



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 07:12 am GMT

PDB ID : 7O7S
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)

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<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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

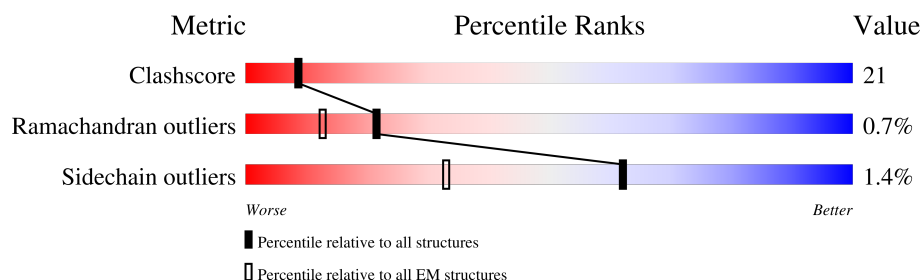
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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>50%</div> <div>36%</div> <div>13%</div> </div>
1	B	1474	<div> <div>24%</div> <div>53%</div> <div>33%</div> <div>13%</div> </div>
1	C	1474	<div> <div>32%</div> <div>52%</div> <div>34%</div> <div>13%</div> </div>
1	D	1474	<div> <div>48%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
2	E	2	<div> <div>50%</div> <div>100%</div> </div>
2	G	2	<div> <div>100%</div> </div>
2	I	2	<div> <div>50%</div> <div>50%</div> </div>
2	K	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
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.

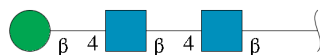
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	0	0
			9958	6331	1672	1912	43		
1	B	1276	Total	C	N	O	S	0	0
			9958	6331	1672	1912	43		
1	C	1277	Total	C	N	O	S	0	0
			9967	6336	1673	1915	43		
1	D	1407	Total	C	N	O	S	0	0
			10985	6988	1836	2113	48		

- 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.



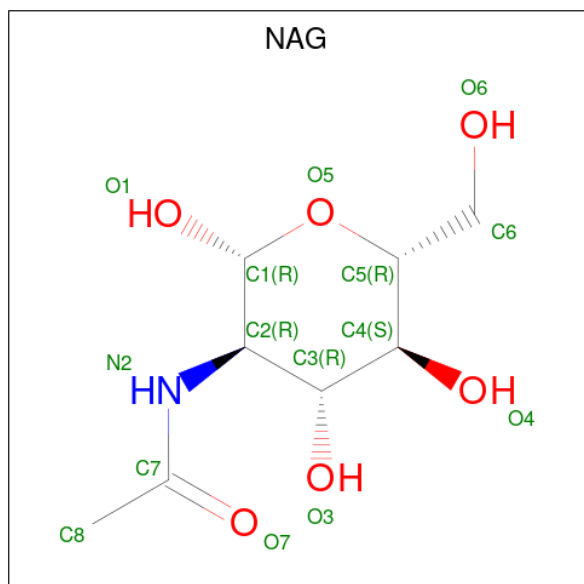
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	H	3	Total	C	N	O	0	0
			39	22	2	15		
3	J	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		

- 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 (three-letter code: 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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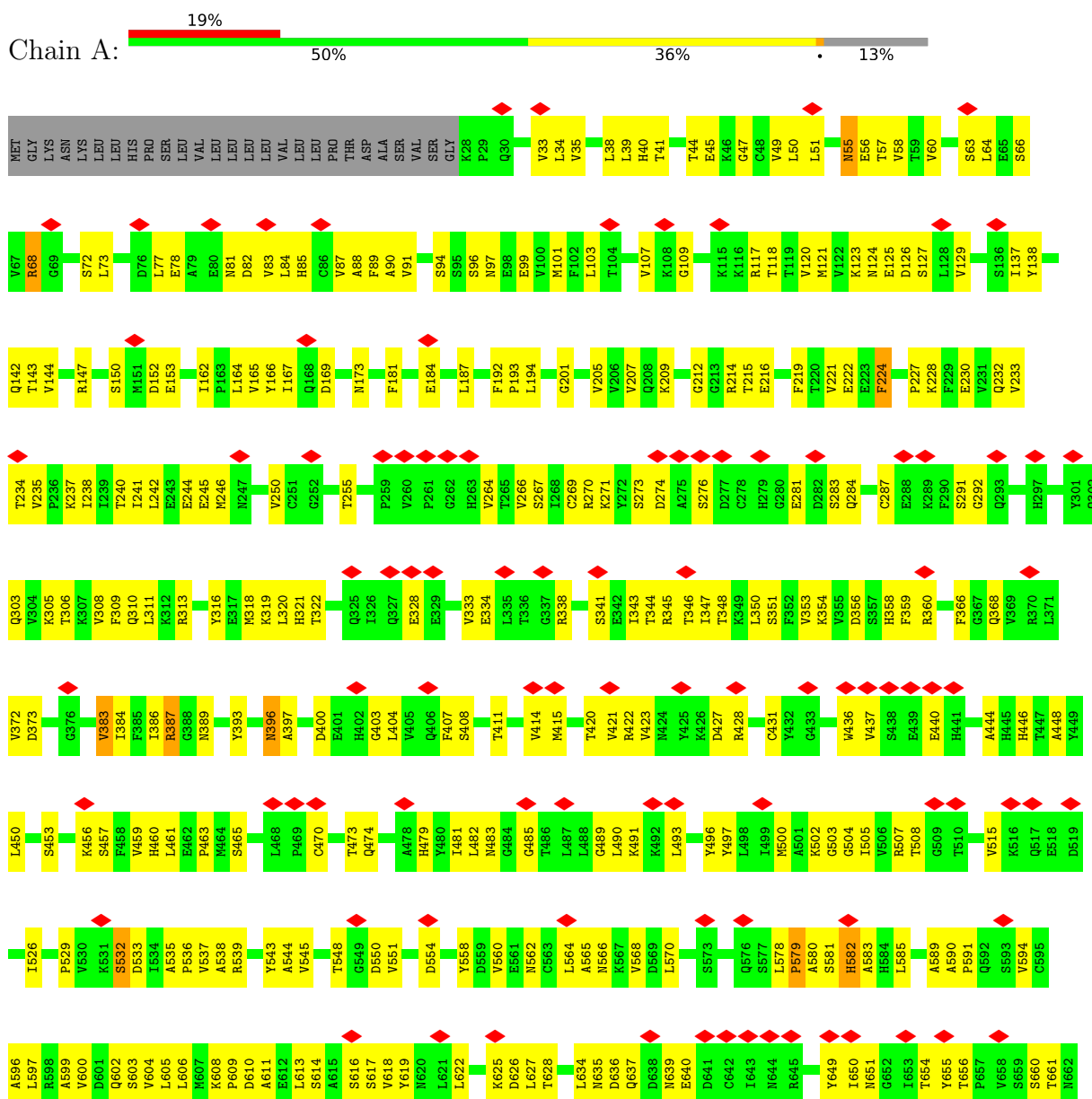
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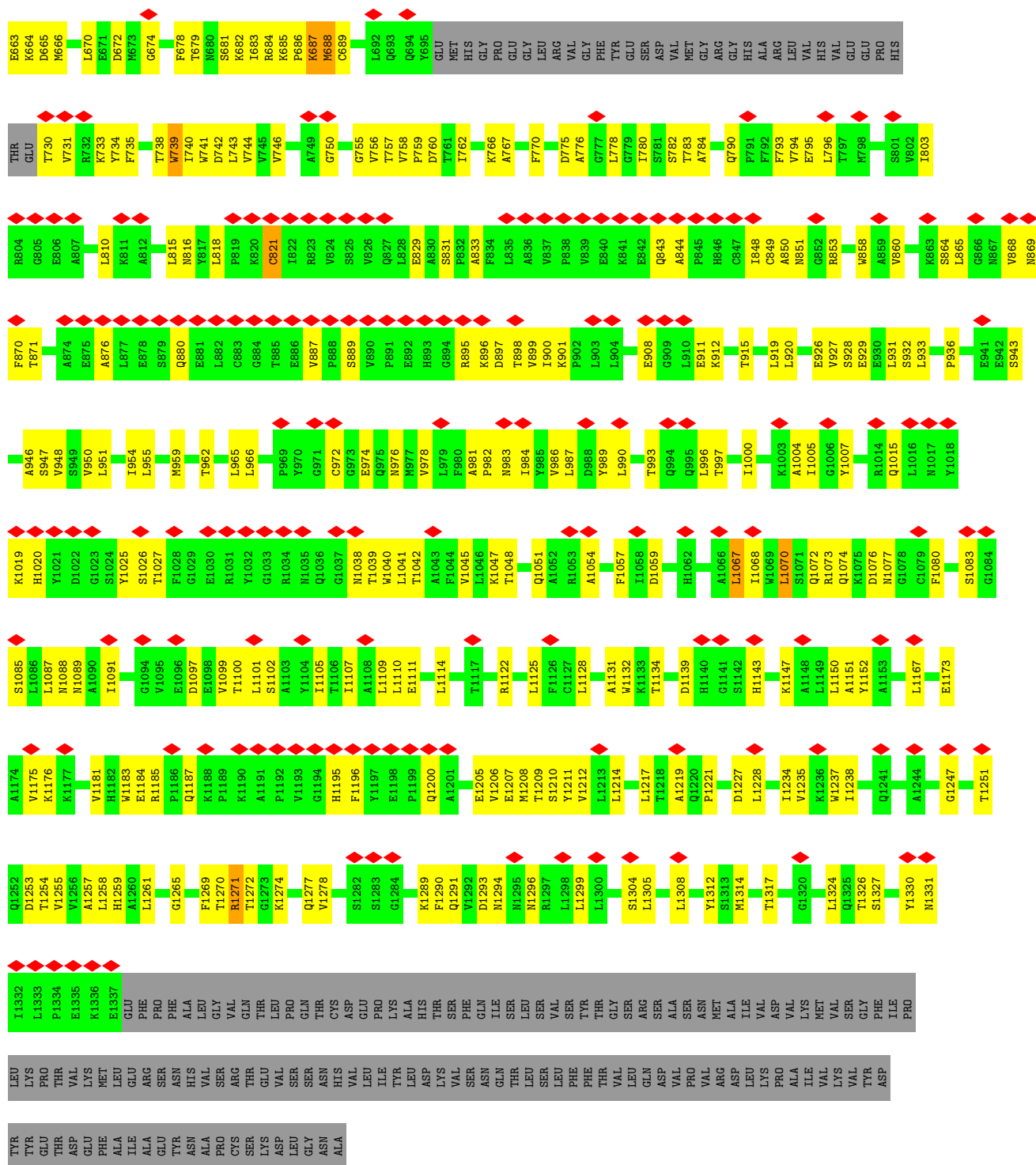
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	A	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	B	1	Total 14	C 8	N 1	O 5	0
5	C	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

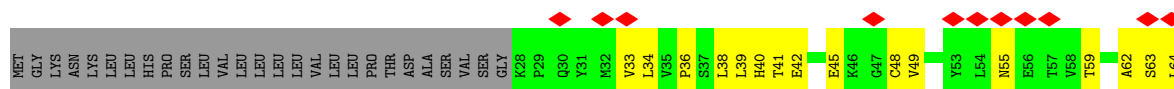
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

