



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:34 PM UTC

PDB ID : 8YT8 / pdb_00008yt8
EMDB ID : EMD-39568
Title : Cryo-EM structure of the dystrophin glycoprotein complex
Authors : Wu, J.P.; Yan, Z.; Wan, L.
Deposited on : 2024-03-25
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

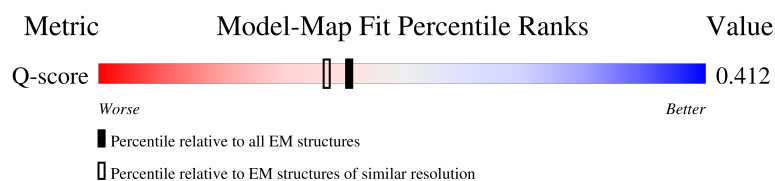
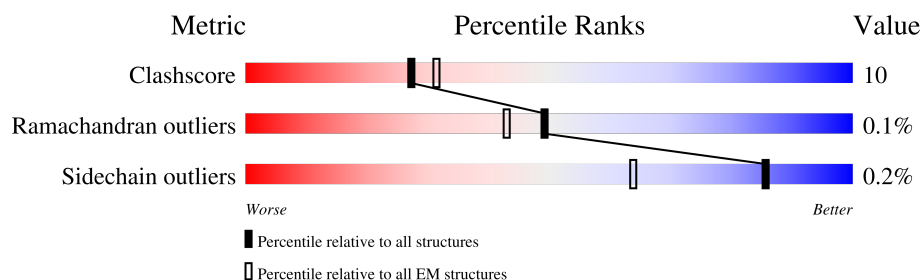
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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	13950 (3.00 - 4.00)

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	291	
2	B	263	
3	C	206	
4	D	263	

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Mol	Chain	Length	Quality of chain
5	E	331	 8% 62% 38%
6	G	265	 78% 22%
7	I	5	 80% 20%
8	O	289	 78% 22%
9	S	179	 74% 26%
10	F	3	 100%
10	K	3	 100%
10	L	3	 100%
10	M	3	 100%
10	N	3	 100%
11	H	3	 67% 33%
12	J	2	 100%
12	Q	2	 100%
13	P	3	 100%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16309 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-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	291	Total	C	N	O	S	0	0
			2296	1481	389	418	8		

- Molecule 2 is a protein called Beta-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	263	Total	C	N	O	S	0	0
			2009	1259	357	379	14		

- Molecule 3 is a protein called Dystrobrevin alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1078	649	215	213	1		

- Molecule 4 is a protein called Delta-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	263	Total	C	N	O	S	0	0
			2045	1303	354	376	12		

- Molecule 5 is a protein called Dystrophin.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	331	Total	C	N	O	S	0	0
			2686	1705	479	478	24		

- Molecule 6 is a protein called Gamma-sarcoglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	265	Total	C	N	O	S	0	0
			2031	1284	349	387	11		

- Molecule 7 is a protein called unknown segment.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	5	Total	C	N	O	S	0	0
			37	25	6	5	1		

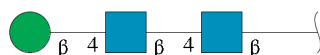
- Molecule 8 is a protein called Beta-dystroglycan.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	O	289	Total	C	N	O	S	0	0
			2247	1423	399	418	7		

- Molecule 9 is a protein called Sarcospan.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S	179	Total	C	N	O	S	0	0
			1390	921	217	233	19		

- Molecule 10 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
10	F	3	Total	C	N	O		0	0
			39	22	2	15			
10	K	3	Total	C	N	O		0	0
			39	22	2	15			
10	L	3	Total	C	N	O		0	0
			39	22	2	15			
10	M	3	Total	C	N	O		0	0
			39	22	2	15			
10	N	3	Total	C	N	O		0	0
			39	22	2	15			

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



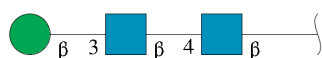
Mol	Chain	Residues	Atoms				AltConf	Trace
11	H	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 12 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



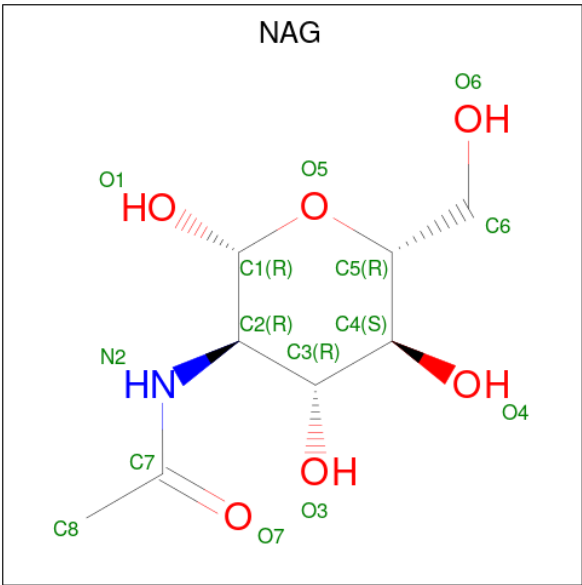
Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	2	Total	C	N	O	0	0
			28	16	2	10		
12	Q	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 13 is an oligosaccharide called beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



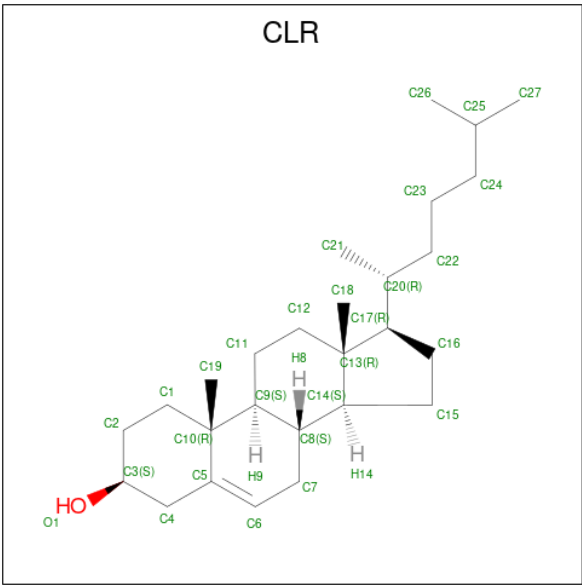
Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 15 is CHOLESTEROL (CCD ID: CLR) (formula: C₂₇H₄₆O).



Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total	C	O	0
			28	27	1	

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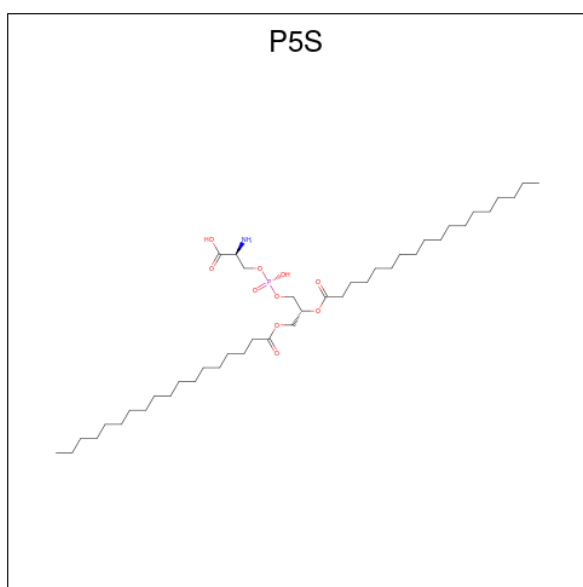
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Mol	Chain	Residues	Atoms			AltConf
15	D	1	Total	C	O	0
			28	27	1	
15	S	1	Total	C	O	0
			28	27	1	

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	E	1	Total	Zn	0
			1	1	

- Molecule 17 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (CCD ID: P5S) (formula: C₄₂H₈₂NO₁₀P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	G	1	Total	C	N	O	P	0
			33	21	1	10	1	

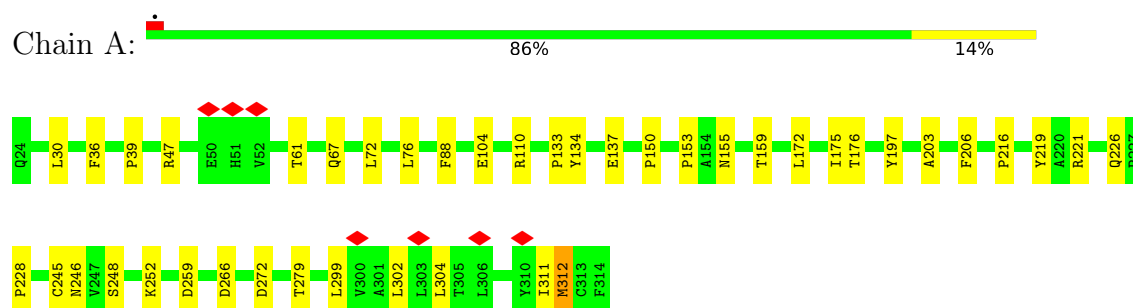
- Molecule 18 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
18	O	1	Total	Ca	0
			1	1	

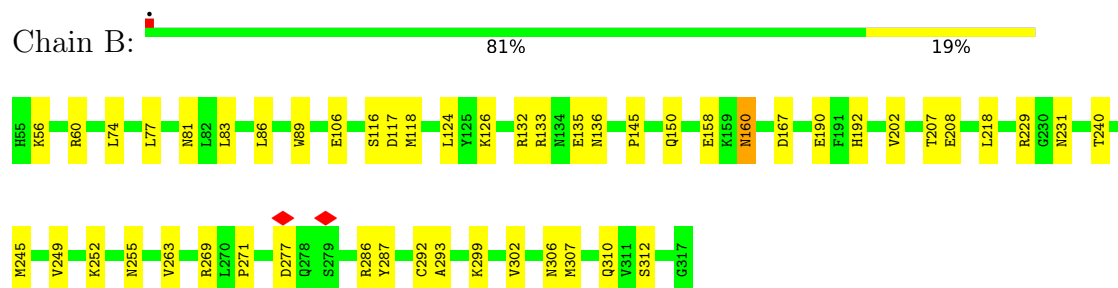
3 Residue-property plots

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.

