83	1 (4%)
1	PSU	A2	119	1	18,21,22	1.39	2 (11%)	21,30,33	2.02	3 (14%)
39	OMC	B5	3573	39	19,22,23	0.77	0	25,31,34	0.84	0
39	PSU	B5	4042	39	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
39	OMG	B5	2267	39	23,26,27	1.20	3 (13%)	32,38,41	1.98	6 (18%)
39	PSU	B5	1721	39	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
39	PSU	B5	3496	39	18,21,22	1.38	2 (11%)	21,30,33	2.07	4 (19%)
39	OMG	B5	3359	39	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
39	A2M	B5	2658	39,89	22,25,26	1.50	4 (18%)	30,36,39	2.08	9 (30%)
39	OMU	B5	4244	39	19,22,23	1.22	3 (15%)	25,31,34	1.76	5 (20%)
39	PSU	B5	4267	39,89	18,21,22	1.37	2 (11%)	21,30,33	2.08	5 (23%)
39	PSU	B5	1799	39	18,21,22	1.37	2 (11%)	21,30,33	2.06	4 (19%)
39	OMC	B5	4202	39	19,22,23	0.76	0	25,31,34	0.76	0
1	A2M	A2	99	1,89	22,25,26	1.51	4 (18%)	30,36,39	2.12	9 (30%)
69	MLZ	Bb	5	69	8,9,10	0.50	0	4,9,11	0.19	0
1	7MG	A2	1640	1,11	23,26,27	1.32	3 (13%)	27,39,42	2.63	7 (25%)
1	B8N	A2	1249	1	25,29,30	1.44	4 (16%)	28,42,45	1.38	3 (10%)
1	PSU	A2	815	1	18,21,22	1.35	2 (11%)	21,30,33	2.06	4 (19%)
1	PSU	A2	682	1	18,21,22	1.37	2 (11%)	21,30,33	2.04	4 (19%)
1	PSU	A2	1046	1	18,21,22	1.35	2 (11%)	21,30,33	2.05	4 (19%)
1	OMU	A2	1805	1	19,22,23	1.24	4 (21%)	25,31,34	1.79	4 (16%)
1	PSU	A2	1047	1	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
1	OMC	A2	1704	1	19,22,23	0.78	0	25,31,34	0.85	1 (4%)
1	PSU	A2	407	1	18,21,22	1.37	2 (11%)	21,30,33	2.09	4 (19%)
39	PSU	B5	4419	39	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
39	PSU	B5	1718	39	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
1	PSU	A2	652	1	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
39	OMU	B5	3973	39	19,22,23	1.27	3 (15%)	25,31,34	1.81	4 (16%)
1	A2M	A2	159	1	22,25,26	1.51	4 (18%)	30,36,39	2.17	10 (33%)
1	PSU	A2	109	1	18,21,22	1.36	2 (11%)	21,30,33	2.03	4 (19%)
31	NMM	As	67	31	8,11,12	0.53	0	7,12,14	0.45	0
39	A2M	B5	2206	39,89	22,25,26	1.51	4 (18%)	30,36,39	2.08	9 (30%)
1	PSU	A2	823	1	18,21,22	1.38	2 (11%)	21,30,33	2.08	4 (19%)
39	PSU	B5	4435	39	18,21,22	1.38	2 (11%)	21,30,33	2.06	4 (19%)
1	OMG	A2	1491	1,89	23,26,27	1.19	3 (13%)	32,38,41	2.01	6 (18%)
39	A2M	B5	1810	39,89	22,25,26	1.49	4 (18%)	30,36,39	2.18	9 (30%)
39	A2M	B5	3599	39	22,25,26	1.50	4 (18%)	30,36,39	2.03	8 (26%)
68	V5N	Ba	39	68	8,11,12	2.09	2 (25%)	8,14,16	1.74	2 (25%)
39	A2M	B5	1489	39,89	22,25,26	1.51	4 (18%)	30,36,39	2.07	9 (30%)
1	PSU	A2	1239	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)
1	A2M	A2	591	1	22,25,26	1.52	4 (18%)	30,36,39	2.17	7 (23%)
39	PSU	B5	1731	39	18,21,22	1.35	2 (11%)	21,30,33	2.02	4 (19%)
39	PSU	B5	1537	39	18,21,22	1.39	2 (11%)	21,30,33	2.03	4 (19%)
39	OMU	B5	2680	39	19,22,23	1.25	3 (15%)	25,31,34	1.89	5 (20%)
1	PSU	A2	1005	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
12	SAC	AZ	2	12	7,8,9	0.56	0	7,9,11	0.96	1 (14%)
39	PSU	B5	3500	39	18,21,22	1.38	2 (11%)	21,30,33	2.04	4 (19%)
39	PSU	B5	4177	39	18,21,22	1.38	2 (11%)	21,30,33	2.05	4 (19%)
39	OMG	B5	3676	39	23,26,27	1.19	3 (13%)	32,38,41	2.00	6 (18%)
39	UR3	B5	4276	39	19,22,23	1.00	1 (5%)	26,32,35	1.75	3 (11%)
1	A2M	A2	513	1	22,25,26	1.50	4 (18%)	30,36,39	2.14	9 (30%)
39	5MC	B5	4193	39	19,22,23	1.69	3 (15%)	26,32,35	1.19	2 (7%)
1	PSU	A2	1175	1	18,21,22	1.36	2 (11%)	21,30,33	2.06	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	OMC	B5	4282	39,89	-	0/9/27/28	0/2/2/2
39	OMC	B5	2667	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	577	1	-	2/9/27/28	0/3/3/3
39	OMG	B5	3631	39	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	210	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4217	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4269	39,89	-	0/9/27/28	0/3/3/3
42	V5N	BA	216	42	-	1/9/10/12	0/1/1/1
39	PSU	B5	2351	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	93	1	-	0/7/25/26	0/2/2/2
11	H2U	AT	16	11	-	1/7/38/39	0/2/2/2
39	PSU	B5	4107	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4245	39	-	1/9/27/28	0/3/3/3
39	A2M	B5	400	39	-	0/9/27/28	0/3/3/3
1	OMU	A2	1443	1,89	-	1/9/27/28	0/2/2/2
39	OMG	B5	3942	39,11	-	0/9/27/28	0/3/3/3
1	OMU	A2	1289	1	-	1/9/27/28	0/2/2/2
39	OMC	B5	3601	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	4240	39	-	0/9/27/28	0/3/3/3
39	OMC	B5	3540	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3554	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1644	1,89	-	0/7/25/26	0/2/2/2
1	PSU	A2	218	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1683	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1368	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	2704	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	2719	39	-	0/9/27/28	0/3/3/3
1	A2M	A2	469	1	-	1/9/27/28	0/3/3/3
1	PSU	A2	1178	1	-	0/7/25/26	0/2/2/2
39	OMG	B5	4383	39	-	0/9/27/28	0/3/3/3
11	H2U	AT	17	11	-	6/7/38/39	0/2/2/2
1	PSU	A2	1245	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	1329	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	4246	39	-	1/7/25/26	0/2/2/2
1	PSU	A2	1057	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	1801	39	-	0/7/25/26	0/2/2/2
41	PSU	B8	69	41	-	0/7/25/26	0/2/2/2
39	1MA	B5	1266	39,89	-	1/7/25/26	0/3/3/3
39	OMG	B5	1580	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	3427	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3585	39,89	-	0/7/25/26	0/2/2/2
39	PSU	B5	3616	39	-	0/7/25/26	0/2/2/2
11	PSU	AT	39	11	-	0/7/25/26	0/2/2/2
33	AME	Au	1	33	-	2/9/10/12	-
1	A2M	A2	1032	1	-	0/9/27/28	0/3/3/3
39	OMU	B5	4366	39	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	3494	39	-	2/7/25/26	0/2/2/2
1	PSU	A2	864	1	-	0/7/25/26	0/2/2/2
11	PSU	AT	55	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	4298	39	-	0/7/25/26	0/2/2/2
39	A2M	B5	4317	39	-	0/9/27/28	0/3/3/3
11	OMC	AT	32	11	-	0/9/27/28	0/2/2/2
1	A2M	A2	27	1,89	-	0/9/27/28	0/3/3/3
44	AYA	BC	2	44	-	2/5/6/8	-
39	A2M	B5	2244	39,89	-	0/9/27/28	0/3/3/3
39	PSU	B5	4278	39	-	0/7/25/26	0/2/2/2
1	MA6	A2	1852	1	-	1/11/29/30	0/3/3/3
39	A2M	B5	4336	39	-	1/9/27/28	0/3/3/3
39	A2M	B5	3517	39	-	2/9/27/28	0/3/3/3
39	OMG	B5	3974	39	-	0/9/27/28	0/3/3/3
39	OMC	B5	2647	39	-	0/9/27/28	0/2/2/2
1	PSU	A2	967	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	1384	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	4099	39	-	0/7/25/26	0/2/2/2
39	5MC	B5	3514	39,89	-	0/7/25/26	0/2/2/2
1	OMG	A2	684	1	-	0/9/27/28	0/3/3/3
39	A2M	B5	3456	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	2475	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4149	39	-	0/7/25/26	0/2/2/2
11	PSU	AT	28	11	-	0/7/25/26	0/2/2/2
1	A2M	A2	669	1,89	-	3/9/27/28	0/3/3/3
11	YYG	AT	37	11	-	1/24/42/43	0/4/4/4
40	GTP	B7	1	40	-	0/22/38/38	0/3/3/3
39	PSU	B5	1491	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1638	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	573	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	645	1	-	4/9/27/28	0/3/3/3
1	PSU	A2	1626	1	-	0/7/25/26	0/2/2/2
39	A2M	B5	398	39	-	2/9/27/28	0/3/3/3
39	A2M	B5	3562	39	-	0/9/27/28	0/3/3/3
39	OMG	B5	4369	39	-	0/9/27/28	0/3/3/3
41	PSU	B8	55	41	-	0/7/25/26	0/2/2/2
39	A2M	B5	3557	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	4169	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	628	1	-	4/9/27/28	0/2/2/2
11	5MC	AT	49	11	-	0/7/25/26	0/2/2/2
1	PSU	A2	867	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	6MZ	B5	3966	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	34	1	-	0/7/25/26	0/2/2/2
1	4AC	A2	1843	1	-	2/11/29/30	0/2/2/2
1	OMU	A2	1327	1,89	-	0/9/27/28	0/2/2/2
1	PSU	A2	36	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3490	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	868	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	3369	39	-	0/7/25/26	0/2/2/2
81	MLZ	Bo	53	81	-	0/7/8/10	-
39	PSU	B5	3462	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	510	1,89	-	0/9/27/28	0/3/3/3
39	A2M	B5	3492	39,1	-	0/9/27/28	0/3/3/3
80	M3L	Bm	98	80	-	0/9/10/12	-
1	PSU	A2	1233	1	-	0/7/25/26	0/2/2/2
11	1MA	AT	14	11	-	0/7/25/26	0/3/3/3
39	PSU	B5	4039	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1446	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	4052	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	3652	39,89	-	0/7/25/26	0/2/2/2
11	M2G	AT	26	11	-	0/11/29/30	0/3/3/3
39	OMG	B5	4138	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	1720	39	-	0/7/25/26	0/2/2/2
11	2MG	AT	10	11	-	0/9/27/28	0/3/3/3
83	SAC	Br	2	83	-	0/7/8/10	-
1	A2M	A2	1679	1	-	0/9/27/28	0/3/3/3
1	PSU	A2	816	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1693	1	-	0/7/25/26	0/2/2/2
1	OMG	A2	437	1	-	0/9/27/28	0/3/3/3
39	A2M	B5	3450	39	-	0/9/27/28	0/3/3/3
1	6MZ	A2	1833	1,89	-	2/9/27/28	0/3/3/3
39	OMG	B5	1260	39	-	0/9/27/28	0/3/3/3
39	OMC	B5	2208	39,89	-	0/9/27/28	0/2/2/2
39	OMC	B5	2194	39,89	-	2/9/27/28	0/2/2/2
1	PSU	A2	687	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	2258	39	-	1/9/27/28	0/2/2/2
39	PSU	B5	3447	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	1082	1	-	1/7/25/26	0/2/2/2
1	OMU	A2	121	1	-	0/9/27/28	0/2/2/2
11	OMG	AT	34	9,11	-	1/9/27/28	0/3/3/3
39	PSU	B5	4166	39	-	0/7/25/26	0/2/2/2
35	HY3	Aw	62	35	-	1/1/12/14	0/1/1/1
1	OMG	A2	602	1	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A2	802	1	-	2/7/25/26	0/2/2/2
39	A2M	B5	1479	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	4382	39	-	3/7/25/26	0/2/2/2
39	PSU	B5	3576	39	-	1/7/25/26	0/2/2/2
39	PSU	B5	4740	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4749	39	-	0/7/25/26	0/2/2/2
11	5MU	AT	54	11	-	0/7/25/26	0/2/2/2
30	SAC	Ar	2	30	-	0/7/8/10	-
39	OMG	B5	4364	39	-	0/9/27/28	0/3/3/3
1	PSU	A2	650	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	463	1	-	1/9/27/28	0/2/2/2
11	1MA	AT	58	11	-	0/7/25/26	0/3/3/3
39	PSU	B5	4203	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4374	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3476	39	-	0/9/27/28	0/3/3/3
1	OMU	A2	116	1	-	1/9/27/28	0/2/2/2
11	7MG	AT	46	11	-	1/7/37/38	0/3/3/3
39	UY1	B5	3550	39	-	3/9/27/28	0/2/2/2
39	PSU	B5	4325	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	1477	39	-	1/9/27/28	0/3/3/3
1	OMC	A2	518	1	-	1/9/27/28	0/2/2/2
39	PSU	B5	4322	39	-	0/7/25/26	0/2/2/2
1	4AC	A2	1338	1	-	4/11/29/30	0/2/2/2
39	OMC	B5	3619	39	-	1/9/27/28	0/2/2/2
39	OMC	B5	1284	39	-	0/9/27/28	0/2/2/2
1	OMU	A2	429	1	-	4/9/27/28	0/2/2/2
1	OMU	A2	355	1	-	0/9/27/28	0/2/2/2
1	A2M	A2	166	1	-	0/9/27/28	0/3/3/3
1	MA6	A2	1851	1	-	0/11/29/30	0/3/3/3
1	PSU	A2	1348	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	1820	39,89	-	0/9/27/28	0/2/2/2
39	PSU	B5	1632	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4058	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	105	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	3583	39	-	2/7/25/26	0/2/2/2
39	PSU	B5	3371	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4188	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	3657	39	-	0/9/27/28	0/2/2/2
39	OMG	B5	2207	39	-	2/9/27/28	0/3/3/3
39	PSU	B5	3502	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	4116	39	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	HIC	BB	245	43	-	0/5/6/8	0/1/1/1
1	OMC	A2	1392	1	-	1/9/27/28	0/2/2/2
39	A2M	B5	2630	39,89	-	3/9/27/28	0/3/3/3
1	A2M	A2	485	1	-	0/9/27/28	0/3/3/3
39	PSU	B5	4045	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	610	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3433	39	-	4/9/27/28	0/2/2/2
1	OMC	A2	174	1,89	-	0/9/27/28	0/2/2/2
39	A2M	B5	1270	39	-	1/9/27/28	0/3/3/3
39	PSU	B5	4711	39	-	0/7/25/26	0/2/2/2
1	OMU	A2	172	1	-	0/9/27/28	0/2/2/2
41	OMG	B8	75	41	-	0/9/27/28	0/3/3/3
11	PSU	AT	27	11	-	0/7/25/26	0/2/2/2
39	PSU	B5	3466	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3524	39	-	1/9/27/28	0/3/3/3
1	OMG	A2	1448	1	-	3/9/27/28	0/3/3/3
39	OMC	B5	2265	39,89	-	2/9/27/28	0/2/2/2
1	PSU	A2	119	1	-	0/7/25/26	0/2/2/2
39	OMC	B5	3573	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4042	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	2267	39	-	0/9/27/28	0/3/3/3
39	PSU	B5	1721	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	3496	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3359	39	-	0/9/27/28	0/3/3/3
39	A2M	B5	2658	39,89	-	1/9/27/28	0/3/3/3
39	OMU	B5	4244	39	-	0/9/27/28	0/2/2/2
39	PSU	B5	4267	39,89	-	1/7/25/26	0/2/2/2
39	PSU	B5	1799	39	-	0/7/25/26	0/2/2/2
39	OMC	B5	4202	39	-	2/9/27/28	0/2/2/2
1	A2M	A2	99	1,89	-	1/9/27/28	0/3/3/3
69	MLZ	Bb	5	69	-	1/7/8/10	-
1	7MG	A2	1640	1,11	-	0/7/37/38	0/3/3/3
1	B8N	A2	1249	1	-	4/16/34/35	0/2/2/2
1	PSU	A2	815	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	682	1	-	0/7/25/26	0/2/2/2
1	PSU	A2	1046	1	-	0/7/25/26	0/2/2/2
1	OMU	A2	1805	1	-	0/9/27/28	0/2/2/2
1	PSU	A2	1047	1	-	0/7/25/26	0/2/2/2
1	OMC	A2	1704	1	-	1/9/27/28	0/2/2/2
1	PSU	A2	407	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4419	39	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PSU	B5	1718	39	-	0/7/25/26	0/2/2/2
1	PSU	A2	652	1	-	0/7/25/26	0/2/2/2
39	OMU	B5	3973	39	-	0/9/27/28	0/2/2/2
1	A2M	A2	159	1	-	2/9/27/28	0/3/3/3
1	PSU	A2	109	1	-	0/7/25/26	0/2/2/2
31	NMM	As	67	31	-	0/9/11/13	-
39	A2M	B5	2206	39,89	-	0/9/27/28	0/3/3/3
1	PSU	A2	823	1	-	0/7/25/26	0/2/2/2
39	PSU	B5	4435	39	-	0/7/25/26	0/2/2/2
1	OMG	A2	1491	1,89	-	1/9/27/28	0/3/3/3
39	A2M	B5	1810	39,89	-	0/9/27/28	0/3/3/3
39	A2M	B5	3599	39	-	2/9/27/28	0/3/3/3
68	V5N	Ba	39	68	-	0/9/10/12	0/1/1/1
39	A2M	B5	1489	39,89	-	1/9/27/28	0/3/3/3
1	PSU	A2	1239	1	-	0/7/25/26	0/2/2/2
1	A2M	A2	591	1	-	3/9/27/28	0/3/3/3
39	PSU	B5	1731	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	1537	39	-	0/7/25/26	0/2/2/2
39	OMU	B5	2680	39	-	1/9/27/28	0/2/2/2
1	PSU	A2	1005	1	-	0/7/25/26	0/2/2/2
12	SAC	AZ	2	12	-	2/7/8/10	-
39	PSU	B5	3500	39	-	0/7/25/26	0/2/2/2
39	PSU	B5	4177	39	-	0/7/25/26	0/2/2/2
39	OMG	B5	3676	39	-	0/9/27/28	0/3/3/3
39	UR3	B5	4276	39	-	0/7/25/26	0/2/2/2
1	A2M	A2	513	1	-	3/9/27/28	0/3/3/3
39	5MC	B5	4193	39	-	4/7/25/26	0/2/2/2
1	PSU	A2	1175	1	-	0/7/25/26	0/2/2/2