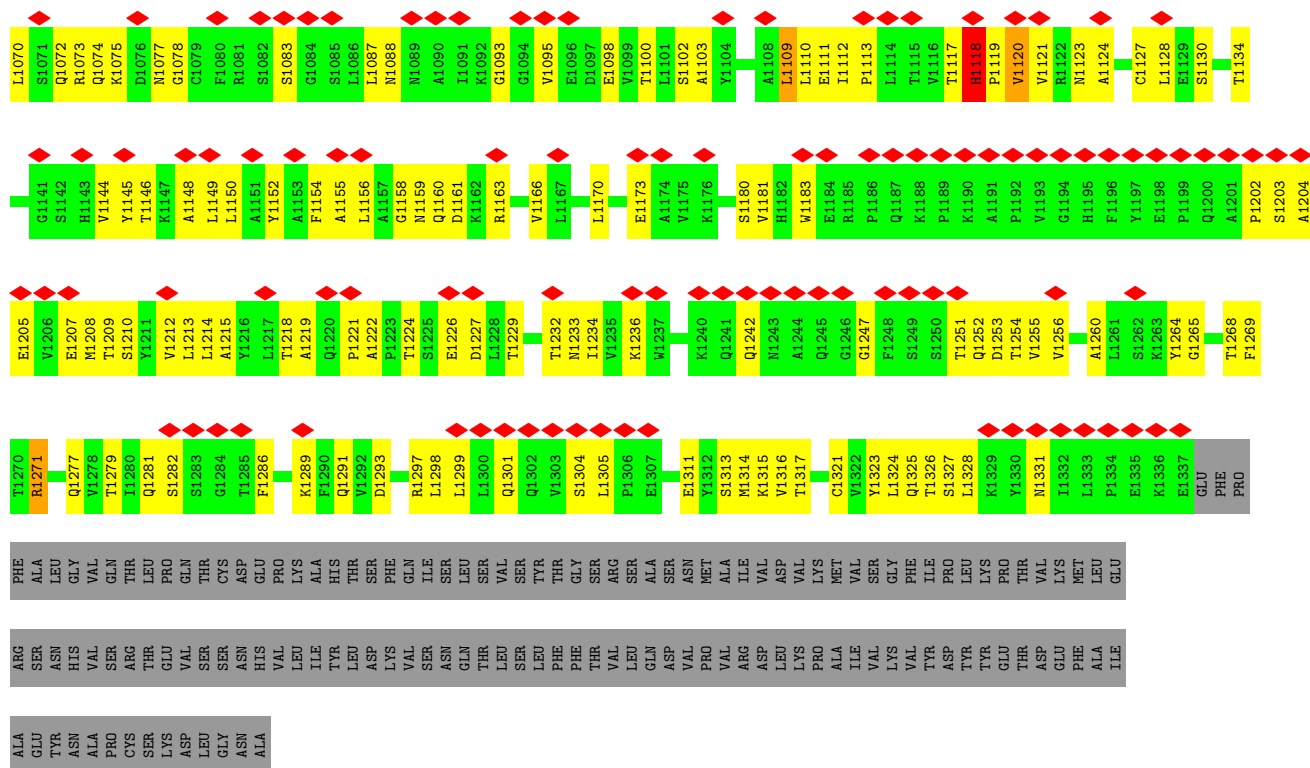




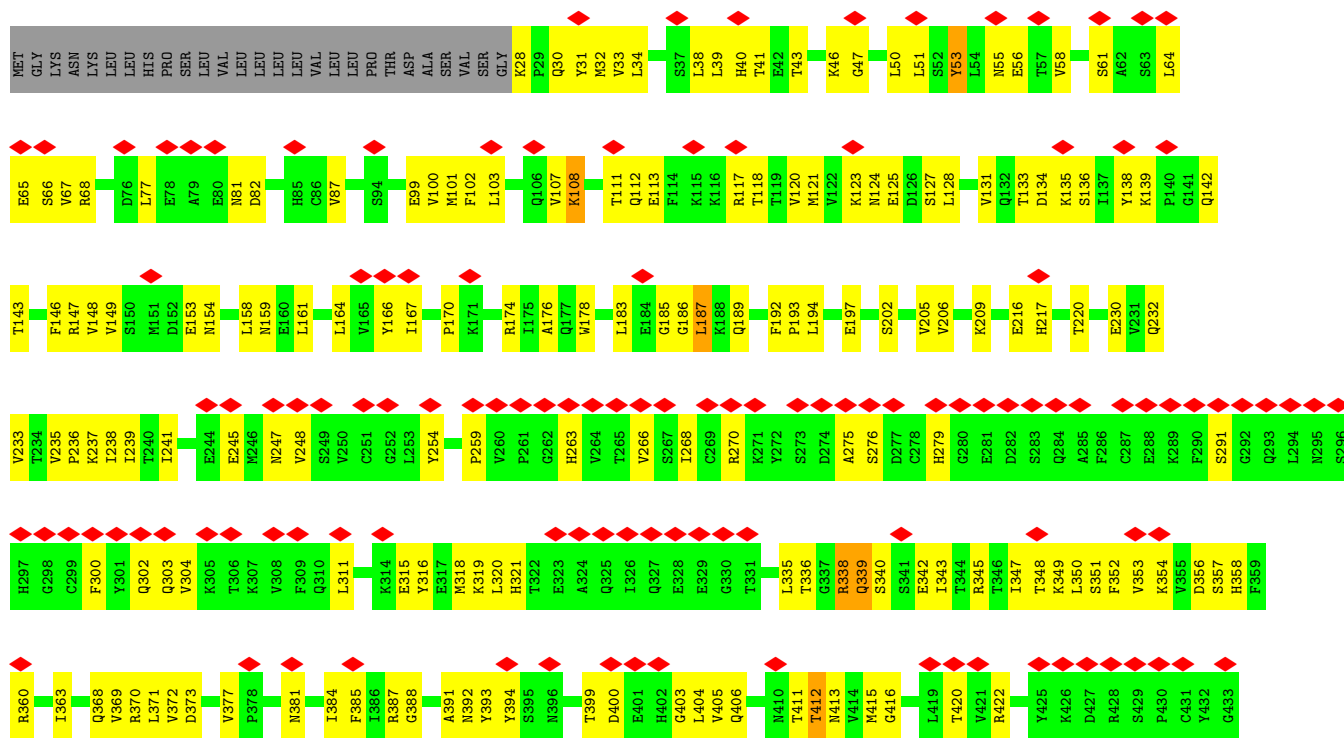
• Molecule 1: Alpha-2-macroglobulin





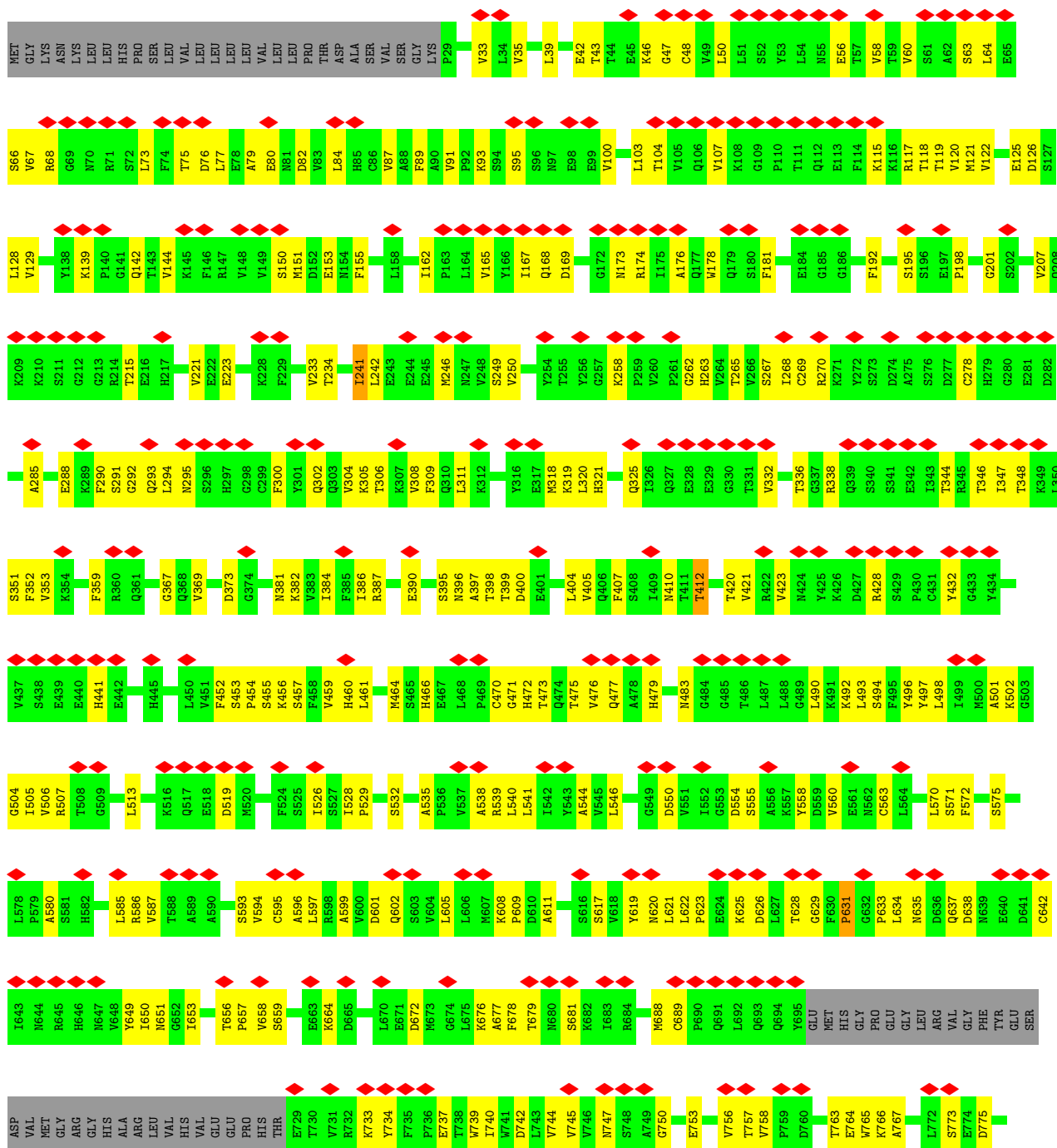


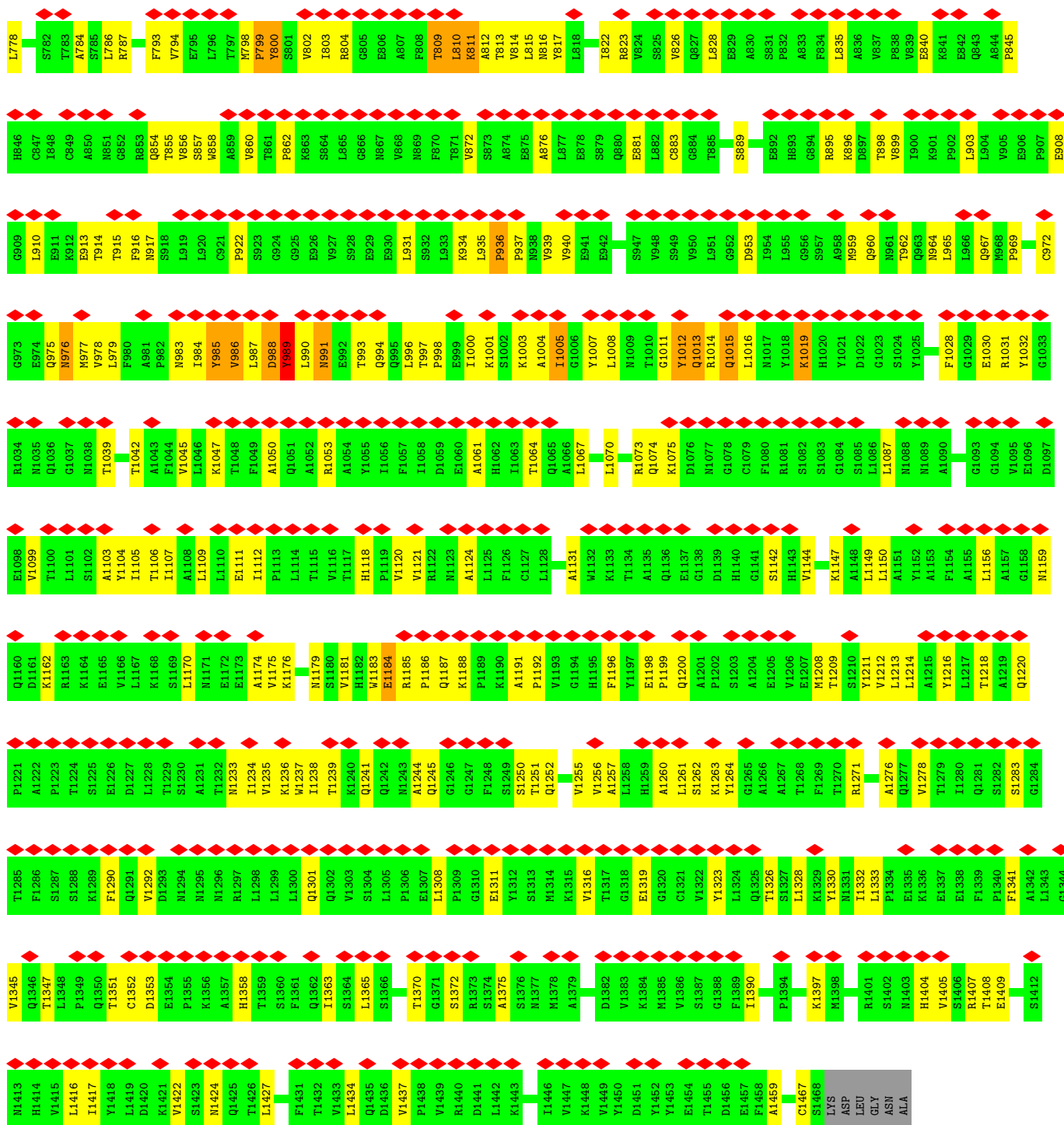
• Molecule 1: Alpha-2-macroglobulin



PHE	R1271	R1272	G1273	Q1277	T1278	T1279	T1280	Q1281	S1282	S1283	ASP	GLU	PRO	LYS	HIS	THR	SER	GLN	ILE	SER	LEU	SER	VAL	SER	THR	GLY	GLY	ARG	SER	ALA	ASN	MET	ALA	ILE	ASP	VAL	VAL	LYS	MET	GLY	SER	GLY	PHE	ILE	PRO	LEU	LEU	VAL	LYS	MET	LEU	LEU	GLU					
E1205	V1206	E1207	M1208	T1209	S1210	Y1211	V1212	L1213	L1217	T1218	F1219	A1220	P1221	A1222	S1225	E1226	D1227	L1228	T1229	S1230	A1231	T1232	M1233	L1234	V1235	I1238	T1239	K1240	Q1241	Q1242	M1243	A1244	Q1245	G1246	G1247	F1248	S1249	S1250	T1251	Q1252	D1253	T1254	V1255	V1256	A1257	L1258	H1259	A1260	L1261	S1262	K1263	G1265	A1266	A1267				
L1070	S1071	Q1072	D1076	G1084	S1085	L1086	L1087	M1088	M1089	A1090	T1091	K1092	G1093	G1094	V1095	V1099	T1100	L1101	S1102	A1103	Y1104	T1105	K1106	L1107	A1108	L1109	L1110	E1111	P1112	P1113	L1114	T1115	V1116	T1117	H1118	P1119	V1120	A1124	L1125	F1126	C1127	L1128	S1130	A1131	K1133	Q1136	E1137	D1138	G1139	H1140	G1141	S1142						
T993	Q994	Q995	L996	T1000	K1001	S1002	K1003	A1004	T1005	L1008	N1009	T1010	G1011	Q1015	Y1018	D1022	G1023	S1024	S1025	S1026	T1027	R1031	Y1032	G1033	R1034	G1037	N1038	T1039	W1040	L1041	T1042	A1043	F1044	V1045	L1046	K1047	T1048	F1049	A1052	R1053	Y1055	I1056	F1057	I1058	N1059	T1061	H1062	I1063	A1066									
L920	Y927	S928	E929	E930	L931	S932	L933	Y934	L935	P936	P937	N938	Y939	Y940	E941	E942	R945	A946	S947	Y948	S949	Y950	L951	G952	N959	Q960	N961	T962	Q963	N964	L965	L966	P969	Y970	G971	C972	G973	E974	Q975	N976	N977	Y978	P980	A981	P982	N983	T984	Y985	V986	L987	P988	Y989	E992					
W858	A859	W860	T861	P862	K863	S864	L865	C866	N867	W868	N869	F870	T871	W872	S873	A874	E875	A876	L877	E878	S879	Q880	E881	L882	C883	G884	T885	E886	W887	P888	S889	W890	H893	G894	R895	K896	D897	T898	W899	I900	K901	P902	L903	L904	V905	E906	P907	E908	G909	L910	E911	K912	E913	T914	T915	F916	N917	
L796	T797	M798	V802	L803	R804	G805	E806	A807	F808	T809	L810	K811	A812	T813	V814	L815	N816	Y817	L818	P819	K820	C821	T822	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	N851	G852	R853	Q854	T855	W856	S857
LEU	VAL	HIS	VAL	GLU	PRD	THR	GLY	T730	T731	R732	K733	T738	W739	I740	D742	L743	V744	V745	V746	N747	S748	A749	G750	V751	A752	E753	T757	I762	T763	E764	A767	G768	C771	L772	S773	E774	D775	A776	G777	L778	A784	R787	A788	F789	Q790	F791	F792	F793										
I653	T654	Y655	T656	P657	V658	S659	T661	N662	E663	K664	D665	D672	M673	G674	L675	K676	A677	F678	C679	N680	S681	R684	K687	M688	C689	P690	S614	A615	S616	S617	V618	Y619	N620	E624	K625	D626	L627	G628	G629	L634	N635	D636	Q637	I643	N644	V645	H646	N647	V648	Y649	I650							
S573	P574	S575	Q576	S577	L578	S579	A580	S581	H582	L585	R586	V587	T588	A590	P591	S592	S593	V594	C595	A596	L597	R598	Q602	S603	K608	S614	A615	S616	S617	V618	Y619	N620	E624	K625	D626	L627	G628	G629	L634	N635	D636	Q637	I643	N644	V645	H646	N647	V648	Y649	I650								
G503	G504	Y505	V506	R507	H511	G512	L513	L514	V515	K516	Q517	E518	D519	M520	F524	S525	I526	S527	I528	P529	V530	K531	S532	D533	I534	A535	P536	V537	A538	R539	C470	G471	H472	T473	Q474	T475	V476	Q477	A478	H479	Y480	I481	L482	H483	L488	K491	K492	L493	S494	F495	Y496	Y497	L498	I499	M500	K502		

- Molecule 1: Alpha-2-macroglobulin





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



NAG1
NAG2

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

Chain G:  100%



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

Chain I:  50% 50%



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

Chain K:  50% 50%



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

Chain F:  33% 67% 33%



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

Chain H:  33% 33% 33% 33%



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

