



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 10:56 PM UTC

PDB ID : 7O7S / pdb_00007o7s
EMDB ID : EMD-12755
Title : (h-alpha2M)4 plasmin-activated II state
Authors : Luque, D.; Goulas, T.; Mata, C.P.; Mendes, S.R.; Gomis-Ruth, F.X.; Caston, J.R.
Deposited on : 2021-04-13
Resolution : 4.30 Å(reported)

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

We welcome your comments at 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>.

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

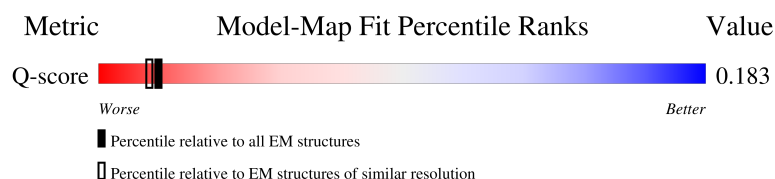
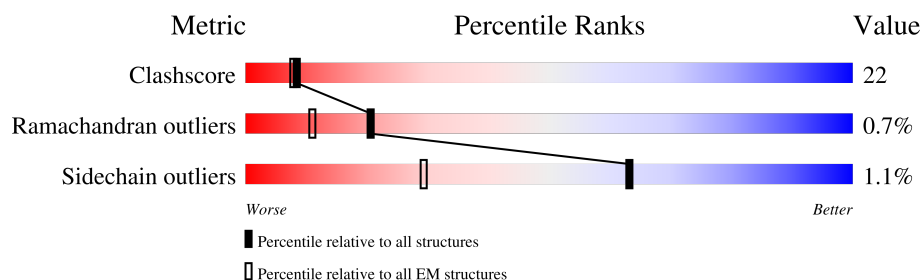
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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.




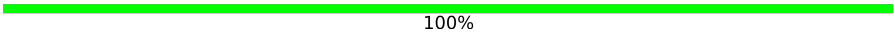
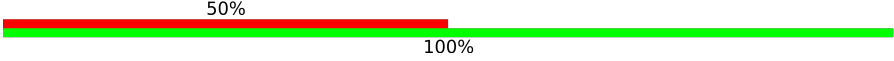


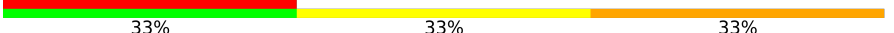



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 (3.80 - 4.80)

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 ≥ 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>19%</div> <div>49%</div> <div>36%</div> <div>•</div> <div>13%</div> </div>
1	B	1474	<div> <div>24%</div> <div>53%</div> <div>33%</div> <div>•</div> <div>13%</div> </div>
1	C	1474	<div> <div>32%</div> <div>51%</div> <div>35%</div> <div>•</div> <div>13%</div> </div>
1	D	1474	<div> <div>48%</div> <div>60%</div> <div>34%</div> <div>•</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	2	
2	G	2	
2	I	2	
2	K	2	
3	F	3	
3	H	3	
3	J	3	
3	M	3	
4	L	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	C	2004	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 41466 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.

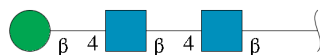
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0
			9958	6331	1672	1912	43		
1	B	1276	Total	C	N	O	S	0	0
			9958	6331	1672	1912	43		
1	C	1277	Total	C	N	O	S	0	0
			9967	6336	1673	1915	43		
1	D	1407	Total	C	N	O	S	0	0
			10985	6988	1836	2113	48		

- Molecule 2 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
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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.



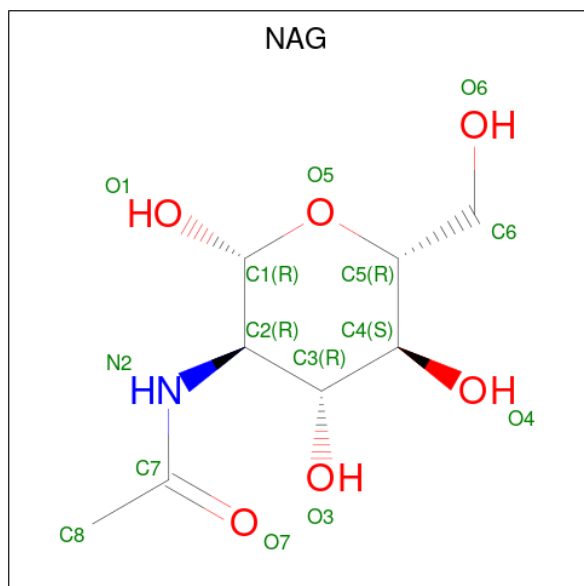
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 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
4	L	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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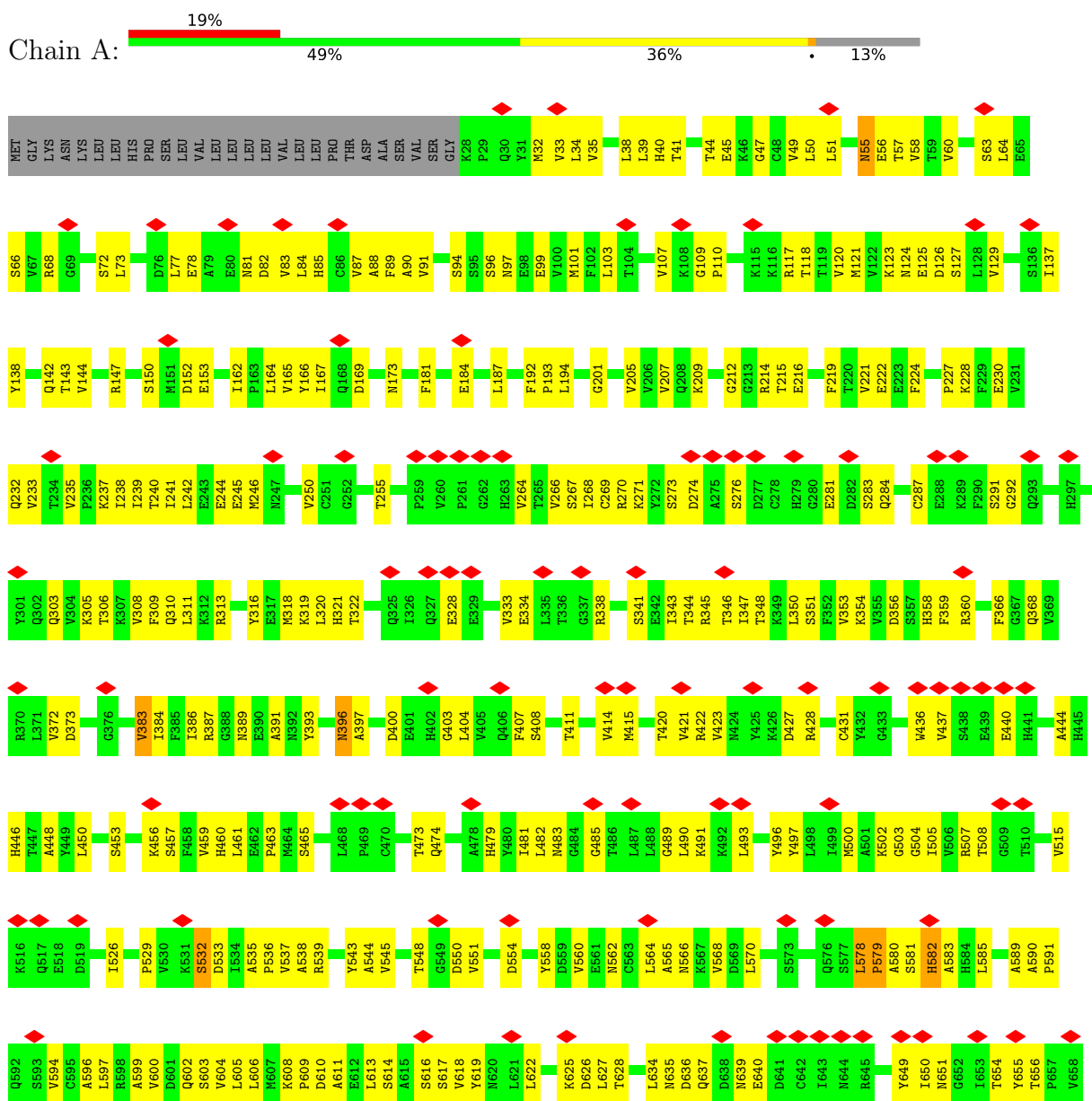
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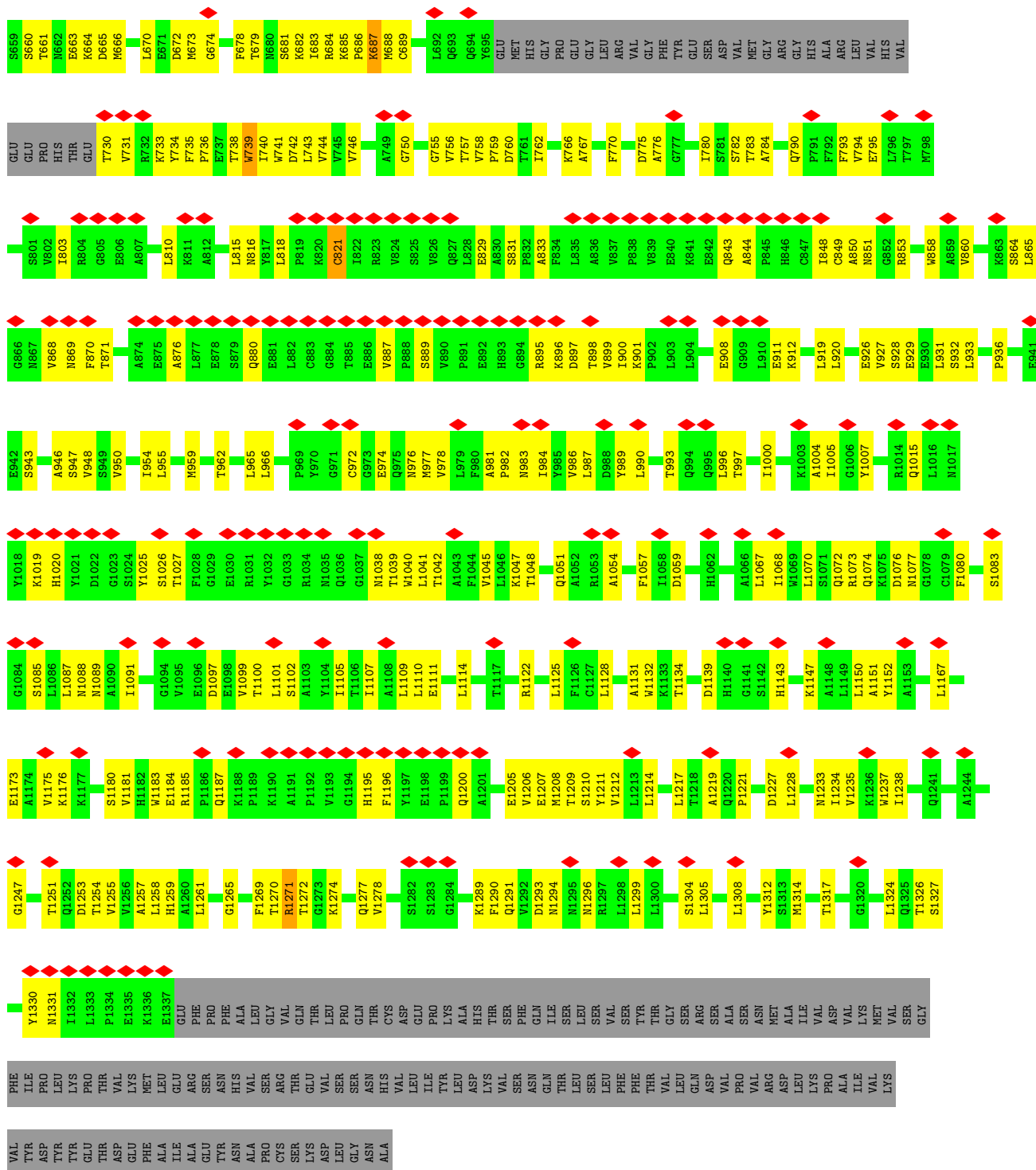
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C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

3 Residue-property plots

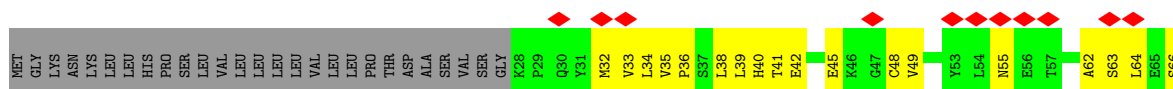
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

