



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:12 AM UTC

PDB ID : 7O7R / pdb_00007o7r
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:

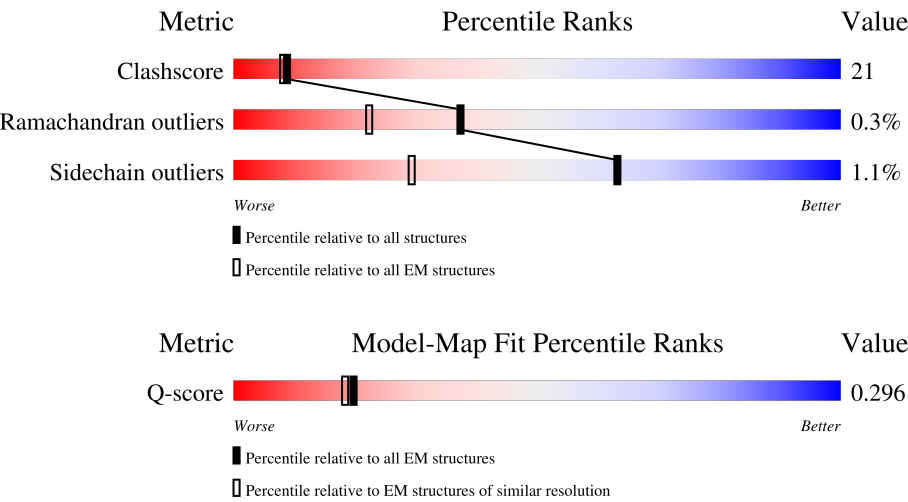
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	
1	B	1474	
1	C	1474	
1	D	1474	

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Mol	Chain	Length	Quality of chain
2	E	2	<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>
3	F	3	<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.

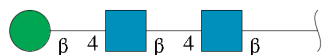
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	B	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		
1	C	1285	Total	C	N	O	S	0	0
			10023	6375	1681	1924	43		
1	D	1278	Total	C	N	O	S	0	0
			9968	6336	1674	1915	43		

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



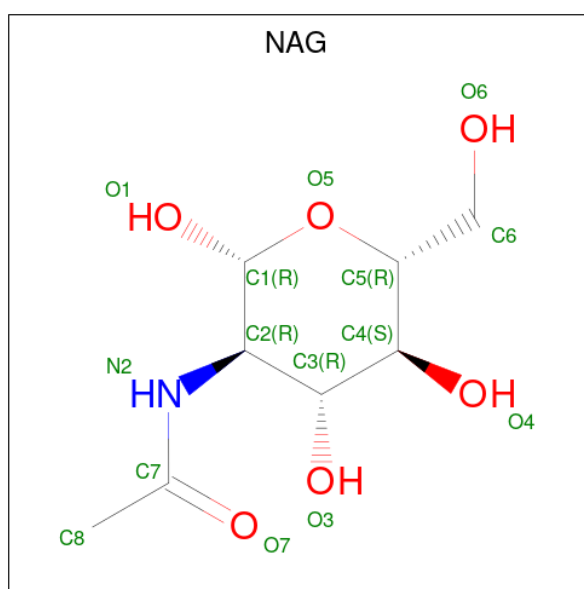
Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	I	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		

- 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 (CCD ID: 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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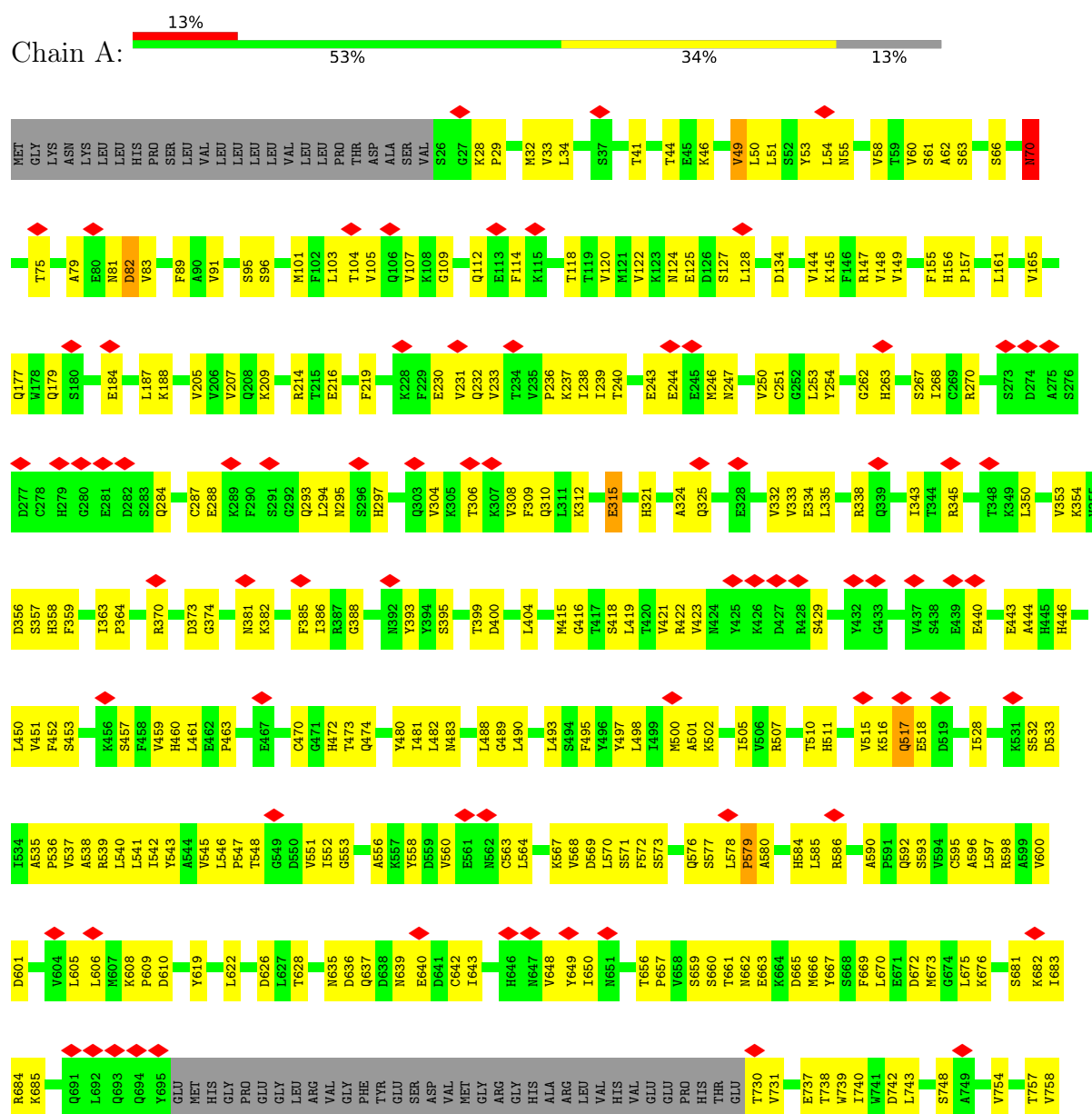
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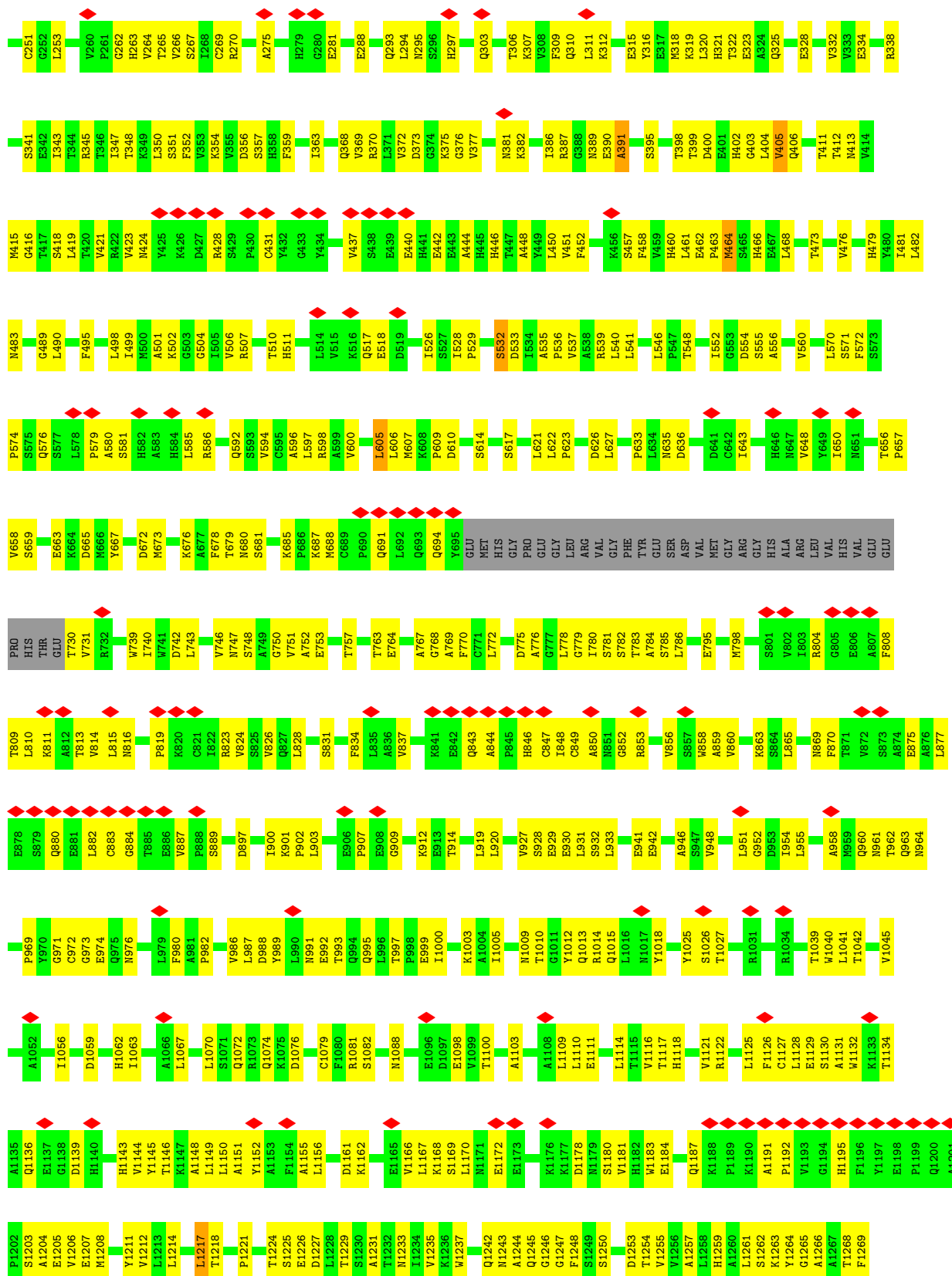
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	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	

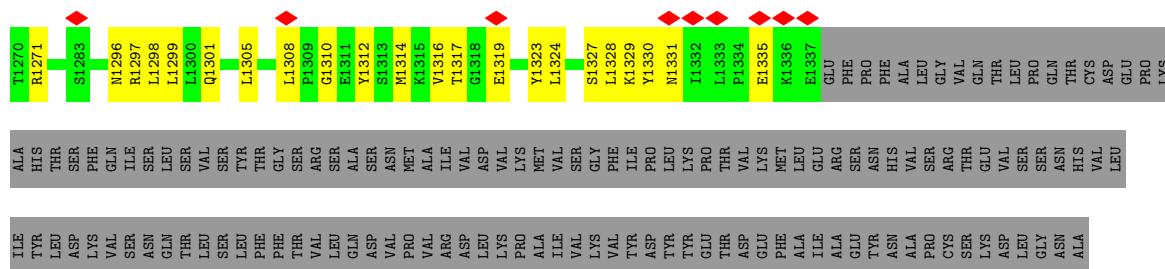
3 Residue-property plots

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.

