



## Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 01:59 PM UTC

PDB ID : 7O7M / pdb\_00007o7m  
EMDB ID : EMD-12748  
Title : (h-alpha2M)4 native II  
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.  
Deposited on : 2021-04-13  
Resolution : 6.60 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:

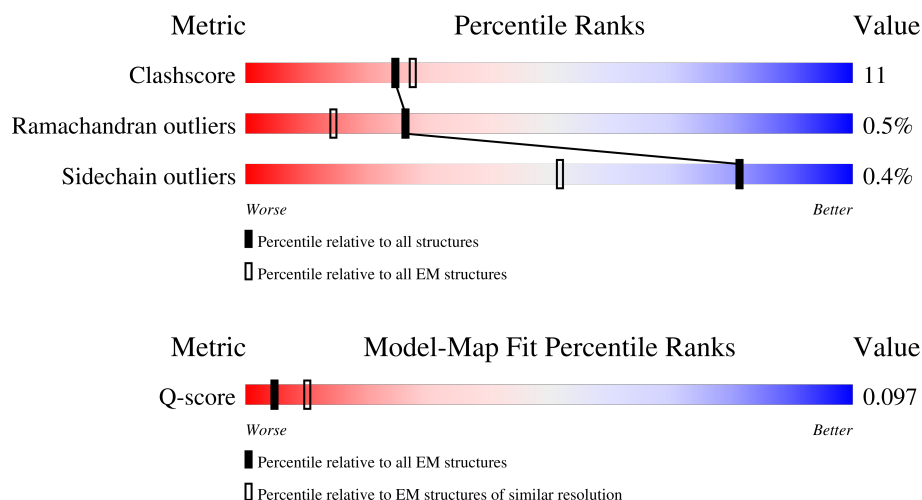
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 6.60 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	-
Q-score	-	25397	531 ( 6.10 - 7.10 )

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	A	1474	<div> <div>73%</div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	B	1474	<div> <div>29%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
1	C	1474	<div> <div>73%</div> <div>76%</div> <div>19%</div> <div>.</div> </div>
1	D	1474	<div> <div>29%</div> <div>69%</div> <div>26%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	4	<div><div></div><div>25%</div><div>50%</div><div>25%</div></div>
2	H	4	<div><div></div><div>25%</div><div>50%</div><div>25%</div></div>
3	F	3	<div><div></div><div>33%</div><div>67%</div></div>
3	I	3	<div><div></div><div>33%</div><div>67%</div></div>
4	G	2	<div><div></div><div>100%</div></div>
4	J	2	<div><div></div><div>100%</div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 44614 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 protein called Alpha-2-macroglobulin.

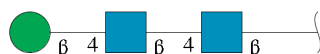
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	B	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	C	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		
1	D	1410	Total	C	N	O	S	0	0
			11004	6999	1840	2117	48		

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	4	Total	C	N	O	0	0
			50	28	2	20		
2	H	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		

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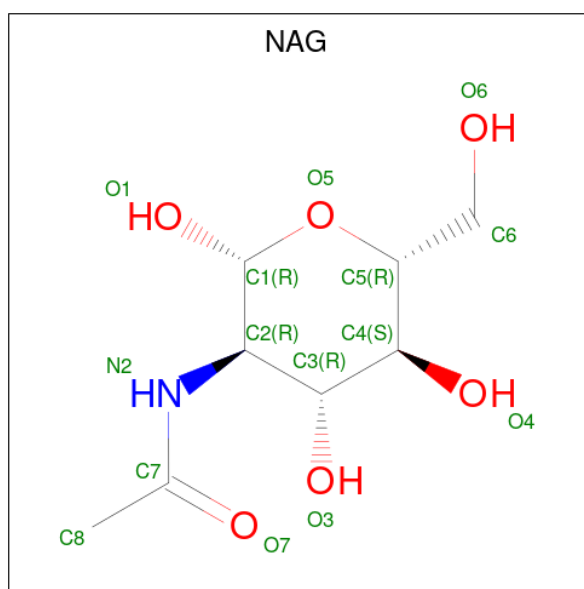
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	C	1	Total 14	C 8	N 1	O 5	0
5	D	1	Total 14	C 8	N 1	O 5	0
5	D	1	Total 14	C 8	N 1	O 5	0
5	D	1	Total 14	C 8	N 1	O 5	0

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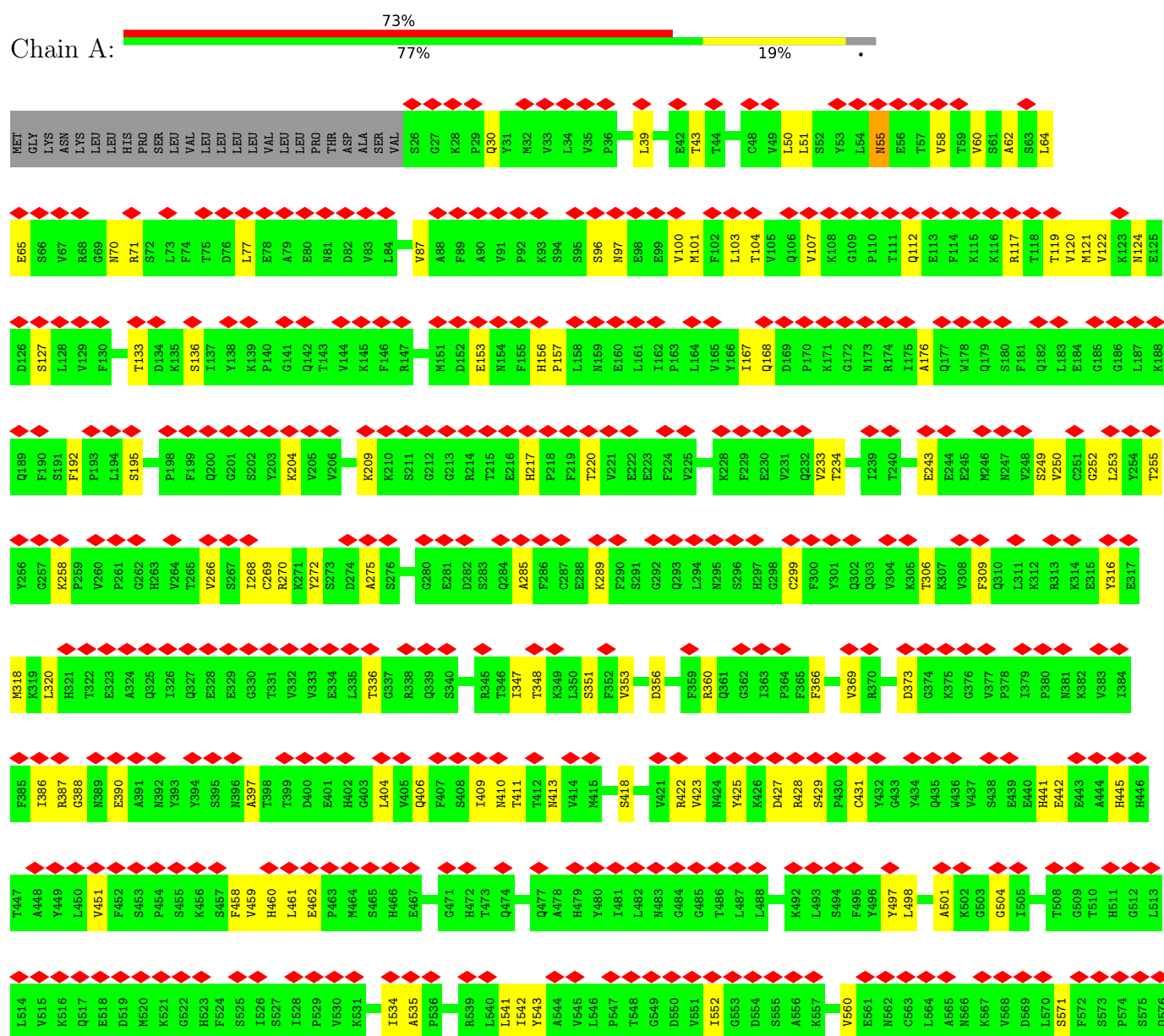
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Mol	Chain	Residues	Atoms				AltConf
5	D	1	Total	C	N	O	0
			14	8	1	5	
5	D	1	Total	C	N	O	0
			14	8	1	5	

### 3 Residue-property plots

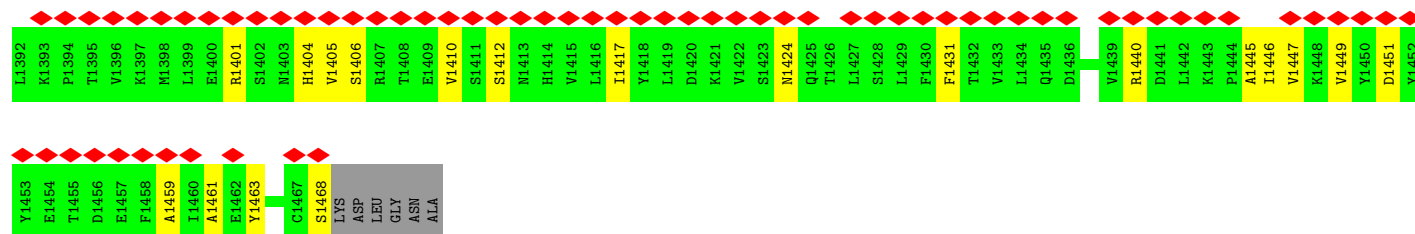
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Alpha-2-macroglobulin

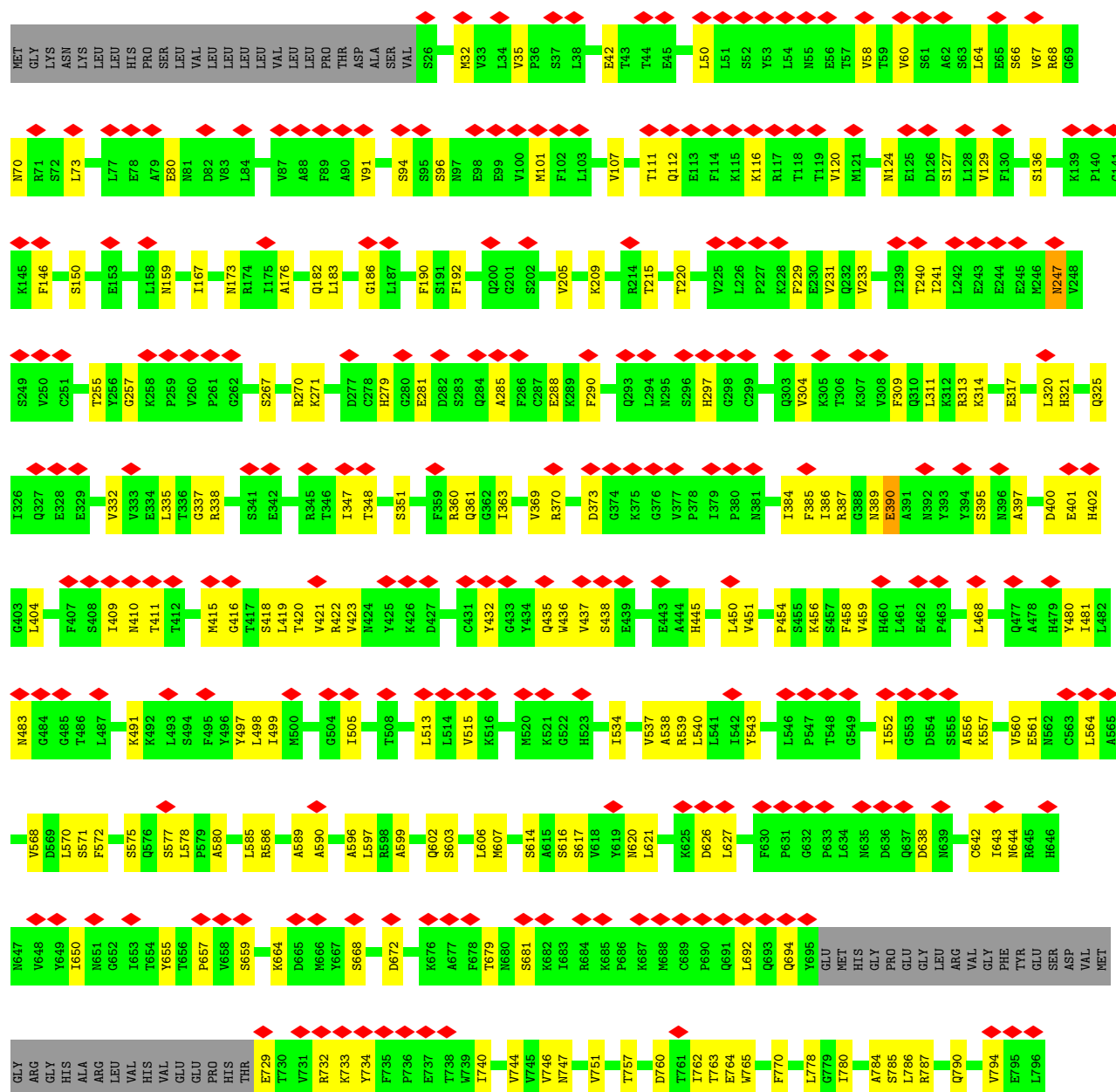




M1331	I1332	L1333	P1334	E1335	K1336	E1337	E1338	F1339	P1340	F1341	A1342	L1343	Q1346	T1347	L1348	P1349	Q1350	T1351	C1352	D1353	E1354	P1355	K1356	A1357	H1358	T1359	S1360	F1361	Q1362	L1363	S1364	L1365	S1366	V1367	S1368	V1369	T1370	G1371	S1372	A1373	S1374	A1375	S1376	M1377	M1378	I1380	V1381	D1382	V1383	K1384	M1385	V1386	S1387	G1388	F1389	I1390	P1391		
F1269	T1270	R1271	T1272	G1273	K1274	A1275	A1276	Q1277	V1278	T1279	I1280	Q1281	S1282	S1283	T1284	F1286	S1287	S1288	K1289	F1290	Q1291	V1292	D1293	N1294	N1295	N1296	L1299	L1300	Q1301	Q1302	V1303	N1304	L1305	P1306	V1307	T1370	G1371	S1372	A1373	S1374	A1375	S1376	M1377	M1378	I1380	V1381	D1382	V1383	K1384	M1385	V1386	S1387	G1388	F1389	I1390	P1391			
M1208	T1209	S1210	Y1211	V1212	L1213	L1214	A1215	Y1216	L1217	T1218	A1219	Q1220	P1221	A1222	P1223	T1224	D1227	L1228	T1229	A1230	A1231	N1232	N1233	I1234	V1235	K1236	W1237	I1238	T1239	K1240	Q1241	Q1242	N1243	A1244	G1245	G1246	G1247	F1248	S1249	S1250	T1251	Q1252	D1253	P1189	K1190	A1191	P1192	V1193	G1194	H1195	F1196	Y1197	A1201	P1202	S1203	A1204	E1205	V1206	E1207
G1084	S1085	L1086	L1087	N1088	A1089	I1091	K1092	G1093	G1094	V1095	E1096	D1097	E1098	V1099	T1100	L1101	S1102	A1103	Y1104	I1105	L1106	I1107	A1108	L1109	L1110	I1111	I1112	P1113	L1114	T1115	V1116	T1117	H1118	P1119	V1120	W1121	V1122	N1123	A1124	L1125	F1126	C1127	L1128	E1129	A1130	W1132	A1135	Q1136	E1137	G1138	D1139	H1140	H1143	V1144	Y1145				
Y1018	K1019	H1020	Y1021	D1022	G1023	S1024	Y1025	S1026	T1027	F1028	G1029	E1030	P1031	Y1032	G1033	N1034	N1035	Q1036	G1037	M1038	W1040	L1041	T1042	A1043	F1044	V1045	L1046	K1047	T1048	F1049	A1050	Q1051	L1052	R1053	A1054	Y1055	I1056	F1057	I1058	D1059	E1060	A1061	H1062	I1063	T1064	Q1065	L1070	S1071	Q1072	R1073	Q1074	C1079	F1080	R1081	S1082	S1083			
G956	S957	A958	M959	Q960	N961	T962	Q963	N964	L965	L966	Q967	M968	P969	Y970	G971	C972	G973	E974	Q975	N976	F980	A981	P982	N983	I984	Y985	V986	L987	D988	Y989	L990	N991	E992	T993	Q994	Q995	L996	T997	P998	E999	I1000	K1001	S1002	K1003	A1004	L1005	G1006	Y1007	L1008	N1009	T1010	G1011	Y1012	Q1013	R1014	Q1015	L1016	N1017	
H893	G894	R895	K896	D897	T898	V899	I900	K901	P902	L903	L904	V905	E906	P907	E908	E911	K912	E913	T914	T915	F916	N917	S918	L919	L920	C921	P922	S923	G924	G925	E926	V927	S928	E929	Q930	L931	S932	L933	K934	L935	P936	P937	N938	V939	Y940	E941	E942	A946	S947	V948	T949	Y950	L951	G952	D953	L954	L955		
P832	A833	F834	L835	A836	V839	E840	K841	E842	Q843	A844	P845	H846	C847	I848	C849	A850	N851	G852	R853	Q854	T855	S856	S857	W858	A859	V860	T861	P862	K863	S864	L865	G866	N867	V868	N869	F870	T871	V872	S873	A874	E875	A876	L877	E878	S879	Q880	E881	L882	C883	G884	T885	E886	V887	P888	S889	V890	P891	E892	
C771	L772	S773	E774	D775	A776	G777	L778	G779	I780	S781	S782	L783	A784	S785	L786	R787	A788	F789	Q790	F791	F792	F793	F794	E795	L796	T797	N798	P799	Y800	S801	Y802	I803	R804	G805	E806	A807	F808	T809	L810	K811	A812	T813	V814	L815	N816	Y817	L818	P819	K820	C821	I822	R823	V824	S825	L828	E829	A830	S831	
TR	GLU	SER	ASP	VAL	MET	GLY	ARG	GLY	HIS	ALA	ARG	LEU	VAL	HIS	VAL	GLU	GLU	PRO	HIS	THR	E729	T730	V731	K733	Y734	F735	P736	E737	T738	W739	I740	W741	D742	L743	V746	N747	S748	A749	G750	V751	A752	E753	V754	G755	V756	T757	V758	P759	D760	E764	W765	K766	A767	G768	VAL	GLY	F770		
E640	D641	N644	R645	H646	M647	I650	N651	G652	I653	T654	Y655	T656	P657	V658	T661	N662	D665	S668	F669	L670	E671	D672	M673	F678	T679	N680	S681	K682	I683	R684	K685	P686	K687	M688	C689	Q690	Q691	L692	Q693	Q694	Y695	GLU	MET	HIS	GLY	PHE													