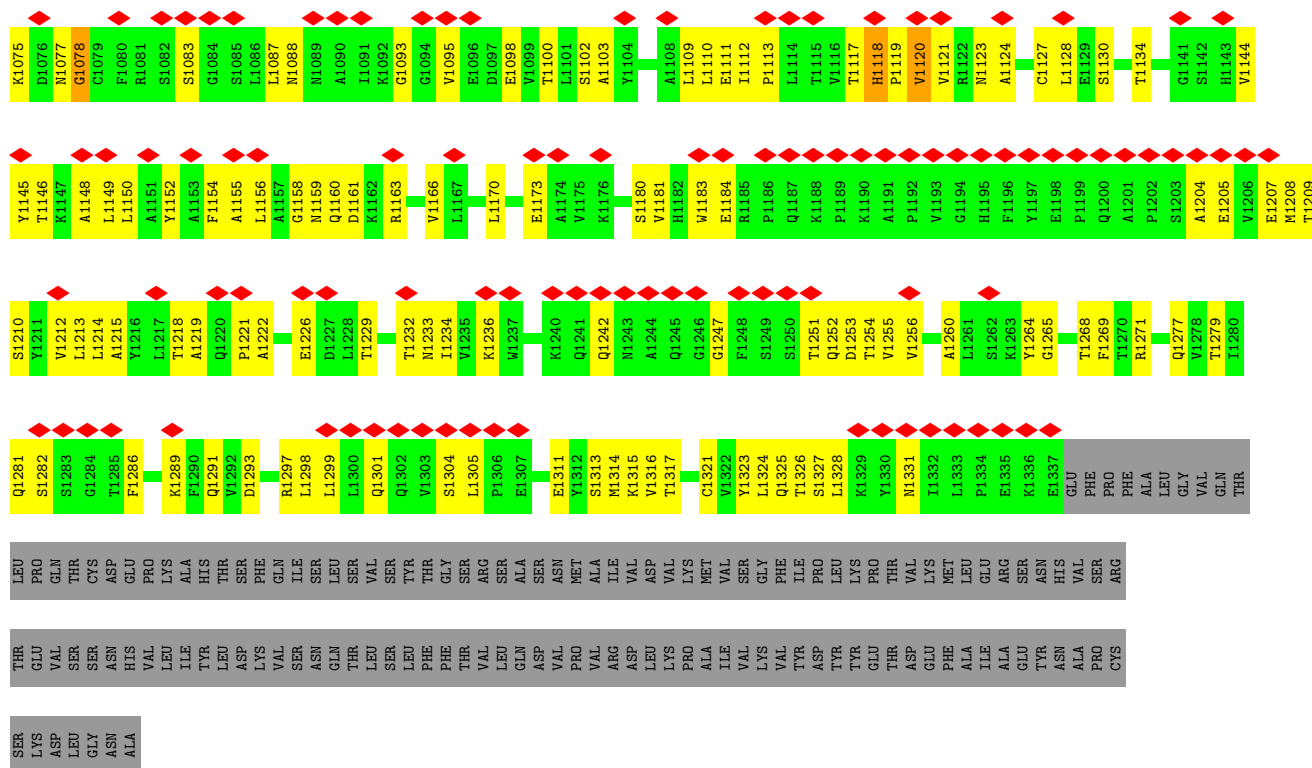




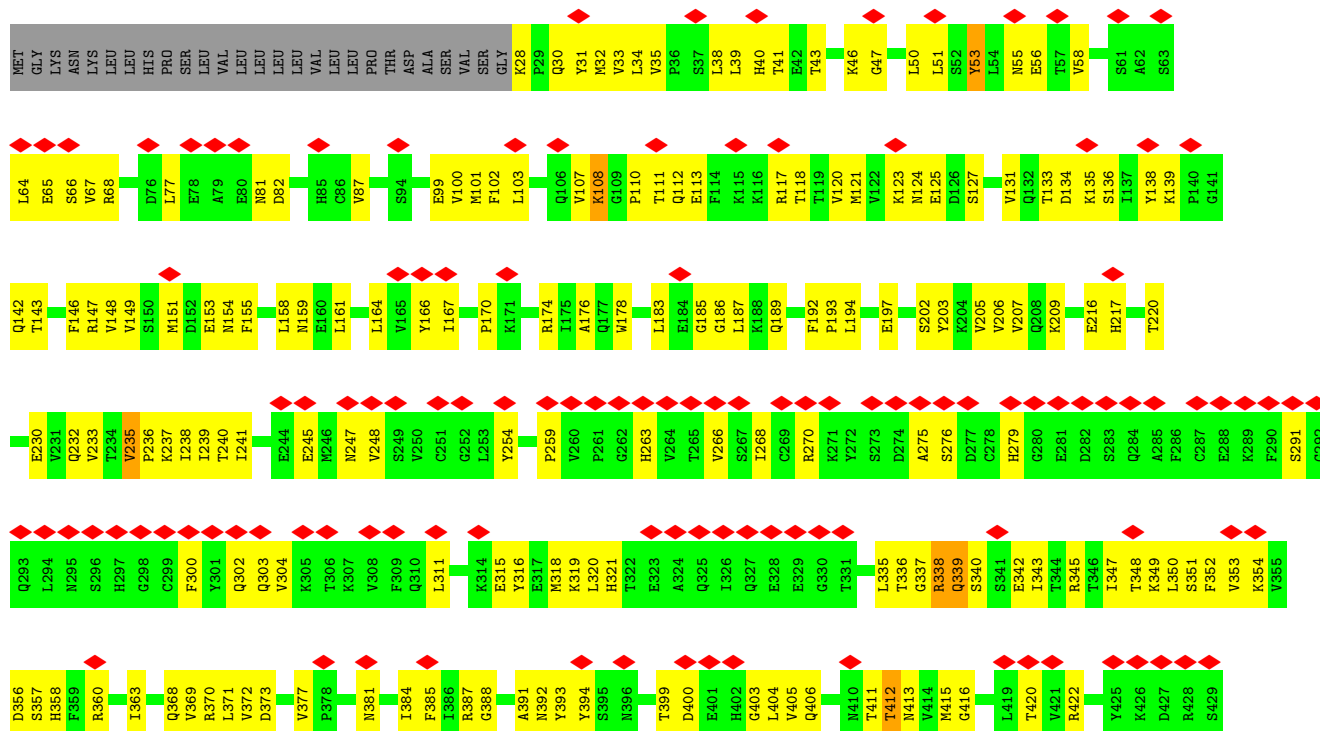
• Molecule 1: Alpha-2-macroglobulin



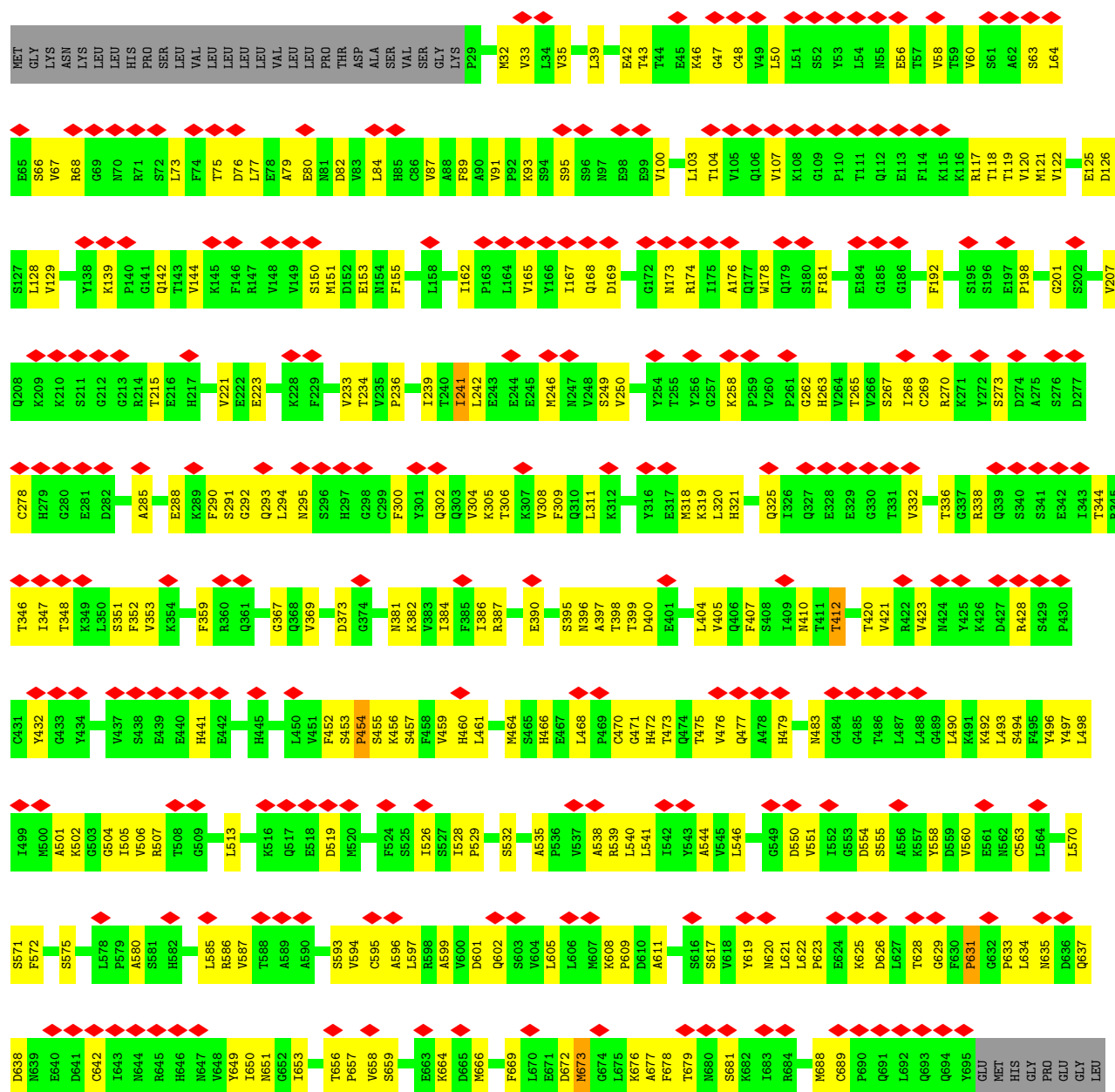


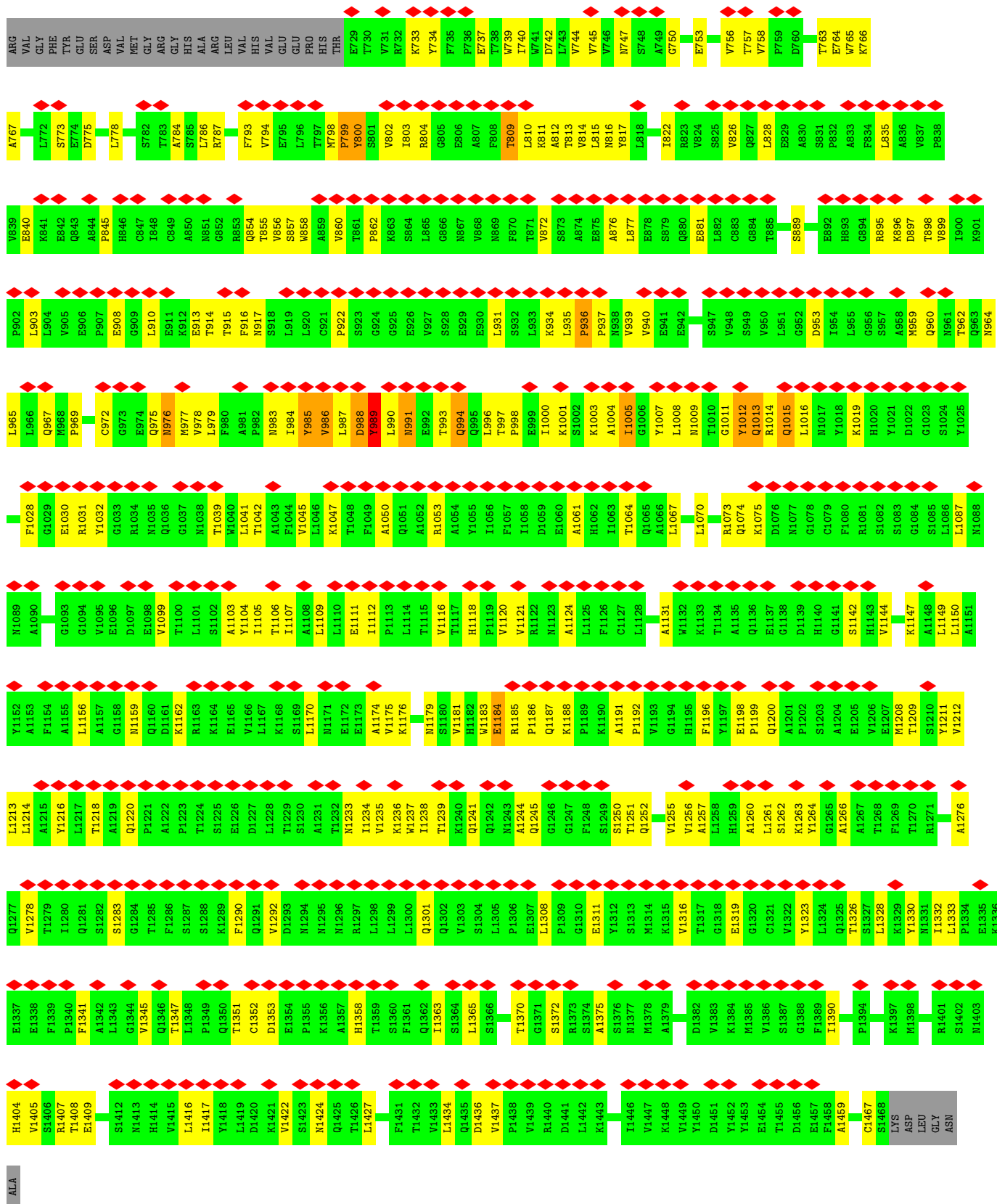


• Molecule 1: Alpha-2-macroglobulin



H1259	A1260	L1261	S1262	K1263	Y1264	G1265	A1266	A1267	R1271	T1272	G1273	Q1277	V1278	T1279	I1280	Q1281	S1282	S1283	G1284	T1285	F1286	S1287	S1288	K1289	F1290	Q1291	V1292	N1296	R1297	L1298	L1299	Q1302	V1303	S1304	L1305	P1306	E1307	L1308	P1309	G1310	E1311	Y1312	S1313	K1314	V1316	G1320	Y1323	L1324	Q1325	T1326	S1327	L1328						
H1195	F1196	Y1197	E1198	F1199	Q1200	A1201	P1202	S1203	A1204	E1205	V1206	M1207	T1209	S1210	Y1211	V1212	L1213	L1217	T1216	A1219	Q1220	P1221	A1222	S1225	I1226	D1227	L1228	T1229	S1230	A1231	T1232	N1233	L1234	V1235	I1238	T1239	K1240	Q1241	Q1242	N1243	A1244	Q1245	G1246	G1247	F1248	S1249	T1250	T1251	Q1252	D1253	T1254	V1255	V1256	A1257	L1258			
W1132	K1133	Q1136	E1137	G1138	D1139	H1140	G1141	S1142	H1143	V1144	Y1145	T1146	K1147	A1148	L1149	L1150	A1151	Y1152	L1153	F1154	A1155	L1156	A1157	G1158	N1159	Q1160	D1161	K1162	R1163	K1164	E1165	V1166	L1167	K1168	S1169	L1170	N1171	E1172	E1173	A1174	V1175	K1176	K1177	V1181	H1182	V1183	E1184	R1185	P1186	Q1187	P1188	K1189	P1190	A1191	P1192	V1193	G1194	
I1056	F1057	I1058	H1062	I1063	T1064	Q1065	A1066	L1070	S1071	Q1072	D1076	G1084	S1085	L1086	L1087	N1088	N1089	A1090	I1091	K1092	G1093	G1094	V1095	V1099	T1100	L1101	S1102	A1103	Y1104	I1105	T1106	I1107	A1108	L1109	L1110	E1111	I1112	P1113	L1114	T1115	V1116	T1117	H1118	P1119	V1120	A1124	L1125	F1126	C1127	L1128	E1129	S1130	A1131					
I984	Y985	V986	L987	D988	Y989	E992	T993	Q994	Q995	L996	I1000	K1001	S1002	A1004	I1005	G1006	Y1007	L1008	N1009	T1010	G1011	Q1015	Y1018	D1022	G1023	S1024	Y1025	S1026	T1027	R1031	Y1032	G1033	R1034	G1037	N1038	T1039	Y1040	L1041	T1042	A1043	F1044	V1045	L1046	K1047	T1048	F1049	A1052	R1053	A1054	Y1055								
K912	E913	T915	F916	N917	L920	V927	S928	E929	L931	S932	R934	L935	P936	P937	N938	V939	V940	E941	E942	R945	A946	S947	V948	S949	V950	L951	G952	N959	Q960	N961	T962	Q963	N964	L965	N967	N968	P969	V970	G971	C972	E974	Q975	N976	V977	V978	L979	F980	A981	P982	N983								
N851	G852	R853	L987	Q854	T855	V856	S857	W858	A859	V860	T861	P862	K863	S864	L865	G866	N867	V868	N869	F870	T871	V872	S873	A874	E875	A876	L877	E878	Q880	E881	L882	C883	G884	T885	E886	V887	P888	S889	V890	H893	G894	R895	K896	D897	T898	V899	I900	K901	P902	L903	L904	V905	E906	P907	E908	G909	L910	E911
A788	F789	Q790	P791	F792	F793	L796	T797	M798	V802	L803	R804	G805	E806	A807	F808	T809	L810	K811	A812	T813	V814	L815	N816	Y817	L818	P819	K820	C821	L822	R823	V824	S825	V826	Q827	L828	E829	A830	S831	P832	A833	F834	L835	A836	V837	P838	V839	E840	K841	E842	Q843	A844	P845	H846	C847	T848	C849	A850	
MET	GLY	ARG	GLY	HIS	ALA	ARG	LEU	VAL	HIS	VAL	GLU	GLU	PRO	HIS	THR	GLU	T730	V731	R732	K733	T738	W739	I740	W741	D742	L743	V744	V745	V746	N747	S748	A749	G750	V751	A752	E753	T757	I762	T763	E764	A767	G768	C771	L772	S773	E774	D775	A776	L778	A784	R787							
R645	H646	Q647	V648	Y649	I650	I653	T654	Y655	T656	P657	V658	S659	S660	T661	N662	E663	K664	D665	P669	Q602	S603	K608	P609	S614	A615	S616	S617	V618	Y619	N620	E624	K625	D626	L627	T628	G629	F630	P631	L634	N635	D636	Q637	I643	N644														
I499	M500	A501	K502	G503	G504	S575	Q576	S577	L578	P579	A580	S581	H582	L585	R586	V587	T588	A589	P590	Q592	S593	V594	C595	A596	L597	R598	Q602	S603	K608	P609	S614	A615	S616	S617	V618	Y619	N620	E624	K625	D626	L627	T628	G629	F630	P631	L634	N635	D636	Q637	I643	N644							
P430	C431	Y432	G433	Y434	Q435	W436	V437	S438	E439	E440	H441	E442	E443	A444	A448	Y449	L450	V451	K456	S457	F458	V459	H460	L461	E462	P463	M464	H466	E467	L468	P469	C470	G471	H472	T473	Q474	T475	V476	Q477	A478	H479	Y480	I481	L482	H483	L488	K491	K492	L493	S494	F495	Y496	Y497	L498				





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



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



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



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

Chain J:  33% 67%



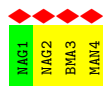
- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  33% 67% 67%



- Molecule 4: 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

Chain L:  25% 75% 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	466082	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 ($e^-/\text{\AA}^2$)	38.7	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.003	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (\AA)	336.64, 336.64, 336.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.052, 1.052, 1.052	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/10179	0.76	3/13829 (0.0%)