All (570) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	37	YYG	O23-C21	6.85	1.45	1.34
39	B5	3514	5MC	C5-C4	6.09	1.48	1.44
39	B5	4193	5MC	C5-C4	6.09	1.48	1.44
11	AT	49	5MC	C5-C4	5.97	1.48	1.44
11	AT	37	YYG	O18-C16	5.15	1.45	1.33
42	BA	216	V5N	CG-ND1	-4.94	1.33	1.37
68	Ba	39	V5N	CG-ND1	-4.89	1.33	1.37
1	A2	591	A2M	C5-C4	4.83	1.47	1.39
1	A2	1851	MA6	C5-C4	4.80	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1852	MA6	C5-C4	4.77	1.47	1.39
1	A2	1833	6MZ	C5-C4	4.77	1.47	1.39
39	B5	2630	A2M	C5-C4	4.76	1.47	1.39
39	B5	4336	A2M	C5-C4	4.73	1.47	1.39
39	B5	398	A2M	C5-C4	4.71	1.47	1.39
1	A2	159	A2M	C5-C4	4.71	1.47	1.39
1	A2	166	A2M	C5-C4	4.70	1.47	1.39
39	B5	3966	6MZ	C5-C4	4.69	1.47	1.39
39	B5	2244	A2M	C5-C4	4.68	1.47	1.39
1	A2	99	A2M	C5-C4	4.68	1.47	1.39
1	A2	485	A2M	C5-C4	4.68	1.47	1.39
39	B5	2206	A2M	C5-C4	4.68	1.47	1.39
1	A2	1384	A2M	C5-C4	4.68	1.47	1.39
1	A2	513	A2M	C5-C4	4.67	1.47	1.39
39	B5	1270	A2M	C5-C4	4.66	1.47	1.39
39	B5	2658	A2M	C5-C4	4.66	1.47	1.39
39	B5	4317	A2M	C5-C4	4.66	1.47	1.39
39	B5	3599	A2M	C5-C4	4.66	1.47	1.39
39	B5	1489	A2M	C5-C4	4.66	1.47	1.39
39	B5	4269	A2M	C5-C4	4.66	1.47	1.39
1	A2	469	A2M	C5-C4	4.66	1.47	1.39
1	A2	1679	A2M	C5-C4	4.66	1.47	1.39
1	A2	577	A2M	C5-C4	4.65	1.47	1.39
39	B5	3492	A2M	C5-C4	4.65	1.47	1.39
39	B5	3450	A2M	C5-C4	4.64	1.47	1.39
39	B5	1479	A2M	C5-C4	4.63	1.47	1.39
39	B5	400	A2M	C5-C4	4.62	1.47	1.39
39	B5	3456	A2M	C5-C4	4.62	1.47	1.39
1	A2	669	A2M	C5-C4	4.61	1.47	1.39
1	A2	1032	A2M	C5-C4	4.60	1.47	1.39
39	B5	3562	A2M	C5-C4	4.60	1.47	1.39
39	B5	1810	A2M	C5-C4	4.59	1.47	1.39
1	A2	27	A2M	C5-C4	4.57	1.47	1.39
39	B5	3557	A2M	C5-C4	4.53	1.47	1.39
39	B5	3517	A2M	C5-C4	4.38	1.46	1.39
35	Aw	62	HY3	C3-CA	-4.37	1.50	1.55
11	AT	37	YYG	C5-C4	4.18	1.48	1.38
39	B5	3550	UY1	C6-C5	3.67	1.39	1.35
1	A2	1249	B8N	C4-C5	-3.61	1.39	1.47
39	B5	3576	PSU	C6-C5	3.49	1.39	1.35
39	B5	4166	PSU	C6-C5	3.48	1.39	1.35
39	B5	4382	PSU	C6-C5	3.48	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4711	PSU	C6-C5	3.48	1.39	1.35
1	A2	1178	PSU	C6-C5	3.46	1.39	1.35
39	B5	4435	PSU	C6-C5	3.46	1.39	1.35
11	AT	37	YYG	C6-N1	-3.46	1.34	1.42
1	A2	682	PSU	C6-C5	3.45	1.39	1.35
39	B5	4419	PSU	C6-C5	3.45	1.39	1.35
1	A2	652	PSU	C6-C5	3.44	1.39	1.35
39	B5	4217	PSU	C6-C5	3.44	1.39	1.35
39	B5	4278	PSU	C6-C5	3.44	1.39	1.35
1	A2	119	PSU	C6-C5	3.44	1.39	1.35
39	B5	4374	PSU	C6-C5	3.44	1.39	1.35
39	B5	3652	PSU	C6-C5	3.43	1.39	1.35
39	B5	4267	PSU	C6-C5	3.43	1.39	1.35
1	A2	93	PSU	C6-C5	3.43	1.39	1.35
39	B5	3494	PSU	C6-C5	3.42	1.39	1.35
1	A2	1005	PSU	C6-C5	3.42	1.39	1.35
1	A2	816	PSU	C6-C5	3.42	1.39	1.35
39	B5	3466	PSU	C6-C5	3.42	1.39	1.35
1	A2	1245	PSU	C6-C5	3.41	1.39	1.35
39	B5	3371	PSU	C6-C5	3.41	1.39	1.35
1	A2	573	PSU	C6-C5	3.41	1.39	1.35
1	A2	34	PSU	C6-C5	3.40	1.39	1.35
39	B5	3500	PSU	C6-C5	3.40	1.39	1.35
39	B5	1721	PSU	C6-C5	3.40	1.39	1.35
39	B5	3490	PSU	C6-C5	3.40	1.39	1.35
1	A2	210	PSU	C6-C5	3.40	1.39	1.35
39	B5	1537	PSU	C6-C5	3.39	1.39	1.35
39	B5	3583	PSU	C6-C5	3.39	1.39	1.35
1	A2	864	PSU	C6-C5	3.39	1.39	1.35
1	A2	1082	PSU	C6-C5	3.38	1.39	1.35
39	B5	3616	PSU	C6-C5	3.38	1.39	1.35
1	A2	1057	PSU	C6-C5	3.38	1.39	1.35
39	B5	4188	PSU	C6-C5	3.38	1.39	1.35
1	A2	610	PSU	C6-C5	3.38	1.39	1.35
1	A2	802	PSU	C6-C5	3.38	1.39	1.35
39	B5	4298	PSU	C6-C5	3.38	1.39	1.35
39	B5	4322	PSU	C6-C5	3.37	1.39	1.35
1	A2	105	PSU	C6-C5	3.37	1.39	1.35
1	A2	687	PSU	C6-C5	3.36	1.39	1.35
1	A2	1233	PSU	C6-C5	3.36	1.39	1.35
39	B5	1683	PSU	C6-C5	3.36	1.39	1.35
39	B5	4177	PSU	C6-C5	3.36	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1047	PSU	C6-C5	3.36	1.39	1.35
1	A2	1239	PSU	C6-C5	3.36	1.39	1.35
39	B5	3427	PSU	C6-C5	3.35	1.39	1.35
39	B5	2475	PSU	C6-C5	3.35	1.39	1.35
39	B5	4042	PSU	C6-C5	3.35	1.39	1.35
39	B5	1638	PSU	C6-C5	3.35	1.39	1.35
41	B8	69	PSU	C6-C5	3.35	1.39	1.35
1	A2	867	PSU	C6-C5	3.35	1.39	1.35
39	B5	1720	PSU	C6-C5	3.34	1.39	1.35
39	B5	3554	PSU	C6-C5	3.34	1.39	1.35
11	AT	27	PSU	C6-C5	3.34	1.39	1.35
1	A2	1368	PSU	C6-C5	3.34	1.39	1.35
1	A2	1693	PSU	C6-C5	3.34	1.39	1.35
39	B5	4740	PSU	C6-C5	3.34	1.39	1.35
39	B5	1491	PSU	C6-C5	3.33	1.39	1.35
39	B5	1718	PSU	C6-C5	3.33	1.39	1.35
1	A2	967	PSU	C6-C5	3.32	1.39	1.35
1	A2	109	PSU	C6-C5	3.32	1.39	1.35
39	B5	3462	PSU	C6-C5	3.32	1.39	1.35
39	B5	3369	PSU	C6-C5	3.32	1.39	1.35
39	B5	4749	PSU	C6-C5	3.31	1.39	1.35
1	A2	1640	7MG	C5-C4	3.31	1.47	1.37
39	B5	1799	PSU	C6-C5	3.30	1.38	1.35
11	AT	28	PSU	C6-C5	3.30	1.38	1.35
1	A2	1175	PSU	C6-C5	3.30	1.38	1.35
39	B5	4045	PSU	C6-C5	3.30	1.38	1.35
39	B5	1632	PSU	C6-C5	3.29	1.38	1.35
1	A2	650	PSU	C6-C5	3.29	1.38	1.35
1	A2	1446	PSU	C6-C5	3.29	1.38	1.35
1	A2	1644	PSU	C6-C5	3.29	1.38	1.35
39	B5	4099	PSU	C6-C5	3.29	1.38	1.35
11	AT	39	PSU	C6-C5	3.29	1.38	1.35
41	B8	55	PSU	C6-C5	3.29	1.38	1.35
1	A2	407	PSU	C6-C5	3.28	1.38	1.35
39	B5	4149	PSU	C6-C5	3.28	1.38	1.35
11	AT	58	1MA	C6-N6	3.28	1.35	1.28
39	B5	4039	PSU	C6-C5	3.28	1.38	1.35
1	A2	1249	B8N	C4-N3	-3.27	1.34	1.40
39	B5	4107	PSU	C6-C5	3.27	1.38	1.35
1	A2	36	PSU	C6-C5	3.27	1.38	1.35
39	B5	3496	PSU	C6-C5	3.27	1.38	1.35
39	B5	2351	PSU	C6-C5	3.27	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	815	PSU	C6-C5	3.26	1.38	1.35
39	B5	4203	PSU	C6-C5	3.26	1.38	1.35
39	B5	1731	PSU	C6-C5	3.26	1.38	1.35
1	A2	823	PSU	C6-C5	3.25	1.38	1.35
1	A2	218	PSU	C6-C5	3.25	1.38	1.35
1	A2	1626	PSU	C6-C5	3.25	1.38	1.35
39	B5	3447	PSU	C6-C5	3.25	1.38	1.35
11	AT	46	7MG	C5-C4	3.24	1.47	1.37
11	AT	55	PSU	C6-C5	3.24	1.38	1.35
39	B5	4325	PSU	C6-C5	3.23	1.38	1.35
11	AT	58	1MA	C5-C4	3.23	1.47	1.38
1	A2	1046	PSU	C6-C5	3.23	1.38	1.35
39	B5	3502	PSU	C6-C5	3.21	1.38	1.35
39	B5	4058	PSU	C6-C5	3.21	1.38	1.35
39	B5	2267	OMG	C5-C4	3.21	1.47	1.38
39	B5	4246	PSU	C6-C5	3.20	1.38	1.35
39	B5	1801	PSU	C6-C5	3.20	1.38	1.35
11	AT	14	1MA	C6-N6	3.20	1.35	1.28
1	A2	1448	OMG	C5-C4	3.19	1.47	1.38
11	AT	14	1MA	C5-C4	3.19	1.47	1.38
1	A2	1348	PSU	C6-C5	3.19	1.38	1.35
39	B5	2719	OMG	C5-C4	3.18	1.47	1.38
39	B5	4169	PSU	C6-C5	3.18	1.38	1.35
39	B5	1580	OMG	C5-C4	3.18	1.47	1.38
39	B5	3585	PSU	C6-C5	3.18	1.38	1.35
39	B5	4138	OMG	C5-C4	3.18	1.47	1.38
11	AT	10	2MG	C5-C4	3.17	1.47	1.38
39	B5	3524	OMG	C5-C4	3.16	1.47	1.38
39	B5	3942	OMG	C5-C4	3.16	1.47	1.38
11	AT	34	OMG	C5-C4	3.14	1.47	1.38
39	B5	1266	1MA	C6-N6	3.14	1.35	1.28
1	A2	1491	OMG	C5-C4	3.13	1.47	1.38
1	A2	510	OMG	C5-C4	3.13	1.47	1.38
1	A2	1329	OMG	C5-C4	3.13	1.47	1.38
1	A2	437	OMG	C5-C4	3.13	1.47	1.38
1	A2	602	OMG	C5-C4	3.13	1.47	1.38
39	B5	2207	OMG	C5-C4	3.12	1.47	1.38
39	B5	3476	OMG	C5-C4	3.12	1.47	1.38
1	A2	645	OMG	C5-C4	3.11	1.47	1.38
1	A2	868	OMG	C5-C4	3.10	1.47	1.38
39	B5	4245	OMG	C5-C4	3.10	1.47	1.38
39	B5	4240	OMG	C5-C4	3.09	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4369	OMG	C5-C4	3.09	1.47	1.38
1	A2	1851	MA6	C5-C6	3.09	1.49	1.41
39	B5	3676	OMG	C5-C4	3.08	1.47	1.38
39	B5	1266	1MA	C5-C4	3.08	1.47	1.38
39	B5	4116	OMG	C5-C4	3.08	1.47	1.38
39	B5	1260	OMG	C5-C4	3.07	1.47	1.38
39	B5	1477	OMG	C5-C4	3.07	1.47	1.38
41	B8	75	OMG	C5-C4	3.07	1.47	1.38
39	B5	4383	OMG	C5-C4	3.07	1.47	1.38
1	A2	684	OMG	C5-C4	3.06	1.47	1.38
11	AT	26	M2G	C5-C4	3.06	1.47	1.38
11	AT	46	7MG	C4-N9	-3.06	1.34	1.37
39	B5	3359	OMG	C5-C4	3.06	1.47	1.38
39	B5	3974	OMG	C5-C4	3.06	1.47	1.38
39	B5	4364	OMG	C5-C4	3.03	1.47	1.38
1	A2	1852	MA6	C5-C6	3.02	1.49	1.41
39	B5	3631	OMG	C5-C4	3.01	1.47	1.38
11	AT	26	M2G	C2-N2	2.91	1.40	1.35
1	A2	1833	6MZ	C5-C6	2.91	1.48	1.41
39	B5	3550	UY1	C2-N1	2.89	1.40	1.36
39	B5	4193	5MC	C6-C5	2.86	1.39	1.34
1	A2	1338	4AC	C4-N4	-2.84	1.35	1.39
39	B5	3514	5MC	C6-C5	2.82	1.39	1.34
39	B5	4052	OMU	C4-N3	-2.82	1.33	1.38
1	A2	1640	7MG	C4-N9	-2.81	1.34	1.37
1	A2	1249	B8N	C6-C5	2.80	1.39	1.35
39	B5	4039	PSU	C4-N3	-2.79	1.33	1.38
39	B5	2351	PSU	C4-N3	-2.78	1.33	1.38
39	B5	3369	PSU	C4-N3	-2.77	1.33	1.38
1	A2	159	A2M	C5-C6	2.77	1.48	1.41
1	A2	166	A2M	C5-C6	2.77	1.48	1.41
1	A2	469	A2M	C5-C6	2.77	1.48	1.41
39	B5	1489	A2M	C5-C6	2.76	1.48	1.41
39	B5	2680	OMU	C4-N3	-2.76	1.33	1.38
39	B5	4711	PSU	C4-N3	-2.76	1.33	1.38
39	B5	3973	OMU	C4-N3	-2.76	1.33	1.38
1	A2	669	A2M	C5-C6	2.75	1.48	1.41
39	B5	398	A2M	C5-C6	2.75	1.48	1.41
39	B5	1731	PSU	C4-N3	-2.75	1.33	1.38
39	B5	3490	PSU	C4-N3	-2.75	1.33	1.38
39	B5	2658	A2M	C5-C6	2.74	1.48	1.41
39	B5	4298	PSU	C4-N3	-2.74	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	1801	PSU	C4-N3	-2.74	1.33	1.38
39	B5	3657	OMU	C4-N3	-2.74	1.33	1.38
39	B5	1799	PSU	C4-N3	-2.74	1.33	1.38
1	A2	591	A2M	C5-C6	2.73	1.48	1.41
1	A2	1178	PSU	C4-N3	-2.73	1.33	1.38
39	B5	4099	PSU	C4-N3	-2.73	1.33	1.38
1	A2	1644	PSU	C4-N3	-2.73	1.33	1.38
1	A2	1384	A2M	C5-C6	2.73	1.48	1.41
1	A2	967	PSU	C4-N3	-2.73	1.33	1.38
1	A2	513	A2M	C5-C6	2.73	1.48	1.41
11	AT	28	PSU	C4-N3	-2.73	1.33	1.38
39	B5	3562	A2M	C5-C6	2.73	1.48	1.41
39	B5	4366	OMU	C4-N3	-2.72	1.33	1.38
39	B5	1537	PSU	C4-N3	-2.72	1.33	1.38
1	A2	1057	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4322	PSU	C4-N3	-2.72	1.33	1.38
39	B5	4177	PSU	C4-N3	-2.72	1.33	1.38
1	A2	27	A2M	C5-C6	2.72	1.48	1.41
39	B5	4382	PSU	C4-N3	-2.71	1.33	1.38
39	B5	400	A2M	C5-C6	2.71	1.48	1.41
1	A2	650	PSU	C4-N3	-2.71	1.33	1.38
1	A2	407	PSU	C4-N3	-2.71	1.33	1.38
1	A2	355	OMU	C4-N3	-2.71	1.34	1.38
1	A2	577	A2M	C5-C6	2.71	1.48	1.41
1	A2	1175	PSU	C4-N3	-2.71	1.33	1.38
1	A2	1005	PSU	C4-N3	-2.71	1.33	1.38
39	B5	1491	PSU	C4-N3	-2.71	1.33	1.38
41	B8	55	PSU	C4-N3	-2.71	1.33	1.38
11	AT	39	PSU	C4-N3	-2.71	1.33	1.38
1	A2	218	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4246	PSU	C4-N3	-2.70	1.33	1.38
41	B8	69	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1082	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3371	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3496	PSU	C4-N3	-2.70	1.33	1.38
39	B5	1810	A2M	C5-C6	2.70	1.48	1.41
39	B5	4336	A2M	C5-C6	2.70	1.48	1.41
1	A2	867	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4045	PSU	C4-N3	-2.70	1.33	1.38
1	A2	1233	PSU	C4-N3	-2.70	1.33	1.38
39	B5	4374	PSU	C4-N3	-2.70	1.33	1.38
39	B5	3450	A2M	C5-C6	2.70	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	2475	PSU	C4-N3	-2.69	1.33	1.38
39	B5	2206	A2M	C5-C6	2.69	1.48	1.41
1	A2	93	PSU	C4-N3	-2.69	1.33	1.38
1	A2	109	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4740	PSU	C4-N3	-2.69	1.33	1.38
11	AT	37	YYG	C2-N3	-2.69	1.34	1.38
39	B5	4107	PSU	C4-N3	-2.69	1.33	1.38
39	B5	2244	A2M	C5-C6	2.69	1.48	1.41
39	B5	4169	PSU	C4-N3	-2.69	1.33	1.38
39	B5	1721	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4278	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4317	A2M	C5-C6	2.69	1.48	1.41
1	A2	1245	PSU	C4-N3	-2.69	1.33	1.38
39	B5	4435	PSU	C4-N3	-2.69	1.33	1.38
1	A2	687	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3576	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4217	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4042	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4749	PSU	C4-N3	-2.68	1.33	1.38
39	B5	1683	PSU	C4-N3	-2.68	1.33	1.38
11	AT	55	PSU	C4-N3	-2.68	1.33	1.38
39	B5	1720	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4166	PSU	C4-N3	-2.68	1.33	1.38
1	A2	1693	PSU	C4-N3	-2.68	1.33	1.38
39	B5	4244	OMU	C4-N3	-2.68	1.34	1.38
1	A2	1047	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3502	PSU	C4-N3	-2.68	1.33	1.38
39	B5	3500	PSU	C4-N3	-2.68	1.33	1.38
11	AT	49	5MC	C6-C5	2.68	1.39	1.34
1	A2	1679	A2M	C5-C6	2.68	1.48	1.41
1	A2	105	PSU	C4-N3	-2.67	1.33	1.38
39	B5	3554	PSU	C4-N3	-2.67	1.33	1.38
39	B5	3585	PSU	C4-N3	-2.67	1.33	1.38
1	A2	119	PSU	C4-N3	-2.67	1.33	1.38
39	B5	4267	PSU	C4-N3	-2.67	1.33	1.38
1	A2	573	PSU	C4-N3	-2.67	1.33	1.38
1	A2	172	OMU	C4-N3	-2.67	1.34	1.38
39	B5	1479	A2M	C5-C6	2.67	1.48	1.41
39	B5	3447	PSU	C4-N3	-2.67	1.33	1.38
1	A2	864	PSU	C4-N3	-2.66	1.33	1.38
1	A2	1327	OMU	C4-N3	-2.66	1.34	1.38
39	B5	1638	PSU	C4-N3	-2.66	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	1348	PSU	C4-N3	-2.66	1.33	1.38
1	A2	815	PSU	C4-N3	-2.66	1.33	1.38
1	A2	121	OMU	C4-N3	-2.66	1.34	1.38
39	B5	3456	A2M	C5-C6	2.66	1.48	1.41
1	A2	682	PSU	C4-N3	-2.66	1.33	1.38
39	B5	1270	A2M	C5-C6	2.66	1.48	1.41
39	B5	3599	A2M	C5-C6	2.66	1.48	1.41
39	B5	4325	PSU	C4-N3	-2.66	1.33	1.38
39	B5	3966	6MZ	C5-C6	2.66	1.48	1.41
1	A2	1239	PSU	C4-N3	-2.66	1.33	1.38
1	A2	485	A2M	C5-C6	2.65	1.48	1.41
39	B5	4203	PSU	C4-N3	-2.65	1.33	1.38
1	A2	99	A2M	C5-C6	2.65	1.48	1.41
1	A2	1851	MA6	C6-N6	2.65	1.44	1.36
1	A2	1446	PSU	C4-N3	-2.65	1.33	1.38
39	B5	3492	A2M	C5-C6	2.65	1.48	1.41
39	B5	3466	PSU	C4-N3	-2.65	1.33	1.38
39	B5	3557	A2M	C5-C6	2.65	1.48	1.41
39	B5	4149	PSU	C4-N3	-2.64	1.33	1.38
11	AT	54	5MU	C6-C5	2.64	1.38	1.34
11	AT	27	PSU	C4-N3	-2.64	1.33	1.38
39	B5	3583	PSU	C4-N3	-2.64	1.33	1.38
1	A2	1443	OMU	C4-N3	-2.64	1.34	1.38
1	A2	816	PSU	C4-N3	-2.64	1.33	1.38
1	A2	802	PSU	C4-N3	-2.64	1.33	1.38
39	B5	1718	PSU	C4-N3	-2.64	1.33	1.38
39	B5	3427	PSU	C4-N3	-2.63	1.33	1.38
1	A2	1626	PSU	C4-N3	-2.63	1.33	1.38
39	B5	2258	OMU	C4-N3	-2.63	1.34	1.38
39	B5	3616	PSU	C4-N3	-2.63	1.33	1.38
39	B5	3462	PSU	C4-N3	-2.63	1.33	1.38
1	A2	1046	PSU	C4-N3	-2.63	1.33	1.38
1	A2	652	PSU	C4-N3	-2.62	1.33	1.38
39	B5	4269	A2M	C5-C6	2.62	1.48	1.41
1	A2	823	PSU	C4-N3	-2.62	1.33	1.38
39	B5	2630	A2M	C5-C6	2.62	1.48	1.41
1	A2	1032	A2M	C5-C6	2.62	1.48	1.41
1	A2	34	PSU	C4-N3	-2.62	1.33	1.38
39	B5	2719	OMG	C6-N1	-2.62	1.33	1.38
39	B5	4419	PSU	C4-N3	-2.62	1.33	1.38
1	A2	36	PSU	C4-N3	-2.62	1.34	1.38
39	B5	4188	PSU	C4-N3	-2.62	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	4058	PSU	C4-N3	-2.61	1.34	1.38
1	A2	1368	PSU	C4-N3	-2.61	1.34	1.38
1	A2	1843	4AC	C4-N4	-2.61	1.36	1.39
39	B5	3652	PSU	C4-N3	-2.61	1.34	1.38
1	A2	116	OMU	C4-N3	-2.60	1.34	1.38
1	A2	1289	OMU	C4-N3	-2.59	1.34	1.38
1	A2	610	PSU	C4-N3	-2.59	1.34	1.38
39	B5	3494	PSU	C4-N3	-2.59	1.34	1.38
1	A2	1805	OMU	C4-N3	-2.59	1.34	1.38
39	B5	1632	PSU	C4-N3	-2.58	1.34	1.38
11	AT	37	YYG	C12-N1	-2.58	1.34	1.40
1	A2	429	OMU	C4-N3	-2.58	1.34	1.38
11	AT	17	H2U	C2-N3	-2.58	1.33	1.38
1	A2	210	PSU	C4-N3	-2.58	1.34	1.38
39	B5	2267	OMG	C6-N1	-2.56	1.34	1.38
11	AT	16	H2U	C2-N3	-2.56	1.33	1.38
39	B5	2207	OMG	C6-N1	-2.56	1.34	1.38
39	B5	3517	A2M	C5-C6	2.56	1.48	1.41
39	B5	3524	OMG	C6-N1	-2.55	1.34	1.38
1	A2	1852	MA6	C6-N6	2.55	1.43	1.36
39	B5	3476	OMG	C6-N1	-2.55	1.34	1.38
1	A2	510	OMG	C6-N1	-2.55	1.34	1.38
39	B5	1580	OMG	C6-N1	-2.54	1.34	1.38
1	A2	628	OMU	C4-N3	-2.54	1.34	1.38
11	AT	54	5MU	C4-N3	-2.53	1.34	1.38
1	A2	602	OMG	C6-N1	-2.52	1.34	1.38
39	B5	3942	OMG	C6-N1	-2.52	1.34	1.38
39	B5	3359	OMG	C6-N1	-2.52	1.34	1.38
39	B5	3676	OMG	C6-N1	-2.52	1.34	1.38
1	A2	1329	OMG	C6-N1	-2.51	1.34	1.38
1	A2	1491	OMG	C6-N1	-2.50	1.34	1.38
39	B5	4240	OMG	C6-N1	-2.50	1.34	1.38
39	B5	4383	OMG	C6-N1	-2.50	1.34	1.38
42	BA	216	V5N	CD2-NE2	-2.49	1.33	1.37
1	A2	1448	OMG	C6-N1	-2.49	1.34	1.38
39	B5	1477	OMG	C6-N1	-2.48	1.34	1.38
39	B5	1260	OMG	C6-N1	-2.48	1.34	1.38
39	B5	3974	OMG	C6-N1	-2.48	1.34	1.38
39	B5	4245	OMG	C6-N1	-2.48	1.34	1.38
39	B5	4364	OMG	C6-N1	-2.47	1.34	1.38
39	B5	2630	A2M	C5-N7	-2.47	1.34	1.39
1	A2	1249	B8N	C2-N3	-2.46	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	645	OMG	C6-N1	-2.46	1.34	1.38
39	B5	4138	OMG	C6-N1	-2.46	1.34	1.38
39	B5	398	A2M	C5-N7	-2.45	1.34	1.39
39	B5	1270	A2M	C5-N7	-2.44	1.34	1.39
11	AT	26	M2G	C6-N1	-2.44	1.34	1.38
1	A2	684	OMG	C6-N1	-2.44	1.34	1.38
68	Ba	39	V5N	CD2-NE2	-2.44	1.33	1.37
11	AT	34	OMG	C6-N1	-2.43	1.34	1.38
1	A2	868	OMG	C6-N1	-2.42	1.34	1.38
1	A2	437	OMG	C6-N1	-2.42	1.34	1.38
1	A2	1640	7MG	C6-N1	-2.41	1.34	1.38
39	B5	4116	OMG	C6-N1	-2.41	1.34	1.38
41	B8	75	OMG	C6-N1	-2.41	1.34	1.38
1	A2	99	A2M	C5-N7	-2.41	1.34	1.39
1	A2	669	A2M	C8-N7	2.40	1.36	1.31
39	B5	3631	OMG	C6-N1	-2.40	1.34	1.38
39	B5	2206	A2M	C5-N7	-2.40	1.34	1.39
39	B5	3966	6MZ	C5-N7	-2.40	1.34	1.39
11	AT	58	1MA	C2-N3	2.40	1.35	1.30
39	B5	4369	OMG	C6-N1	-2.39	1.34	1.38
1	A2	485	A2M	C5-N7	-2.39	1.34	1.39
11	AT	17	H2U	C4-N3	-2.38	1.33	1.37
39	B5	4269	A2M	C5-N7	-2.38	1.34	1.39
1	A2	591	A2M	C5-N7	-2.37	1.34	1.39
1	A2	159	A2M	C8-N7	2.37	1.36	1.31
39	B5	3557	A2M	C5-N7	-2.37	1.34	1.39
39	B5	3562	A2M	C5-N7	-2.37	1.34	1.39
11	AT	10	2MG	C6-N1	-2.36	1.34	1.38
1	A2	469	A2M	C8-N7	2.36	1.36	1.31
39	B5	4317	A2M	C5-N7	-2.36	1.34	1.39
1	A2	1384	A2M	C8-N7	2.35	1.36	1.31
1	A2	1833	6MZ	C5-N7	-2.35	1.34	1.39
39	B5	3550	UY1	C6-N1	-2.35	1.32	1.36
39	B5	1479	A2M	C5-N7	-2.34	1.34	1.39
1	A2	1032	A2M	C5-N7	-2.34	1.34	1.39
39	B5	2244	A2M	C5-N7	-2.33	1.34	1.39
39	B5	3450	A2M	C5-N7	-2.33	1.34	1.39
39	B5	3456	A2M	C8-N7	2.33	1.36	1.31
39	B5	2658	A2M	C5-N7	-2.33	1.34	1.39
39	B5	400	A2M	C5-N7	-2.33	1.34	1.39
39	B5	3599	A2M	C5-N7	-2.32	1.34	1.39
1	A2	513	A2M	C8-N7	2.32	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	16	H2U	C4-N3	-2.32	1.33	1.37
39	B5	4336	A2M	C5-N7	-2.32	1.34	1.39
39	B5	1810	A2M	C5-N7	-2.32	1.34	1.39
1	A2	166	A2M	C8-N7	2.32	1.36	1.31
1	A2	1679	A2M	C5-N7	-2.31	1.34	1.39
1	A2	27	A2M	C5-N7	-2.31	1.34	1.39
1	A2	1384	A2M	C5-N7	-2.31	1.34	1.39
11	AT	54	5MU	C4-C5	2.30	1.48	1.44
39	B5	3492	A2M	C8-N7	2.30	1.36	1.31
1	A2	166	A2M	C5-N7	-2.30	1.34	1.39
11	AT	14	1MA	C2-N3	2.30	1.34	1.30
1	A2	577	A2M	C5-N7	-2.30	1.34	1.39
1	A2	469	A2M	C5-N7	-2.30	1.34	1.39
39	B5	4336	A2M	C8-N7	2.29	1.36	1.31
1	A2	1679	A2M	C8-N7	2.29	1.36	1.31
11	AT	46	7MG	C6-N1	-2.29	1.34	1.38
1	A2	577	A2M	C8-N7	2.29	1.36	1.31
39	B5	2680	OMU	C2-N3	-2.28	1.34	1.38
1	A2	27	A2M	C8-N7	2.28	1.36	1.31
1	A2	1327	OMU	C2-N3	-2.28	1.34	1.38
39	B5	3492	A2M	C5-N7	-2.28	1.34	1.39
1	A2	513	A2M	C5-N7	-2.27	1.34	1.39
39	B5	4244	OMU	C2-N3	-2.26	1.34	1.38
39	B5	4366	OMU	C2-N3	-2.26	1.34	1.38
1	A2	99	A2M	C8-N7	2.26	1.36	1.31
39	B5	4317	A2M	C8-N7	2.26	1.36	1.31
39	B5	398	A2M	C8-N7	2.26	1.36	1.31
1	A2	1289	OMU	C2-N1	2.26	1.42	1.38
39	B5	2658	A2M	C8-N7	2.26	1.36	1.31
39	B5	3517	A2M	C8-N7	2.26	1.36	1.31
39	B5	400	A2M	C8-N7	2.26	1.36	1.31
39	B5	3456	A2M	C5-N7	-2.25	1.35	1.39
39	B5	1489	A2M	C5-N7	-2.25	1.35	1.39
1	A2	159	A2M	C5-N7	-2.25	1.35	1.39
39	B5	3973	OMU	C2-N3	-2.25	1.34	1.38
1	A2	121	OMU	C2-N3	-2.25	1.34	1.38
1	A2	669	A2M	C5-N7	-2.25	1.35	1.39
11	AT	54	5MU	C6-N1	-2.24	1.34	1.38
11	AT	37	YYG	C2-N1	-2.24	1.34	1.38
39	B5	3657	OMU	C2-N3	-2.24	1.34	1.38
39	B5	3517	A2M	C5-N7	-2.23	1.35	1.39
39	B5	1489	A2M	C8-N7	2.23	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	AT	54	5MU	C2-N1	2.23	1.42	1.38
39	B5	2206	A2M	C8-N7	2.23	1.36	1.31
1	A2	1833	6MZ	C8-N7	2.23	1.36	1.31
39	B5	1810	A2M	C8-N7	2.23	1.36	1.31
11	AT	10	2MG	C2-N3	2.22	1.36	1.32
39	B5	2244	A2M	C8-N7	2.22	1.35	1.31
11	AT	49	5MC	C6-N1	-2.22	1.34	1.38
1	A2	591	A2M	C8-N7	2.22	1.35	1.31
39	B5	2258	OMU	C2-N3	-2.22	1.34	1.38
11	AT	37	YYG	C5-N7	-2.22	1.34	1.39
1	A2	1805	OMU	C2-N3	-2.21	1.34	1.38
39	B5	3524	OMG	C5-N7	-2.21	1.34	1.39
39	B5	3942	OMG	C5-N7	-2.21	1.34	1.39
39	B5	3557	A2M	C8-N7	2.21	1.35	1.31
1	A2	172	OMU	C2-N3	-2.21	1.34	1.38
39	B5	4269	A2M	C8-N7	2.21	1.35	1.31
39	B5	2267	OMG	C5-N7	-2.20	1.34	1.39
1	A2	1852	MA6	C8-N7	2.20	1.35	1.31
39	B5	3973	OMU	C2-N1	2.20	1.41	1.38
39	B5	2630	A2M	C8-N7	2.19	1.35	1.31
1	A2	355	OMU	C2-N3	-2.19	1.34	1.38
1	A2	1289	OMU	C2-N3	-2.19	1.34	1.38
39	B5	3450	A2M	C8-N7	2.19	1.35	1.31
39	B5	1270	A2M	C8-N7	2.19	1.35	1.31
39	B5	4052	OMU	C2-N3	-2.18	1.34	1.38
39	B5	4193	5MC	C6-N1	-2.18	1.34	1.38
39	B5	3562	A2M	C8-N7	2.18	1.35	1.31
39	B5	4276	UR3	C2-N1	2.18	1.41	1.38
1	A2	1852	MA6	C5-N7	-2.18	1.35	1.39
1	A2	485	A2M	C8-N7	2.18	1.35	1.31
39	B5	2719	OMG	C5-N7	-2.18	1.34	1.39
1	A2	1851	MA6	C8-N7	2.17	1.35	1.31
39	B5	1266	1MA	C5-N7	-2.17	1.34	1.39
39	B5	1479	A2M	C8-N7	2.17	1.35	1.31
1	A2	1443	OMU	C2-N3	-2.17	1.34	1.38
1	A2	429	OMU	C2-N3	-2.17	1.34	1.38
39	B5	3517	A2M	C4-N9	-2.17	1.33	1.37
39	B5	1580	OMG	C5-N7	-2.17	1.34	1.39
39	B5	3599	A2M	C8-N7	2.17	1.35	1.31
39	B5	4240	OMG	C5-N7	-2.16	1.34	1.39
1	A2	116	OMU	C2-N3	-2.16	1.34	1.38
1	A2	1032	A2M	C8-N7	2.16	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A2	602	OMG	C5-N7	-2.15	1.34	1.39
39	B5	3966	6MZ	C8-N7	2.15	1.35	1.31
39	B5	1260	OMG	C5-N7	-2.15	1.34	1.39
1	A2	1805	OMU	C2-N1	2.14	1.41	1.38
1	A2	1491	OMG	C5-N7	-2.14	1.34	1.39
1	A2	1448	OMG	C5-N7	-2.14	1.34	1.39
39	B5	3476	OMG	C5-N7	-2.13	1.34	1.39
39	B5	4052	OMU	C2-N1	2.13	1.41	1.38
1	A2	628	OMU	C2-N3	-2.13	1.34	1.38
1	A2	510	OMG	C5-N7	-2.12	1.34	1.39
1	A2	1851	MA6	C5-N7	-2.12	1.35	1.39
39	B5	1632	PSU	O4'-C1'	-2.12	1.40	1.43
39	B5	3359	OMG	C5-N7	-2.12	1.34	1.39
39	B5	4245	OMG	C5-N7	-2.11	1.34	1.39
1	A2	437	OMG	C5-N7	-2.11	1.34	1.39
39	B5	3631	OMG	C5-N7	-2.11	1.34	1.39
39	B5	4116	OMG	C5-N7	-2.11	1.34	1.39
1	A2	116	OMU	C5-C4	-2.11	1.39	1.43
39	B5	3514	5MC	C6-N1	-2.10	1.34	1.38
39	B5	4138	OMG	C5-N7	-2.10	1.34	1.39
11	AT	14	1MA	C5-N7	-2.10	1.34	1.39
1	A2	645	OMG	C5-N7	-2.10	1.34	1.39
39	B5	1266	1MA	C2-N3	2.10	1.34	1.30
11	AT	58	1MA	C5-N7	-2.09	1.34	1.39
39	B5	4383	OMG	C5-N7	-2.09	1.34	1.39
11	AT	34	OMG	C5-N7	-2.08	1.34	1.39
1	A2	121	OMU	C5-C4	-2.08	1.39	1.43
1	A2	1032	A2M	C4-N9	-2.07	1.33	1.37
11	AT	10	2MG	C5-N7	-2.07	1.34	1.39
41	B8	75	OMG	C5-N7	-2.07	1.34	1.39
1	A2	684	OMG	C5-N7	-2.06	1.34	1.39
39	B5	4052	OMU	C5-C4	-2.06	1.39	1.43
1	A2	868	OMG	C5-N7	-2.06	1.34	1.39
39	B5	4244	OMU	C5-C4	-2.06	1.39	1.43
39	B5	2207	OMG	C5-N7	-2.06	1.34	1.39
39	B5	4369	OMG	C5-N7	-2.06	1.35	1.39
1	A2	1443	OMU	C2-N1	2.05	1.41	1.38
39	B5	3676	OMG	C5-N7	-2.05	1.35	1.39
11	AT	26	M2G	C5-N7	-2.05	1.35	1.39
1	A2	1443	OMU	C5-C4	-2.04	1.39	1.43
39	B5	2258	OMU	C5-C4	-2.04	1.39	1.43
1	A2	1289	OMU	C5-C4	-2.04	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B5	3369	PSU	C2-N3	-2.04	1.34	1.37
11	AT	54	5MU	C2-N3	-2.04	1.34	1.38
1	A2	121	OMU	C2-N1	2.03	1.41	1.38
39	B5	4366	OMU	C2-N1	2.03	1.41	1.38
39	B5	1477	OMG	C5-N7	-2.03	1.35	1.39
1	A2	669	A2M	C4-N9	-2.03	1.33	1.37
1	A2	1851	MA6	C4-N9	-2.03	1.33	1.37
39	B5	4364	OMG	C5-N7	-2.03	1.35	1.39
1	A2	1805	OMU	C5-C4	-2.02	1.39	1.43
1	A2	1329	OMG	C5-N7	-2.02	1.35	1.39
39	B5	2258	OMU	C2-N1	2.02	1.41	1.38
1	A2	355	OMU	C5-C4	-2.01	1.39	1.43
39	B5	2680	OMU	C2-N1	2.01	1.41	1.38
1	A2	1327	OMU	C5-C4	-2.01	1.39	1.43
39	B5	4269	A2M	C4-N9	-2.00	1.33	1.37