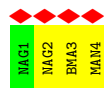
Chain J:  33% 67%



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



- 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



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: BMA, MAN, NAG

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	0.49	0/10179	0.74	4/13829 (0.0%)
1	B	0.42	0/10179	0.71	5/13829 (0.0%)
1	C	0.46	0/10188	0.74	5/13841 (0.0%)
1	D	0.39	0/11230	0.67	1/15261 (0.0%)
All	All	0.44	0/41776	0.71	15/56760 (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 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1120	VAL	CG1-CB-CG2	7.29	122.56	110.90
1	B	1120	VAL	CA-CB-CG2	7.28	121.82	110.90
1	D	989	TYR	CB-CA-C	-6.94	96.52	110.40
1	A	1070	LEU	CA-CB-CG	6.74	130.80	115.30
1	C	598	ARG	NE-CZ-NH1	6.25	123.42	120.30

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	452	0
1	B	9958	0	9859	413	0
1	C	9967	0	9865	436	0
1	D	10985	0	10870	439	0
2	E	28	0	25	0	0
2	G	28	0	25	0	0
2	I	28	0	25	1	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	2	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	11	0
5	D	70	0	65	1	0
All	All	41466	0	40992	1717	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 21.

The worst 5 of 1717 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%)	19	56
1	B	1272/1474 (86%)	1033 (81%)	230 (18%)	9 (1%)	19	56
1	C	1273/1474 (86%)	992 (78%)	274 (22%)	7 (0%)	25	63
1	D	1403/1474 (95%)	1122 (80%)	270 (19%)	11 (1%)	16	53
All	All	5220/5896 (88%)	4133 (79%)	1051 (20%)	36 (1%)	21	56

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%)	1099 (99%)	15 (1%)	65	77
1	B	1114/1290 (86%)	1100 (99%)	14 (1%)	65	77
1	C	1115/1290 (86%)	1103 (99%)	12 (1%)	70	80
1	D	1234/1290 (96%)	1213 (98%)	21 (2%)	56	73
All	All	4577/5160 (89%)	4515 (99%)	62 (1%)	62	76

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1271	ARG
1	D	1013	GLN
1	C	654	THR
1	D	1012	TYR
1	D	1245	GLN

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	511	HIS
1	C	1242	GLN
1	D	1051	GLN
1	C	584	HIS
1	C	867	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	1,2	14,14,15	0.25	0	17,19,21	0.52	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.56	0
3	NAG	F	1	3,1	14,14,15	0.37	0	17,19,21	1.23	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	0.76	0
3	BMA	F	3	3	11,11,12	0.24	0	15,15,17	0.76	0
2	NAG	G	1	1,2	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	H	1	3,1	14,14,15	0.37	0	17,19,21	1.03	2 (11%)
3	NAG	H	2	3	14,14,15	0.44	0	17,19,21	1.24	2 (11%)
3	BMA	H	3	3	11,11,12	0.22	0	15,15,17	0.52	0
2	NAG	I	1	1,2	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.52	0
3	NAG	J	1	3,1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
3	NAG	J	2	3	14,14,15	0.34	0	17,19,21	0.73	0
3	BMA	J	3	3	11,11,12	0.23	0	15,15,17	0.57	0
2	NAG	K	1	1,2	14,14,15	0.29	0	17,19,21	0.82	1 (5%)
2	NAG	K	2	2	14,14,15	0.30	0	17,19,21	0.64	0
4	NAG	L	1	1,4	14,14,15	0.32	0	17,19,21	0.50	0
4	NAG	L	2	4	14,14,15	0.37	0	17,19,21	0.79	0
4	BMA	L	3	4	11,11,12	0.24	0	15,15,17	0.55	0
4	MAN	L	4	4	11,11,12	0.26	0	15,15,17	0.60	0
3	NAG	M	1	3,1	14,14,15	0.37	0	17,19,21	0.80	0
3	NAG	M	2	3	14,14,15	0.37	0	17,19,21	0.68	0
3	BMA	M	3	3	11,11,12	0.22	0	15,15,17	0.63	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	1,2	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	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	1,2	-	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	1,2	-	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	1,2	-	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	1,4	-	4/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	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	-	4/6/23/26	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	3.65	117.14	112.19
3	F	1	NAG	C1-O5-C5	2.78	115.96	112.19
3	J	1	NAG	C1-O5-C5	2.58	115.69	112.19
3	H	1	NAG	C1-O5-C5	2.39	115.43	112.19
3	F	1	NAG	C3-C4-C5	2.31	114.36	110.24