1	B	0.42	0/10179	0.73	11/13829 (0.1%)
1	C	0.46	0/10188	0.76	4/13841 (0.0%)
1	D	0.40	0/11230	0.70	5/15261 (0.0%)
All	All	0.44	0/41776	0.74	23/56760 (0.0%)

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
1	D	0	1

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	454	PRO	N-CA-C	-10.28	100.39	114.27
1	D	989	TYR	CB-CA-C	-9.14	96.52	110.88
1	B	391	ALA	N-CA-C	-8.99	102.31	113.28
1	C	609	PRO	N-CA-C	-7.47	99.52	110.80
1	D	1116	VAL	N-CA-C	-7.07	105.73	111.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	985	TYR	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	A	9958	0	9859	468	0
1	B	9958	0	9859	418	0
1	C	9967	0	9865	451	0
1	D	10985	0	10870	467	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	0	0
2	K	28	0	25	0	0
3	F	39	0	34	0	0
3	H	39	0	34	3	0
3	J	39	0	34	1	0
3	M	39	0	34	1	0
4	L	50	0	43	2	0
5	A	70	0	65	2	0
5	B	70	0	65	3	0
5	C	70	0	65	10	0
5	D	70	0	65	0	0
All	All	41466	0	40992	1776	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 22.

The worst 5 of 1776 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:B:1118:HIS:ND1	1:B:1119:PRO:HD2	1.49	1.26
1:B:1118:HIS:HB2	1:B:1119:PRO:HD3	1.24	1.11
1:B:1118:HIS:ND1	1:B:1119:PRO:CD	2.20	1.03
1:B:101:MET:HG3	1:B:122:VAL:HG13	1.36	1.03
1:B:1118:HIS:CB	1:B:1119:PRO:HD3	1.90	1.01

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	1272/1474 (86%)	986 (78%)	277 (22%)	9 (1%)	18	55
1	B	1272/1474 (86%)	1033 (81%)	230 (18%)	9 (1%)	18	55
1	C	1273/1474 (86%)	992 (78%)	274 (22%)	7 (0%)	24	62
1	D	1403/1474 (95%)	1122 (80%)	270 (19%)	11 (1%)	16	52
All	All	5220/5896 (88%)	4133 (79%)	1051 (20%)	36 (1%)	20	55

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	B	1118	HIS
1	C	339	GLN
1	C	412	THR
1	D	412	THR

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	1114/1290 (86%)	1104 (99%)	10 (1%)	70	76
1	B	1114/1290 (86%)	1105 (99%)	9 (1%)	73	77
1	C	1115/1290 (86%)	1098 (98%)	17 (2%)	57	70
1	D	1234/1290 (96%)	1220 (99%)	14 (1%)	65	74
All	All	4577/5160 (89%)	4527 (99%)	50 (1%)	63	74

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	654	THR
1	C	1195	HIS
1	D	1245	GLN
1	C	867	ASN
1	C	966	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	303	GLN
1	C	867	ASN
1	D	1015	GLN
1	C	413	ASN
1	C	620	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 ⓘ

24 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	2,1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	F	1	3,1	14,14,15	0.37	0	17,19,21	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	F	2	3	14,14,15	0.35	0	17,19,21	0.74	0
3	BMA	F	3	3	11,11,12	0.24	0	15,15,17	0.67	0
2	NAG	G	1	2,1	14,14,15	0.32	0	17,19,21	0.59	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.60	0
3	NAG	H	1	3,1	14,14,15	0.37	0	17,19,21	1.04	2 (11%)
3	NAG	H	2	3	14,14,15	0.46	0	17,19,21	1.22	2 (11%)
3	BMA	H	3	3	11,11,12	0.22	0	15,15,17	0.44	0
2	NAG	I	1	2,1	14,14,15	0.32	0	17,19,21	0.46	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.47	0
3	NAG	J	1	3,1	14,14,15	0.34	0	17,19,21	0.93	1 (5%)
3	NAG	J	2	3	14,14,15	0.35	0	17,19,21	0.71	0
3	BMA	J	3	3	11,11,12	0.22	0	15,15,17	0.49	0
2	NAG	K	1	2,1	14,14,15	0.29	0	17,19,21	0.81	1 (5%)
2	NAG	K	2	2	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	L	1	4,1	14,14,15	0.32	0	17,19,21	0.48	0
4	NAG	L	2	4	14,14,15	0.37	0	17,19,21	0.77	0
4	BMA	L	3	4	11,11,12	0.24	0	15,15,17	0.50	0
4	MAN	L	4	4	11,11,12	0.25	0	15,15,17	0.49	0
3	NAG	M	1	3,1	14,14,15	0.36	0	17,19,21	0.81	0
3	NAG	M	2	3	14,14,15	0.37	0	17,19,21	0.67	0
3	BMA	M	3	3	11,11,12	0.21	0	15,15,17	0.57	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
2	NAG	E	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	NAG	F	2	3	-	3/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	5/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	H	2	3	-	4/6/23/26	0/1/1/1
3	BMA	H	3	3	-	0/2/19/22	0/1/1/1
2	NAG	I	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
4	NAG	L	1	4,1	-	3/6/23/26	0/1/1/1
4	NAG	L	2	4	-	4/6/23/26	0/1/1/1
4	BMA	L	3	4	-	2/2/19/22	0/1/1/1
4	MAN	L	4	4	-	1/2/19/22	0/1/1/1
3	NAG	M	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	M	2	3	-	3/6/23/26	0/1/1/1
3	BMA	M	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	2	NAG	C1-O5-C5	3.69	117.14	112.19
3	F	1	NAG	C1-O5-C5	2.82	115.96	112.19
3	J	1	NAG	C1-O5-C5	2.62	115.69	112.19
3	H	1	NAG	C1-O5-C5	2.42	115.43	112.19
3	F	1	NAG	C3-C4-C5	2.28	114.36	110.23