All (1104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	AT	37	YYG	C5-C4-N3	-9.17	116.55	123.99
1	A2	1640	7MG	N9-C4-N3	9.13	138.85	125.46
11	AT	46	7MG	N9-C4-N3	9.01	138.66	125.46
11	AT	10	2MG	C2-N3-C4	7.20	121.01	112.00
39	B5	4276	UR3	C4-N3-C2	-6.86	119.06	124.58
39	B5	4374	PSU	N1-C2-N3	6.77	122.31	115.17
1	A2	1057	PSU	N1-C2-N3	6.70	122.24	115.17
39	B5	3369	PSU	N1-C2-N3	6.66	122.20	115.17
39	B5	4039	PSU	N1-C2-N3	6.64	122.17	115.17
39	B5	3585	PSU	N1-C2-N3	6.59	122.12	115.17
1	A2	591	A2M	C5-C4-N3	-6.57	117.67	126.72
1	A2	1233	PSU	N1-C2-N3	6.55	122.08	115.17
41	B8	69	PSU	N1-C2-N3	6.55	122.07	115.17
1	A2	1368	PSU	N1-C2-N3	6.54	122.07	115.17
39	B5	4435	PSU	N1-C2-N3	6.54	122.07	115.17
39	B5	4246	PSU	N1-C2-N3	6.54	122.07	115.17
39	B5	1721	PSU	N1-C2-N3	6.54	122.06	115.17
39	B5	1491	PSU	N1-C2-N3	6.54	122.06	115.17
39	B5	1799	PSU	N1-C2-N3	6.54	122.06	115.17
1	A2	407	PSU	N1-C2-N3	6.53	122.06	115.17
39	B5	4267	PSU	N1-C2-N3	6.52	122.05	115.17
39	B5	1801	PSU	N1-C2-N3	6.52	122.05	115.17
39	B5	4045	PSU	N1-C2-N3	6.52	122.05	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1005	PSU	N1-C2-N3	6.52	122.05	115.17
39	B5	4217	PSU	N1-C2-N3	6.52	122.05	115.17
39	B5	4382	PSU	N1-C2-N3	6.51	122.04	115.17
39	B5	1683	PSU	N1-C2-N3	6.51	122.04	115.17
39	B5	4149	PSU	N1-C2-N3	6.51	122.03	115.17
1	A2	823	PSU	N1-C2-N3	6.51	122.03	115.17
39	B5	4325	PSU	N1-C2-N3	6.50	122.02	115.17
39	B5	3496	PSU	N1-C2-N3	6.49	122.02	115.17
39	B5	3502	PSU	N1-C2-N3	6.49	122.02	115.17
39	B5	4099	PSU	N1-C2-N3	6.49	122.01	115.17
39	B5	4188	PSU	N1-C2-N3	6.48	122.01	115.17
39	B5	1632	PSU	N1-C2-N3	6.48	122.00	115.17
11	AT	28	PSU	N1-C2-N3	6.48	122.00	115.17
1	A2	573	PSU	N1-C2-N3	6.47	121.99	115.17
39	B5	2719	OMG	C5-C4-N3	-6.47	118.10	128.39
1	A2	1047	PSU	N1-C2-N3	6.46	121.99	115.17
1	A2	967	PSU	N1-C2-N3	6.46	121.98	115.17
39	B5	4278	PSU	N1-C2-N3	6.46	121.98	115.17
39	B5	4711	PSU	N1-C2-N3	6.46	121.98	115.17
39	B5	4740	PSU	N1-C2-N3	6.46	121.98	115.17
11	AT	55	PSU	N1-C2-N3	6.46	121.98	115.17
39	B5	3490	PSU	N1-C2-N3	6.46	121.98	115.17
39	B5	4177	PSU	N1-C2-N3	6.46	121.98	115.17
1	A2	864	PSU	N1-C2-N3	6.45	121.98	115.17
39	B5	3583	PSU	N1-C2-N3	6.45	121.98	115.17
1	A2	218	PSU	N1-C2-N3	6.45	121.97	115.17
1	A2	105	PSU	N1-C2-N3	6.45	121.97	115.17
39	B5	4298	PSU	N1-C2-N3	6.45	121.97	115.17
1	A2	652	PSU	N1-C2-N3	6.45	121.97	115.17
1	A2	119	PSU	N1-C2-N3	6.44	121.97	115.17
1	A2	1175	PSU	N1-C2-N3	6.44	121.97	115.17
39	B5	4749	PSU	N1-C2-N3	6.44	121.97	115.17
39	B5	1537	PSU	N1-C2-N3	6.44	121.96	115.17
39	B5	3942	OMG	C5-C4-N3	-6.44	118.14	128.39
39	B5	3447	PSU	N1-C2-N3	6.44	121.96	115.17
39	B5	3500	PSU	N1-C2-N3	6.43	121.95	115.17
1	A2	1245	PSU	N1-C2-N3	6.43	121.95	115.17
39	B5	2351	PSU	N1-C2-N3	6.42	121.94	115.17
39	B5	2267	OMG	C5-C4-N3	-6.42	118.17	128.39
1	A2	93	PSU	N1-C2-N3	6.42	121.94	115.17
1	A2	687	PSU	N1-C2-N3	6.42	121.94	115.17
1	A2	34	PSU	N1-C2-N3	6.42	121.94	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1082	PSU	N1-C2-N3	6.42	121.94	115.17
1	A2	867	PSU	N1-C2-N3	6.42	121.94	115.17
1	A2	1239	PSU	N1-C2-N3	6.42	121.94	115.17
39	B5	4107	PSU	N1-C2-N3	6.41	121.93	115.17
39	B5	4419	PSU	N1-C2-N3	6.41	121.93	115.17
11	AT	27	PSU	N1-C2-N3	6.41	121.93	115.17
1	A2	1046	PSU	N1-C2-N3	6.41	121.93	115.17
1	A2	1178	PSU	N1-C2-N3	6.41	121.93	115.17
39	B5	1718	PSU	N1-C2-N3	6.41	121.93	115.17
1	A2	1348	PSU	N1-C2-N3	6.41	121.93	115.17
39	B5	4042	PSU	N1-C2-N3	6.40	121.92	115.17
39	B5	3371	PSU	N1-C2-N3	6.40	121.92	115.17
39	B5	3466	PSU	N1-C2-N3	6.39	121.91	115.17
1	A2	610	PSU	N1-C2-N3	6.39	121.91	115.17
1	A2	815	PSU	N1-C2-N3	6.39	121.91	115.17
39	B5	3462	PSU	N1-C2-N3	6.39	121.91	115.17
11	AT	39	PSU	N1-C2-N3	6.39	121.91	115.17
1	A2	36	PSU	N1-C2-N3	6.39	121.90	115.17
39	B5	3576	PSU	N1-C2-N3	6.38	121.90	115.17
39	B5	4058	PSU	N1-C2-N3	6.38	121.90	115.17
1	A2	1448	OMG	C5-C4-N3	-6.38	118.23	128.39
39	B5	3494	PSU	N1-C2-N3	6.38	121.89	115.17
39	B5	4322	PSU	N1-C2-N3	6.37	121.89	115.17
1	A2	816	PSU	N1-C2-N3	6.37	121.89	115.17
41	B8	55	PSU	N1-C2-N3	6.37	121.89	115.17
1	A2	1491	OMG	C5-C4-N3	-6.37	118.26	128.39
1	A2	1446	PSU	N1-C2-N3	6.36	121.88	115.17
39	B5	2475	PSU	N1-C2-N3	6.36	121.88	115.17
1	A2	682	PSU	N1-C2-N3	6.36	121.87	115.17
1	A2	650	PSU	N1-C2-N3	6.35	121.87	115.17
39	B5	4169	PSU	N1-C2-N3	6.35	121.87	115.17
1	A2	802	PSU	N1-C2-N3	6.35	121.86	115.17
1	A2	109	PSU	N1-C2-N3	6.35	121.86	115.17
39	B5	3616	PSU	N1-C2-N3	6.34	121.86	115.17
1	A2	1626	PSU	N1-C2-N3	6.34	121.86	115.17
39	B5	1731	PSU	N1-C2-N3	6.34	121.85	115.17
1	A2	1693	PSU	N1-C2-N3	6.34	121.85	115.17
39	B5	3554	PSU	N1-C2-N3	6.33	121.84	115.17
39	B5	1720	PSU	N1-C2-N3	6.32	121.84	115.17
39	B5	3652	PSU	N1-C2-N3	6.32	121.84	115.17
1	A2	210	PSU	N1-C2-N3	6.32	121.83	115.17
39	B5	1580	OMG	C5-C4-N3	-6.30	118.36	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3427	PSU	N1-C2-N3	6.30	121.81	115.17
39	B5	1638	PSU	N1-C2-N3	6.28	121.80	115.17
39	B5	4203	PSU	N1-C2-N3	6.28	121.80	115.17
1	A2	645	OMG	C5-C4-N3	-6.28	118.39	128.39
39	B5	3524	OMG	C5-C4-N3	-6.27	118.42	128.39
1	A2	1644	PSU	N1-C2-N3	6.26	121.77	115.17
39	B5	4166	PSU	N1-C2-N3	6.25	121.76	115.17
1	A2	510	OMG	C5-C4-N3	-6.22	118.50	128.39
11	AT	34	OMG	C5-C4-N3	-6.18	118.56	128.39
39	B5	4240	OMG	C5-C4-N3	-6.17	118.57	128.39
39	B5	1260	OMG	C5-C4-N3	-6.15	118.59	128.39
1	A2	602	OMG	C5-C4-N3	-6.15	118.61	128.39
39	B5	2207	OMG	C5-C4-N3	-6.15	118.61	128.39
41	B8	75	OMG	C5-C4-N3	-6.14	118.61	128.39
11	AT	10	2MG	C5-C4-N3	-6.14	118.61	128.39
1	A2	1329	OMG	C5-C4-N3	-6.12	118.65	128.39
39	B5	3476	OMG	C5-C4-N3	-6.11	118.66	128.39
39	B5	4364	OMG	C5-C4-N3	-6.09	118.69	128.39
39	B5	3676	OMG	C5-C4-N3	-6.09	118.69	128.39
39	B5	4383	OMG	C5-C4-N3	-6.09	118.69	128.39
1	A2	437	OMG	C5-C4-N3	-6.09	118.70	128.39
39	B5	4369	OMG	C5-C4-N3	-6.08	118.71	128.39
39	B5	4116	OMG	C5-C4-N3	-6.06	118.75	128.39
39	B5	4245	OMG	C5-C4-N3	-6.05	118.77	128.39
11	AT	26	M2G	C5-C4-N3	-6.04	118.77	128.39
1	A2	684	OMG	C5-C4-N3	-6.04	118.78	128.39
39	B5	4336	A2M	C5-C4-N3	-6.03	118.42	126.72
1	A2	868	OMG	C5-C4-N3	-6.02	118.80	128.39
39	B5	398	A2M	C5-C4-N3	-5.99	118.46	126.72
1	A2	1384	A2M	C5-C4-N3	-5.98	118.48	126.72
39	B5	2630	A2M	C5-C4-N3	-5.97	118.49	126.72
39	B5	3359	OMG	C5-C4-N3	-5.96	118.90	128.39
39	B5	4138	OMG	C5-C4-N3	-5.94	118.93	128.39
39	B5	1270	A2M	C5-C4-N3	-5.93	118.55	126.72
1	A2	166	A2M	C5-C4-N3	-5.92	118.56	126.72
39	B5	1477	OMG	C5-C4-N3	-5.92	118.97	128.39
39	B5	3631	OMG	C5-C4-N3	-5.90	118.99	128.39
1	A2	485	A2M	C5-C4-N3	-5.89	118.60	126.72
39	B5	2658	A2M	C5-C4-N3	-5.89	118.60	126.72
35	Aw	62	HY3	C4-C3-CA	-5.86	96.14	102.51
39	B5	2244	A2M	C5-C4-N3	-5.86	118.65	126.72
1	A2	469	A2M	C5-C4-N3	-5.85	118.66	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1479	A2M	C5-C4-N3	-5.85	118.66	126.72
39	B5	3966	6MZ	C5-C4-N3	-5.85	118.66	126.72
39	B5	2206	A2M	C5-C4-N3	-5.84	118.67	126.72
1	A2	1679	A2M	C5-C4-N3	-5.84	118.67	126.72
1	A2	99	A2M	C5-C4-N3	-5.84	118.68	126.72
1	A2	513	A2M	C5-C4-N3	-5.83	118.69	126.72
39	B5	4317	A2M	C5-C4-N3	-5.82	118.70	126.72
39	B5	3599	A2M	C5-C4-N3	-5.82	118.71	126.72
1	A2	159	A2M	C5-C4-N3	-5.81	118.72	126.72
1	A2	27	A2M	C5-C4-N3	-5.81	118.72	126.72
39	B5	3974	OMG	C5-C4-N3	-5.78	119.19	128.39
39	B5	3557	A2M	C5-C4-N3	-5.78	118.76	126.72
39	B5	3456	A2M	C5-C4-N3	-5.77	118.77	126.72
1	A2	1833	6MZ	C5-C4-N3	-5.76	118.78	126.72
39	B5	3562	A2M	C5-C4-N3	-5.74	118.82	126.72
1	A2	577	A2M	C5-C4-N3	-5.73	118.83	126.72
39	B5	3450	A2M	C5-C4-N3	-5.72	118.84	126.72
39	B5	3492	A2M	C5-C4-N3	-5.69	118.89	126.72
39	B5	1810	A2M	C5-C4-N3	-5.68	118.90	126.72
39	B5	4269	A2M	C5-C4-N3	-5.66	118.92	126.72
39	B5	400	A2M	C5-C4-N3	-5.64	118.95	126.72
11	AT	37	YYG	N9-C4-N3	5.64	138.57	129.45
39	B5	1489	A2M	C5-C4-N3	-5.62	118.98	126.72
39	B5	3550	UY1	C4-N3-C2	-5.60	118.65	126.37
1	A2	1640	7MG	C5-C4-N3	-5.57	117.67	128.13
11	AT	58	1MA	C5-C4-N3	-5.56	119.08	127.27
1	A2	669	A2M	C5-C4-N3	-5.54	119.09	126.72
1	A2	1032	A2M	C5-C4-N3	-5.51	119.14	126.72
11	AT	14	1MA	C5-C4-N3	-5.49	119.19	127.27
11	AT	46	7MG	C5-C4-N3	-5.42	117.97	128.13
11	AT	46	7MG	N9-C8-N7	-5.41	95.71	103.37
39	B5	3517	A2M	C5-C4-N3	-5.40	119.29	126.72
1	A2	1851	MA6	C5-C4-N3	-5.36	119.34	126.72
1	A2	1852	MA6	C5-C4-N3	-5.35	119.35	126.72
1	A2	591	A2M	N3-C4-N9	5.29	136.17	127.17
39	B5	3942	OMG	C2-N3-C4	5.19	121.25	112.30
39	B5	2719	OMG	C2-N3-C4	5.18	121.22	112.30
39	B5	1266	1MA	C5-C4-N3	-5.17	119.66	127.27
1	A2	1491	OMG	C2-N3-C4	5.16	121.18	112.30
39	B5	4364	OMG	C2-N3-C4	5.15	121.16	112.30
1	A2	1448	OMG	C2-N3-C4	5.13	121.13	112.30
1	A2	645	OMG	C2-N3-C4	5.12	121.12	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4116	OMG	C2-N3-C4	5.10	121.09	112.30
39	B5	4369	OMG	C2-N3-C4	5.10	121.09	112.30
39	B5	4383	OMG	C2-N3-C4	5.10	121.09	112.30
11	AT	34	OMG	C2-N3-C4	5.08	121.05	112.30
41	B8	75	OMG	C2-N3-C4	5.08	121.05	112.30
39	B5	2267	OMG	C2-N3-C4	5.07	121.03	112.30
39	B5	3676	OMG	C2-N3-C4	5.06	121.02	112.30
39	B5	3476	OMG	C2-N3-C4	5.06	121.02	112.30
1	A2	437	OMG	C2-N3-C4	5.06	121.01	112.30
39	B5	4240	OMG	C2-N3-C4	5.05	121.00	112.30
39	B5	1260	OMG	C2-N3-C4	5.05	120.99	112.30
1	A2	602	OMG	C2-N3-C4	5.04	120.99	112.30
1	A2	1640	7MG	N9-C8-N7	-5.04	96.23	103.37
1	A2	684	OMG	C2-N3-C4	5.04	120.98	112.30
39	B5	3524	OMG	C2-N3-C4	5.04	120.98	112.30
1	A2	510	OMG	C2-N3-C4	5.03	120.97	112.30
39	B5	1580	OMG	C2-N3-C4	5.02	120.94	112.30
39	B5	2680	OMU	C4-N3-C2	-5.02	120.38	126.61
1	A2	1329	OMG	C2-N3-C4	5.02	120.94	112.30
39	B5	3631	OMG	C2-N3-C4	5.01	120.94	112.30
1	A2	868	OMG	C2-N3-C4	5.00	120.92	112.30
39	B5	3359	OMG	C2-N3-C4	5.00	120.92	112.30
39	B5	2207	OMG	C2-N3-C4	4.99	120.89	112.30
11	AT	54	5MU	C4-N3-C2	-4.98	120.81	127.34
39	B5	4138	OMG	C2-N3-C4	4.97	120.87	112.30
39	B5	4245	OMG	C2-N3-C4	4.97	120.86	112.30
39	B5	3974	OMG	C2-N3-C4	4.96	120.83	112.30
39	B5	1477	OMG	C2-N3-C4	4.92	120.77	112.30
1	A2	429	OMU	C4-N3-C2	-4.90	120.53	126.61
39	B5	3973	OMU	C4-N3-C2	-4.88	120.55	126.61
39	B5	3657	OMU	C4-N3-C2	-4.88	120.55	126.61
39	B5	1580	OMG	N9-C4-N3	4.87	135.69	125.95
11	AT	54	5MU	N3-C2-N1	4.86	121.22	114.89
39	B5	2719	OMG	N9-C4-N3	4.85	135.65	125.95
1	A2	1327	OMU	C4-N3-C2	-4.84	120.60	126.61
1	A2	628	OMU	C4-N3-C2	-4.82	120.63	126.61
1	A2	1491	OMG	N9-C4-N3	4.81	135.57	125.95
39	B5	3942	OMG	N9-C4-N3	4.80	135.55	125.95
39	B5	1270	A2M	N3-C4-N9	4.80	135.32	127.17
1	A2	172	OMU	C4-N3-C2	-4.80	120.66	126.61
39	B5	3524	OMG	N9-C4-N3	4.78	135.52	125.95
1	A2	1448	OMG	N9-C4-N3	4.77	135.49	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4336	A2M	N3-C4-N9	4.77	135.28	127.17
1	A2	355	OMU	C4-N3-C2	-4.74	120.72	126.61
39	B5	2258	OMU	C4-N3-C2	-4.74	120.73	126.61
39	B5	2267	OMG	N9-C4-N3	4.74	135.43	125.95
39	B5	2206	A2M	N3-C4-N9	4.73	135.21	127.17
39	B5	3550	UY1	N1-C2-N3	4.70	120.13	115.17
39	B5	2244	A2M	N3-C4-N9	4.70	135.16	127.17
1	A2	116	OMU	C4-N3-C2	-4.70	120.78	126.61
39	B5	398	A2M	N3-C4-N9	4.70	135.15	127.17
1	A2	1384	A2M	N3-C4-N9	4.69	135.15	127.17
1	A2	1443	OMU	C4-N3-C2	-4.69	120.79	126.61
1	A2	99	A2M	N3-C4-N9	4.69	135.15	127.17
39	B5	2630	A2M	N3-C4-N9	4.69	135.14	127.17
1	A2	166	A2M	N3-C4-N9	4.69	135.14	127.17
1	A2	485	A2M	N3-C4-N9	4.68	135.13	127.17
39	B5	1479	A2M	N3-C4-N9	4.68	135.12	127.17
39	B5	3966	6MZ	N3-C4-N9	4.67	135.12	127.17
39	B5	3599	A2M	N3-C4-N9	4.67	135.12	127.17
39	B5	4366	OMU	C4-N3-C2	-4.66	120.82	126.61
1	A2	1679	A2M	N3-C4-N9	4.66	135.10	127.17
39	B5	4244	OMU	C4-N3-C2	-4.65	120.83	126.61
39	B5	4317	A2M	N3-C4-N9	4.65	135.08	127.17
11	AT	14	1MA	C2-N3-C4	4.65	121.64	112.53
1	A2	1805	OMU	C4-N3-C2	-4.65	120.84	126.61
11	AT	10	2MG	N9-C4-N3	4.64	135.24	125.95
1	A2	510	OMG	N9-C4-N3	4.63	135.20	125.95
1	A2	469	A2M	N3-C4-N9	4.62	135.03	127.17
39	B5	4052	OMU	C4-N3-C2	-4.62	120.88	126.61
11	AT	58	1MA	C2-N3-C4	4.62	121.58	112.53
39	B5	2658	A2M	N3-C4-N9	4.61	135.01	127.17
1	A2	577	A2M	N3-C4-N9	4.61	135.00	127.17
1	A2	602	OMG	N9-C4-N3	4.61	135.16	125.95
11	AT	26	M2G	C2-N3-C4	4.60	121.02	112.51
1	A2	121	OMU	C4-N3-C2	-4.60	120.91	126.61
1	A2	27	A2M	N3-C4-N9	4.59	134.98	127.17
1	A2	513	A2M	N3-C4-N9	4.59	134.98	127.17
1	A2	645	OMG	N9-C4-N3	4.59	135.13	125.95
39	B5	3557	A2M	N3-C4-N9	4.59	134.97	127.17
11	AT	34	OMG	N9-C4-N3	4.58	135.11	125.95
39	B5	4116	OMG	N9-C4-N3	4.58	135.10	125.95
39	B5	3562	A2M	C2'-C1'-N9	-4.57	106.24	113.75
39	B5	4240	OMG	N9-C4-N3	4.57	135.08	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4269	A2M	N3-C4-N9	4.56	134.92	127.17
1	A2	1289	OMU	C4-N3-C2	-4.55	120.97	126.61
41	B8	75	OMG	N9-C4-N3	4.55	135.04	125.95
39	B5	3492	A2M	N3-C4-N9	4.54	134.89	127.17
39	B5	3456	A2M	N3-C4-N9	4.54	134.89	127.17
39	B5	3562	A2M	N3-C4-N9	4.54	134.88	127.17
39	B5	2680	OMU	N3-C2-N1	4.53	120.79	114.89
39	B5	3476	OMG	N9-C4-N3	4.53	135.02	125.95
39	B5	1266	1MA	C2-N3-C4	4.53	121.41	112.53
1	A2	437	OMG	N9-C4-N3	4.52	134.99	125.95
39	B5	400	A2M	N3-C4-N9	4.52	134.85	127.17
39	B5	3450	A2M	N3-C4-N9	4.52	134.85	127.17
1	A2	159	A2M	N3-C4-N9	4.51	134.83	127.17
39	B5	2207	OMG	N9-C4-N3	4.50	134.95	125.95
1	A2	1833	6MZ	N3-C4-N9	4.49	134.80	127.17
39	B5	4245	OMG	N9-C4-N3	4.49	134.93	125.95
1	A2	1851	MA6	C2-N1-C6	4.48	122.77	111.83
39	B5	1810	A2M	N3-C4-N9	4.48	134.78	127.17
39	B5	1260	OMG	N9-C4-N3	4.48	134.91	125.95
1	A2	1329	OMG	N9-C4-N3	4.47	134.88	125.95
39	B5	1810	A2M	C2'-C1'-N9	-4.46	106.41	113.75
1	A2	868	OMG	N9-C4-N3	4.46	134.88	125.95
11	AT	46	7MG	C2-N3-C4	4.45	119.97	112.30
1	A2	1640	7MG	C2-N3-C4	4.44	119.95	112.30
39	B5	4369	OMG	N9-C4-N3	4.44	134.83	125.95
39	B5	3676	OMG	N9-C4-N3	4.44	134.83	125.95
1	A2	1032	A2M	N3-C4-N9	4.43	134.69	127.17
11	AT	26	M2G	N9-C4-N3	4.42	134.80	125.95
1	A2	684	OMG	N9-C4-N3	4.42	134.80	125.95
39	B5	4138	OMG	N9-C4-N3	4.40	134.75	125.95
39	B5	3517	A2M	N3-C4-N9	4.38	134.61	127.17
39	B5	1477	OMG	N9-C4-N3	4.38	134.70	125.95
11	AT	37	YYG	O23-C21-N20	4.38	118.13	110.77
39	B5	1489	A2M	N3-C4-N9	4.37	134.60	127.17
39	B5	4383	OMG	N9-C4-N3	4.37	134.69	125.95
39	B5	3631	OMG	N9-C4-N3	4.36	134.67	125.95
39	B5	3359	OMG	N9-C4-N3	4.35	134.65	125.95
11	AT	54	5MU	C5-C4-N3	4.34	119.09	115.32
1	A2	1852	MA6	C2-N1-C6	4.34	122.43	111.83
39	B5	4364	OMG	N9-C4-N3	4.33	134.61	125.95
39	B5	3973	OMU	N3-C2-N1	4.31	120.50	114.89
39	B5	3502	PSU	C4-N3-C2	-4.30	120.44	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3657	OMU	N3-C2-N1	4.30	120.49	114.89
39	B5	4366	OMU	N3-C2-N1	4.28	120.46	114.89
39	B5	1491	PSU	C4-N3-C2	-4.28	120.48	126.37
39	B5	4039	PSU	C4-N3-C2	-4.27	120.49	126.37
39	B5	4042	PSU	C4-N3-C2	-4.27	120.49	126.37
39	B5	4269	A2M	C2'-C1'-N9	-4.25	106.75	113.75
1	A2	1348	PSU	C4-N3-C2	-4.25	120.51	126.37
1	A2	815	PSU	C4-N3-C2	-4.25	120.51	126.37
39	B5	3557	A2M	C2'-C1'-N9	-4.25	106.76	113.75
39	B5	4267	PSU	C4-N3-C2	-4.25	120.52	126.37
1	A2	429	OMU	N3-C2-N1	4.25	120.42	114.89
1	A2	1233	PSU	C4-N3-C2	-4.24	120.54	126.37
11	AT	55	PSU	C4-N3-C2	-4.24	120.54	126.37
1	A2	1368	PSU	C4-N3-C2	-4.23	120.54	126.37
39	B5	4149	PSU	C4-N3-C2	-4.23	120.54	126.37
39	B5	4052	OMU	N3-C2-N1	4.23	120.40	114.89
39	B5	3447	PSU	C4-N3-C2	-4.23	120.55	126.37
1	A2	355	OMU	N3-C2-N1	4.22	120.39	114.89
1	A2	1239	PSU	C4-N3-C2	-4.22	120.55	126.37
39	B5	4374	PSU	C4-N3-C2	-4.22	120.56	126.37
1	A2	407	PSU	C4-N3-C2	-4.22	120.56	126.37
39	B5	3585	PSU	C4-N3-C2	-4.22	120.56	126.37
39	B5	4099	PSU	C4-N3-C2	-4.21	120.56	126.37
39	B5	4298	PSU	C4-N3-C2	-4.21	120.57	126.37
39	B5	4325	PSU	C4-N3-C2	-4.21	120.57	126.37
39	B5	4749	PSU	C4-N3-C2	-4.21	120.57	126.37
1	A2	1047	PSU	C4-N3-C2	-4.21	120.57	126.37
39	B5	2351	PSU	C4-N3-C2	-4.21	120.57	126.37
1	A2	1057	PSU	C4-N3-C2	-4.21	120.57	126.37
41	B8	69	PSU	C4-N3-C2	-4.20	120.58	126.37
1	A2	116	OMU	N3-C2-N1	4.20	120.36	114.89
1	A2	573	PSU	C4-N3-C2	-4.20	120.59	126.37
1	A2	1327	OMU	N3-C2-N1	4.20	120.35	114.89
41	B8	55	PSU	C4-N3-C2	-4.19	120.60	126.37
39	B5	4045	PSU	C4-N3-C2	-4.19	120.60	126.37
1	A2	669	A2M	N3-C4-N9	4.19	134.29	127.17
1	A2	172	OMU	N3-C2-N1	4.19	120.34	114.89
39	B5	3427	PSU	C4-N3-C2	-4.19	120.60	126.37
39	B5	3490	PSU	C4-N3-C2	-4.19	120.61	126.37
39	B5	3496	PSU	C4-N3-C2	-4.18	120.61	126.37
39	B5	3369	PSU	C4-N3-C2	-4.17	120.62	126.37
39	B5	4177	PSU	C4-N3-C2	-4.17	120.62	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	218	PSU	C4-N3-C2	-4.17	120.63	126.37
39	B5	4419	PSU	C4-N3-C2	-4.17	120.63	126.37
1	A2	1032	A2M	C2'-C1'-N9	-4.17	106.89	113.75
39	B5	1683	PSU	C4-N3-C2	-4.17	120.63	126.37
1	A2	682	PSU	C4-N3-C2	-4.16	120.63	126.37
1	A2	867	PSU	C4-N3-C2	-4.16	120.64	126.37
39	B5	4246	PSU	C4-N3-C2	-4.16	120.64	126.37
1	A2	93	PSU	C4-N3-C2	-4.16	120.65	126.37
1	A2	1005	PSU	C4-N3-C2	-4.15	120.65	126.37
39	B5	3974	OMG	N9-C4-N3	4.15	134.26	125.95
39	B5	4711	PSU	C4-N3-C2	-4.15	120.65	126.37
11	AT	28	PSU	C4-N3-C2	-4.15	120.66	126.37
39	B5	3371	PSU	C4-N3-C2	-4.14	120.66	126.37
1	A2	1851	MA6	C4-C5-N7	-4.14	105.84	110.58
39	B5	4107	PSU	C4-N3-C2	-4.14	120.67	126.37
39	B5	3462	PSU	C4-N3-C2	-4.14	120.67	126.37
1	A2	36	PSU	C4-N3-C2	-4.14	120.67	126.37
1	A2	1175	PSU	C4-N3-C2	-4.14	120.67	126.37
39	B5	1721	PSU	C4-N3-C2	-4.14	120.67	126.37
1	A2	105	PSU	C4-N3-C2	-4.14	120.67	126.37
1	A2	577	A2M	C2'-C1'-N9	-4.13	106.95	113.75
1	A2	967	PSU	C4-N3-C2	-4.13	120.68	126.37
1	A2	816	PSU	C4-N3-C2	-4.13	120.68	126.37
1	A2	652	PSU	C4-N3-C2	-4.13	120.68	126.37
39	B5	1801	PSU	C4-N3-C2	-4.13	120.69	126.37
1	A2	1046	PSU	C4-N3-C2	-4.12	120.69	126.37
1	A2	864	PSU	C4-N3-C2	-4.12	120.69	126.37
1	A2	1693	PSU	C4-N3-C2	-4.12	120.69	126.37
39	B5	4740	PSU	C4-N3-C2	-4.12	120.69	126.37
39	B5	3583	PSU	C4-N3-C2	-4.12	120.70	126.37
39	B5	4435	PSU	C4-N3-C2	-4.12	120.70	126.37
39	B5	3517	A2M	O4'-C1'-N9	4.11	115.99	108.09
39	B5	4244	OMU	N3-C2-N1	4.11	120.25	114.89
1	A2	109	PSU	C4-N3-C2	-4.11	120.71	126.37
39	B5	1638	PSU	C4-N3-C2	-4.11	120.71	126.37
1	A2	1446	PSU	C4-N3-C2	-4.11	120.72	126.37
1	A2	121	OMU	N3-C2-N1	4.10	120.23	114.89
39	B5	4169	PSU	C4-N3-C2	-4.10	120.72	126.37
1	A2	610	PSU	C4-N3-C2	-4.10	120.72	126.37