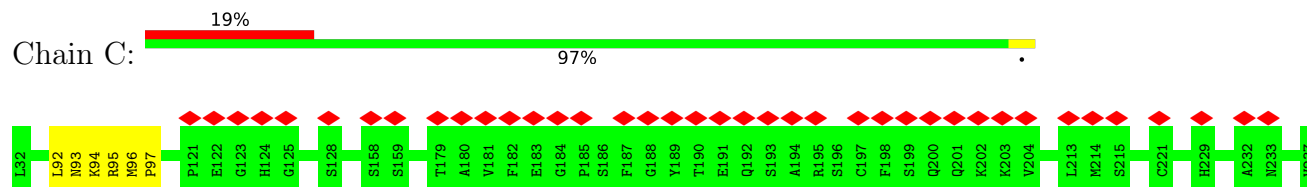
• Molecule 1: Alpha-sarcoglycan



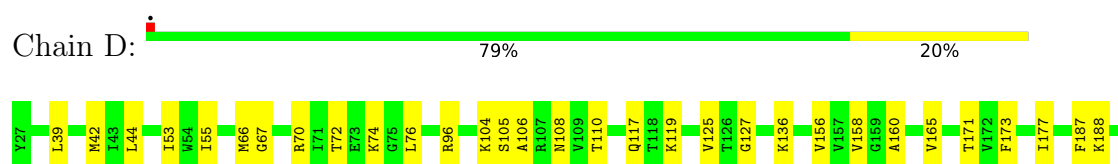
• Molecule 2: Beta-sarcoglycan

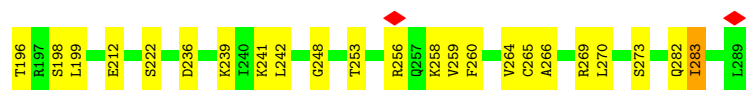


• Molecule 3: Dystrobrevin alpha

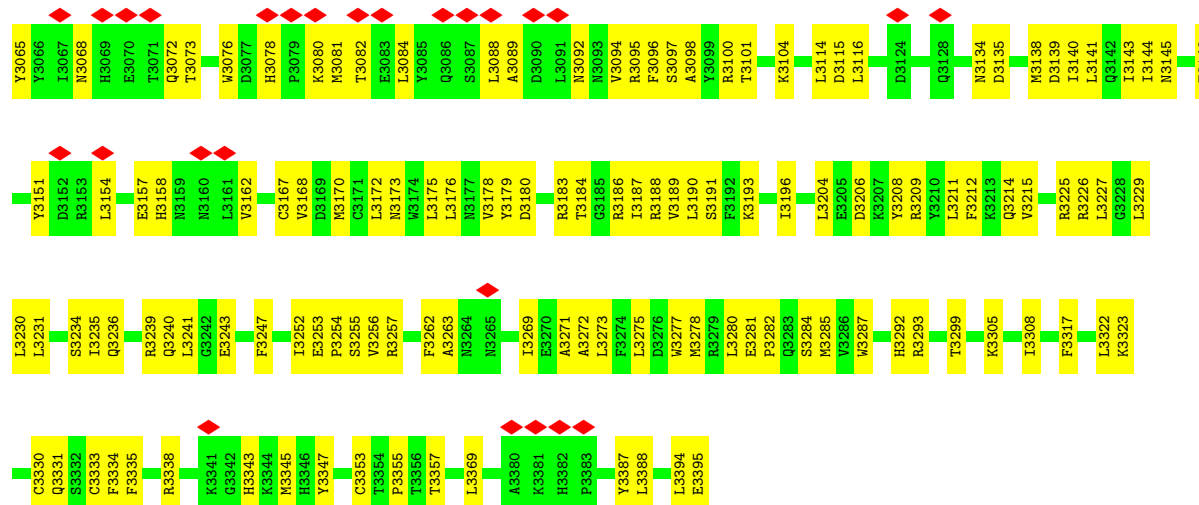


• Molecule 4: Delta-sarcoglycan

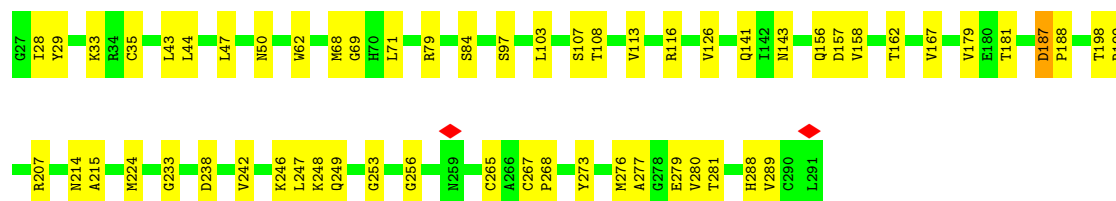
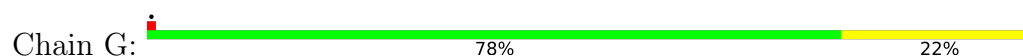




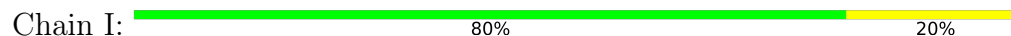
- Molecule 5: Dystrophin



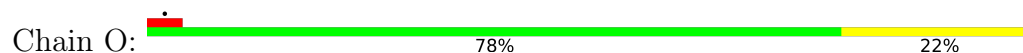
- Molecule 6: Gamma-sarcoglycan

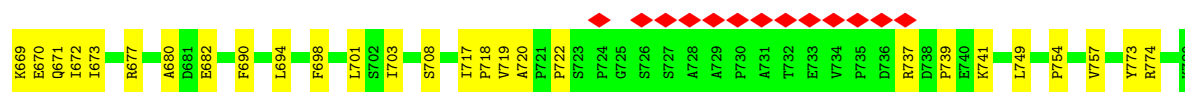


- Molecule 7: unknown segment



- Molecule 8: Beta-dystroglycan





- Molecule 9: Sarcospan



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 11: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 67% 33%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 12: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 100%



- Molecule 13: beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	499658	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.341	Depositor
Minimum map value	-1.909	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.28	Depositor
Map size ($\text{\AA}$)	469.584, 469.584, 469.584	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.087, 1.087, 1.087	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, CA, NAG, CLR, ZN, P5S

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	0.14	0/2366	0.34	1/3248 (0.0%)
2	B	0.14	0/2042	0.29	0/2758
3	C	0.07	0/1082	0.21	0/1503
4	D	0.15	0/2076	0.29	0/2799
5	E	0.14	0/2747	0.40	0/3713
6	G	0.16	0/2067	0.33	0/2799
7	I	0.14	0/37	0.37	0/48
8	O	0.12	0/2299	0.29	0/3119
9	S	0.14	0/1422	0.39	0/1934
All	All	0.14	0/16138	0.33	1/21921 (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	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	MET	N-CA-C	-8.11	105.37	114.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	311	ILE	Peptide

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	2296	0	2269	31	0
2	B	2009	0	2022	44	0
3	C	1078	0	556	5	0
4	D	2045	0	2129	44	0
5	E	2686	0	2678	107	0
6	G	2031	0	2039	53	0
7	I	37	0	44	1	0
8	O	2247	0	2257	48	0
9	S	1390	0	1434	32	0
10	F	39	0	34	0	0
10	K	39	0	34	0	0
10	L	39	0	34	0	0
10	M	39	0	34	0	0
10	N	39	0	34	0	0
11	H	39	0	34	2	0
12	J	28	0	25	0	0
12	Q	28	0	25	0	0
13	P	39	0	34	0	0
14	A	28	0	26	2	0
14	O	14	0	13	1	0
15	D	56	0	92	3	0
15	S	28	0	46	4	0
16	E	1	0	0	0	0
17	G	33	0	32	3	0
18	O	1	0	0	0	0
All	All	16309	0	15925	316	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 10.