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

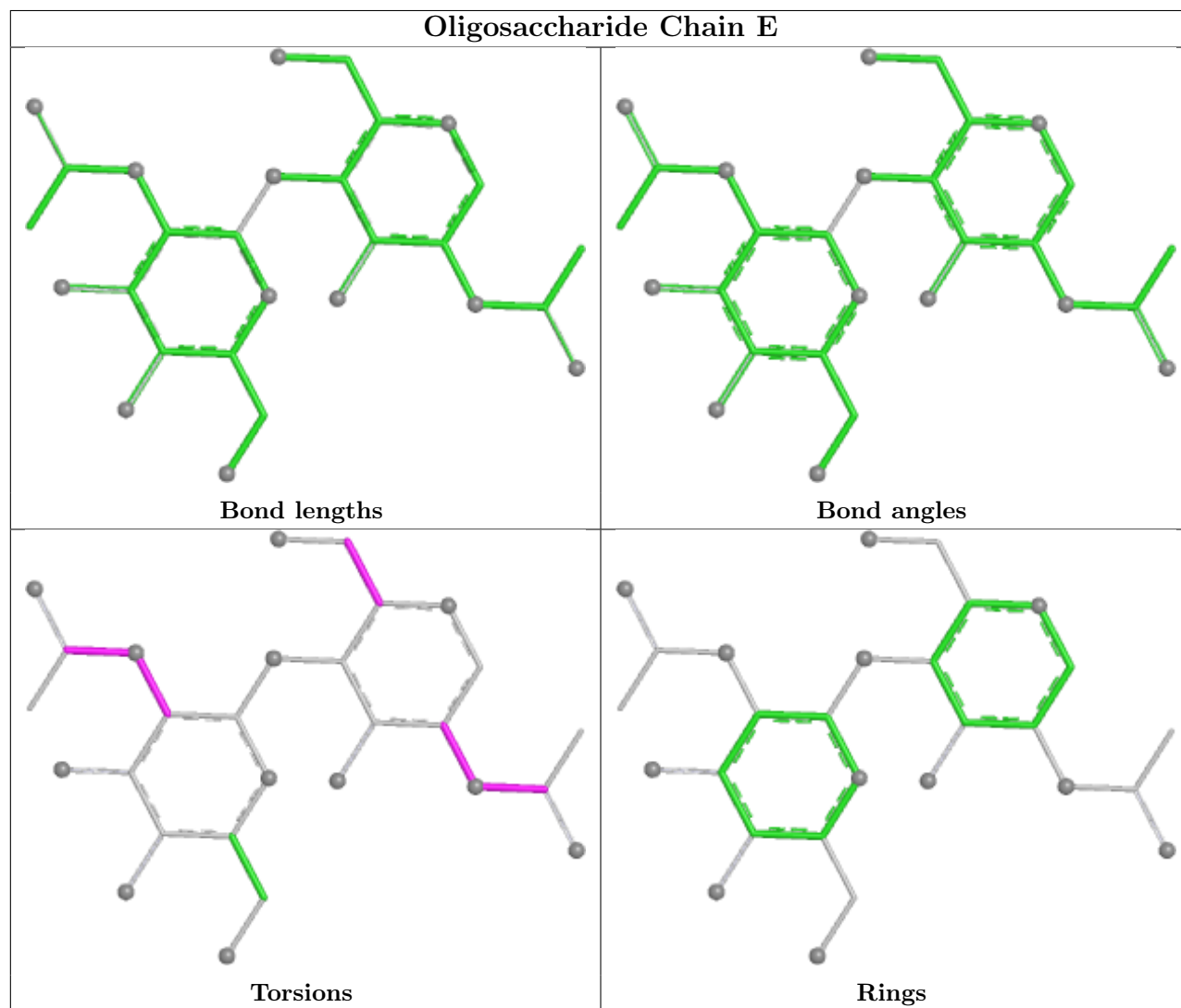
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C1-C2-N2-C7
2	E	2	NAG	C3-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2

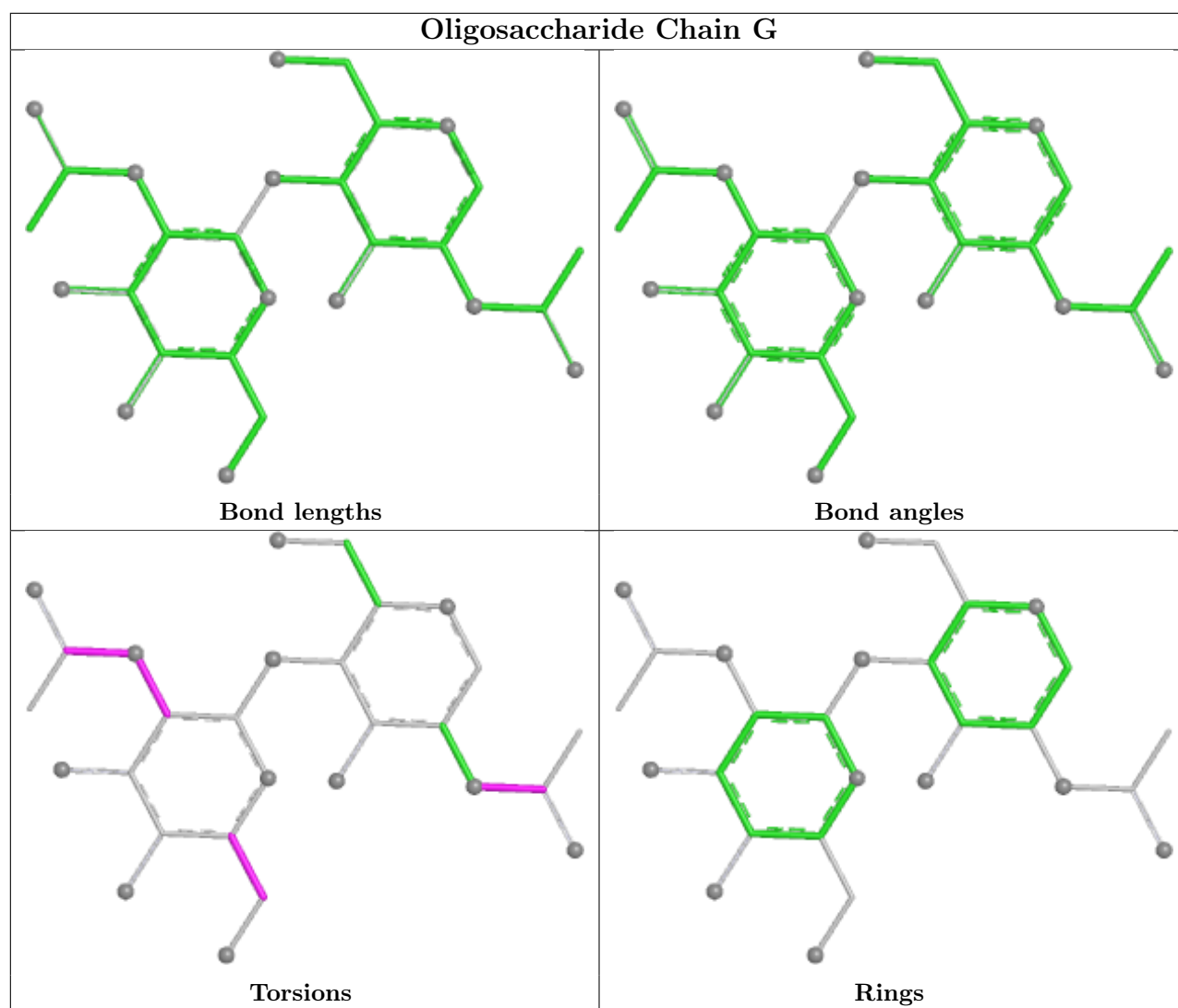
There are no ring outliers.

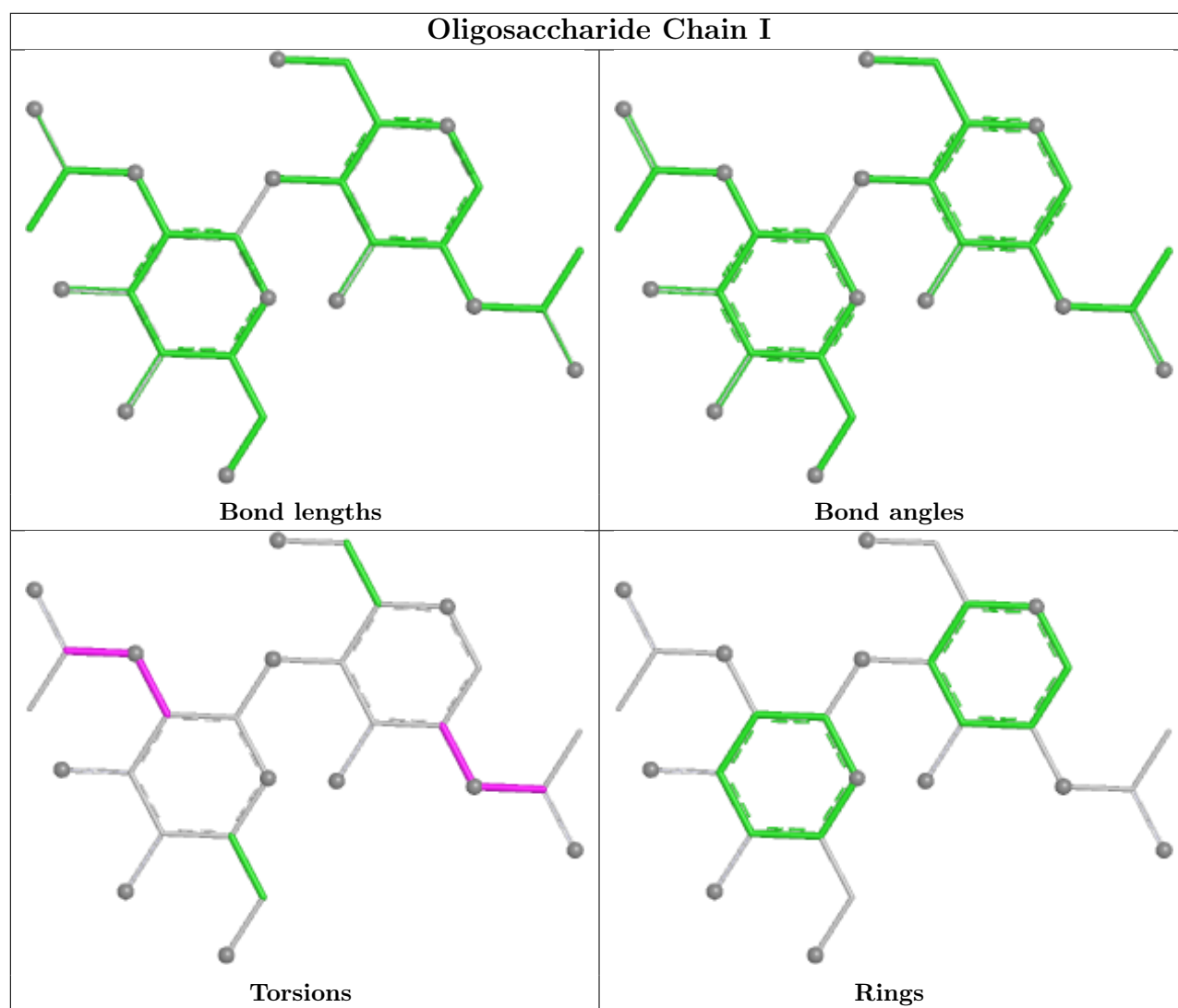
7 monomers are involved in 7 short contacts:

