



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 05:13 am GMT

PDB ID : 7O7R
EMDB ID : EMD-12754
Title : (h-alpha2M)4 plasmin-activated I 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 : 3.90 Å(reported)

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

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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.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

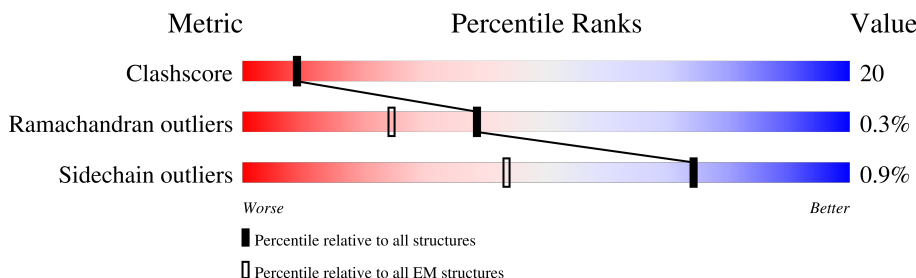
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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>13%</div> <div>54%</div> <div>33%</div> <div>•</div> <div>13%</div> </div>
1	B	1474	<div> <div>9%</div> <div>49%</div> <div>37%</div> <div>13%</div> </div>
1	C	1474	<div> <div>12%</div> <div>53%</div> <div>34%</div> <div>•</div> <div>13%</div> </div>
1	D	1474	<div> <div>10%</div> <div>51%</div> <div>35%</div> <div>•</div> <div>13%</div> </div>
2	E	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>
2	G	2	<div> <div>50%</div> <div>100%</div> </div>
2	I	2	<div> <div>100%</div> </div>
2	K	2	<div> <div>50%</div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	3	<div> <div>33%</div> <div>33%</div> <div>67%</div> </div>
3	H	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>
3	J	3	<div> <div>33%</div> <div>100%</div> </div>
3	L	3	<div> <div>33%</div> <div>33%</div> <div>33%</div> </div>

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
3	NAG	H	1	-	-	X	-

2 Entry composition [i](#)

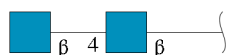
There are 4 unique types of molecules in this entry. The entry contains 40530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

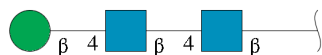
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	B	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		
1	C	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	D	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		

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



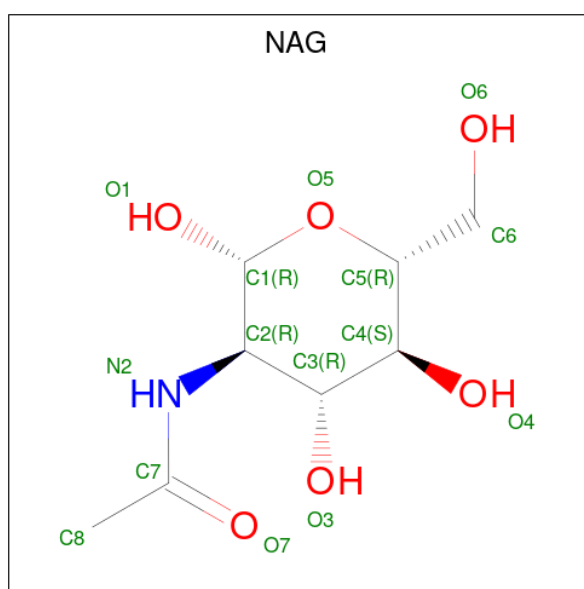
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	L	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

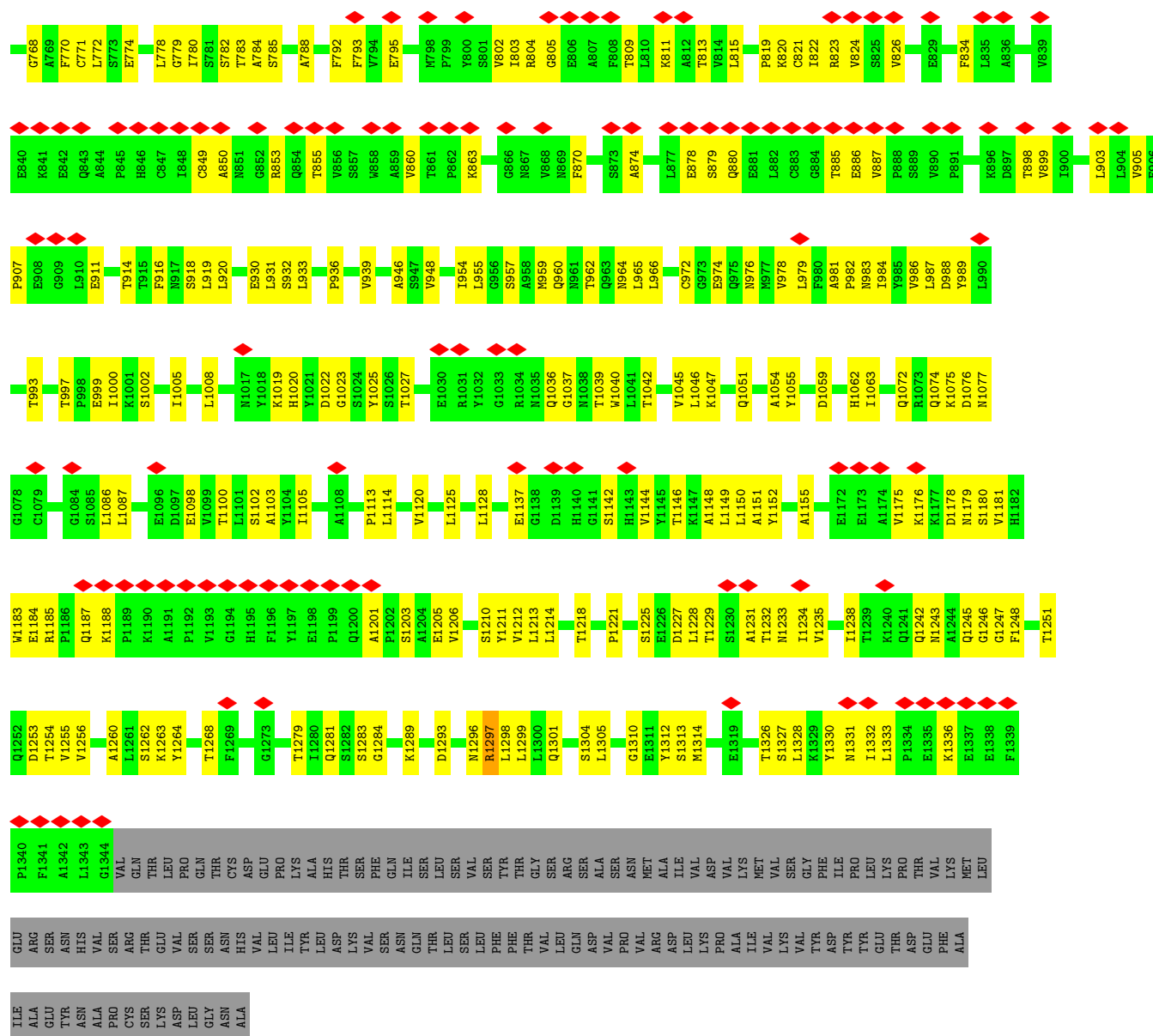


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

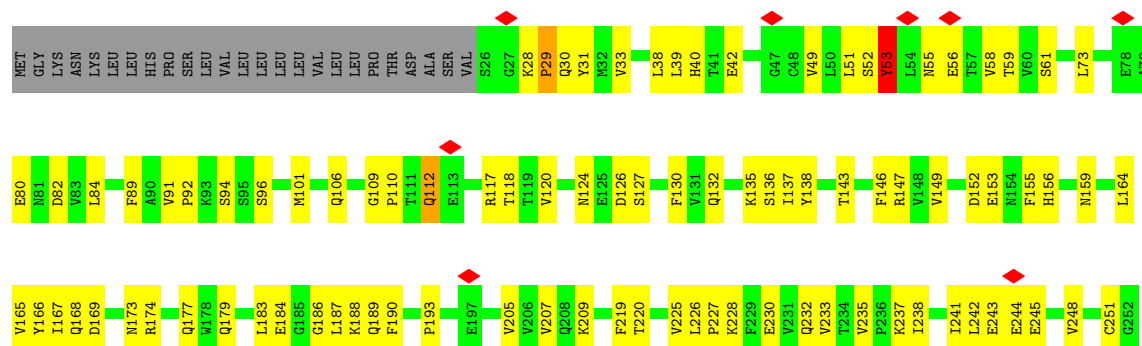
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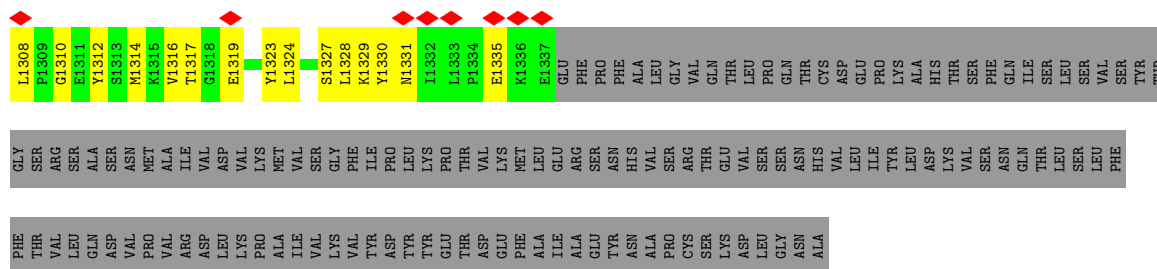
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4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