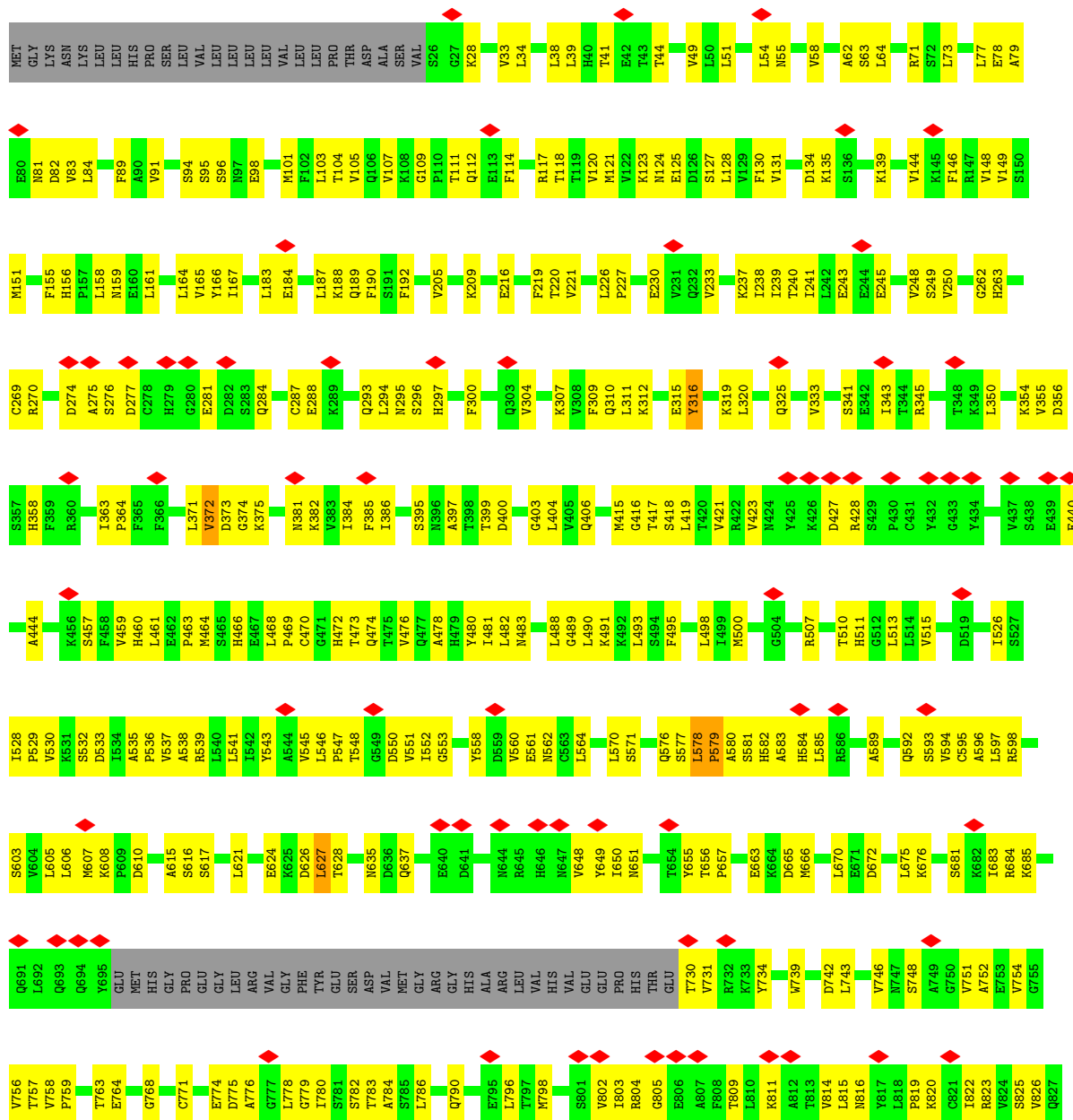
• Molecule 1: Alpha-2-macroglobulin

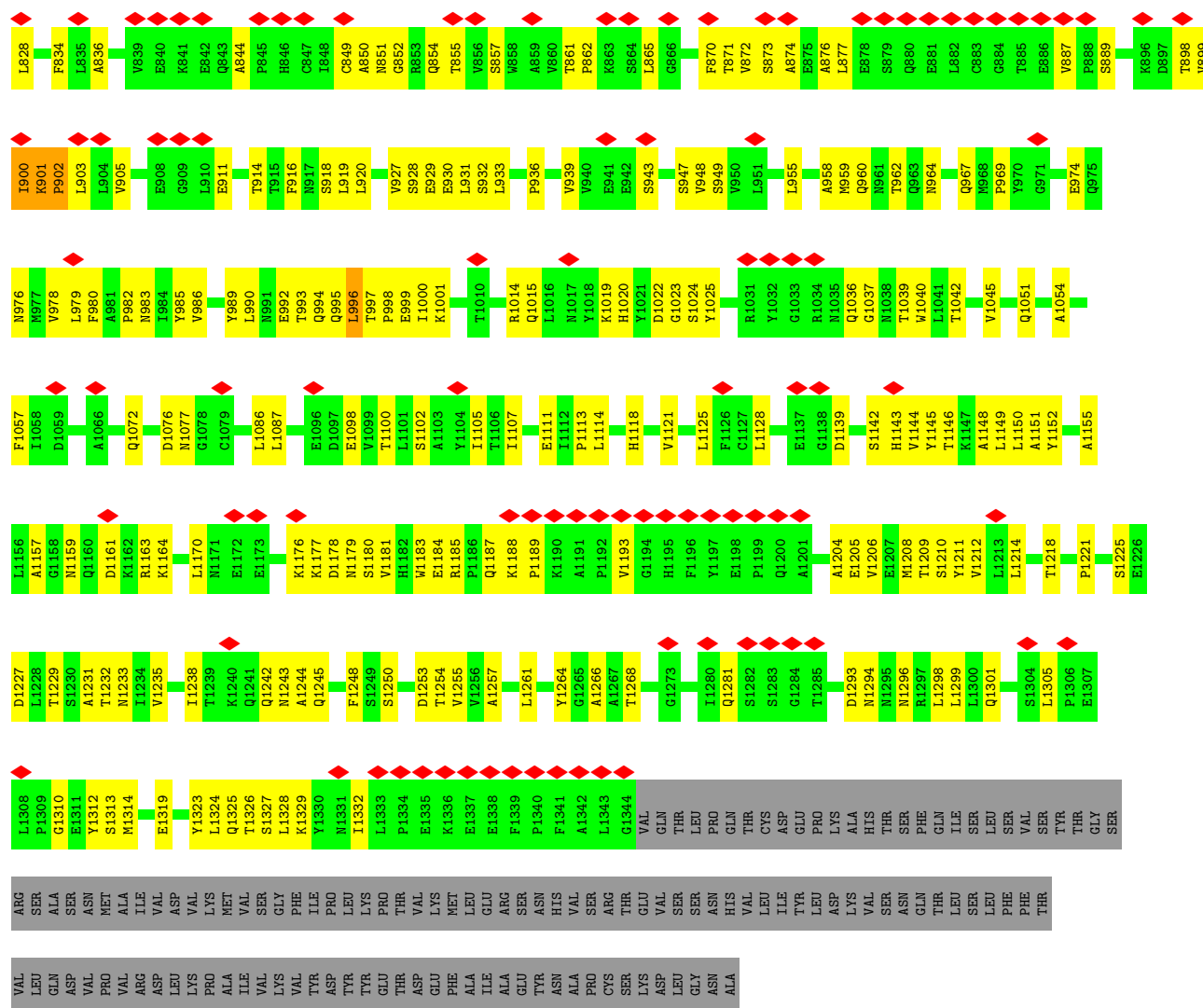




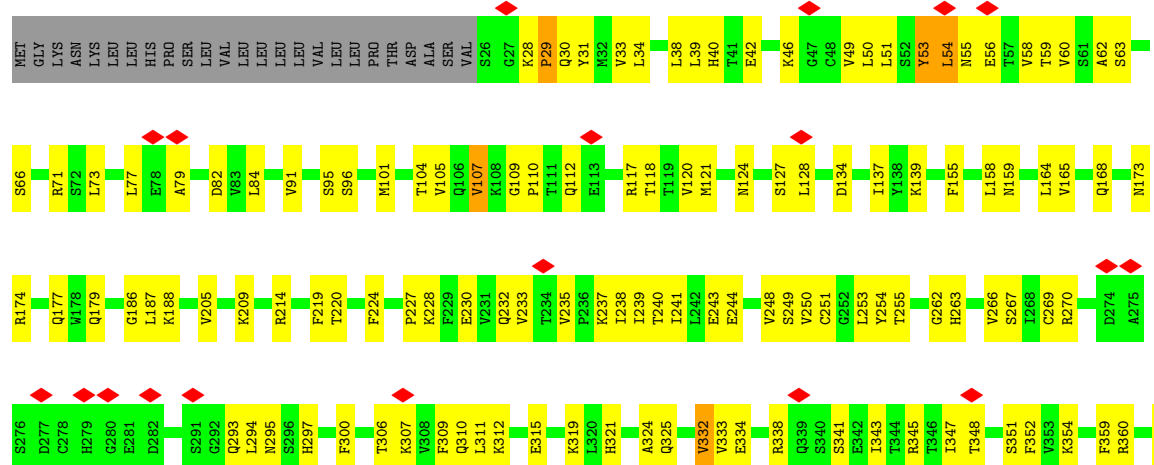


• Molecule 1: Alpha-2-macroglobulin





• Molecule 1: Alpha-2-macroglobulin



VAL	T1232	L1067	L903	E753	Q693	E612	D533	L450	V369
SER	M1233	I1068	L904	V756	Q694	L613	I534	L451	V370
GLY	I1234	L979	V905	T757	Y695	S614	A535	V451	D373
PHE	K1235	E906	E906	V756	GLU	S617	P536	S453	
ILE	K1236	Q1072	P907	D760	MET	L621	V537	K456	N381
PRO	M1237	R1073	E908	T761	HIS	L622	A538	V457	K382
LEU	I1238	Q1074	G909	I762	GLY	P623	L540	V458	V383
LYS	I1332	D1075	L910	T763	PRO	L541	L541	V459	I384
PRO	K1239	D1076	E911	E764	GLY	P631	I542	V460	F385
THR	K1168	Q1077	E912	W765	LEU	G632	V545	I386	I387
VAL	Q1241	Q1078	K912		ARG	P633	L546	I387	G388
VAL	Q1242	L996	E913	G768	VAL	D636	P547	L461	
LYS	N1243	T997	E914	A769	GLY	Q637	M464	E462	Y393
LEU	A1244	I1000	T915	C771	PHE	D638	S465	S465	Y394
GLU	G1247	I1001	F916	L772	TYR	C642	H466	E467	S395
PHE	T1251	K1001	N917	L778	SER	H645	I481	L468	N396
ASN	G1252	K1002	S918	G779	ASP	N647	T473	V476	A397
ALA	D1253	K1003	L919	S781	VAL	M647	Q474	V476	T399
VAL	T1254	K1004	L920	T783	GLY	V648	T475	V476	D400
SER	V1255	I1005		A784	ARG	Y649	T476	V476	E401
ARG	H1259			S785	ALA	I650	T481	V476	H402
THR	S1262	L1008	Y927	L786	VAL	N651	L482	V476	G403
VAL	K1263	N1009	S928	R787	MET	T654	T486	V476	L404
PRO	K1263	N1010	E929	A788	GLY	Y655	L486	V476	V405
GLN	G1265	T1010	T930	Q790	GLY	T656	L486	V476	T411
THR	G1265	G1011	Y939	P791	THR	Y657	L486	V476	T412
ASN	G1265	G1012	V940	L796	GLU	P657	L486	V476	M415
CYS	T1268	G1013	E941	L797	PRO	S659	L486	V476	T417
ASP	T1269	R1014	E942	W797	HIS	S660	L486	V476	S418
GLU	T1270	L1015	S943	M798	THR	T661	L486	V476	L419
LEU	R1271	L1016	A944	L798	GLU	N662	L486	V476	T420
LYS	F1196	N1017		L799	THR	E663	L486	V476	V421
ALA	T1272	Y1025		L799	GLU	K664	L486	V476	R422
THR	G1273	S1026		L799	THR	D665	L486	V476	R423
VAL	V1278	T1027		L799	GLU	F669	L486	V476	M424
GLN	T1279	E1030		L799	THR	M673	L486	V476	Y425
ILE	I1280	R1031		L799	GLU	G674	L486	V476	K426
LEU	Q1281	F1126		L799	THR	L675	L486	V476	D427
SER	G1284	C1127		L799	GLU	K676	L486	V476	R428
VAL	R1297	L1128		L799	THR	A677	L486	V476	S429
PHE	L1298	E1129		L799	GLU	N681	L486	V476	P430
THR	Q1301	S1130		L799	THR	K685	L486	V476	C431
VAL	L1305	A1131		L799	GLU	P686	L486	V476	Y432
GLN	L1305	T1134		L799	THR	K687	L486	V476	G433
ASP	Y1312	E1137		L799	GLU	M688	L486	V476	Y434
PRO	S1313	H1140		L799	THR	S689	L486	V476	Q435
VAL	M1314	V1144		L799	GLU	K689	L486	V476	Q436
VAL	K1315	T1145		L799	THR	M689	L486	V476	Y437
ARG	V1316	L1146		L799	GLU	C689	L486	V476	S438
ASP	T1317	A1148		L799	THR	P690	L486	V476	E439
LEU	L1324	L1149		L799	GLU	Q691	L486	V476	E440
LYS	Y1323	H1062		L799	THR	L692	L486	V476	E443
PRO	S1325	I1063		L799	GLU		L486	V476	A444
ALA	Q1325	Y1152		L799	THR		L486	V476	
VAL				L799	GLU		L486	V476	
MET				L799	THR		L486	V476	

ILE VAL LYS VAL TYR ASP TYR GLU THR ASP GLU PHE ALA ILE 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.60	0/10247	0.76	2/13921 (0.0%)
1	B	0.67	3/10189 (0.0%)	0.81	10/13842 (0.1%)
1	C	0.68	3/10247 (0.0%)	0.80	5/13921 (0.0%)
1	D	0.68	4/10189 (0.0%)	0.80	9/13842 (0.1%)
All	All	0.66	10/40872 (0.0%)	0.79	26/55526 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	902	PRO	N-CA	22.76	1.70	1.47