All (316) 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)
9:S:77:MET:HE1	9:S:94:MET:HG2	1.49	0.94
6:G:35:CYS:SG	17:G:301:P5S:H21A	2.11	0.90
6:G:187:ASP:HB2	6:G:188:PRO:HD2	1.61	0.81
5:E:3104:LYS:HD3	5:E:3241:LEU:HD21	1.67	0.76
4:D:265:CYS:SG	4:D:266:ALA:N	2.57	0.76
6:G:141:GLN:NE2	6:G:143:ASN:OD1	2.19	0.76
5:E:3141:LEU:O	5:E:3145:ASN:ND2	2.21	0.74
1:A:304:LEU:HG	4:D:42:MET:HE1	1.69	0.73
4:D:42:MET:HB2	6:G:43:LEU:HD11	1.71	0.72
5:E:3081:MET:HB2	5:E:3170:MET:HE1	1.71	0.72
5:E:3092:ASN:OD1	5:E:3104:LYS:NZ	2.17	0.71
1:A:228:PRO:HB3	1:A:245:CYS:HB3	1.73	0.70
4:D:173:PHE:HB2	6:G:181:THR:HG22	1.72	0.70
2:B:145:PRO:HB3	2:B:158:GLU:HG3	1.71	0.70
9:S:77:MET:HE3	9:S:95:LYS:HD2	1.74	0.69
2:B:116:SER:HB3	2:B:118:MET:HE3	1.75	0.69
2:B:208:GLU:HG3	4:D:188:LYS:HD2	1.73	0.69
8:O:737:ARG:HG3	8:O:739:PRO:HD3	1.75	0.68
5:E:3282:PRO:HG2	5:E:3285:MET:HB2	1.76	0.68
6:G:157:ASP:OD1	6:G:158:VAL:N	2.27	0.68
5:E:3227:LEU:HD11	5:E:3256:VAL:HG13	1.77	0.67
1:A:72:LEU:HD22	1:A:76:LEU:HD23	1.76	0.67
6:G:35:CYS:SG	17:G:301:P5S:O18	2.53	0.66
7:I:213:LEU:O	8:O:773:TYR:OH	2.13	0.66
5:E:3098:ALA:HB3	5:E:3388:LEU:HG	1.77	0.65
5:E:3236:GLN:HA	5:E:3239:ARG:HE	1.58	0.65
5:E:3293:ARG:NH1	5:E:3353:CYS:SG	2.70	0.65
5:E:3208:TYR:CG	5:E:3278:MET:HE1	2.32	0.64
2:B:229:ARG:NH1	4:D:212:GLU:OE2	2.30	0.64
5:E:3285:MET:HE3	5:E:3285:MET:HA	1.80	0.64
4:D:53:ILE:HD12	15:D:302:CLR:H183	1.80	0.63
1:A:133:PRO:HD2	1:A:203:ALA:HA	1.79	0.63
5:E:3078:HIS:O	5:E:3082:THR:N	2.30	0.63
4:D:110:THR:HG23	4:D:125:VAL:HG22	1.81	0.62
2:B:263:VAL:HG21	4:D:242:LEU:HD23	1.81	0.62
1:A:272:ASP:OD2	6:G:116:ARG:NH2	2.32	0.62
9:S:27:LEU:HA	9:S:78:LEU:HD13	1.81	0.61
5:E:3178:VAL:HG12	5:E:3240:GLN:HG3	1.81	0.61
6:G:62:TRP:O	6:G:69:GLY:N	2.29	0.61
9:S:88:THR:HG22	9:S:91:GLN:HG2	1.81	0.61
6:G:187:ASP:HB2	6:G:188:PRO:CD	2.30	0.61
5:E:3333:CYS:SG	5:E:3338:ARG:NH1	2.71	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:135:CYS:HB2	9:S:154:VAL:HG21	1.81	0.61
6:G:279:GLU:HG2	6:G:280:VAL:HG13	1.83	0.60
8:O:609:ARG:HD2	8:O:701:LEU:HD11	1.82	0.60
2:B:292:CYS:SG	2:B:293:ALA:N	2.74	0.60
6:G:107:SER:OG	6:G:108:THR:N	2.34	0.60
5:E:3115:ASP:N	5:E:3115:ASP:OD1	2.33	0.60
5:E:3231:LEU:O	5:E:3235:ILE:HG12	2.02	0.59
5:E:3252:ILE:O	5:E:3255:SER:OG	2.20	0.59
2:B:269:ARG:NH1	6:G:238:ASP:OD1	2.32	0.59
5:E:3176:LEU:HD12	5:E:3180:ASP:HB3	1.85	0.59
2:B:74:LEU:HD11	6:G:44:LEU:HD12	1.85	0.59
5:E:3184:THR:HG23	5:E:3186:ARG:H	1.68	0.59
9:S:120:TYR:HB2	9:S:168:LEU:HD23	1.85	0.59
5:E:3135:ASP:HA	5:E:3188:ARG:HD2	1.84	0.58
5:E:3135:ASP:O	5:E:3188:ARG:NH1	2.36	0.58
2:B:150:GLN:NE2	6:G:108:THR:O	2.37	0.58
1:A:221:ARG:HH11	1:A:226:GLN:HB3	1.69	0.57
4:D:66:MET:HE1	6:G:68:MET:HE1	1.84	0.57
5:E:3272:ALA:HA	5:E:3275:LEU:HD12	1.86	0.57
6:G:248:LYS:NZ	6:G:249:GLN:O	2.37	0.57
2:B:245:MET:HE3	2:B:245:MET:HA	1.85	0.57
8:O:663:PRO:HD2	8:O:668:PRO:HG3	1.85	0.57
9:S:51:SER:OG	9:S:53:SER:OG	2.23	0.57
1:A:67:GLN:NE2	1:A:104:GLU:OE2	2.30	0.57
5:E:3068:ASN:O	5:E:3072:GLN:N	2.37	0.57
5:E:3154:LEU:O	5:E:3158:HIS:ND1	2.31	0.57
4:D:76:LEU:HD11	6:G:71:LEU:HD12	1.86	0.57
2:B:207:THR:OG1	2:B:208:GLU:N	2.37	0.57
9:S:91:GLN:O	9:S:95:LYS:HG2	2.06	0.56
9:S:60:PRO:HG2	9:S:171:GLN:HE22	1.70	0.56
8:O:671:GLN:H	8:O:671:GLN:CD	2.13	0.56
5:E:3104:LYS:NZ	5:E:3241:LEU:HD11	2.21	0.55
4:D:187:PHE:O	6:G:199:ARG:NH1	2.39	0.55
1:A:312:MET:HE3	1:A:312:MET:O	2.06	0.55
5:E:3104:LYS:HZ1	5:E:3241:LEU:HD11	1.72	0.55
8:O:530:ASP:HA	8:O:557:GLN:HE22	1.72	0.54
8:O:673:ILE:O	8:O:677:ARG:HG2	2.07	0.54
9:S:70:VAL:HG22	9:S:101:LEU:HG	1.89	0.54
1:A:266:ASP:OD1	1:A:266:ASP:N	2.41	0.54
5:E:3076:TRP:O	5:E:3173:ASN:ND2	2.40	0.54
5:E:3154:LEU:O	5:E:3158:HIS:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:HA	1:A:252:LYS:HB2	1.90	0.54
2:B:77:LEU:HD23	6:G:47:LEU:HD21	1.89	0.54
2:B:277:ASP:HB3	4:D:283:ILE:HG23	1.89	0.53
5:E:3254:PRO:HA	5:E:3257:ARG:HD2	1.89	0.53
5:E:3134:ASN:ND2	5:E:3214:GLN:OE1	2.41	0.53
9:S:102:SER:OG	9:S:186:CYS:SG	2.59	0.53
4:D:248:GLY:HA2	6:G:289:VAL:HG11	1.91	0.53
8:O:529:THR:HA	8:O:532:LEU:HD12	1.89	0.53
8:O:680:ALA:HB2	8:O:703:ILE:HD11	1.89	0.53
5:E:3206:ASP:OD1	5:E:3206:ASP:N	2.39	0.52
6:G:113:VAL:HB	6:G:126:VAL:HG22	1.91	0.52
8:O:717:ILE:HG12	8:O:719:VAL:HG22	1.90	0.52
2:B:135:GLU:HG3	2:B:136:ASN:H	1.74	0.52
5:E:3287:TRP:H	5:E:3287:TRP:CD1	2.28	0.52
5:E:3084:LEU:O	5:E:3088:LEU:HG	2.10	0.52
9:S:53:SER:HA	9:S:152:ARG:HH11	1.75	0.51
9:S:92:PHE:HE1	15:S:301:CLR:H152	1.74	0.51
4:D:177:ILE:HD11	6:G:179:VAL:HG11	1.92	0.51
5:E:3151:TYR:CE2	5:E:3167:CYS:HB3	2.46	0.51
5:E:3157:GLU:HB2	5:E:3158:HIS:CE1	2.46	0.51
5:E:3226:ARG:O	5:E:3230:LEU:HG	2.11	0.51
8:O:610:LEU:HB2	8:O:653:ILE:HB	1.93	0.51
1:A:137:GLU:HB3	1:A:248:SER:HB2	1.92	0.51
4:D:253:THR:O	4:D:256:ARG:NH2	2.44	0.51
5:E:3080:LYS:O	5:E:3084:LEU:HG	2.10	0.51
5:E:3116:LEU:HD23	5:E:3116:LEU:H	1.76	0.50
8:O:670:GLU:HG2	8:O:671:GLN:N	2.25	0.50
4:D:158:VAL:HG12	4:D:160:ALA:H	1.75	0.50
9:S:96:VAL:HG23	15:S:301:CLR:H182	1.93	0.50
5:E:3100:ARG:NH2	5:E:3243:GLU:OE2	2.40	0.50
2:B:56:LYS:O	2:B:60:ARG:NH1	2.45	0.50
2:B:190:GLU:OE2	2:B:192:HIS:NE2	2.45	0.50
8:O:741:LYS:HB2	9:S:145:LEU:HD12	1.93	0.50
2:B:124:LEU:HD23	4:D:96:ARG:HG3	1.92	0.49
8:O:549:TRP:CD1	8:O:549:TRP:H	2.29	0.49
2:B:312:SER:HB3	6:G:253:GLY:HA3	1.93	0.49
5:E:3076:TRP:HZ2	5:E:3183:ARG:HG2	1.77	0.49
5:E:3269:ILE:HG23	5:E:3273:LEU:HD22	1.93	0.49
5:E:3204:LEU:HD21	5:E:3292:HIS:CD2	2.47	0.49
4:D:117:GLN:HE22	4:D:119:LYS:HB3	1.76	0.49
15:D:301:CLR:H3	15:D:302:CLR:H12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3193:LYS:HA	5:E:3196:ILE:HG22	1.95	0.49
1:A:246:ASN:HD21	11:H:1:NAG:C7	2.26	0.49
1:A:246:ASN:HB2	11:H:1:NAG:O5	2.13	0.49
9:S:139:LEU:HD13	9:S:140:PRO:HD2	1.95	0.49
2:B:167:ASP:OD1	2:B:167:ASP:N	2.34	0.49
5:E:3095:ARG:NH2	5:E:3334:PHE:O	2.46	0.49
5:E:3189:VAL:O	5:E:3193:LYS:HG2	2.13	0.49
2:B:132:ARG:NH1	2:B:135:GLU:OE2	2.46	0.48
5:E:3144:ILE:O	5:E:3148:THR:OG1	2.29	0.48
2:B:271:PRO:HG3	4:D:269:ARG:HH21	1.78	0.48
3:C:94:LYS:O	5:E:3092:ASN:ND2	2.42	0.48
8:O:598:GLN:NE2	8:O:660:ASN:OD1	2.46	0.48
8:O:720:ALA:O	8:O:722:PRO:HD3	2.13	0.48
1:A:176:THR:HG23	1:A:197:TYR:HB2	1.96	0.48
9:S:60:PRO:HG2	9:S:171:GLN:NE2	2.28	0.48
2:B:255:ASN:HB2	6:G:224:MET:O	2.14	0.48
8:O:504:VAL:HB	8:O:591:ILE:HG12	1.96	0.48
3:C:92:LEU:HA	3:C:95:ARG:HE	1.80	0.47
4:D:165:VAL:HG11	4:D:171:THR:HG21	1.96	0.47
4:D:222:SER:O	6:G:233:GLY:HA3	2.14	0.47
5:E:3241:LEU:HD12	5:E:3241:LEU:O	2.14	0.47
5:E:3333:CYS:SG	5:E:3338:ARG:HD2	2.54	0.47
8:O:526:ASP:N	8:O:526:ASP:OD1	2.47	0.47
8:O:668:PRO:HB2	8:O:671:GLN:OE1	2.14	0.47
4:D:239:LYS:HD2	4:D:241:LYS:HE2	1.95	0.47
5:E:3094:VAL:O	5:E:3100:ARG:NH1	2.48	0.47
4:D:105:SER:OG	4:D:106:ALA:N	2.48	0.47
9:S:106:LEU:HB2	9:S:182:CYS:HB3	1.96	0.47
4:D:260:PHE:HA	4:D:273:SER:O	2.15	0.47
5:E:3148:THR:HA	5:E:3168:VAL:HG11	1.96	0.47
1:A:216:PRO:HA	1:A:219:TYR:HD2	1.80	0.47
2:B:252:LYS:HG2	4:D:236:ASP:HB2	1.96	0.47
5:E:3116:LEU:HD12	5:E:3158:HIS:CD2	2.50	0.47
6:G:198:THR:OG1	8:O:502:ASP:OD1	2.33	0.47
8:O:668:PRO:HB2	8:O:671:GLN:CD	2.38	0.47
2:B:81:ASN:ND2	6:G:50:ASN:OD1	2.32	0.47
5:E:3271:ALA:O	5:E:3275:LEU:HG	2.15	0.47
9:S:74:GLY:HA2	9:S:98:TYR:HE2	1.78	0.47
1:A:172:LEU:HD13	1:A:175:ILE:HD11	1.97	0.47
9:S:31:LEU:O	9:S:34:LEU:HG	2.15	0.47
9:S:54:LEU:HD12	9:S:55:LEU:O	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3138:MET:HE2	5:E:3138:MET:HA	1.96	0.46