1	A2	1082	PSU	C4-N3-C2	-4.10	120.73	126.37
1	A2	1805	OMU	N3-C2-N1	4.09	120.22	114.89
1	A2	628	OMU	N3-C2-N1	4.09	120.22	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3500	PSU	C4-N3-C2	-4.09	120.73	126.37
39	B5	1799	PSU	C4-N3-C2	-4.09	120.73	126.37
39	B5	4203	PSU	C4-N3-C2	-4.09	120.74	126.37
39	B5	2258	OMU	N3-C2-N1	4.09	120.21	114.89
1	A2	1644	PSU	C4-N3-C2	-4.09	120.74	126.37
1	A2	34	PSU	C4-N3-C2	-4.09	120.74	126.37
11	AT	27	PSU	C4-N3-C2	-4.08	120.74	126.37
39	B5	4188	PSU	C4-N3-C2	-4.08	120.75	126.37
1	A2	687	PSU	C4-N3-C2	-4.08	120.75	126.37
1	A2	1178	PSU	C4-N3-C2	-4.08	120.75	126.37
39	B5	3652	PSU	C4-N3-C2	-4.08	120.76	126.37
1	A2	823	PSU	C4-N3-C2	-4.07	120.76	126.37
11	AT	39	PSU	C4-N3-C2	-4.07	120.76	126.37
1	A2	1443	OMU	N3-C2-N1	4.07	120.19	114.89
39	B5	1718	PSU	C4-N3-C2	-4.07	120.76	126.37
1	A2	1245	PSU	C4-N3-C2	-4.07	120.76	126.37
39	B5	1720	PSU	C4-N3-C2	-4.07	120.77	126.37
39	B5	4322	PSU	C4-N3-C2	-4.07	120.77	126.37
1	A2	1626	PSU	C4-N3-C2	-4.06	120.77	126.37
39	B5	1537	PSU	C4-N3-C2	-4.06	120.77	126.37
39	B5	3466	PSU	C4-N3-C2	-4.06	120.77	126.37
1	A2	650	PSU	C4-N3-C2	-4.05	120.79	126.37
39	B5	4058	PSU	C4-N3-C2	-4.05	120.79	126.37
39	B5	4278	PSU	C4-N3-C2	-4.05	120.79	126.37
39	B5	1731	PSU	C4-N3-C2	-4.05	120.80	126.37
1	A2	1851	MA6	N3-C4-N9	4.05	134.05	127.17
1	A2	1852	MA6	N3-C4-N9	4.05	134.05	127.17
1	A2	802	PSU	C4-N3-C2	-4.04	120.81	126.37
39	B5	3616	PSU	C4-N3-C2	-4.03	120.82	126.37
11	AT	37	YYG	N3-C2-N2	-4.00	121.10	126.62
39	B5	3554	PSU	C4-N3-C2	-4.00	120.86	126.37
1	A2	591	A2M	C2-N3-C4	4.00	121.59	111.83
1	A2	1047	PSU	O2-C2-N1	-4.00	118.67	122.79
39	B5	4217	PSU	C4-N3-C2	-3.99	120.87	126.37
39	B5	2475	PSU	C4-N3-C2	-3.98	120.88	126.37
1	A2	210	PSU	C4-N3-C2	-3.98	120.89	126.37
1	A2	1289	OMU	N3-C2-N1	3.98	120.07	114.89
11	AT	54	5MU	O4-C4-C5	-3.98	120.37	124.92
39	B5	3494	PSU	C4-N3-C2	-3.96	120.92	126.37
39	B5	4382	PSU	C4-N3-C2	-3.96	120.92	126.37
1	A2	119	PSU	C4-N3-C2	-3.96	120.92	126.37
1	A2	1852	MA6	C4-C5-N7	-3.95	106.06	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3576	PSU	C4-N3-C2	-3.94	120.95	126.37
39	B5	4166	PSU	C4-N3-C2	-3.92	120.98	126.37
39	B5	4193	5MC	C5-C6-N1	-3.91	119.06	123.31
39	B5	2258	OMU	C5-C4-N3	3.91	120.28	114.80
39	B5	4374	PSU	O2-C2-N1	-3.90	118.76	122.79
1	A2	429	OMU	C5-C4-N3	3.90	120.27	114.80
39	B5	1632	PSU	C4-N3-C2	-3.90	121.00	126.37
39	B5	2680	OMU	C5-C4-N3	3.90	120.26	114.80
1	A2	1327	OMU	C5-C4-N3	3.90	120.26	114.80
1	A2	628	OMU	C5-C4-N3	3.89	120.25	114.80
39	B5	3657	OMU	C5-C4-N3	3.89	120.24	114.80
39	B5	1632	PSU	O2-C2-N1	-3.89	118.78	122.79
1	A2	1289	OMU	C5-C4-N3	3.88	120.23	114.80
39	B5	3973	OMU	C5-C4-N3	3.88	120.23	114.80
39	B5	4325	PSU	O2-C2-N1	-3.87	118.79	122.79
11	AT	37	YYG	C24-O23-C21	3.86	120.10	115.63
1	A2	1443	OMU	C5-C4-N3	3.86	120.21	114.80
1	A2	116	OMU	C5-C4-N3	3.86	120.20	114.80
1	A2	355	OMU	C5-C4-N3	3.85	120.20	114.80
11	AT	37	YYG	O23-C21-O22	-3.85	119.01	124.62
1	A2	823	PSU	O2-C2-N1	-3.85	118.82	122.79
1	A2	1805	OMU	C5-C4-N3	3.84	120.18	114.80
39	B5	4244	OMU	C5-C4-N3	3.84	120.18	114.80
1	A2	172	OMU	C5-C4-N3	3.82	120.16	114.80
39	B5	4366	OMU	C5-C4-N3	3.80	120.13	114.80
39	B5	4419	PSU	O2-C2-N1	-3.80	118.87	122.79
39	B5	4052	OMU	C5-C4-N3	3.79	120.11	114.80
1	A2	1626	PSU	O2-C2-N1	-3.78	118.89	122.79
1	A2	121	OMU	C5-C4-N3	3.78	120.10	114.80
1	A2	1057	PSU	O2-C2-N1	-3.77	118.90	122.79
1	A2	1233	PSU	O2-C2-N1	-3.76	118.91	122.79
39	B5	3450	A2M	C2'-C1'-N9	-3.75	107.57	113.75
1	A2	669	A2M	C4-C5-N7	-3.75	106.30	110.58
1	A2	159	A2M	C2'-C1'-N9	-3.75	107.59	113.75
1	A2	469	A2M	C2-N3-C4	3.75	120.98	111.83
1	A2	166	A2M	C2-N3-C4	3.75	120.98	111.83
39	B5	2630	A2M	C2-N3-C4	3.74	120.98	111.83
39	B5	4336	A2M	C2-N3-C4	3.74	120.98	111.83
39	B5	3550	UY1	CM2-O2'-C2'	-3.74	104.86	114.47
39	B5	2658	A2M	C2-N3-C4	3.74	120.97	111.83
1	A2	1679	A2M	C2-N3-C4	3.74	120.96	111.83
39	B5	4058	PSU	O2-C2-N1	-3.73	118.94	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1338	4AC	N4-C4-N3	3.73	119.93	113.87
11	AT	37	YYG	C10-C11-N2	3.73	126.81	119.32
39	B5	3496	PSU	O2-C2-N1	-3.73	118.94	122.79
1	A2	513	A2M	C2-N3-C4	3.73	120.94	111.83
39	B5	4246	PSU	O2-C2-N1	-3.73	118.94	122.79
1	A2	27	A2M	C2-N3-C4	3.72	120.92	111.83
39	B5	4188	PSU	O2-C2-N1	-3.72	118.95	122.79
1	A2	36	PSU	O2-C2-N1	-3.72	118.95	122.79
39	B5	3456	A2M	C2-N3-C4	3.72	120.91	111.83
1	A2	1384	A2M	C2-N3-C4	3.72	120.91	111.83
39	B5	3557	A2M	C2-N3-C4	3.71	120.88	111.83
1	A2	218	PSU	O2-C2-N1	-3.70	118.97	122.79
11	AT	27	PSU	O2-C2-N1	-3.70	118.97	122.79
39	B5	398	A2M	C2-N3-C4	3.70	120.87	111.83
39	B5	2244	A2M	C2-N3-C4	3.70	120.87	111.83
39	B5	3966	6MZ	C2-N3-C4	3.70	120.86	111.83
39	B5	4039	PSU	O2-C2-N1	-3.70	118.97	122.79
1	A2	159	A2M	C2-N3-C4	3.70	120.86	111.83
1	A2	1833	6MZ	C4-C5-N7	-3.70	106.36	110.58
39	B5	1683	PSU	O2-C2-N1	-3.69	118.98	122.79
1	A2	93	PSU	O2-C2-N1	-3.69	118.98	122.79
1	A2	610	PSU	O2-C2-N1	-3.69	118.98	122.79
1	A2	1046	PSU	O2-C2-N1	-3.69	118.99	122.79
1	A2	1833	6MZ	C2-N3-C4	3.68	120.83	111.83
39	B5	3562	A2M	C2-N3-C4	3.68	120.81	111.83
1	A2	1175	PSU	O2-C2-N1	-3.68	119.00	122.79
39	B5	4317	A2M	C2-N3-C4	3.68	120.81	111.83
1	A2	485	A2M	C2-N3-C4	3.68	120.81	111.83
1	A2	650	PSU	O2-C2-N1	-3.67	119.00	122.79
1	A2	1368	PSU	O2-C2-N1	-3.67	119.00	122.79
39	B5	3494	PSU	O2-C2-N1	-3.67	119.00	122.79
39	B5	1270	A2M	C2-N3-C4	3.67	120.80	111.83
39	B5	1721	PSU	O2-C2-N1	-3.67	119.00	122.79
39	B5	1801	PSU	O2-C2-N1	-3.67	119.01	122.79
39	B5	2206	A2M	C2-N3-C4	3.67	120.78	111.83
1	A2	99	A2M	C2-N3-C4	3.66	120.78	111.83
39	B5	400	A2M	C2-N3-C4	3.66	120.78	111.83
39	B5	1489	A2M	C2-N3-C4	3.66	120.78	111.83
39	B5	1489	A2M	C4-C5-N7	-3.66	106.39	110.58
39	B5	1479	A2M	C2-N3-C4	3.65	120.75	111.83
1	A2	577	A2M	C2-N3-C4	3.65	120.75	111.83
39	B5	3599	A2M	C2-N3-C4	3.65	120.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3462	PSU	O2-C2-N1	-3.65	119.03	122.79
39	B5	4749	PSU	O2-C2-N1	-3.64	119.03	122.79
39	B5	1810	A2M	C2-N3-C4	3.64	120.73	111.83
1	A2	1249	B8N	C4-N3-C2	-3.64	121.14	125.62
1	A2	1446	PSU	O2-C2-N1	-3.64	119.04	122.79
1	A2	513	A2M	C2'-C1'-N9	-3.63	107.77	113.75
39	B5	4045	PSU	O2-C2-N1	-3.63	119.04	122.79
1	A2	573	PSU	O2-C2-N1	-3.63	119.04	122.79
1	A2	1851	MA6	C2-N3-C4	3.63	120.70	111.83
1	A2	407	PSU	O2-C2-N1	-3.63	119.05	122.79
39	B5	3554	PSU	O2-C2-N1	-3.63	119.05	122.79
39	B5	4278	PSU	O2-C2-N1	-3.62	119.05	122.79
39	B5	3517	A2M	C2-N3-C4	3.62	120.67	111.83
1	A2	105	PSU	O2-C2-N1	-3.62	119.06	122.79
11	AT	39	PSU	O2-C2-N1	-3.62	119.06	122.79
39	B5	3447	PSU	O2-C2-N1	-3.62	119.06	122.79
39	B5	3502	PSU	O2-C2-N1	-3.61	119.06	122.79
39	B5	4267	PSU	O2-C2-N1	-3.61	119.06	122.79
1	A2	802	PSU	O2-C2-N1	-3.61	119.06	122.79
39	B5	3492	A2M	C2-N3-C4	3.61	120.65	111.83
39	B5	3450	A2M	C2-N3-C4	3.61	120.64	111.83
1	A2	1032	A2M	C2-N3-C4	3.61	120.64	111.83
1	A2	1249	B8N	N3-C2-N1	3.60	121.12	116.72
1	A2	669	A2M	C2-N3-C4	3.60	120.63	111.83
1	A2	1082	PSU	O2-C2-N1	-3.60	119.07	122.79
1	A2	159	A2M	C4-C5-N7	-3.60	106.47	110.58
39	B5	4107	PSU	O2-C2-N1	-3.60	119.08	122.79
39	B5	4382	PSU	O2-C2-N1	-3.60	119.08	122.79
1	A2	1239	PSU	O2-C2-N1	-3.60	119.08	122.79
1	A2	1348	PSU	O2-C2-N1	-3.59	119.08	122.79
1	A2	815	PSU	O2-C2-N1	-3.59	119.09	122.79
41	B8	69	PSU	O2-C2-N1	-3.59	119.09	122.79
1	A2	816	PSU	O2-C2-N1	-3.58	119.10	122.79
1	A2	1852	MA6	C2-N3-C4	3.58	120.57	111.83
39	B5	3974	OMG	C6-C5-N7	3.57	136.80	130.29
1	A2	1005	PSU	O2-C2-N1	-3.57	119.10	122.79
39	B5	3585	PSU	O2-C2-N1	-3.57	119.11	122.79
39	B5	4149	PSU	O2-C2-N1	-3.57	119.11	122.79
39	B5	1491	PSU	O2-C2-N1	-3.57	119.11	122.79
1	A2	864	PSU	O2-C2-N1	-3.57	119.11	122.79
1	A2	687	PSU	O2-C2-N1	-3.56	119.12	122.79
39	B5	4169	PSU	O2-C2-N1	-3.56	119.12	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1718	PSU	O2-C2-N1	-3.56	119.12	122.79
39	B5	3427	PSU	O2-C2-N1	-3.55	119.13	122.79
39	B5	3583	PSU	O2-C2-N1	-3.55	119.13	122.79
39	B5	3631	OMG	C6-C5-N7	3.55	136.74	130.29
39	B5	3562	A2M	C4-C5-N7	-3.55	106.53	110.58
1	A2	652	PSU	O2-C2-N1	-3.54	119.13	122.79
39	B5	4203	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A2	1833	6MZ	C6-C5-N7	3.54	136.29	132.43
1	A2	109	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A2	1245	PSU	O2-C2-N1	-3.54	119.14	122.79
39	B5	1799	PSU	O2-C2-N1	-3.54	119.14	122.79
39	B5	3466	PSU	O2-C2-N1	-3.54	119.14	122.79
39	B5	3500	PSU	O2-C2-N1	-3.54	119.14	122.79
1	A2	119	PSU	O2-C2-N1	-3.53	119.15	122.79
1	A2	210	PSU	O2-C2-N1	-3.53	119.15	122.79
39	B5	4298	PSU	O2-C2-N1	-3.53	119.15	122.79
11	AT	28	PSU	O2-C2-N1	-3.53	119.15	122.79
1	A2	1644	PSU	O2-C2-N1	-3.52	119.16	122.79
1	A2	34	PSU	O2-C2-N1	-3.52	119.16	122.79
39	B5	2658	A2M	C4-C5-N7	-3.52	106.56	110.58
1	A2	1384	A2M	C4-C5-N7	-3.51	106.57	110.58
39	B5	4269	A2M	C2-N3-C4	3.51	120.39	111.83
1	A2	166	A2M	C4-C5-N7	-3.50	106.58	110.58
1	A2	867	PSU	O2-C2-N1	-3.50	119.18	122.79
39	B5	4217	PSU	O2-C2-N1	-3.50	119.18	122.79
39	B5	4336	A2M	C4-C5-N7	-3.49	106.59	110.58
39	B5	4364	OMG	C6-C5-N7	3.49	136.64	130.29
1	A2	513	A2M	C4-C5-N7	-3.49	106.59	110.58
39	B5	1537	PSU	O2-C2-N1	-3.49	119.19	122.79
39	B5	4177	PSU	O2-C2-N1	-3.49	119.19	122.79
39	B5	398	A2M	C4-C5-N7	-3.48	106.60	110.58
11	AT	55	PSU	O2-C2-N1	-3.48	119.20	122.79
39	B5	4383	OMG	C6-C5-N7	3.48	136.62	130.29
39	B5	4099	PSU	O2-C2-N1	-3.48	119.20	122.79
39	B5	1731	PSU	O2-C2-N1	-3.47	119.21	122.79
1	A2	469	A2M	C4-C5-N7	-3.47	106.62	110.58
1	A2	682	PSU	O2-C2-N1	-3.47	119.21	122.79
39	B5	4435	PSU	O2-C2-N1	-3.47	119.21	122.79
39	B5	4322	PSU	O2-C2-N1	-3.47	119.21	122.79
1	A2	1032	A2M	N3-C2-N1	-3.47	123.34	128.58
39	B5	1720	PSU	O2-C2-N1	-3.46	119.22	122.79
39	B5	1810	A2M	C4-C5-N7	-3.46	106.63	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1479	A2M	C4-C5-N7	-3.45	106.64	110.58
39	B5	3359	OMG	C6-C5-N7	3.45	136.56	130.29
41	B8	55	PSU	O2-C2-N1	-3.44	119.24	122.79
39	B5	2475	PSU	O2-C2-N1	-3.44	119.24	122.79
1	A2	1679	A2M	C4-C5-N7	-3.44	106.65	110.58
1	A2	27	A2M	C4-C5-N7	-3.44	106.65	110.58
39	B5	3652	PSU	O2-C2-N1	-3.43	119.25	122.79
1	A2	1851	MA6	N1-C2-N3	-3.43	123.39	128.58
39	B5	2244	A2M	C4-C5-N7	-3.43	106.66	110.58
39	B5	4711	PSU	O2-C2-N1	-3.43	119.25	122.79
39	B5	3456	A2M	C4-C5-N7	-3.43	106.67	110.58
1	A2	1693	PSU	O2-C2-N1	-3.43	119.26	122.79
1	A2	1032	A2M	C4-C5-N7	-3.42	106.67	110.58
11	AT	14	1MA	N9-C4-N3	3.42	134.70	126.90
39	B5	2206	A2M	C4-C5-N7	-3.42	106.67	110.58
1	A2	1833	6MZ	N1-C2-N3	-3.42	123.41	128.58
1	A2	967	PSU	O2-C2-N1	-3.42	119.27	122.79
39	B5	3450	A2M	C4-C5-N7	-3.41	106.68	110.58
1	A2	1178	PSU	O2-C2-N1	-3.41	119.27	122.79
39	B5	2351	PSU	O2-C2-N1	-3.41	119.28	122.79
39	B5	3490	PSU	O2-C2-N1	-3.41	119.28	122.79
11	AT	37	YYG	O18-C16-C15	3.40	120.14	111.49
39	B5	1638	PSU	O2-C2-N1	-3.40	119.29	122.79
39	B5	4042	PSU	O2-C2-N1	-3.39	119.29	122.79
39	B5	4269	A2M	C4-C5-N7	-3.39	106.70	110.58
11	AT	58	1MA	N9-C4-N3	3.39	134.63	126.90
39	B5	3599	A2M	C4-C5-N7	-3.39	106.70	110.58
1	A2	577	A2M	C4-C5-N7	-3.39	106.71	110.58
1	A2	684	OMG	C6-C5-N7	3.39	136.46	130.29
39	B5	3369	PSU	O2-C2-N1	-3.39	119.29	122.79
39	B5	4369	OMG	C6-C5-N7	3.38	136.44	130.29
39	B5	4317	A2M	C4-C5-N7	-3.38	106.72	110.58
11	AT	26	M2G	C6-C5-N7	3.37	136.43	130.29
39	B5	3557	A2M	C4-C5-N7	-3.37	106.73	110.58
39	B5	2207	OMG	C6-C5-N7	3.37	136.42	130.29
1	A2	99	A2M	C2'-C1'-N9	-3.37	108.21	113.75
39	B5	3576	PSU	O2-C2-N1	-3.37	119.32	122.79
1	A2	485	A2M	C4-C5-N7	-3.37	106.73	110.58
1	A2	99	A2M	C4-C5-N7	-3.37	106.73	110.58
39	B5	3492	A2M	C4-C5-N7	-3.37	106.73	110.58
39	B5	400	A2M	C4-C5-N7	-3.36	106.74	110.58
39	B5	3517	A2M	C4-C5-N7	-3.36	106.74	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	166	A2M	C2'-C1'-N9	-3.36	108.23	113.75
39	B5	4166	PSU	O2-C2-N1	-3.36	119.33	122.79
39	B5	1260	OMG	C6-C5-N7	3.35	136.39	130.29
39	B5	3676	OMG	C6-C5-N7	3.34	136.38	130.29
39	B5	3966	6MZ	C4-C5-N7	-3.34	106.77	110.58
39	B5	4138	OMG	C6-C5-N7	3.33	136.36	130.29
39	B5	2630	A2M	C4-C5-N7	-3.33	106.77	110.58
1	A2	591	A2M	C4-C5-N7	-3.33	106.77	110.58
1	A2	1329	OMG	C6-C5-N7	3.33	136.35	130.29
39	B5	4740	PSU	O2-C2-N1	-3.33	119.36	122.79
39	B5	3517	A2M	N3-C2-N1	-3.33	123.54	128.58
39	B5	1477	OMG	C6-C5-N7	3.33	136.34	130.29
42	BA	216	V5N	CD2-CG-ND1	3.32	110.24	105.76
39	B5	2630	A2M	N3-C2-N1	-3.32	123.56	128.58
1	A2	1679	A2M	N3-C2-N1	-3.32	123.56	128.58
39	B5	1270	A2M	C4-C5-N7	-3.31	106.79	110.58
39	B5	3476	OMG	C6-C5-N7	3.31	136.32	130.29
39	B5	400	A2M	N3-C2-N1	-3.31	123.57	128.58
39	B5	3456	A2M	N3-C2-N1	-3.31	123.57	128.58
1	A2	1852	MA6	N1-C2-N3	-3.31	123.58	128.58
39	B5	1810	A2M	N3-C2-N1	-3.30	123.58	128.58
39	B5	1266	1MA	N9-C4-N3	3.30	134.42	126.90
39	B5	3557	A2M	N3-C2-N1	-3.30	123.59	128.58
39	B5	398	A2M	C2'-C1'-N9	-3.29	108.33	113.75
39	B5	3550	UY1	C6-C5-C4	3.29	120.39	118.17
39	B5	3562	A2M	N3-C2-N1	-3.29	123.60	128.58
1	A2	27	A2M	N3-C2-N1	-3.29	123.61	128.58
39	B5	4276	UR3	C5-C4-N3	3.28	119.36	115.04
1	A2	469	A2M	N3-C2-N1	-3.27	123.63	128.58
39	B5	4245	OMG	C6-C5-N7	3.27	136.24	130.29
39	B5	4116	OMG	C6-C5-N7	3.27	136.24	130.29
39	B5	3966	6MZ	N1-C2-N3	-3.27	123.64	128.58
1	A2	868	OMG	C6-C5-N7	3.26	136.23	130.29
39	B5	1489	A2M	N3-C2-N1	-3.26	123.65	128.58
11	AT	34	OMG	C6-C5-N7	3.26	136.22	130.29
1	A2	437	OMG	C6-C5-N7	3.26	136.22	130.29
39	B5	3966	6MZ	C9-N6-C6	-3.25	119.83	122.85
39	B5	3514	5MC	C5-C6-N1	-3.25	119.78	123.31
1	A2	513	A2M	N3-C2-N1	-3.24	123.67	128.58
1	A2	577	A2M	N3-C2-N1	-3.24	123.67	128.58
11	AT	54	5MU	C5-C6-N1	-3.24	119.79	123.31
1	A2	645	OMG	C6-C5-N7	3.23	136.17	130.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	591	A2M	N3-C2-N1	-3.23	123.69	128.58
39	B5	4240	OMG	C6-C5-N7	3.23	136.17	130.29
68	Ba	39	V5N	CD2-CG-ND1	3.23	110.11	105.76
41	B8	75	OMG	C6-C5-N7	3.22	136.16	130.29
39	B5	2658	A2M	N3-C2-N1	-3.22	123.71	128.58
39	B5	3517	A2M	C4-N9-C8	3.22	109.12	105.74
1	A2	602	OMG	C6-C5-N7	3.22	136.15	130.29
1	A2	669	A2M	N3-C2-N1	-3.22	123.72	128.58
39	B5	4317	A2M	N3-C2-N1	-3.21	123.73	128.58
39	B5	4336	A2M	N3-C2-N1	-3.20	123.73	128.58
1	A2	166	A2M	N3-C2-N1	-3.20	123.73	128.58
39	B5	3492	A2M	N3-C2-N1	-3.20	123.74	128.58
1	A2	99	A2M	N3-C2-N1	-3.19	123.75	128.58
39	B5	3966	6MZ	C6-C5-N7	3.19	135.91	132.43
1	A2	510	OMG	C6-C5-N7	3.19	136.10	130.29
39	B5	3371	PSU	O2-C2-N1	-3.19	119.50	122.79
39	B5	3616	PSU	O2-C2-N1	-3.19	119.50	122.79
1	A2	159	A2M	N3-C2-N1	-3.19	123.76	128.58
39	B5	2206	A2M	N3-C2-N1	-3.18	123.76	128.58
1	A2	628	OMU	O4-C4-C5	-3.18	119.67	125.16
1	A2	485	A2M	N3-C2-N1	-3.18	123.77	128.58
39	B5	2244	A2M	N3-C2-N1	-3.18	123.77	128.58
39	B5	3599	A2M	N3-C2-N1	-3.17	123.78	128.58
1	A2	1384	A2M	N3-C2-N1	-3.14	123.82	128.58
39	B5	398	A2M	N3-C2-N1	-3.14	123.83	128.58
11	AT	10	2MG	C6-C5-N7	3.14	136.00	130.29
39	B5	1270	A2M	N3-C2-N1	-3.14	123.84	128.58
39	B5	3492	A2M	C2'-C1'-N9	-3.13	108.61	113.75
39	B5	3450	A2M	N3-C2-N1	-3.11	123.87	128.58
1	A2	1443	OMU	O4-C4-C5	-3.10	119.81	125.16
39	B5	1479	A2M	N3-C2-N1	-3.10	123.89	128.58
39	B5	4269	A2M	N3-C2-N1	-3.09	123.91	128.58
1	A2	116	OMU	O4-C4-C5	-3.09	119.83	125.16
1	A2	1679	A2M	C2'-C1'-N9	-3.09	108.67	113.75
39	B5	2258	OMU	O4-C4-C5	-3.08	119.85	125.16
1	A2	429	OMU	O4-C4-C5	-3.08	119.85	125.16
1	A2	1491	OMG	C6-C5-N7	3.06	135.86	130.29
39	B5	3524	OMG	C6-C5-N7	3.05	135.85	130.29
39	B5	2719	OMG	C6-C5-N7	3.05	135.84	130.29
11	AT	49	5MC	C5-C6-N1	-3.03	120.02	123.31
1	A2	1448	OMG	C6-C5-N7	3.03	135.80	130.29
1	A2	1289	OMU	O4-C4-C5	-3.02	119.95	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	121	OMU	O4-C4-C5	-3.02	119.95	125.16
39	B5	4244	OMU	O4-C4-C5	-3.01	119.96	125.16
39	B5	2267	OMG	C6-C5-N7	3.01	135.76	130.29
1	A2	1805	OMU	O4-C4-C5	-3.00	119.98	125.16
39	B5	3942	OMG	C6-C5-N7	3.00	135.75	130.29
1	A2	172	OMU	O4-C4-C5	-2.98	120.02	125.16
39	B5	3456	A2M	C2'-C1'-N9	-2.98	108.84	113.75
39	B5	4336	A2M	C2'-C1'-N9	-2.94	108.92	113.75
39	B5	2680	OMU	O4-C4-C5	-2.94	120.10	125.16
1	A2	355	OMU	O4-C4-C5	-2.93	120.10	125.16
1	A2	1327	OMU	O4-C4-C5	-2.93	120.11	125.16
1	A2	1851	MA6	C5-N7-C8	2.92	108.04	103.45
39	B5	3657	OMU	O4-C4-C5	-2.92	120.13	125.16
39	B5	3973	OMU	O4-C4-C5	-2.90	120.16	125.16
1	A2	27	A2M	C2'-C1'-N9	-2.89	109.00	113.75
39	B5	1580	OMG	C6-C5-N7	2.88	135.54	130.29
39	B5	4366	OMU	O4-C4-C5	-2.87	120.22	125.16
39	B5	2244	A2M	C2'-C1'-N9	-2.85	109.06	113.75
39	B5	4052	OMU	O4-C4-C5	-2.83	120.27	125.16
1	A2	1851	MA6	C4-N9-C8	2.83	108.71	105.74
1	A2	1032	A2M	C4-N9-C8	2.83	108.71	105.74
1	A2	469	A2M	C2'-C1'-N9	-2.82	109.11	113.75
1	A2	1843	4AC	N4-C4-N3	2.81	118.43	113.87
39	B5	4269	A2M	C4-N9-C8	2.77	108.64	105.74
1	A2	1852	MA6	C5-N7-C8	2.77	107.80	103.45
1	A2	577	A2M	C4-N9-C8	2.76	108.64	105.74
11	AT	46	7MG	C5-C6-N1	2.75	115.79	110.94
39	B5	3517	A2M	C2'-C1'-N9	-2.75	109.23	113.75
39	B5	2206	A2M	C4-N9-C8	2.75	108.62	105.74
39	B5	4364	OMG	C4-C5-N7	-2.74	106.32	110.67
39	B5	3514	5MC	C5-C4-N3	-2.74	118.95	121.75
39	B5	4383	OMG	C4-C5-N7	-2.74	106.34	110.67
39	B5	3631	OMG	C4-C5-N7	-2.73	106.34	110.67
39	B5	400	A2M	C4-N9-C8	2.73	108.60	105.74
39	B5	2207	OMG	C4-C5-N7	-2.72	106.36	110.67
11	AT	49	5MC	C5-C4-N3	-2.72	118.97	121.75
39	B5	4193	5MC	C5-C4-N3	-2.72	118.97	121.75
39	B5	3492	A2M	C4-N9-C8	2.71	108.59	105.74
39	B5	1260	OMG	C4-C5-N7	-2.71	106.37	110.67
1	A2	1338	4AC	C6-C5-C4	2.71	120.27	117.00
39	B5	3974	OMG	C4-C5-N7	-2.71	106.38	110.67
1	A2	669	A2M	C4-N9-C8	2.70	108.57	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	1833	6MZ	C5-N7-C8	2.69	107.69	103.45
39	B5	2244	A2M	C4-N9-C8	2.69	108.56	105.74
1	A2	1679	A2M	C4-N9-C8	2.69	108.56	105.74
1	A2	1640	7MG	C5-C6-N1	2.68	115.66	110.94
39	B5	1489	A2M	C4-N9-C8	2.68	108.55	105.74
68	Ba	39	V5N	O-C-CA	-2.68	117.88	124.77
1	A2	645	OMG	C4-C5-N7	-2.67	106.44	110.67
42	BA	216	V5N	O-C-CA	-2.66	117.93	124.77
39	B5	3599	A2M	C4-N9-C8	2.66	108.53	105.74
1	A2	1329	OMG	C4-C5-N7	-2.66	106.46	110.67
1	A2	669	A2M	C5-N7-C8	2.65	107.61	103.45
1	A2	684	OMG	C4-C5-N7	-2.65	106.47	110.67
39	B5	3562	A2M	C4-N9-C8	2.65	108.52	105.74
39	B5	3359	OMG	C4-C5-N7	-2.65	106.48	110.67