1	B	29	PRO	N-CA	18.84	1.71	1.47
1	D	29	PRO	N-CA	18.55	1.71	1.47
1	D	168	GLN	C-N	-10.66	1.16	1.33
1	C	967	GLN	C-N	-8.26	1.21	1.33

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	LYS	CA-C-N	15.13	138.75	119.84
1	B	28	LYS	C-N-CA	15.13	138.75	119.84
1	D	28	LYS	CA-C-N	15.02	138.61	119.84
1	D	28	LYS	C-N-CA	15.02	138.61	119.84
1	C	901	LYS	CA-C-N	14.79	140.01	120.79

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	407	0
1	B	9968	0	9866	425	0
1	C	10023	0	9917	421	0
1	D	9968	0	9866	415	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	1694	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 1694 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:N	1:C:902:PRO:CA	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%)	24	59
1	B	1274/1474 (86%)	1057 (83%)	214 (17%)	3 (0%)	43	74
1	C	1281/1474 (87%)	1036 (81%)	239 (19%)	6 (0%)	24	59
1	D	1274/1474 (86%)	1041 (82%)	231 (18%)	2 (0%)	43	74
All	All	5110/5896 (87%)	4159 (81%)	934 (18%)	17 (0%)	37	69

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%)	1111 (99%)	9 (1%)	73	77
1	B	1115/1290 (86%)	1099 (99%)	16 (1%)	59	71
1	C	1120/1290 (87%)	1111 (99%)	9 (1%)	73	77
1	D	1115/1290 (86%)	1101 (99%)	14 (1%)	61	71
All	All	4470/5160 (87%)	4422 (99%)	48 (1%)	63	74

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	245	GLU
1	D	107	VAL
1	C	372	VAL
1	C	996	LEU
1	D	396	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1187	GLN
1	D	1038	ASN
1	C	389	ASN
1	D	994	GLN
1	D	1187	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	0.27	0	17,19,21	0.75	1 (5%)
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.57	0
3	NAG	F	1	1,3	14,14,15	0.30	0	17,19,21	0.65	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	0.34	0	17,19,21	0.60	0
3	BMA	F	3	3	11,11,12	0.25	0	15,15,17	0.47	0
2	NAG	G	1	2,1	14,14,15	0.30	0	17,19,21	0.69	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.60	0
3	NAG	H	1	1,3	14,14,15	0.36	0	17,19,21	1.40	2 (11%)
3	NAG	H	2	3	14,14,15	0.34	0	17,19,21	0.57	0
3	BMA	H	3	3	11,11,12	0.24	0	15,15,17	0.51	0
2	NAG	I	1	2,1	14,14,15	0.28	0	17,19,21	0.49	0
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.56	0
3	NAG	J	1	1,3	14,14,15	0.31	0	17,19,21	0.63	0
3	NAG	J	2	3	14,14,15	0.32	0	17,19,21	0.66	0
3	BMA	J	3	3	11,11,12	0.26	0	15,15,17	0.49	0
2	NAG	K	1	2,1	14,14,15	0.32	0	17,19,21	0.80	0
2	NAG	K	2	2	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	L	1	1,3	14,14,15	0.49	0	17,19,21	1.42	2 (11%)
3	NAG	L	2	3	14,14,15	0.36	0	17,19,21	0.70	0
3	BMA	L	3	3	11,11,12	0.25	0	15,15,17	0.52	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	1,3	-	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	1,3	-	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	-	4/6/23/26	0/1/1/1
3	NAG	J	1	1,3	-	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	1,3	-	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	4.36	118.04	111.29
3	H	1	NAG	C1-O5-C5	3.87	117.37	112.19
3	H	1	NAG	O5-C1-C2	3.08	116.05	111.29
3	L	1	NAG	C1-O5-C5	2.36	115.34	112.19
2	E	1	NAG	C4-C3-C2	-2.07	107.98	111.02

There are no chirality outliers.

5 of 54 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:

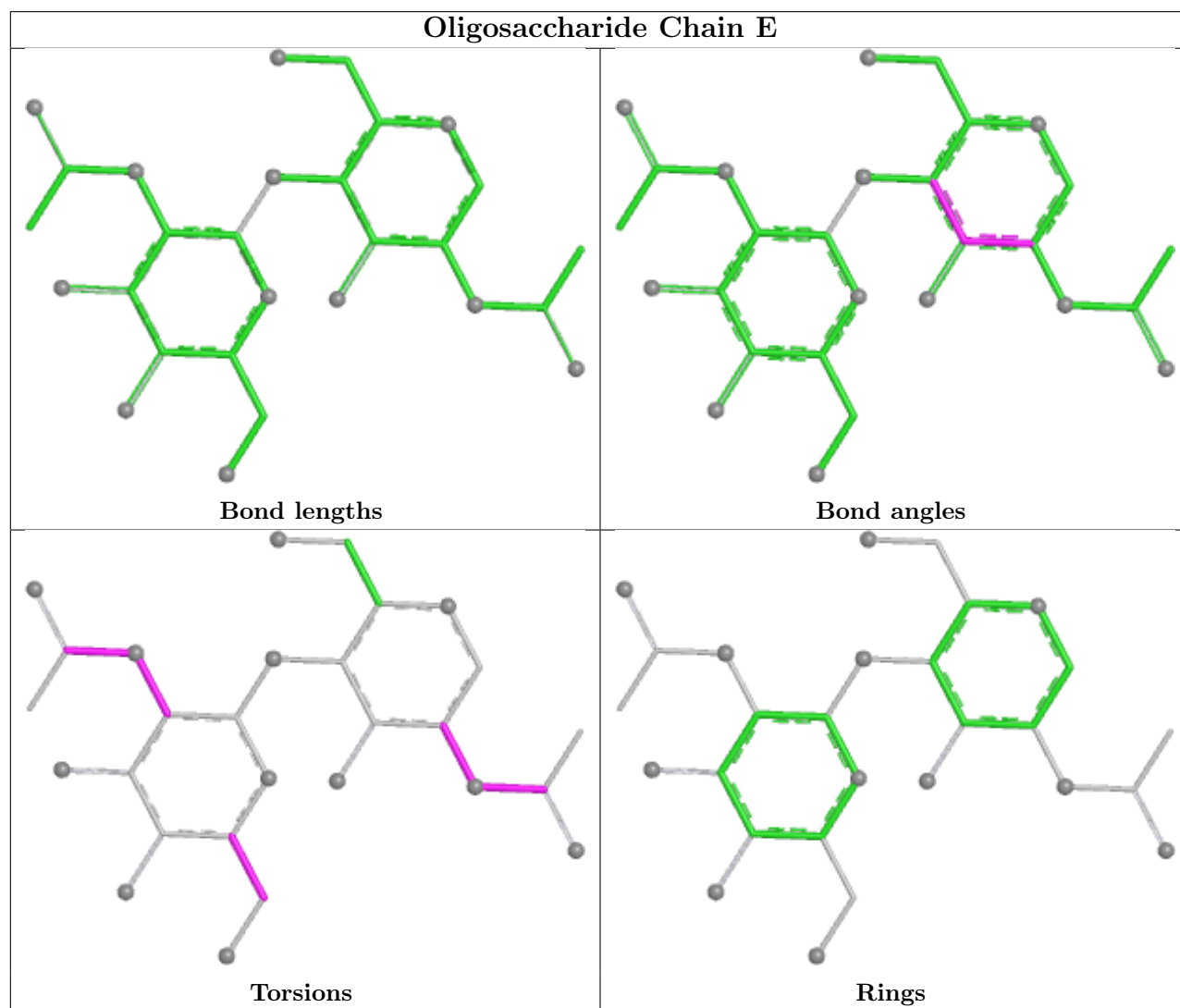
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2	NAG	6	0
2	K	2	NAG	1	0
2	I	1	NAG	2	0
3	J	3	BMA	1	0
2	E	1	NAG	1	0
3	L	2	NAG	2	0
3	L	1	NAG	2	0
3	H	1	NAG	9	0
2	I	2	NAG	2	0
3	J	2	NAG	5	0