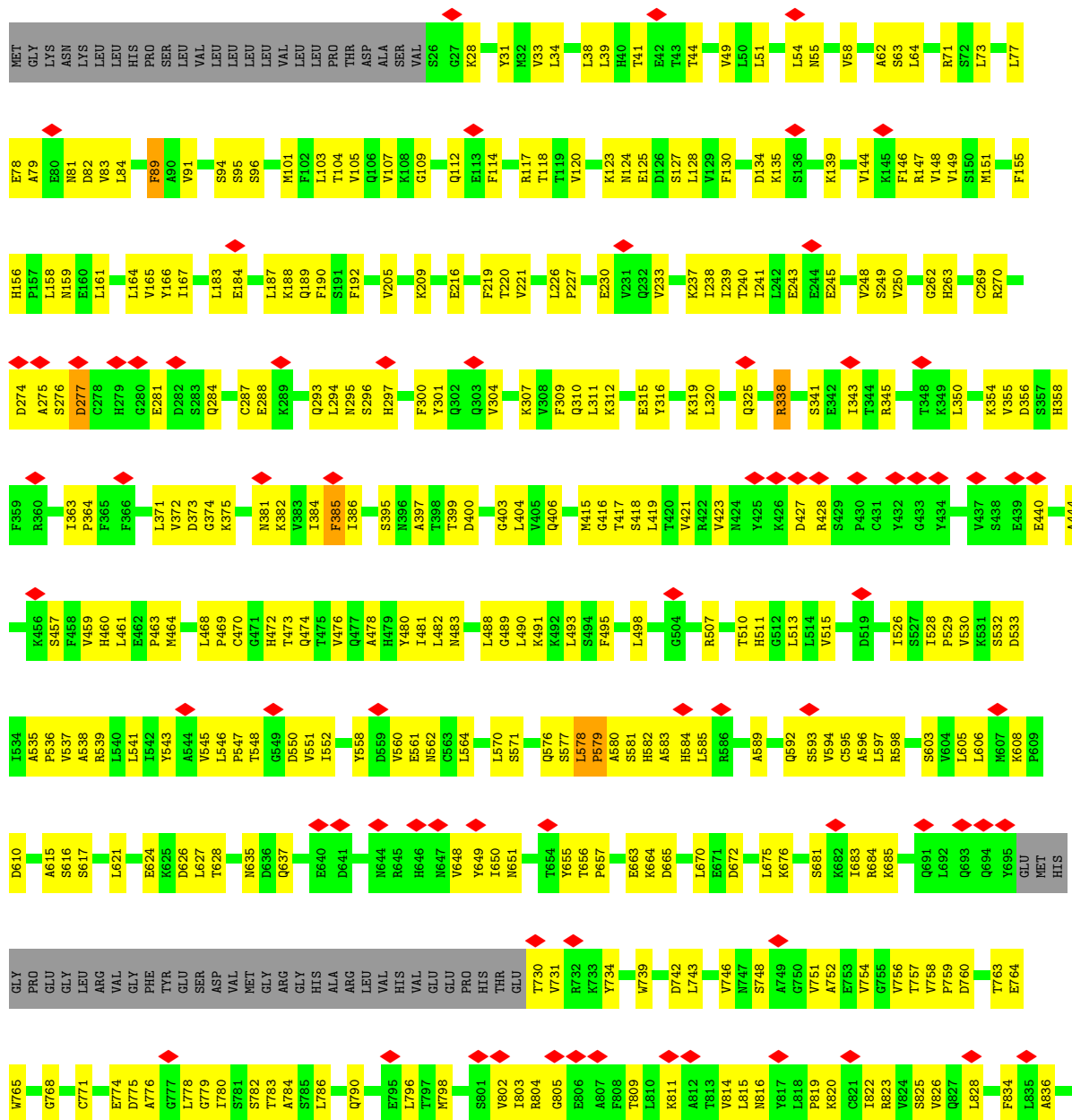
• Molecule 1: Alpha-2-macroglobulin

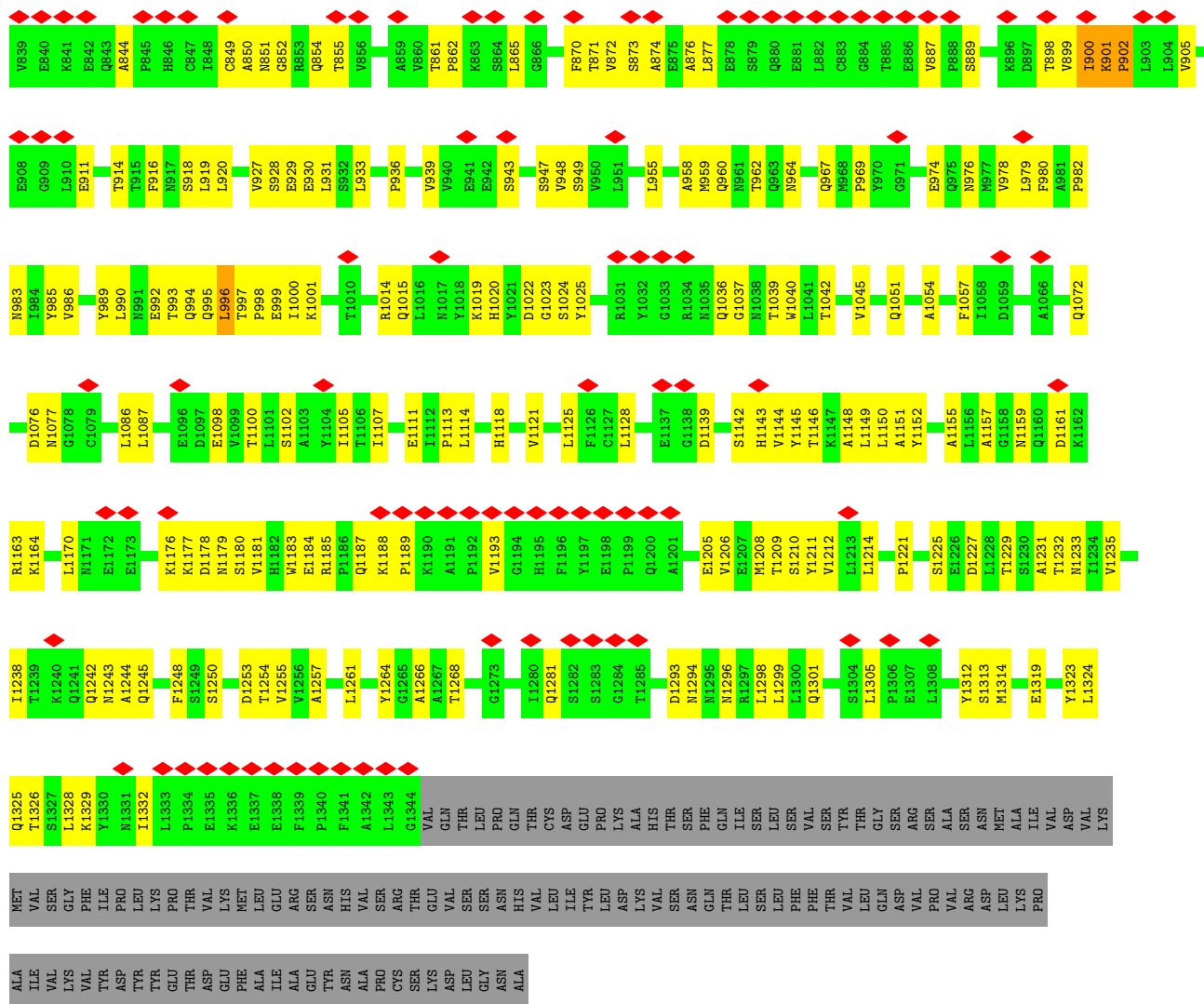


T1218	L1150	Q1072	V986	D897	R823	D742	K676	S581	L498	T420	I343	L953
A1151	A1151	R1073	L987	R901	W824	L743	A677	H582	L999	V421	I344	V260
Y1152	Y1152	Q1074	D988	P902	S825	N747	F678	A583	M500	R422	R345	P261
A1153	A1153	K1075	Y989	F902	W826	S748	T679	H584	A501	V423	R346	G262
F1154	F1154	D1076	L990	E906	Q827	A749	N680	L585	K502	N424	I347	G263
A1155	A1155	C1079	N991	P907	L828	G750	S681	R586	G503	Y425	T348	H264
E1156	E1156	F1080	E992	P907	S831	V751	K685	Q592	G504	K426	L350	V265
D1161	D1161	Q1081	Q993	E908	S831	A752	K686	K593	R507	D427	F352	V266
K1162	K1162	S1082	Q995	G909	F834	E753	K687	Q594	R507	R428	V353	S267
E1165	E1165	N1088	L996	R912	L835	T757	K688	C595	T510	S429	K354	I268
V1166	V1166	E1096	T997	T914	A836	T763	P690	A596	H511	P430	V355	C269
L1167	L1167	D1097	P998	E913	W837	E764	Q691	L597	C431	C431	D858	R270
K1168	K1168	E1098	I1000	T914	R841	W765	L692	R599	L514	G433	F359	A275
S1169	S1169	Y1099	K1003	L919	Q842	K766	L693	V600	V515	G433	I363	S276
L1170	L1170	T1100	A1004	L920	Q843	A767	Q694	L605	K516	Y434	D277	D277
N1171	N1171	L1101	N1005	V927	Q844	G768	Q695	L606	Q517	V437	Q368	C278
E1172	E1172	E1102	N1009	E929	P845	A769	Y695	L606	Q518	S438	V369	H279
E1173	E1173	A1103	T1010	E930	H846	F770	GLU	P609	D519	E439	R370	G280
K1176	K1176	A1108	G1011	L931	C847	L771	MET	D610	I526	H441	V372	E281
R1177	R1177	Y1012	Y1012	S932	T848	G777	HIS	D510	S527	E440	D373	E288
D1178	D1178	Q1013	Q1013	L933	C849	L778	GLY	S614	I528	H441	G374	Q293
N1179	N1179	R1014	Q1015	E941	A850	L778	PRO	S617	P529	E442	E443	L294
S1180	S1180	L1016	L1016	E942	R851	G777	GLY	S617	S532	H444	G376	N295
V1181	V1181	Y1017	N1017	A946	C852	L778	LEU	L621	D533	H445	K381	S296
H1182	H1182	Y1018	Y1018	V947	R853	G779	ARG	L622	I534	H446	K382	H297
E1184	E1184	Y1018	Y1018	V948	R853	L780	VAL	P623	A535	L450	I386	Q303
Q1187	Q1187	Y1025	Y1025	L951	V856	S782	PHE	D626	P536	V451	R387	T306
K1188	K1188	S1026	S1026	L951	S857	L783	TYR	L627	A539	F452	G388	K307
P1189	P1189	T1027	T1027	G952	W858	A784	GLU	R539	R389	K456	N389	V308
K1190	K1190	R1031	R1031	D953	A859	S785	SER	N635	L540	S457	E390	F309
A1191	A1191	R1034	R1034	E954	V860	L786	ASP	D636	L541	F458	A391	Q310
Y1192	Y1192	T1039	T1039	A958	R863	E795	MET	D641	L546	L461	S395	L311
V1193	V1193	W1040	W1040	G959	S864	S801	GLY	C642	P947	E462	T398	E315
G1194	G1194	L1041	L1041	N961	L865	V802	ARG	I643	T548	P463	T399	Y316
A1195	A1195	T1042	T1042	T962	N869	R803	HIS	H646	I552	M464	D400	E317
F1196	F1196	V1045	V1045	Q963	F870	G805	ALA	N647	G553	S465	E401	M318
Y1197	Y1197	A1045	A1045	N964	W872	E806	ARG	V648	D554	H466	H402	K319
E1198	E1198	A1052	A1052	P969	S873	A807	LEU	Y649	S555	E467	L404	L320
P1199	P1199	I1056	I1056	G970	A874	A807	VAL	I650	A556	T473	L405	H321
Q1200	Q1200	I1056	I1056	G971	E875	F808	VAL	N651	V560	V476	T322	T322
P1202	P1202	D1059	D1059	C972	L877	T809	GLU	T656	L570	V476	E323	E323
S1203	S1203	H1062	H1062	G973	E878	L810	PRO	P657	S571	H479	T411	A324
A1204	A1204	I1063	I1063	E974	S879	K811	HIS	V658	F572	Y480	T412	Q325
E1205	E1205	H1143	H1143	G975	Q880	A812	THR	S659	S574	I481	M413	E328
V1206	V1206	Y1144	Y1144	N976	E881	W814	GLU	P574	G575	L482	V414	E328
E1207	E1207	A1066	A1066	L979	L862	L815	TYR	E663	Q576	N483	M415	V332
M1208	M1208	L1067	L1067	F980	C883	N816	VAL	K664	Q576	L482	G416	V333
Y1211	Y1211	L1070	L1070	A981	C884	N816	VAL	D665	S577	N483	T417	E334
L1212	L1212	S1071	S1071	P982	T885	P819	GLU	Y667	L578	G489	S418	R338
L1213	L1213	L1149	L1149		E886	K820	GLU	W739	L578	L490	L419	
L1214	L1214				V887	C821	GLU	I740	A580	K492		
L1217	L1217				S889	L822	GLU	W741		F495		