39	B5	1479	A2M	C4-N9-C8	2.64	108.52	105.74
1	A2	1843	4AC	C6-C5-C4	2.64	120.19	117.00
11	AT	26	M2G	C4-C5-N7	-2.64	106.48	110.67
1	A2	469	A2M	C4-N9-C8	2.64	108.51	105.74
1	A2	1852	MA6	C4-N9-C8	2.64	108.51	105.74
39	B5	3562	A2M	C5-N7-C8	2.63	107.58	103.45
1	A2	99	A2M	C4-N9-C8	2.63	108.50	105.74
39	B5	3557	A2M	C4-N9-C8	2.62	108.49	105.74
39	B5	3676	OMG	C4-C5-N7	-2.62	106.52	110.67
11	AT	37	YYG	C3-N3-C2	-2.62	115.03	120.32
1	A2	27	A2M	C4-N9-C8	2.62	108.49	105.74
39	B5	1810	A2M	C4-N9-C8	2.62	108.49	105.74
39	B5	3456	A2M	C4-N9-C8	2.62	108.49	105.74
1	A2	513	A2M	C4-N9-C8	2.61	108.48	105.74
39	B5	1489	A2M	C5-N7-C8	2.61	107.55	103.45
39	B5	1270	A2M	C4-N9-C8	2.61	108.48	105.74
1	A2	159	A2M	C5-N7-C8	2.61	107.55	103.45
39	B5	4240	OMG	C4-C5-N7	-2.60	106.54	110.67
39	B5	4369	OMG	C4-C5-N7	-2.60	106.54	110.67
1	A2	159	A2M	C4-N9-C8	2.60	108.47	105.74
39	B5	3476	OMG	C4-C5-N7	-2.60	106.55	110.67
39	B5	4317	A2M	C4-N9-C8	2.59	108.46	105.74
1	A2	166	A2M	C5-N7-C8	2.59	107.52	103.45
11	AT	58	1MA	C4-C5-N7	-2.59	106.57	110.67
39	B5	1270	A2M	C2'-C1'-N9	-2.59	109.49	113.75
11	AT	34	OMG	C4-C5-N7	-2.59	106.57	110.67
39	B5	4336	A2M	C5-N7-C8	2.58	107.51	103.45
39	B5	400	A2M	C2'-C1'-N9	-2.58	109.50	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3517	A2M	C5-N7-C8	2.58	107.50	103.45
39	B5	4138	OMG	C4-C5-N7	-2.57	106.60	110.67
41	B8	75	OMG	C4-C5-N7	-2.57	106.60	110.67
1	A2	513	A2M	C5-N7-C8	2.57	107.49	103.45
1	A2	166	A2M	C4-N9-C8	2.57	108.43	105.74
39	B5	2658	A2M	C5-N7-C8	2.57	107.48	103.45
39	B5	2206	A2M	C5-N7-C8	2.56	107.48	103.45
39	B5	2244	A2M	C5-N7-C8	2.56	107.48	103.45
39	B5	4245	OMG	C4-C5-N7	-2.56	106.61	110.67
1	A2	1679	A2M	C5-N7-C8	2.56	107.47	103.45
1	A2	469	A2M	C5-N7-C8	2.56	107.47	103.45
1	A2	1384	A2M	C5-N7-C8	2.55	107.46	103.45
1	A2	868	OMG	C4-C5-N7	-2.55	106.63	110.67
39	B5	1810	A2M	C5-N7-C8	2.55	107.46	103.45
39	B5	1477	OMG	C4-C5-N7	-2.55	106.63	110.67
1	A2	510	OMG	C4-C5-N7	-2.55	106.64	110.67
39	B5	1479	A2M	C5-N7-C8	2.54	107.45	103.45
1	A2	1833	6MZ	C4-N9-C8	2.54	108.41	105.74
1	A2	437	OMG	C4-C5-N7	-2.54	106.65	110.67
39	B5	2194	OMC	O2-C2-N3	-2.54	118.33	122.33
1	A2	1384	A2M	C4-N9-C8	2.54	108.40	105.74
1	A2	27	A2M	C5-N7-C8	2.53	107.43	103.45
1	A2	577	A2M	C5-N7-C8	2.53	107.43	103.45
39	B5	398	A2M	C5-N7-C8	2.53	107.43	103.45
33	Au	1	AME	O-C-CA	-2.53	118.27	124.77
11	AT	16	H2U	C5-C6-N1	-2.52	103.88	111.52
39	B5	1270	A2M	C5-N7-C8	2.52	107.41	103.45
39	B5	2267	OMG	C4-C5-N7	-2.51	106.69	110.67
39	B5	4336	A2M	C4-N9-C8	2.51	108.37	105.74
39	B5	2719	OMG	C4-C5-N7	-2.50	106.70	110.67
39	B5	4269	A2M	C5-N7-C8	2.50	107.38	103.45
39	B5	400	A2M	C5-N7-C8	2.50	107.38	103.45
39	B5	3942	OMG	C4-C5-N7	-2.50	106.71	110.67
1	A2	602	OMG	C4-C5-N7	-2.50	106.71	110.67
39	B5	3557	A2M	C5-N7-C8	2.50	107.38	103.45
1	A2	1032	A2M	C5-N7-C8	2.50	107.38	103.45
1	A2	99	A2M	C5-N7-C8	2.50	107.37	103.45
39	B5	3450	A2M	C5-N7-C8	2.50	107.37	103.45
1	A2	591	A2M	C5-N7-C8	2.49	107.37	103.45
11	AT	37	YYG	O18-C16-O17	-2.49	119.01	123.85
1	A2	1448	OMG	C4-C5-N7	-2.48	106.74	110.67
11	AT	10	2MG	C4-C5-N7	-2.48	106.74	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4317	A2M	C5-N7-C8	2.47	107.34	103.45
1	A2	1851	MA6	N1-C6-N6	2.47	119.87	116.86
39	B5	3599	A2M	C5-N7-C8	2.47	107.33	103.45
39	B5	3450	A2M	C4-N9-C8	2.47	108.33	105.74
39	B5	3492	A2M	C5-N7-C8	2.46	107.32	103.45
39	B5	3456	A2M	C5-N7-C8	2.46	107.32	103.45
39	B5	4116	OMG	C4-C5-N7	-2.46	106.77	110.67
1	A2	1491	OMG	C4-C5-N7	-2.46	106.78	110.67
11	AT	14	1MA	C4-C5-N7	-2.45	106.79	110.67
39	B5	3966	6MZ	C5-N7-C8	2.45	107.30	103.45
1	A2	485	A2M	C4-N9-C8	2.45	108.31	105.74
39	B5	2658	A2M	C4-N9-C8	2.45	108.31	105.74
1	A2	485	A2M	C5-N7-C8	2.44	107.29	103.45
39	B5	3524	OMG	C4-C5-N7	-2.44	106.80	110.67
39	B5	3550	UY1	O2-C2-N1	-2.44	120.28	122.79
1	A2	485	A2M	C2'-C1'-N9	-2.44	109.74	113.75
39	B5	3966	6MZ	C4-N9-C8	2.44	108.30	105.74
1	A2	1384	A2M	C2'-C1'-N9	-2.43	109.75	113.75
1	A2	1851	MA6	C6-C5-N7	2.43	137.31	133.43
30	Ar	2	SAC	O-C-CA	-2.42	118.54	124.77
12	AZ	2	SAC	O-C-CA	-2.42	118.55	124.77
39	B5	3517	A2M	N9-C8-N7	-2.40	110.53	113.94
39	B5	2630	A2M	C5-N7-C8	2.39	107.21	103.45
39	B5	398	A2M	C4-N9-C8	2.37	108.22	105.74
35	Aw	62	HY3	O-C-CA	-2.35	118.64	124.86
1	A2	669	A2M	C6-C5-N7	2.35	136.62	132.09
39	B5	4149	PSU	C5-C6-N1	-2.35	118.88	122.14
1	A2	628	OMU	O2-C2-N1	-2.35	119.74	122.80
39	B5	2206	A2M	C2'-C1'-N9	-2.34	109.90	113.75
39	B5	4317	A2M	C2'-C1'-N9	-2.34	109.90	113.75
39	B5	1489	A2M	C6-C5-N7	2.34	136.60	132.09
39	B5	4267	PSU	C5-C6-N1	-2.34	118.89	122.14
39	B5	3517	A2M	C6-C5-N7	2.34	136.59	132.09
39	B5	4042	PSU	C5-C6-N1	-2.33	118.90	122.14
39	B5	4099	PSU	C5-C6-N1	-2.33	118.90	122.14
83	Br	2	SAC	O-C-CA	-2.33	118.78	124.77
39	B5	1580	OMG	C4-C5-N7	-2.33	106.98	110.67
39	B5	4177	PSU	C5-C6-N1	-2.33	118.91	122.14
1	A2	429	OMU	O2-C2-N1	-2.31	119.78	122.80
11	AT	46	7MG	C5-C4-N9	-2.31	103.37	106.33
1	A2	407	PSU	C5-C6-N1	-2.30	118.94	122.14
39	B5	1266	1MA	C4-C5-N7	-2.30	107.02	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	2658	A2M	C2'-C1'-N9	-2.30	109.97	113.75
39	B5	3492	A2M	O4'-C1'-N9	2.29	112.48	108.09
39	B5	3657	OMU	O2-C2-N1	-2.28	119.83	122.80
39	B5	1491	PSU	C5-C6-N1	-2.28	118.98	122.14
41	B8	55	PSU	C5-C6-N1	-2.27	118.99	122.14
11	AT	54	5MU	O2-C2-N1	-2.27	119.84	122.80
1	A2	1032	A2M	C2-N1-C6	2.27	122.46	118.73
1	A2	1239	PSU	C5-C6-N1	-2.26	119.00	122.14
39	B5	3502	PSU	C5-C6-N1	-2.26	119.00	122.14
39	B5	3447	PSU	C5-C6-N1	-2.26	119.00	122.14
39	B5	3631	OMG	C2'-C1'-N9	-2.26	109.96	114.24
1	A2	1289	OMU	C1'-N1-C2	2.25	121.64	117.59
39	B5	3490	PSU	C5-C6-N1	-2.25	119.01	122.14
1	A2	1327	OMU	O2-C2-N1	-2.25	119.86	122.80
39	B5	3371	PSU	C5-C6-N1	-2.25	119.02	122.14
11	AT	17	H2U	C5-C6-N1	-2.25	104.72	111.52
41	B8	69	PSU	C5-C6-N1	-2.25	119.02	122.14
11	AT	49	5MC	O2-C2-N3	-2.24	118.80	122.33
11	AT	55	PSU	C5-C6-N1	-2.24	119.03	122.14
39	B5	2680	OMU	O2-C2-N1	-2.24	119.88	122.80
1	A2	1640	7MG	C5-C4-N9	-2.23	103.48	106.33
39	B5	4116	OMG	O6-C6-C5	-2.23	120.64	126.53
1	A2	1852	MA6	C6-C5-N7	2.23	136.99	133.43
1	A2	1392	OMC	O2-C2-N3	-2.23	118.82	122.33
39	B5	3631	OMG	O6-C6-C5	-2.23	120.65	126.53
1	A2	815	PSU	C5-C6-N1	-2.22	119.06	122.14
1	A2	1833	6MZ	C2-N1-C6	2.22	122.59	115.24
1	A2	1851	MA6	N9-C8-N7	-2.22	110.79	113.94
1	A2	823	PSU	O4'-C1'-C2'	2.21	108.21	105.15
39	B5	3369	PSU	C5-C6-N1	-2.21	119.07	122.14
39	B5	1632	PSU	O4'-C1'-C2'	2.21	108.21	105.15
1	A2	591	A2M	C4-N9-C8	2.21	108.06	105.74
39	B5	4419	PSU	C5-C6-N1	-2.21	119.07	122.14
1	A2	573	PSU	C5-C6-N1	-2.21	119.07	122.14
1	A2	1368	PSU	C5-C6-N1	-2.21	119.07	122.14
39	B5	3496	PSU	C5-C6-N1	-2.21	119.07	122.14
11	AT	37	YYG	C8-N9-C4	2.21	108.66	106.54
1	A2	1491	OMG	O6-C6-C5	-2.21	120.71	126.53
1	A2	1233	PSU	C5-C6-N1	-2.20	119.08	122.14
1	A2	1843	4AC	C5-C4-N3	-2.20	119.15	122.60
1	A2	816	PSU	C5-C6-N1	-2.20	119.09	122.14
39	B5	4240	OMG	O6-C6-C5	-2.20	120.73	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	3524	OMG	O6-C6-C5	-2.20	120.73	126.53
39	B5	4711	PSU	C5-C6-N1	-2.19	119.10	122.14
39	B5	2630	A2M	C4-N9-C8	2.19	108.03	105.74
39	B5	1721	PSU	C5-C6-N1	-2.18	119.11	122.14
39	B5	3514	5MC	O2-C2-N3	-2.18	118.89	122.33
1	A2	159	A2M	C6-C5-N7	2.18	136.30	132.09
39	B5	1683	PSU	C5-C6-N1	-2.18	119.11	122.14
1	A2	1348	PSU	C5-C6-N1	-2.18	119.12	122.14
39	B5	4245	OMG	O6-C6-C5	-2.18	120.79	126.53
39	B5	3562	A2M	C6-C5-N7	2.18	136.28	132.09
39	B5	2351	PSU	C5-C6-N1	-2.17	119.12	122.14
39	B5	4749	PSU	C5-C6-N1	-2.17	119.12	122.14
1	A2	1005	PSU	C5-C6-N1	-2.17	119.12	122.14
11	AT	46	7MG	O6-C6-C5	-2.17	122.28	127.62
39	B5	4039	PSU	C5-C6-N1	-2.17	119.12	122.14
39	B5	4045	PSU	C5-C6-N1	-2.17	119.13	122.14
39	B5	4298	PSU	C5-C6-N1	-2.17	119.13	122.14
1	A2	172	OMU	O2-C2-N1	-2.17	119.97	122.80
11	AT	58	1MA	C6-C5-N7	2.17	136.00	132.16
1	A2	1178	PSU	C5-C6-N1	-2.17	119.13	122.14
39	B5	4325	PSU	C5-C6-N1	-2.17	119.13	122.14
1	A2	1446	PSU	C5-C6-N1	-2.17	119.14	122.14
39	B5	3500	PSU	C5-C6-N1	-2.16	119.14	122.14
1	A2	1032	A2M	C6-C5-N7	2.16	136.26	132.09
11	AT	28	PSU	C5-C6-N1	-2.16	119.14	122.14
39	B5	4374	PSU	C5-C6-N1	-2.16	119.14	122.14
11	AT	10	2MG	O6-C6-C5	-2.16	120.84	126.53
39	B5	2658	A2M	C6-C5-N7	2.15	136.24	132.09
1	A2	682	PSU	C5-C6-N1	-2.15	119.16	122.14
1	A2	1175	PSU	C5-C6-N1	-2.15	119.16	122.14
41	B8	69	PSU	O4'-C1'-C2'	2.15	108.12	105.15
39	B5	1720	PSU	C5-C6-N1	-2.14	119.17	122.14
39	B5	4435	PSU	C5-C6-N1	-2.14	119.17	122.14
1	A2	868	OMG	O6-C6-C5	-2.14	120.88	126.53
39	B5	3456	A2M	C6-C5-N7	2.14	136.21	132.09
1	A2	1640	7MG	O6-C6-C5	-2.14	122.38	127.62
39	B5	4166	PSU	O4'-C1'-C2'	2.13	108.11	105.15
1	A2	669	A2M	N9-C8-N7	-2.13	110.91	113.94
1	A2	513	A2M	C6-C5-N7	2.13	136.20	132.09
39	B5	3462	PSU	C5-C6-N1	-2.13	119.19	122.14
39	B5	3583	PSU	C5-C6-N1	-2.13	119.19	122.14
39	B5	1638	PSU	C5-C6-N1	-2.13	119.19	122.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	B8	75	OMG	O6-C6-C5	-2.13	120.92	126.53
39	B5	3676	OMG	O6-C6-C5	-2.12	120.92	126.53
1	A2	652	PSU	C5-C6-N1	-2.12	119.19	122.14
1	A2	1704	OMC	O2-C2-N3	-2.12	118.98	122.33
39	B5	3359	OMG	O6-C6-C5	-2.12	120.93	126.53
1	A2	602	OMG	O6-C6-C5	-2.12	120.93	126.53
39	B5	1718	PSU	C5-C6-N1	-2.12	119.19	122.14
1	A2	116	OMU	O2-C2-N1	-2.12	120.04	122.80
39	B5	4276	UR3	C6-N1-C2	-2.12	120.07	121.80
1	A2	437	OMG	O6-C6-C5	-2.12	120.95	126.53
39	B5	1266	1MA	C6-C5-N7	2.12	135.90	132.16
11	AT	26	M2G	O6-C6-C5	-2.11	120.95	126.53
1	A2	1249	B8N	C5-C4-N3	2.11	119.99	116.15
1	A2	218	PSU	C5-C6-N1	-2.11	119.21	122.14
39	B5	1580	OMG	O6-C6-C5	-2.11	120.95	126.53
1	A2	1448	OMG	O6-C6-C5	-2.11	120.96	126.53
11	AT	54	5MU	C5M-C5-C4	2.11	121.04	118.78
39	B5	1799	PSU	C5-C6-N1	-2.11	119.21	122.14
11	AT	14	1MA	C6-C5-N7	2.10	135.88	132.16
1	A2	1057	PSU	C5-C6-N1	-2.10	119.22	122.14
39	B5	1537	PSU	C5-C6-N1	-2.10	119.22	122.14
39	B5	4322	PSU	C5-C6-N1	-2.10	119.22	122.14
39	B5	2244	A2M	C6-C5-N7	2.10	136.13	132.09
1	A2	867	PSU	C5-C6-N1	-2.09	119.23	122.14
39	B5	1801	PSU	C5-C6-N1	-2.09	119.23	122.14
39	B5	4369	OMG	O6-C6-C5	-2.09	121.00	126.53
1	A2	1679	A2M	C6-C5-N7	2.09	136.12	132.09
1	A2	645	OMG	O6-C6-C5	-2.09	121.01	126.53
39	B5	4188	PSU	C5-C6-N1	-2.09	119.24	122.14
39	B5	3942	OMG	O6-C6-C5	-2.09	121.01	126.53
39	B5	1260	OMG	O6-C6-C5	-2.09	121.02	126.53
1	A2	469	A2M	C6-C5-N7	2.09	136.11	132.09
1	A2	1245	PSU	C5-C6-N1	-2.08	119.25	122.14
1	A2	166	A2M	C6-C5-N7	2.08	136.11	132.09
11	AT	39	PSU	C5-C6-N1	-2.08	119.25	122.14
39	B5	400	A2M	C6-C5-N7	2.08	136.10	132.09
39	B5	1810	A2M	C6-C5-N7	2.08	136.10	132.09
11	AT	34	OMG	O6-C6-C5	-2.08	121.05	126.53
39	B5	3427	PSU	C5-C6-N1	-2.08	119.26	122.14
39	B5	3466	PSU	C5-C6-N1	-2.08	119.26	122.14
1	A2	1644	PSU	C5-C6-N1	-2.08	119.26	122.14
39	B5	4138	OMG	O6-C6-C5	-2.07	121.06	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	1477	OMG	O6-C6-C5	-2.07	121.06	126.53
1	A2	105	PSU	C5-C6-N1	-2.07	119.27	122.14
1	A2	93	PSU	C5-C6-N1	-2.07	119.27	122.14
1	A2	864	PSU	C5-C6-N1	-2.07	119.27	122.14
1	A2	34	PSU	C5-C6-N1	-2.07	119.27	122.14
1	A2	1082	PSU	O4'-C1'-C2'	2.07	108.01	105.15
1	A2	27	A2M	C6-C5-N7	2.07	136.07	132.09
1	A2	36	PSU	C5-C6-N1	-2.06	119.28	122.14
39	B5	2267	OMG	O6-C6-C5	-2.06	121.08	126.53
11	AT	10	2MG	N1-C2-N2	2.06	118.67	116.56
39	B5	3619	OMC	O2-C2-N3	-2.06	119.08	122.33
39	B5	4382	PSU	O4'-C1'-C2'	2.06	108.00	105.15
1	A2	1384	A2M	C6-C5-N7	2.06	136.06	132.09
1	A2	1693	PSU	C5-C6-N1	-2.06	119.28	122.14
1	A2	577	A2M	C6-C5-N7	2.06	136.06	132.09
39	B5	2667	OMC	O2-C2-N3	-2.06	119.09	122.33
1	A2	1852	MA6	N9-C8-N7	-2.06	111.02	113.94
39	B5	3599	A2M	C6-C5-N7	2.06	136.06	132.09
1	A2	967	PSU	C5-C6-N1	-2.06	119.29	122.14
39	B5	4244	OMU	O2-C2-N1	-2.05	120.12	122.80
1	A2	1626	PSU	C5-C6-N1	-2.05	119.29	122.14
39	B5	4169	PSU	C5-C6-N1	-2.05	119.29	122.14
39	B5	3450	A2M	C6-C5-N7	2.05	136.04	132.09
1	A2	1329	OMG	O6-C6-C5	-2.05	121.12	126.53
1	A2	1046	PSU	C5-C6-N1	-2.05	119.30	122.14
39	B5	4203	PSU	O4'-C1'-C2'	2.05	107.99	105.15
1	A2	650	PSU	C5-C6-N1	-2.05	119.30	122.14
39	B5	4364	OMG	O6-C6-C5	-2.05	121.13	126.53
39	B5	4246	PSU	C5-C6-N1	-2.05	119.30	122.14
39	B5	2265	OMC	O2-C2-N3	-2.05	119.11	122.33
1	A2	684	OMG	O6-C6-C5	-2.05	121.13	126.53
1	A2	687	PSU	C5-C6-N1	-2.05	119.30	122.14
1	A2	510	OMG	O6-C6-C5	-2.04	121.14	126.53
1	A2	109	PSU	C5-C6-N1	-2.04	119.31	122.14
11	AT	27	PSU	C5-C6-N1	-2.04	119.31	122.14
1	A2	802	PSU	C5-C6-N1	-2.04	119.31	122.14
1	A2	1392	OMC	C1'-N1-C2	2.04	122.94	118.44
39	B5	1731	PSU	C5-C6-N1	-2.03	119.32	122.14
39	B5	1266	1MA	N1-C2-N3	-2.03	123.58	126.00
1	A2	577	A2M	N9-C8-N7	-2.03	111.05	113.94
39	B5	4267	PSU	O4'-C1'-C2'	2.03	107.96	105.15
39	B5	1479	A2M	C6-C5-N7	2.03	136.00	132.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B5	4107	PSU	C5-C6-N1	-2.03	119.33	122.14
39	B5	3557	A2M	C6-C5-N7	2.02	135.99	132.09
39	B5	3447	PSU	O4'-C1'-C2'	2.02	107.95	105.15
1	A2	159	A2M	N9-C8-N7	-2.02	111.07	113.94
39	B5	400	A2M	N9-C8-N7	-2.02	111.07	113.94
39	B5	4336	A2M	C6-C5-N7	2.02	135.98	132.09
39	B5	3974	OMG	O6-C6-C5	-2.02	121.21	126.53
39	B5	3554	PSU	O4'-C1'-C2'	2.02	107.94	105.15
39	B5	2475	PSU	C5-C6-N1	-2.02	119.34	122.14
39	B5	4740	PSU	C5-C6-N1	-2.02	119.34	122.14
39	B5	2207	OMG	O6-C6-C5	-2.02	121.21	126.53
39	B5	1489	A2M	N9-C8-N7	-2.02	111.08	113.94
39	B5	4188	PSU	O4'-C1'-C2'	2.02	107.94	105.15
1	A2	1047	PSU	C5-C6-N1	-2.02	119.34	122.14
39	B5	4317	A2M	C6-C5-N7	2.01	135.97	132.09
1	A2	1032	A2M	N9-C8-N7	-2.01	111.08	113.94
39	B5	2719	OMG	O6-C6-C5	-2.01	121.22	126.53
39	B5	3562	A2M	N9-C8-N7	-2.01	111.08	113.94
39	B5	4058	PSU	C5-C6-N1	-2.01	119.35	122.14
39	B5	4203	PSU	C5-C6-N1	-2.01	119.35	122.14
1	A2	1679	A2M	N9-C8-N7	-2.01	111.08	113.94
39	B5	3616	PSU	C5-C6-N1	-2.01	119.35	122.14
39	B5	4383	OMG	O6-C6-C5	-2.01	121.23	126.53
39	B5	3492	A2M	C6-C5-N7	2.01	135.96	132.09
39	B5	3476	OMG	O6-C6-C5	-2.00	121.24	126.53
39	B5	3652	PSU	C5-C6-N1	-2.00	119.36	122.14
39	B5	3466	PSU	O4'-C1'-C2'	2.00	107.92	105.15
1	A2	469	A2M	N9-C8-N7	-2.00	111.09	113.94
1	A2	99	A2M	C6-C5-N7	2.00	135.95	132.09
1	A2	610	PSU	C5-C6-N1	-2.00	119.36	122.14
39	B5	2206	A2M	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (123) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A2	429	OMU	C2'-C1'-N1-C6
1	A2	645	OMG	O4'-C4'-C5'-O5'
1	A2	1833	6MZ	C5-C6-N6-C9
1	A2	1833	6MZ	N1-C6-N6-C9
39	B5	3433	OMC	C2'-C1'-N1-C6
39	B5	4336	A2M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
39	B5	4382	PSU	O4'-C1'-C5-C6
1	A2	1249	B8N	N34-C33-C34-O35
1	A2	1338	4AC	N3-C4-N4-C7
1	A2	1338	4AC	C5-C4-N4-C7
1	A2	1338	4AC	O7-C7-N4-C4
1	A2	1338	4AC	CM7-C7-N4-C4
11	AT	17	H2U	O4'-C4'-C5'-O5'
11	AT	17	H2U	O4'-C1'-N1-C6
11	AT	17	H2U	C2'-C1'-N1-C2
11	AT	17	H2U	C2'-C1'-N1-C6
42	BA	216	V5N	O-C-CA-CB
39	B5	3433	OMC	C2'-C1'-N1-C2
1	A2	513	A2M	O4'-C4'-C5'-O5'
1	A2	645	OMG	C3'-C4'-C5'-O5'
39	B5	4382	PSU	C3'-C4'-C5'-O5'
33	Au	1	AME	CT2-CT1-N-CA
33	Au	1	AME	OT-CT1-N-CA
1	A2	429	OMU	C2'-C1'-N1-C2
1	A2	669	A2M	O4'-C4'-C5'-O5'
1	A2	802	PSU	C3'-C4'-C5'-O5'
39	B5	2207	OMG	O4'-C4'-C5'-O5'
39	B5	4382	PSU	O4'-C4'-C5'-O5'
1	A2	1249	B8N	N34-C33-C34-O36
39	B5	4193	5MC	C2'-C1'-N1-C6
1	A2	669	A2M	C3'-C4'-C5'-O5'
1	A2	1448	OMG	C3'-C4'-C5'-O5'
39	B5	3599	A2M	C3'-C4'-C5'-O5'
11	AT	17	H2U	C3'-C4'-C5'-O5'
1	A2	577	A2M	C3'-C4'-C5'-O5'
39	B5	3517	A2M	O4'-C4'-C5'-O5'
39	B5	3517	A2M	C3'-C4'-C5'-O5'
39	B5	3583	PSU	C3'-C4'-C5'-O5'
1	A2	628	OMU	C2'-C1'-N1-C6
39	B5	4193	5MC	C2'-C1'-N1-C2
1	A2	99	A2M	O4'-C4'-C5'-O5'
1	A2	577	A2M	O4'-C4'-C5'-O5'
1	A2	802	PSU	O4'-C4'-C5'-O5'
39	B5	398	A2M	O4'-C4'-C5'-O5'
1	A2	513	A2M	C3'-C4'-C5'-O5'
39	B5	2265	OMC	O4'-C4'-C5'-O5'
39	B5	3494	PSU	C3'-C4'-C5'-O5'
39	B5	2630	A2M	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
1	A2	1448	OMG	O4'-C4'-C5'-O5'
39	B5	2207	OMG	C3'-C4'-C5'-O5'
39	B5	2265	OMC	C3'-C4'-C5'-O5'
11	AT	17	H2U	O4'-C1'-N1-C2
1	A2	1843	4AC	C5-C4-N4-C7
1	A2	1249	B8N	C32-C33-C34-O36
39	B5	4193	5MC	O4'-C1'-N1-C2
1	A2	645	OMG	C4'-C5'-O5'-P
69	Bb	5	MLZ	N-CA-CB-CG
1	A2	628	OMU	O4'-C1'-N1-C6
39	B5	3494	PSU	O4'-C4'-C5'-O5'
39	B5	3583	PSU	O4'-C4'-C5'-O5'
39	B5	3599	A2M	O4'-C4'-C5'-O5'
12	AZ	2	SAC	CB-CA-N-C1A
1	A2	1249	B8N	C32-C33-C34-O35
39	B5	4246	PSU	C4'-C5'-O5'-P
39	B5	3550	UY1	C4'-C5'-O5'-P
39	B5	4193	5MC	O4'-C1'-N1-C6
1	A2	628	OMU	C2'-C1'-N1-C2
1	A2	159	A2M	C3'-C2'-O2'-CM'
1	A2	469	A2M	C3'-C2'-O2'-CM'
1	A2	1289	OMU	C3'-C2'-O2'-CM2
1	A2	1443	OMU	C3'-C2'-O2'-CM2
39	B5	2658	A2M	C3'-C2'-O2'-CM'
39	B5	3524	OMG	C3'-C2'-O2'-CM2
11	AT	34	OMG	C3'-C2'-O2'-CM2
39	B5	4267	PSU	O4'-C1'-C5-C4
39	B5	3550	UY1	O4'-C1'-C5-C4
1	A2	591	A2M	C2'-C1'-N9-C4
39	B5	2630	A2M	C2'-C1'-N9-C4
1	A2	429	OMU	O4'-C1'-N1-C2
11	AT	46	7MG	C2'-C1'-N9-C8
1	A2	429	OMU	O4'-C1'-N1-C6
1	A2	1852	MA6	C4'-C5'-O5'-P
11	AT	37	YYG	C13-C14-C15-C16
39	B5	3433	OMC	O4'-C1'-N1-C6
1	A2	591	A2M	C2'-C1'-N9-C8
44	BC	2	AYA	C-CA-N-CT
39	B5	3433	OMC	O4'-C1'-N1-C2
1	A2	116	OMU	C3'-C2'-O2'-CM2
1	A2	463	OMC	C3'-C2'-O2'-CM2
1	A2	518	OMC	C3'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
39	B5	4202	OMC	C3'-C2'-O2'-CM2
12	AZ	2	SAC	C-CA-N-C1A
39	B5	1270	A2M	C4'-C5'-O5'-P
1	A2	159	A2M	O4'-C4'-C5'-O5'
1	A2	628	OMU	O4'-C1'-N1-C2
1	A2	591	A2M	O4'-C1'-N9-C8
1	A2	1491	OMG	C4'-C5'-O5'-P
11	AT	16	H2U	C4'-C5'-O5'-P
39	B5	1266	1MA	C2'-C1'-N9-C8
35	Aw	62	HY3	O-C-CA-C3
39	B5	4202	OMC	C1'-C2'-O2'-CM2
39	B5	3576	PSU	C4'-C5'-O5'-P
39	B5	3550	UY1	O4'-C1'-C5-C6
39	B5	2630	A2M	O4'-C1'-N9-C8
1	A2	513	A2M	C3'-C2'-O2'-CM'
1	A2	602	OMG	C3'-C2'-O2'-CM2
1	A2	645	OMG	C3'-C2'-O2'-CM2
39	B5	2680	OMU	C3'-C2'-O2'-CM2
39	B5	4245	OMG	C3'-C2'-O2'-CM2
39	B5	3619	OMC	C4'-C5'-O5'-P
1	A2	1704	OMC	O4'-C4'-C5'-O5'
39	B5	1489	A2M	O4'-C4'-C5'-O5'
39	B5	1477	OMG	C3'-C2'-O2'-CM2
39	B5	2258	OMU	C3'-C2'-O2'-CM2
39	B5	398	A2M	C3'-C4'-C5'-O5'
44	BC	2	AYA	CB-CA-N-CT
1	A2	669	A2M	C2'-C1'-N9-C8
1	A2	1843	4AC	N3-C4-N4-C7
1	A2	1082	PSU	C4'-C5'-O5'-P
1	A2	1448	OMG	C4'-C5'-O5'-P
1	A2	1392	OMC	C2'-C1'-N1-C2
39	B5	2194	OMC	C2'-C1'-N1-C2
39	B5	2194	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