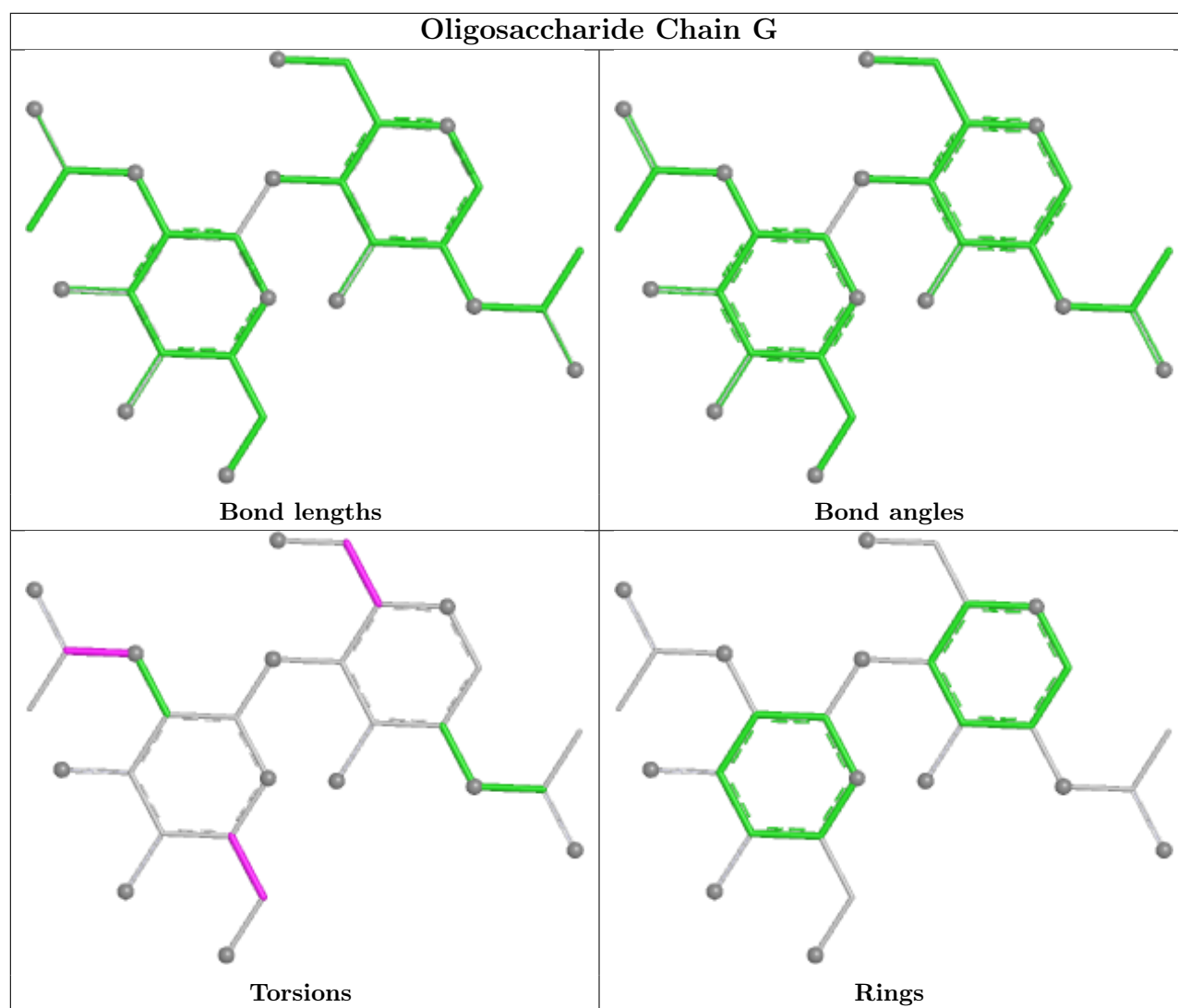
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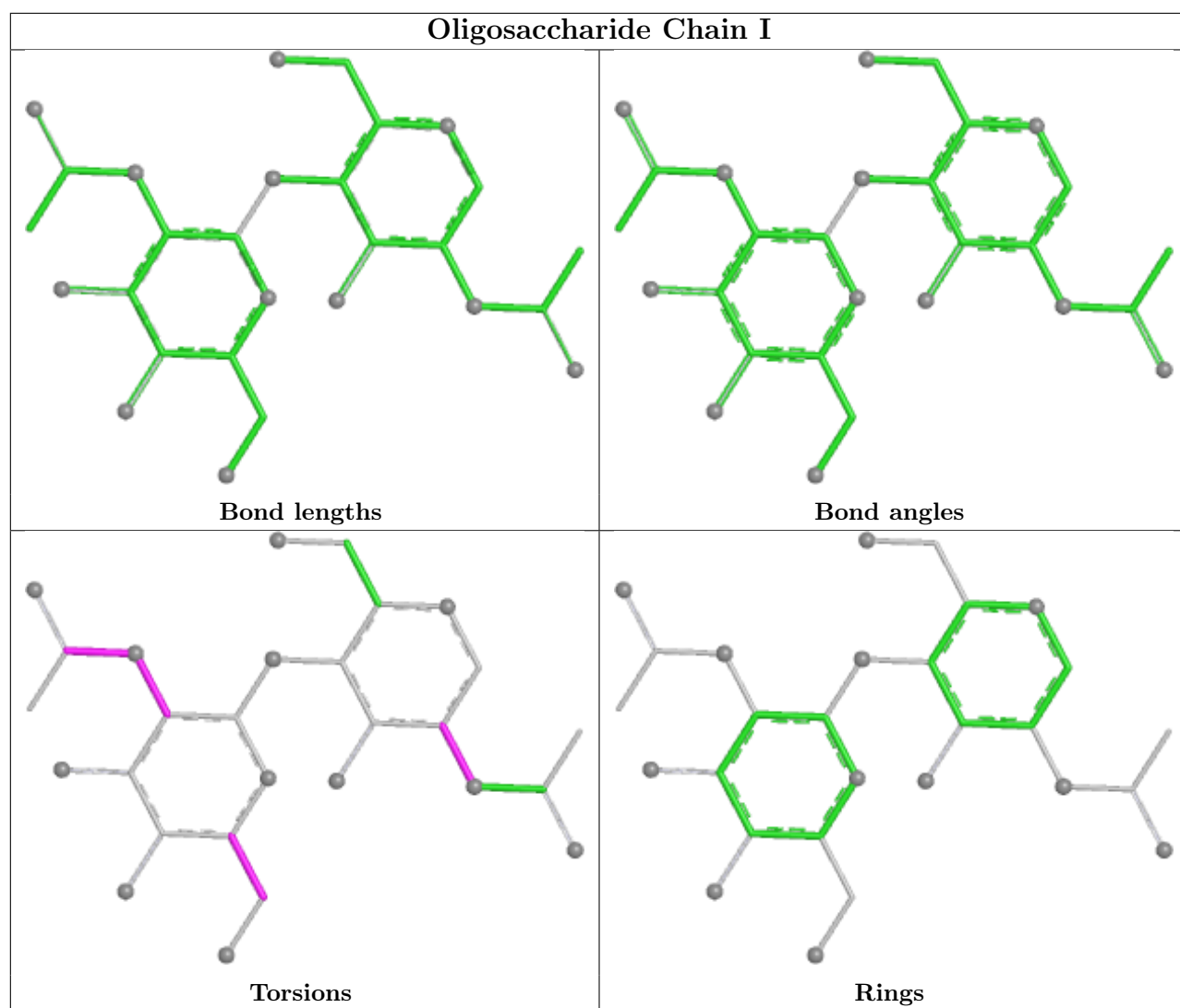
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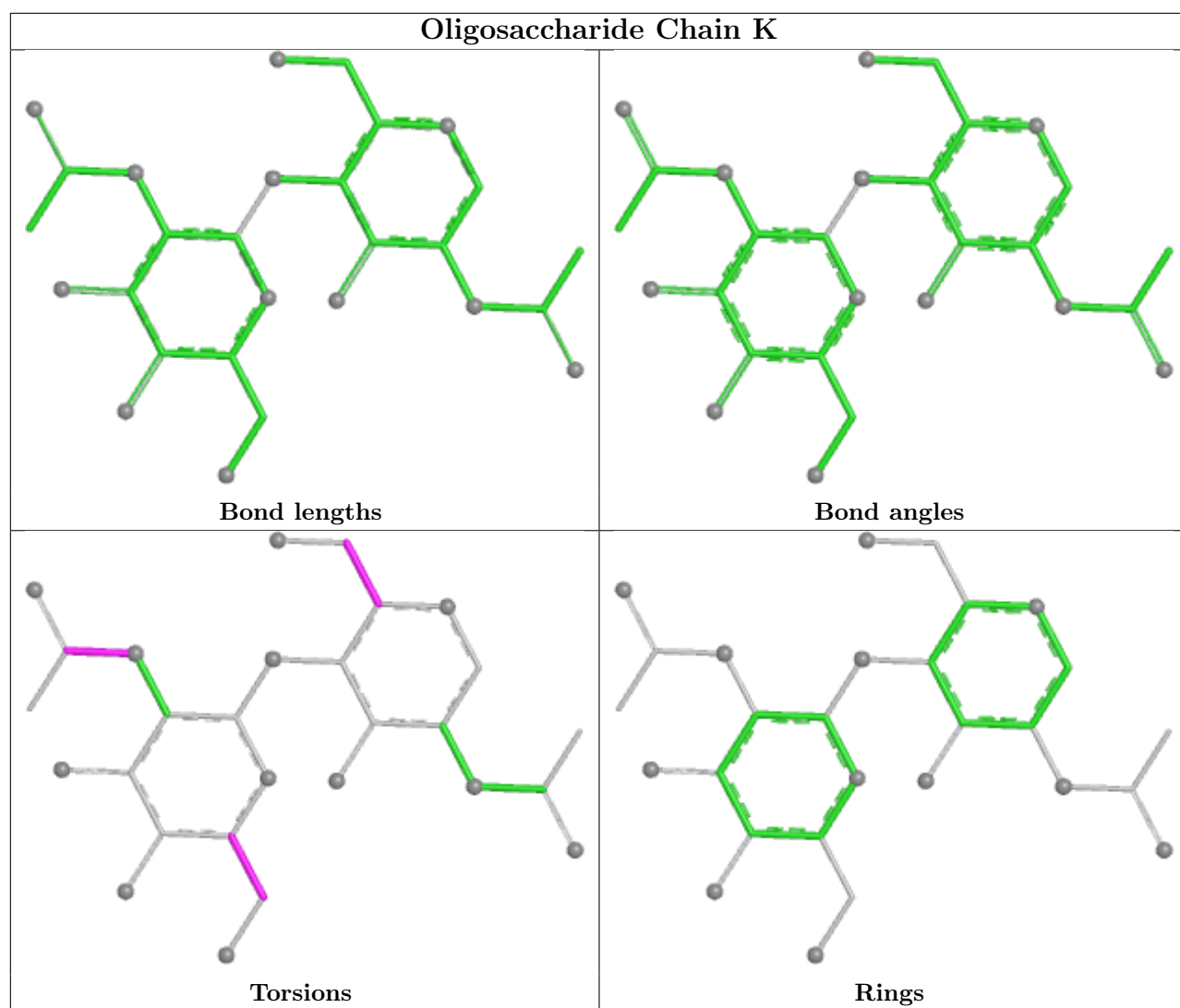
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	NAG	2	0
3	H	2	NAG	4	0
3	J	1	NAG	1	0