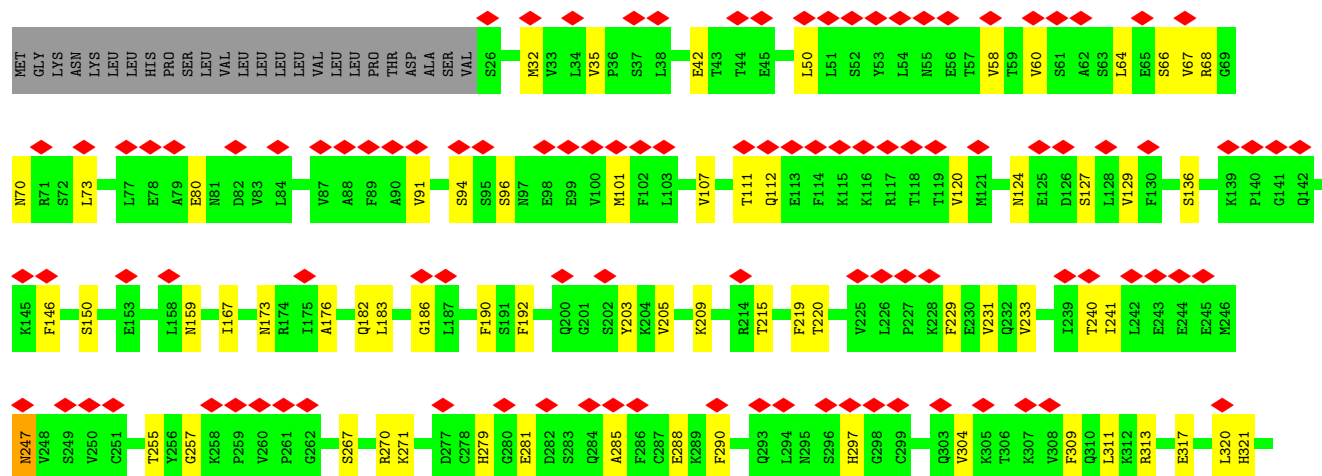


• Molecule 1: Alpha-2-macroglobulin

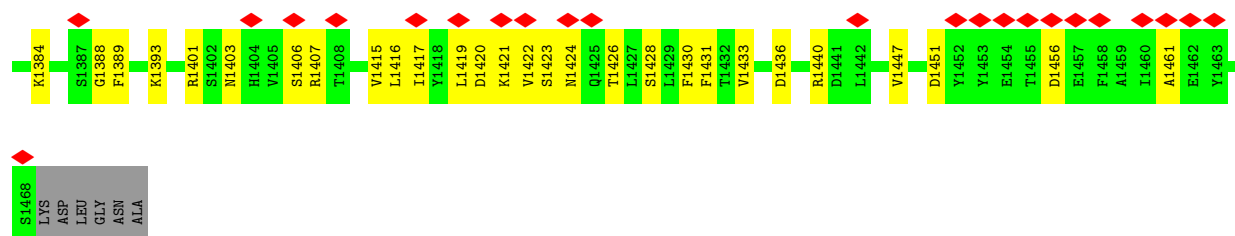




L955	G956	S957	A958	N959	Q960	N961	T962	Q963	N964	L965	L966	Q967	N968	P969	Q970	Q971	C972	G973	E974	Q975	N976		F980	A981	P982	N983	L984	Y985	V986	L987	D988	Y989	L990	N991	E992	T993	Q994	Q995	L996	T997	P998	E999	T1000	K1001	S1002	K1003	A1004	I1005	G1006	Y1007	L1008	N1009	T1010	G1011	Y1012	Q1013	R1014	Q1015	L1016		
E892	H893	G894	R895	K896	D897	T898	V899	I900	K901	P902	L903	L904	P845	H846	C947	I948	C949	A850	N851	G852	R853	Q854	T855	V856	N917	S918	L919	A859	L920	C921	P922	S923	G924	G925	E926	V927	T993	E929	E930	L931	S932	L933	K934	L935	P936	P937	N938	V939	V940	E941	E942		A946	S947	V948	S949	V950	L951	G952	D953	I954
S831	P832	G894	F834	L835	A836		V839	Q963	K941	E942	Q943	A844	P845	H846	C947	I948	C949	A850	N851	G852	R853	Q854	T855	V856	N917	S918	L919	A859	L920	C921	P922	S923	G924	G925	E926	V927	T993	E929	E930	L931	S932	L933	K934	L935	P936	P937	N938	V939	V940	E941	E942		A946	S947	V948	S949	V950	L951	G952	D953	I954
F770	C771	L772	S773	E774	D775	A776	G777	L778	G779	I780	S781	S782	T783	A784	S785	L786	R787	A788	F789	Q790	P791	F792	F793	V794	E795	L796	T797	W798	F799	Y800	S801	V802	I803	R804	G805	E806	A807	F808	T809	L810	K811	A812	E875	A876	L877	E878	S879	Q880	E881	L882	C883	G884	T885	E886	V887	P888	V889	P891			
PHE	TYR	SER	ASP	VAL	MET	GLY	ARG	HIS	ALA	ARG	LEU	VAL	HIS	VAL	GLU	GLU	THR	E729	T730	V731	R732	K733	Y734	F735	F736	E737	T738	W739	I740	W741	D742	L743	W746	N747	S748	A749	G750	V751	A752	E753	V754	G755	V756	T757	V758	P759	D760		E764	W765	K766	A767	G768	A769		L828	E829	A830			
N639	E640	D641	N644	R645	H646	N647	T650	N651	G652	L653	T654	Y655	T656	P657	V658	T661	N662	D665	S668	F669	L670	E671	D672	H673	F678	T679	N680	S681	K682	L683	R684	K685	P686	K687	H688	C689	P690	Q691	L692	V695	GLU	MET	HIS	GLY	PRO	GLU	LEU	ARG	VAL	GLY		L828	E829	A830							
Q576	S577	L578	P579	A580	S581	H582	A583	H584	L585	R586	V587	T588	S593	V594	C595	A596	L597	R598	A599	V600	D601	Q602	S603	V604	L605	L606	H607	K608	P609	D610	A611	E612	G613	S614	A615	S616	S617	V618	Y619	N620	L621	L622	P623	E624	K625	D626	L627	T628	G629	F630	P631	G632	P633	L634	N635	D636	Q637	D638			
L513	L514	V515	K516	Q517	E518	D519	K521	G522	H523	F524	S525	I526	S527	I528	P529	V530	K531	I534	A535	P536	R539	L540	L541	I542	Y543	A544	V545	L546	P547	T548	G549	D550	V551	I552	G553	D554	S555	A556	K557	V560	E561	N562	C563	L564	A565	N566	K567	V568	D569	L570	S571	F572	S573	P574	S575						
H446	T447	A448	Y449	L450	V451	F452	S453	P454	S455	K456	S457	F458	V459	H460	L461	E462	P463	M464	S465	H466	E467	G471	H472	T473	Q474	Q477	A478	H479	Y480	I481	L482	M483	G484	G485	T486	L487	L488	K492	L493	S494	F495	Y496	Y497	L498	A501	K502	G503	G504	I505	T508	G509	T510	H511	G512							
E317	M318	K319	L320	H321	T322	A324	Q325	I326	Q327	E328	E329	G330	T331	V332	V333	E334	L335	T336	G337	R338	Q339	S340	K345	T346	I347	T348	K349	L350	S351	F352	V353	D356	F359	Q361	G362	I363	F364	F365	F366	V369	R370	D373	G374	K375	G376	V377	P378	I379	P380	N381	K382	V383									
T255	Y256	G257	K258	P259	V260	P261	G262	H263	V264	T265	V266	S267	I268	C269	R270	K271	S272	S273	D274	A275	S276	G280	E281	D282	S283	Q284	A285	F286	C287	L288	K289	F290	S291	Q292	Q293	L294	N295	S296	H297	G298	C299	F300	Y301	Q302	Q303	V304	K305	T306	K307	V308	F309	Q310	L311	K312	R313	K314	E315	Y316			
K188	Q189	F190	S191	F192	P193	L194	S195		P198	F199	Q200	G201	S202	Y203	K204	V205	V206		K209	K210	S211	G212	G213	R214	T215	E216	H217	P218	F219	T220	V221	E222	E223	F224	V225		K228	F229	E230	V231	Q232	V233	T234		T239	T240		E243	E244	E245	M246	N247	V248	S249	C250	C251	G252	L253	Y254		







- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	30618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	39.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	47775	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0135	Depositor
Map size ( $\text{\AA}$ )	335.04, 335.04, 335.04	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.047, 1.047, 1.047	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	A	0.27	0/11249	0.56	5/15286 (0.0%)
1	B	0.27	0/11248	0.57	5/15283 (0.0%)
1	C	0.27	0/11249	0.56	5/15286 (0.0%)
1	D	0.27	0/11248	0.57	5/15283 (0.0%)
All	All	0.27	0/44994	0.56	20/61138 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	801	SER	N-CA-C	-9.41	93.27	108.41
1	D	801	SER	N-CA-C	-9.41	93.27	108.41
1	B	423	VAL	N-CA-C	-7.13	106.13	111.90
1	D	423	VAL	N-CA-C	-7.13	106.13	111.90
1	A	1116	VAL	N-CA-C	-6.84	106.12	112.96
1	C	1116	VAL	N-CA-C	-6.84	106.12	112.96
1	A	55	ASN	CB-CA-C	6.54	123.43	110.42
1	C	55	ASN	CB-CA-C	6.54	123.43	110.42
1	A	656	THR	CB-CA-C	6.07	122.14	110.17
1	C	656	THR	CB-CA-C	6.07	122.14	110.17
1	B	577	SER	CA-C-N	5.87	126.35	119.83
1	B	577	SER	C-N-CA	5.87	126.35	119.83
1	D	577	SER	CA-C-N	5.87	126.35	119.83
1	D	577	SER	C-N-CA	5.87	126.35	119.83
1	B	953	ASP	N-CA-C	5.85	118.54	110.35
1	D	953	ASP	N-CA-C	5.85	118.54	110.35
1	A	657	PRO	N-CA-C	5.61	119.90	111.14
1	C	657	PRO	N-CA-C	5.61	119.90	111.14
1	A	1184	GLU	N-CA-C	5.10	121.66	110.80
1	C	1184	GLU	N-CA-C	5.10	121.66	110.80

There are no chirality outliers.

There are no planarity outliers.

## 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	A	11004	0	10891	194	0
1	B	11004	0	10888	275	0
1	C	11004	0	10891	198	0
1	D	11004	0	10888	269	0
2	E	50	0	43	3	0
2	H	50	0	43	3	0
3	F	39	0	34	1	0
3	I	39	0	34	1	0
4	G	28	0	25	3	0
4	J	28	0	25	3	0
5	A	112	0	104	6	0
5	B	70	0	65	6	0
5	C	112	0	104	6	0
5	D	70	0	65	6	0
All	All	44614	0	44100	936	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 11.