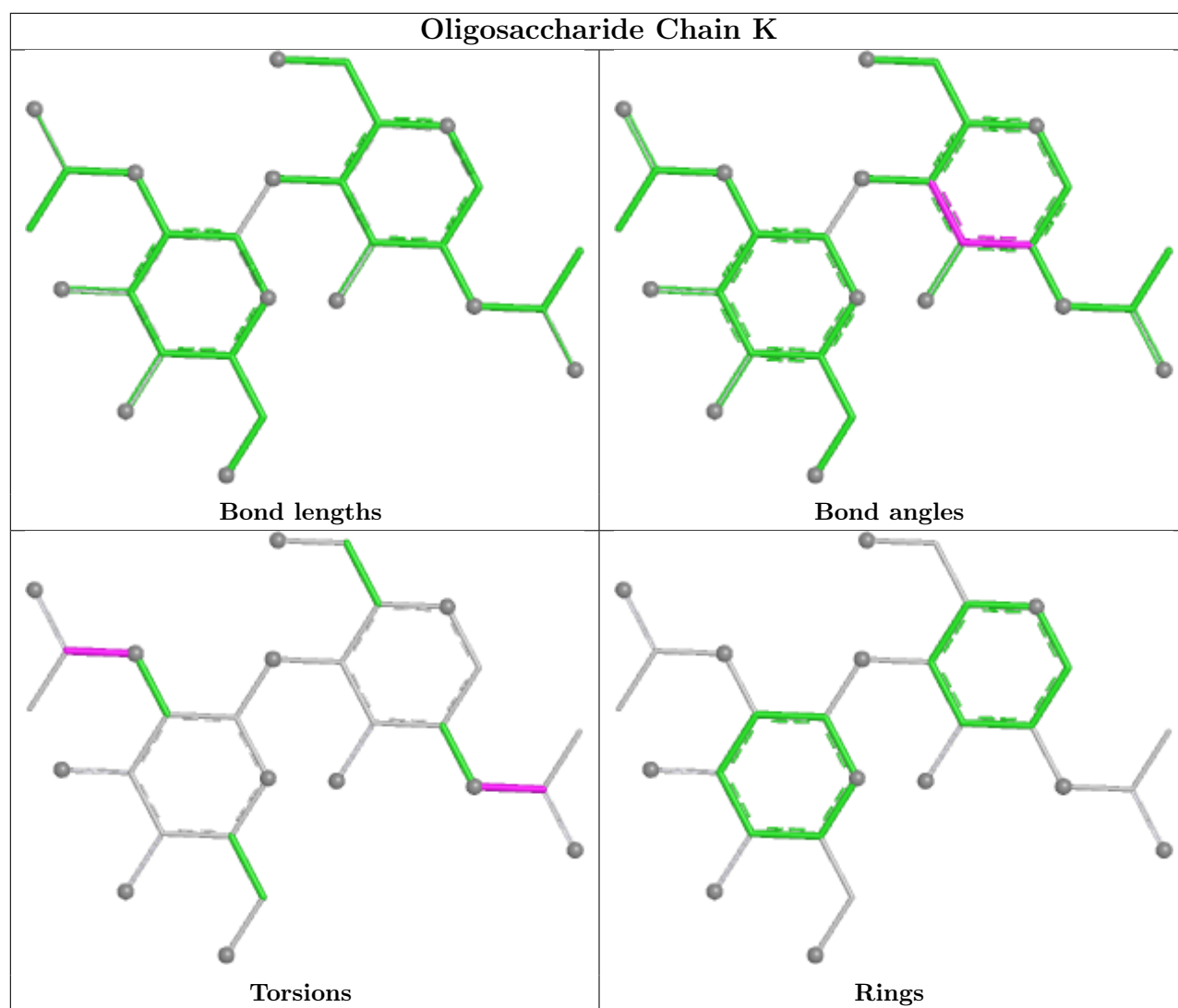
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	2	NAG	1	0
4	L	2	NAG	1	0
3	H	2	NAG	3	0
4	L	4	MAN	1	0
4	L	3	BMA	1	0
3	M	1	NAG	1	0
3	M	2	NAG	1	0

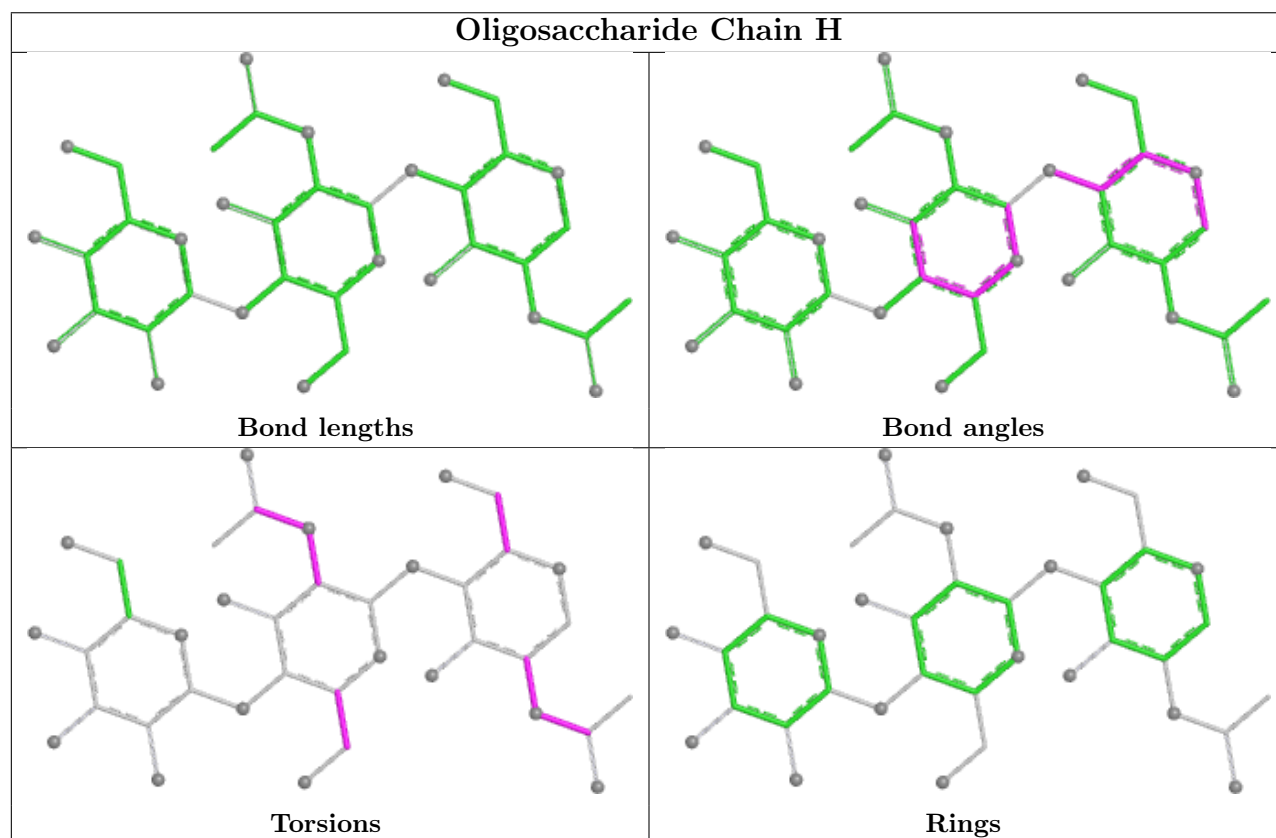
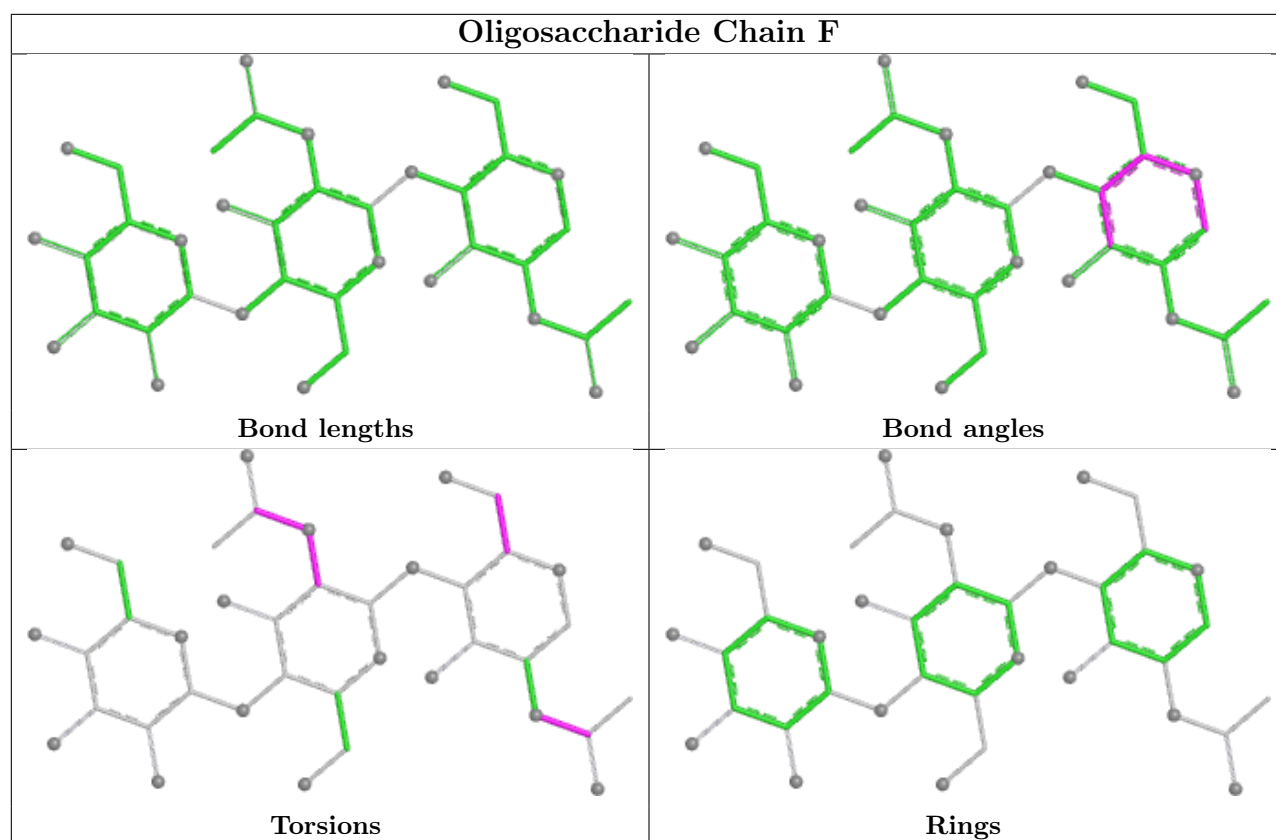
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