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

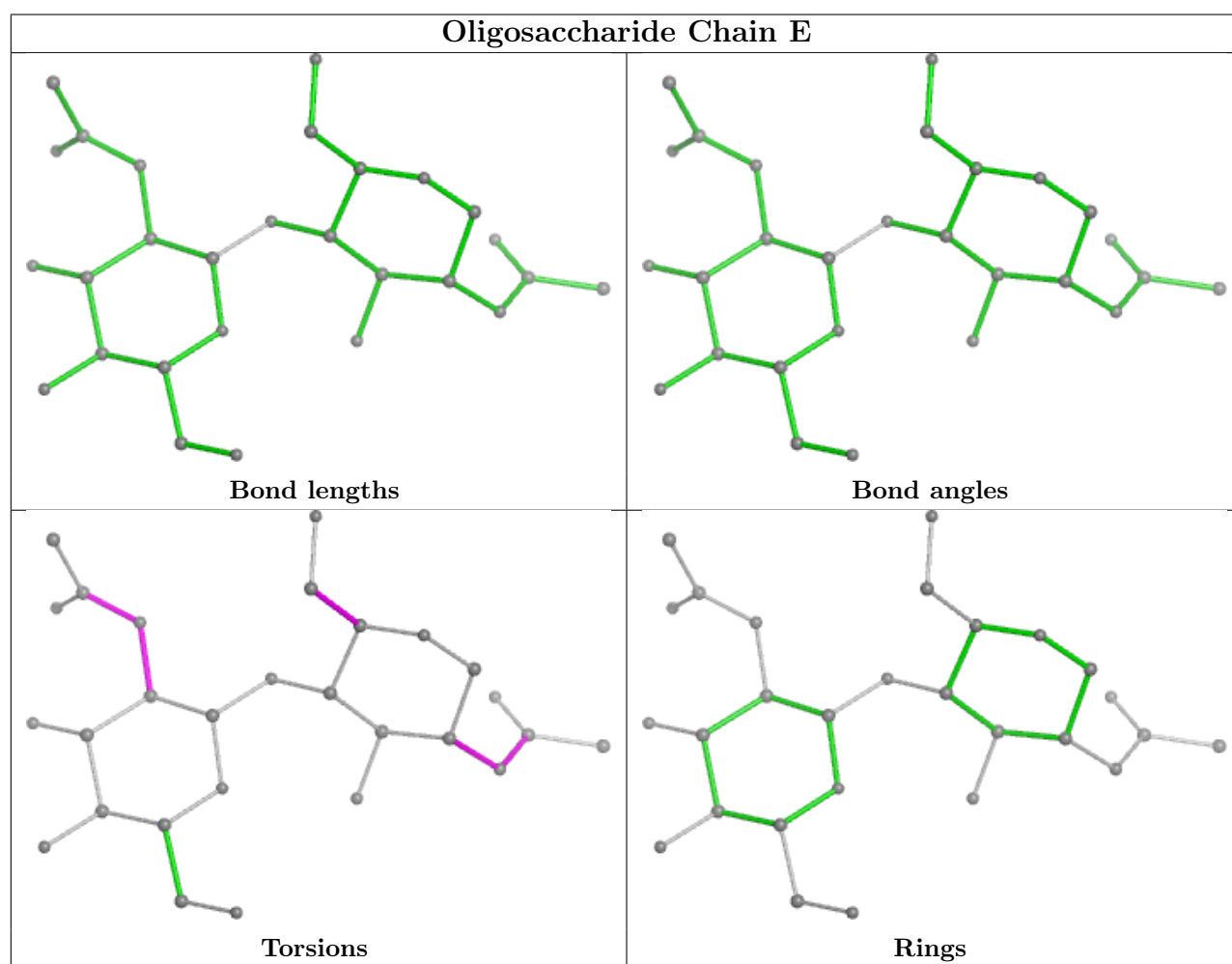
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C3-C2-N2-C7
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C1-C2-N2-C7
2	G	2	NAG	C8-C7-N2-C2

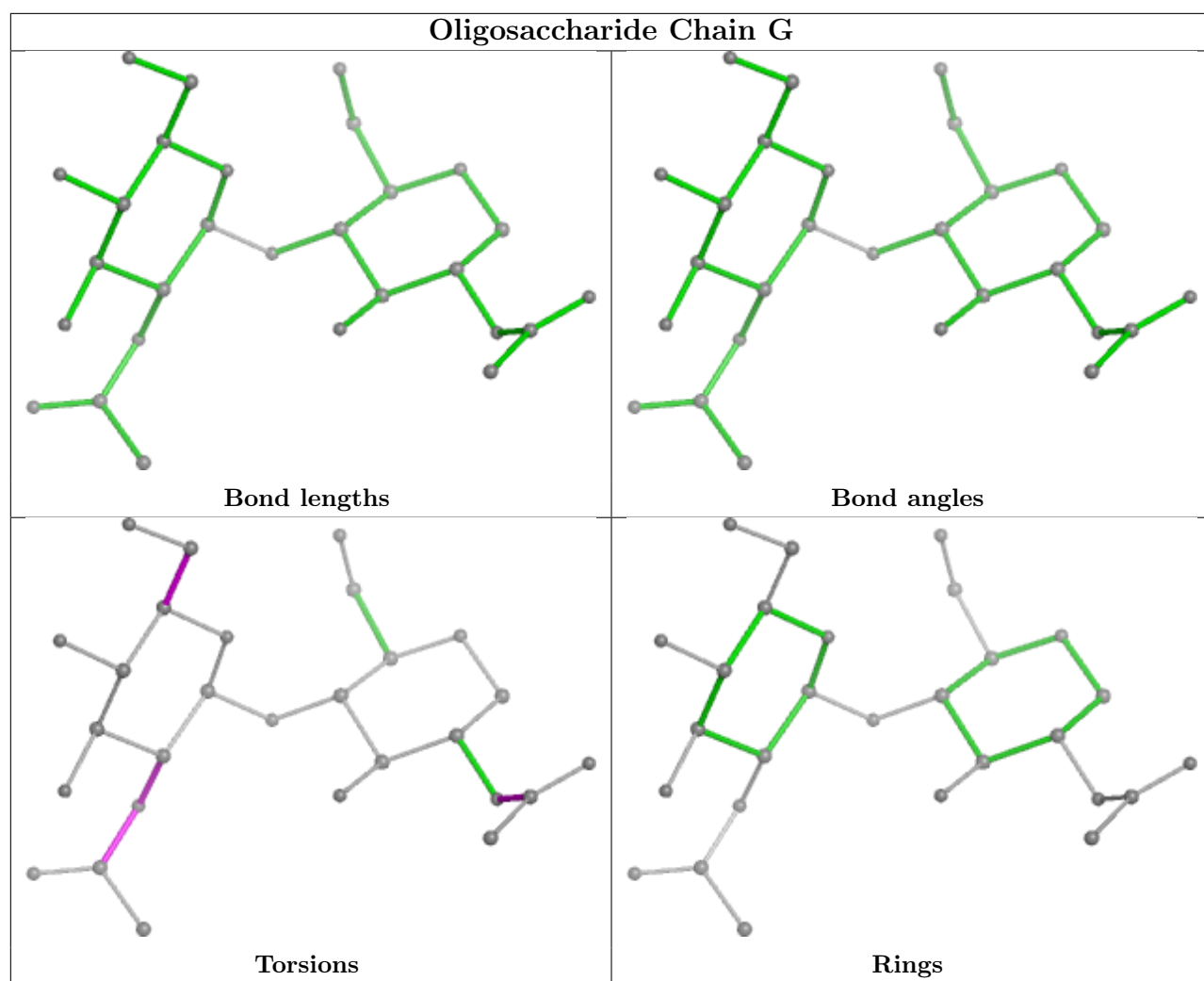
There are no ring outliers.

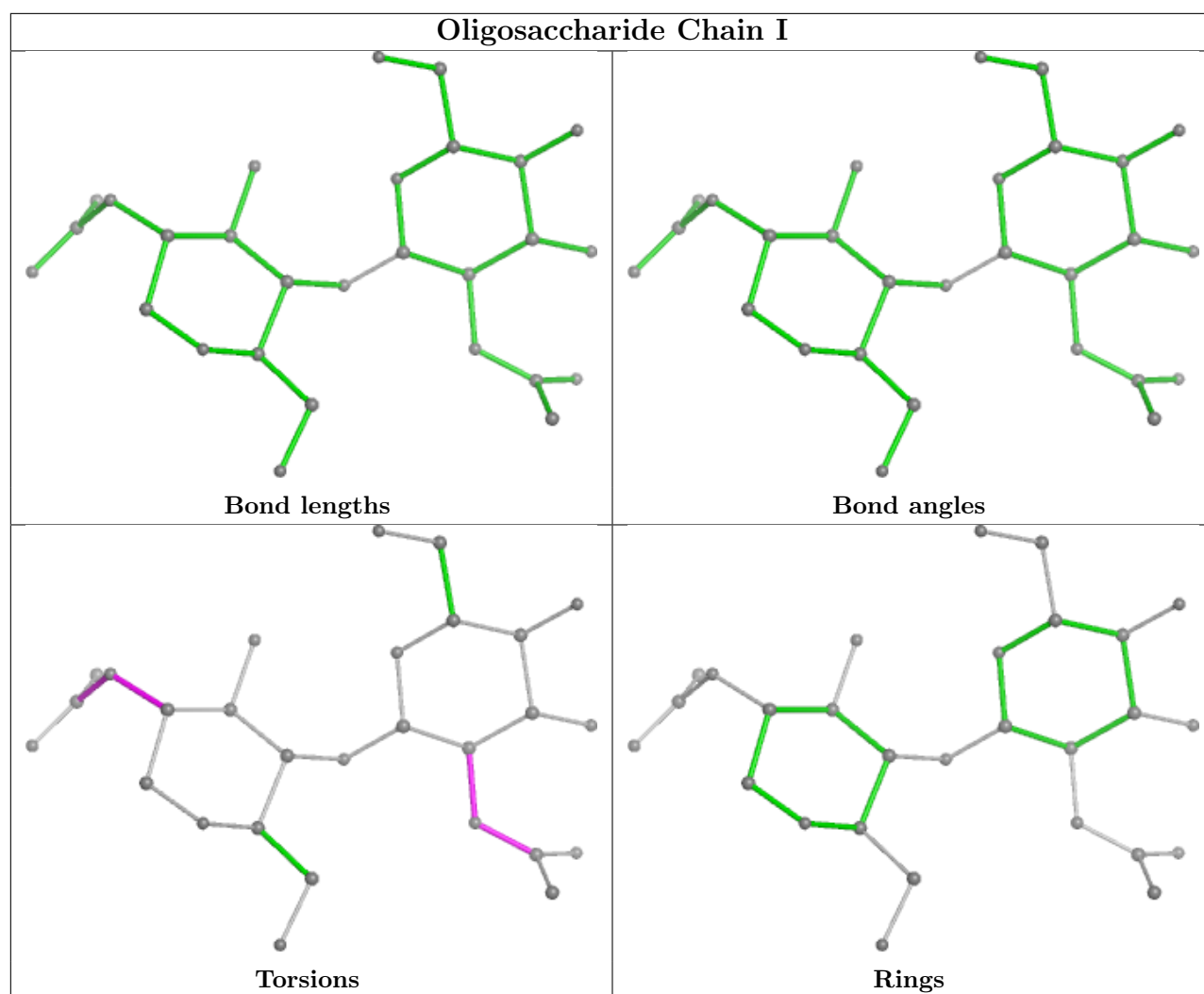
8 monomers are involved in 9 short contacts:

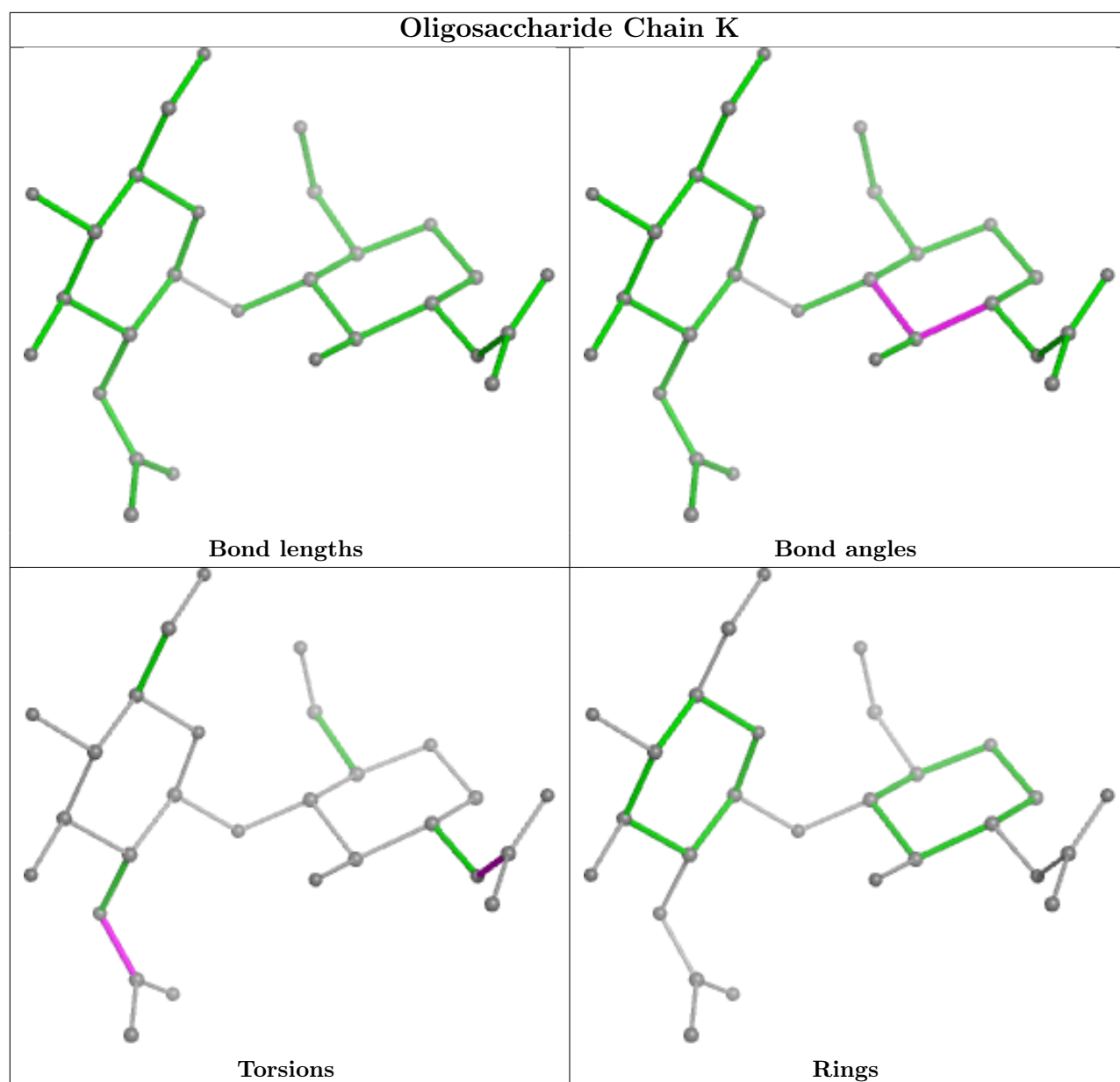
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	4	MAN	1	0
2	I	2	NAG	1	0
4	L	2	NAG	1	0
3	M	2	NAG	1	0
3	H	2	NAG	3	0
4	L	3	BMA	1	0
3	M	1	NAG	2	0
3	J	2	NAG	1	0