9:S:47:MET:HE1	9:S:167:PHE:HB3	1.97	0.46
2:B:106:GLU:CD	2:B:106:GLU:H	2.23	0.46
5:E:3206:ASP:O	5:E:3209:ARG:HG3	2.14	0.46
5:E:3208:TYR:CD2	5:E:3278:MET:HE1	2.51	0.46
6:G:35:CYS:HB3	17:G:301:P5S:H43	1.96	0.46
5:E:3247:PHE:HB3	5:E:3284:SER:HA	1.98	0.46
6:G:156:GLN:NE2	6:G:157:ASP:HB3	2.30	0.46
9:S:193:ARG:HG2	15:S:301:CLR:H161	1.97	0.46
1:A:134:TYR:HB3	1:A:206:PHE:CE1	2.50	0.46
5:E:3212:PHE:CE2	5:E:3271:ALA:HB2	2.50	0.46
1:A:279:THR:HB	14:A:401:NAG:C7	2.46	0.46
3:C:96:MET:HE3	3:C:97:PRO:O	2.16	0.46
8:O:602:ALA:O	8:O:708:SER:OG	2.28	0.46
9:S:72:TYR:O	9:S:75:LEU:HG	2.15	0.46
2:B:287:TYR:HB3	2:B:299:LYS:HB2	1.98	0.46
5:E:3088:LEU:HD22	5:E:3104:LYS:HG2	1.97	0.46
5:E:3179:TYR:HB3	5:E:3187:ILE:HG12	1.98	0.46
5:E:3253:GLU:CD	5:E:3253:GLU:H	2.22	0.46
8:O:694:LEU:HD21	8:O:698:PHE:HB2	1.98	0.46
6:G:97:SER:HB2	6:G:103:LEU:HB2	1.97	0.46
2:B:245:MET:HG3	2:B:249:VAL:HG22	1.98	0.46
5:E:3305:LYS:HD2	6:G:29:TYR:HE2	1.81	0.46
2:B:306:ASN:HA	6:G:281:THR:HG23	1.99	0.45
2:B:287:TYR:HB2	4:D:264:VAL:HG13	1.99	0.45
5:E:3225:ARG:O	5:E:3229:LEU:HG	2.17	0.45
8:O:682:GLU:HB2	8:O:718:PRO:HB2	1.97	0.45
2:B:89:TRP:CD1	4:D:55:ILE:HD11	2.52	0.45
5:E:3088:LEU:HB3	5:E:3104:LYS:HE2	1.99	0.45
4:D:259:VAL:HG12	6:G:267:CYS:HB2	1.99	0.45
1:A:39:PRO:HB3	1:A:88:PHE:CE1	2.52	0.45
5:E:3263:ALA:HB2	5:E:3273:LEU:HD21	1.99	0.45
1:A:302:LEU:HA	1:A:302:LEU:HD23	1.79	0.45
8:O:598:GLN:HE22	8:O:660:ASN:HA	1.82	0.45
2:B:86:LEU:HD23	2:B:86:LEU:HA	1.81	0.44
5:E:3355:PRO:HB2	9:S:197:PHE:HE2	1.81	0.44
5:E:3097:SER:O	5:E:3101:THR:HG23	2.18	0.44
9:S:47:MET:HE2	9:S:167:PHE:HD2	1.81	0.44
2:B:231:ASN:ND2	8:O:572:GLU:OE1	2.41	0.44
4:D:72:THR:HG21	4:D:74:LYS:HZ2	1.83	0.44
5:E:3097:SER:HA	5:E:3100:ARG:HH21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3322:LEU:HD23	5:E:3322:LEU:HA	1.83	0.44
8:O:539:ARG:NH1	8:O:572:GLU:OE2	2.50	0.44
5:E:3208:TYR:O	5:E:3211:LEU:HD12	2.18	0.44
4:D:196:THR:HG22	4:D:196:THR:O	2.18	0.44
5:E:3114:LEU:HD11	5:E:3196:ILE:HD11	1.98	0.44
2:B:302:VAL:HG12	2:B:307:MET:SD	2.57	0.44
6:G:198:THR:OG1	6:G:198:THR:O	2.33	0.44
1:A:279:THR:HB	14:A:401:NAG:N2	2.32	0.44
6:G:28:ILE:HG22	6:G:33:LYS:HB2	2.00	0.44
5:E:3175:LEU:HA	5:E:3178:VAL:HG22	2.00	0.43
5:E:3065:TYR:HB3	5:E:3076:TRP:CD1	2.53	0.43
5:E:3262:PHE:CD1	5:E:3262:PHE:C	2.94	0.43
8:O:549:TRP:CE3	8:O:550:VAL:HG23	2.53	0.43
8:O:690:PHE:HE2	8:O:703:ILE:HG21	1.82	0.43
5:E:3144:ILE:HG22	5:E:3172:LEU:HD22	1.99	0.43
5:E:3317:PHE:HB2	5:E:3331:GLN:HB3	2.00	0.43
8:O:717:ILE:O	8:O:719:VAL:N	2.45	0.43
2:B:135:GLU:HG3	2:B:136:ASN:N	2.34	0.43
2:B:312:SER:HA	6:G:256:GLY:HA3	2.00	0.43
1:A:30:LEU:HD21	1:A:36:PHE:CD2	2.53	0.43
2:B:218:LEU:HD23	4:D:199:LEU:HD12	2.00	0.43
8:O:511:TYR:HD1	8:O:625:ILE:HD12	1.83	0.43
5:E:3096:PHE:HE2	5:E:3387:TYR:HB3	1.82	0.43
1:A:150:PRO:O	1:A:153:PRO:HD2	2.18	0.43
4:D:177:ILE:HG13	6:G:181:THR:HG21	2.01	0.43
3:C:93:ASN:HA	3:C:96:MET:HB3	2.00	0.43
8:O:562:LEU:HB2	8:O:625:ILE:HD11	2.01	0.43
4:D:104:LYS:HD3	6:G:116:ARG:HH22	1.84	0.43
5:E:3323:LYS:HE3	5:E:3343:HIS:NE2	2.34	0.43
2:B:133:ARG:HA	2:B:133:ARG:HD3	1.88	0.42
4:D:260:PHE:HE2	6:G:268:PRO:HA	1.83	0.42
5:E:3068:ASN:ND2	5:E:3073:THR:OG1	2.30	0.42
5:E:3098:ALA:HB3	5:E:3388:LEU:CG	2.48	0.42
5:E:3305:LYS:HE3	5:E:3305:LYS:HB2	1.78	0.42
9:S:46:LEU:O	9:S:50:ILE:HG12	2.19	0.42
2:B:83:LEU:HD23	2:B:83:LEU:HA	1.89	0.42
3:C:97:PRO:HA	5:E:3089:ALA:O	2.19	0.42
1:A:61:THR:HG21	1:A:110:ARG:HE	1.84	0.42
5:E:3154:LEU:C	5:E:3158:HIS:HD1	2.25	0.42
5:E:3175:LEU:HA	5:E:3175:LEU:HD23	1.81	0.42
5:E:3235:ILE:O	5:E:3239:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:580:LYS:HE3	8:O:580:LYS:HB3	1.82	0.42
2:B:286:ARG:HD3	4:D:282:GLN:HE22	1.84	0.42
5:E:3215:VAL:CG2	5:E:3230:LEU:HD21	2.49	0.42
8:O:649:THR:HB	14:O:801:NAG:H81	2.02	0.42
8:O:650:ARG:HD2	8:O:650:ARG:HA	1.76	0.42
2:B:126:LYS:HA	2:B:126:LYS:HD3	1.78	0.42
5:E:3234:SER:HB2	5:E:3287:TRP:HZ2	1.85	0.42
8:O:595:LYS:HD2	8:O:595:LYS:HA	1.74	0.42
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.74	0.42
4:D:136:LYS:HB3	4:D:136:LYS:HE2	1.80	0.42
6:G:187:ASP:OD1	6:G:187:ASP:N	2.52	0.42
8:O:492:ASN:ND2	8:O:525:GLU:OE1	2.52	0.42
8:O:749:LEU:HD23	8:O:749:LEU:HA	1.81	0.42
1:A:259:ASP:OD1	1:A:259:ASP:N	2.42	0.42
2:B:202:VAL:HG12	6:G:167:VAL:HB	2.01	0.42
4:D:67:GLY:O	4:D:70:ARG:NH1	2.52	0.42
4:D:258:LYS:HD2	4:D:258:LYS:HA	1.87	0.42
6:G:84:SER:O	6:G:84:SER:OG	2.34	0.42
9:S:58:ASP:OD2	9:S:119:HIS:ND1	2.52	0.42
4:D:270:LEU:HB2	6:G:242:VAL:HG13	2.01	0.42
6:G:214:ASN:OD1	6:G:215:ALA:N	2.53	0.42
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.87	0.41
5:E:3141:LEU:O	5:E:3144:ILE:HG12	2.18	0.41
5:E:3323:LYS:HE2	5:E:3347:TYR:CD1	2.55	0.41
5:E:3330:CYS:SG	5:E:3333:CYS:HB2	2.59	0.41
5:E:3394:LEU:O	5:E:3395:GLU:HG3	2.20	0.41
5:E:3179:TYR:CE1	5:E:3191:SER:HB3	2.55	0.41
8:O:669:LYS:HA	8:O:672:ILE:HD12	2.02	0.41
8:O:682:GLU:HA	8:O:718:PRO:HD2	2.01	0.41
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.93	0.41
1:A:155:ASN:O	1:A:159:THR:HG23	2.20	0.41
5:E:3299:THR:O	5:E:3299:THR:OG1	2.36	0.41
6:G:276:MET:SD	6:G:277:ALA:N	2.93	0.41
4:D:156:VAL:HG23	6:G:162:THR:HG21	2.02	0.41
5:E:3094:VAL:HB	5:E:3100:ARG:HB2	2.02	0.41
5:E:3387:TYR:O	5:E:3387:TYR:CG	2.73	0.41
8:O:564:ASP:OD1	8:O:565:SER:N	2.52	0.41
5:E:3139:ASP:O	5:E:3143:ILE:HG22	2.21	0.41
5:E:3369:LEU:HD23	5:E:3369:LEU:HA	1.80	0.41
9:S:110:MET:HE2	9:S:110:MET:HB2	1.94	0.41
5:E:3140:ILE:O	5:E:3144:ILE:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3151:TYR:CZ	5:E:3167:CYS:HB3	2.56	0.41
5:E:3280:LEU:C	5:E:3281:GLU:HG3	2.45	0.41
5:E:3158:HIS:HB2	5:E:3162:VAL:HG23	2.02	0.41
1:A:221:ARG:NH1	1:A:226:GLN:HB3	2.35	0.41
4:D:198:SER:HB3	6:G:207:ARG:HB3	2.02	0.41
5:E:3094:VAL:HG13	5:E:3335:PHE:HB3	2.03	0.41
5:E:3190:LEU:HA	5:E:3193:LYS:HE2	2.03	0.41
6:G:246:LYS:HD2	6:G:247:LEU:N	2.36	0.41
8:O:526:ASP:HB3	8:O:531:LYS:HB2	2.02	0.41
9:S:92:PHE:CE1	15:S:301:CLR:H152	2.55	0.41
4:D:108:ASN:OD1	4:D:127:GLY:HA2	2.21	0.41
15:D:302:CLR:H222	15:D:302:CLR:H162	1.84	0.41
5:E:3308:ILE:HG21	5:E:3338:ARG:HB3	2.01	0.41
2:B:117:ASP:HB3	6:G:79:ARG:HA	2.03	0.40
8:O:498:LYS:HA	8:O:498:LYS:HD3	1.68	0.40
2:B:299:LYS:HG2	6:G:248:LYS:O	2.21	0.40
4:D:44:LEU:HD23	4:D:44:LEU:HA	1.86	0.40
5:E:3262:PHE:CD2	5:E:3277:TRP:HB2	2.56	0.40
5:E:3345:MET:HE2	5:E:3345:MET:N	2.36	0.40
6:G:265:CYS:HB2	6:G:273:TYR:CZ	2.57	0.40
9:S:193:ARG:HG3	9:S:194:TYR:CD1	2.56	0.40
8:O:754:PRO:HG3	9:S:111:LEU:HD11	2.03	0.40
2:B:310:GLN:NE2	6:G:253:GLY:O	2.54	0.40
8:O:608:ALA:HA	8:O:703:ILE:HG22	2.02	0.40
1:A:252:LYS:HA	1:A:252:LYS:HD2	1.87	0.40
5:E:3357:THR:OG1	8:O:774:ARG:O	2.36	0.40
8:O:601:LYS:HB2	8:O:664:LEU:HD11	2.03	0.40
8:O:754:PRO:O	8:O:757:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	289/291 (99%)	275 (95%)	14 (5%)	0	100	100
2	B	261/263 (99%)	241 (92%)	19 (7%)	1 (0%)	30	62
3	C	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
4	D	261/263 (99%)	230 (88%)	30 (12%)	1 (0%)	30	62
5	E	329/331 (99%)	307 (93%)	22 (7%)	0	100	100
6	G	263/265 (99%)	249 (95%)	13 (5%)	1 (0%)	30	62
7	I	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
8	O	287/289 (99%)	272 (95%)	15 (5%)	0	100	100
9	S	177/179 (99%)	171 (97%)	6 (3%)	0	100	100
All	All	2074/2092 (99%)	1948 (94%)	123 (6%)	3 (0%)	49	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	187	ASP
2	B	160	ASN
4	D	283	ILE