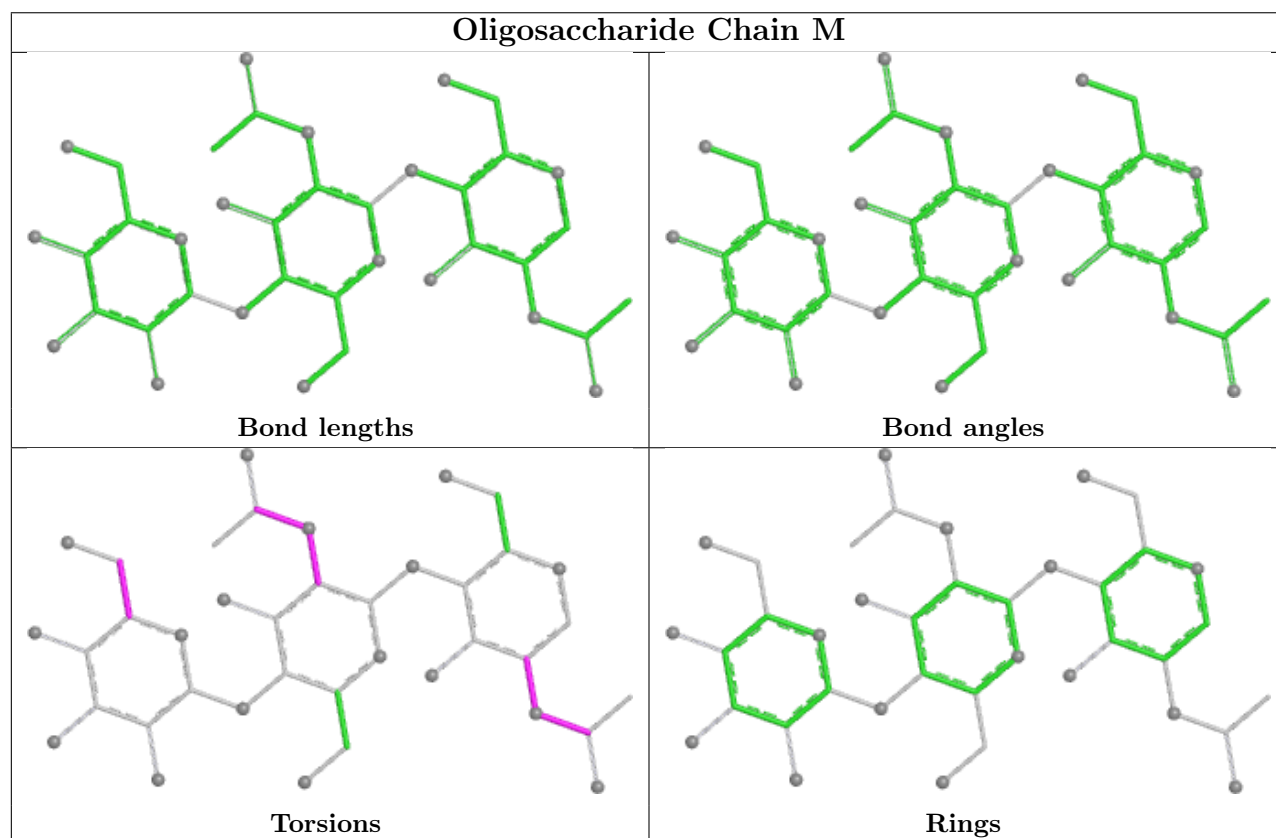
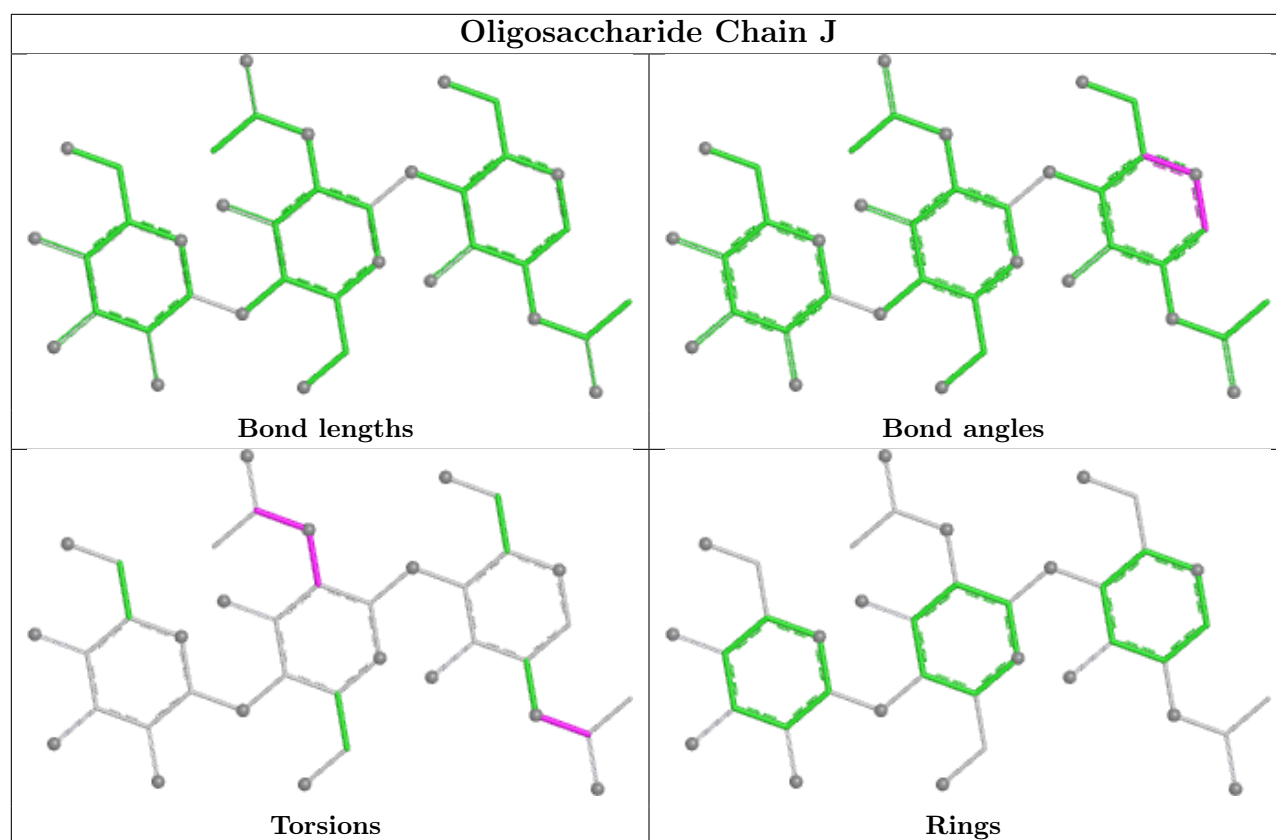


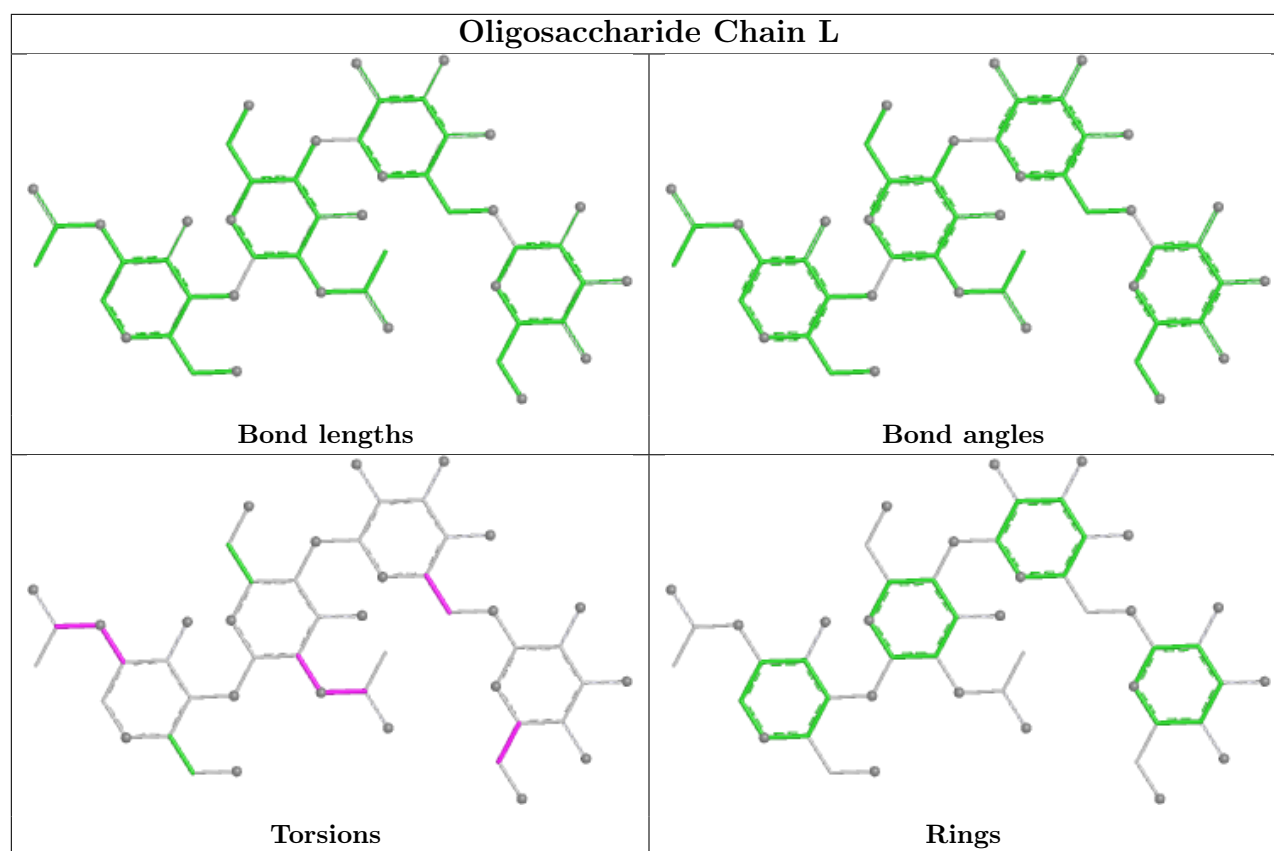












5.6 Ligand geometry [i](#)

20 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	D	2004	1	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	B	2001	1	14,14,15	0.33	0	17,19,21	0.72	0
5	NAG	D	2001	1	14,14,15	0.28	0	17,19,21	0.60	0
5	NAG	D	2003	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	B	2004	1	14,14,15	0.27	0	17,19,21	0.57	0
5	NAG	C	2004	1	14,14,15	0.28	0	17,19,21	0.53	0
5	NAG	A	2002	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	C	2002	1	14,14,15	0.35	0	17,19,21	0.79	1 (5%)
5	NAG	D	2005	1	14,14,15	0.27	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.49	0
5	NAG	C	2003	1	14,14,15	0.27	0	17,19,21	0.48	0
5	NAG	D	2002	1	14,14,15	0.28	0	17,19,21	0.48	0
5	NAG	A	2003	1	14,14,15	0.30	0	17,19,21	0.39	0
5	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	B	2003	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	2001	1	14,14,15	0.41	0	17,19,21	0.66	0
5	NAG	A	2001	1	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	A	2004	1	14,14,15	0.29	0	17,19,21	0.52	0
5	NAG	B	2002	1	14,14,15	0.29	0	17,19,21	0.64	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
5	NAG	D	2004	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2001	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2004	1	-	5/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	4/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	3/6/23/26	0/1/1/1
5	NAG	A	2001	1	-	3/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2002	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	C	2002	NAG	C1-O5-C5	2.20	115.13	112.19

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2001	NAG	C3-C2-N2-C7
5	A	2001	NAG	C8-C7-N2-C2
5	A	2001	NAG	O7-C7-N2-C2
5	A	2002	NAG	O7-C7-N2-C2
5	A	2003	NAG	C1-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	3	0
5	C	2004	NAG	7	0
5	A	2005	NAG	1	0
5	C	2003	NAG	1	0
5	A	2003	NAG	1	0
5	C	2001	NAG	2	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.

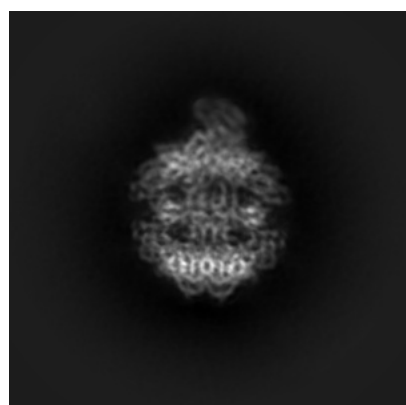
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12755. These allow visual inspection of the internal detail of the map and identification of artifacts.

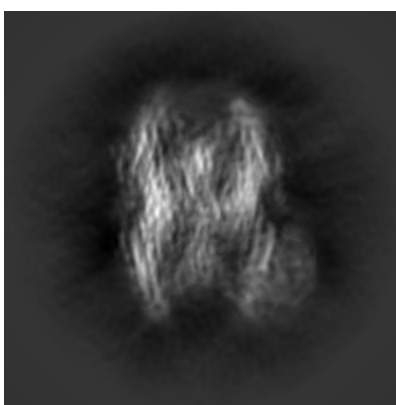
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

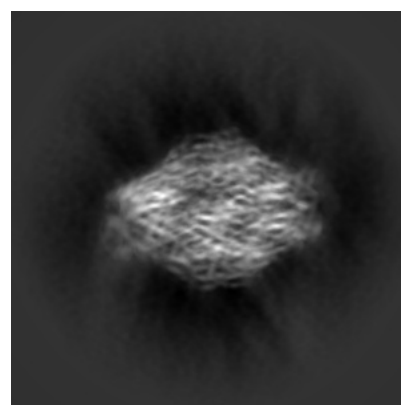
6.1.1 Primary map



X



Y

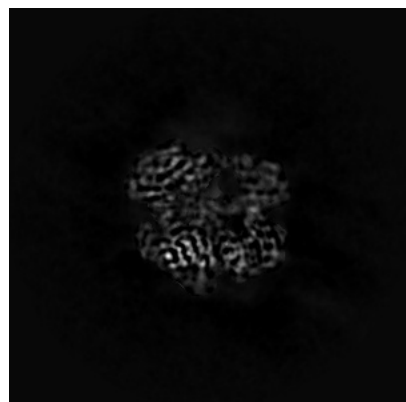


Z

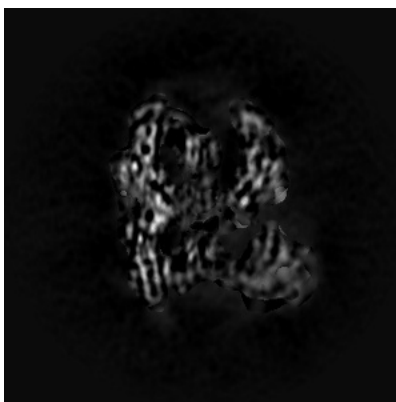
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