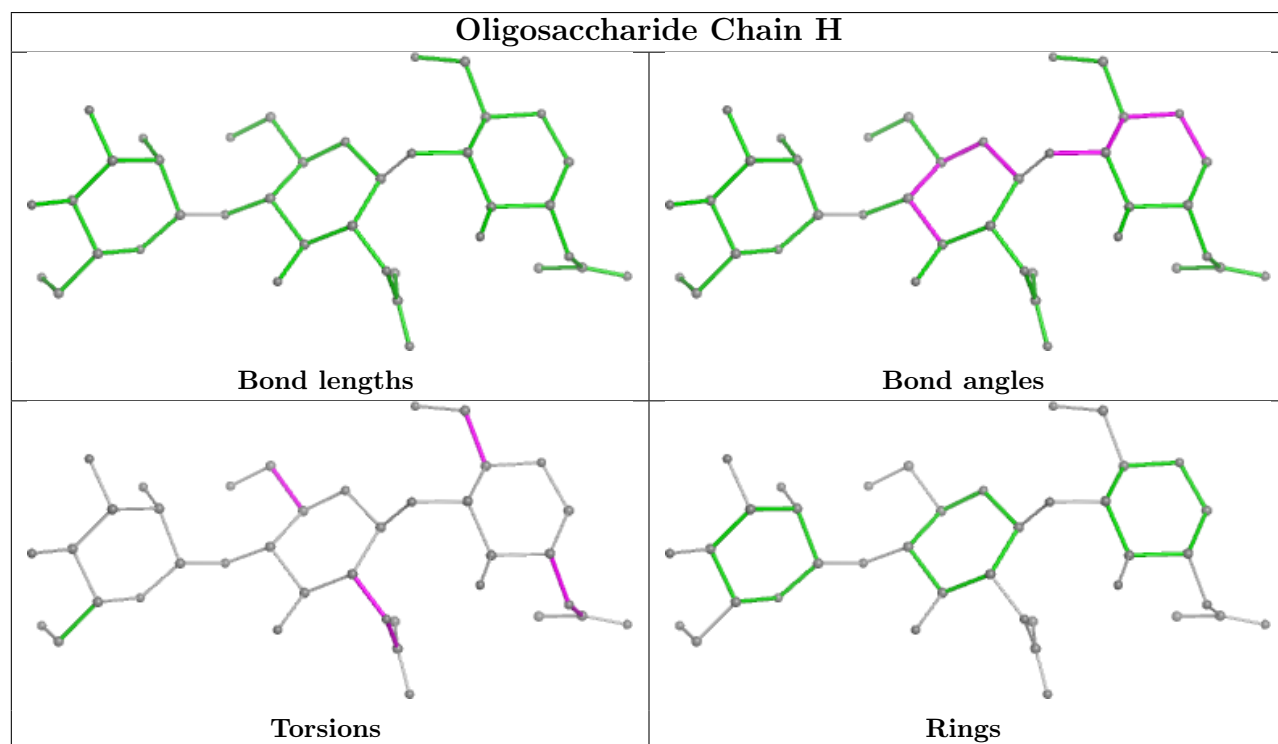
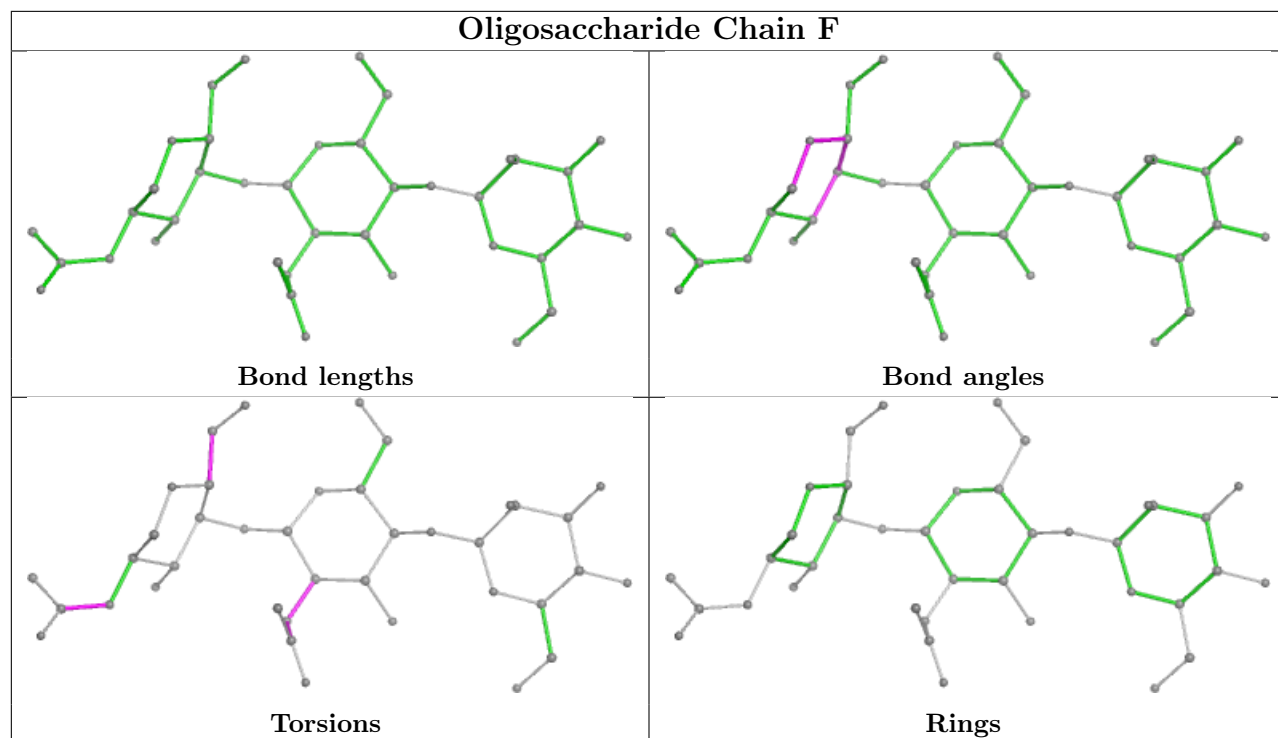
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

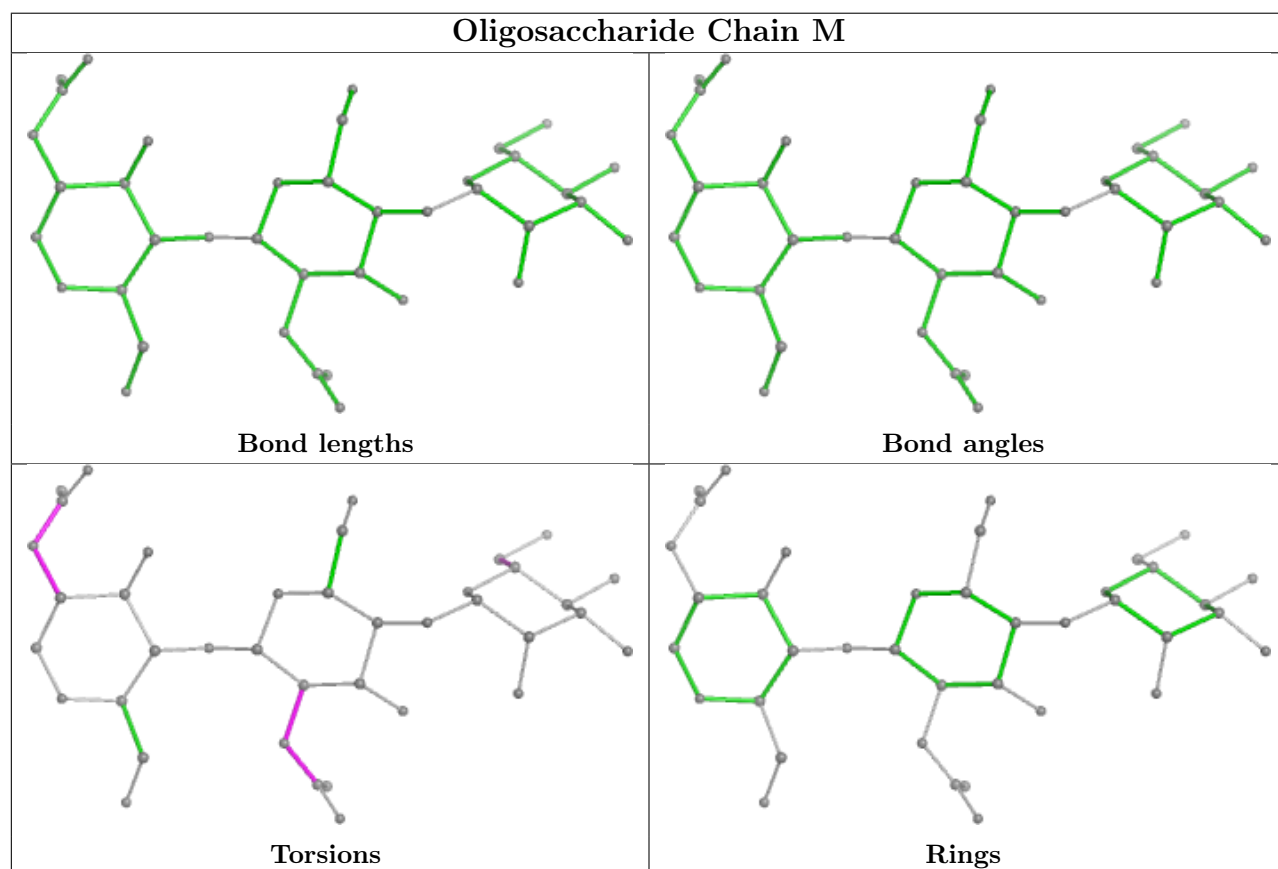
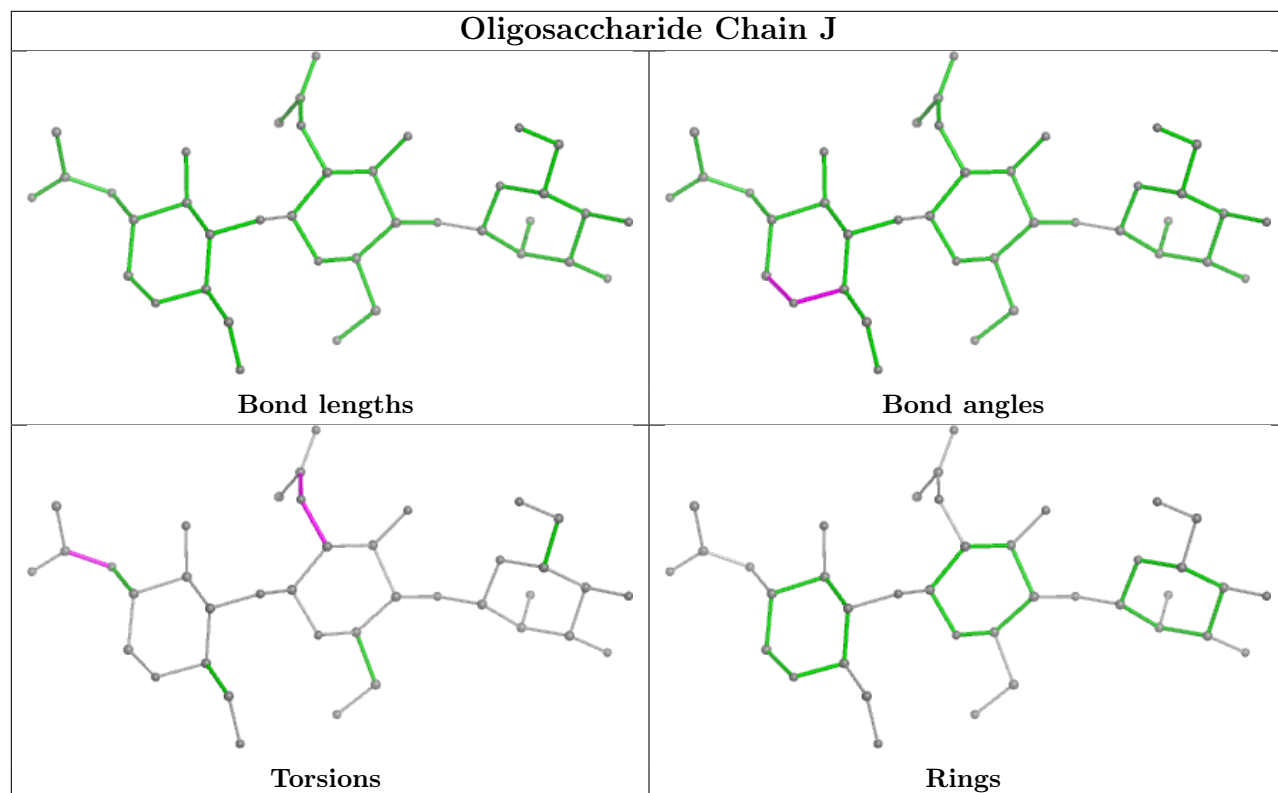