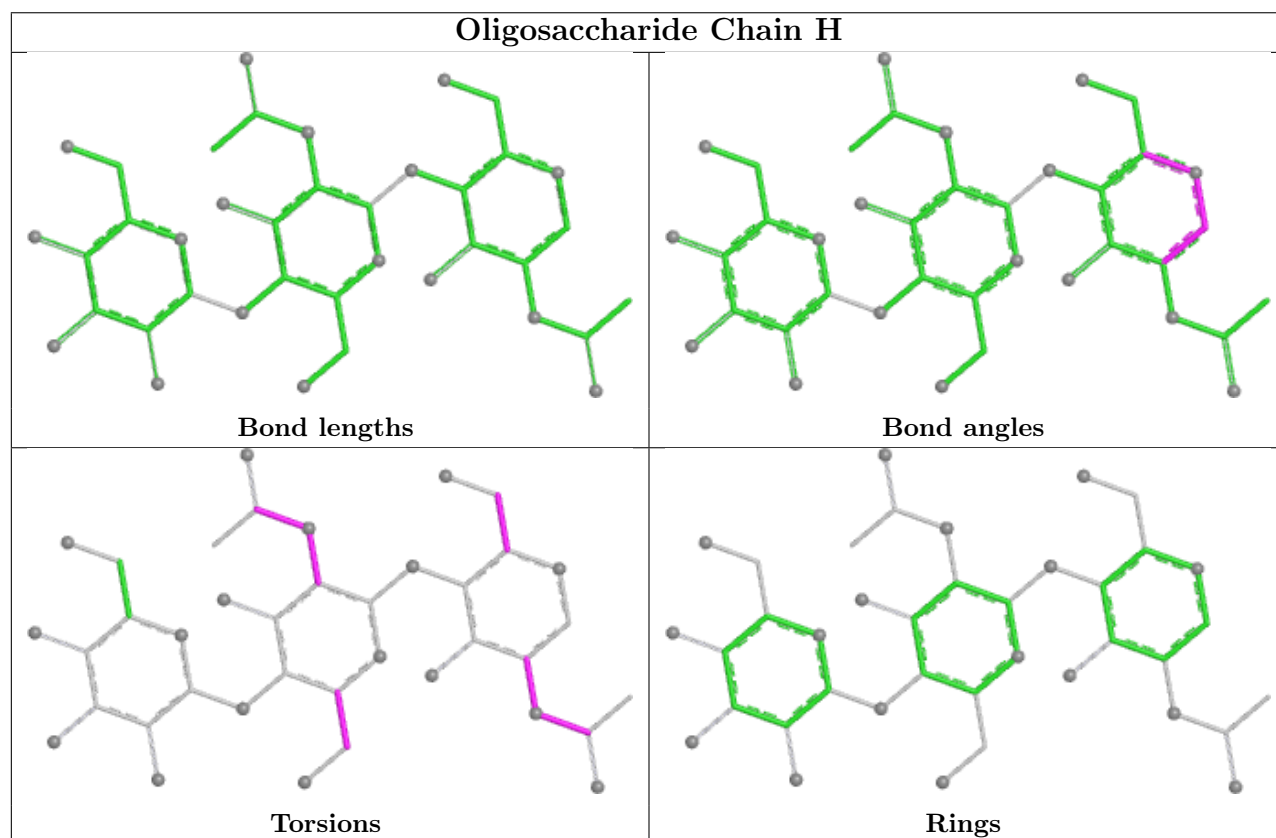
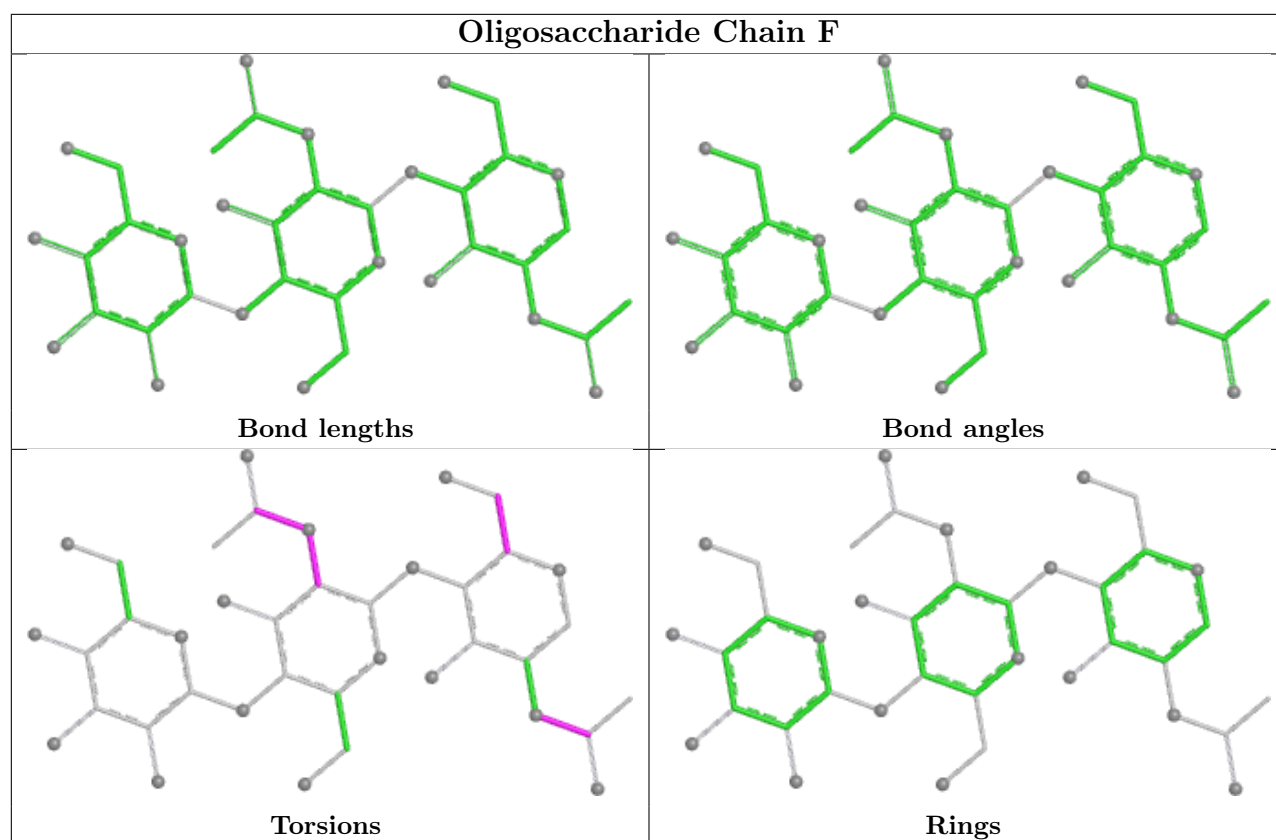
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

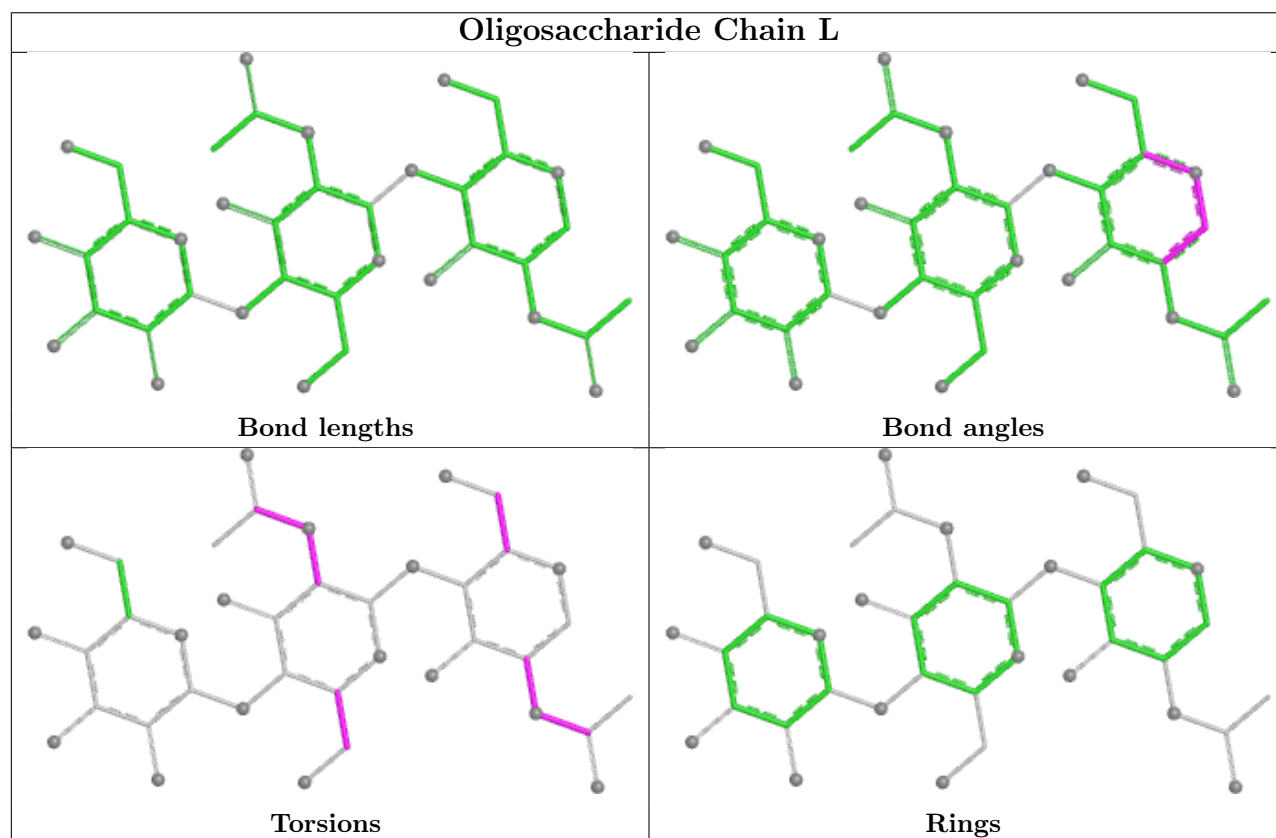
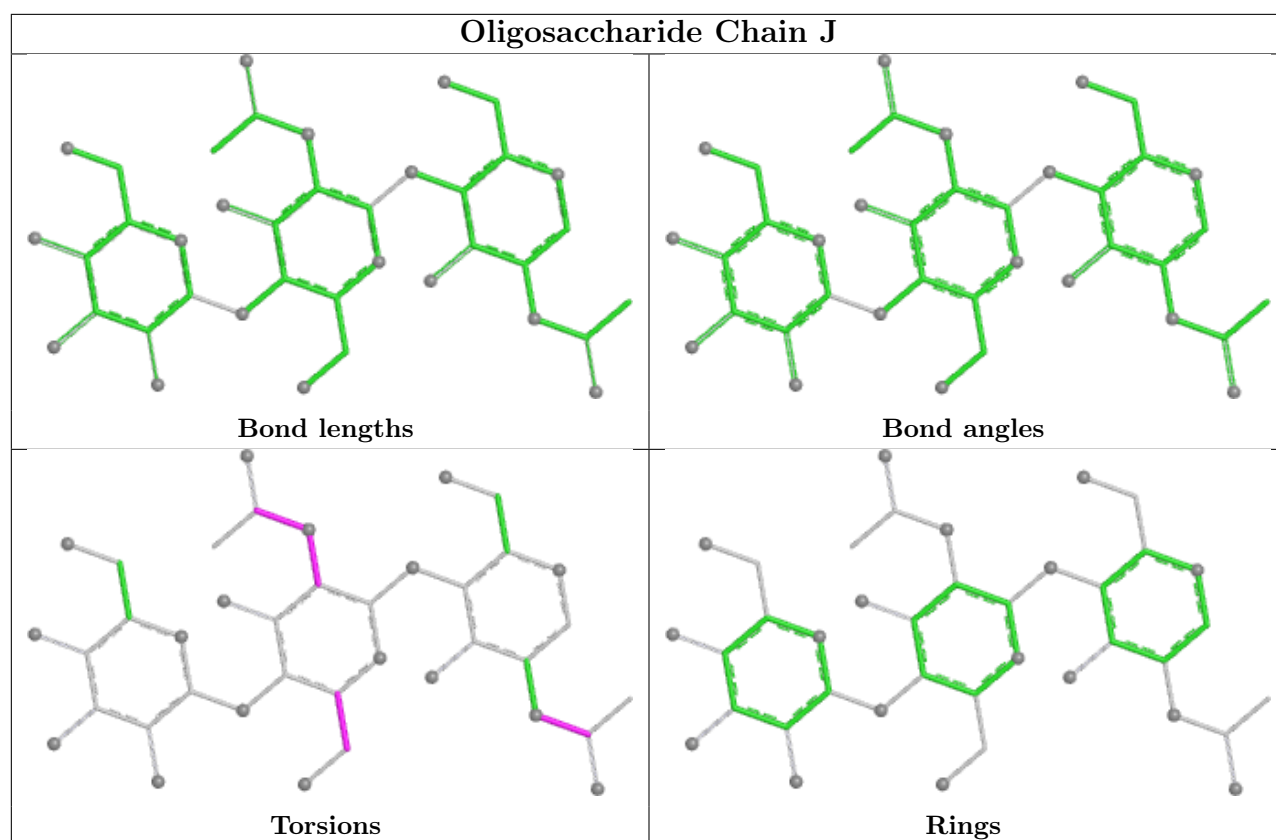