All (936) 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:C:55:ASN:HD22	5:C:2001:NAG:C1	1.06	1.57
1:A:55:ASN:HD22	5:A:2001:NAG:C1	1.06	1.55
1:B:1424:ASN:ND2	4:G:1:NAG:C1	1.70	1.52
1:D:1424:ASN:ND2	4:J:1:NAG:C1	1.70	1.51
1:B:247:ASN:HD21	5:B:2003:NAG:C1	1.27	1.45
1:D:247:ASN:HD21	5:D:2003:NAG:C1	1.27	1.45
1:A:55:ASN:ND2	5:A:2001:NAG:C1	1.79	1.43
1:C:55:ASN:ND2	5:C:2001:NAG:C1	1.79	1.40
1:D:247:ASN:ND2	5:D:2003:NAG:C1	2.08	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:ND2	5:B:2003:NAG:C1	2.08	1.13
1:B:1424:ASN:ND2	4:G:1:NAG:O5	2.08	0.87
1:D:1424:ASN:ND2	4:J:1:NAG:O5	2.08	0.84
1:A:55:ASN:HB2	5:A:2001:NAG:C7	2.09	0.82
1:C:55:ASN:HB2	5:C:2001:NAG:C7	2.09	0.82
1:A:270:ARG:NE	1:A:316:TYR:O	2.14	0.81
1:C:270:ARG:NE	1:C:316:TYR:O	2.14	0.81
1:D:1159:ASN:O	1:D:1162:LYS:NZ	2.15	0.79
1:D:956:GLY:O	1:D:995:GLN:NE2	2.15	0.79
1:B:956:GLY:O	1:B:995:GLN:NE2	2.15	0.79
1:B:1159:ASN:O	1:B:1162:LYS:NZ	2.15	0.78
1:D:642:CYS:SG	1:D:643:ILE:N	2.57	0.78
1:B:642:CYS:SG	1:B:643:ILE:N	2.57	0.78
1:D:127:SER:O	1:D:209:LYS:NZ	2.17	0.77
1:A:1177:LYS:N	1:A:1180:SER:O	2.18	0.76
1:B:127:SER:O	1:B:209:LYS:NZ	2.17	0.76
1:B:843:GLN:NE2	1:B:844:ALA:O	2.19	0.76
1:C:1177:LYS:N	1:C:1180:SER:O	2.18	0.75
1:D:580:ALA:O	1:D:757:THR:OG1	2.04	0.75
1:B:1401:ARG:NH2	1:B:1428:SER:O	2.19	0.75
1:D:843:GLN:NE2	1:D:844:ALA:O	2.19	0.75
1:D:1401:ARG:NH2	1:D:1428:SER:O	2.19	0.75
1:D:1420:ASP:O	1:D:1421:LYS:NZ	2.18	0.74
1:A:127:SER:O	1:A:209:LYS:NZ	2.21	0.74
1:A:976:ASN:OD1	1:A:1014:ARG:NH1	2.22	0.73
1:C:127:SER:O	1:C:209:LYS:NZ	2.21	0.73
1:D:540:LEU:O	1:D:556:ALA:N	2.22	0.73
1:B:540:LEU:O	1:B:556:ALA:N	2.22	0.73
1:D:94:SER:OG	1:D:96:SER:O	2.07	0.73
1:A:1128:LEU:HD21	1:A:1150:LEU:HD21	1.71	0.73
1:C:976:ASN:OD1	1:C:1014:ARG:NH1	2.22	0.72
1:C:1128:LEU:HD21	1:C:1150:LEU:HD21	1.71	0.72
1:D:1346:GLN:NE2	1:D:1348:LEU:O	2.24	0.71
1:B:94:SER:OG	1:B:96:SER:O	2.07	0.71
1:B:400:ASP:OD1	1:B:404:LEU:N	2.23	0.71
1:B:1346:GLN:NE2	1:B:1348:LEU:O	2.24	0.71
1:A:43:THR:OG1	1:A:153:GLU:OE1	2.07	0.70
1:C:1179:ASN:ND2	1:C:1233:ASN:O	2.24	0.70
1:A:1179:ASN:ND2	1:A:1233:ASN:O	2.24	0.70
1:B:313:ARG:NH2	1:B:436:TRP:O	2.24	0.70
1:D:400:ASP:OD1	1:D:404:LEU:N	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:ASP:OD1	1:D:1062:HIS:N	2.25	0.70
1:B:616:SER:O	1:B:620:ASN:ND2	2.25	0.70
1:D:313:ARG:NH2	1:D:436:TRP:O	2.24	0.70
1:D:570:LEU:HD21	1:D:784:ALA:HB3	1.74	0.70
1:B:1059:ASP:OD1	1:B:1062:HIS:N	2.25	0.69
1:D:616:SER:O	1:D:620:ASN:ND2	2.25	0.69
1:B:570:LEU:HD21	1:B:784:ALA:HB3	1.74	0.69
1:A:823:ARG:NH1	1:A:846:HIS:O	2.25	0.69
1:B:270:ARG:NH1	1:B:309:PHE:O	2.26	0.69
1:C:43:THR:OG1	1:C:153:GLU:OE1	2.07	0.69
1:D:1106:THR:HG21	1:D:1124:ALA:HB3	1.74	0.69
1:C:823:ARG:NH1	1:C:846:HIS:O	2.25	0.68
1:D:270:ARG:NH1	1:D:309:PHE:O	2.26	0.68
1:B:580:ALA:O	1:B:757:THR:OG1	2.04	0.68
1:B:1420:ASP:O	1:B:1421:LYS:NZ	2.18	0.68
1:B:1106:THR:HG21	1:B:1124:ALA:HB3	1.74	0.68
1:C:1106:THR:HG21	1:C:1124:ALA:HB3	1.75	0.68
1:B:1099:VAL:O	1:B:1102:SER:OG	2.09	0.67
1:A:912:LYS:HE2	1:A:1184:GLU:HB3	1.75	0.67
1:A:1106:THR:HG21	1:A:1124:ALA:HB3	1.75	0.67
1:C:912:LYS:HE2	1:C:1184:GLU:HB3	1.75	0.67
1:A:411:THR:OG1	1:A:413:ASN:OD1	2.13	0.67
1:C:665:ASP:OD1	1:C:668:SER:N	2.28	0.67
1:D:401:GLU:OE1	1:D:402:HIS:ND1	2.27	0.67
1:D:1045:VAL:O	1:D:1048:THR:N	2.28	0.67
1:B:182:GLN:NE2	1:B:183:LEU:O	2.29	0.67
1:B:401:GLU:OE1	1:B:402:HIS:ND1	2.27	0.67
1:B:1109:LEU:HD12	1:B:1117:THR:HG23	1.77	0.67
1:C:112:GLN:NE2	5:C:2001:NAG:O4	2.29	0.67
1:C:411:THR:OG1	1:C:413:ASN:OD1	2.13	0.67
1:A:665:ASP:OD1	1:A:668:SER:N	2.28	0.66
1:B:926:GLU:OE2	1:B:1315:LYS:NZ	2.28	0.66
1:D:182:GLN:NE2	1:D:183:LEU:O	2.29	0.66
1:A:112:GLN:NE2	5:A:2001:NAG:O4	2.29	0.66
1:A:928:SER:OG	1:A:1314:MET:O	2.09	0.66
1:A:860:VAL:HG22	1:A:862:PRO:HD3	1.77	0.66
1:B:1045:VAL:O	1:B:1048:THR:N	2.28	0.66
1:B:825:SER:N	1:B:875:GLU:O	2.29	0.66
1:C:928:SER:OG	1:C:1314:MET:O	2.09	0.66
1:C:96:SER:O	1:C:124:ASN:ND2	2.30	0.65
1:C:915:THR:OG1	1:C:1326:THR:O	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:O	1:A:124:ASN:ND2	2.30	0.65
1:D:1109:LEU:HD12	1:D:1117:THR:HG23	1.77	0.65
1:B:981:ALA:HB3	1:B:982:PRO:HD3	1.79	0.65
1:A:428:ARG:NH2	1:A:441:HIS:O	2.29	0.65
1:D:129:VAL:HG23	1:D:215:THR:HG21	1.79	0.65
1:D:571:SER:O	1:D:586:ARG:N	2.30	0.65
1:D:860:VAL:HG22	1:D:862:PRO:HD3	1.79	0.65
1:B:571:SER:O	1:B:586:ARG:N	2.30	0.65
1:B:1125:LEU:O	1:B:1129:GLU:N	2.30	0.65
1:D:926:GLU:OE2	1:D:1315:LYS:NZ	2.28	0.65
1:C:638:ASP:OD2	1:C:641:ASP:N	2.30	0.65
1:A:800:TYR:O	1:A:802:VAL:HG13	1.96	0.64
1:A:1336:LYS:NZ	1:A:1337:GLU:OE1	2.25	0.64
1:D:1099:VAL:O	1:D:1102:SER:OG	2.09	0.64
1:B:279:HIS:NE2	1:B:281:GLU:O	2.30	0.64
1:C:1213:LEU:HD23	1:C:1260:ALA:HA	1.80	0.64
1:D:1403:ASN:ND2	1:D:1420:ASP:OD2	2.31	0.64
1:D:233:VAL:HG21	1:D:320:LEU:HD21	1.79	0.64
1:D:981:ALA:HB3	1:D:982:PRO:HD3	1.79	0.64
1:B:823:ARG:NH1	1:B:846:HIS:O	2.31	0.64
1:B:860:VAL:HG22	1:B:862:PRO:HD3	1.79	0.64
1:D:279:HIS:NE2	1:D:281:GLU:O	2.30	0.64
1:D:999:GLU:O	1:D:1003:LYS:N	2.30	0.64
1:C:428:ARG:NH2	1:C:441:HIS:O	2.29	0.64
1:D:816:ASN:ND2	1:D:820:LYS:O	2.31	0.64
1:D:1125:LEU:O	1:D:1129:GLU:N	2.30	0.64
1:C:272:TYR:HB2	1:C:275:ALA:HB2	1.80	0.64
1:C:860:VAL:HG22	1:C:862:PRO:HD3	1.77	0.64
1:D:825:SER:N	1:D:875:GLU:O	2.29	0.64
1:A:638:ASP:OD2	1:A:641:ASP:N	2.30	0.64
1:B:159:ASN:OD1	1:B:186:GLY:N	2.31	0.64
1:C:800:TYR:O	1:C:802:VAL:HG13	1.96	0.64
1:B:999:GLU:O	1:B:1003:LYS:N	2.30	0.64
1:A:913:GLU:OE1	1:A:1327:SER:OG	2.16	0.63
1:B:816:ASN:ND2	1:B:820:LYS:O	2.31	0.63
1:B:1424:ASN:CG	4:G:1:NAG:C1	2.67	0.63
1:A:272:TYR:HB2	1:A:275:ALA:HB2	1.80	0.63
1:D:823:ARG:NH1	1:D:846:HIS:O	2.31	0.63
1:A:915:THR:OG1	1:A:1326:THR:O	2.09	0.63
1:C:913:GLU:OE1	1:C:1327:SER:OG	2.16	0.63
1:D:564:LEU:HD11	1:D:778:LEU:HD21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:SER:OG	1:B:787:ARG:O	2.08	0.63
1:B:1344:GLY:O	1:B:1366:SER:N	2.31	0.63
1:B:1403:ASN:ND2	1:B:1420:ASP:OD2	2.31	0.63
1:B:129:VAL:HG23	1:B:215:THR:HG21	1.79	0.63
1:C:55:ASN:ND2	5:C:2001:NAG:O5	2.30	0.63
1:C:843:GLN:NE2	1:C:844:ALA:O	2.32	0.63
1:A:1213:LEU:HD23	1:A:1260:ALA:HA	1.80	0.62
1:B:480:TYR:CZ	1:B:513:LEU:HD21	2.34	0.62
1:B:564:LEU:HD11	1:B:778:LEU:HD21	1.80	0.62
1:C:387:ARG:HB3	1:C:423:VAL:HG11	1.81	0.62
1:D:159:ASN:OD1	1:D:186:GLY:N	2.31	0.62
1:C:353:VAL:HG21	1:C:404:LEU:HD13	1.81	0.62
1:A:390:GLU:OE2	1:A:413:ASN:ND2	2.33	0.62
1:A:656:THR:HB	1:A:657:PRO:CD	2.30	0.62
1:B:233:VAL:HG21	1:B:320:LEU:HD21	1.79	0.62
1:A:843:GLN:NE2	1:A:844:ALA:O	2.32	0.62
1:B:314:LYS:HZ1	1:B:437:VAL:HG12	1.64	0.62
1:C:1336:LYS:NZ	1:C:1337:GLU:OE1	2.25	0.62
1:A:65:GLU:OE2	1:A:104:THR:OG1	2.17	0.62
1:D:1344:GLY:O	1:D:1366:SER:N	2.31	0.62
1:A:55:ASN:ND2	5:A:2001:NAG:O5	2.30	0.62
1:C:422:ARG:NH1	1:C:442:GLU:O	2.32	0.62
1:B:1237:TRP:O	1:B:1241:GLN:N	2.33	0.62
1:C:65:GLU:OE2	1:C:104:THR:OG1	2.17	0.62
1:A:422:ARG:NH1	1:A:442:GLU:O	2.32	0.62
1:C:620:ASN:O	1:C:625:LYS:NZ	2.28	0.62
1:A:353:VAL:HG21	1:A:404:LEU:HD13	1.81	0.61
1:A:387:ARG:HB3	1:A:423:VAL:HG11	1.81	0.61
1:C:656:THR:HB	1:C:657:PRO:CD	2.30	0.61
1:D:969:PRO:HD3	1:D:979:LEU:HD11	1.82	0.61
1:D:480:TYR:CZ	1:D:513:LEU:HD21	2.34	0.61
1:A:501:ALA:N	1:A:504:GLY:O	2.34	0.61
1:A:1013:GLN:O	1:A:1017:ASN:ND2	2.33	0.61
1:C:390:GLU:OE2	1:C:413:ASN:ND2	2.33	0.61
1:A:451:VAL:HG23	1:A:669:PHE:CZ	2.35	0.61
1:A:620:ASN:O	1:A:625:LYS:NZ	2.28	0.61
1:C:418:SER:OG	1:C:445:HIS:NE2	2.34	0.61
1:A:269:CYS:SG	1:A:289:LYS:NZ	2.74	0.61
1:B:960:GLN:OE1	1:B:1242:GLN:NE2	2.34	0.61
1:A:404:LEU:O	1:A:406:GLN:NE2	2.34	0.61
1:B:969:PRO:HD3	1:B:979:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:CYS:SG	1:C:289:LYS:NZ	2.74	0.61
1:D:1237:TRP:O	1:D:1241:GLN:N	2.33	0.61
1:B:454:PRO:HD2	1:B:552:ILE:HD11	1.83	0.61
1:C:1013:GLN:O	1:C:1017:ASN:ND2	2.33	0.61
1:D:960:GLN:OE1	1:D:1242:GLN:NE2	2.34	0.61
1:B:959:MET:O	1:B:962:THR:OG1	2.18	0.60
1:B:1384:LYS:H	1:B:1447:VAL:HG11	1.66	0.60
1:C:451:VAL:HG23	1:C:669:PHE:CZ	2.35	0.60
1:C:501:ALA:N	1:C:504:GLY:O	2.34	0.60
1:D:575:SER:OG	1:D:787:ARG:O	2.08	0.60
1:D:1424:ASN:CG	4:J:1:NAG:C1	2.67	0.60
1:A:599:ALA:HB3	1:A:740:ILE:CG1	2.32	0.60
1:B:1388:GLY:O	1:B:1436:ASP:N	2.34	0.60
1:B:94:SER:OG	1:B:124:ASN:ND2	2.34	0.60
1:B:597:LEU:HD11	1:B:744:VAL:HG22	1.83	0.60
1:B:802:VAL:O	1:B:906:GLU:N	2.35	0.60
1:C:451:VAL:HG23	1:C:669:PHE:HZ	1.67	0.60
1:D:454:PRO:HD2	1:D:552:ILE:HD11	1.83	0.60
1:A:418:SER:OG	1:A:445:HIS:NE2	2.34	0.60
1:C:404:LEU:O	1:C:406:GLN:NE2	2.34	0.60
1:B:785:SER:OG	1:B:786:LEU:N	2.35	0.60
1:D:384:ILE:HD12	1:D:421:VAL:HG11	1.84	0.60
1:C:599:ALA:HB3	1:C:740:ILE:CG1	2.32	0.59
1:D:785:SER:OG	1:D:786:LEU:N	2.35	0.59
1:A:451:VAL:HG23	1:A:669:PHE:HZ	1.67	0.59
1:A:959:MET:SD	1:A:959:MET:N	2.75	0.59
1:D:94:SER:OG	1:D:124:ASN:ND2	2.34	0.59
1:B:596:ALA:N	1:B:770:PHE:O	2.34	0.59
1:A:1106:THR:HG21	1:A:1124:ALA:CB	2.33	0.59
2:E:2:NAG:H3	2:E:2:NAG:C8	2.32	0.59
2:H:2:NAG:C8	2:H:2:NAG:H3	2.32	0.59
1:A:599:ALA:HB3	1:A:740:ILE:HG13	1.83	0.59
1:D:599:ALA:HB3	1:D:740:ILE:HB	1.85	0.59
1:D:1384:LYS:H	1:D:1447:VAL:HG11	1.66	0.59
1:C:959:MET:SD	1:C:959:MET:N	2.75	0.59
1:B:384:ILE:HD12	1:B:421:VAL:HG11	1.84	0.59
1:C:1106:THR:HG21	1:C:1124:ALA:CB	2.33	0.59
1:A:665:ASP:O	1:A:668:SER:OG	2.21	0.58
1:B:603:SER:OG	1:B:763:THR:OG1	2.19	0.58
1:C:195:SER:OG	1:C:1244:ALA:O	2.14	0.58
1:D:233:VAL:HG13	1:D:338:ARG:HD3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:THR:HG21	1:C:635:ASN:HB3	1.85	0.58
1:C:912:LYS:NZ	1:C:913:GLU:O	2.36	0.58
1:C:96:SER:OG	1:C:97:ASN:N	2.36	0.58
1:B:385:PHE:N	1:B:422:ARG:O	2.37	0.58
1:D:596:ALA:N	1:D:770:PHE:O	2.34	0.58
1:A:96:SER:OG	1:A:97:ASN:N	2.36	0.58
1:C:599:ALA:HB3	1:C:740:ILE:HG13	1.83	0.58
1:A:195:SER:OG	1:A:1244:ALA:O	2.14	0.58
1:D:1388:GLY:O	1:D:1436:ASP:N	2.34	0.58
1:D:597:LEU:HD11	1:D:744:VAL:HG22	1.83	0.58
1:B:499:ILE:O	1:B:505:ILE:HG23	2.04	0.58
1:A:912:LYS:NZ	1:A:913:GLU:O	2.36	0.58
1:B:599:ALA:HB3	1:B:740:ILE:HB	1.85	0.58
1:D:802:VAL:O	1:D:906:GLU:N	2.35	0.58
1:A:119:THR:HG21	1:A:635:ASN:HB3	1.85	0.58
1:B:1156:LEU:O	1:B:1220:GLN:NE2	2.37	0.58
1:C:498:LEU:O	1:C:541:LEU:N	2.36	0.57
1:C:811:LYS:NZ	1:C:813:THR:OG1	2.35	0.57
1:D:499:ILE:O	1:D:505:ILE:HG23	2.04	0.57
1:D:614:SER:O	1:D:617:SER:OG	2.11	0.57
1:B:418:SER:OG	1:B:445:HIS:NE2	2.36	0.57
1:D:959:MET:O	1:D:962:THR:OG1	2.18	0.57
1:D:1156:LEU:O	1:D:1220:GLN:NE2	2.37	0.57
1:C:534:ILE:HG23	1:C:560:VAL:HG11	1.86	0.57
1:A:534:ILE:HG23	1:A:560:VAL:HG11	1.86	0.57
1:D:418:SER:OG	1:D:445:HIS:NE2	2.36	0.57
1:D:603:SER:OG	1:D:763:THR:OG1	2.19	0.57
1:B:233:VAL:HG13	1:B:338:ARG:HD3	1.84	0.57
1:B:570:LEU:HD13	1:B:585:LEU:HD11	1.85	0.57
1:B:435:GLN:O	1:B:438:SER:OG	2.22	0.57
1:A:100:VAL:HG12	1:A:121:MET:HE1	1.87	0.57
1:C:799:PRO:O	1:C:800:TYR:HB2	2.04	0.57
1:D:570:LEU:HD13	1:D:585:LEU:HD11	1.85	0.57
1:B:564:LEU:HD11	1:B:778:LEU:CD2	2.35	0.57
1:D:385:PHE:N	1:D:422:ARG:O	2.37	0.57
1:B:607:MET:HE1	1:B:733:LYS:HZ3	1.69	0.56
1:B:1098:GLU:O	1:B:1102:SER:N	2.37	0.56
1:C:268:ILE:HG22	1:C:320:LEU:HA	1.86	0.56
1:C:665:ASP:O	1:C:668:SER:OG	2.21	0.56
1:D:692:LEU:O	1:D:694:GLN:NE2	2.38	0.56
1:A:799:PRO:O	1:A:800:TYR:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD11	1:B:762:ILE:CG2	2.35	0.56
1:C:55:ASN:CG	5:C:2001:NAG:C1	2.74	0.56
1:C:100:VAL:HG12	1:C:121:MET:HE1	1.87	0.56
1:D:435:GLN:O	1:D:438:SER:OG	2.22	0.56
1:D:570:LEU:CD2	1:D:784:ALA:HB3	2.36	0.56
1:A:498:LEU:O	1:A:541:LEU:N	2.36	0.56
1:B:692:LEU:O	1:B:694:GLN:NE2	2.38	0.56
1:D:363:ILE:O	1:D:411:THR:HG21	2.06	0.56
1:A:811:LYS:NZ	1:A:813:THR:OG1	2.35	0.56
1:D:578:LEU:HD11	1:D:762:ILE:CG2	2.35	0.56
1:D:1098:GLU:O	1:D:1102:SER:N	2.37	0.56
1:B:68:ARG:NH2	1:B:70:ASN:OD1	2.39	0.56
1:B:363:ILE:O	1:B:411:THR:HG21	2.06	0.56
1:B:998:PRO:O	1:B:1002:SER:N	2.36	0.56
1:D:68:ARG:NH2	1:D:70:ASN:OD1	2.39	0.56
1:B:570:LEU:CD2	1:B:784:ALA:HB3	2.36	0.56
1:B:1347:THR:HA	1:B:1363:ILE:HG23	1.87	0.56
1:C:268:ILE:HD12	1:C:318:MET:HE3	1.88	0.56
1:B:1118:HIS:O	1:B:1121:VAL:HG22	2.06	0.56
1:D:1167:LEU:O	1:D:1171:ASN:ND2	2.39	0.56
1:B:915:THR:HG21	1:B:1177:LYS:NZ	2.21	0.56
1:B:816:ASN:O	1:B:851:ASN:N	2.38	0.55
1:D:564:LEU:HD11	1:D:778:LEU:CD2	2.35	0.55
1:B:534:ILE:HG23	1:B:560:VAL:HG11	1.89	0.55
1:B:1128:LEU:O	1:B:1132:TRP:N	2.39	0.55
1:B:1167:LEU:O	1:B:1171:ASN:ND2	2.39	0.55
1:D:1364:SER:C	1:D:1365:LEU:HD12	2.31	0.55
1:A:351:SER:O	1:A:369:VAL:HG13	2.07	0.55
1:C:960:GLN:O	1:C:1244:ALA:HB2	2.07	0.55
1:A:960:GLN:O	1:A:1244:ALA:HB2	2.07	0.55
1:B:1364:SER:C	1:B:1365:LEU:HD12	2.31	0.55
1:C:1128:LEU:HD21	1:C:1150:LEU:CD2	2.36	0.55
1:D:805:GLY:O	1:D:1440:ARG:NH2	2.39	0.55
1:A:268:ILE:HD12	1:A:318:MET:HE3	1.88	0.55
1:B:910:LEU:HD23	1:B:911:GLU:N	2.22	0.55
1:C:60:VAL:HG12	1:C:107:VAL:HA	1.89	0.55
1:C:874:ALA:N	1:C:897:ASP:O	2.39	0.55
1:C:963:GLN:O	1:C:1244:ALA:HB1	2.06	0.55
1:D:816:ASN:O	1:D:851:ASN:N	2.38	0.55
1:D:1118:HIS:O	1:D:1121:VAL:HG22	2.06	0.55
1:A:60:VAL:HG12	1:A:107:VAL:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:VAL:HG12	1:B:60:VAL:HG13	1.89	0.55
1:B:267:SER:HG	1:B:321:HIS:CD2	2.23	0.55
1:D:915:THR:HG21	1:D:1177:LYS:NZ	2.21	0.55
1:D:1293:ASP:O	1:D:1297:ARG:N	2.40	0.55
1:A:268:ILE:HG22	1:A:320:LEU:HA	1.86	0.55
1:D:910:LEU:HD23	1:D:911:GLU:N	2.22	0.55
1:D:1128:LEU:O	1:D:1132:TRP:N	2.39	0.55
1:D:1347:THR:HA	1:D:1363:ILE:HG23	1.87	0.55
1:A:387:ARG:CB	1:A:423:VAL:HG11	2.37	0.55
1:A:874:ALA:N	1:A:897:ASP:O	2.39	0.55
1:A:963:GLN:O	1:A:1244:ALA:HB1	2.06	0.55
1:D:360:ARG:NE	1:D:459:VAL:O	2.39	0.55
1:D:992:GLU:OE1	5:D:2005:NAG:O6	2.24	0.55
1:C:351:SER:O	1:C:369:VAL:HG13	2.07	0.55
1:B:614:SER:O	1:B:617:SER:OG	2.11	0.55
1:B:1293:ASP:O	1:B:1297:ARG:N	2.40	0.55
1:D:267:SER:HG	1:D:321:HIS:CD2	2.24	0.55
1:B:360:ARG:NE	1:B:459:VAL:O	2.39	0.54
1:B:992:GLU:OE1	5:B:2005:NAG:O6	2.24	0.54
1:D:534:ILE:HG23	1:D:560:VAL:HG11	1.89	0.54