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	256/256 (100%)	256 (100%)	0	100	100
2	B	228/228 (100%)	226 (99%)	2 (1%)	70	76
3	C	16/184 (9%)	16 (100%)	0	100	100
4	D	225/225 (100%)	224 (100%)	1 (0%)	84	81
5	E	297/297 (100%)	297 (100%)	0	100	100
6	G	224/224 (100%)	223 (100%)	1 (0%)	84	81
7	I	4/4 (100%)	4 (100%)	0	100	100
8	O	246/246 (100%)	246 (100%)	0	100	100
9	S	157/157 (100%)	157 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1653/1821 (91%)	1649 (100%)	4 (0%)	85 85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	160	ASN
2	B	240	THR
4	D	39	LEU
6	G	288	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
2	B	219	ASN
2	B	310	GLN
3	C	93	ASN
4	D	210	ASN
5	E	3068	ASN
5	E	3145	ASN
5	E	3265	ASN
6	G	141	GLN
6	G	143	ASN
8	O	576	HIS
9	S	33	GLN
9	S	83	GLN
9	S	91	GLN
9	S	195	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

25 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	$\# Z > 2$
10	NAG	F	1	1,10	14,14,15	0.23	0	17,19,21	0.45	0
10	NAG	F	2	10	14,14,15	0.23	0	17,19,21	0.45	0
10	BMA	F	3	10	11,11,12	0.64	0	15,15,17	0.67	0
11	NAG	H	1	11,1	14,14,15	0.35	0	17,19,21	0.39	0
11	NAG	H	2	11	14,14,15	0.30	0	17,19,21	0.39	0
11	BMA	H	3	11	11,11,12	0.61	0	15,15,17	0.68	0
12	NAG	J	1	2,12	14,14,15	0.16	0	17,19,21	0.46	0
12	NAG	J	2	12	14,14,15	0.22	0	17,19,21	0.45	0
10	NAG	K	1	2,10	14,14,15	0.31	0	17,19,21	0.42	0
10	NAG	K	2	10	14,14,15	0.22	0	17,19,21	0.36	0
10	BMA	K	3	10	11,11,12	0.57	0	15,15,17	0.73	0
10	NAG	L	1	2,10	14,14,15	0.21	0	17,19,21	0.43	0
10	NAG	L	2	10	14,14,15	0.22	0	17,19,21	0.43	0
10	BMA	L	3	10	11,11,12	0.56	0	15,15,17	0.71	0
10	NAG	M	1	4,10	14,14,15	0.29	0	17,19,21	0.43	0
10	NAG	M	2	10	14,14,15	0.18	0	17,19,21	0.46	0
10	BMA	M	3	10	11,11,12	0.55	0	15,15,17	0.72	0
10	NAG	N	1	6,10	14,14,15	0.18	0	17,19,21	0.42	0
10	NAG	N	2	10	14,14,15	0.19	0	17,19,21	0.41	0
10	BMA	N	3	10	11,11,12	0.58	0	15,15,17	0.68	0
13	NAG	P	1	13,8	14,14,15	0.21	0	17,19,21	0.46	0
13	NAG	P	2	13	14,14,15	0.23	0	17,19,21	0.47	0
13	BMA	P	3	13	11,11,12	0.54	0	15,15,17	0.81	0
12	NAG	Q	1	12,8	14,14,15	0.22	0	17,19,21	0.50	0
12	NAG	Q	2	12	14,14,15	0.29	0	17,19,21	0.44	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
10	NAG	F	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	1/2/19/22	0/1/1/1
11	NAG	H	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	H	2	11	-	2/6/23/26	0/1/1/1
11	BMA	H	3	11	-	1/2/19/22	0/1/1/1
12	NAG	J	1	2,12	-	0/6/23/26	0/1/1/1
12	NAG	J	2	12	-	2/6/23/26	0/1/1/1
10	NAG	K	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	K	2	10	-	3/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	NAG	L	1	2,10	-	2/6/23/26	0/1/1/1
10	NAG	L	2	10	-	2/6/23/26	0/1/1/1
10	BMA	L	3	10	-	0/2/19/22	0/1/1/1
10	NAG	M	1	4,10	-	0/6/23/26	0/1/1/1
10	NAG	M	2	10	-	2/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
10	NAG	N	1	6,10	-	2/6/23/26	0/1/1/1
10	NAG	N	2	10	-	2/6/23/26	0/1/1/1
10	BMA	N	3	10	-	1/2/19/22	0/1/1/1
13	NAG	P	1	13,8	-	2/6/23/26	0/1/1/1
13	NAG	P	2	13	-	2/6/23/26	0/1/1/1
13	BMA	P	3	13	-	0/2/19/22	0/1/1/1
12	NAG	Q	1	12,8	-	2/6/23/26	0/1/1/1
12	NAG	Q	2	12	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	1	NAG	O5-C5-C6-O6
12	Q	1	NAG	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
12	Q	2	NAG	O5-C5-C6-O6
13	P	2	NAG	O5-C5-C6-O6
12	J	2	NAG	O5-C5-C6-O6
13	P	1	NAG	O5-C5-C6-O6