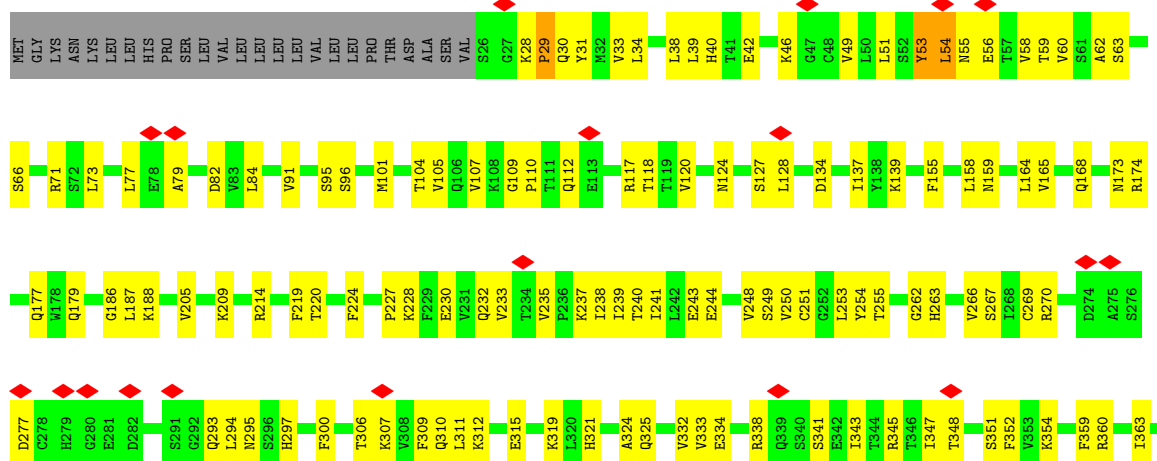


Molecule 1: Alpha-2-macroglobulin





• Molecule 1: Alpha-2-macroglobulin





GLU
THR
ASP
GLU
PHE
ALA
TLE
ALA
GLU
TYR
ASN
ALA
PRO
CYS
SER
LYS
ASP
LEU
GLY
ASN
ALA

- 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



- Molecule 3: 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	121437	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	0.081	Depositor
Minimum map value	-0.002	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	1/10247 (0.0%)	0.74	6/13921 (0.0%)
1	B	0.64	4/10189 (0.0%)	0.74	5/13842 (0.0%)
1	C	0.64	4/10247 (0.0%)	0.74	4/13921 (0.0%)
1	D	0.65	4/10189 (0.0%)	0.72	2/13842 (0.0%)
All	All	0.63	13/40872 (0.0%)	0.74	17/55526 (0.0%)

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	PRO	N-CA	14.23	1.71	1.47
1	D	29	PRO	N-CA	14.01	1.71	1.47
1	C	902	PRO	N-CA	13.62	1.70	1.47
1	D	168	GLN	C-N	-7.58	1.16	1.34
1	D	28	LYS	C-N	6.17	1.46	1.34

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	902	PRO	CA-N-CD	-9.30	98.49	111.50
1	C	277	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	277	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	29	PRO	CA-N-CD	-7.62	100.84	111.50
1	D	29	PRO	CA-N-CD	-7.53	100.96	111.50

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	10023	0	9917	386	0
1	B	9968	0	9866	417	0
1	C	10023	0	9917	408	0
1	D	9968	0	9866	407	0
2	E	28	0	25	1	0
2	G	28	0	25	0	0
2	I	28	0	25	3	0
2	K	28	0	25	1	0
3	F	39	0	34	6	0
3	H	39	0	34	13	0
3	J	39	0	34	5	0
3	L	39	0	34	4	0
4	A	70	0	65	13	0
4	B	70	0	65	1	0
4	C	70	0	65	5	0
4	D	70	0	65	5	0
All	All	40530	0	40062	1644	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 20.

The worst 5 of 1644 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:D:29:PRO:N	1:D:29:PRO:CA	1.71	1.46
1:C:902:PRO:CA	1:C:902:PRO:N	1.70	1.46
1:B:29:PRO:N	1:B:29:PRO:CA	1.71	1.39
1:C:871:THR:HG22	1:C:900:ILE:HG23	1.15	1.10
4:A:2001:NAG:H3	4:A:2001:NAG:H83	1.34	1.08

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	1281/1474 (87%)	1025 (80%)	250 (20%)	6 (0%)	25	60
1	B	1274/1474 (86%)	1057 (83%)	214 (17%)	3 (0%)	44	75
1	C	1281/1474 (87%)	1036 (81%)	239 (19%)	6 (0%)	25	60
1	D	1274/1474 (86%)	1041 (82%)	231 (18%)	2 (0%)	44	75
All	All	5110/5896 (87%)	4159 (81%)	934 (18%)	17 (0%)	38	70

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	PRO
1	C	579	PRO
1	C	651	ASN
1	D	53	TYR
1	A	54	LEU

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	1120/1290 (87%)	1112 (99%)	8 (1%)	81	86
1	B	1115/1290 (86%)	1105 (99%)	10 (1%)	75	83
1	C	1120/1290 (87%)	1111 (99%)	9 (1%)	79	84
1	D	1115/1290 (86%)	1102 (99%)	13 (1%)	67	78
All	All	4470/5160 (87%)	4430 (99%)	40 (1%)	74	83

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	396	ASN
1	D	763	THR
1	D	426	LYS
1	D	492	LYS
1	D	992	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	310	GLN
1	C	1013	GLN
1	D	1035	ASN
1	C	361	GLN
1	C	694	GLN

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 ⓘ

20 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	0.26	0	17,19,21	0.80	1 (5%)
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	F	1	3,1	14,14,15	0.31	0	17,19,21	0.66	0

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	0.33	0	17,19,21	0.64	0
3	BMA	F	3	3	11,11,12	0.25	0	15,15,17	0.59	0
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.65	0
3	NAG	H	1	3,1	14,14,15	0.36	0	17,19,21	1.38	2 (11%)
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	0.62	0
3	BMA	H	3	3	11,11,12	0.25	0	15,15,17	0.62	0
2	NAG	I	1	2,1	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	I	2	2	14,14,15	0.29	0	17,19,21	0.62	0
3	NAG	J	1	3,1	14,14,15	0.32	0	17,19,21	0.68	0
3	NAG	J	2	3	14,14,15	0.31	0	17,19,21	0.71	0
3	BMA	J	3	3	11,11,12	0.26	0	15,15,17	0.60	0
2	NAG	K	1	2,1	14,14,15	0.32	0	17,19,21	0.83	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.68	0
3	NAG	L	1	3,1	14,14,15	0.47	0	17,19,21	1.43	2 (11%)
3	NAG	L	2	3	14,14,15	0.35	0	17,19,21	0.75	0
3	BMA	L	3	3	11,11,12	0.26	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	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	3/6/23/26	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	-	3/6/23/26	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	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	5/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	BMA	J	3	3	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	K	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	3/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	5/6/23/26	0/1/1/1
3	NAG	L	2	3	-	5/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1	NAG	O5-C1-C2	4.27	118.04	111.29
3	H	1	NAG	C1-O5-C5	3.82	117.37	112.19
3	H	1	NAG	O5-C1-C2	3.02	116.05	111.29
3	L	1	NAG	C1-O5-C5	2.33	115.34	112.19
2	E	1	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

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

There are no ring outliers.

13 monomers are involved in 33 short contacts:

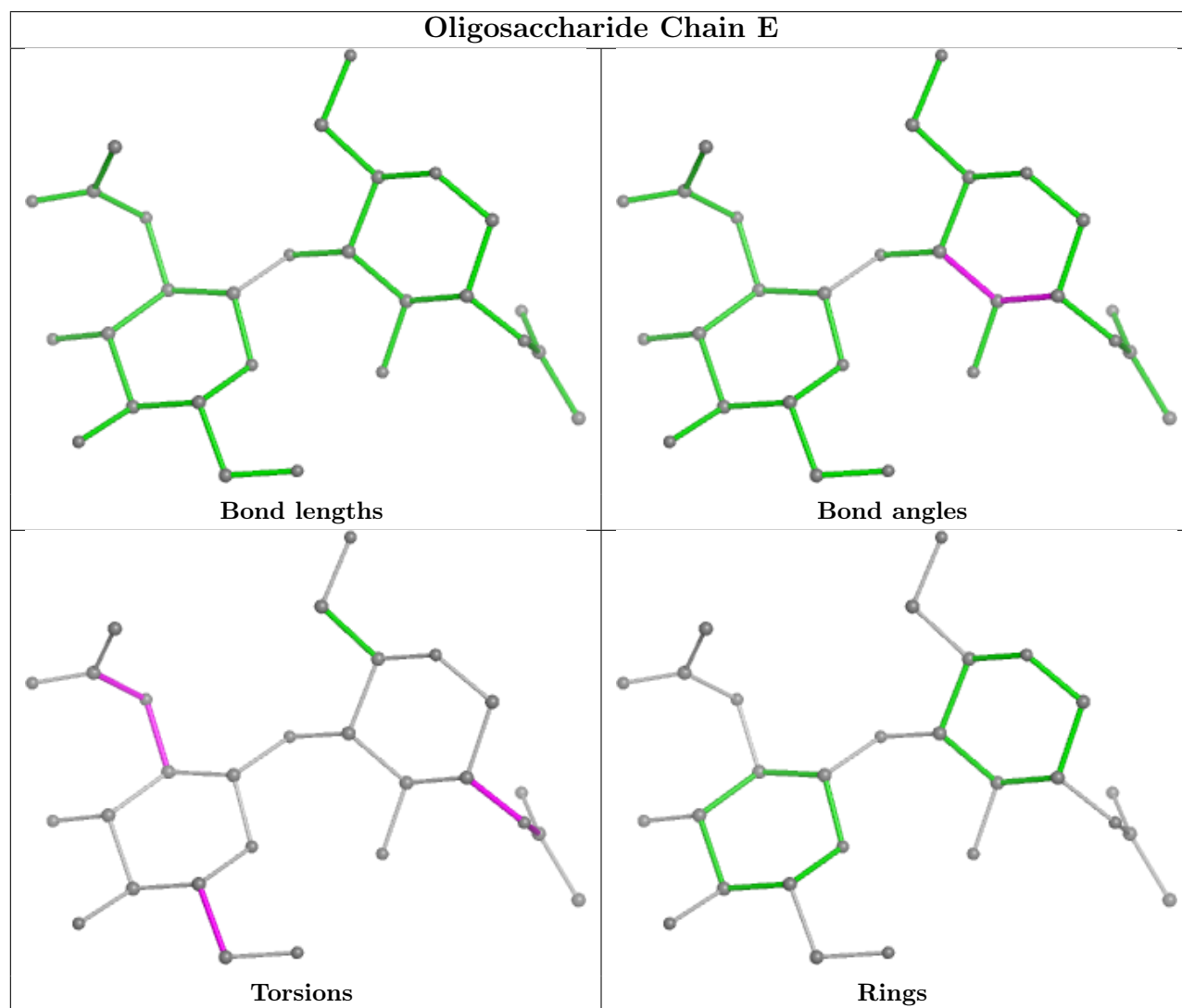
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2	NAG	4	0
3	J	3	BMA	1	0
3	J	2	NAG	5	0
3	H	1	NAG	9	0
2	K	2	NAG	1	0
3	J	1	NAG	1	0
2	I	2	NAG	2	0
3	L	2	NAG	2	0
3	F	1	NAG	2	0
2	I	1	NAG	2	0