5.6 Ligand geometry

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	B	2005	1	14,14,15	0.30	0	17,19,21	0.55	0
4	NAG	A	2001	1	14,14,15	0.69	0	17,19,21	0.85	0
4	NAG	B	2001	1	14,14,15	0.30	0	17,19,21	0.48	0
4	NAG	C	2001	1	14,14,15	1.14	1 (7%)	17,19,21	1.82	5 (29%)
4	NAG	B	2002	1	14,14,15	0.31	0	17,19,21	0.56	0
4	NAG	D	2003	1	14,14,15	0.29	0	17,19,21	0.51	0
4	NAG	D	2004	1	14,14,15	0.50	0	17,19,21	1.41	3 (17%)
4	NAG	A	2005	1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	A	2003	1	14,14,15	0.28	0	17,19,21	0.59	0
4	NAG	C	2002	1	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	A	2004	1	14,14,15	0.28	0	17,19,21	0.65	0
4	NAG	D	2001	1	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	B	2004	1	14,14,15	0.30	0	17,19,21	0.61	0
4	NAG	C	2004	1	14,14,15	0.29	0	17,19,21	0.74	1 (5%)
4	NAG	D	2002	1	14,14,15	0.34	0	17,19,21	0.58	0
4	NAG	C	2003	1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	B	2003	1	14,14,15	0.30	0	17,19,21	0.52	0
4	NAG	A	2002	1	14,14,15	0.31	0	17,19,21	0.58	0
4	NAG	D	2005	1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	C	2005	1	14,14,15	0.29	0	17,19,21	0.65	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	B	2005	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	5/6/23/26	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	C	2001	1	-	4/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	1/6/23/26	0/1/1/1
4	NAG	D	2003	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	4/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	4/6/23/26	0/1/1/1
4	NAG	D	2001	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	D	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	3/6/23/26	0/1/1/1
4	NAG	D	2005	1	-	3/6/23/26	0/1/1/1
4	NAG	C	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	2.81	1.49	1.43

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	NAG	C1-O5-C5	3.84	117.34	112.19
4	D	2004	NAG	C1-O5-C5	3.59	116.99	112.19
4	C	2001	NAG	C4-C3-C2	3.41	116.02	111.02
4	C	2001	NAG	C3-C4-C5	-3.10	104.61	110.23
4	C	2001	NAG	O4-C4-C5	2.86	116.36	109.32

There are no chirality outliers.

5 of 58 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2003	NAG	C1-C2-N2-C7
4	A	2003	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	B	2001	NAG	C3-C2-N2-C7
4	B	2002	NAG	C3-C2-N2-C7
4	B	2003	NAG	C1-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 24 short contacts:

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

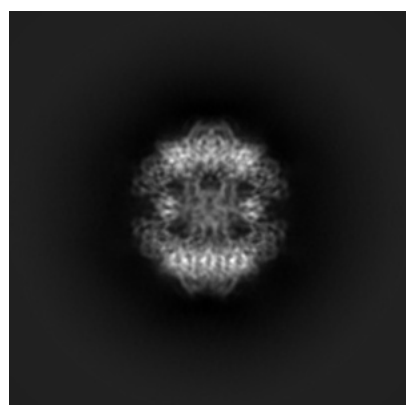
6 Map visualisation [i](#)

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.

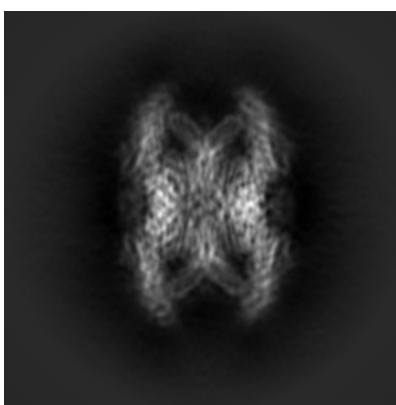
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

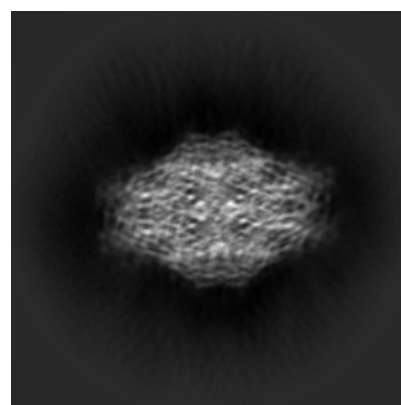
6.1.1 Primary map



X



Y

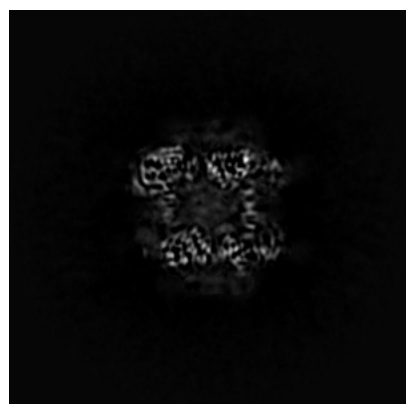


Z

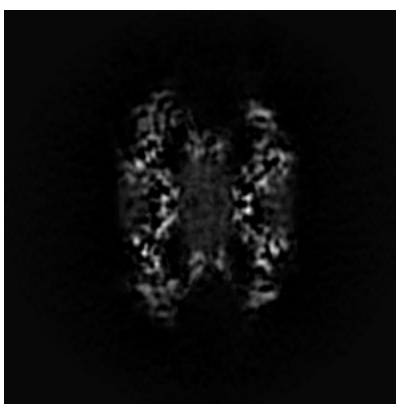
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