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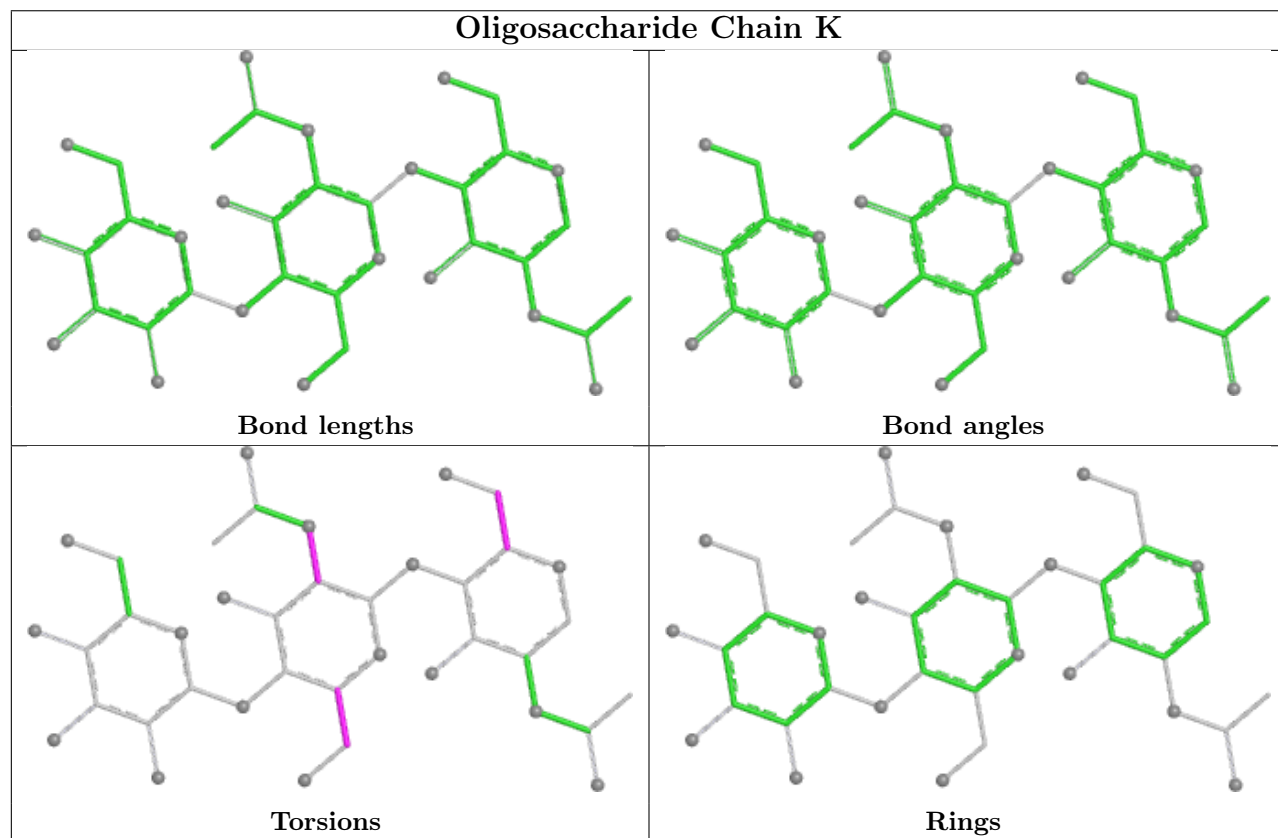
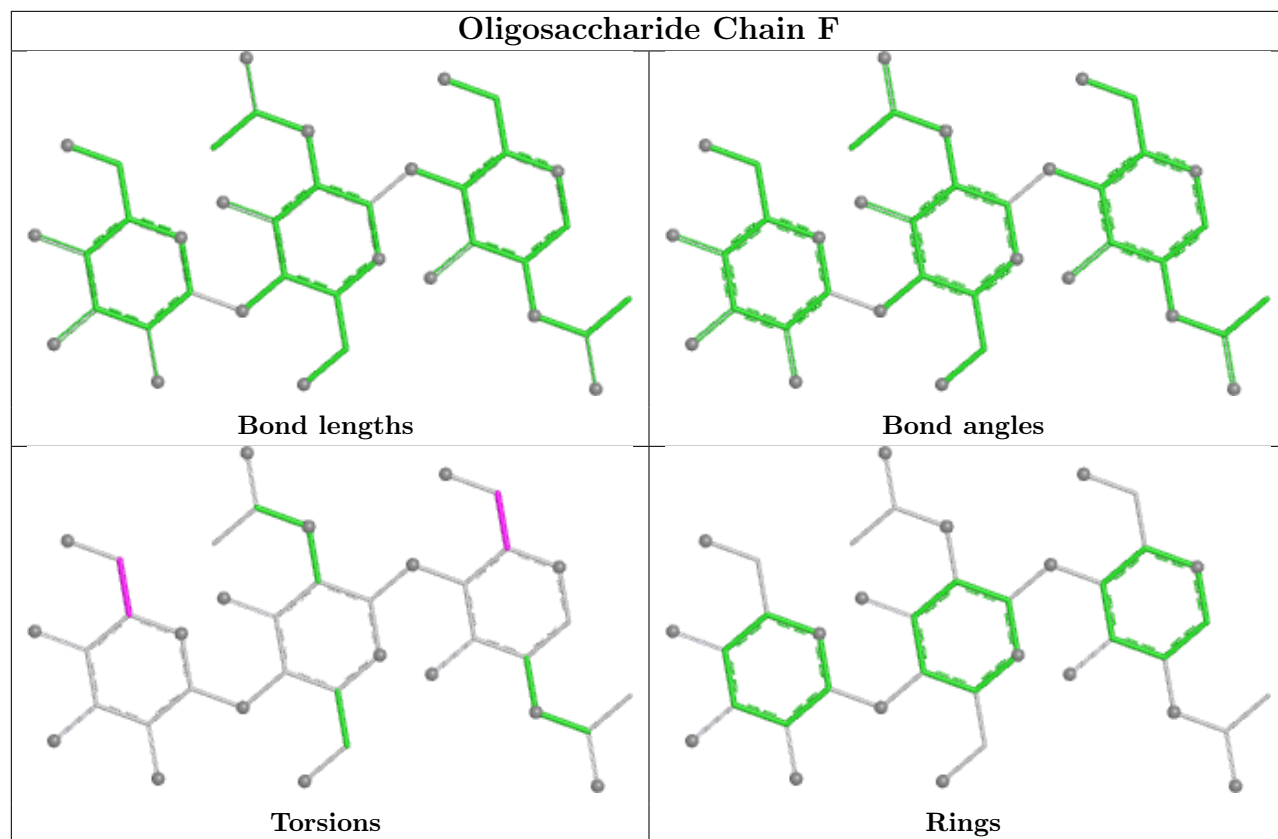
Mol	Chain	Res	Type	Atoms
12	Q	1	NAG	C4-C5-C6-O6
11	H	1	NAG	C4-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
13	P	1	NAG	C4-C5-C6-O6
12	J	2	NAG	C4-C5-C6-O6
13	P	2	NAG	C4-C5-C6-O6
12	Q	2	NAG	C4-C5-C6-O6
10	M	2	NAG	C8-C7-N2-C2
10	M	2	NAG	O7-C7-N2-C2
12	Q	2	NAG	C8-C7-N2-C2
12	Q	2	NAG	O7-C7-N2-C2
11	H	2	NAG	O5-C5-C6-O6
10	K	1	NAG	O5-C5-C6-O6
10	N	1	NAG	C4-C5-C6-O6
10	N	1	NAG	O5-C5-C6-O6
10	L	1	NAG	C4-C5-C6-O6
10	N	2	NAG	C4-C5-C6-O6
10	F	1	NAG	O5-C5-C6-O6
11	H	3	BMA	O5-C5-C6-O6
10	N	3	BMA	O5-C5-C6-O6
11	H	2	NAG	C4-C5-C6-O6
10	L	1	NAG	O5-C5-C6-O6
10	N	2	NAG	O5-C5-C6-O6
10	K	1	NAG	C4-C5-C6-O6
10	L	2	NAG	C4-C5-C6-O6
10	L	2	NAG	O5-C5-C6-O6
10	K	2	NAG	C1-C2-N2-C7
10	F	3	BMA	C4-C5-C6-O6