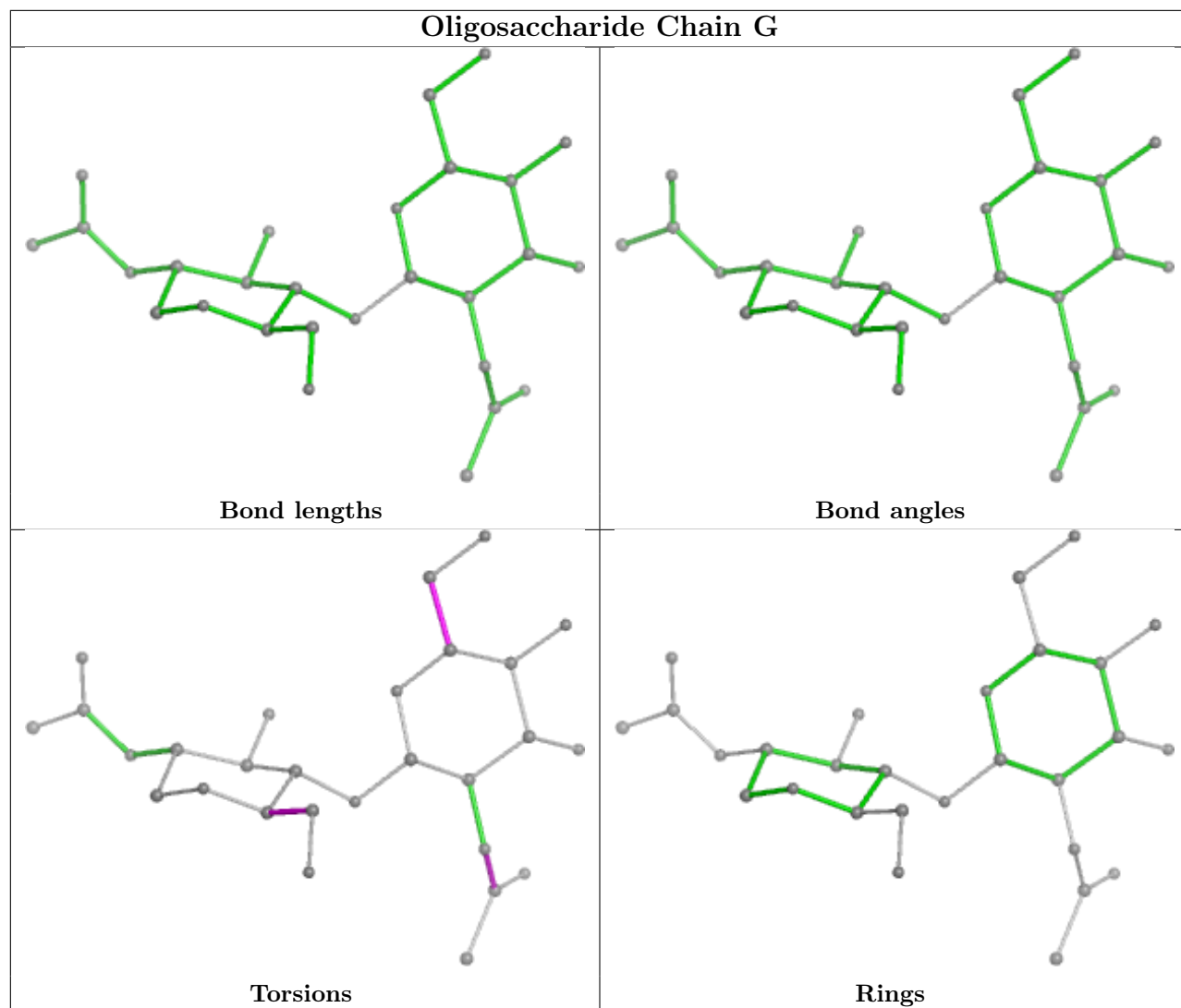
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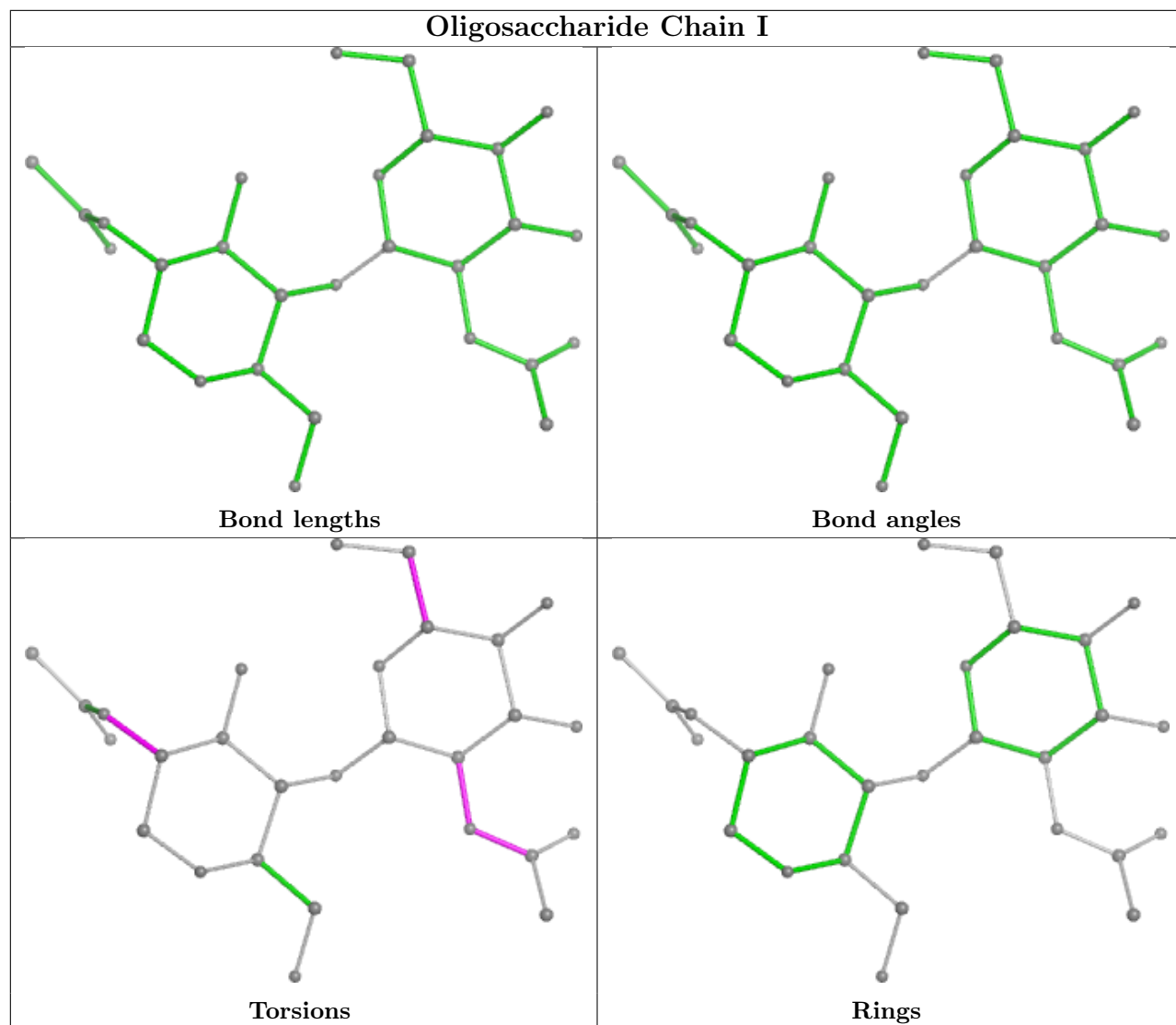
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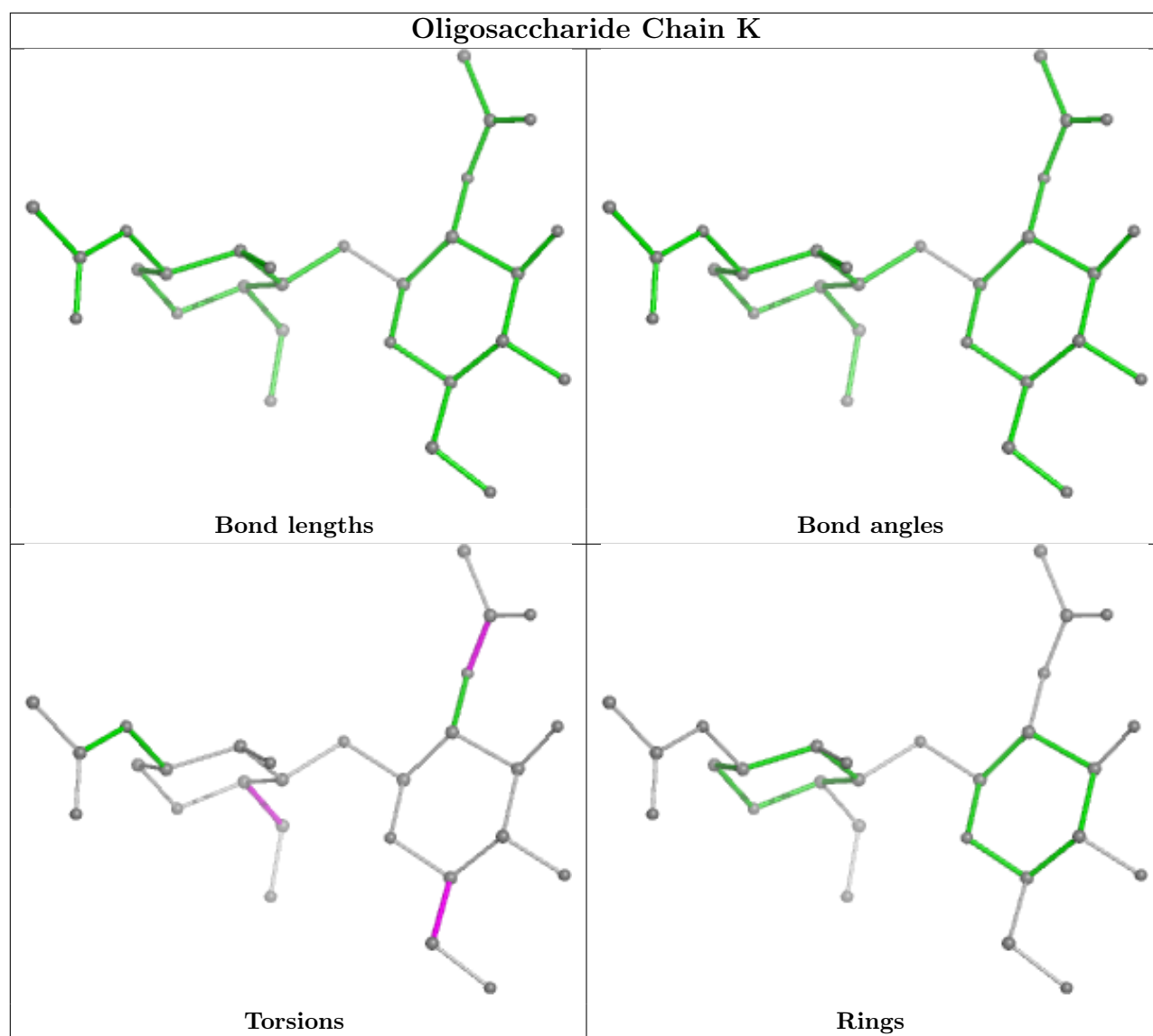
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	6	0
3	L	1	NAG	2	0
2	E	1	NAG	1	0