1:D:60:VAL:HG12	1:D:107:VAL:HA	1.89	0.54
1:D:1363:ILE:HG22	1:D:1365:LEU:HD11	1.88	0.54
1:C:387:ARG:CB	1:C:423:VAL:HG11	2.37	0.54
1:A:55:ASN:CG	5:A:2001:NAG:C1	2.74	0.54
1:B:578:LEU:HD13	1:B:790:GLN:HB2	1.88	0.54
1:A:1128:LEU:HD21	1:A:1150:LEU:CD2	2.36	0.54
1:B:1369:TYR:OH	1:B:1456:ASP:OD2	2.20	0.54
1:B:491:LYS:HA	1:B:515:VAL:HG13	1.90	0.54
1:D:607:MET:HE1	1:D:733:LYS:HZ3	1.71	0.54
1:D:614:SER:OG	1:D:617:SER:N	2.41	0.54
1:D:1393:LYS:NZ	1:D:1430:PHE:O	2.40	0.54
1:D:1351:THR:OG1	1:D:1353:ASP:OD1	2.26	0.54
1:D:578:LEU:HD13	1:D:790:GLN:HB2	1.88	0.54
1:A:1127:CYS:O	1:A:1130:SER:OG	2.16	0.54
1:B:805:GLY:O	1:B:1440:ARG:NH2	2.39	0.54
1:B:1406:SER:OG	1:B:1417:ILE:HD12	2.08	0.54
1:D:58:VAL:HG12	1:D:60:VAL:HG13	1.89	0.54
1:D:491:LYS:HA	1:D:515:VAL:HG13	1.90	0.54
1:D:931:LEU:O	1:D:1312:TYR:N	2.41	0.54
1:D:998:PRO:O	1:D:1002:SER:N	2.36	0.54
1:A:268:ILE:HD12	1:A:318:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:THR:OG1	1:D:657:PRO:HD2	2.08	0.53
1:B:1378:MET:SD	1:B:1378:MET:N	2.81	0.53
1:C:268:ILE:HD12	1:C:318:MET:CE	2.38	0.53
1:D:271:LYS:N	1:D:317:GLU:O	2.40	0.53
1:B:1363:ILE:HG22	1:B:1365:LEU:HD11	1.88	0.53
1:B:1393:LYS:NZ	1:B:1430:PHE:O	2.40	0.53
1:B:657:PRO:HD2	1:C:656:THR:OG1	2.08	0.53
1:A:571:SER:O	1:A:586:ARG:N	2.41	0.53
1:B:60:VAL:HG12	1:B:107:VAL:HA	1.89	0.53
1:B:1351:THR:OG1	1:B:1353:ASP:OD1	2.26	0.53
1:C:1343:LEU:H	1:C:1461:ALA:HB3	1.74	0.53
1:D:1406:SER:OG	1:D:1417:ILE:HD12	2.08	0.53
1:A:156:HIS:ND1	1:A:157:PRO:O	2.42	0.53
1:D:1229:THR:HG21	1:D:1322:VAL:HG23	1.90	0.53
1:D:1369:TYR:OH	1:D:1456:ASP:OD2	2.20	0.53
1:B:931:LEU:O	1:B:1312:TYR:N	2.41	0.53
1:D:910:LEU:N	1:D:1332:ILE:O	2.42	0.53
1:A:58:VAL:HG12	1:A:60:VAL:HG13	1.91	0.53
1:B:167:ILE:HD12	1:B:176:ALA:CB	2.39	0.53
1:D:167:ILE:HD12	1:D:176:ALA:HB3	1.91	0.53
1:C:347:ILE:HG22	1:C:348:THR:HG23	1.91	0.53
1:B:167:ILE:HD12	1:B:176:ALA:HB3	1.91	0.53
1:C:1341:PHE:O	1:C:1461:ALA:HB2	2.09	0.53
1:D:167:ILE:HD12	1:D:176:ALA:CB	2.39	0.53
1:A:665:ASP:N	1:A:668:SER:OG	2.42	0.52
1:D:1378:MET:N	1:D:1378:MET:SD	2.81	0.52
1:A:981:ALA:HB3	1:A:982:PRO:HD3	1.91	0.52
1:A:1341:PHE:O	1:A:1461:ALA:HB2	2.09	0.52
1:B:247:ASN:HD21	5:B:2003:NAG:C2	2.13	0.52
1:C:156:HIS:ND1	1:C:157:PRO:O	2.42	0.52
1:C:571:SER:O	1:C:586:ARG:N	2.41	0.52
1:C:1347:THR:HA	1:C:1363:ILE:HG23	1.92	0.52
1:B:311:LEU:HD12	1:B:311:LEU:O	2.10	0.52
1:C:360:ARG:NH1	1:C:459:VAL:O	2.43	0.52
1:C:836:ALA:HA	1:C:860:VAL:HG23	1.91	0.52
1:D:1208:MET:SD	1:D:1209:THR:N	2.83	0.52
1:A:1343:LEU:H	1:A:1461:ALA:HB3	1.74	0.52
1:B:950:VAL:HG23	1:B:1323:TYR:O	2.09	0.52
1:A:360:ARG:NH1	1:A:459:VAL:O	2.43	0.52
1:D:231:VAL:HG23	1:D:335:LEU:HD13	1.91	0.52
1:A:1347:THR:HA	1:A:1363:ILE:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:THR:HG21	1:B:1322:VAL:HG23	1.90	0.52
1:B:136:SER:O	1:B:220:THR:N	2.43	0.52
1:B:288:GLU:N	1:B:288:GLU:OE1	2.43	0.52
1:B:959:MET:SD	1:B:959:MET:N	2.83	0.52
1:D:910:LEU:O	1:D:1332:ILE:N	2.38	0.52
1:D:950:VAL:HG23	1:D:1323:TYR:O	2.09	0.52
1:A:347:ILE:HG22	1:A:348:THR:HG23	1.91	0.52
1:B:129:VAL:HG12	1:B:150:SER:CB	2.40	0.52
1:D:129:VAL:HG12	1:D:150:SER:CB	2.40	0.52
1:D:311:LEU:HD12	1:D:311:LEU:O	2.10	0.52
1:D:983:ASN:O	1:D:986:VAL:HG22	2.10	0.52
1:A:836:ALA:HA	1:A:860:VAL:HG23	1.91	0.52
1:B:1208:MET:SD	1:B:1209:THR:N	2.83	0.52
1:B:1372:SER:CB	1:B:1422:VAL:HG11	2.40	0.52
1:D:959:MET:SD	1:D:959:MET:N	2.83	0.52
1:D:288:GLU:OE1	1:D:288:GLU:N	2.43	0.51
1:A:360:ARG:HH21	1:A:451:VAL:HG21	1.75	0.51
1:B:231:VAL:HG23	1:B:335:LEU:HD13	1.91	0.51
1:C:50:LEU:HD11	1:C:543:TYR:CE1	2.45	0.51
1:C:58:VAL:HG12	1:C:60:VAL:HG13	1.91	0.51
1:B:320:LEU:HD22	1:B:337:GLY:O	2.11	0.51
1:D:746:VAL:HG23	1:D:751:VAL:H	1.76	0.51
1:C:739:TRP:NE1	1:C:756:VAL:O	2.41	0.51
1:C:981:ALA:HB3	1:C:982:PRO:HD3	1.91	0.51
1:D:626:ASP:OD1	1:D:627:LEU:N	2.44	0.51
1:A:50:LEU:HD11	1:A:543:TYR:CE1	2.45	0.51
1:A:801:SER:OG	1:A:904:LEU:HD23	2.10	0.51
1:B:42:GLU:N	1:B:91:VAL:O	2.37	0.51
1:B:746:VAL:HG23	1:B:751:VAL:H	1.76	0.51
1:B:983:ASN:O	1:B:986:VAL:HG22	2.10	0.51
1:D:1372:SER:CB	1:D:1422:VAL:HG11	2.40	0.51
1:A:268:ILE:HD11	1:A:309:PHE:CE1	2.45	0.51
1:A:366:PHE:N	1:A:462:GLU:OE2	2.44	0.51
1:C:176:ALA:HB2	1:C:192:PHE:CZ	2.46	0.51
1:C:268:ILE:HD11	1:C:309:PHE:CE1	2.45	0.51
1:B:614:SER:OG	1:B:617:SER:N	2.41	0.51
1:C:366:PHE:N	1:C:462:GLU:OE2	2.44	0.51
1:C:665:ASP:N	1:C:668:SER:OG	2.42	0.51
1:D:136:SER:O	1:D:220:THR:N	2.43	0.51
1:D:320:LEU:HD22	1:D:337:GLY:O	2.11	0.51
1:D:361:GLN:HB3	1:D:450:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:ARG:HB3	1:D:404:LEU:HD23	1.93	0.51
1:D:951:LEU:HD21	1:D:953:ASP:OD2	2.11	0.51
1:A:71:ARG:HG2	1:A:101:MET:HE3	1.91	0.51
1:A:1151:ALA:HB2	1:A:1167:LEU:HD11	1.93	0.51
1:B:578:LEU:O	1:B:757:THR:HG21	2.10	0.51
1:C:71:ARG:HG2	1:C:101:MET:HE3	1.91	0.51
1:C:1050:ALA:O	1:C:1053:ARG:NH1	2.43	0.51
1:D:813:THR:HG22	1:D:854:GLN:O	2.11	0.51
1:B:910:LEU:N	1:B:1332:ILE:O	2.42	0.51
1:B:1191:ALA:HB3	1:B:1192:PRO:HD3	1.92	0.51
1:C:801:SER:OG	1:C:904:LEU:HD23	2.10	0.51
1:D:1191:ALA:HB3	1:D:1192:PRO:HD3	1.92	0.50
1:A:176:ALA:HB2	1:A:192:PHE:CZ	2.46	0.50
1:B:1091:ILE:HG23	1:B:1092:LYS:HG2	1.93	0.50
1:D:578:LEU:O	1:D:757:THR:HG21	2.10	0.50
1:D:912:LYS:NZ	1:D:913:GLU:O	2.44	0.50
1:A:62:ALA:HB1	1:A:103:LEU:HD11	1.94	0.50
1:A:1401:ARG:HG3	1:A:1417:ILE:HG21	1.94	0.50
1:B:271:LYS:N	1:B:317:GLU:O	2.40	0.50
1:C:360:ARG:HH21	1:C:451:VAL:HG21	1.75	0.50
1:D:409:ILE:HD13	1:D:419:LEU:HD21	1.93	0.50
1:A:580:ALA:O	1:A:757:THR:OG1	2.23	0.50
1:A:1168:LYS:NZ	1:A:1172:GLU:OE2	2.31	0.50
1:B:910:LEU:O	1:B:1332:ILE:N	2.38	0.50
1:C:1401:ARG:HG3	1:C:1417:ILE:HG21	1.94	0.50
1:C:425:TYR:OH	1:C:428:ARG:NE	2.45	0.50
1:C:1109:LEU:HD12	1:C:1117:THR:HG23	1.94	0.50
1:B:836:ALA:HA	1:B:860:VAL:HG23	1.94	0.50
1:B:912:LYS:NZ	1:B:913:GLU:O	2.44	0.50
1:D:247:ASN:HD21	5:D:2003:NAG:C2	2.13	0.50
1:A:425:TYR:OH	1:A:428:ARG:NE	2.45	0.50
1:A:1050:ALA:O	1:A:1053:ARG:NH1	2.43	0.50
1:B:599:ALA:O	1:B:740:ILE:N	2.44	0.50
1:B:813:THR:HG22	1:B:854:GLN:O	2.11	0.50
1:D:66:SER:OG	1:D:67:VAL:N	2.45	0.50
1:D:1415:VAL:C	1:D:1416:LEU:HD12	2.37	0.50
1:A:825:SER:N	1:A:875:GLU:O	2.45	0.50
1:B:571:SER:N	1:B:586:ARG:O	2.45	0.50
1:B:1415:VAL:C	1:B:1416:LEU:HD12	2.37	0.50
1:C:62:ALA:HB1	1:C:103:LEU:HD11	1.94	0.50
1:C:571:SER:N	1:C:586:ARG:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:SER:N	1:C:875:GLU:O	2.45	0.50
1:D:42:GLU:N	1:D:91:VAL:O	2.37	0.50
1:D:836:ALA:HA	1:D:860:VAL:HG23	1.94	0.50
1:B:370:ARG:HB3	1:B:404:LEU:HD23	1.93	0.50
1:C:1168:LYS:NZ	1:C:1172:GLU:OE2	2.31	0.50
1:B:66:SER:OG	1:B:67:VAL:N	2.45	0.49
1:B:626:ASP:OD1	1:B:627:LEU:N	2.44	0.49
1:B:1183:TRP:O	1:B:1184:GLU:HB2	2.12	0.49
1:B:668:SER:O	1:B:672:ASP:N	2.42	0.49
1:D:571:SER:N	1:D:586:ARG:O	2.45	0.49
1:D:1004:ALA:O	1:D:1008:LEU:N	2.44	0.49
1:A:571:SER:N	1:A:586:ARG:O	2.45	0.49
1:B:32:MET:HG3	1:B:679:THR:HG23	1.93	0.49
1:B:361:GLN:HB3	1:B:450:LEU:HD11	1.93	0.49
1:B:409:ILE:HD13	1:B:419:LEU:HD21	1.93	0.49
1:B:951:LEU:HD21	1:B:953:ASP:OD2	2.11	0.49
1:C:671:GLU:OE1	1:C:685:LYS:NZ	2.45	0.49
1:C:1151:ALA:HB2	1:C:1167:LEU:HD11	1.93	0.49
1:D:1183:TRP:O	1:D:1184:GLU:HB2	2.12	0.49
1:D:799:PRO:HB2	1:D:802:VAL:HG11	1.94	0.49
1:B:173:ASN:N	1:B:173:ASN:OD1	2.45	0.49
1:C:812:ALA:N	1:C:856:VAL:O	2.46	0.49
1:D:325:GLN:HA	1:D:332:VAL:HG13	1.93	0.49
1:D:874:ALA:O	1:D:897:ASP:N	2.46	0.49
1:B:1367:VAL:O	1:B:1426:THR:OG1	2.24	0.49
1:C:1451:ASP:OD1	1:C:1451:ASP:N	2.45	0.49
1:D:599:ALA:O	1:D:740:ILE:N	2.44	0.49
1:B:732:ARG:NH2	1:B:734:TYR:OH	2.46	0.49
1:D:1091:ILE:HG23	1:D:1092:LYS:HG2	1.93	0.49
1:B:325:GLN:HA	1:B:332:VAL:HG13	1.93	0.49
1:B:537:VAL:HG21	1:B:557:LYS:HD2	1.94	0.49
1:B:765:TRP:O	1:B:786:LEU:N	2.46	0.49
1:B:874:ALA:O	1:B:897:ASP:N	2.46	0.49
1:D:32:MET:HG3	1:D:679:THR:HG23	1.93	0.49
1:D:537:VAL:HG21	1:D:557:LYS:HD2	1.94	0.49
1:B:389:ASN:O	1:B:390:GLU:HB2	2.13	0.49
1:D:389:ASN:O	1:D:390:GLU:HB2	2.13	0.49
1:D:1367:VAL:O	1:D:1426:THR:OG1	2.24	0.49
1:A:812:ALA:N	1:A:856:VAL:O	2.46	0.49
1:C:1228:LEU:O	1:C:1232:THR:HG23	2.13	0.49
1:B:799:PRO:HB2	1:B:802:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:SER:O	1:D:672:ASP:N	2.42	0.48
1:D:732:ARG:NH2	1:D:734:TYR:OH	2.46	0.48
1:D:1171:ASN:OD1	1:D:1216:TYR:OH	2.13	0.48
1:A:1109:LEU:HD12	1:A:1117:THR:HG23	1.94	0.48
1:C:429:SER:O	1:C:431:CYS:N	2.44	0.48
1:D:173:ASN:N	1:D:173:ASN:OD1	2.45	0.48
1:D:373:ASP:OD1	1:D:373:ASP:N	2.45	0.48
1:D:914:THR:O	1:D:1328:LEU:N	2.43	0.48
1:D:992:GLU:OE2	1:D:1266:ALA:N	2.46	0.48
1:D:1020:HIS:N	1:D:1024:SER:O	2.46	0.48
1:A:656:THR:OG1	1:D:657:PRO:CD	2.62	0.48
1:B:456:LYS:O	1:B:483:ASN:N	2.46	0.48
1:B:992:GLU:OE2	1:B:1266:ALA:N	2.46	0.48
1:B:1047:LYS:O	1:B:1050:ALA:HB3	2.13	0.48
1:A:585:LEU:HD21	1:A:599:ALA:HB2	1.96	0.48
1:D:290:PHE:CG	1:D:304:VAL:HG12	2.49	0.48
1:D:387:ARG:HB2	1:D:420:THR:HG23	1.95	0.48
1:D:1422:VAL:HG13	1:D:1423:SER:H	1.79	0.48
1:C:136:SER:O	1:C:220:THR:N	2.47	0.48
1:A:136:SER:O	1:A:220:THR:N	2.47	0.48
1:A:1228:LEU:O	1:A:1232:THR:HG23	2.13	0.48
1:B:657:PRO:CD	1:C:656:THR:OG1	2.62	0.48
1:A:1451:ASP:N	1:A:1451:ASP:OD1	2.45	0.48
1:B:387:ARG:HB2	1:B:420:THR:HG23	1.95	0.48
1:D:1047:LYS:O	1:D:1050:ALA:HB3	2.13	0.48
1:A:1410:VAL:HG22	1:A:1412:SER:H	1.78	0.48
1:B:657:PRO:N	1:C:656:THR:OG1	2.46	0.48
1:B:1352:CYS:SG	1:B:1358:HIS:N	2.87	0.48
1:C:1440:ARG:NH2	1:C:1468:SER:OG	2.47	0.48
1:C:1410:VAL:HG22	1:C:1412:SER:H	1.78	0.48
1:D:765:TRP:O	1:D:786:LEU:N	2.46	0.48
1:D:1372:SER:HB3	1:D:1422:VAL:HG11	1.96	0.48
1:A:429:SER:O	1:A:431:CYS:N	2.44	0.47
1:B:497:TYR:C	1:B:498:LEU:HD22	2.39	0.47
1:D:1181:VAL:HG11	1:D:1208:MET:HE3	1.96	0.47
1:A:656:THR:OG1	1:D:657:PRO:N	2.46	0.47
1:A:739:TRP:NE1	1:A:756:VAL:O	2.41	0.47
1:B:1181:VAL:HG11	1:B:1208:MET:HE3	1.96	0.47
1:B:1451:ASP:OD1	1:B:1451:ASP:N	2.47	0.47
1:C:64:LEU:HD12	1:C:103:LEU:HD13	1.95	0.47
1:D:247:ASN:ND2	5:D:2003:NAG:C2	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:TYR:C	1:A:498:LEU:HD22	2.39	0.47
1:B:974:GLU:N	1:B:974:GLU:OE2	2.48	0.47
1:B:1372:SER:HB3	1:B:1422:VAL:HG11	1.96	0.47
1:A:1440:ARG:NH2	1:A:1468:SER:OG	2.47	0.47
1:C:1252:GLN:O	1:C:1255:VAL:HG22	2.14	0.47
1:D:1176:LYS:HB3	1:D:1181:VAL:HG13	1.96	0.47
1:D:1420:ASP:OD1	1:D:1420:ASP:N	2.47	0.47
1:B:290:PHE:CG	1:B:304:VAL:HG12	2.49	0.47
1:B:602:GLN:O	1:B:606:LEU:N	2.42	0.47
1:B:1176:LYS:HB3	1:B:1181:VAL:HG13	1.96	0.47
1:B:1422:VAL:HG13	1:B:1423:SER:H	1.79	0.47
1:D:456:LYS:O	1:D:483:ASN:N	2.46	0.47
1:A:64:LEU:HD12	1:A:103:LEU:HD13	1.95	0.47
1:A:1252:GLN:O	1:A:1255:VAL:HG22	2.14	0.47
1:B:1420:ASP:OD1	1:B:1420:ASP:N	2.47	0.47
1:C:104:THR:HG22	1:C:117:ARG:HA	1.97	0.47
1:C:498:LEU:HD23	1:C:543:TYR:HE2	1.80	0.47
1:D:572:PHE:CG	1:D:786:LEU:HD12	2.50	0.47
1:D:1352:CYS:SG	1:D:1358:HIS:N	2.87	0.47
1:A:498:LEU:HD23	1:A:543:TYR:HE2	1.80	0.47
1:A:641:ASP:O	1:A:658:VAL:HG11	2.15	0.47
1:A:650:ILE:HD13	1:A:655:TYR:HB3	1.96	0.47
1:B:835:LEU:HB2	1:B:861:THR:HG23	1.97	0.47
1:C:641:ASP:O	1:C:658:VAL:HG11	2.15	0.47
1:C:650:ILE:HD13	1:C:655:TYR:HB3	1.96	0.47
1:D:497:TYR:C	1:D:498:LEU:HD22	2.39	0.47
1:D:924:GLY:N	1:D:1318:GLY:O	2.44	0.47
1:D:974:GLU:OE2	1:D:974:GLU:N	2.48	0.47
1:C:585:LEU:HD21	1:C:599:ALA:HB2	1.96	0.47
1:D:1200:GLN:OE1	1:D:1200:GLN:N	2.46	0.47
1:A:960:GLN:OE1	1:A:1242:GLN:NE2	2.48	0.47
1:B:1363:ILE:HG22	1:B:1365:LEU:CD1	2.45	0.47
1:C:497:TYR:C	1:C:498:LEU:HD22	2.39	0.47
1:C:1042:THR:HA	1:C:1045:VAL:HG12	1.97	0.47
1:A:272:TYR:CB	1:A:275:ALA:HB2	2.45	0.47
1:B:1168:LYS:O	1:B:1172:GLU:N	2.40	0.47
1:B:914:THR:O	1:B:1328:LEU:N	2.43	0.46
1:C:270:ARG:O	1:C:285:ALA:N	2.41	0.46
1:D:167:ILE:HG12	1:D:205:VAL:HG22	1.97	0.46
1:D:902:PRO:HG3	5:D:2004:NAG:H61	1.97	0.46
1:B:80:GLU:OE1	1:B:80:GLU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ASP:OD1	1:B:373:ASP:N	2.45	0.46
1:D:835:LEU:HB2	1:D:861:THR:HG23	1.97	0.46
1:D:1451:ASP:N	1:D:1451:ASP:OD1	2.47	0.46
1:A:1042:THR:HA	1:A:1045:VAL:HG12	1.97	0.46
1:B:386:ILE:HA	1:B:421:VAL:HG13	1.97	0.46
1:B:570:LEU:HB2	1:B:585:LEU:HD11	1.98	0.46
1:C:960:GLN:OE1	1:C:1242:GLN:NE2	2.48	0.46
1:A:104:THR:HG22	1:A:117:ARG:HA	1.97	0.46
1:A:982:PRO:HG2	1:A:1255:VAL:HG21	1.97	0.46
1:C:1384:LYS:H	1:C:1447:VAL:HG11	1.81	0.46
1:D:539:ARG:NE	1:D:626:ASP:OD2	2.45	0.46
1:A:1070:LEU:HD12	1:A:1109:LEU:HD22	1.98	0.46
1:C:614:SER:O	1:C:617:SER:OG	2.29	0.46
1:A:356:ASP:OD2	1:A:460:HIS:NE2	2.46	0.46
1:A:671:GLU:OE1	1:A:685:LYS:NZ	2.45	0.46
1:A:1364:SER:C	1:A:1365:LEU:HD12	2.40	0.46
1:B:176:ALA:HB2	1:B:192:PHE:CE1	2.51	0.46
1:B:980:PHE:CE1	1:B:1041:LEU:HD23	2.50	0.46
1:C:120:VAL:C	1:C:121:MET:HE2	2.41	0.46
1:D:50:LEU:HD11	1:D:543:TYR:CZ	2.51	0.46
1:D:80:GLU:OE1	1:D:80:GLU:N	2.48	0.46
1:A:1384:LYS:H	1:A:1447:VAL:HG11	1.81	0.46
1:B:1171:ASN:OD1	1:B:1216:TYR:OH	2.13	0.46
1:C:39:LEU:HD12	1:C:122:VAL:HG12	1.98	0.46
1:C:982:PRO:HG2	1:C:1255:VAL:HG21	1.97	0.46
1:C:1364:SER:C	1:C:1365:LEU:HD12	2.40	0.46
1:D:644:ASN:ND2	1:D:692:LEU:HD13	2.31	0.46
1:A:1163:ARG:HA	1:A:1166:VAL:HG22	1.98	0.46
1:B:50:LEU:HD11	1:B:543:TYR:CZ	2.51	0.46
1:B:572:PHE:CG	1:B:786:LEU:HD12	2.50	0.46
1:C:1232:THR:HG22	1:C:1264:TYR:OH	2.16	0.46
1:D:386:ILE:HA	1:D:421:VAL:HG13	1.97	0.46
1:D:980:PHE:CE1	1:D:1041:LEU:HD23	2.50	0.46
1:B:578:LEU:HD23	1:B:760:ASP:H	1.81	0.46
1:C:1163:ARG:HA	1:C:1166:VAL:HG22	1.98	0.46
1:D:50:LEU:HD11	1:D:543:TYR:CE1	2.51	0.46
1:D:1365:LEU:HD13	1:D:1431:PHE:HE1	1.80	0.46
1:A:243:GLU:CG	1:A:306:THR:HG21	2.46	0.46
1:A:1404:HIS:O	1:A:1405:VAL:HG13	2.16	0.46
1:B:1200:GLN:OE1	1:B:1200:GLN:N	2.46	0.46
1:B:1365:LEU:HD13	1:B:1431:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1070:LEU:HD12	1:C:1109:LEU:HD22	1.98	0.46
1:D:1132:TRP:O	1:D:1136:GLN:N	2.46	0.46
1:B:902:PRO:HG3	5:B:2004:NAG:H61	1.97	0.45
1:B:1004:ALA:O	1:B:1008:LEU:N	2.44	0.45
1:B:1020:HIS:N	1:B:1024:SER:O	2.46	0.45
1:B:1181:VAL:O	1:B:1181:VAL:HG23	2.16	0.45
1:B:1447:VAL:O	1:B:1447:VAL:HG13	2.16	0.45