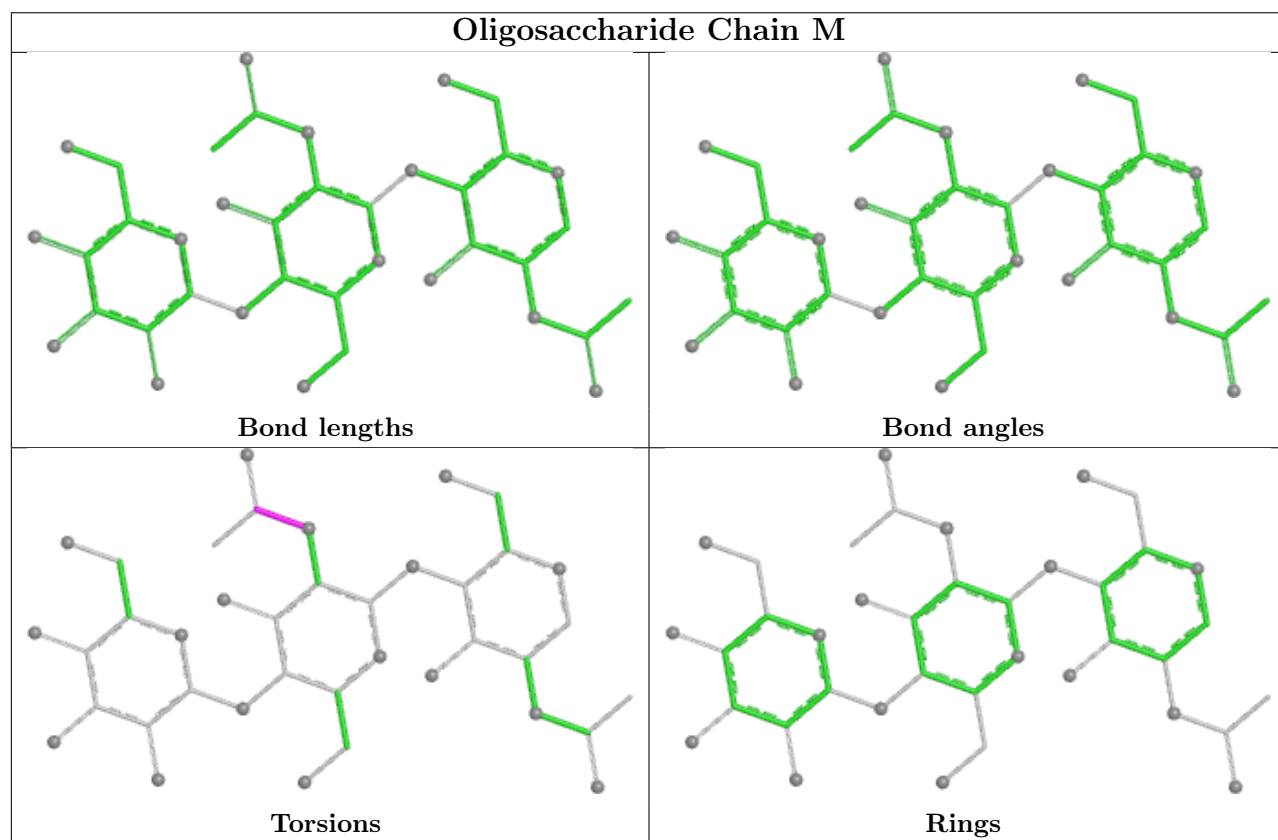
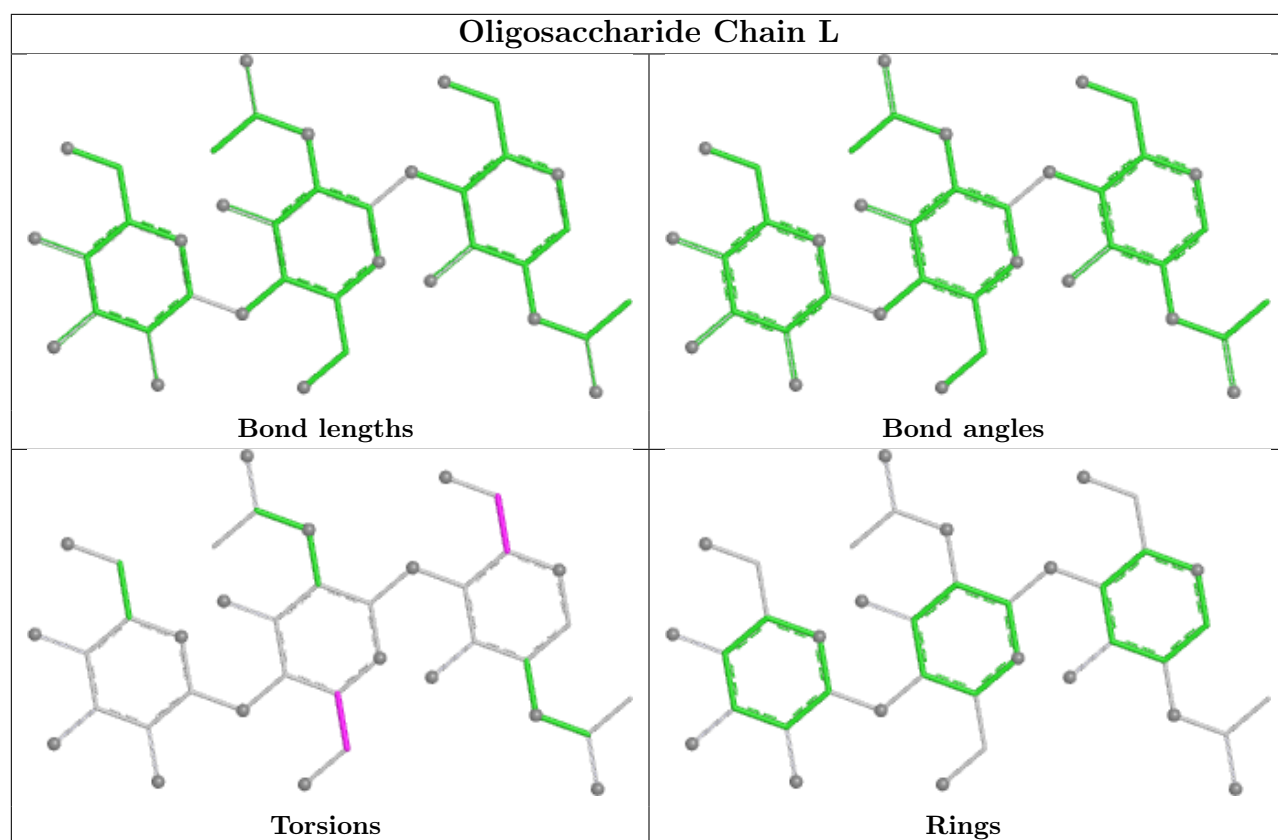
There are no ring outliers.