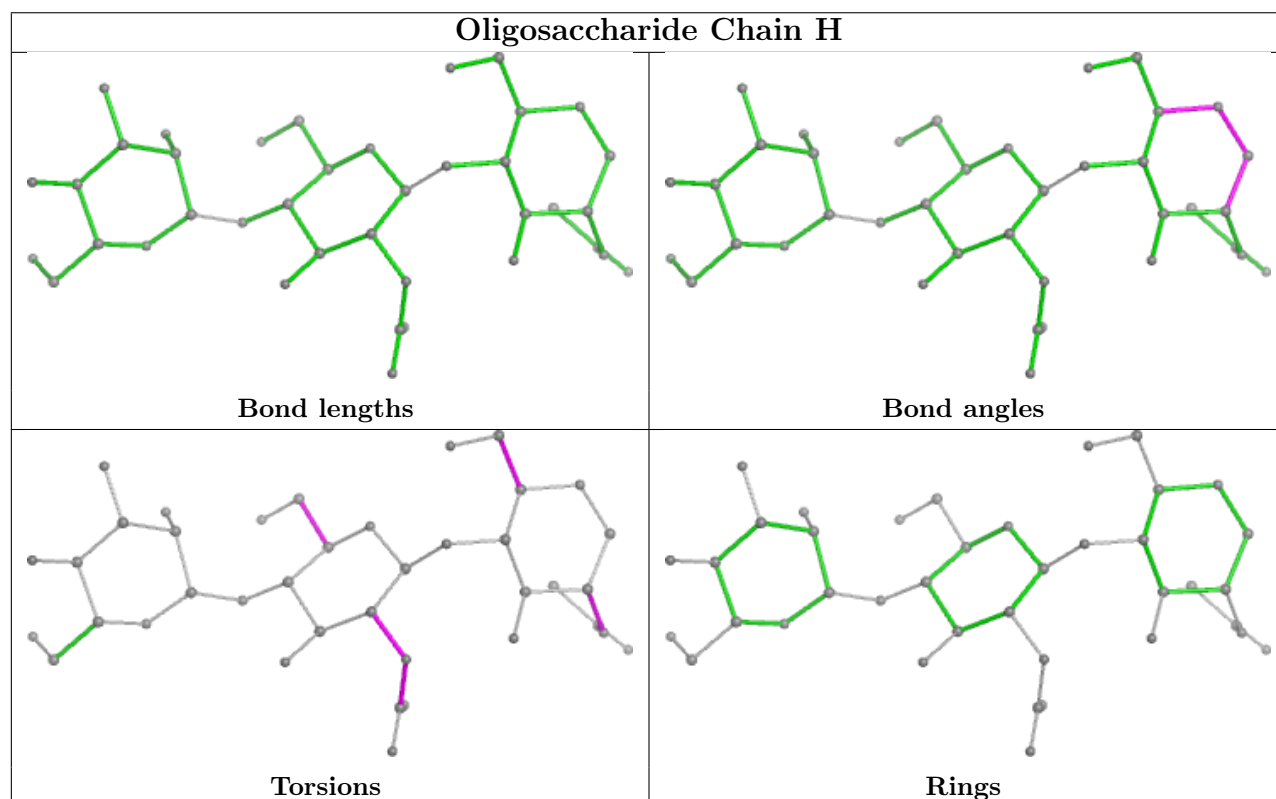
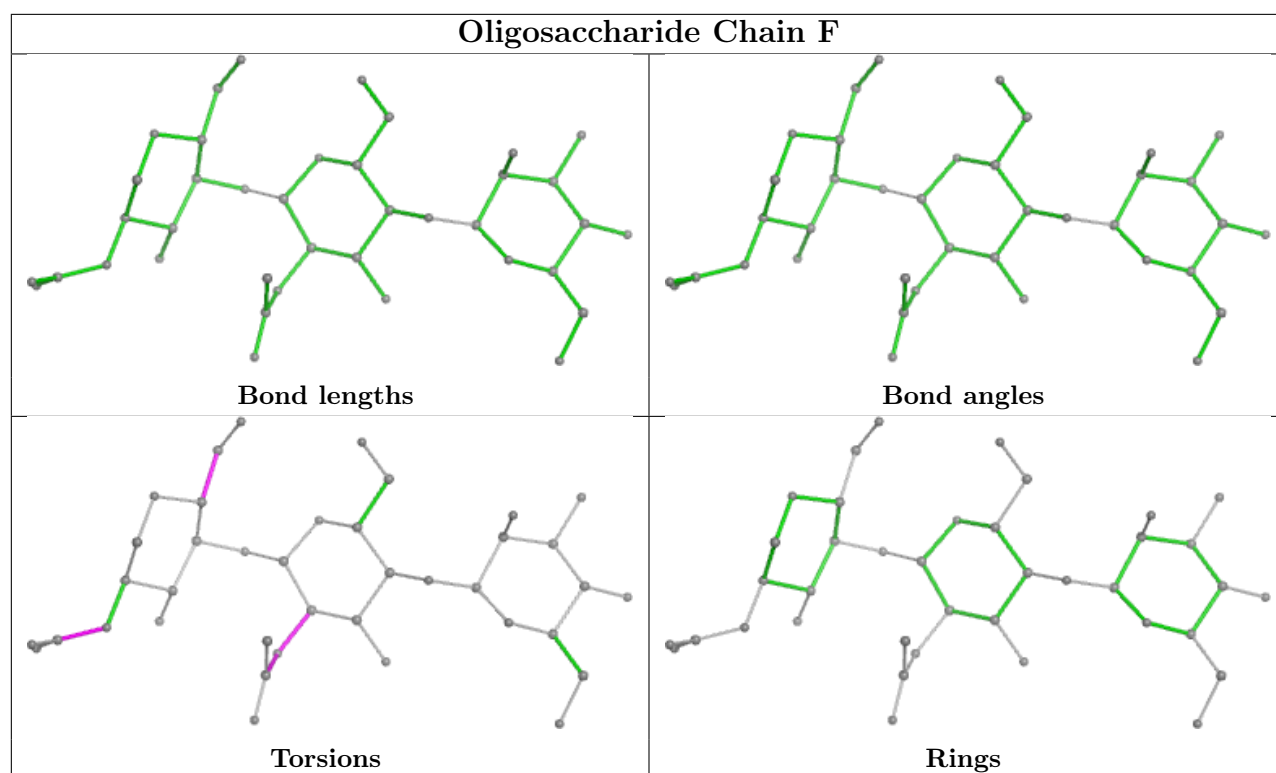
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