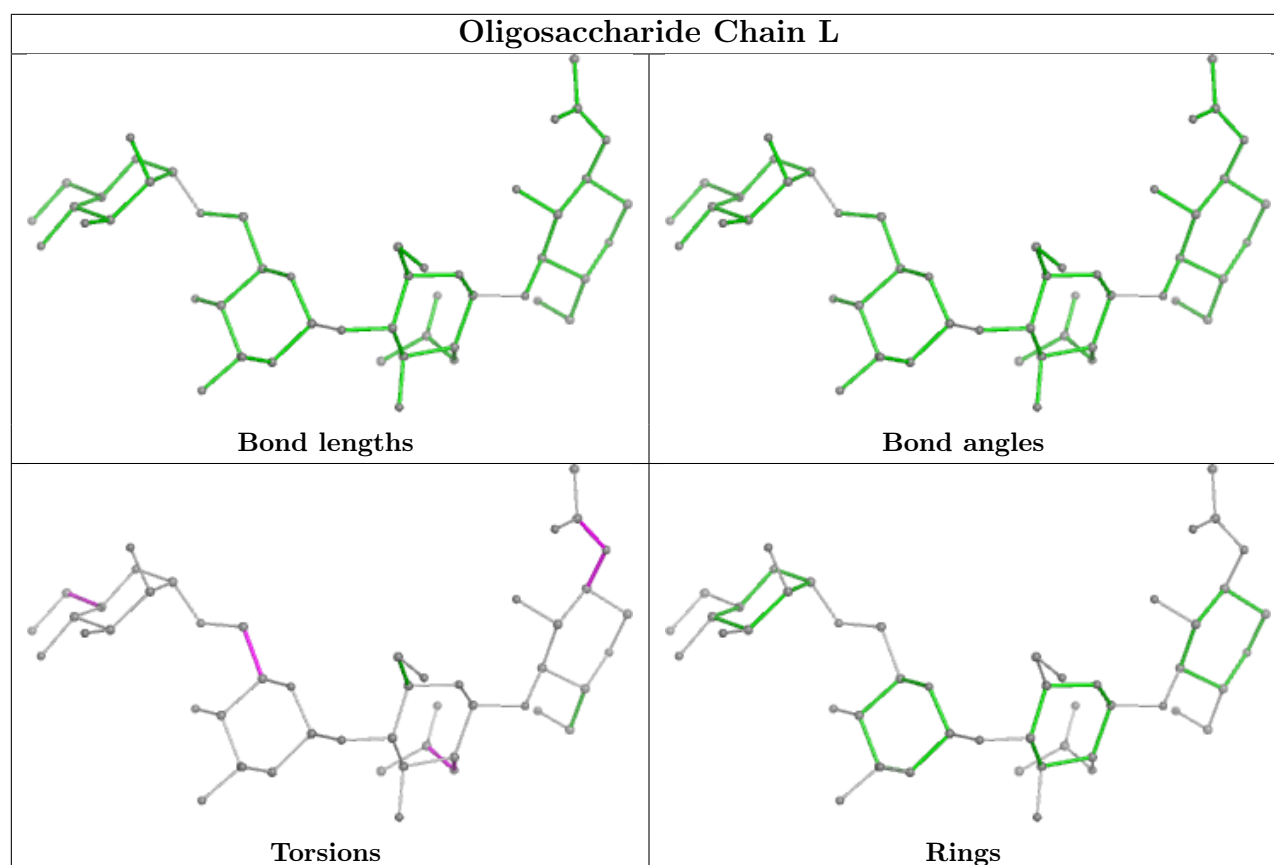












5.6 Ligand geometry [i](#)

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	2002	1	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	B	2002	1	14,14,15	0.29	0	17,19,21	0.66	0
5	NAG	D	2001	1	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
5	NAG	A	2002	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	A	2001	1	14,14,15	0.30	0	17,19,21	0.61	0
5	NAG	A	2003	1	14,14,15	0.30	0	17,19,21	0.45	0
5	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.54	0
5	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	C	2004	1	14,14,15	0.28	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	2005	1	14,14,15	0.29	0	17,19,21	0.62	0
5	NAG	D	2003	1	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	A	2004	1	14,14,15	0.30	0	17,19,21	0.57	0
5	NAG	C	2002	1	14,14,15	0.35	0	17,19,21	0.81	1 (5%)
5	NAG	B	2003	1	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
5	NAG	B	2004	1	14,14,15	0.27	0	17,19,21	0.65	0
5	NAG	C	2001	1	14,14,15	0.40	0	17,19,21	0.70	0
5	NAG	D	2005	1	14,14,15	0.27	0	17,19,21	0.52	0
5	NAG	B	2001	1	14,14,15	0.33	0	17,19,21	0.73	0
5	NAG	C	2003	1	14,14,15	0.26	0	17,19,21	0.53	0
5	NAG	D	2004	1	14,14,15	0.30	0	17,19,21	0.55	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	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	D	2001	1	-	4/6/23/26	0/1/1/1
5	NAG	A	2002	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	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	C	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	2004	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	3/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2003	1	-	3/6/23/26	0/1/1/1
5	NAG	B	2004	1	-	5/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	3/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	4/6/23/26	0/1/1/1
5	NAG	B	2001	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	2004	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2002	NAG	C1-O5-C5	2.17	115.13	112.19
5	B	2003	NAG	O5-C5-C6	2.10	110.49	107.20
5	D	2001	NAG	O5-C5-C6	2.00	110.35	107.20

There are no chirality outliers.

5 of 71 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	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2002	NAG	1	0
5	A	2003	NAG	1	0
5	C	2005	NAG	1	0
5	A	2005	NAG	1	0
5	C	2004	NAG	7	0
5	C	2001	NAG	2	0
5	B	2001	NAG	3	0
5	C	2003	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

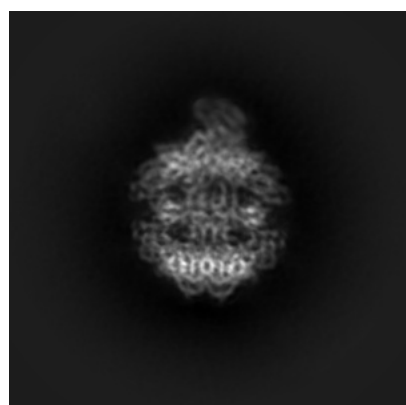
6 Map visualisation [i](#)

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

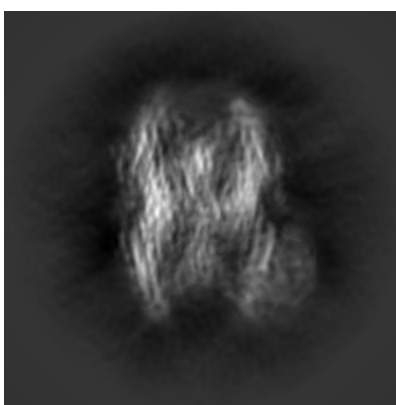
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

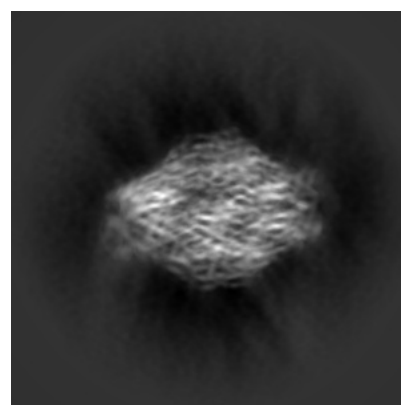
6.1.1 Primary map



X



Y

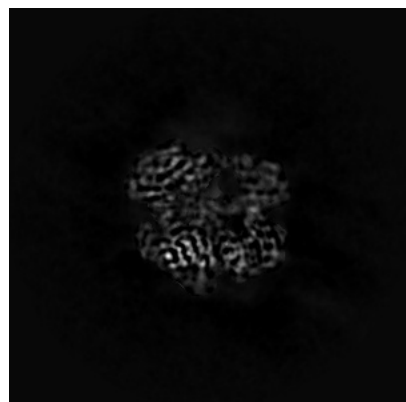


Z

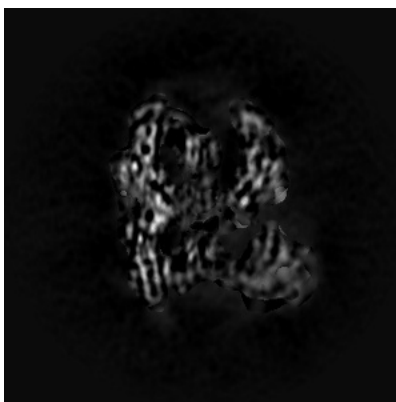
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

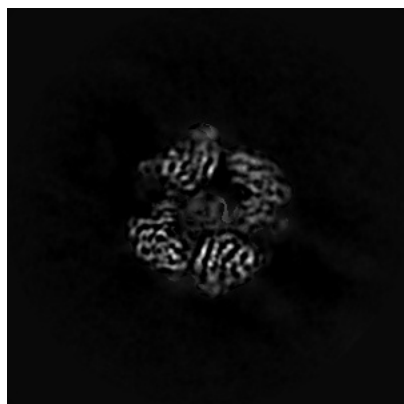


Z Index: 160

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

6.3 Largest variance slices [i](#)

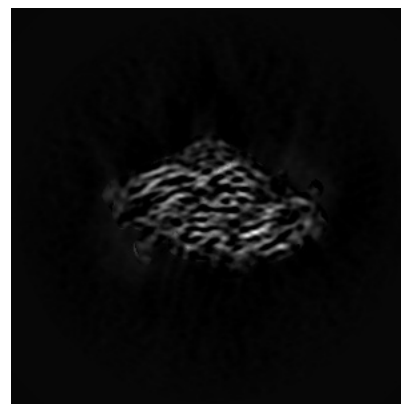
6.3.1 Primary map



X Index: 175



Y Index: 171

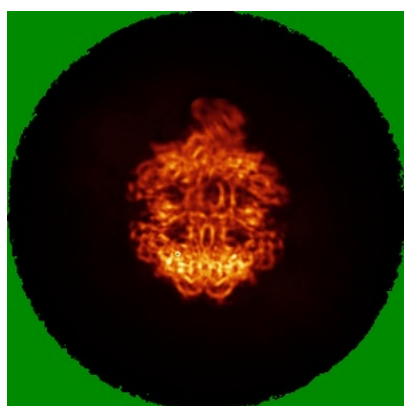


Z Index: 117

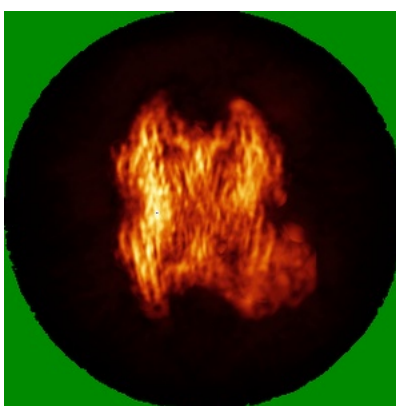
The images above show the largest variance slices of the map in three orthogonal directions.