83 monomers are involved in 112 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B5	4282	OMC	1	0
1	A2	577	A2M	1	0
39	B5	4269	A2M	2	0
1	A2	1443	OMU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	B5	3942	OMG	1	0
1	A2	1289	OMU	2	0
39	B5	3540	OMC	1	0
39	B5	2704	OMC	1	0
39	B5	2719	OMG	1	0
1	A2	469	A2M	1	0
1	A2	1245	PSU	1	0
1	A2	1329	OMG	1	0
39	B5	1266	1MA	1	0
33	Au	1	AME	2	0
1	A2	1032	A2M	2	0
39	B5	4366	OMU	2	0
39	B5	4298	PSU	1	0
11	AT	32	OMC	1	0
39	B5	4336	A2M	1	0
39	B5	3517	A2M	1	0
39	B5	3974	OMG	1	0
39	B5	3456	A2M	2	0
11	AT	37	YYG	1	0
39	B5	1638	PSU	1	0
39	B5	398	A2M	1	0
39	B5	3557	A2M	1	0
39	B5	3966	6MZ	1	0
1	A2	1843	4AC	1	0
1	A2	510	OMG	1	0
39	B5	3492	A2M	1	0
1	A2	1233	PSU	2	0
39	B5	4039	PSU	1	0
1	A2	1446	PSU	2	0
1	A2	1679	A2M	1	0
1	A2	1693	PSU	1	0
1	A2	437	OMG	1	0
39	B5	3450	A2M	3	0
1	A2	1833	6MZ	1	0
39	B5	1260	OMG	1	0
39	B5	2194	OMC	1	0
39	B5	2258	OMU	1	0
11	AT	34	OMG	1	0
1	A2	602	OMG	1	0
39	B5	4382	PSU	2	0
39	B5	4364	OMG	1	0
1	A2	463	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	AT	58	1MA	1	0
39	B5	4203	PSU	2	0
1	A2	116	OMU	2	0
11	AT	46	7MG	1	0
39	B5	3550	UY1	2	0
1	A2	518	OMC	1	0
1	A2	1338	4AC	3	0
39	B5	3619	OMC	2	0
39	B5	1284	OMC	3	0
1	A2	166	A2M	2	0
39	B5	1820	OMC	1	0
39	B5	1632	PSU	1	0
39	B5	3371	PSU	1	0
39	B5	2207	OMG	2	0
39	B5	3502	PSU	1	0
1	A2	1392	OMC	1	0
1	A2	485	A2M	2	0
39	B5	1270	A2M	2	0
1	A2	172	OMU	1	0
41	B8	75	OMG	1	0
39	B5	3466	PSU	1	0
1	A2	1448	OMG	2	0
39	B5	2267	OMG	1	0
39	B5	4202	OMC	2	0
1	A2	99	A2M	2	0
1	A2	1640	7MG	1	0
1	A2	1046	PSU	1	0
1	A2	1805	OMU	1	0
1	A2	1704	OMC	1	0
1	A2	159	A2M	1	0
39	B5	2206	A2M	2	0
1	A2	1491	OMG	1	0
39	B5	1810	A2M	2	0
39	B5	3599	A2M	3	0
39	B5	1489	A2M	2	0
1	A2	513	A2M	1	0
39	B5	4193	5MC	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.