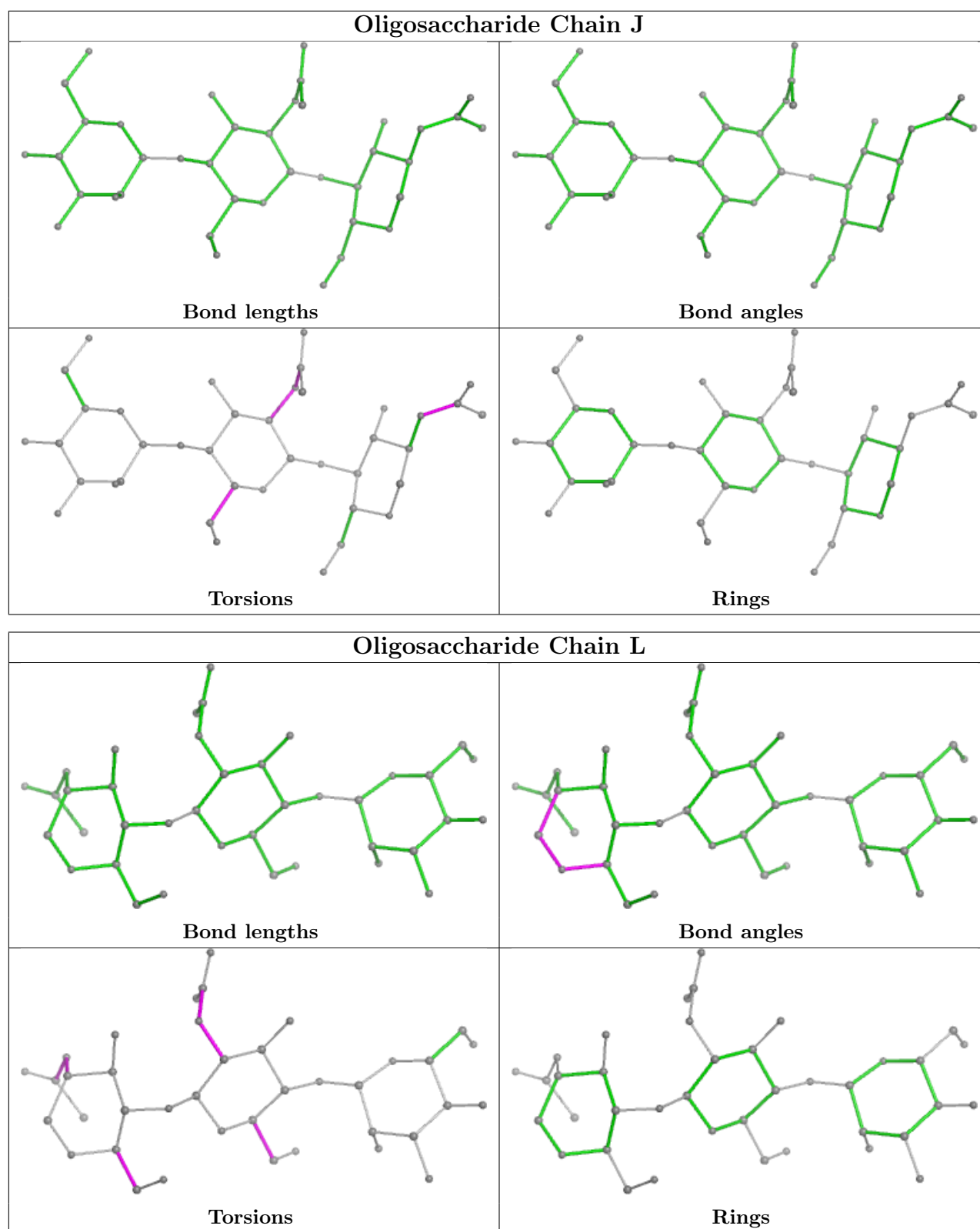












5.6 Ligand geometry [i](#)

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$
4	NAG	A	2002	1	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	A	2003	1	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	A	2004	1	14,14,15	0.28	0	17,19,21	0.70	0
4	NAG	D	2002	1	14,14,15	0.33	0	17,19,21	0.64	0
4	NAG	D	2003	1	14,14,15	0.30	0	17,19,21	0.57	0
4	NAG	B	2001	1	14,14,15	0.29	0	17,19,21	0.55	0
4	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	B	2003	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	B	2004	1	14,14,15	0.30	0	17,19,21	0.67	0
4	NAG	A	2001	1	14,14,15	0.68	0	17,19,21	0.90	0
4	NAG	D	2001	1	14,14,15	0.28	0	17,19,21	0.53	0
4	NAG	C	2002	1	14,14,15	0.29	0	17,19,21	0.54	0
4	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.70	0
4	NAG	D	2004	1	14,14,15	0.48	0	17,19,21	1.42	3 (17%)
4	NAG	C	2004	1	14,14,15	0.29	0	17,19,21	0.78	0
4	NAG	C	2001	1	14,14,15	1.14	1 (7%)	17,19,21	1.83	5 (29%)
4	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.67	0
4	NAG	B	2002	1	14,14,15	0.31	0	17,19,21	0.61	0
4	NAG	C	2003	1	14,14,15	0.28	0	17,19,21	0.61	0
4	NAG	B	2005	1	14,14,15	0.30	0	17,19,21	0.61	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
4	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2003	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	5/6/23/26	0/1/1/1

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2001	NAG	O4-C4	2.94	1.49	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	3.80	117.34	112.19
4	D	2004	NAG	C1-O5-C5	3.54	116.99	112.19
4	C	2001	NAG	C4-C3-C2	3.41	116.02	111.02
4	C	2001	NAG	C3-C4-C5	-3.15	104.61	110.24
4	C	2001	NAG	O4-C4-C5	2.84	116.36	109.30

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2003	NAG	C8-C7-N2-C2
4	B	2001	NAG	C3-C2-N2-C7
4	B	2002	NAG	C3-C2-N2-C7
4	B	2005	NAG	C8-C7-N2-C2
4	B	2005	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	NAG	1	0
4	A	2003	NAG	4	0
4	A	2004	NAG	1	0
4	D	2002	NAG	1	0
4	A	2001	NAG	6	0
4	D	2001	NAG	3	0
4	C	2005	NAG	1	0
4	D	2004	NAG	1	0
4	C	2004	NAG	1	0
4	A	2005	NAG	1	0
4	B	2002	NAG	1	0
4	C	2003	NAG	3	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	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	168:GLN	C	169:ASP	N	1.16

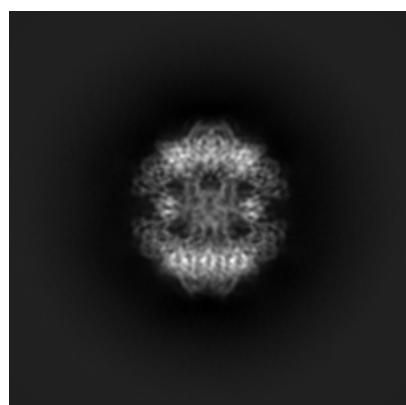
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12754. These allow visual inspection of the internal detail of the map and identification of artifacts.

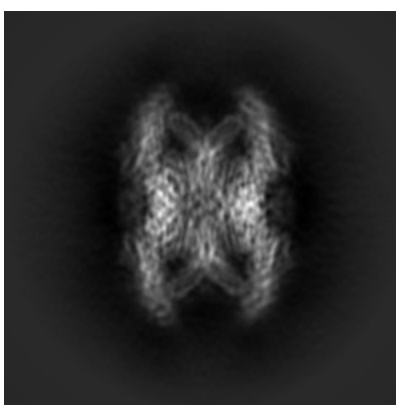
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

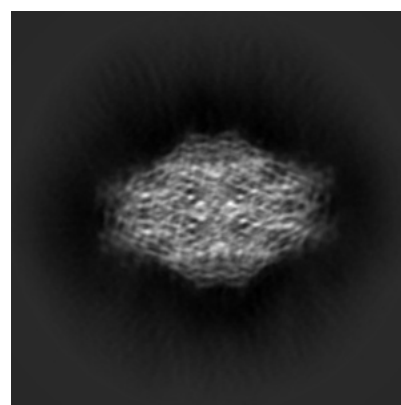
6.1.1 Primary map



X



Y

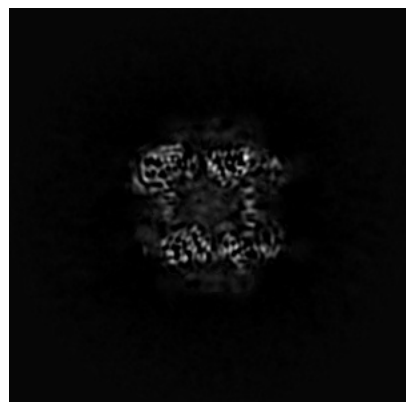


Z

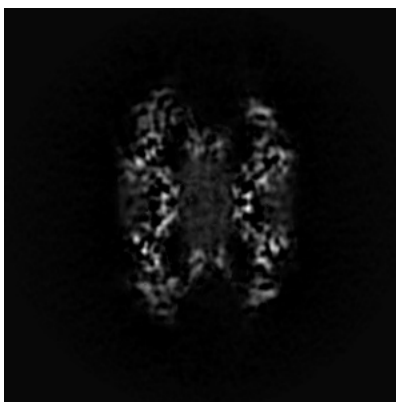
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

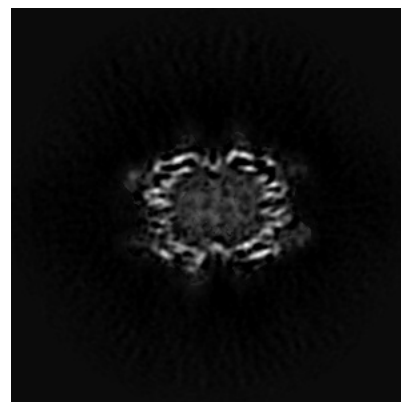
6.2.1 Primary map



X Index: 160



Y Index: 160

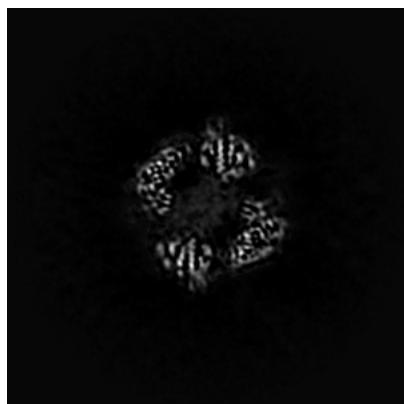


Z Index: 160

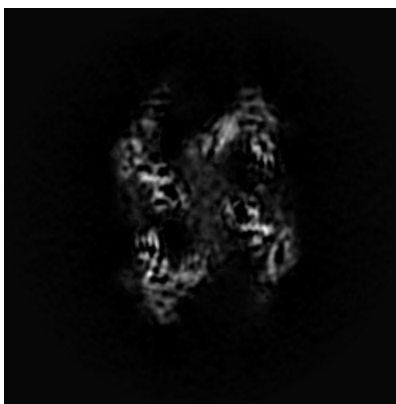
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

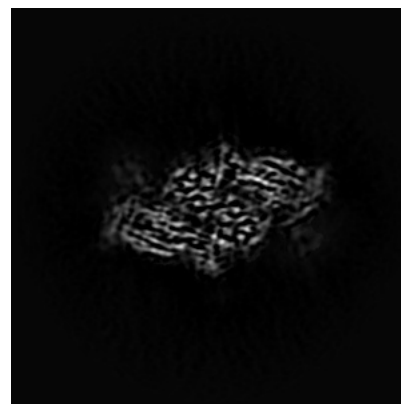
6.3.1 Primary map



X Index: 144



Y Index: 171



Z Index: 202

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

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

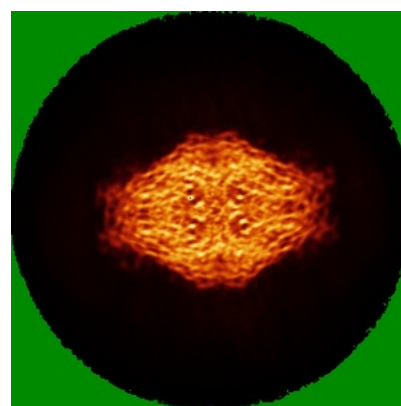
6.4.1 Primary map



X



Y

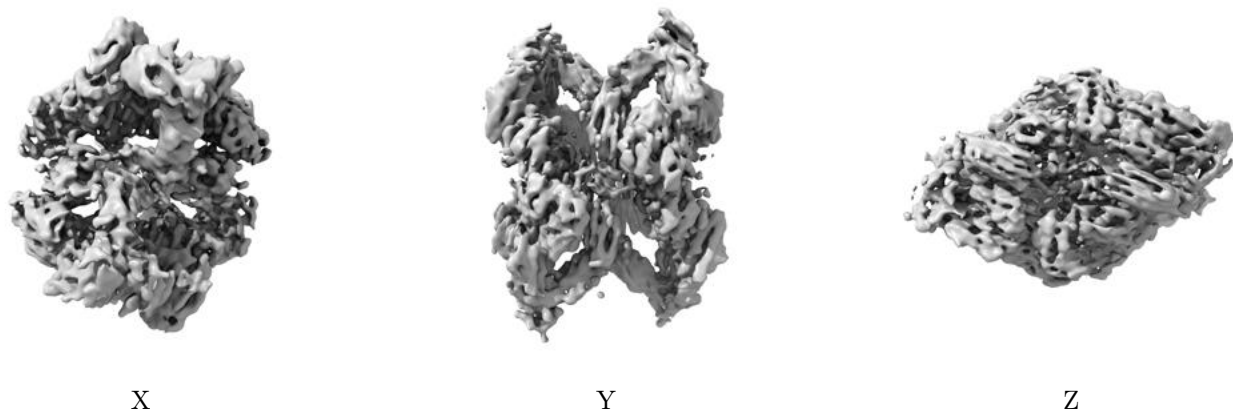


Z

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.