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

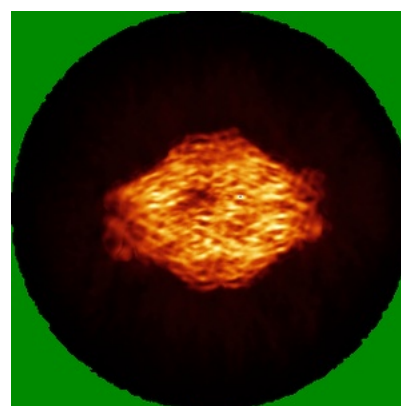
6.4.1 Primary map



X



Y

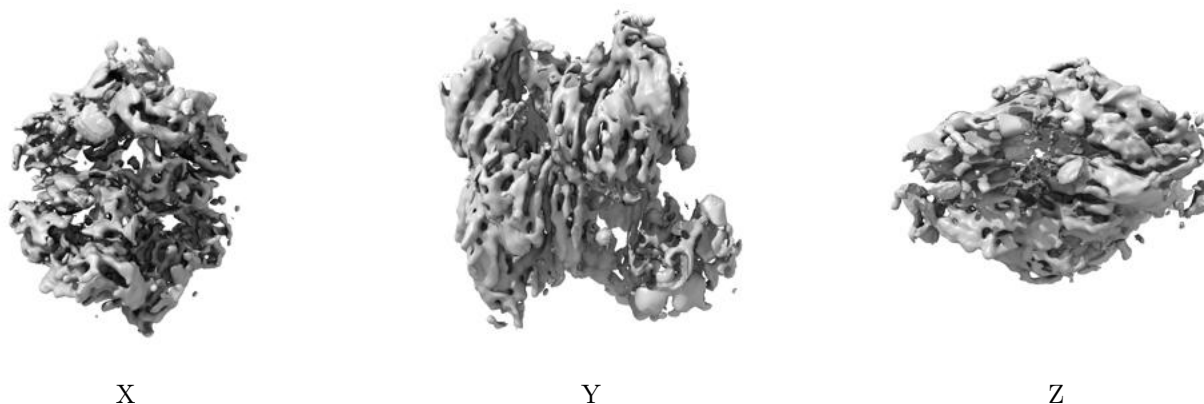


Z

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.

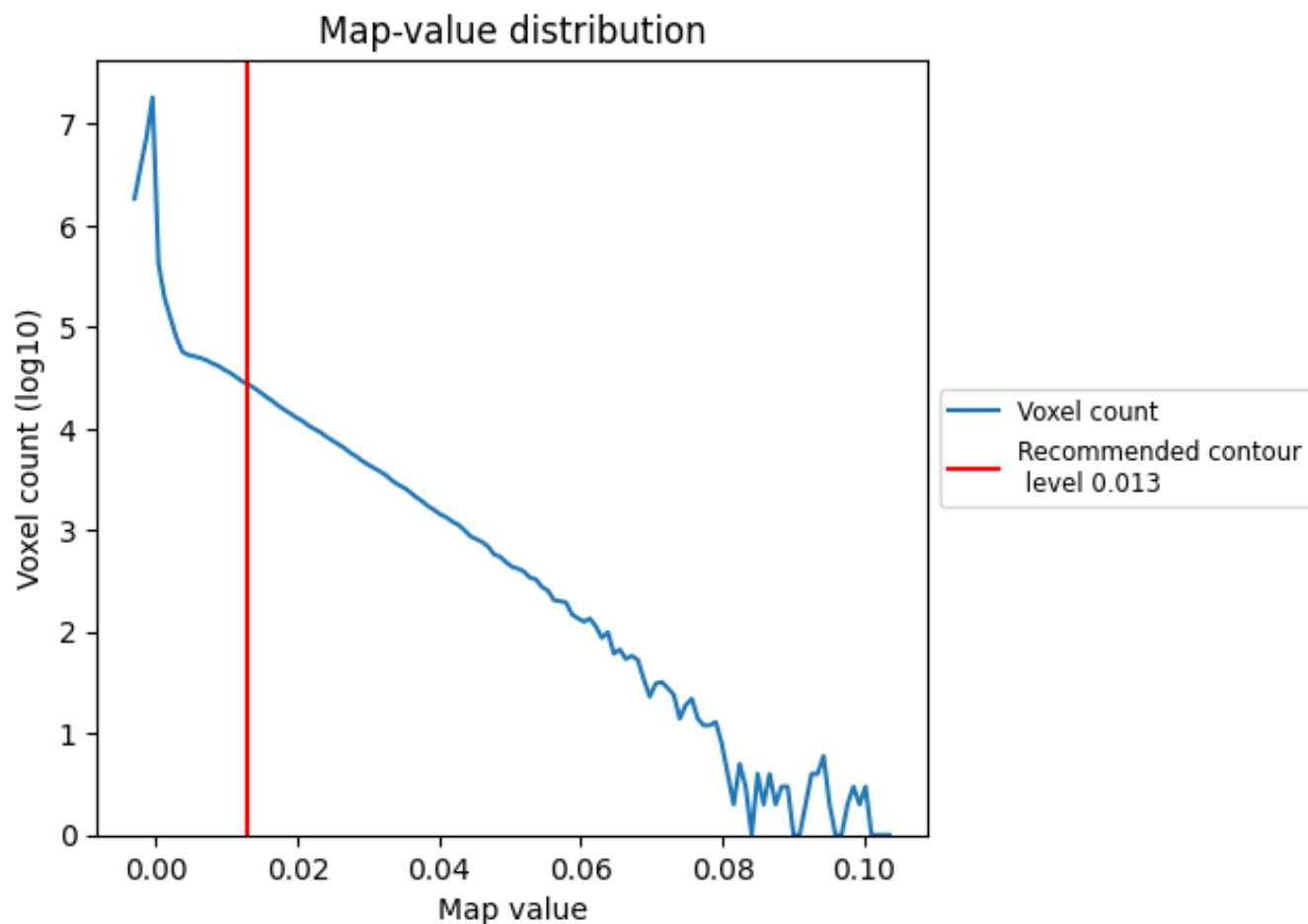
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

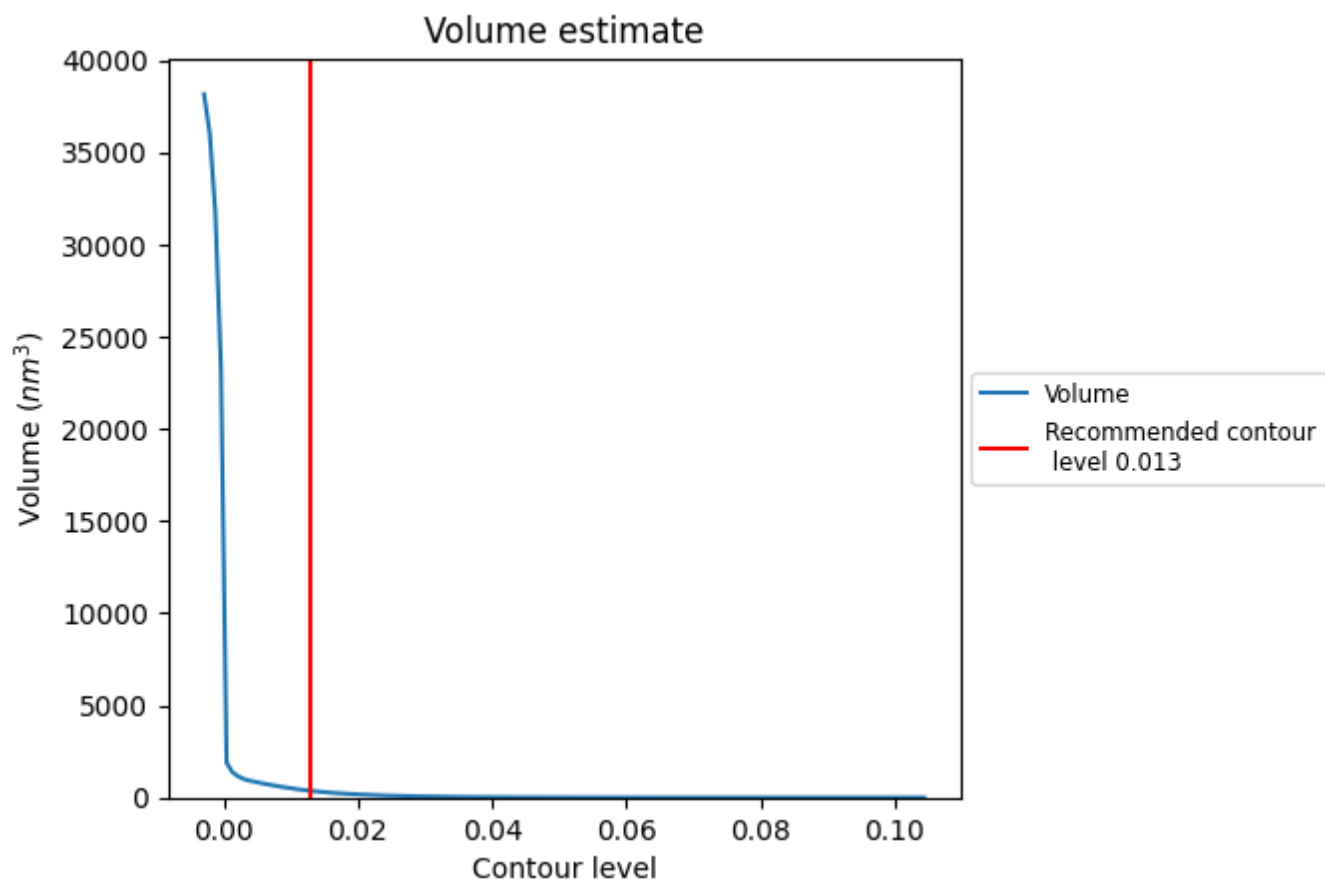
This section contains the results of statistical analysis of the map.

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.