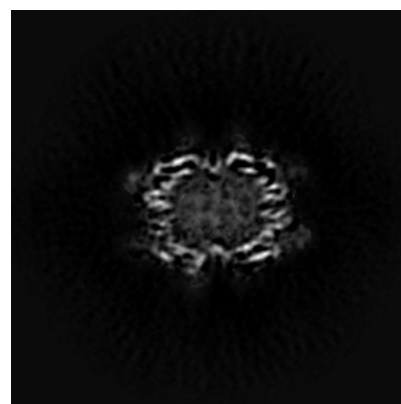
6.2.1 Primary map



X Index: 160



Y Index: 160

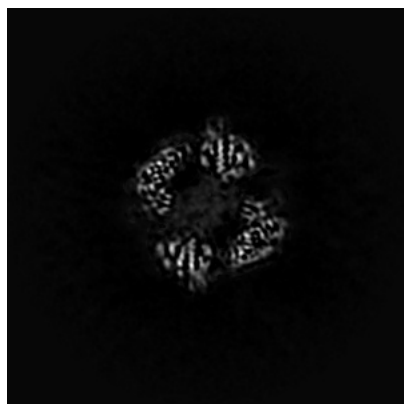


Z Index: 160

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

6.3 Largest variance slices [i](#)

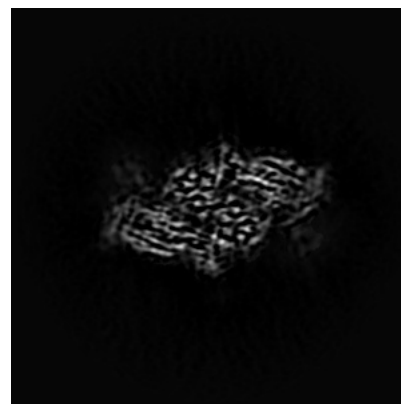
6.3.1 Primary map



X Index: 144



Y Index: 171

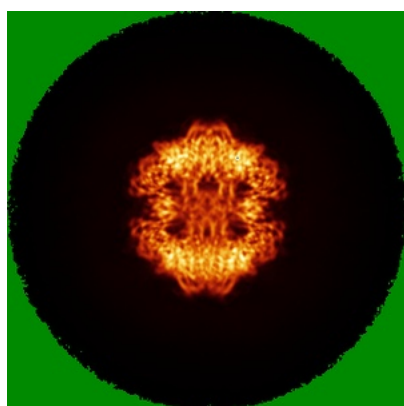


Z Index: 202

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

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

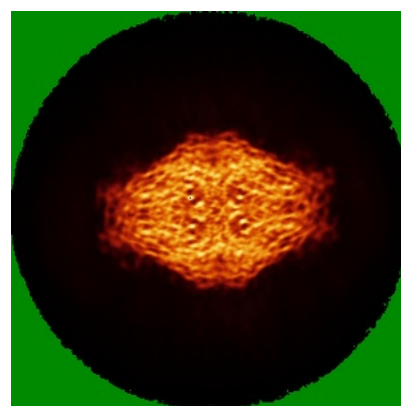
6.4.1 Primary map



X



Y

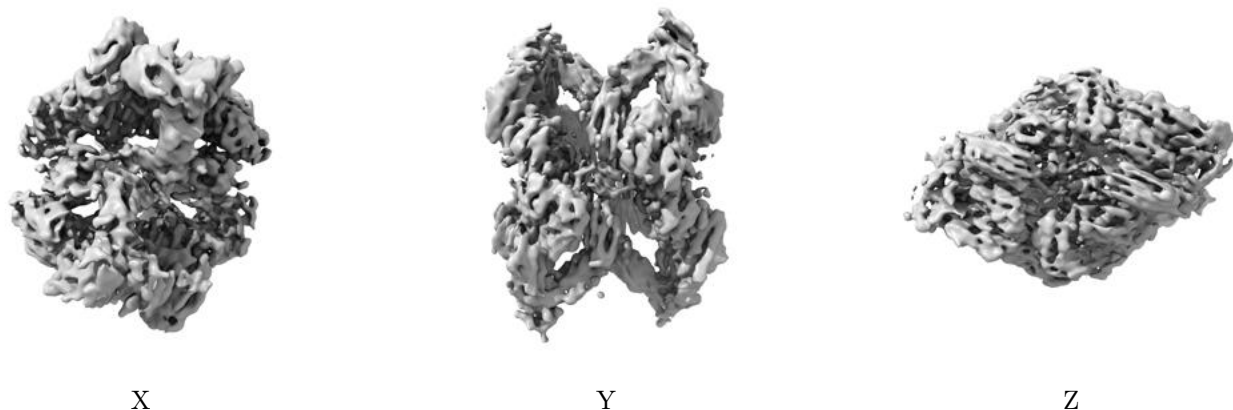


Z

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.

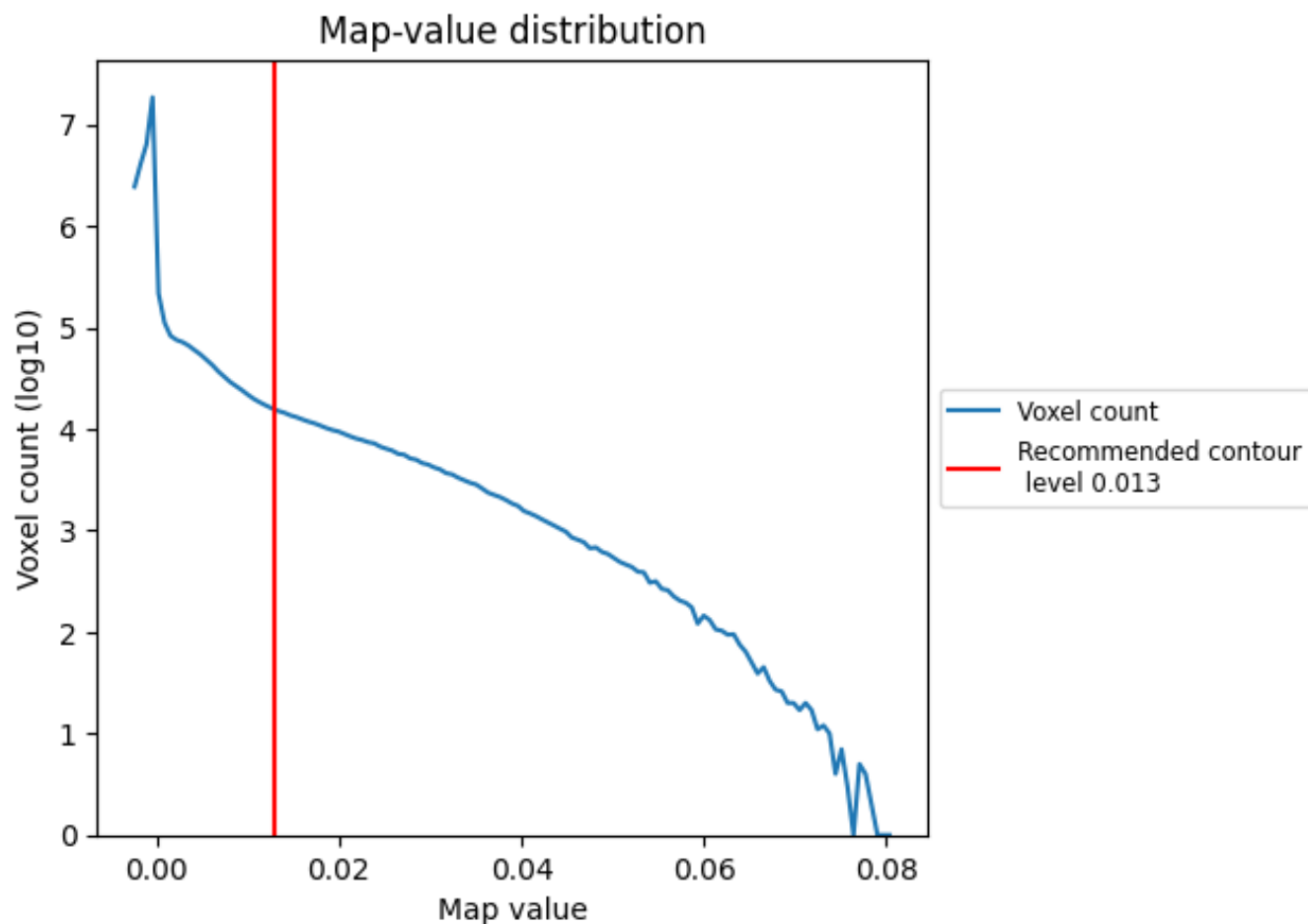
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

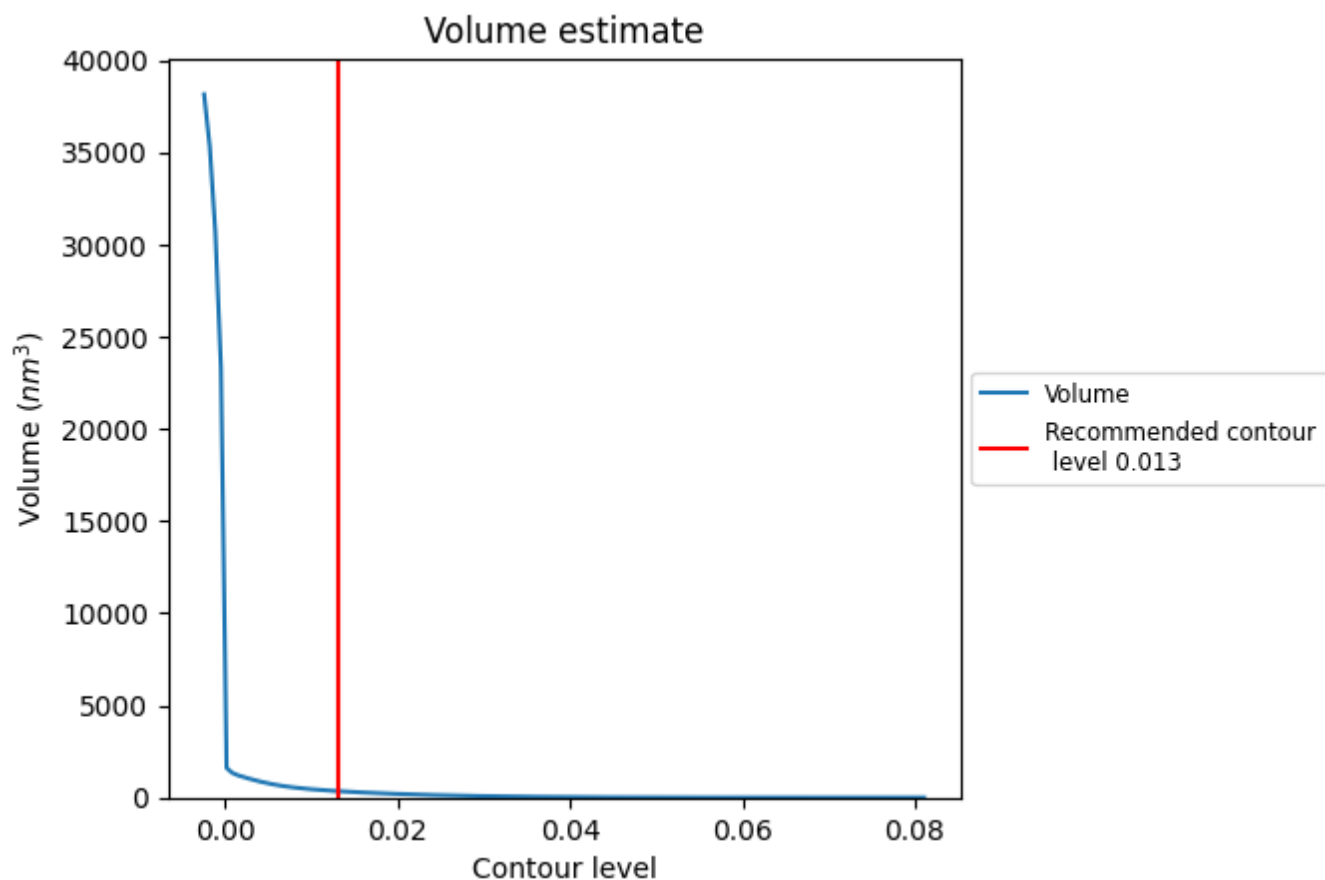
This section contains the results of statistical analysis of the map.

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.