1:C:252:GLY:C	1:C:253:LEU:HD12	2.41	0.45
1:D:578:LEU:HD23	1:D:760:ASP:H	1.81	0.45
1:D:823:ARG:NH1	1:D:824:VAL:O	2.49	0.45
1:B:50:LEU:HD11	1:B:543:TYR:CE1	2.51	0.45
1:C:1125:LEU:HD12	1:C:1128:LEU:HD22	1.98	0.45
1:A:120:VAL:C	1:A:121:MET:HE2	2.41	0.45
1:B:167:ILE:HG12	1:B:205:VAL:HG22	1.97	0.45
1:B:1250:SER:OG	1:B:1251:THR:N	2.49	0.45
1:C:386:ILE:HD11	1:C:397:ALA:HB3	1.98	0.45
1:D:996:LEU:HD23	1:D:997:THR:C	2.41	0.45
1:A:386:ILE:HD11	1:A:397:ALA:HB3	1.98	0.45
1:B:1132:TRP:O	1:B:1136:GLN:N	2.46	0.45
1:D:64:LEU:HD11	1:D:101:MET:CB	2.47	0.45
1:D:602:GLN:O	1:D:606:LEU:N	2.42	0.45
1:D:1363:ILE:HG22	1:D:1365:LEU:CD1	2.45	0.45
1:A:614:SER:O	1:A:617:SER:OG	2.29	0.45
1:A:1125:LEU:HD12	1:A:1128:LEU:HD22	1.98	0.45
1:B:644:ASN:ND2	1:B:692:LEU:HD13	2.31	0.45
1:B:1255:VAL:HG23	1:B:1256:VAL:HG23	1.98	0.45
1:D:1250:SER:OG	1:D:1251:THR:N	2.49	0.45
1:A:39:LEU:HD12	1:A:122:VAL:HG12	1.98	0.45
1:A:599:ALA:HB3	1:A:740:ILE:HB	1.98	0.45
1:B:468:LEU:N	1:B:561:GLU:OE1	2.48	0.45
1:B:823:ARG:NH1	1:B:824:VAL:O	2.49	0.45
1:B:1232:THR:HG22	1:B:1264:TYR:OH	2.17	0.45
1:C:1404:HIS:O	1:C:1405:VAL:HG13	2.16	0.45
1:D:176:ALA:HB2	1:D:192:PHE:CE1	2.51	0.45
1:D:1264:TYR:O	1:D:1267:ALA:N	2.50	0.45
1:A:133:THR:OG1	1:A:217:HIS:NE2	2.36	0.45
1:A:252:GLY:C	1:A:253:LEU:HD12	2.41	0.45
1:A:1232:THR:HG22	1:A:1264:TYR:OH	2.16	0.45
1:B:432:TYR:OH	1:B:437:VAL:HG22	2.17	0.45
1:B:650:ILE:HG21	1:B:655:TYR:CD1	2.52	0.45
1:C:243:GLU:CG	1:C:306:THR:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:SER:O	1:D:124:ASN:ND2	2.50	0.45
1:D:794:VAL:HG21	1:D:899:VAL:HG21	1.99	0.45
1:D:1168:LYS:O	1:D:1172:GLU:N	2.40	0.45
1:B:64:LEU:HD11	1:B:101:MET:CB	2.47	0.45
1:B:270:ARG:O	1:B:285:ALA:N	2.50	0.45
1:B:409:ILE:CD1	1:B:419:LEU:HD21	2.47	0.45
1:B:996:LEU:HD23	1:B:997:THR:C	2.41	0.45
1:C:1144:VAL:HG23	1:C:1145:TYR:CD1	2.52	0.45
1:D:270:ARG:O	1:D:285:ALA:N	2.50	0.45
1:D:1447:VAL:O	1:D:1447:VAL:HG13	2.16	0.45
1:D:432:TYR:OH	1:D:437:VAL:HG22	2.17	0.45
1:D:1181:VAL:HG23	1:D:1181:VAL:O	2.16	0.45
1:B:924:GLY:N	1:B:1318:GLY:O	2.44	0.45
1:C:234:THR:N	1:C:249:SER:O	2.50	0.45
1:C:1163:ARG:O	1:C:1167:LEU:HD13	2.17	0.45
1:A:234:THR:N	1:A:249:SER:O	2.50	0.44
1:A:270:ARG:O	1:A:285:ALA:N	2.41	0.44
1:B:794:VAL:HG21	1:B:899:VAL:HG21	1.99	0.44
1:B:874:ALA:N	1:B:897:ASP:O	2.50	0.44
1:B:1435:GLN:NE2	1:B:1437:VAL:O	2.46	0.44
1:C:599:ALA:HB3	1:C:740:ILE:HB	1.98	0.44
1:D:386:ILE:HD12	1:D:395:SER:O	2.18	0.44
1:D:650:ILE:HG21	1:D:655:TYR:CD1	2.52	0.44
1:D:729:GLU:N	1:D:729:GLU:OE1	2.51	0.44
1:D:1041:LEU:HD11	1:D:1091:ILE:HG12	1.99	0.44
1:A:773:SER:OG	1:A:775:ASP:OD1	2.27	0.44
1:A:1346:GLN:O	1:A:1364:SER:N	2.51	0.44
1:B:96:SER:O	1:B:124:ASN:ND2	2.50	0.44
1:B:386:ILE:HD12	1:B:395:SER:O	2.18	0.44
1:B:1264:TYR:O	1:B:1267:ALA:N	2.50	0.44
1:C:272:TYR:CB	1:C:275:ALA:HB2	2.45	0.44
1:C:356:ASP:OD2	1:C:460:HIS:NE2	2.46	0.44
1:D:361:GLN:OE1	1:D:361:GLN:N	2.50	0.44
1:D:570:LEU:HB2	1:D:585:LEU:HD11	1.98	0.44
1:A:1163:ARG:O	1:A:1167:LEU:HD13	2.17	0.44
1:C:1351:THR:OG1	1:C:1353:ASP:OD1	2.35	0.44
1:D:111:THR:HG23	1:D:112:GLN:HG2	2.00	0.44
1:D:1255:VAL:HG23	1:D:1256:VAL:HG23	1.98	0.44
1:A:427:ASP:OD1	1:A:428:ARG:N	2.51	0.44
1:A:931:LEU:O	1:A:1312:TYR:N	2.50	0.44
1:B:729:GLU:N	1:B:729:GLU:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:ARG:NH1	1:D:672:ASP:O	2.46	0.44
1:B:64:LEU:HD11	1:B:101:MET:HB2	2.00	0.44
1:B:361:GLN:OE1	1:B:361:GLN:N	2.50	0.44
1:B:1416:LEU:O	1:B:1417:ILE:HD13	2.18	0.44
1:C:427:ASP:OD1	1:C:428:ARG:N	2.51	0.44
1:D:451:VAL:HG23	1:D:664:LYS:HZ2	1.83	0.44
1:B:111:THR:HG23	1:B:112:GLN:HG2	2.00	0.44
1:B:947:SER:OG	1:B:948:VAL:N	2.51	0.44
1:B:1048:THR:O	1:B:1052:ALA:N	2.46	0.44
1:A:1144:VAL:HG23	1:A:1145:TYR:CD1	2.52	0.44
1:B:247:ASN:ND2	5:B:2003:NAG:C2	2.75	0.44
1:D:568:VAL:CG2	1:D:589:ALA:HB2	2.47	0.44
1:D:1416:LEU:O	1:D:1417:ILE:HD13	2.18	0.44
1:B:351:SER:O	1:B:369:VAL:HG13	2.18	0.44
1:C:1346:GLN:O	1:C:1364:SER:N	2.51	0.44
1:D:1232:THR:HG22	1:D:1264:TYR:OH	2.17	0.44
1:A:50:LEU:HD11	1:A:543:TYR:CZ	2.53	0.44
1:A:461:LEU:HD11	1:A:542:ILE:HG21	2.00	0.44
1:B:568:VAL:CG2	1:B:589:ALA:HB2	2.47	0.44
1:D:351:SER:O	1:D:369:VAL:HG13	2.18	0.44
1:B:1065:GLN:HA	1:B:1068:ILE:HG22	2.00	0.43
1:B:1251:THR:HG21	1:B:1407:ARG:HG2	1.99	0.43
1:C:167:ILE:HD12	1:C:176:ALA:CB	2.48	0.43
1:C:461:LEU:HD11	1:C:542:ILE:HG21	2.00	0.43
1:C:585:LEU:CD2	1:C:599:ALA:HB2	2.48	0.43
1:C:1041:LEU:HD13	1:C:1091:ILE:HD11	2.00	0.43
1:D:1251:THR:HG21	1:D:1407:ARG:HG2	1.99	0.43
1:B:229:PHE:CD2	1:B:231:VAL:HG22	2.54	0.43
1:B:659:SER:N	1:C:654:THR:HG21	2.34	0.43
1:B:1041:LEU:HD11	1:B:1091:ILE:HG12	1.99	0.43
1:C:580:ALA:O	1:C:757:THR:OG1	2.23	0.43
1:D:537:VAL:HG22	1:D:538:ALA:H	1.83	0.43
1:D:1065:GLN:HA	1:D:1068:ILE:HG22	2.00	0.43
2:H:2:NAG:H3	2:H:2:NAG:H82	1.99	0.43
1:B:590:ALA:O	1:B:746:VAL:HG11	2.19	0.43
1:B:871:THR:HG22	1:B:900:ILE:HG23	2.00	0.43
1:C:614:SER:C	1:C:617:SER:HG	2.23	0.43
1:C:1227:ASP:OD1	1:C:1227:ASP:N	2.52	0.43
1:D:229:PHE:CD2	1:D:231:VAL:HG22	2.54	0.43
1:D:468:LEU:N	1:D:561:GLU:OE1	2.48	0.43
1:D:1000:ILE:HG23	1:D:1001:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:THR:HA	1:A:1042:THR:HG22	2.00	0.43
1:C:233:VAL:HG23	1:C:250:VAL:HG22	2.00	0.43
1:C:498:LEU:HD23	1:C:543:TYR:CE2	2.53	0.43
1:C:1386:VAL:HG13	1:C:1445:ALA:HB3	2.01	0.43
1:D:409:ILE:CD1	1:D:419:LEU:HD21	2.47	0.43
1:D:871:THR:HG22	1:D:900:ILE:HG23	2.00	0.43
1:A:167:ILE:HD12	1:A:176:ALA:CB	2.48	0.43
1:A:498:LEU:HD23	1:A:543:TYR:CE2	2.53	0.43
1:A:1447:VAL:HG13	1:A:1447:VAL:O	2.19	0.43
1:B:480:TYR:CE2	1:B:513:LEU:HD21	2.54	0.43
1:B:1050:ALA:O	1:B:1053:ARG:NH1	2.50	0.43
1:C:50:LEU:HD11	1:C:543:TYR:CZ	2.53	0.43
1:C:1365:LEU:HD13	1:C:1431:PHE:HE1	1.83	0.43
1:D:64:LEU:HD11	1:D:101:MET:HB2	2.00	0.43
1:D:146:PHE:O	1:D:190:PHE:N	2.50	0.43
1:A:585:LEU:CD2	1:A:599:ALA:HB2	2.48	0.43
1:A:926:GLU:OE2	1:A:1315:LYS:NZ	2.49	0.43
1:A:1041:LEU:HD13	1:A:1091:ILE:HD11	2.00	0.43
1:A:1227:ASP:OD1	1:A:1227:ASP:N	2.52	0.43
1:C:1341:PHE:HB2	1:C:1459:ALA:HB1	2.00	0.43
1:D:480:TYR:CE2	1:D:513:LEU:HD21	2.54	0.43
1:A:654:THR:HG21	1:D:659:SER:N	2.34	0.43
1:A:1380:ILE:HD11	1:A:1449:VAL:HG11	2.00	0.43
1:A:1386:VAL:HG13	1:A:1445:ALA:HB3	2.01	0.43
1:B:297:HIS:ND1	1:B:297:HIS:O	2.52	0.43
1:C:742:ASP:OD1	1:C:742:ASP:N	2.52	0.43
1:C:1380:ILE:HD11	1:C:1449:VAL:HG11	2.00	0.43
1:D:614:SER:N	1:D:617:SER:OG	2.49	0.43
2:E:2:NAG:H3	2:E:2:NAG:H82	1.99	0.43
1:A:742:ASP:OD1	1:A:742:ASP:N	2.52	0.43
1:A:765:TRP:HB2	1:A:786:LEU:HD22	2.01	0.43
1:A:1341:PHE:HB2	1:A:1459:ALA:HB1	2.00	0.43
1:C:388:GLY:HA3	1:C:409:ILE:HD13	2.01	0.43
1:A:1351:THR:OG1	1:A:1353:ASP:OD1	2.35	0.43
1:C:1097:ASP:O	1:C:1100:THR:OG1	2.35	0.43
1:D:203:TYR:O	1:D:219:PHE:N	2.47	0.43
1:D:297:HIS:O	1:D:297:HIS:ND1	2.52	0.43
1:A:167:ILE:HB	1:A:176:ALA:HB3	2.01	0.42
1:A:233:VAL:HG23	1:A:250:VAL:HG22	2.00	0.42
1:B:537:VAL:HG22	1:B:538:ALA:H	1.83	0.42
1:B:1341:PHE:O	1:B:1461:ALA:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:GLN:O	1:C:51:LEU:HD12	2.18	0.42
1:C:765:TRP:HB2	1:C:786:LEU:HD22	2.01	0.42
1:A:30:GLN:O	1:A:51:LEU:HD12	2.18	0.42
1:A:336:THR:O	1:A:336:THR:OG1	2.38	0.42
1:B:451:VAL:HG23	1:B:664:LYS:HZ2	1.83	0.42
1:C:931:LEU:O	1:C:1312:TYR:N	2.50	0.42
1:C:1347:THR:HG23	1:C:1463:TYR:CE2	2.54	0.42
1:D:415:MET:SD	1:D:416:GLY:N	2.92	0.42
1:D:874:ALA:N	1:D:897:ASP:O	2.50	0.42
1:A:388:GLY:HA3	1:A:409:ILE:HD13	2.01	0.42
1:B:146:PHE:O	1:B:190:PHE:N	2.50	0.42
1:B:1000:ILE:HG23	1:B:1001:LYS:HD3	2.00	0.42
1:B:1041:LEU:HD11	1:B:1091:ILE:CG1	2.49	0.42
1:C:150:SER:N	1:C:186:GLY:O	2.51	0.42
1:A:1097:ASP:O	1:A:1100:THR:OG1	2.35	0.42
1:A:1347:THR:HG23	1:A:1463:TYR:CE2	2.54	0.42
1:B:415:MET:SD	1:B:416:GLY:N	2.92	0.42
1:C:243:GLU:O	1:C:306:THR:OG1	2.37	0.42
1:C:535:ALA:O	1:C:560:VAL:HG21	2.19	0.42
1:C:679:THR:HG22	1:C:681:SER:H	1.84	0.42
1:C:1191:ALA:HB3	1:C:1192:PRO:HD3	2.01	0.42
1:D:800:TYR:CG	1:D:801:SER:N	2.88	0.42
1:D:1422:VAL:HG13	1:D:1423:SER:N	2.34	0.42
1:B:1422:VAL:HG13	1:B:1423:SER:N	2.34	0.42
1:C:77:LEU:HD22	1:C:87:VAL:HG11	2.02	0.42
1:C:614:SER:OG	1:C:615:ALA:N	2.53	0.42
1:D:1050:ALA:O	1:D:1053:ARG:NH1	2.50	0.42
1:A:243:GLU:O	1:A:306:THR:OG1	2.37	0.42
1:B:116:LYS:NZ	1:B:638:ASP:O	2.50	0.42
1:D:1041:LEU:HD11	1:D:1091:ILE:CG1	2.49	0.42
1:A:77:LEU:HD22	1:A:87:VAL:HG11	2.02	0.42
1:A:535:ALA:O	1:A:560:VAL:HG21	2.19	0.42
1:A:1365:LEU:HD13	1:A:1431:PHE:HE1	1.83	0.42
1:B:614:SER:N	1:B:617:SER:OG	2.49	0.42
1:B:1389:PHE:HB3	1:B:1433:VAL:HG21	2.01	0.42
1:C:1039:THR:HA	1:C:1042:THR:HG22	2.00	0.42
1:C:1447:VAL:O	1:C:1447:VAL:HG13	2.19	0.42
1:D:240:THR:OG1	1:D:241:ILE:N	2.53	0.42
1:A:255:THR:HG22	1:A:258:LYS:HE2	2.02	0.42
1:A:614:SER:OG	1:A:615:ALA:N	2.53	0.42
1:A:874:ALA:O	1:A:897:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1191:ALA:HB3	1:A:1192:PRO:HD3	2.01	0.42
1:B:617:SER:O	1:B:621:LEU:N	2.42	0.42
1:B:934:LYS:NZ	1:B:1308:LEU:O	2.47	0.42
1:A:679:THR:HG22	1:A:681:SER:H	1.84	0.42
1:A:996:LEU:HD23	1:A:997:THR:C	2.45	0.42
1:A:1270:THR:OG1	1:A:1271:ARG:N	2.53	0.42
1:A:1333:LEU:HD22	1:A:1446:ILE:HD11	2.02	0.42
1:B:539:ARG:NE	1:B:626:ASP:OD2	2.45	0.42
1:B:912:LYS:HD2	1:B:1332:ILE:HD13	2.02	0.42
1:C:1333:LEU:HD22	1:C:1446:ILE:HD11	2.02	0.42
1:B:35:VAL:HG23	1:B:35:VAL:O	2.20	0.41
1:B:384:ILE:HD11	1:B:397:ALA:HB3	2.02	0.41
1:B:401:GLU:OE2	1:B:401:GLU:N	2.51	0.41
1:C:656:THR:HB	1:C:657:PRO:HD3	2.02	0.41
1:D:590:ALA:O	1:D:746:VAL:HG11	2.19	0.41
1:D:947:SER:OG	1:D:948:VAL:N	2.51	0.41
1:A:1039:THR:O	1:A:1039:THR:HG22	2.20	0.41
1:C:168:GLN:N	1:C:204:LYS:O	2.44	0.41
1:D:564:LEU:HD22	1:D:780:ILE:HG22	2.02	0.41
3:F:1:NAG:H62	3:F:2:NAG:HN2	1.85	0.41
1:A:373:ASP:OD1	1:A:373:ASP:N	2.53	0.41
1:C:373:ASP:OD1	1:C:373:ASP:N	2.53	0.41
1:C:996:LEU:HD23	1:C:997:THR:C	2.45	0.41
1:D:231:VAL:CG2	1:D:335:LEU:HD13	2.50	0.41
1:D:384:ILE:HD11	1:D:397:ALA:HB3	2.02	0.41
1:D:679:THR:HG22	1:D:681:SER:N	2.35	0.41
1:D:1346:GLN:O	1:D:1364:SER:N	2.52	0.41
1:D:1389:PHE:HB3	1:D:1433:VAL:HG21	2.01	0.41
1:A:1363:ILE:HG22	1:A:1365:LEU:CD1	2.50	0.41
1:B:803:ILE:HG22	1:B:804:ARG:N	2.35	0.41
1:C:250:VAL:HG21	1:C:266:VAL:CG2	2.51	0.41
1:C:1039:THR:HG22	1:C:1039:THR:O	2.20	0.41
1:D:746:VAL:HG22	1:D:747:ASN:O	2.21	0.41
2:H:1:NAG:O3	2:H:1:NAG:C7	2.69	0.41
1:B:240:THR:OG1	1:B:241:ILE:N	2.53	0.41
1:B:458:PHE:CE2	1:B:481:ILE:HD11	2.56	0.41
1:B:733:LYS:NZ	1:B:734:TYR:O	2.53	0.41
1:B:746:VAL:HG22	1:B:747:ASN:O	2.21	0.41
1:C:255:THR:HG22	1:C:258:LYS:HE2	2.02	0.41
1:D:35:VAL:HG23	1:D:35:VAL:O	2.20	0.41
1:D:64:LEU:HD13	1:D:120:VAL:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:THR:HG23	1:D:257:GLY:H	1.85	0.41
1:D:456:LYS:C	1:D:457:SER:HG	2.26	0.41
1:D:1341:PHE:O	1:D:1461:ALA:HB2	2.19	0.41
1:A:168:GLN:N	1:A:204:LYS:O	2.44	0.41
1:B:255:THR:HG23	1:B:257:GLY:H	1.85	0.41
1:C:458:PHE:HB3	1:C:552:ILE:HG21	2.02	0.41
1:C:599:ALA:HB3	1:C:740:ILE:CB	2.51	0.41
1:D:64:LEU:HD11	1:D:101:MET:C	2.46	0.41
1:D:458:PHE:CE2	1:D:481:ILE:HD11	2.56	0.41
1:D:1407:ARG:HB2	1:D:1419:LEU:HD21	2.03	0.41
1:B:231:VAL:CG2	1:B:335:LEU:HD13	2.50	0.41
1:C:1386:VAL:HG12	1:C:1387:SER:H	1.85	0.41
1:D:1024:SER:OG	1:D:1025:TYR:N	2.53	0.41
1:A:195:SER:HA	1:A:1244:ALA:HB3	2.02	0.41
1:A:250:VAL:HG21	1:A:266:VAL:CG2	2.51	0.41
1:A:614:SER:N	1:A:617:SER:OG	2.51	0.41
1:B:679:THR:HG22	1:B:681:SER:N	2.35	0.41
1:C:1091:ILE:HG23	1:C:1092:LYS:N	2.36	0.41
1:D:733:LYS:NZ	1:D:734:TYR:O	2.53	0.41
1:A:1386:VAL:HG12	1:A:1387:SER:H	1.85	0.41
1:B:64:LEU:HD11	1:B:101:MET:C	2.46	0.41
1:B:240:THR:OG1	1:B:347:ILE:HG23	2.21	0.41
1:B:800:TYR:CG	1:B:801:SER:N	2.88	0.41
1:B:1061:ALA:HA	1:B:1064:THR:HG22	2.03	0.41
1:B:1088:ASN:OD1	1:B:1088:ASN:N	2.53	0.41
1:B:1161:ASP:OD1	1:B:1161:ASP:N	2.54	0.41
1:C:33:VAL:O	1:C:33:VAL:HG13	2.21	0.41
1:C:128:LEU:HD11	1:C:623:PRO:CD	2.51	0.41
1:C:167:ILE:HB	1:C:176:ALA:HB3	2.01	0.41
1:C:336:THR:O	1:C:336:THR:OG1	2.38	0.41
1:C:1363:ILE:HG22	1:C:1365:LEU:CD1	2.50	0.41
1:D:763:THR:OG1	1:D:764:GLU:N	2.54	0.41
1:D:1252:GLN:O	1:D:1255:VAL:HG22	2.21	0.41
3:I:1:NAG:H62	3:I:2:NAG:HN2	1.85	0.41
1:A:458:PHE:HB3	1:A:552:ILE:HG21	2.02	0.41
1:A:617:SER:HG	1:A:618:VAL:H	1.69	0.41
1:B:1024:SER:OG	1:B:1025:TYR:N	2.53	0.41
1:C:656:THR:HB	1:C:657:PRO:HD2	2.03	0.41
1:D:803:ILE:HG22	1:D:804:ARG:N	2.35	0.41
1:D:912:LYS:HD2	1:D:1332:ILE:HD13	2.02	0.41
1:A:656:THR:HB	1:A:657:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:LEU:HD11	1:B:1226:GLU:HB3	2.04	0.40
1:C:1398:MET:CG	1:C:1415:VAL:HG13	2.51	0.40
1:D:511:HIS:NE2	1:D:525:SER:OG	2.55	0.40
1:D:952:GLY:N	1:D:1297:ARG:O	2.54	0.40
1:A:1091:ILE:HG23	1:A:1092:LYS:N	2.36	0.40
1:B:64:LEU:HD13	1:B:120:VAL:CG2	2.51	0.40
1:B:73:LEU:HD12	1:B:91:VAL:HG12	2.03	0.40
1:B:539:ARG:NH1	1:B:672:ASP:O	2.46	0.40
1:B:564:LEU:HD22	1:B:780:ILE:HG22	2.02	0.40
1:B:952:GLY:N	1:B:1297:ARG:O	2.54	0.40
1:C:167:ILE:CG1	1:C:176:ALA:HB3	2.52	0.40
1:C:775:ASP:OD1	1:C:776:ALA:N	2.54	0.40
1:D:1061:ALA:HA	1:D:1064:THR:HG22	2.03	0.40
1:B:1346:GLN:O	1:B:1364:SER:N	2.52	0.40
1:B:1407:ARG:HB2	1:B:1419:LEU:HD21	2.03	0.40
1:C:1398:MET:HG3	1:C:1415:VAL:HG13	2.03	0.40
1:A:1405:VAL:O	1:A:1406:SER:OG	2.35	0.40
1:B:763:THR:OG1	1:B:764:GLU:N	2.54	0.40
1:C:195:SER:HA	1:C:1244:ALA:HB3	2.02	0.40
1:C:849:CYS:SG	1:C:850:ALA:N	2.91	0.40
1:C:1270:THR:OG1	1:C:1271:ARG:N	2.53	0.40
1:D:73:LEU:HD12	1:D:91:VAL:HG12	2.03	0.40
2:E:1:NAG:C7	2:E:1:NAG:O3	2.69	0.40
1:C:869:ASN:OD1	1:C:869:ASN:N	2.54	0.40
1:D:461:LEU:HG	1:D:478:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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
1	A	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	24 63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	21	59
1	C	1406/1474 (95%)	1190 (85%)	209 (15%)	7 (0%)	24	63
1	D	1404/1474 (95%)	1163 (83%)	233 (17%)	8 (1%)	21	59
All	All	5620/5896 (95%)	4706 (84%)	884 (16%)	30 (0%)	26	63