## 5.6 Ligand geometry

Of 791 ligands modelled in this entry, 428 are monoatomic and 330 are unknown - leaving 33 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
87	SPD	B5	4917	-	9,9,9	0.14	0	8,8,8	0.17	0
87	SPD	A2	1904	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	A2	1905	-	9,9,9	0.16	0	8,8,8	0.18	0
87	SPD	B5	4921	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4922	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4906	-	9,9,9	0.14	0	8,8,8	0.24	0
87	SPD	B5	4904	-	9,9,9	0.16	0	8,8,8	0.20	0
87	SPD	B5	4910	-	9,9,9	0.14	0	8,8,8	0.16	0
87	SPD	B5	4902	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	A2	1906	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4909	-	9,9,9	0.17	0	8,8,8	0.19	0
87	SPD	B5	4913	-	9,9,9	0.15	0	8,8,8	0.20	0
87	SPD	A2	1903	-	9,9,9	0.16	0	8,8,8	0.16	0
87	SPD	B5	4918	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4920	-	9,9,9	0.15	0	8,8,8	0.27	0
87	SPD	A2	1908	-	9,9,9	0.15	0	8,8,8	0.18	0
87	SPD	B5	4914	-	9,9,9	0.15	0	8,8,8	0.17	0
87	SPD	B5	4905	-	9,9,9	0.14	0	8,8,8	0.17	0
87	SPD	BN	301	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	A2	1902	-	9,9,9	0.15	0	8,8,8	0.16	0
88	SPM	B5	4912	-	13,13,13	0.16	0	12,12,12	0.22	0
87	SPD	B5	4907	-	9,9,9	0.16	0	8,8,8	0.22	0
87	SPD	B5	4923	-	9,9,9	0.15	0	8,8,8	0.20	0
88	SPM	A2	1909	-	13,13,13	0.15	0	12,12,12	0.18	0
87	SPD	B5	4903	-	9,9,9	0.15	0	8,8,8	0.29	0
87	SPD	B5	4924	-	9,9,9	0.15	0	8,8,8	0.15	0
87	SPD	B5	4911	-	9,9,9	0.15	0	8,8,8	0.16	0
87	SPD	B5	4919	-	9,9,9	0.14	0	8,8,8	0.18	0
87	SPD	A2	1901	-	9,9,9	0.16	0	8,8,8	0.18	0
88	SPM	B5	4915	-	13,13,13	0.16	0	12,12,12	0.29	0
87	SPD	A2	1907	-	9,9,9	0.15	0	8,8,8	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
87	SPD	B5	4916	-	9,9,9	0.15	0	8,8,8	0.19	0
87	SPD	B5	4908	-	9,9,9	0.14	0	8,8,8	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
87	SPD	B5	4917	-	-	0/7/7/7	-
87	SPD	A2	1904	-	-	0/7/7/7	-
87	SPD	A2	1905	-	-	0/7/7/7	-
87	SPD	B5	4921	-	-	1/7/7/7	-
87	SPD	B5	4922	-	-	1/7/7/7	-
87	SPD	B5	4906	-	-	0/7/7/7	-
87	SPD	B5	4904	-	-	1/7/7/7	-
87	SPD	B5	4910	-	-	1/7/7/7	-
87	SPD	B5	4902	-	-	1/7/7/7	-
87	SPD	A2	1906	-	-	1/7/7/7	-
87	SPD	B5	4909	-	-	1/7/7/7	-
87	SPD	B5	4913	-	-	0/7/7/7	-
87	SPD	A2	1903	-	-	0/7/7/7	-
87	SPD	B5	4918	-	-	0/7/7/7	-
87	SPD	B5	4920	-	-	0/7/7/7	-
87	SPD	A2	1908	-	-	0/7/7/7	-
87	SPD	B5	4914	-	-	0/7/7/7	-
87	SPD	B5	4905	-	-	0/7/7/7	-
87	SPD	BN	301	-	-	2/7/7/7	-
87	SPD	A2	1902	-	-	0/7/7/7	-
88	SPM	B5	4912	-	-	1/11/11/11	-
87	SPD	B5	4907	-	-	0/7/7/7	-
87	SPD	B5	4923	-	-	0/7/7/7	-
88	SPM	A2	1909	-	-	1/11/11/11	-
87	SPD	B5	4903	-	-	2/7/7/7	-
87	SPD	B5	4924	-	-	1/7/7/7	-
87	SPD	B5	4911	-	-	0/7/7/7	-
87	SPD	B5	4919	-	-	0/7/7/7	-
87	SPD	A2	1901	-	-	1/7/7/7	-
88	SPM	B5	4915	-	-	0/11/11/11	-
87	SPD	A2	1907	-	-	1/7/7/7	-
87	SPD	B5	4916	-	-	0/7/7/7	-
87	SPD	B5	4908	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	A2	1909	SPM	C12-C11-N10-C9
87	B5	4903	SPD	C2-C3-C4-C5
87	B5	4903	SPD	C3-C4-C5-N6
87	B5	4902	SPD	C4-C5-N6-C7
87	B5	4924	SPD	C2-C3-C4-C5
87	B5	4922	SPD	C2-C3-C4-C5
87	A2	1906	SPD	C8-C7-N6-C5
87	B5	4921	SPD	C8-C7-N6-C5
87	B5	4909	SPD	C4-C5-N6-C7
87	B5	4910	SPD	C2-C3-C4-C5
87	A2	1907	SPD	C2-C3-C4-C5
87	A2	1901	SPD	C2-C3-C4-C5
87	BN	301	SPD	C2-C3-C4-C5
87	B5	4904	SPD	C2-C3-C4-C5
87	BN	301	SPD	C4-C5-N6-C7
88	B5	4912	SPM	C8-C9-N10-C11

There are no ring outliers.

18 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
87	B5	4917	SPD	3	0
87	A2	1905	SPD	2	0
87	B5	4921	SPD	1	0
87	B5	4922	SPD	1	0
87	A2	1906	SPD	2	0
87	B5	4909	SPD	1	0
87	B5	4913	SPD	1	0
87	A2	1903	SPD	2	0
87	B5	4920	SPD	2	0
88	B5	4912	SPM	2	0
87	B5	4907	SPD	1	0
87	B5	4923	SPD	1	0
88	A2	1909	SPM	2	0
87	B5	4903	SPD	1	0
87	B5	4924	SPD	4	0
87	B5	4919	SPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	B5	4915	SPM	2	0
87	B5	4916	SPD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

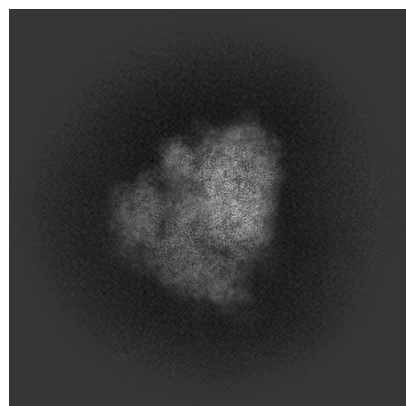
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12756. These allow visual inspection of the internal detail of the map and identification of artifacts.

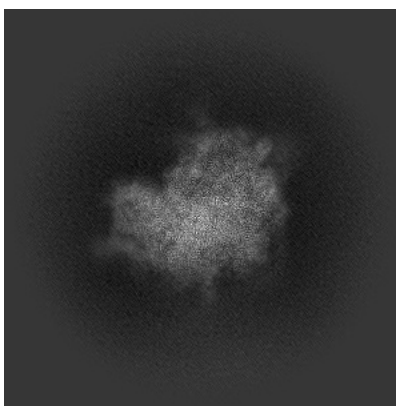
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

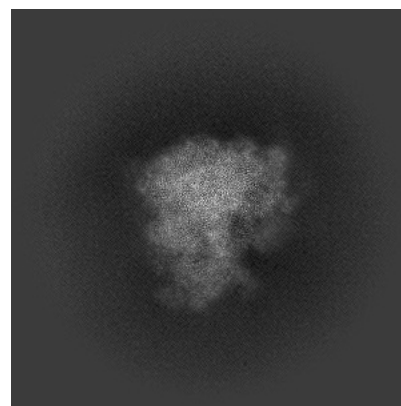
#### 6.1.1 Primary map



X

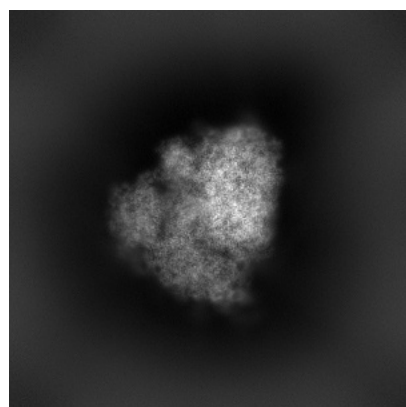


Y

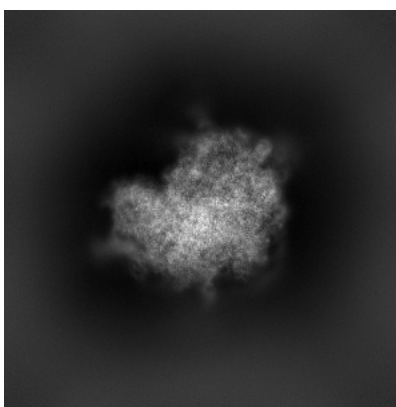


Z

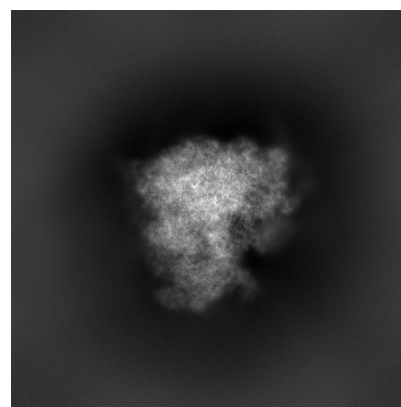
#### 6.1.2 Raw map



X



Y

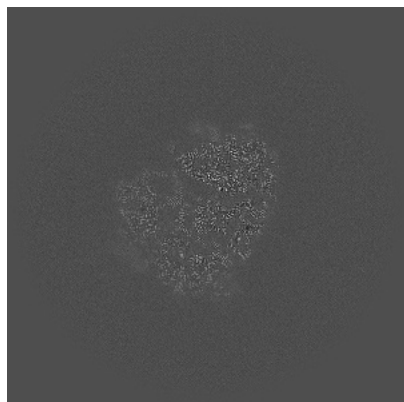


Z

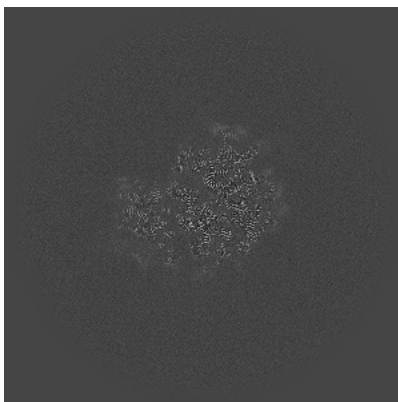
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

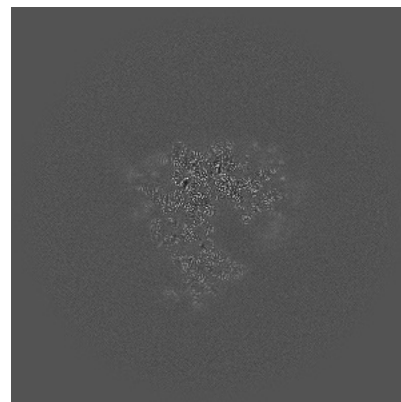
### 6.2.1 Primary map



X Index: 280

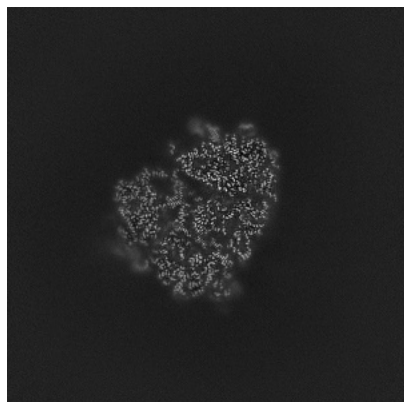


Y Index: 280

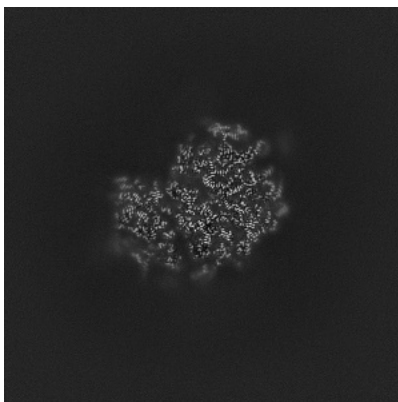


Z Index: 280

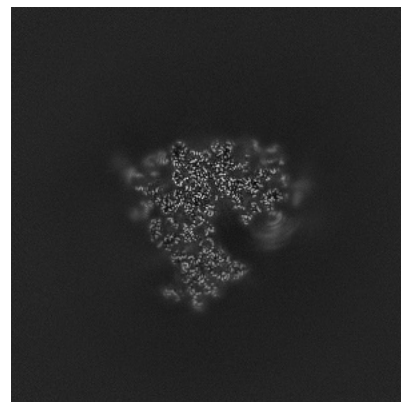
### 6.2.2 Raw map



X Index: 280



Y Index: 280

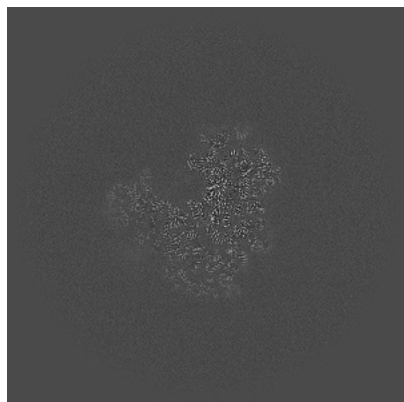


Z Index: 280

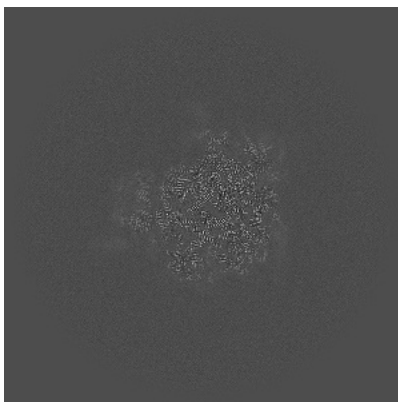
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

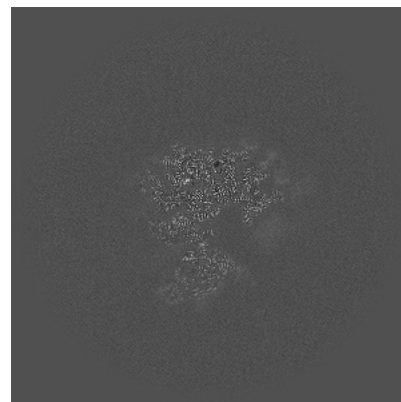
### 6.3.1 Primary map



X Index: 265

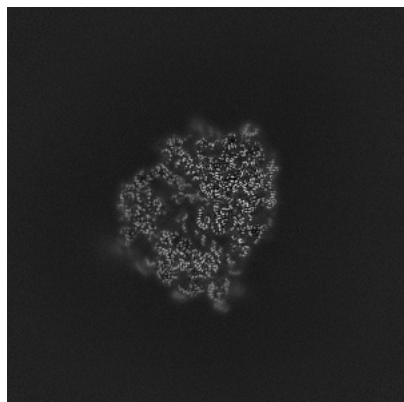


Y Index: 313

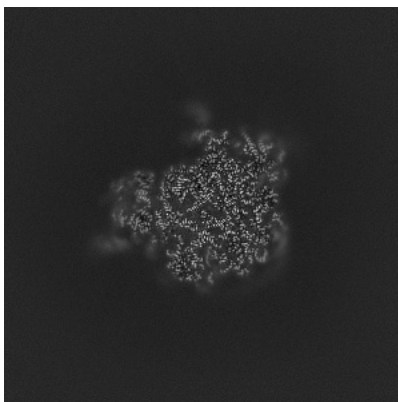


Z Index: 272

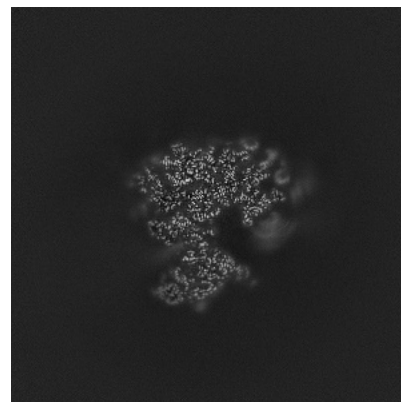
### 6.3.2 Raw map



X Index: 287



Y Index: 313



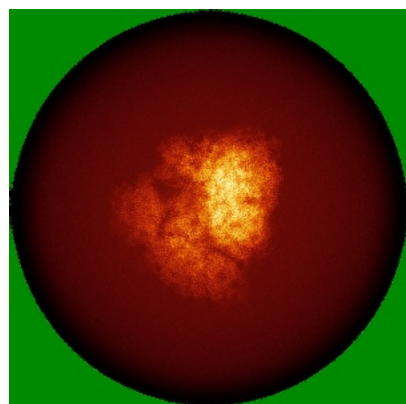
Z Index: 272

The images above show the largest variance slices of the map in three orthogonal directions.

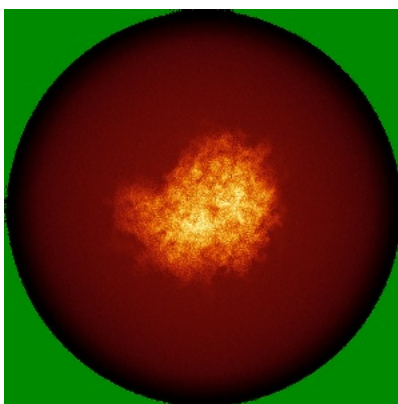


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

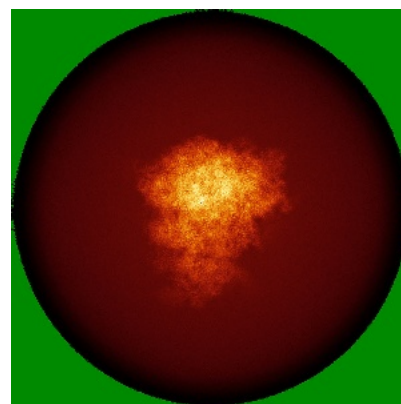
### 6.4.1 Primary map



X

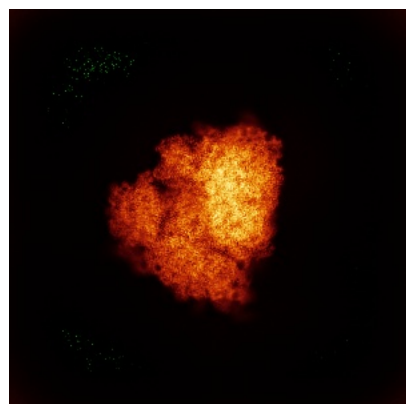


Y

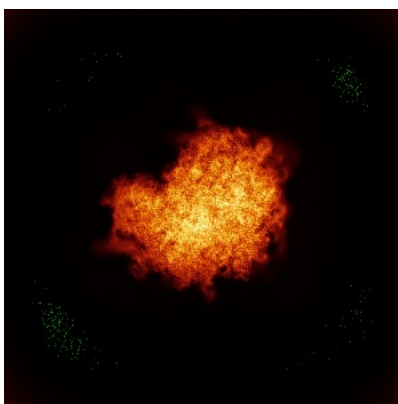


Z

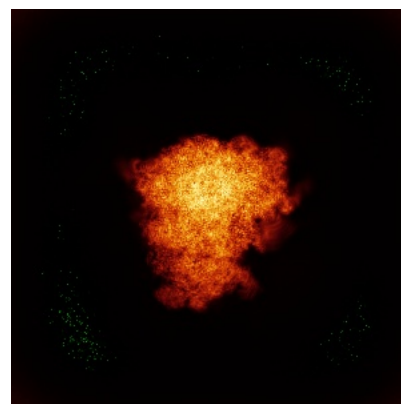
### 6.4.2 Raw map



X



Y



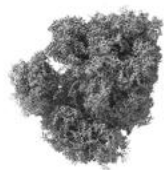
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



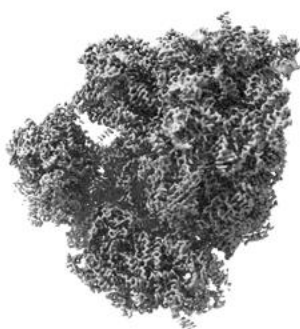
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

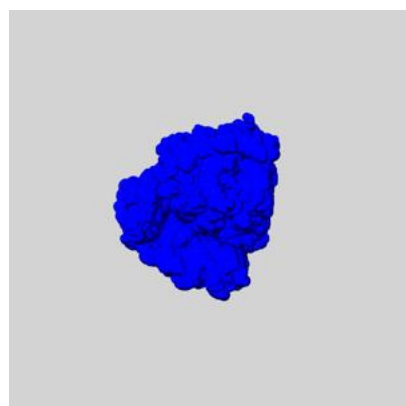
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

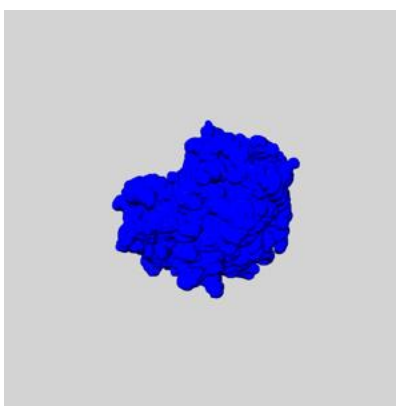
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

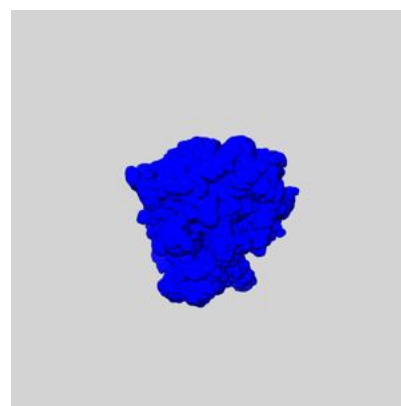
### 6.6.1 emd\_12756\_msk\_1.map [i](#)



X

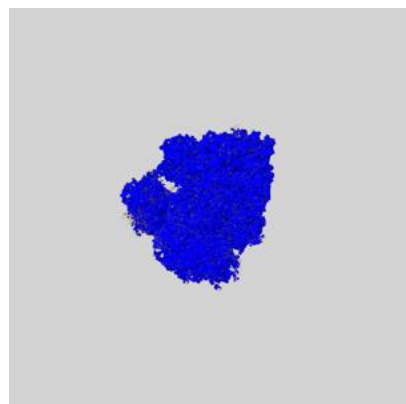


Y

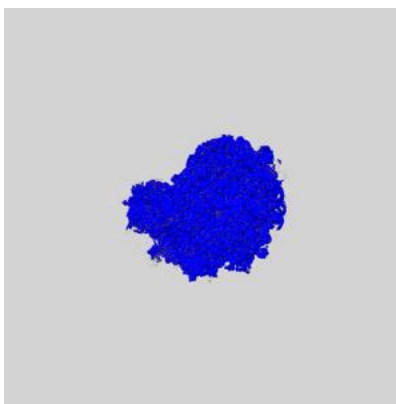


Z

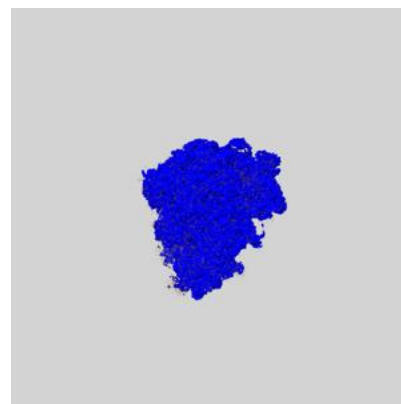
### 6.6.2 emd\_12756\_msk\_2.map [i](#)