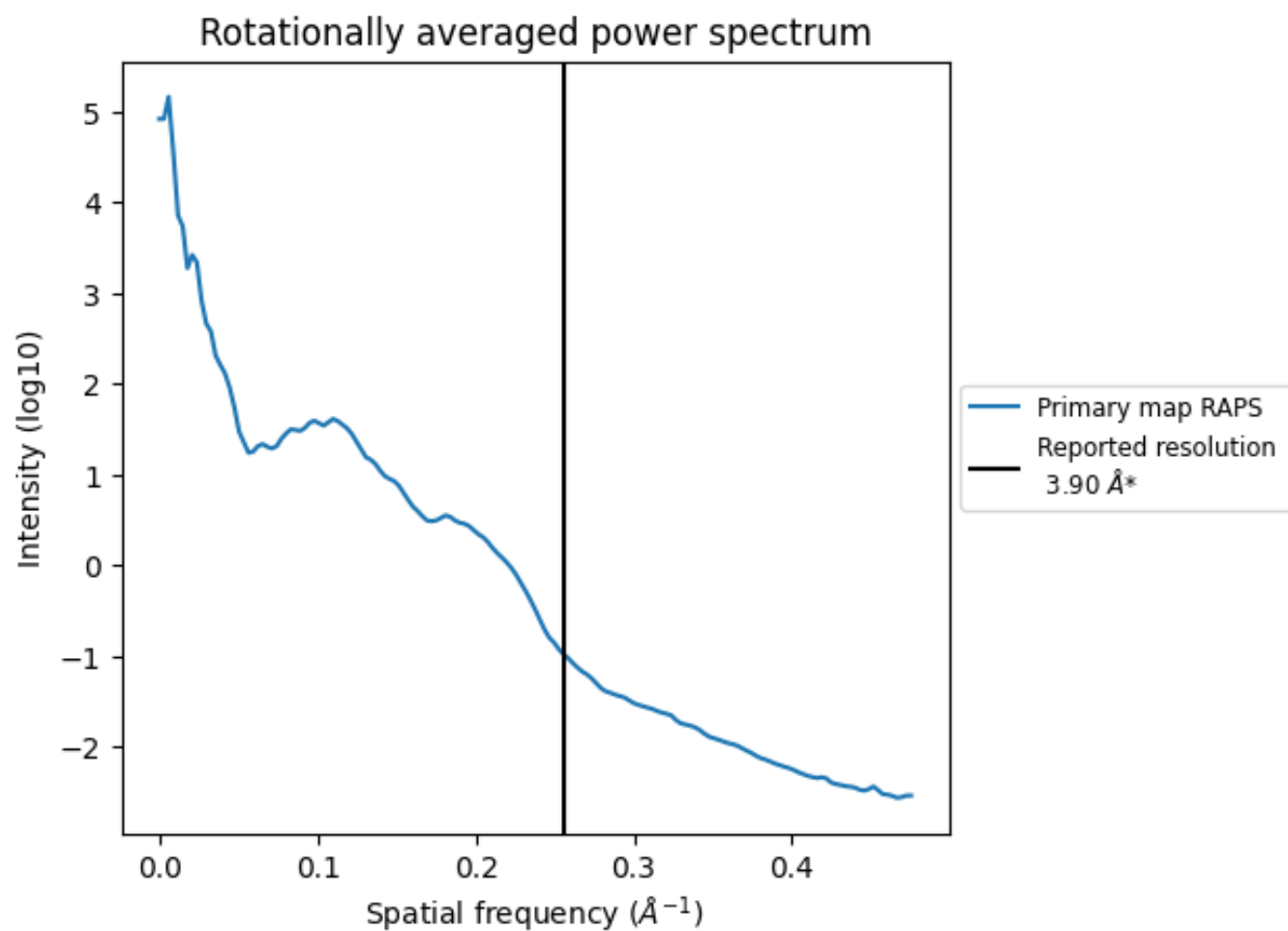
7.2 Volume estimate [i](#)



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}

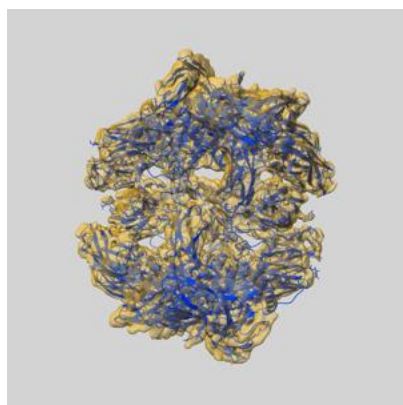
8 Fourier-Shell correlation

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

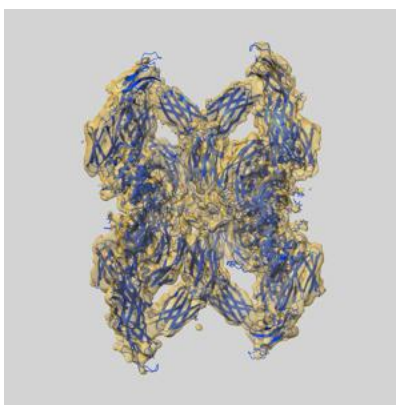
9 Map-model fit [i](#)

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](#).

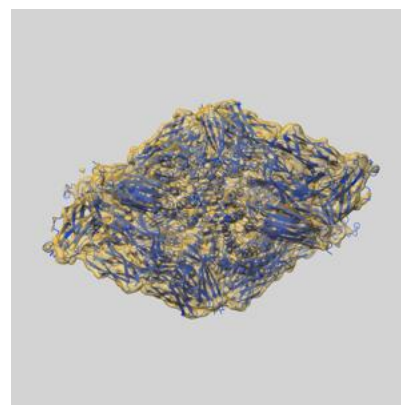
9.1 Map-model overlay [i](#)



X



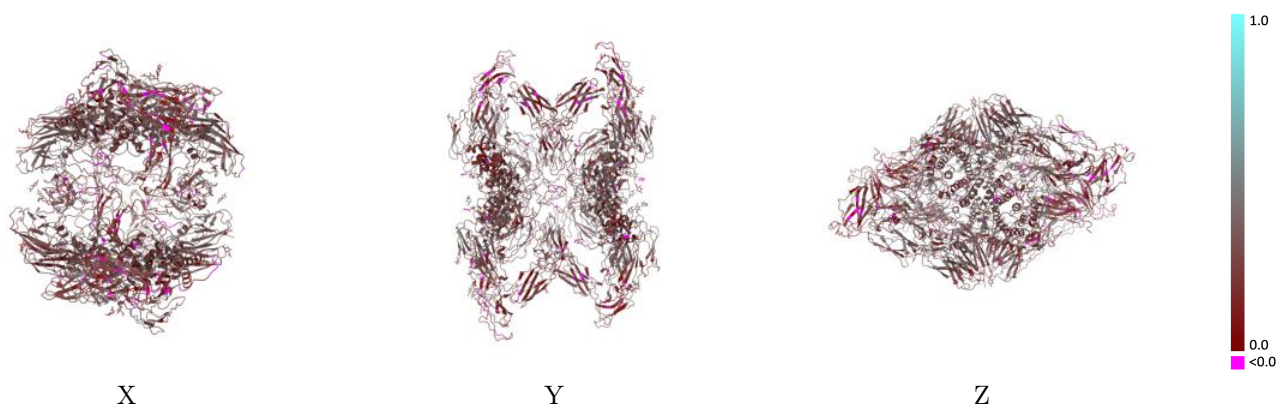
Y



Z

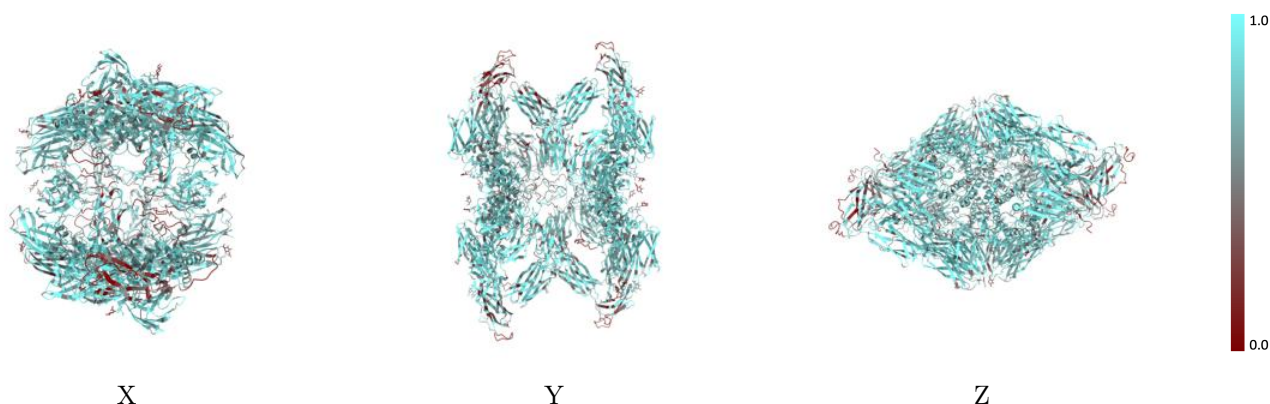
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



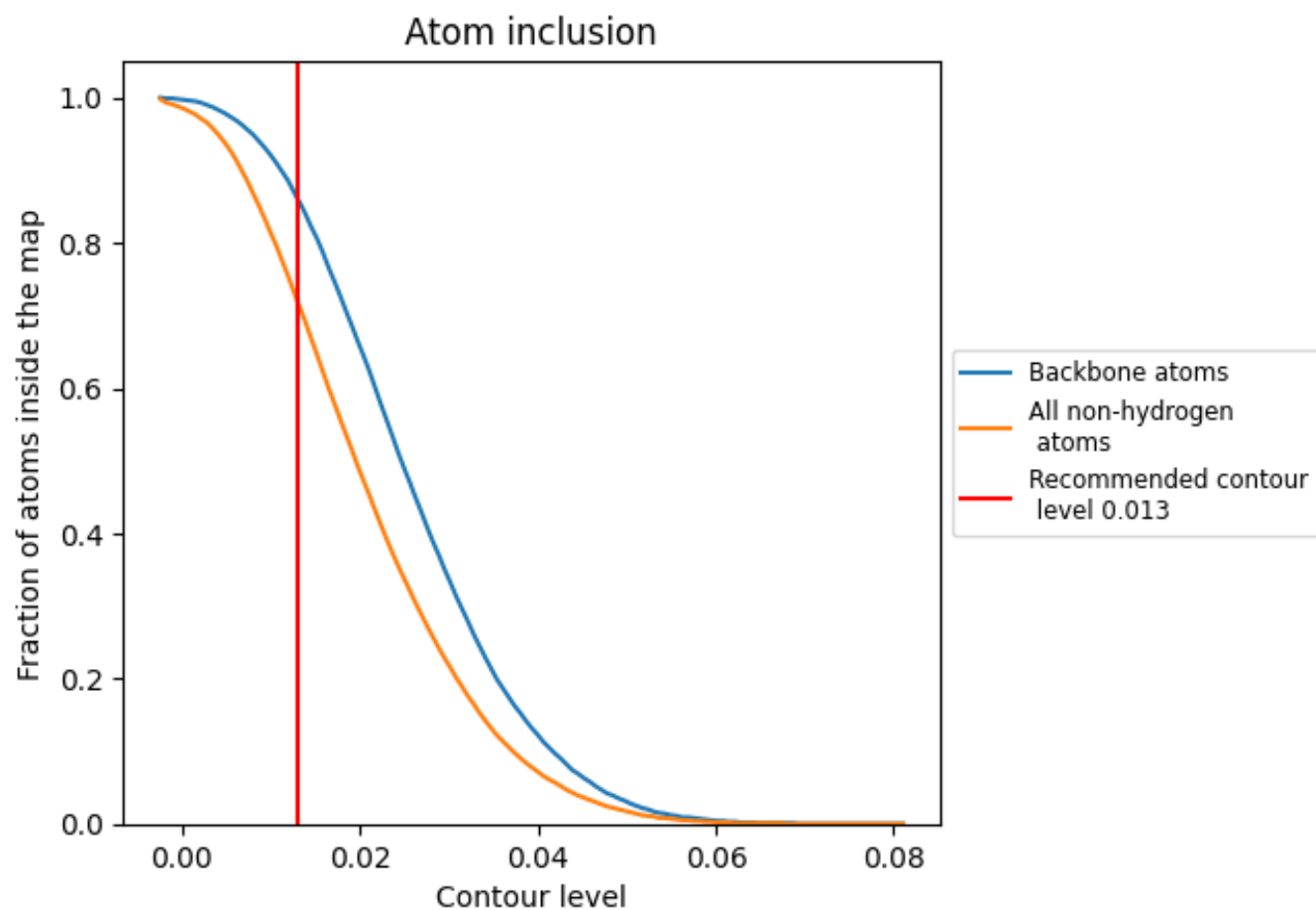
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0