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	800	TYR
1	A	1184	GLU
1	B	1184	GLU
1	C	800	TYR
1	C	1184	GLU
1	D	1184	GLU
1	B	390	GLU
1	B	799	PRO
1	B	800	TYR
1	D	390	GLU
1	D	799	PRO
1	D	800	TYR
1	A	656	THR
1	C	656	THR
1	B	808	PHE
1	B	1182	HIS
1	D	808	PHE
1	D	1182	HIS
1	A	808	PHE
1	A	936	PRO
1	A	1186	PRO
1	C	808	PHE
1	C	936	PRO
1	C	1186	PRO
1	A	809	THR
1	C	809	THR
1	B	936	PRO
1	D	936	PRO
1	B	1186	PRO
1	D	1186	PRO

### 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	
1	A	1236/1290 (96%)	1230 (100%)	6 (0%)	81	83
1	B	1236/1290 (96%)	1233 (100%)	3 (0%)	87	87
1	C	1236/1290 (96%)	1230 (100%)	6 (0%)	81	83
1	D	1236/1290 (96%)	1233 (100%)	3 (0%)	87	87
All	All	4944/5160 (96%)	4926 (100%)	18 (0%)	81	84

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	299	CYS
1	A	410	ASN
1	A	869	ASN
1	A	1184	GLU
1	A	1424	ASN
1	B	247	ASN
1	B	348	THR
1	B	410	ASN
1	C	70	ASN
1	C	299	CYS
1	C	410	ASN
1	C	869	ASN
1	C	1184	GLU
1	C	1424	ASN
1	D	247	ASN
1	D	348	THR
1	D	410	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	142	GLN
1	A	389	ASN
1	A	474	GLN
1	A	816	ASN
1	A	827	GLN
1	A	893	HIS
1	A	964	ASN
1	A	983	ASN
1	A	1179	ASN
1	A	1277	GLN
1	A	1413	ASN
1	B	132	GLN
1	B	247	ASN
1	B	368	GLN
1	B	435	GLN
1	B	474	GLN
1	B	644	ASN
1	B	880	GLN
1	B	976	ASN
1	B	995	GLN
1	B	1159	ASN
1	B	1296	ASN
1	C	55	ASN
1	C	112	GLN
1	C	389	ASN
1	C	474	GLN
1	C	694	GLN
1	C	816	ASN
1	C	827	GLN
1	C	893	HIS
1	C	964	ASN
1	C	1036	GLN
1	C	1179	ASN
1	D	132	GLN
1	D	247	ASN
1	D	368	GLN
1	D	435	GLN
1	D	460	HIS
1	D	474	GLN
1	D	644	ASN
1	D	976	ASN

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Mol	Chain	Res	Type
1	D	995	GLN
1	D	1159	ASN
1	D	1277	GLN
1	D	1296	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

18 monosaccharides 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	$\# Z  > 2$
2	NAG	E	1	2	14,14,15	0.38	0	17,19,21	0.52	0
2	NAG	E	2	2	14,14,15	0.40	0	17,19,21	1.09	1 (5%)
2	BMA	E	3	2	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
2	MAN	E	4	2	11,11,12	0.22	0	15,15,17	0.48	0
3	NAG	F	1	1,3	14,14,15	0.32	0	17,19,21	0.81	0
3	NAG	F	2	3	14,14,15	0.30	0	17,19,21	0.71	0
3	BMA	F	3	3	11,11,12	0.23	0	15,15,17	0.56	0
4	NAG	G	1	4	14,14,15	0.61	0	17,19,21	1.66	4 (23%)
4	NAG	G	2	4	14,14,15	0.37	0	17,19,21	0.81	1 (5%)
2	NAG	H	1	2	14,14,15	0.38	0	17,19,21	0.52	0
2	NAG	H	2	2	14,14,15	0.40	0	17,19,21	1.09	1 (5%)
2	BMA	H	3	2	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
2	MAN	H	4	2	11,11,12	0.22	0	15,15,17	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	1,3	14,14,15	0.32	0	17,19,21	0.81	0
3	NAG	I	2	3	14,14,15	0.30	0	17,19,21	0.71	0
3	BMA	I	3	3	11,11,12	0.23	0	15,15,17	0.56	0
4	NAG	J	1	4	14,14,15	0.61	0	17,19,21	1.66	4 (23%)
4	NAG	J	2	4	14,14,15	0.37	0	17,19,21	0.81	1 (5%)

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
2	NAG	E	1	2	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
2	BMA	E	3	2	-	1/2/19/22	0/1/1/1
2	MAN	E	4	2	-	1/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	BMA	F	3	3	-	1/2/19/22	0/1/1/1
4	NAG	G	1	4	-	4/6/23/26	0/1/1/1
4	NAG	G	2	4	-	5/6/23/26	0/1/1/1
2	NAG	H	1	2	-	3/6/23/26	0/1/1/1
2	NAG	H	2	2	-	3/6/23/26	0/1/1/1
2	BMA	H	3	2	-	1/2/19/22	0/1/1/1
2	MAN	H	4	2	-	1/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	BMA	I	3	3	-	1/2/19/22	0/1/1/1
4	NAG	J	1	4	-	4/6/23/26	0/1/1/1
4	NAG	J	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	O5-C1-C2	-4.08	104.98	111.29
4	J	1	NAG	O5-C1-C2	-4.08	104.98	111.29
2	E	2	NAG	C1-O5-C5	3.47	116.83	112.19
2	H	2	NAG	C1-O5-C5	3.47	116.83	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	NAG	O4-C4-C3	3.24	118.03	110.38
4	J	1	NAG	O4-C4-C3	3.24	118.03	110.38
4	G	1	NAG	C1-O5-C5	2.31	115.28	112.19
4	J	1	NAG	C1-O5-C5	2.31	115.28	112.19
4	G	1	NAG	C4-C3-C2	2.22	114.28	111.02
4	J	1	NAG	C4-C3-C2	2.22	114.28	111.02
2	E	3	BMA	C1-O5-C5	2.11	115.01	112.19
2	H	3	BMA	C1-O5-C5	2.11	115.01	112.19
4	G	2	NAG	C4-C3-C2	2.06	114.03	111.02
4	J	2	NAG	C4-C3-C2	2.06	114.03	111.02

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C1-C2-N2-C7
2	E	2	NAG	C8-C7-N2-C2
2	E	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C3-C2-N2-C7
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	H	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C8-C7-N2-C2
3	F	1	NAG	O7-C7-N2-C2
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	I	1	NAG	C8-C7-N2-C2
3	I	1	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
4	G	1	NAG	C8-C7-N2-C2
4	G	1	NAG	O7-C7-N2-C2
4	G	2	NAG	C3-C2-N2-C7
4	G	2	NAG	C8-C7-N2-C2
4	G	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	J	2	NAG	C3-C2-N2-C7
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
3	F	3	BMA	O5-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
2	E	4	MAN	O5-C5-C6-O6
2	H	4	MAN	O5-C5-C6-O6
3	F	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
4	G	1	NAG	C3-C2-N2-C7
4	J	1	NAG	C3-C2-N2-C7
2	E	3	BMA	O5-C5-C6-O6
2	H	3	BMA	O5-C5-C6-O6
3	F	1	NAG	C1-C2-N2-C7
3	I	1	NAG	C1-C2-N2-C7
3	F	1	NAG	C3-C2-N2-C7
3	I	1	NAG	C3-C2-N2-C7
4	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
3	I	2	NAG	C1-C2-N2-C7

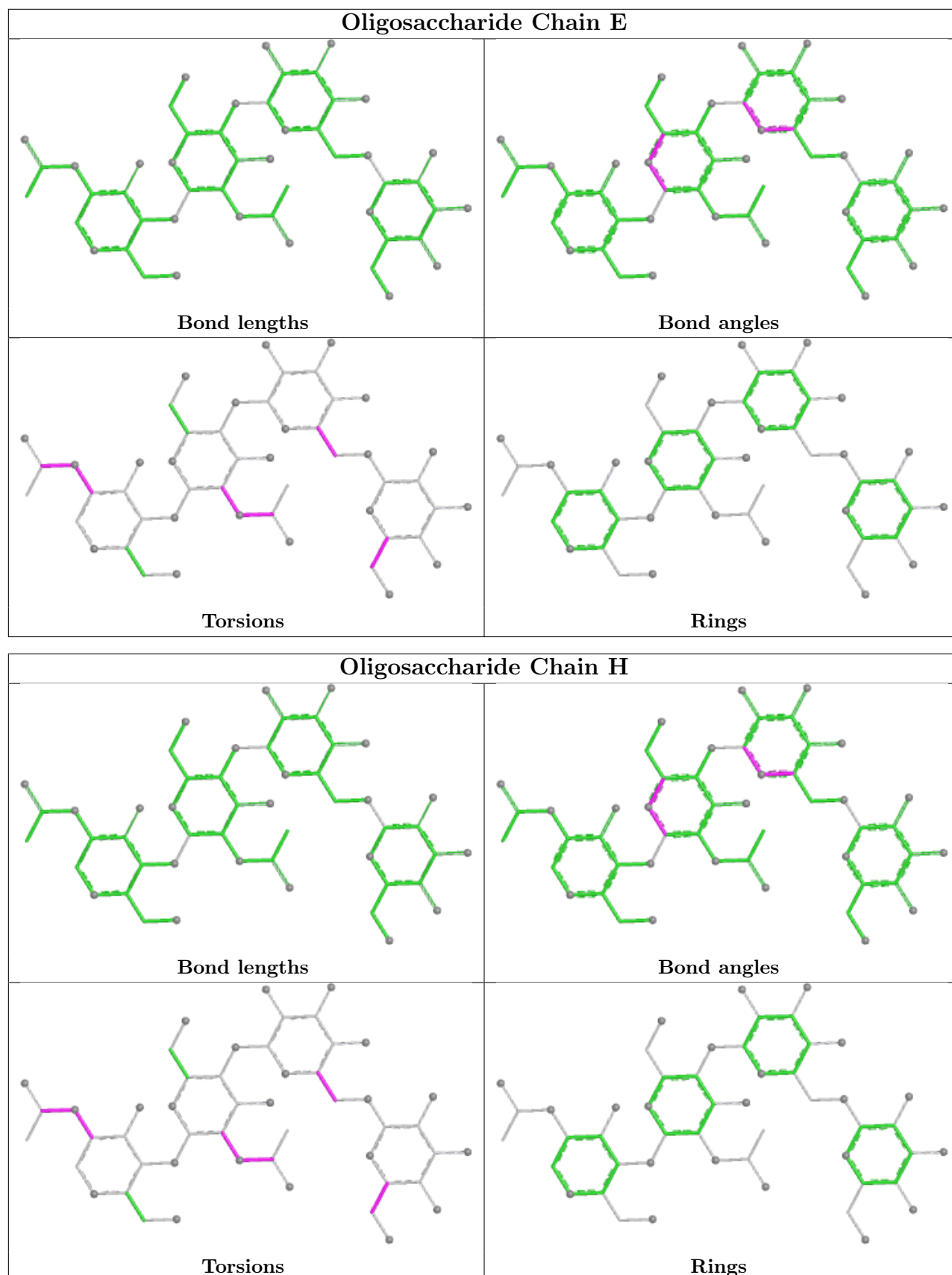
There are no ring outliers.

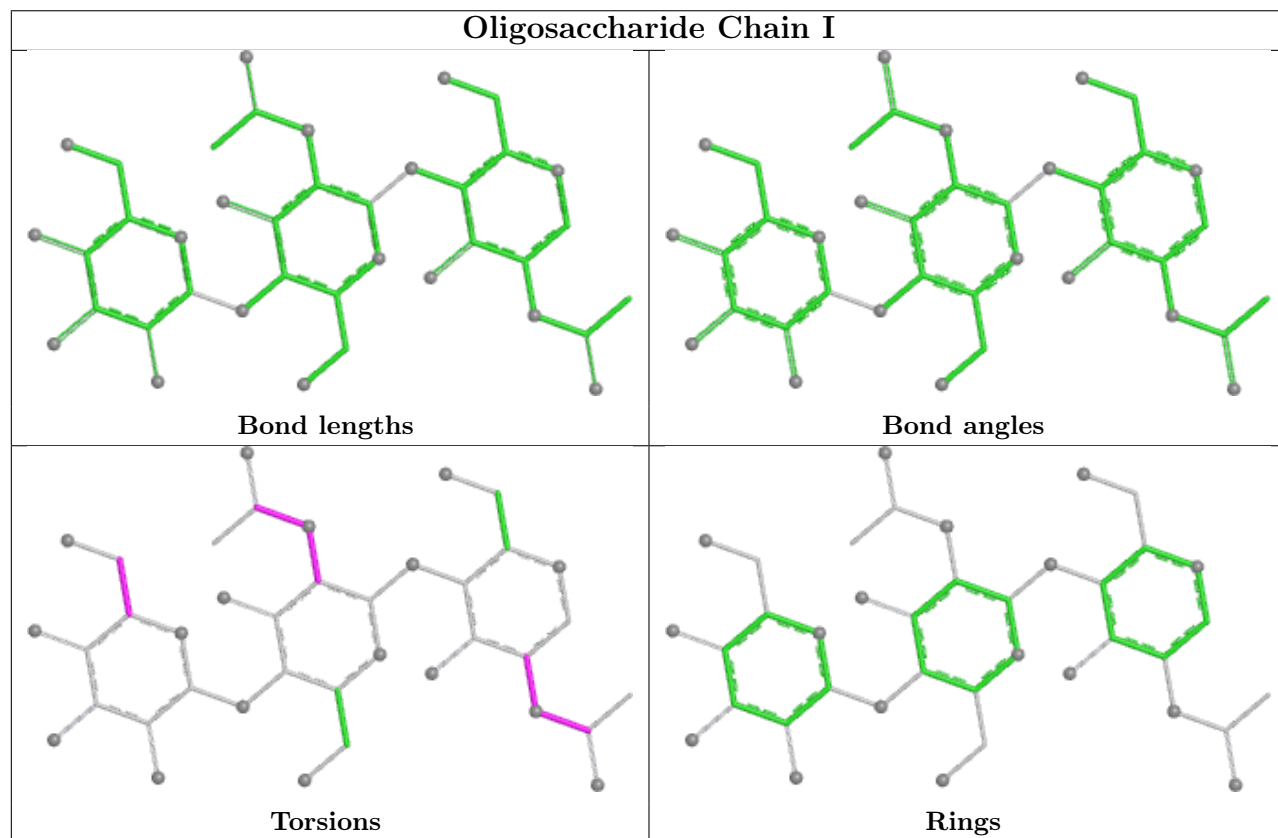
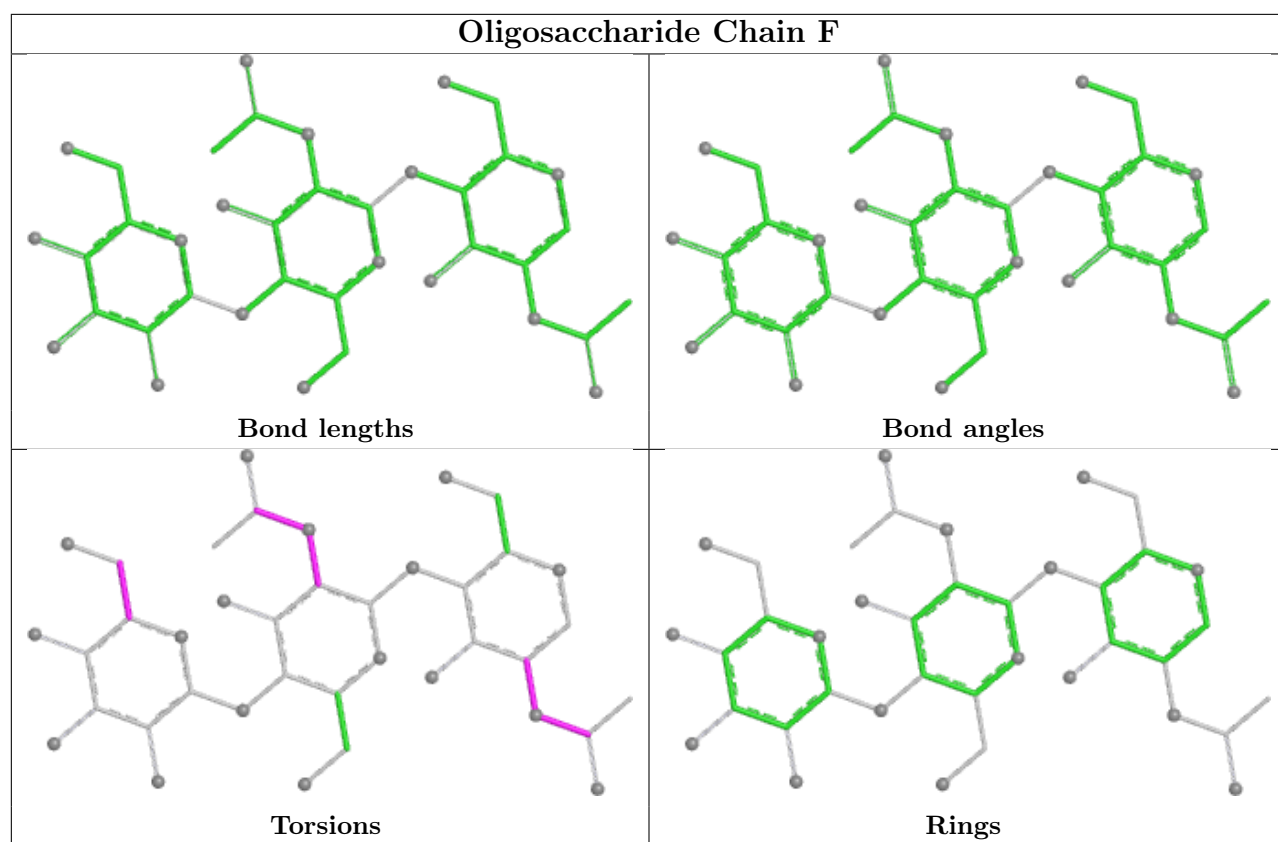
10 monomers are involved in 14 short contacts:

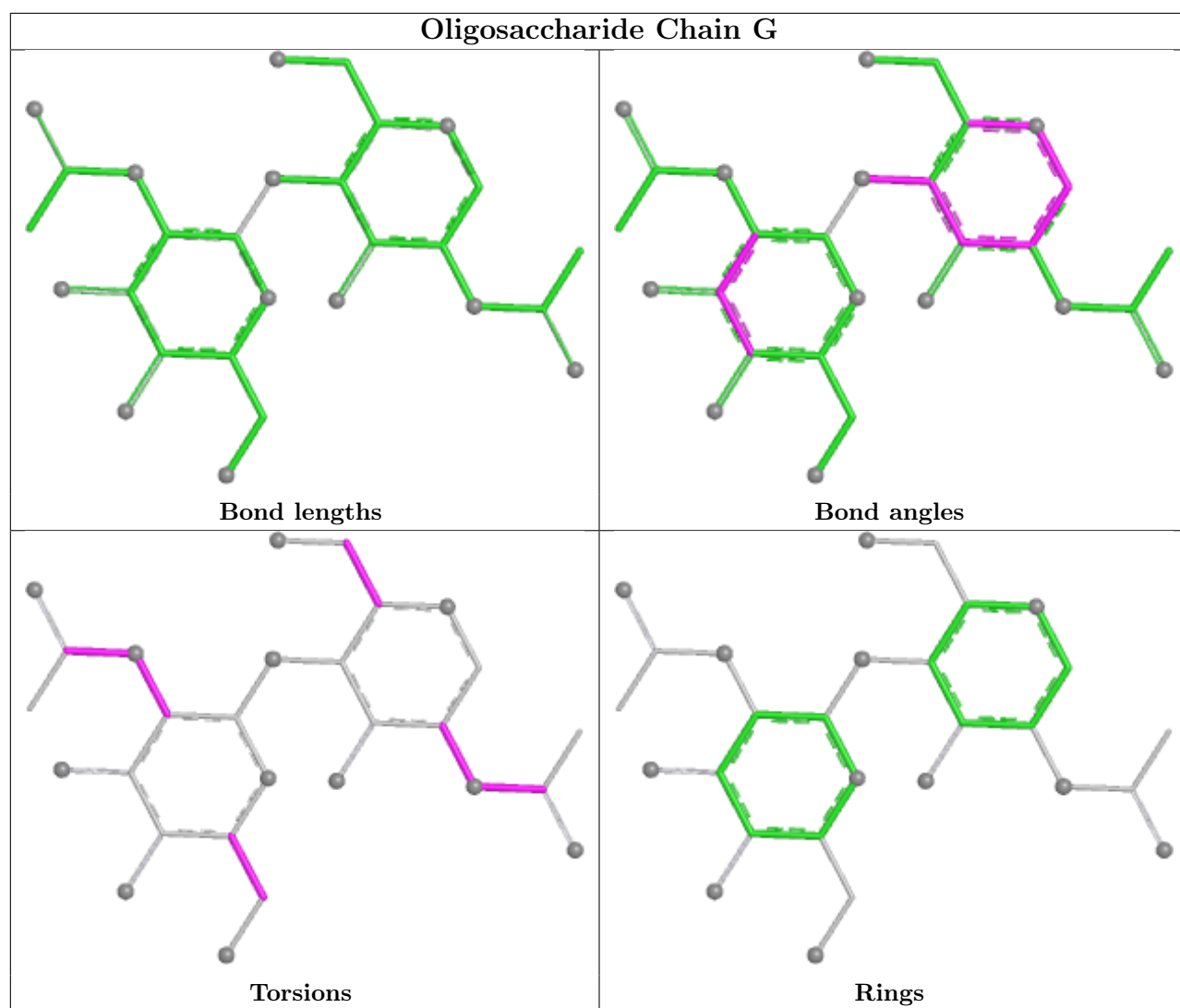
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	1	0
2	H	1	NAG	1	0
2	H	2	NAG	2	0
4	G	1	NAG	3	0
2	E	1	NAG	1	0
3	I	2	NAG	1	0
4	J	1	NAG	3	0
3	F	1	NAG	1	0
2	E	2	NAG	2	0
3	I	1	NAG	1	0

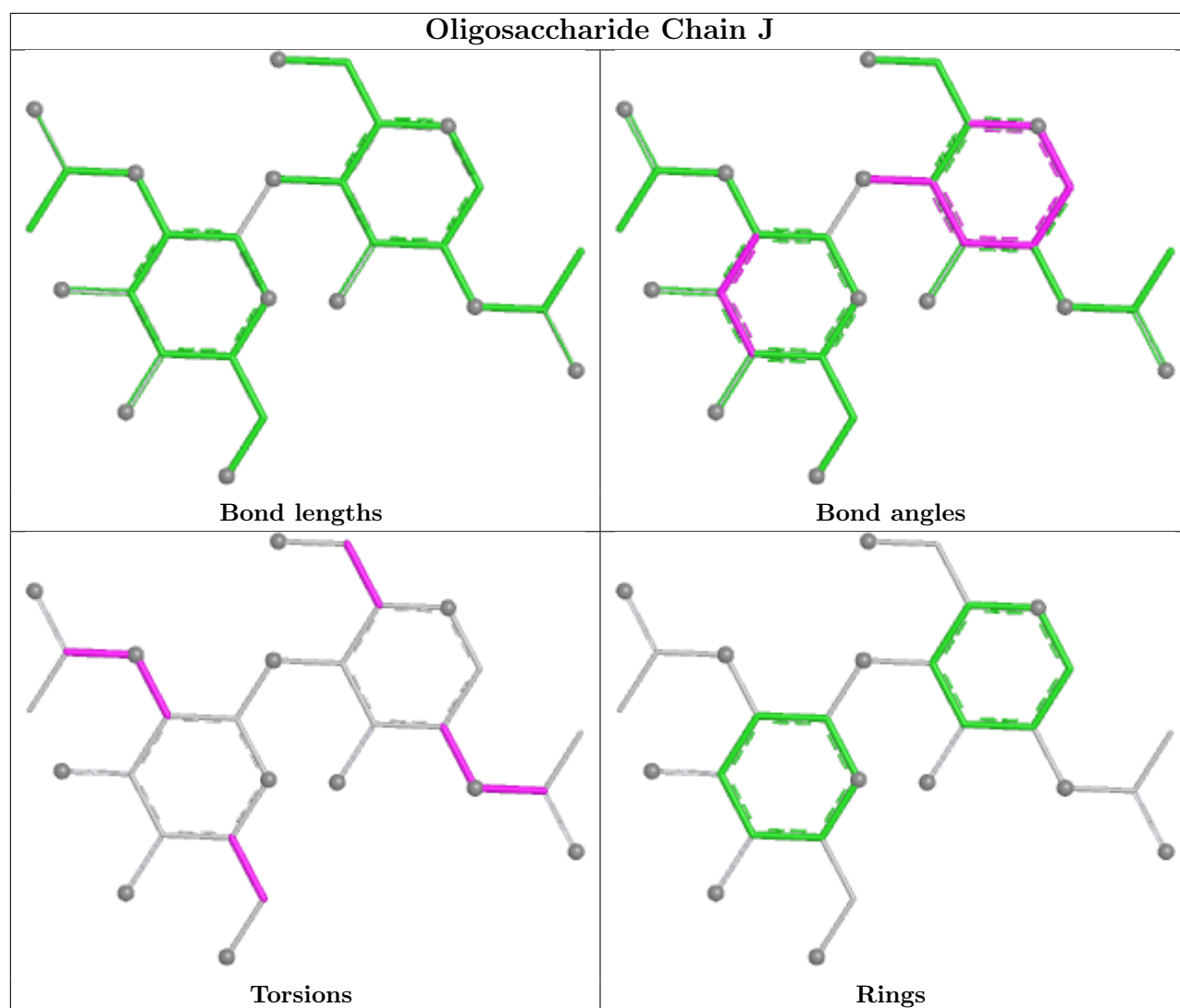
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.









## 5.6 Ligand geometry [i](#)

26 ligands 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	$\# Z  > 2$
5	NAG	A	2003	1	14,14,15	0.29	0	17,19,21	0.91	0
5	NAG	B	2002	-	14,14,15	0.27	0	17,19,21	0.76	0
5	NAG	A	2008	1	14,14,15	0.31	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	2003	-	14,14,15	0.32	0	17,19,21	0.45	0
5	NAG	A	2007	1	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	D	2001	1	14,14,15	0.26	0	17,19,21	1.27	2 (11%)
5	NAG	A	2005	1	14,14,15	0.35	0	17,19,21	0.71	1 (5%)
5	NAG	A	2004	1	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	D	2004	-	14,14,15	0.37	0	17,19,21	0.87	0
5	NAG	A	2002	-	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	2003	1	14,14,15	0.29	0	17,19,21	0.91	0
5	NAG	C	2008	1	14,14,15	0.31	0	17,19,21	0.44	0
5	NAG	A	2001	-	14,14,15	0.27	0	17,19,21	1.28	2 (11%)
5	NAG	C	2002	-	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	2007	1	14,14,15	0.29	0	17,19,21	0.65	0
5	NAG	B	2001	1	14,14,15	0.26	0	17,19,21	1.27	2 (11%)
5	NAG	B	2003	-	14,14,15	0.32	0	17,19,21	0.45	0
5	NAG	C	2004	1	14,14,15	0.33	0	17,19,21	0.59	0
5	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	C	2006	1	14,14,15	0.32	0	17,19,21	0.81	0
5	NAG	D	2002	-	14,14,15	0.27	0	17,19,21	0.76	0
5	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.91	1 (5%)
5	NAG	A	2006	1	14,14,15	0.32	0	17,19,21	0.81	0
5	NAG	B	2004	-	14,14,15	0.37	0	17,19,21	0.87	0
5	NAG	C	2001	-	14,14,15	0.27	0	17,19,21	1.28	2 (11%)
5	NAG	C	2005	1	14,14,15	0.35	0	17,19,21	0.71	1 (5%)

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
5	NAG	A	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	A	2007	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2004	-	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2008	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2001	-	-	2/6/23/26	0/1/1/1
5	NAG	C	2002	-	-	3/6/23/26	0/1/1/1
5	NAG	C	2007	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2003	-	-	4/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	D	2002	-	-	4/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2004	-	-	4/6/23/26	0/1/1/1
5	NAG	C	2001	-	-	2/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2001	NAG	C1-O5-C5	3.94	117.47	112.19
5	C	2001	NAG	C1-O5-C5	3.94	117.47	112.19
5	B	2001	NAG	C1-O5-C5	3.89	117.40	112.19
5	D	2001	NAG	C1-O5-C5	3.89	117.40	112.19
5	B	2005	NAG	C1-O5-C5	2.42	115.43	112.19
5	D	2005	NAG	C1-O5-C5	2.42	115.43	112.19
5	B	2001	NAG	C4-C3-C2	-2.17	107.84	111.02
5	D	2001	NAG	C4-C3-C2	-2.17	107.84	111.02
5	A	2001	NAG	C4-C3-C2	-2.15	107.87	111.02
5	C	2001	NAG	C4-C3-C2	-2.15	107.87	111.02
5	A	2005	NAG	C1-O5-C5	-2.03	109.47	112.19
5	C	2005	NAG	C1-O5-C5	-2.03	109.47	112.19

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2002	NAG	C3-C2-N2-C7
5	A	2002	NAG	C8-C7-N2-C2
5	A	2002	NAG	O7-C7-N2-C2
5	A	2004	NAG	C8-C7-N2-C2
5	A	2004	NAG	O7-C7-N2-C2
5	A	2005	NAG	C3-C2-N2-C7
5	A	2005	NAG	C8-C7-N2-C2
5	A	2005	NAG	O7-C7-N2-C2
5	A	2006	NAG	C8-C7-N2-C2
5	A	2006	NAG	O7-C7-N2-C2
5	A	2007	NAG	C3-C2-N2-C7
5	A	2007	NAG	C8-C7-N2-C2
5	A	2007	NAG	O7-C7-N2-C2
5	A	2008	NAG	C8-C7-N2-C2
5	A	2008	NAG	O7-C7-N2-C2
5	B	2002	NAG	C3-C2-N2-C7
5	B	2002	NAG	C8-C7-N2-C2
5	B	2002	NAG	O7-C7-N2-C2
5	B	2003	NAG	C1-C2-N2-C7
5	B	2003	NAG	C8-C7-N2-C2
5	B	2003	NAG	O7-C7-N2-C2
5	B	2004	NAG	C8-C7-N2-C2
5	B	2004	NAG	O7-C7-N2-C2
5	B	2005	NAG	C8-C7-N2-C2
5	B	2005	NAG	O7-C7-N2-C2
5	C	2002	NAG	C3-C2-N2-C7
5	C	2002	NAG	C8-C7-N2-C2
5	C	2002	NAG	O7-C7-N2-C2
5	C	2004	NAG	C8-C7-N2-C2
5	C	2004	NAG	O7-C7-N2-C2
5	C	2005	NAG	C3-C2-N2-C7
5	C	2005	NAG	C8-C7-N2-C2
5	C	2005	NAG	O7-C7-N2-C2
5	C	2006	NAG	C8-C7-N2-C2
5	C	2006	NAG	O7-C7-N2-C2
5	C	2007	NAG	C3-C2-N2-C7
5	C	2007	NAG	C8-C7-N2-C2
5	C	2007	NAG	O7-C7-N2-C2
5	C	2008	NAG	C8-C7-N2-C2
5	C	2008	NAG	O7-C7-N2-C2
5	D	2002	NAG	C3-C2-N2-C7
5	D	2002	NAG	C8-C7-N2-C2
5	D	2002	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	D	2003	NAG	C1-C2-N2-C7
5	D	2003	NAG	C8-C7-N2-C2
5	D	2003	NAG	O7-C7-N2-C2
5	D	2004	NAG	C8-C7-N2-C2
5	D	2004	NAG	O7-C7-N2-C2
5	D	2005	NAG	C8-C7-N2-C2
5	D	2005	NAG	O7-C7-N2-C2
5	A	2008	NAG	O5-C5-C6-O6
5	C	2008	NAG	O5-C5-C6-O6
5	B	2004	NAG	O5-C5-C6-O6
5	D	2004	NAG	O5-C5-C6-O6
5	B	2002	NAG	O5-C5-C6-O6
5	D	2002	NAG	O5-C5-C6-O6
5	B	2004	NAG	C3-C2-N2-C7
5	D	2004	NAG	C3-C2-N2-C7
5	A	2004	NAG	C4-C5-C6-O6
5	C	2004	NAG	C4-C5-C6-O6
5	A	2001	NAG	C1-C2-N2-C7
5	B	2001	NAG	C1-C2-N2-C7
5	C	2001	NAG	C1-C2-N2-C7
5	D	2001	NAG	C1-C2-N2-C7
5	A	2008	NAG	C3-C2-N2-C7
5	C	2008	NAG	C3-C2-N2-C7
5	A	2004	NAG	O5-C5-C6-O6
5	C	2004	NAG	O5-C5-C6-O6
5	A	2001	NAG	C3-C2-N2-C7
5	B	2001	NAG	C3-C2-N2-C7
5	B	2003	NAG	C3-C2-N2-C7
5	C	2001	NAG	C3-C2-N2-C7
5	D	2001	NAG	C3-C2-N2-C7
5	D	2003	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2003	NAG	4	0
5	D	2004	NAG	1	0
5	A	2001	NAG	6	0
5	B	2003	NAG	4	0
5	B	2005	NAG	1	0
5	D	2005	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2004	NAG	1	0
5	C	2001	NAG	6	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	629:GLY	C	630:PHE	N	5.14
1	D	629:GLY	C	630:PHE	N	5.14

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12748. These allow visual inspection of the internal detail of the map and identification of artifacts.

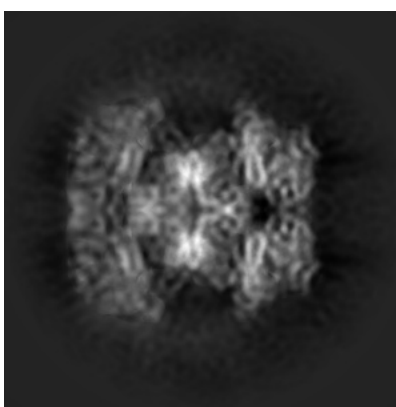
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

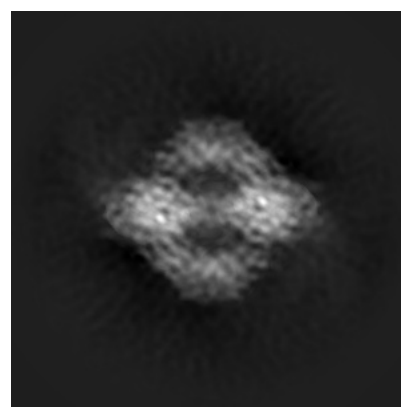
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

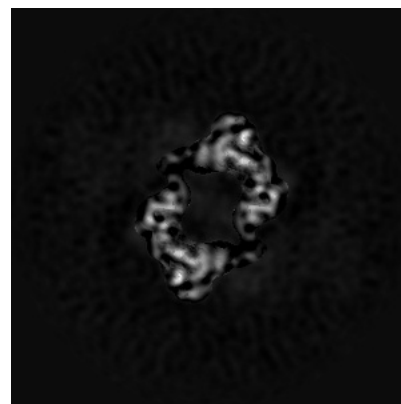
#### 6.2.1 Primary map



X Index: 160



Y Index: 160



Z Index: 160

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: 130



Y Index: 160

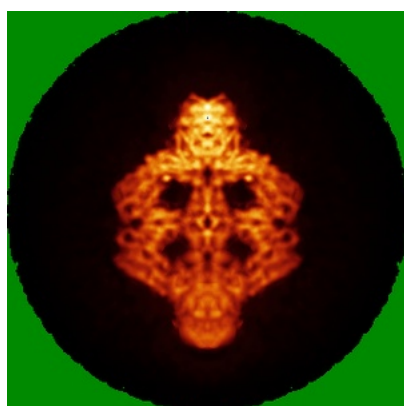


Z Index: 195

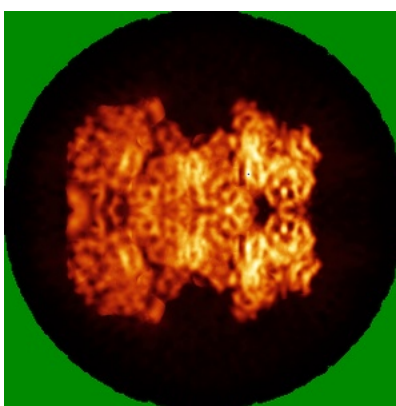
The images above show the largest variance slices of the map in three orthogonal directions.