X



Y

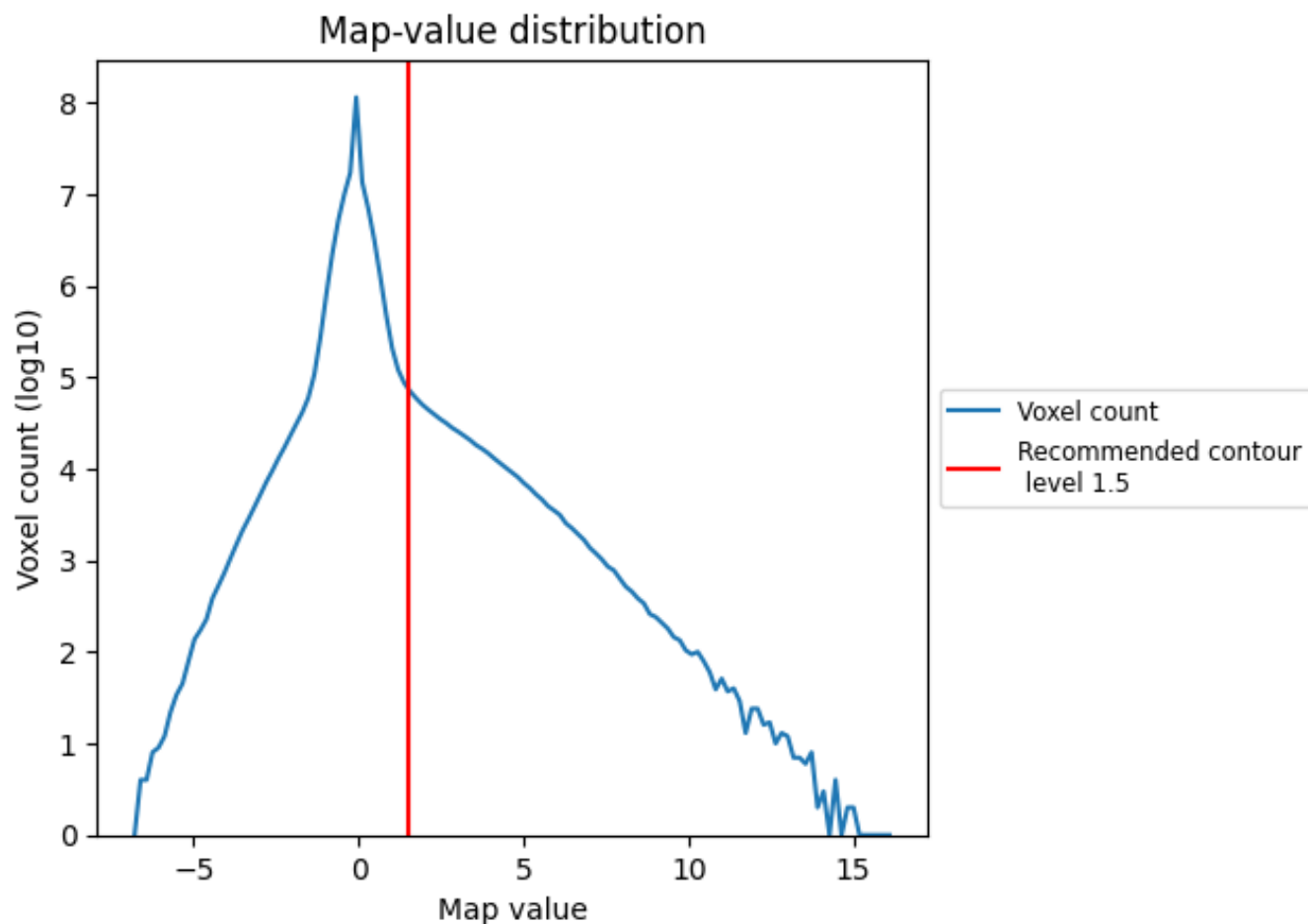


Z

## 7 Map analysis [i](#)

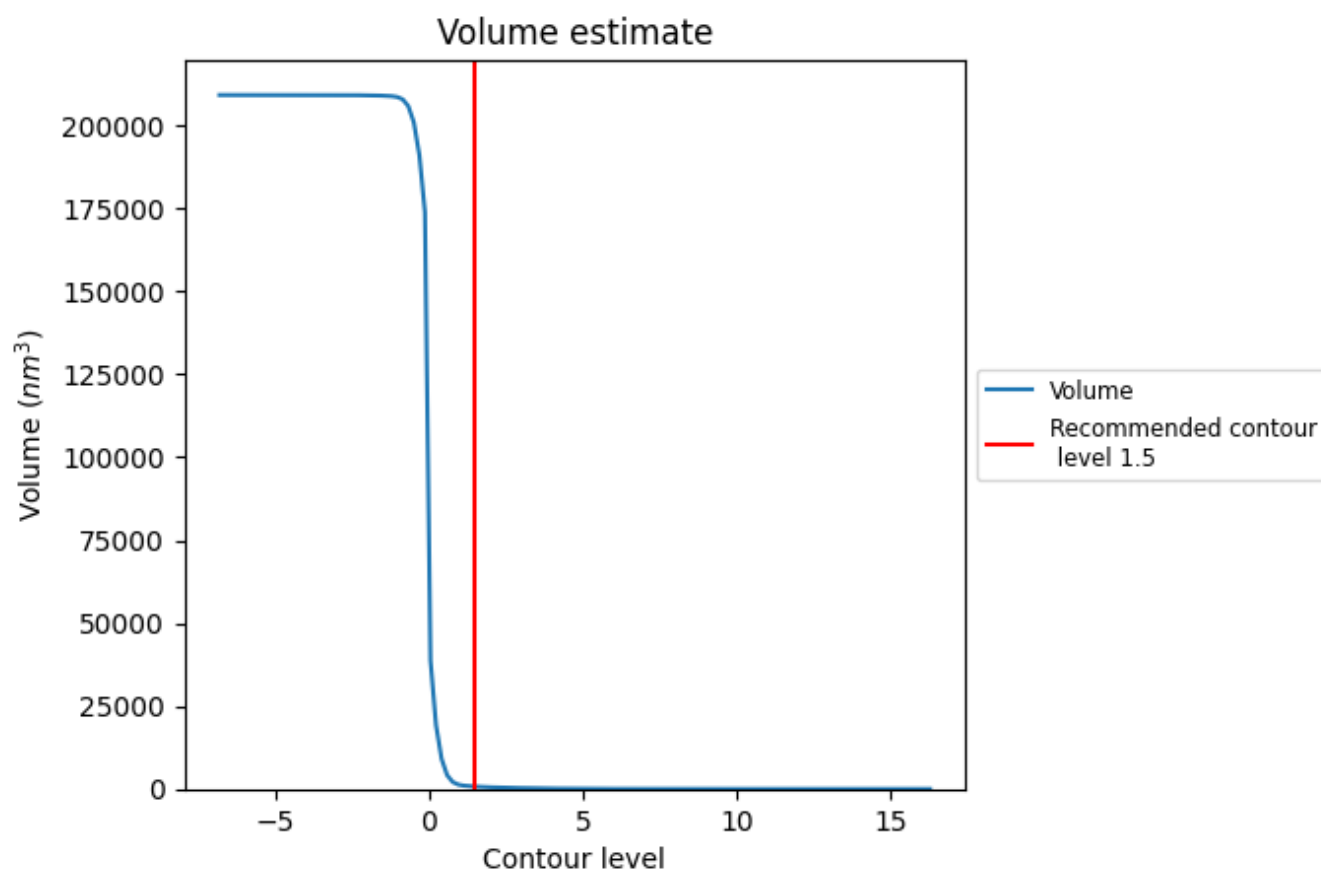
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

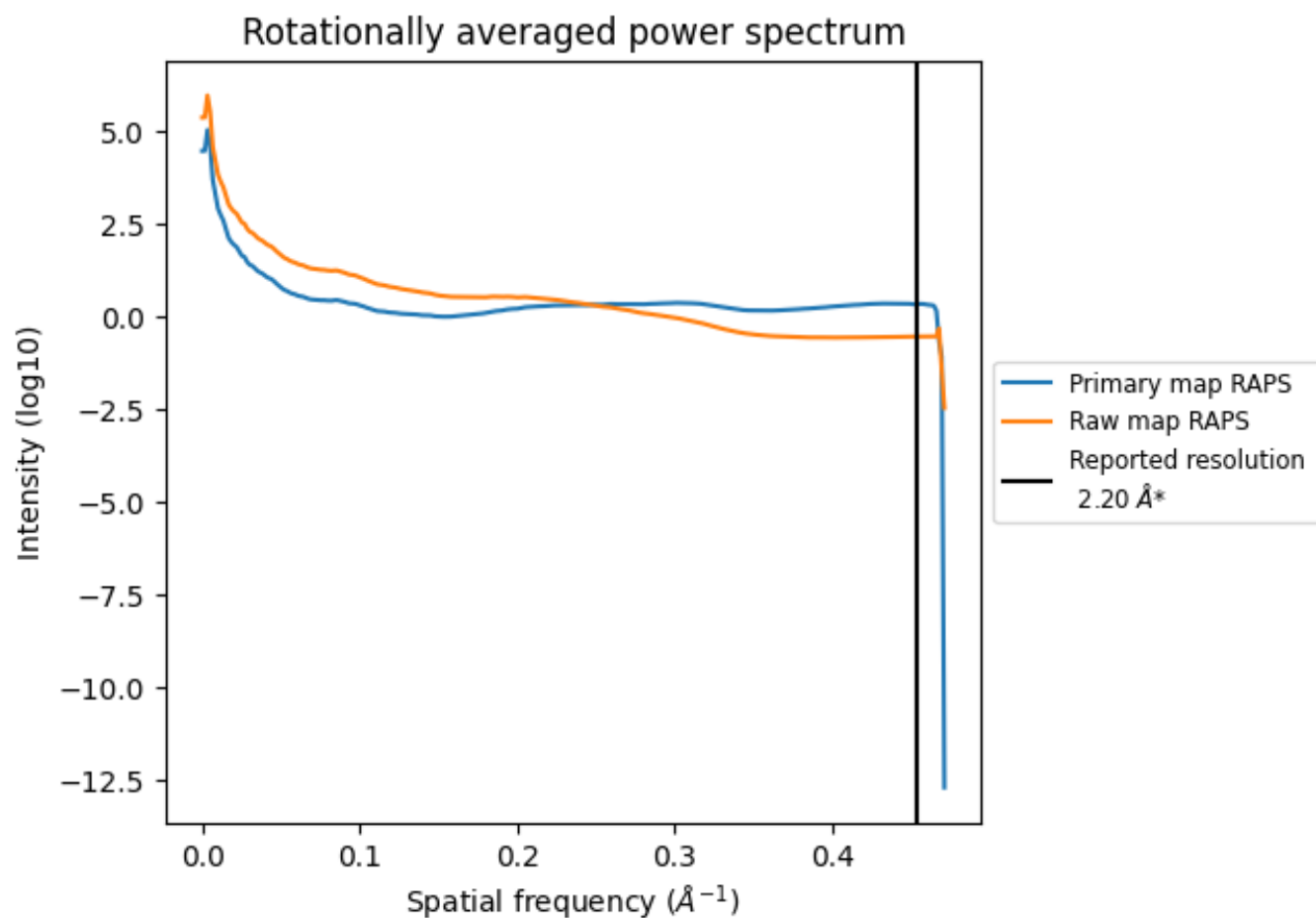
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723  $\text{nm}^3$ ; this corresponds to an approximate mass of 653 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

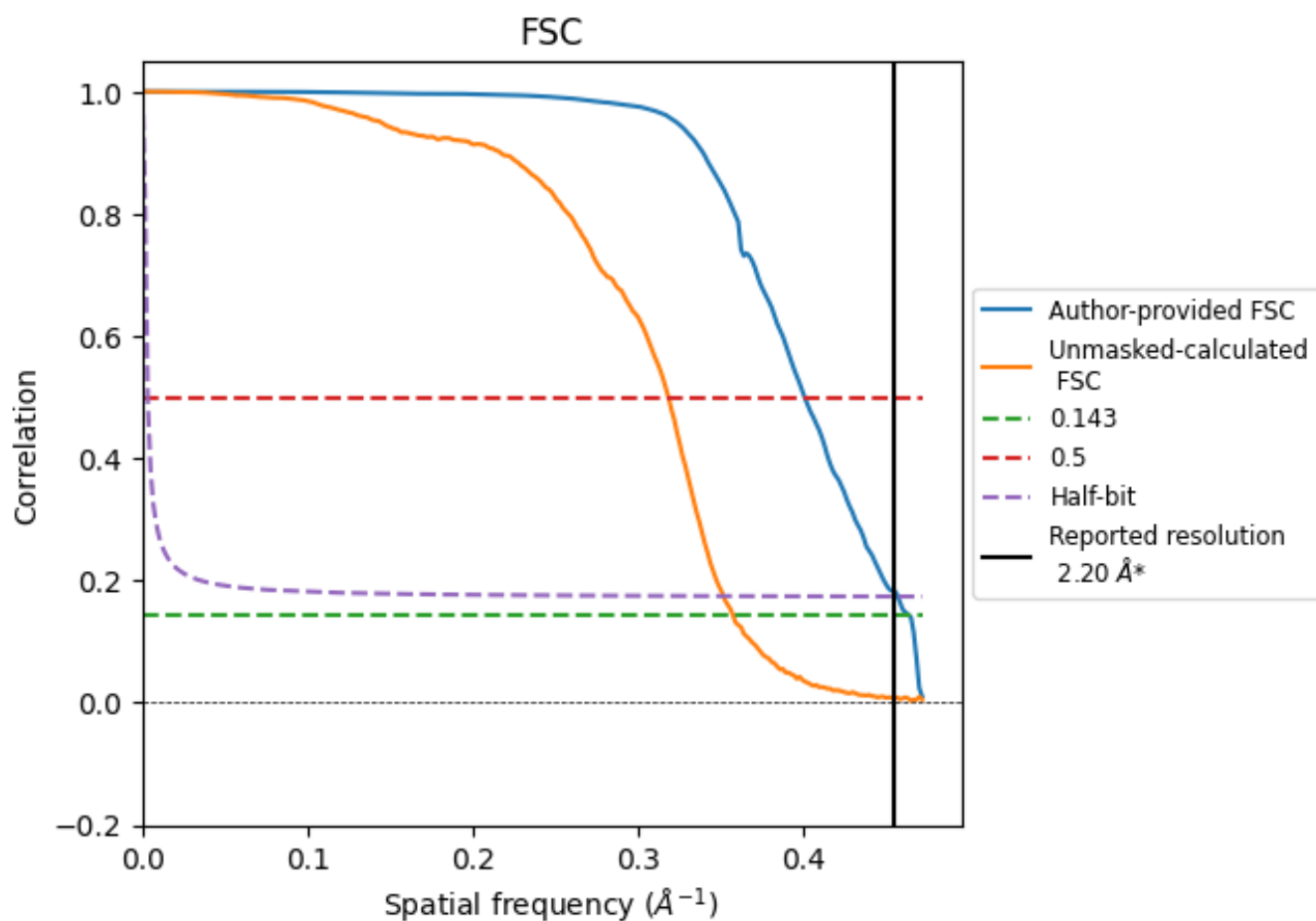


\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.455 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

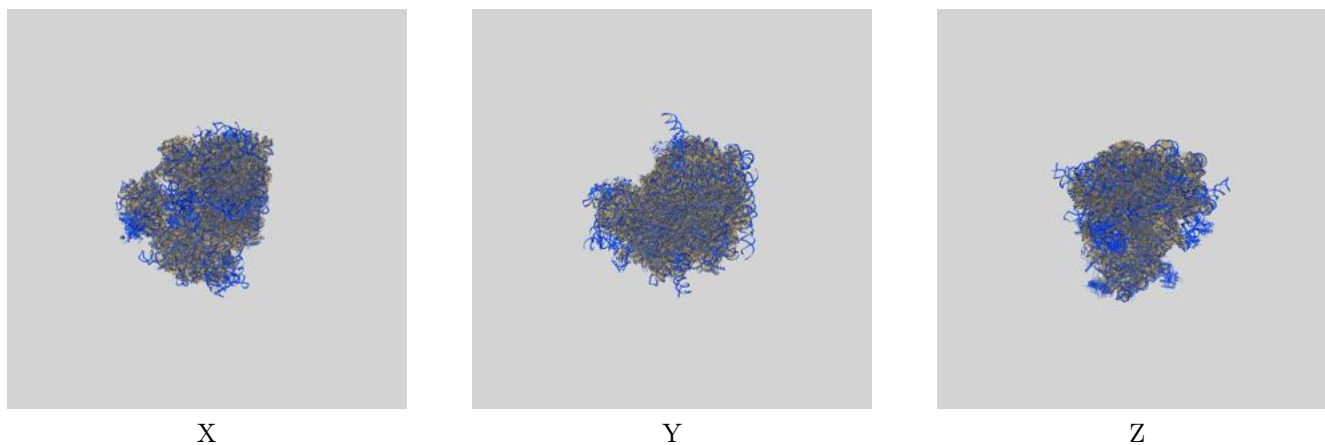
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	2.16	2.50	2.19
Unmasked-calculated*	2.80	3.14	2.84

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.80 differs from the reported value 2.2 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12756 and PDB model 7O7Y. Per-residue inclusion information can be found in [section 3](#) on [page 29](#).

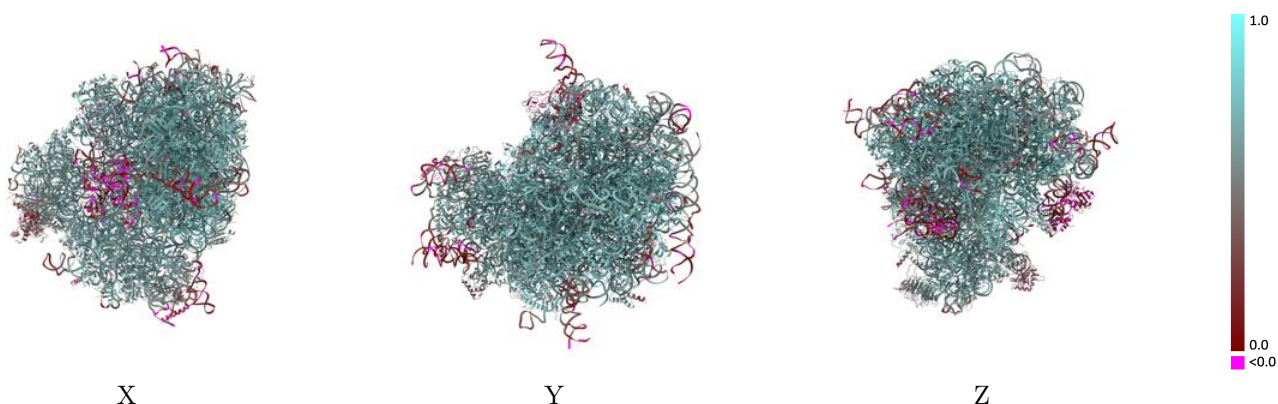
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

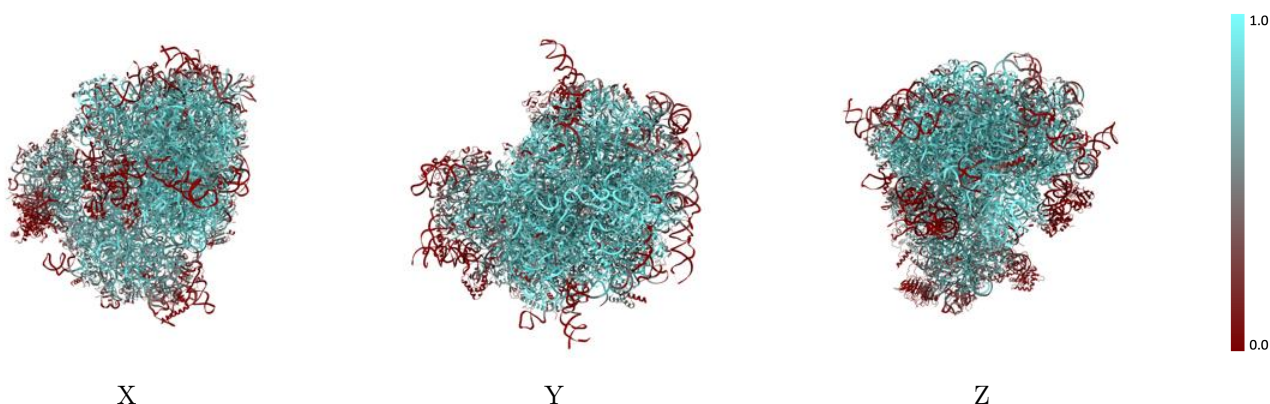


## 9.2 Q-score mapped to coordinate model [i](#)



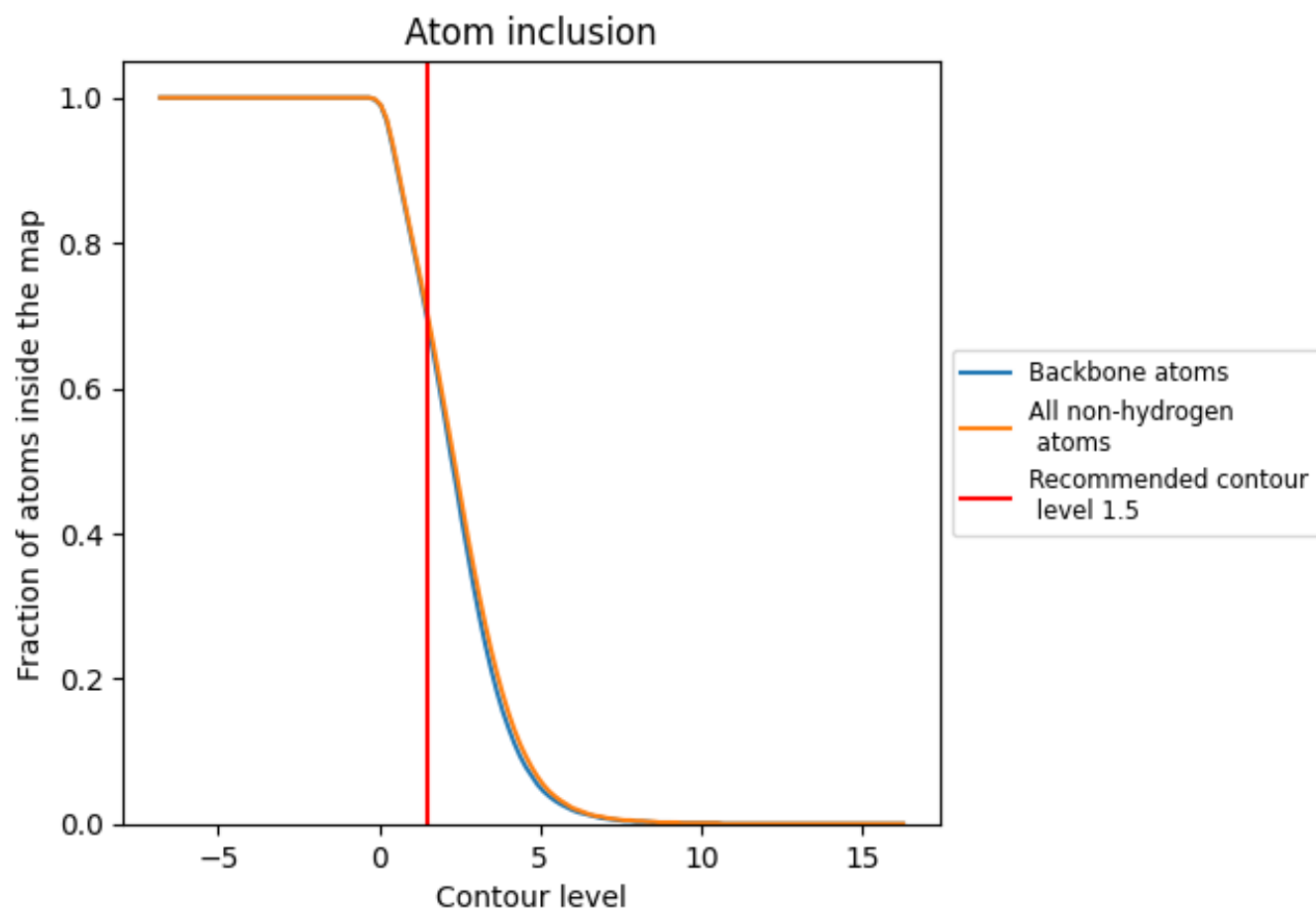
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.5).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7030	 0.6240
A2	 0.7180	 0.6100
AA	 0.5380	 0.6250
AB	 0.5180	 0.6150
AC	 0.0020	 0.2930
AD	 0.4820	 0.5650
AE	 0.7670	 0.6720
AF	 0.1070	 0.4800
AG	 0.7060	 0.6680
AH	 0.9220	 0.7110
AI	 0.1100	 0.2750
AT	 0.6580	 0.6380
AZ	 0.5710	 0.6340
Aa	 0.6610	 0.6540
Ab	 0.7370	 0.6750
Ac	 0.3790	 0.5650
Ad	 0.6380	 0.6530
Ae	 0.6090	 0.6410
Af	 0.2980	 0.5150
Ag	 0.2440	 0.5320
Ah	 0.6860	 0.6420
Ai	 0.6400	 0.6370
Aj	 0.1990	 0.5320
Ak	 0.7380	 0.6480
Al	 0.0000	 0.2330
Am	 0.7760	 0.6910
An	 0.7760	 0.6830
Ao	 0.3980	 0.5730
Ap	 0.5550	 0.6380
Aq	 0.3580	 0.5830
Ar	 0.5060	 0.6230
As	 0.5030	 0.6140
At	 0.3210	 0.5210
Au	 0.5850	 0.6630
Av	 0.8510	 0.7110























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Chain	Atom inclusion	Q-score
Aw	 0.8110	 0.7010
Ax	 0.4420	 0.6050
Ay	 0.3540	 0.5930
Az	 0.8620	 0.7100
B5	 0.7560	 0.6250
B7	 0.9400	 0.7030
B8	 0.8610	 0.6770
BA	 0.9210	 0.7320
BB	 0.8730	 0.7180
BC	 0.8930	 0.7170
BD	 0.7630	 0.6770
BE	 0.6320	 0.6190
BF	 0.9010	 0.7270
BG	 0.6740	 0.6440
BH	 0.7840	 0.6850
BI	 0.8270	 0.7000
BJ	 0.6800	 0.6500
BK	 0.1420	 0.4730
BL	 0.7800	 0.6800
BM	 0.8160	 0.6820
BN	 0.9690	 0.7480
BO	 0.8900	 0.7200
BP	 0.8500	 0.7120
BQ	 0.9210	 0.7300
BR	 0.7540	 0.6740
BS	 0.9120	 0.7230
BT	 0.8030	 0.6900
BU	 0.4910	 0.6040
BV	 0.8530	 0.7080
BW	 0.4520	 0.4730
BX	 0.8170	 0.7030
BY	 0.8150	 0.6930
BZ	 0.7830	 0.6900
Ba	 0.9220	 0.7340
Bb	 0.5760	 0.6030
Bc	 0.7450	 0.6560
Bd	 0.7900	 0.6930
Be	 0.9040	 0.7230
Bf	 0.9240	 0.7360
Bg	 0.8390	 0.6960
Bh	 0.7920	 0.6890
Bi	 0.7650	 0.6830

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Chain	Atom inclusion	Q-score
Bj	 0.9570	 0.7370
Bk	 0.5600	 0.6180
Bl	 0.8550	 0.7020
Bm	 0.8380	 0.7100
Bo	 0.8450	 0.7190
Bp	 0.8750	 0.7160
Br	 0.8730	 0.7110
Bs	 0.0000	 0.0660
Bt	 0.0000	 0.0850
Bv	 0.0000	 0.1340