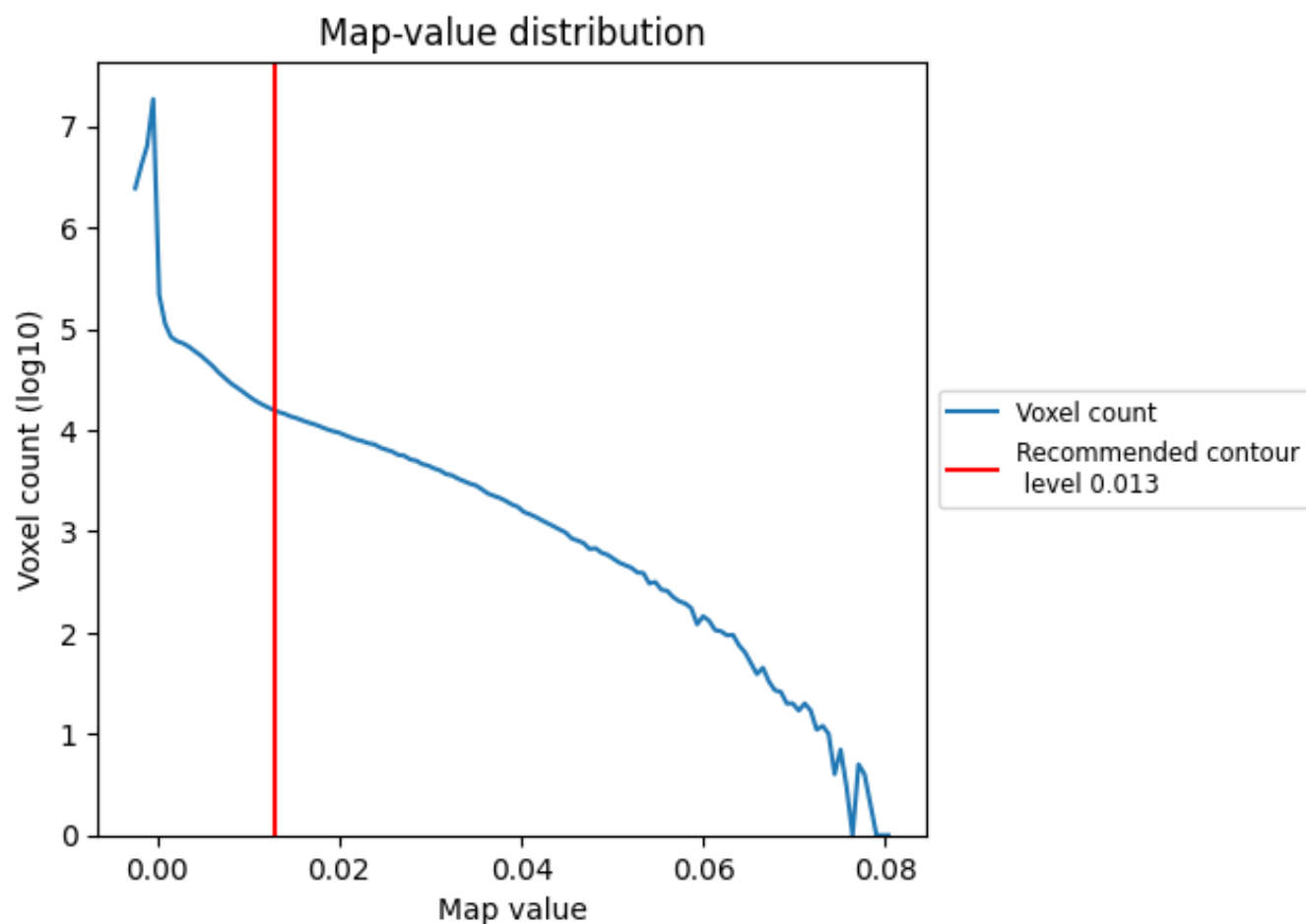
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

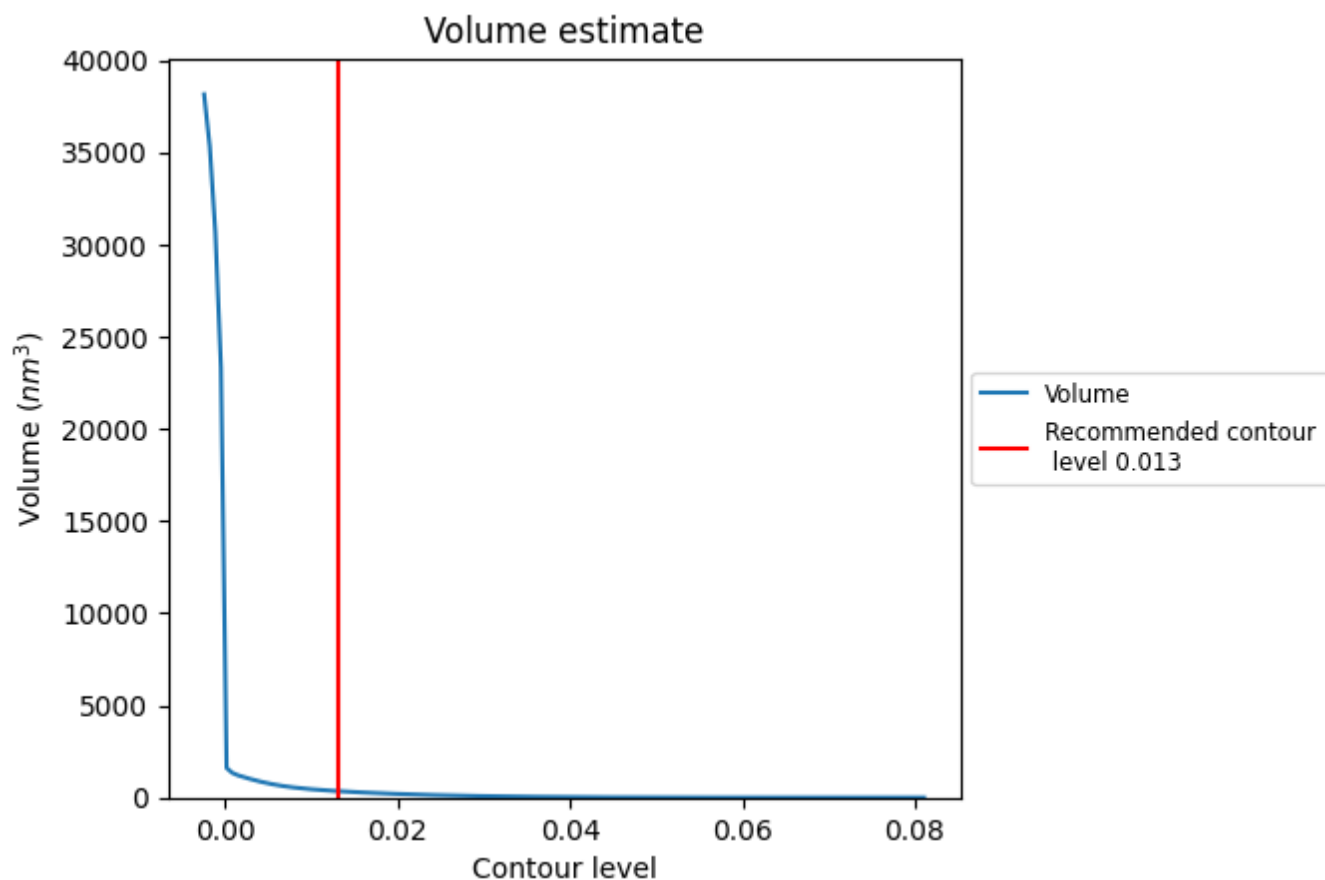
This section contains the results of statistical analysis of the map.

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.

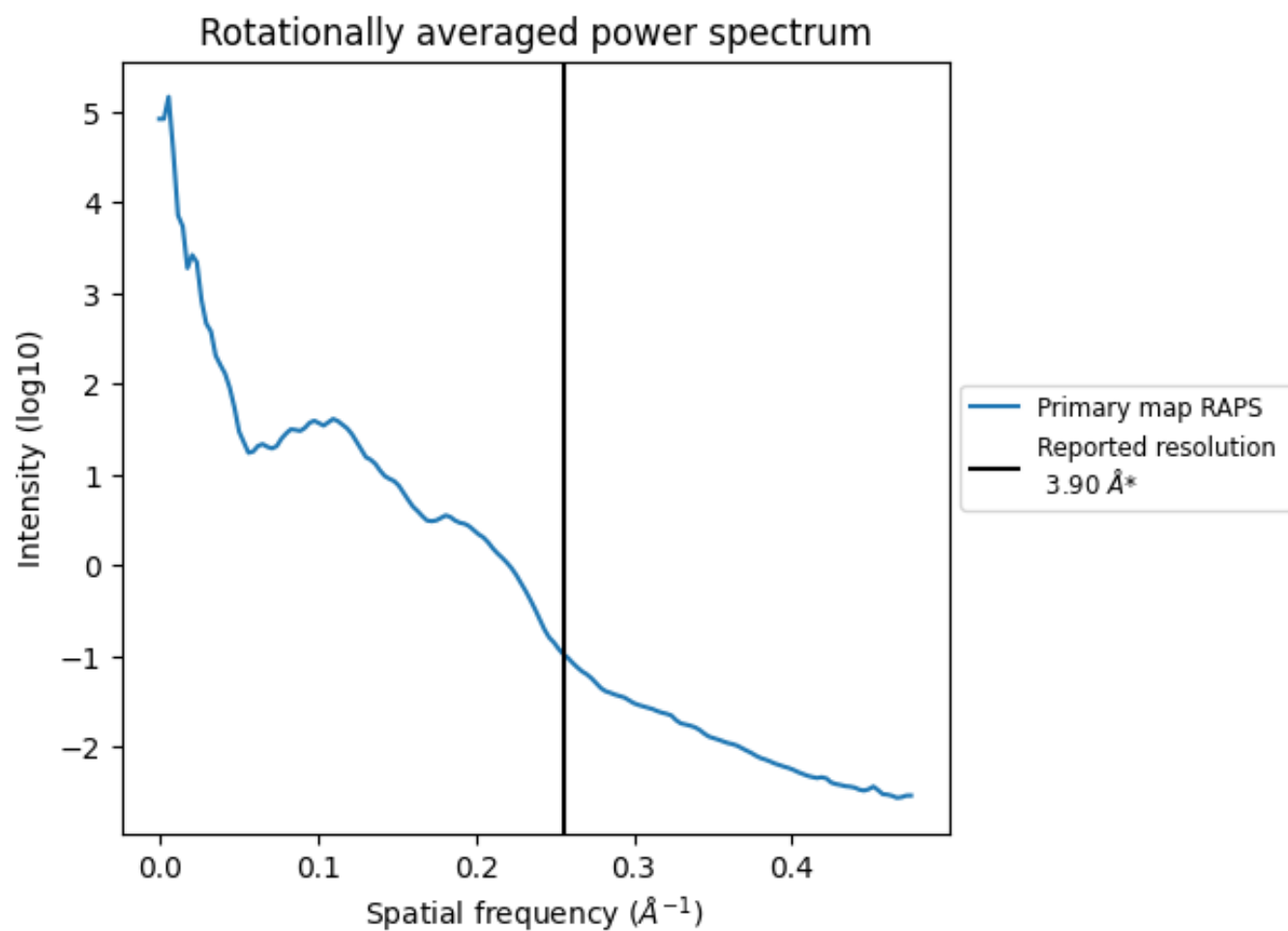
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm³; this corresponds to an approximate mass of 317 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 0.256 \AA^{-1}