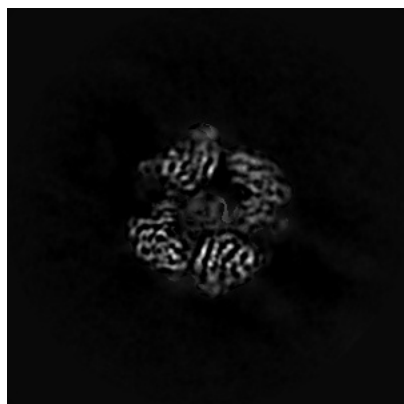


Z Index: 160

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

6.3 Largest variance slices [i](#)

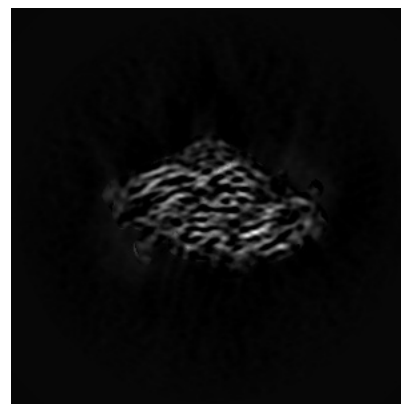
6.3.1 Primary map



X Index: 175



Y Index: 171

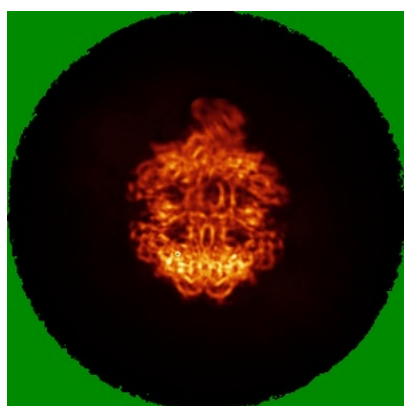


Z Index: 117

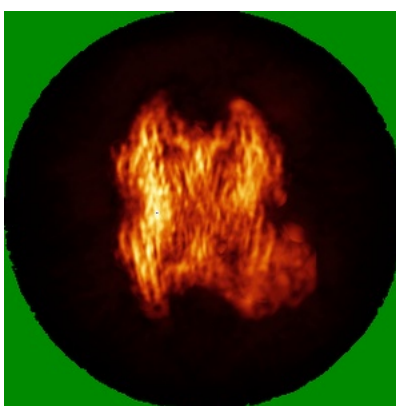
The images above show the largest variance slices of the map in three orthogonal directions.

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

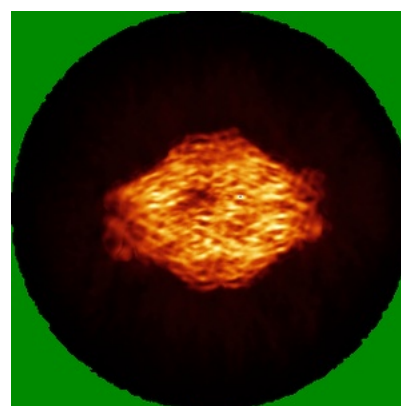
6.4.1 Primary map



X



Y

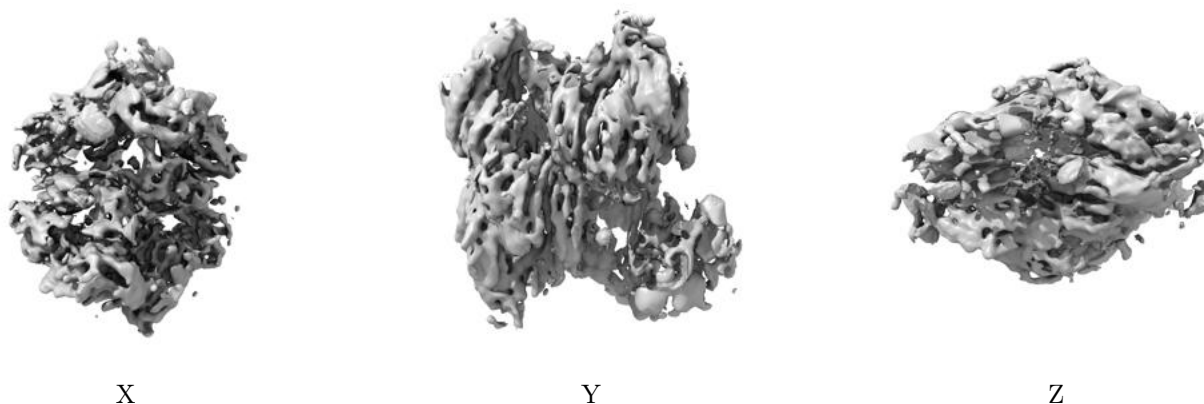


Z

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

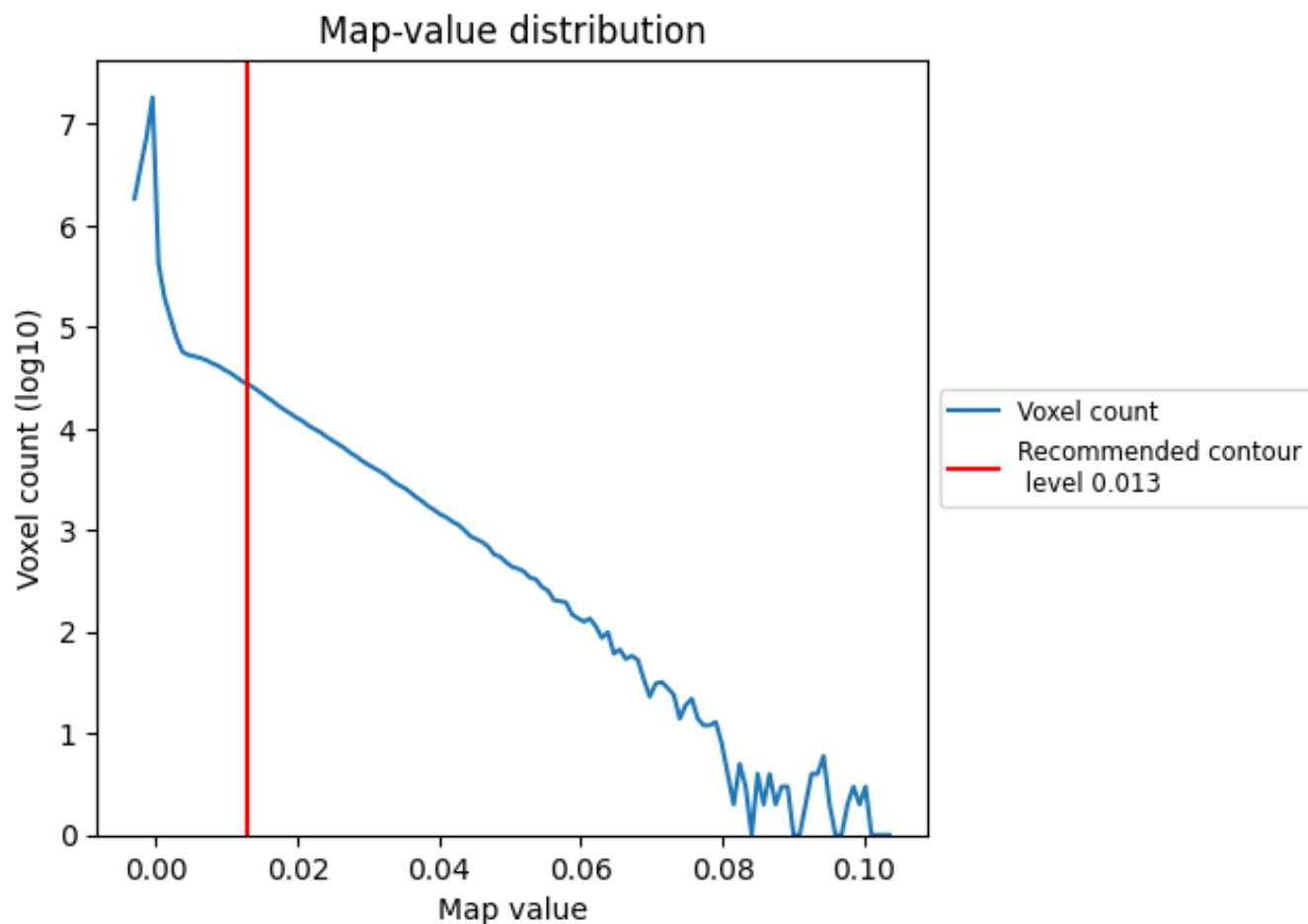
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

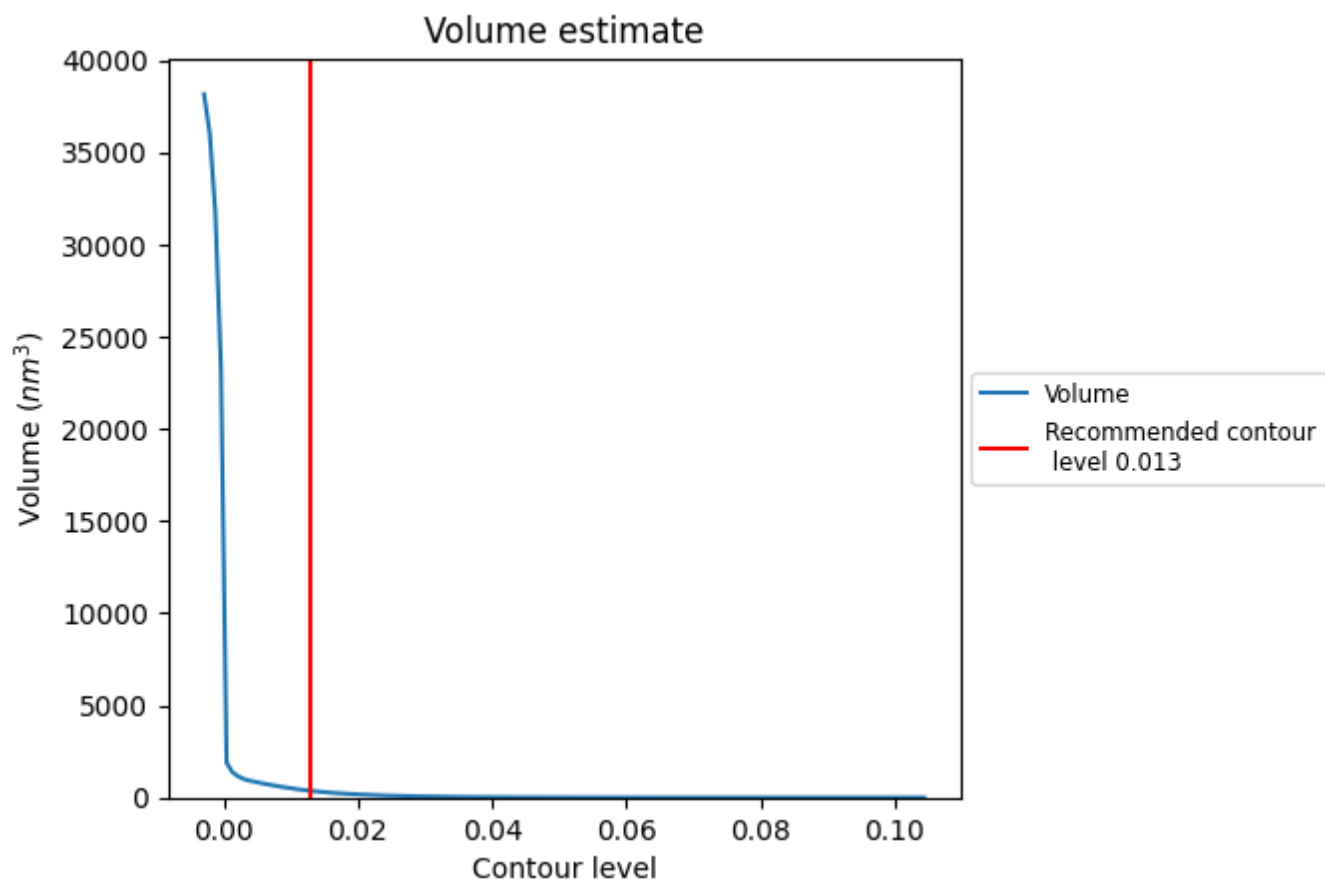
This section contains the results of statistical analysis of the map.

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.