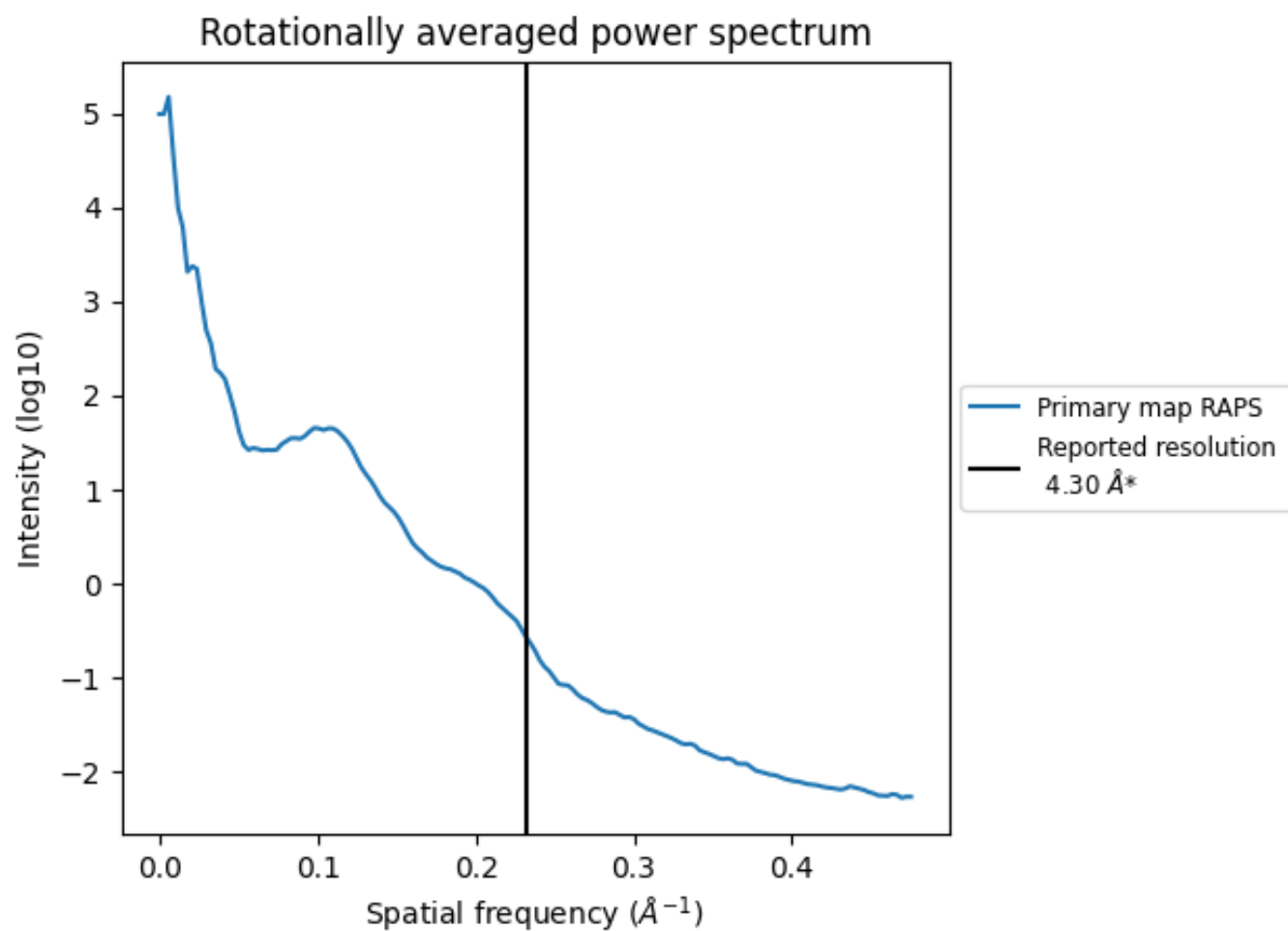
7.2 Volume estimate [i](#)



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 Å⁻¹

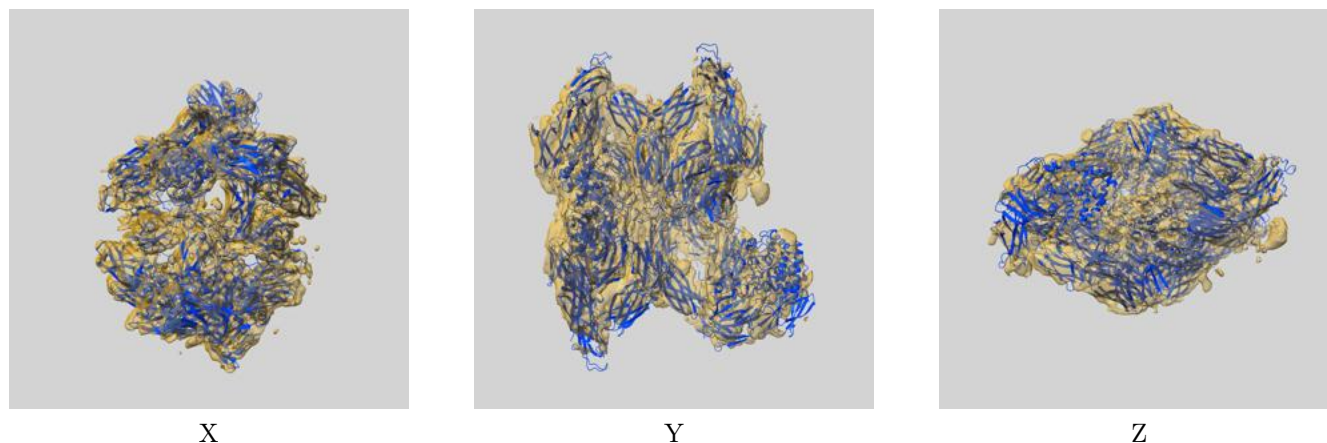
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

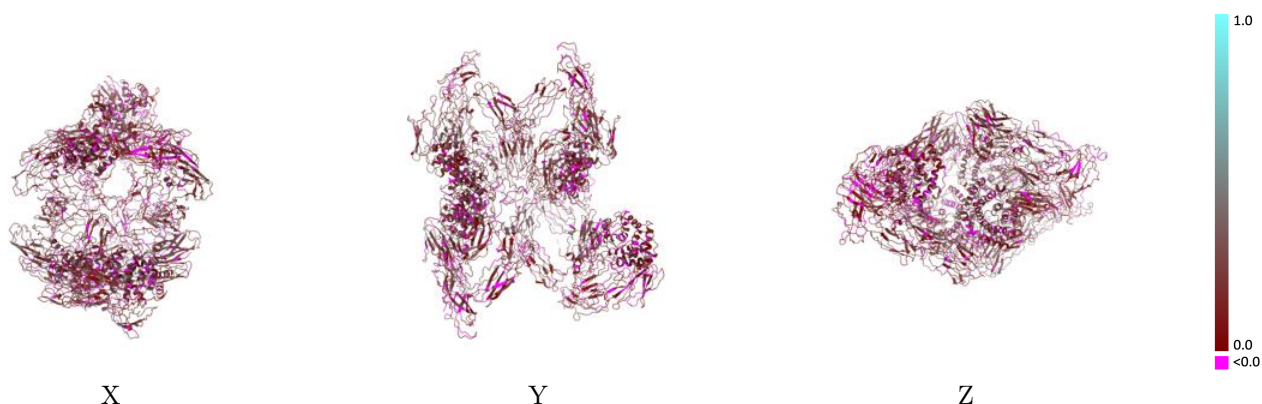
This section contains information regarding the fit between EMDB map EMD-12755 and PDB model 7O7S. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



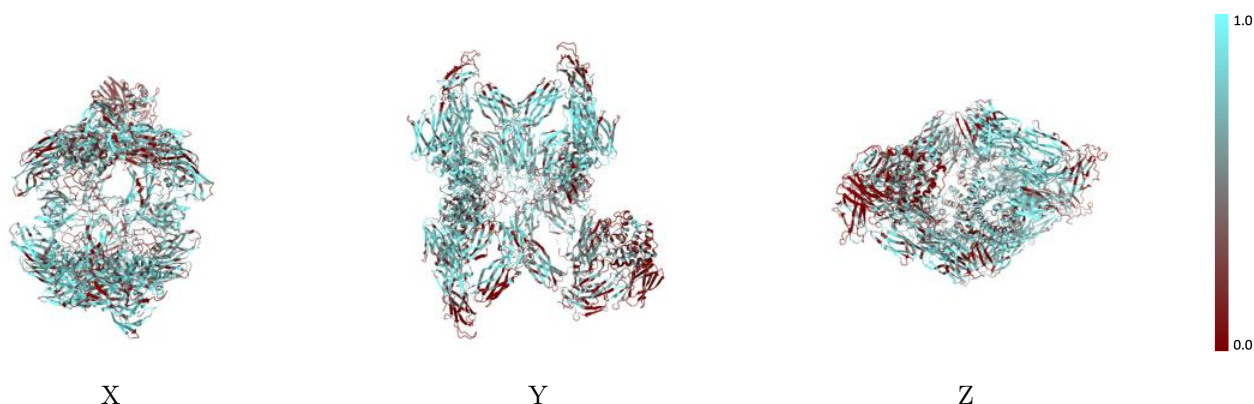
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



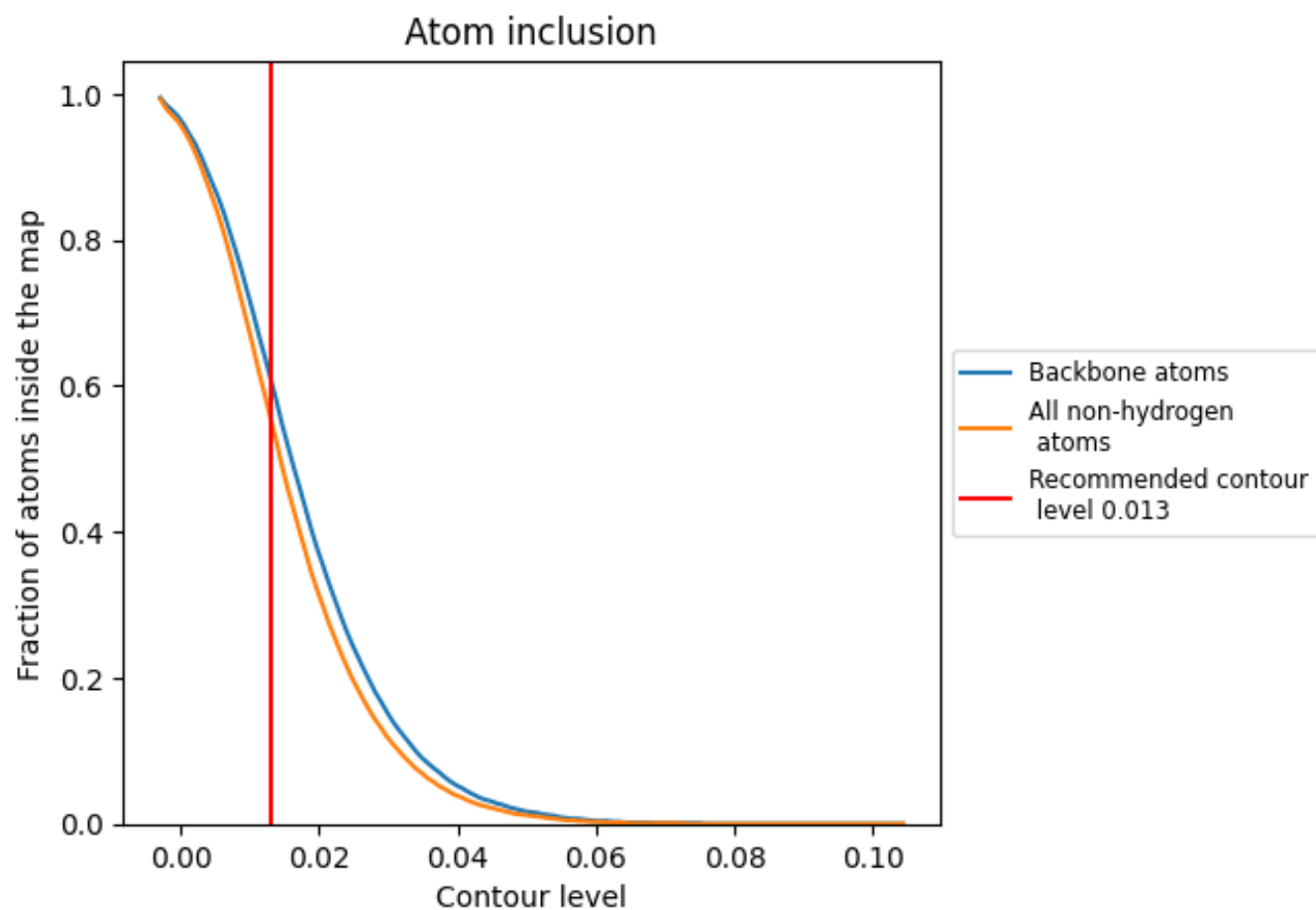
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.1530
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