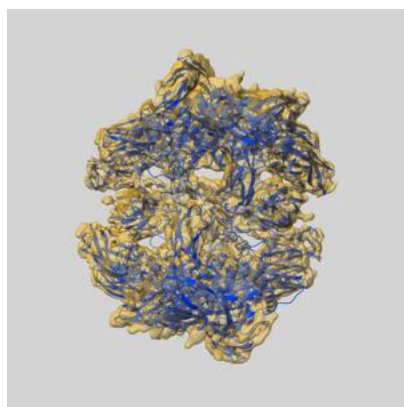
8 Fourier-Shell correlation

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

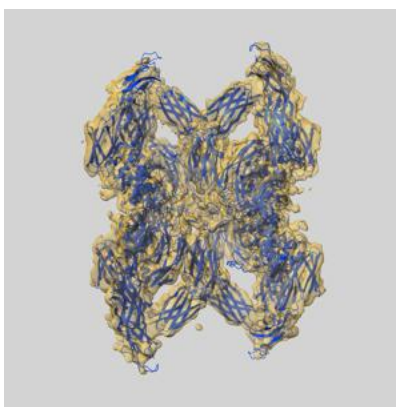
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12754 and PDB model 7O7R. Per-residue inclusion information can be found in section [3](#) on page [7](#).

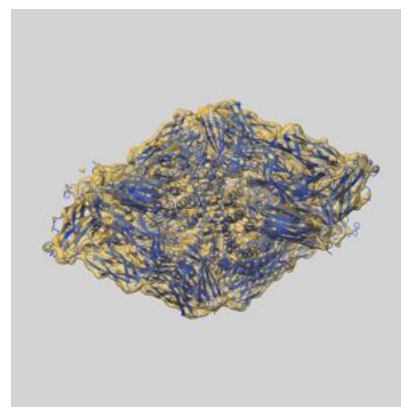
9.1 Map-model overlay [i](#)



X



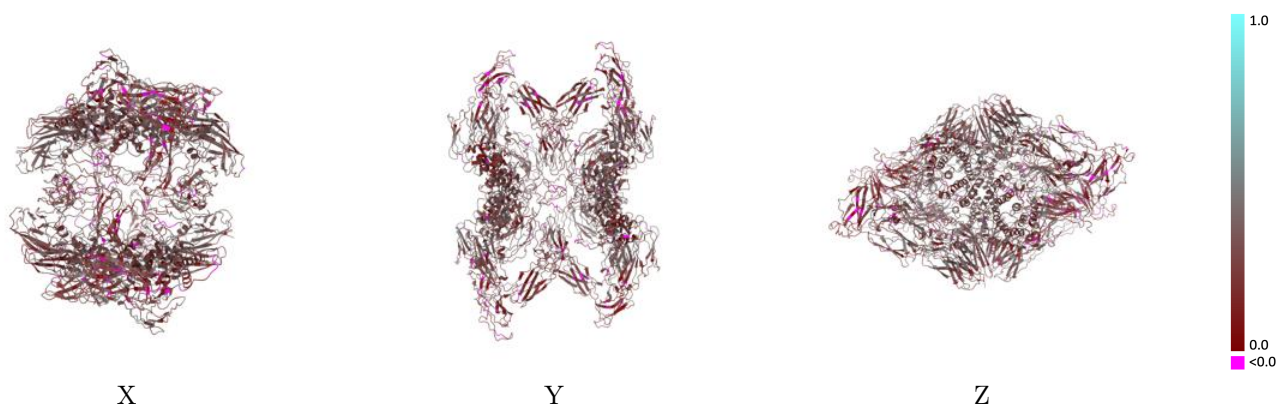
Y



Z

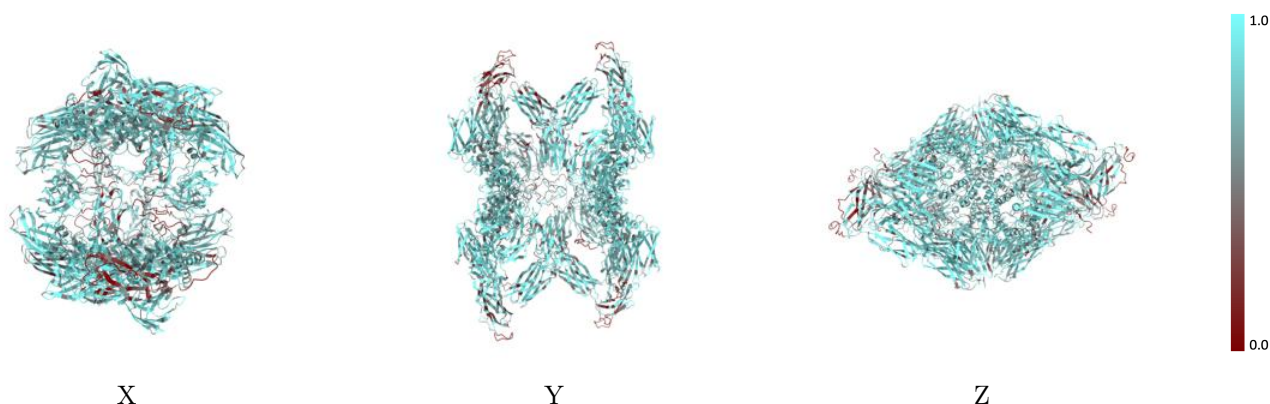
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



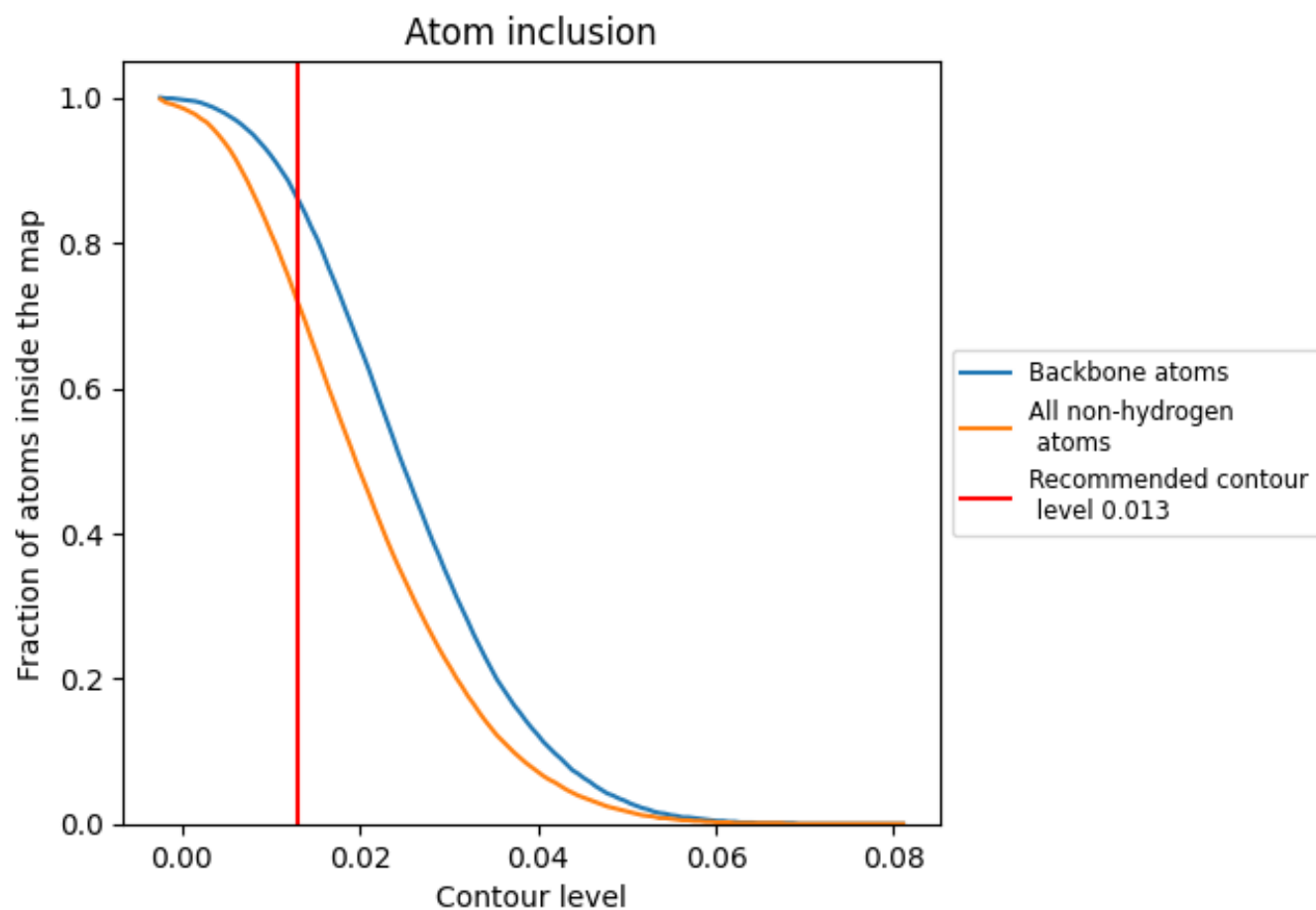
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 86% of all backbone atoms, 72% 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	<div></div> 0.7180	<div></div> 0.2960
A	<div></div> 0.6940	<div></div> 0.2900
B	<div></div> 0.7400	<div></div> 0.3030
C	<div></div> 0.7100	<div></div> 0.2870
D	<div></div> 0.7350	<div></div> 0.3060
E	<div></div> 0.5000	<div></div> 0.2430
F	<div></div> 0.5130	<div></div> 0.1480
G	<div></div> 0.3930	<div></div> 0.1770
H	<div></div> 0.5380	<div></div> 0.1800
I	<div></div> 0.7140	<div></div> 0.3220
J	<div></div> 0.5380	<div></div> 0.1360
K	<div></div> 0.4640	<div></div> 0.2000
L	<div></div> 0.4620	<div></div> 0.2800