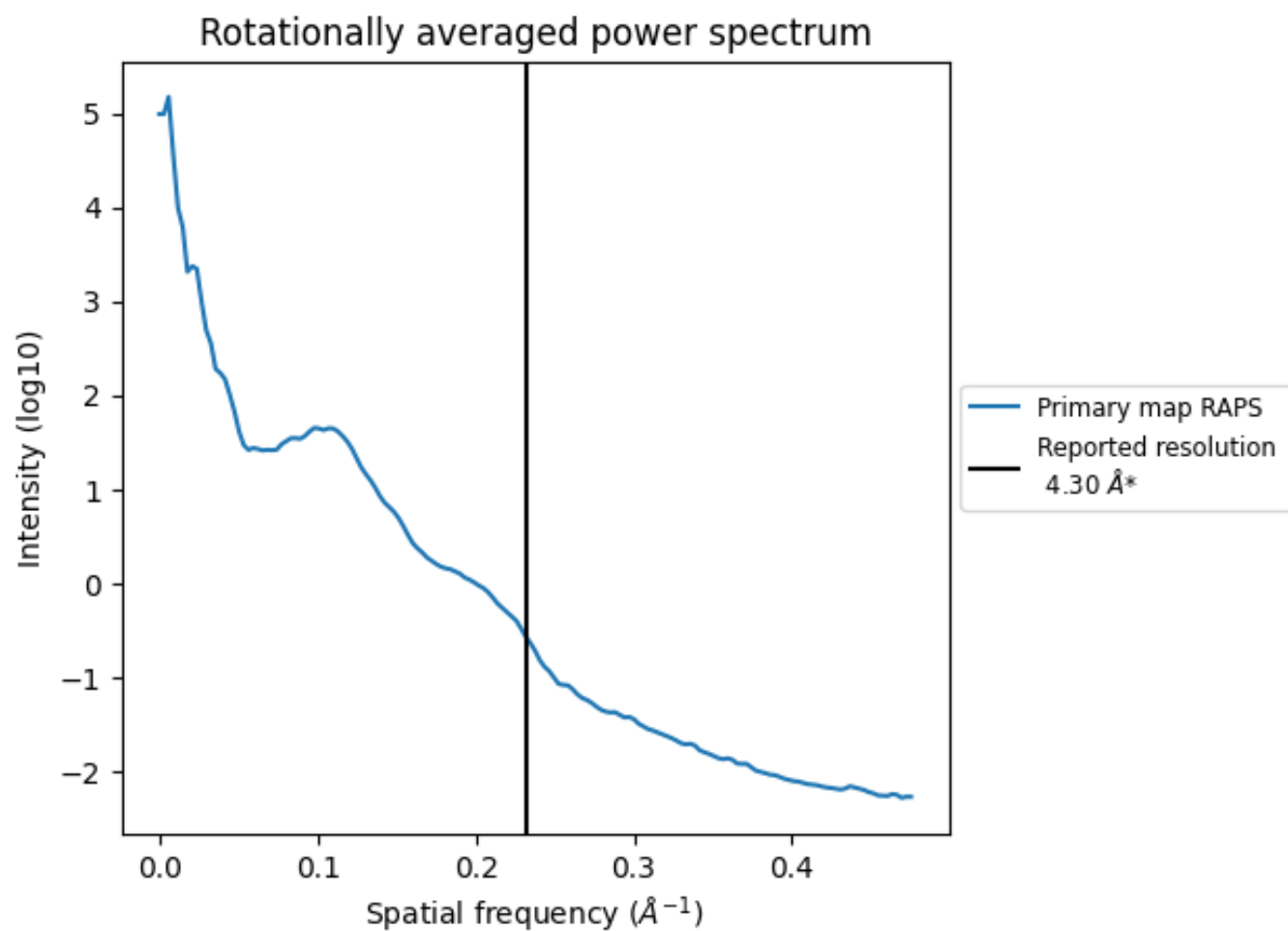
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 365 nm³; this corresponds to an approximate mass of 330 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 0.233 \AA^{-1}

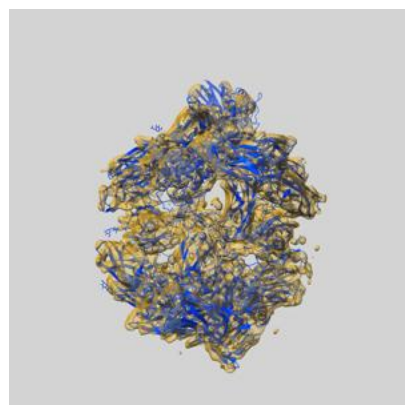
8 Fourier-Shell correlation ⓘ

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

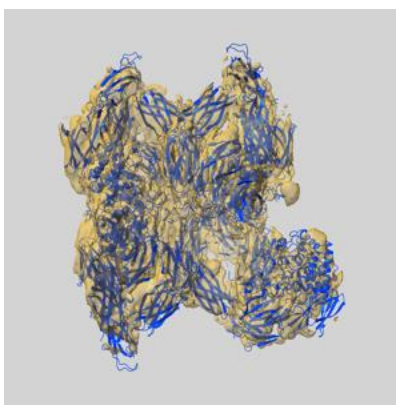
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12755 and PDB model 7O7S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

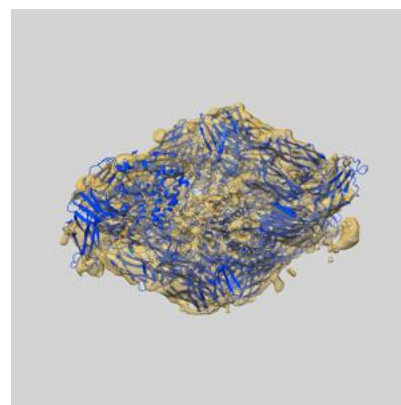
9.1 Map-model overlay [i](#)



X



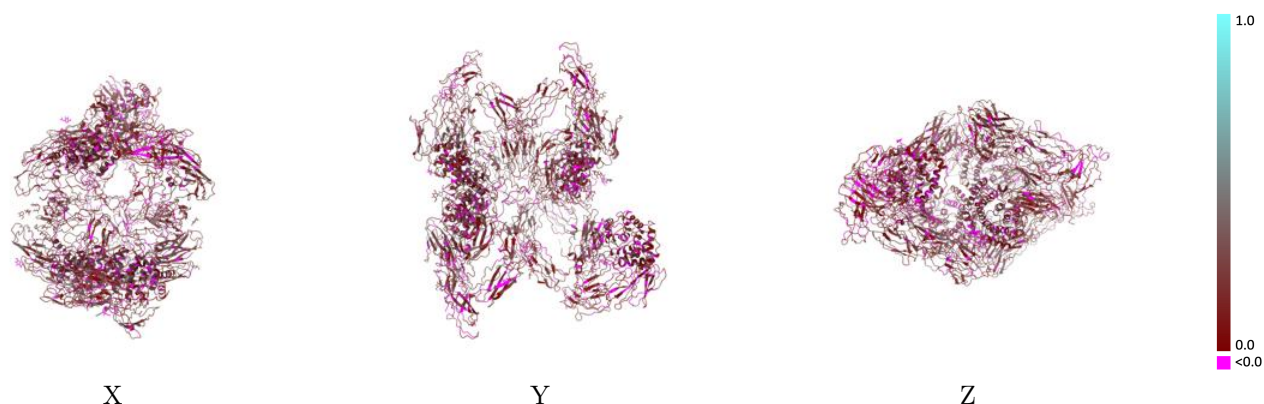
Y



Z

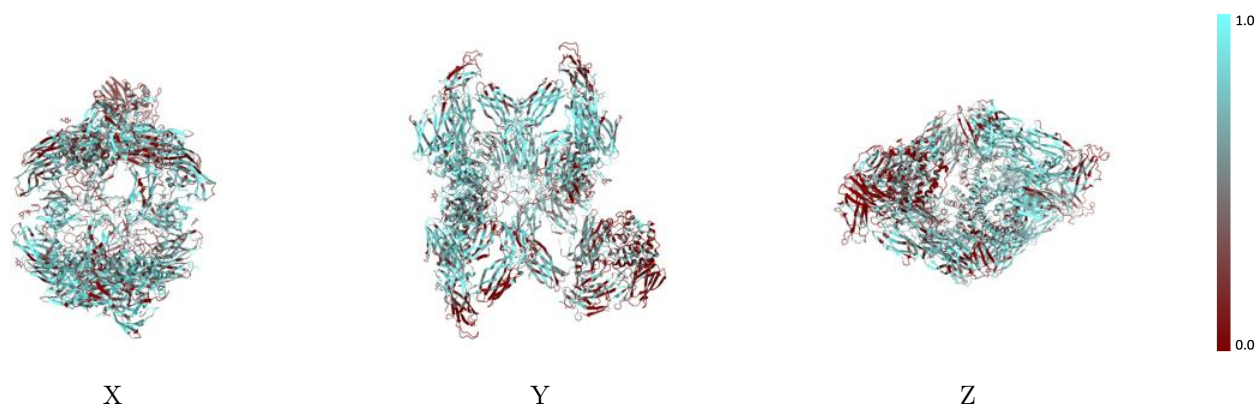
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



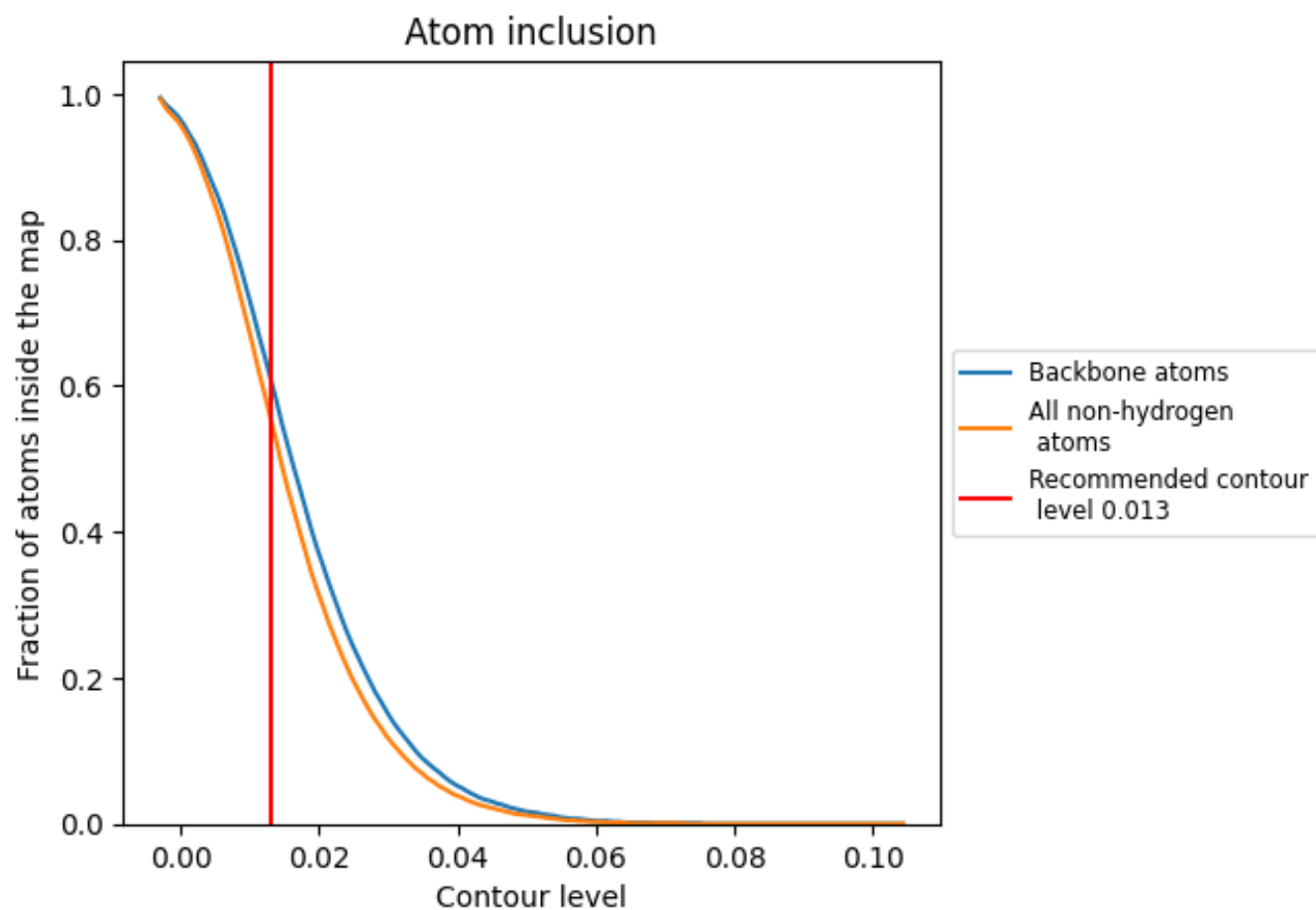
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).





























9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 55% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5540	 0.1830
A	 0.6670	 0.2180
B	 0.6060	 0.1880
C	 0.5400	 0.1770
D	 0.4200	 0.1520
E	 0.5710	 0.2100
F	 0.4870	 0.0030
G	 0.6430	 0.2550
H	 0.6410	 0.1860
I	 0.3570	 0.2860
J	 0.8460	 0.2750
K	 0.6430	 0.1600
L	 0.0000	 0.1340
M	 0.2310	 0.2440