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

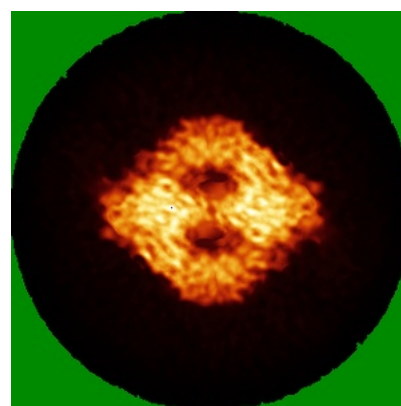
### 6.4.1 Primary map



X



Y

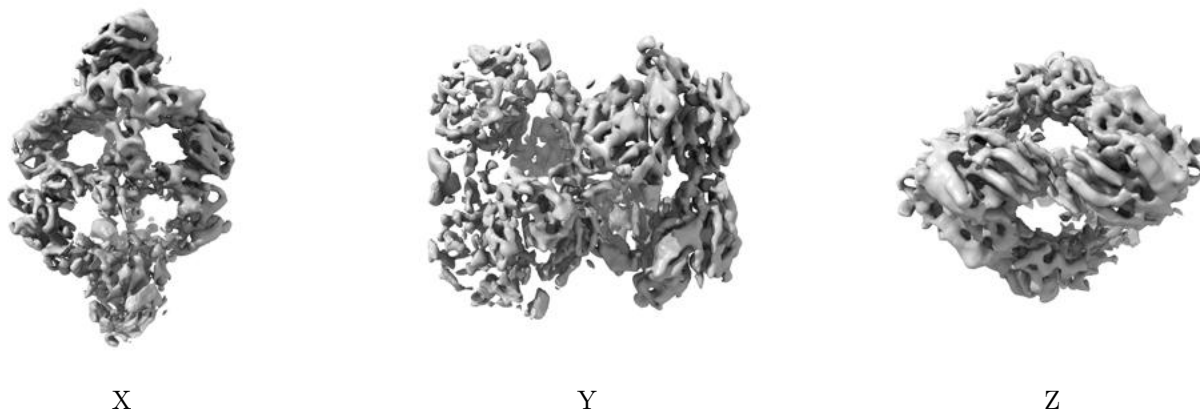


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

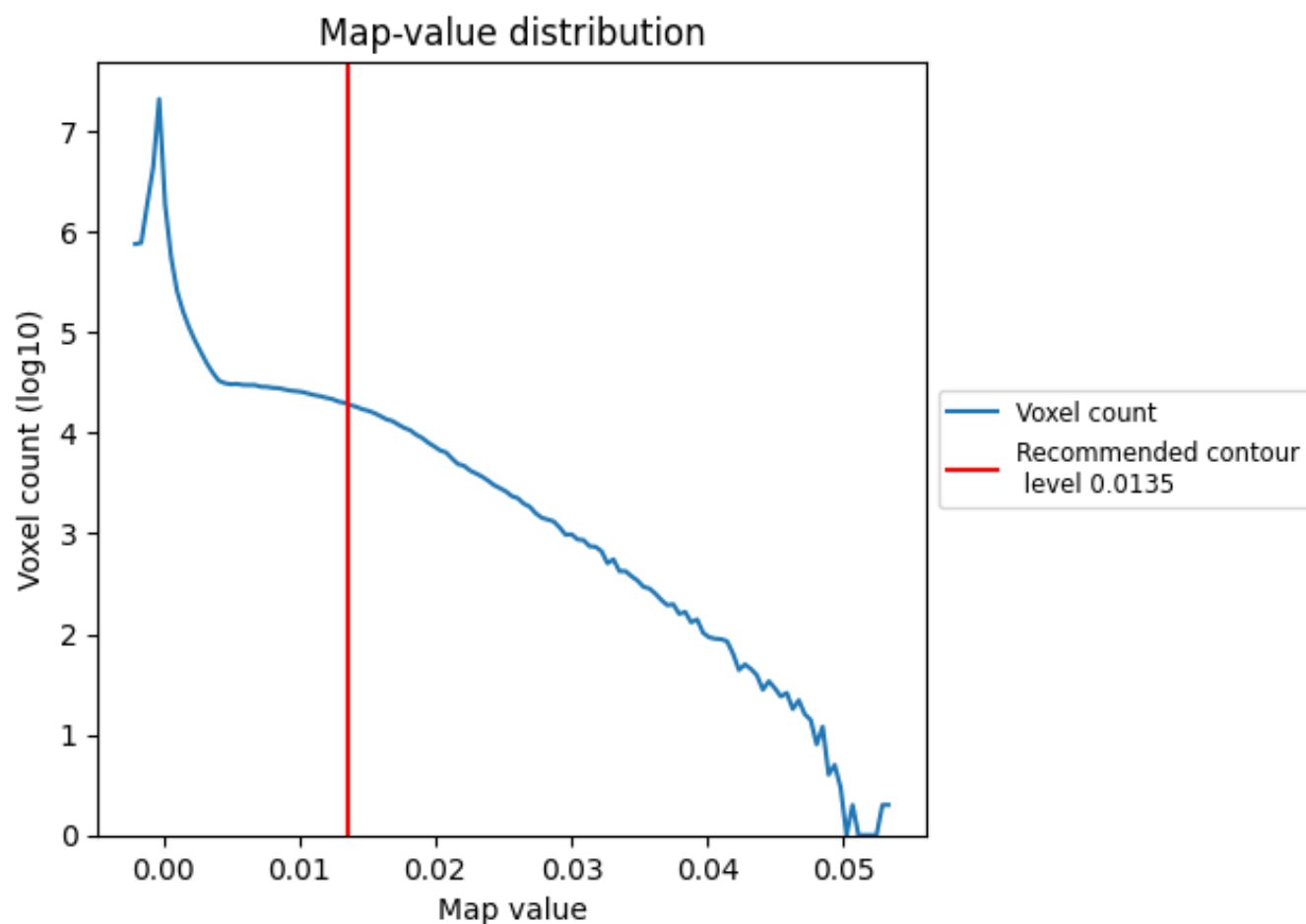
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

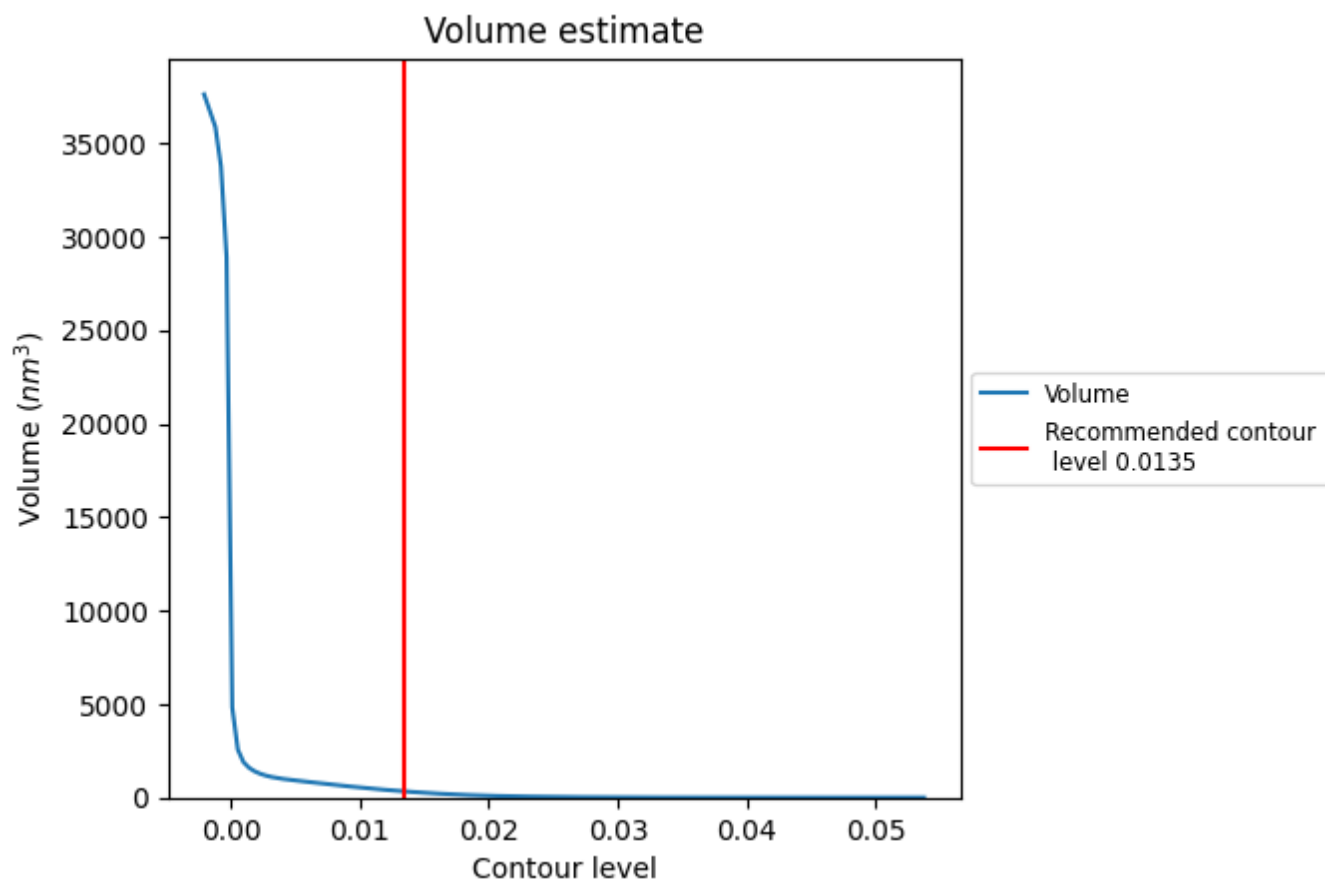
This section contains the results of statistical analysis of the map.

### 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.

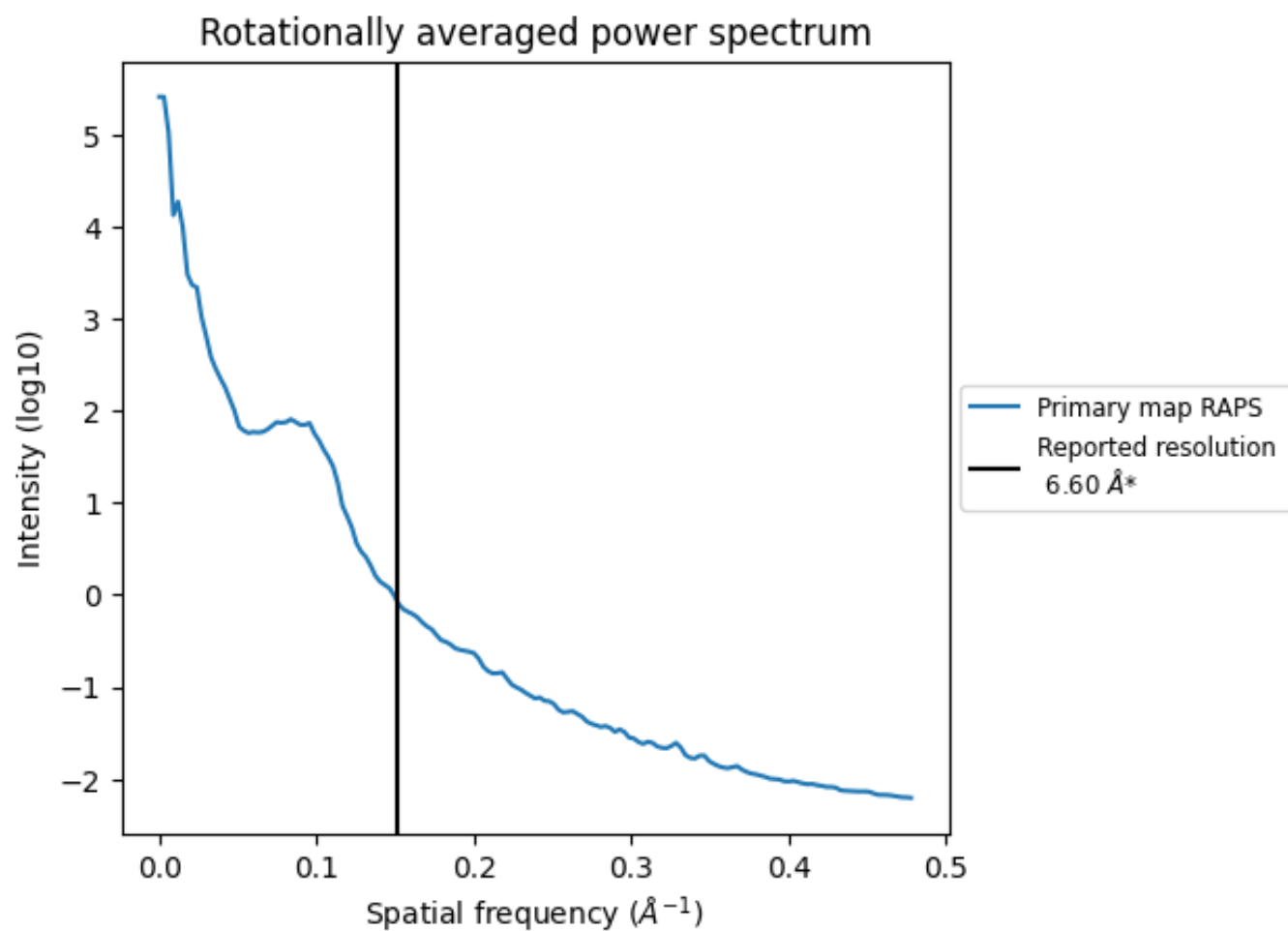
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329  $\text{nm}^3$ ; this corresponds to an approximate mass of 297 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 0.152 Å<sup>-1</sup>



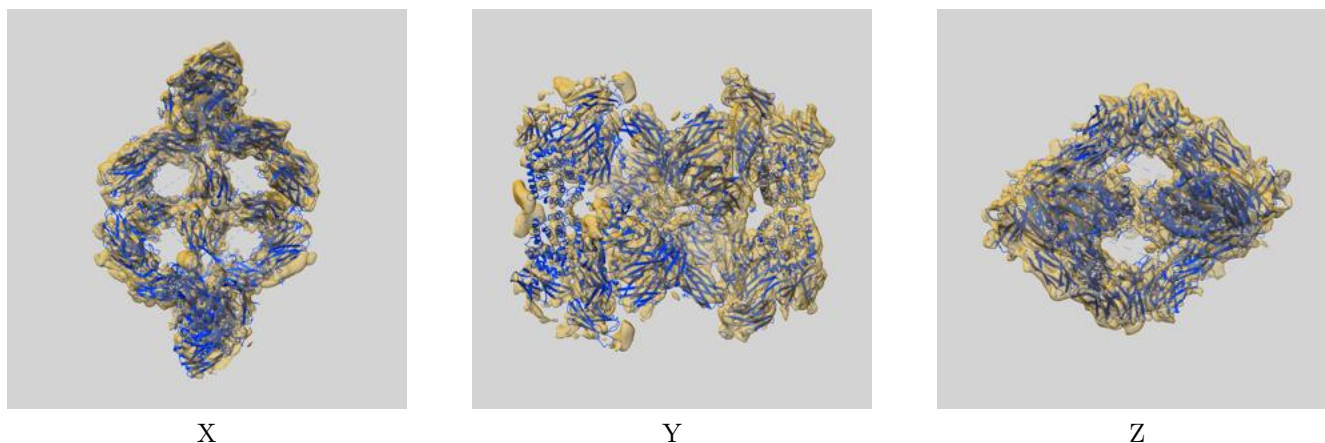
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

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

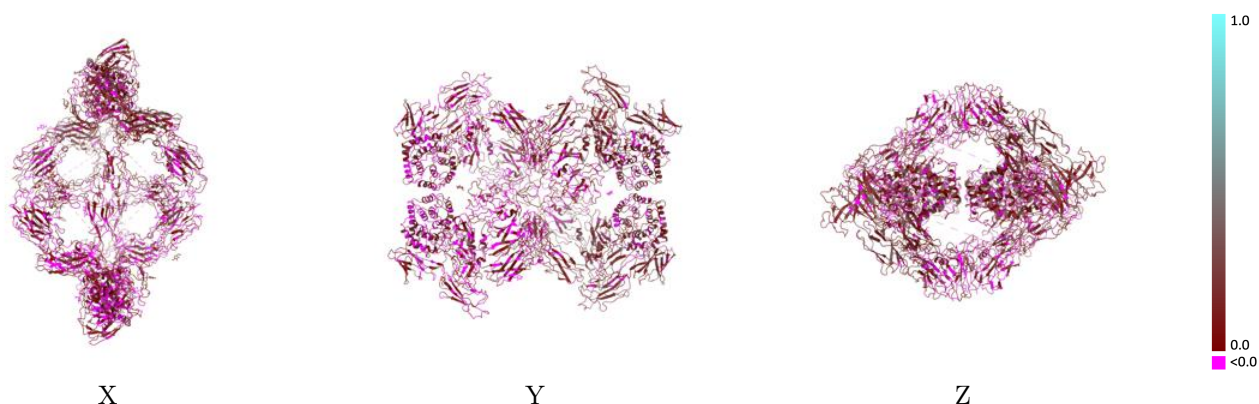
This section contains information regarding the fit between EMDB map EMD-12748 and PDB model 7O7M. Per-residue inclusion information can be found in section [3](#) on page [8](#).

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



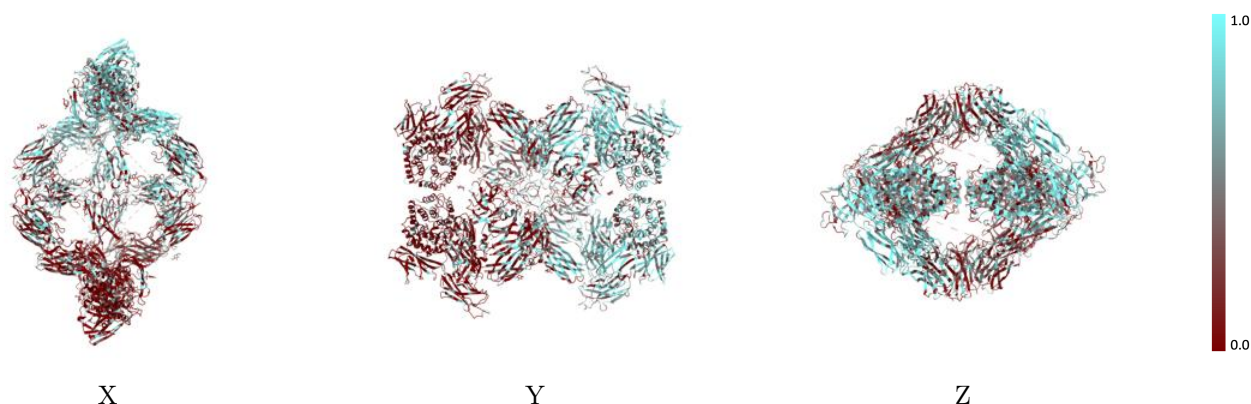
The images above show the 3D surface view of the map at the recommended contour level 0.0135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



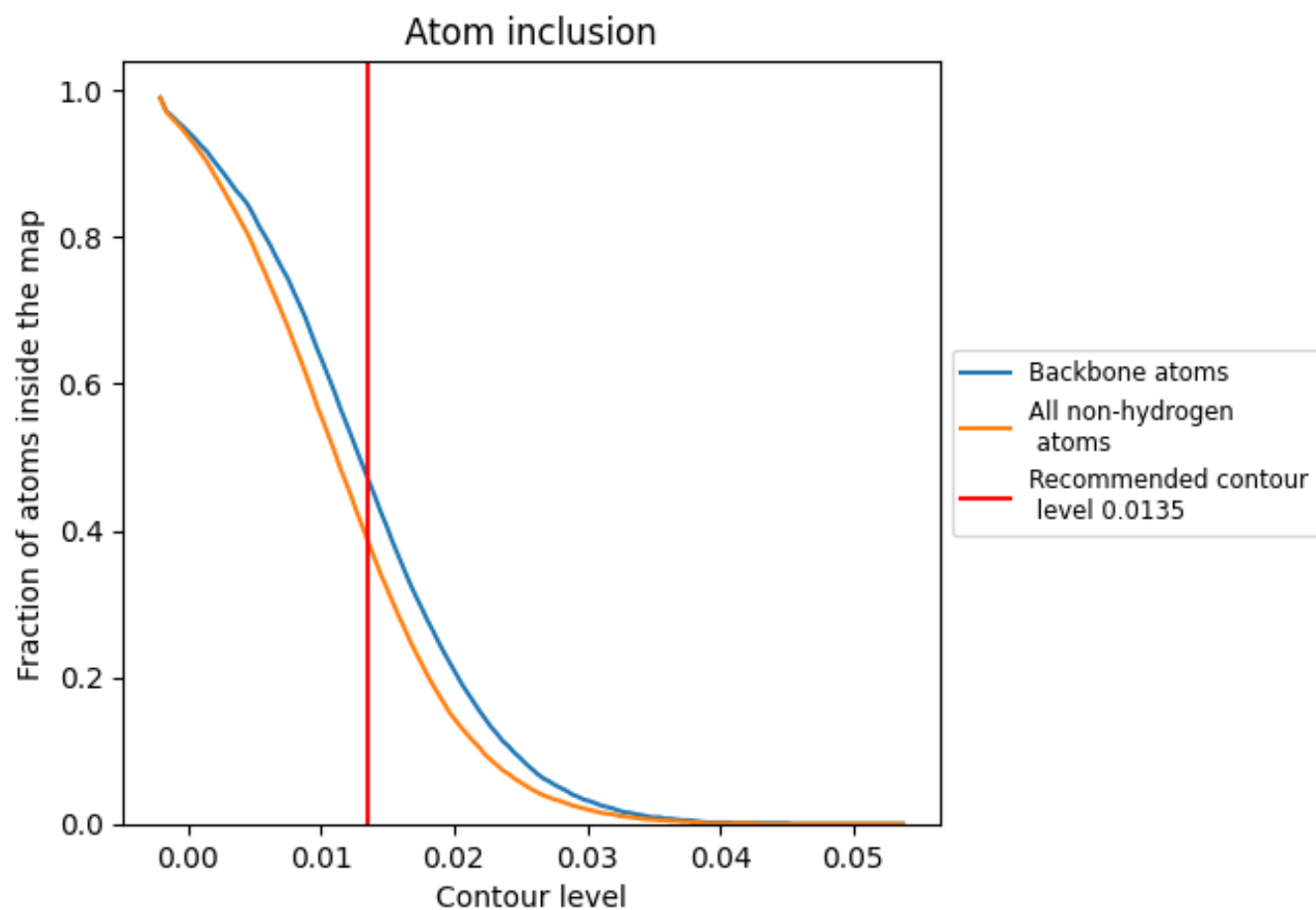
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0135).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 47% of all backbone atoms, 39% 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 (0.0135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3870	<div></div> 0.0970
A	<div></div> 0.2130	<div></div> 0.0550
B	<div></div> 0.5610	<div></div> 0.1380
C	<div></div> 0.2130	<div></div> 0.0530
D	<div></div> 0.5610	<div></div> 0.1390
E	<div></div> 0.5800	<div></div> 0.2000
F	<div></div> 0.3850	<div></div> 0.2290
G	<div></div> 0.1430	<div></div> 0.2210
H	<div></div> 0.5800	<div></div> 0.2060
I	<div></div> 0.3850	<div></div> 0.2110
J	<div></div> 0.1430	<div></div> 0.2120

1.0

0.0

<0.0