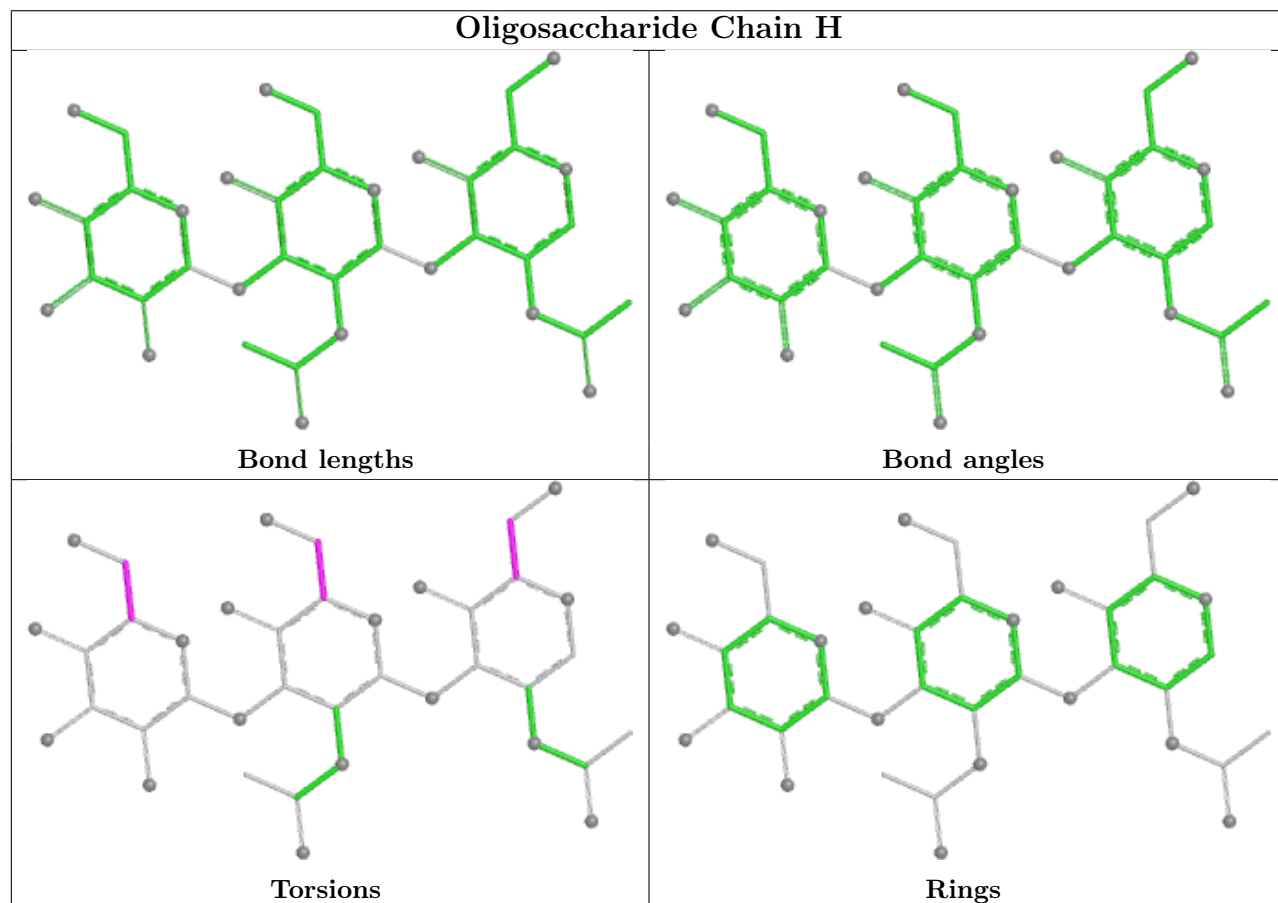
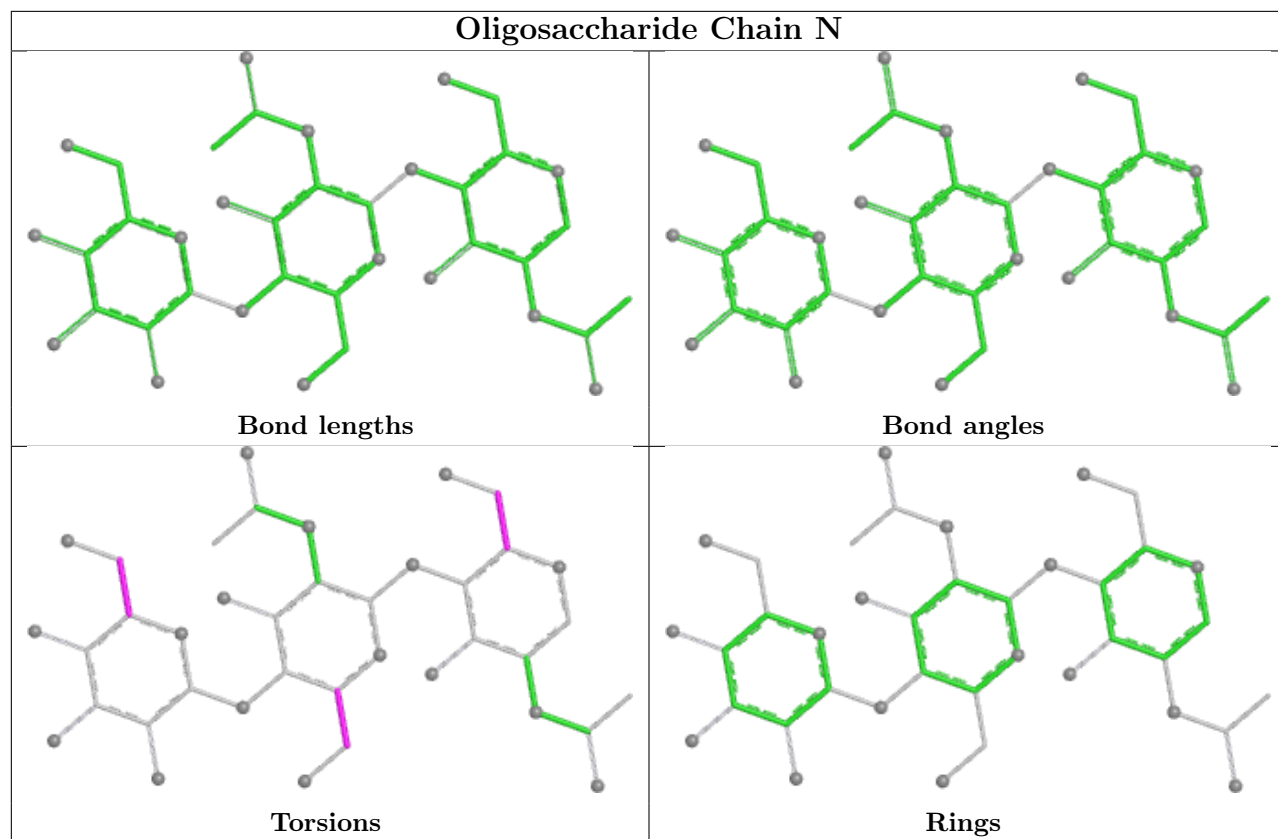
1 monomer is involved in 2 short contacts:

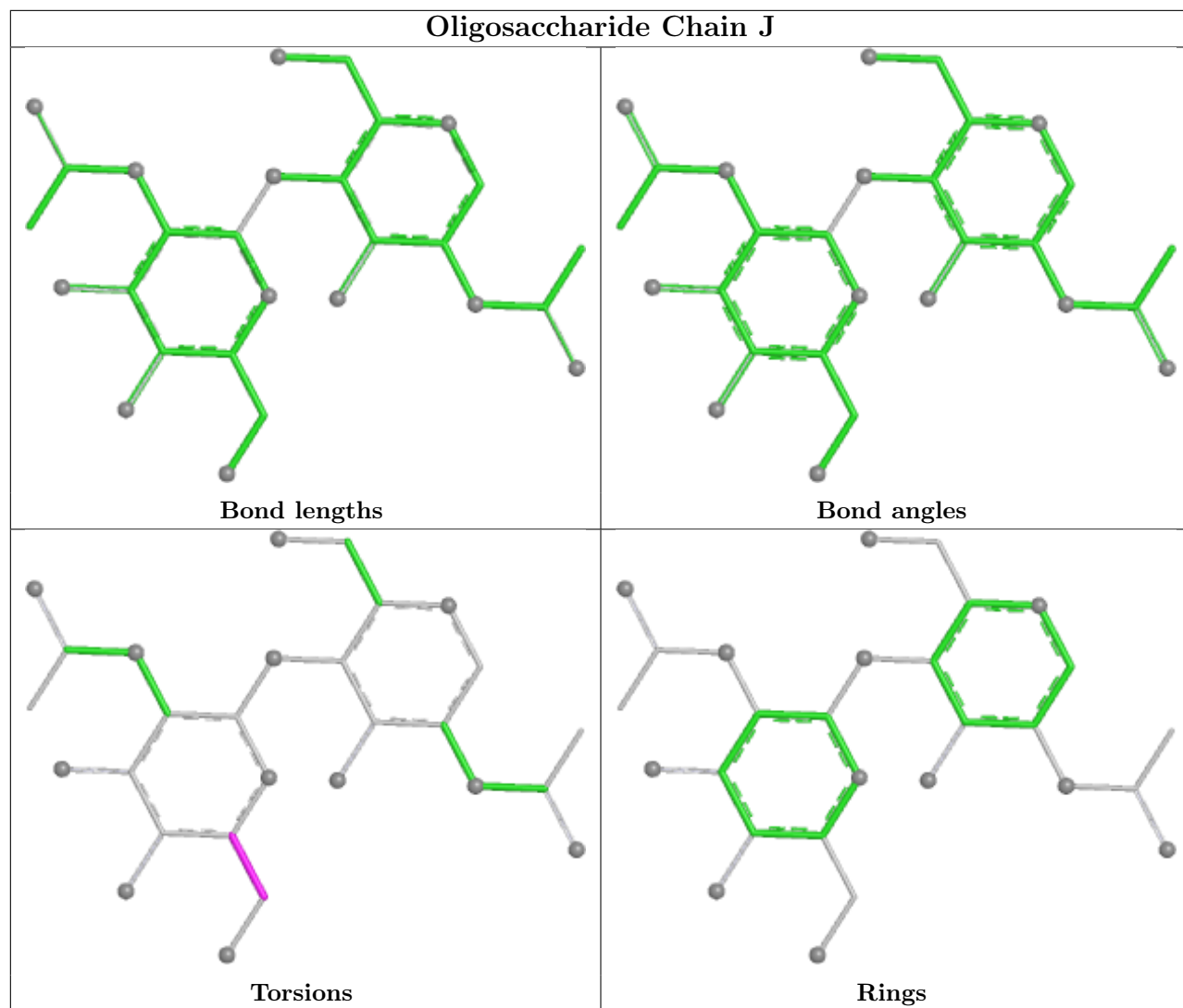
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	H	1	NAG	2	0

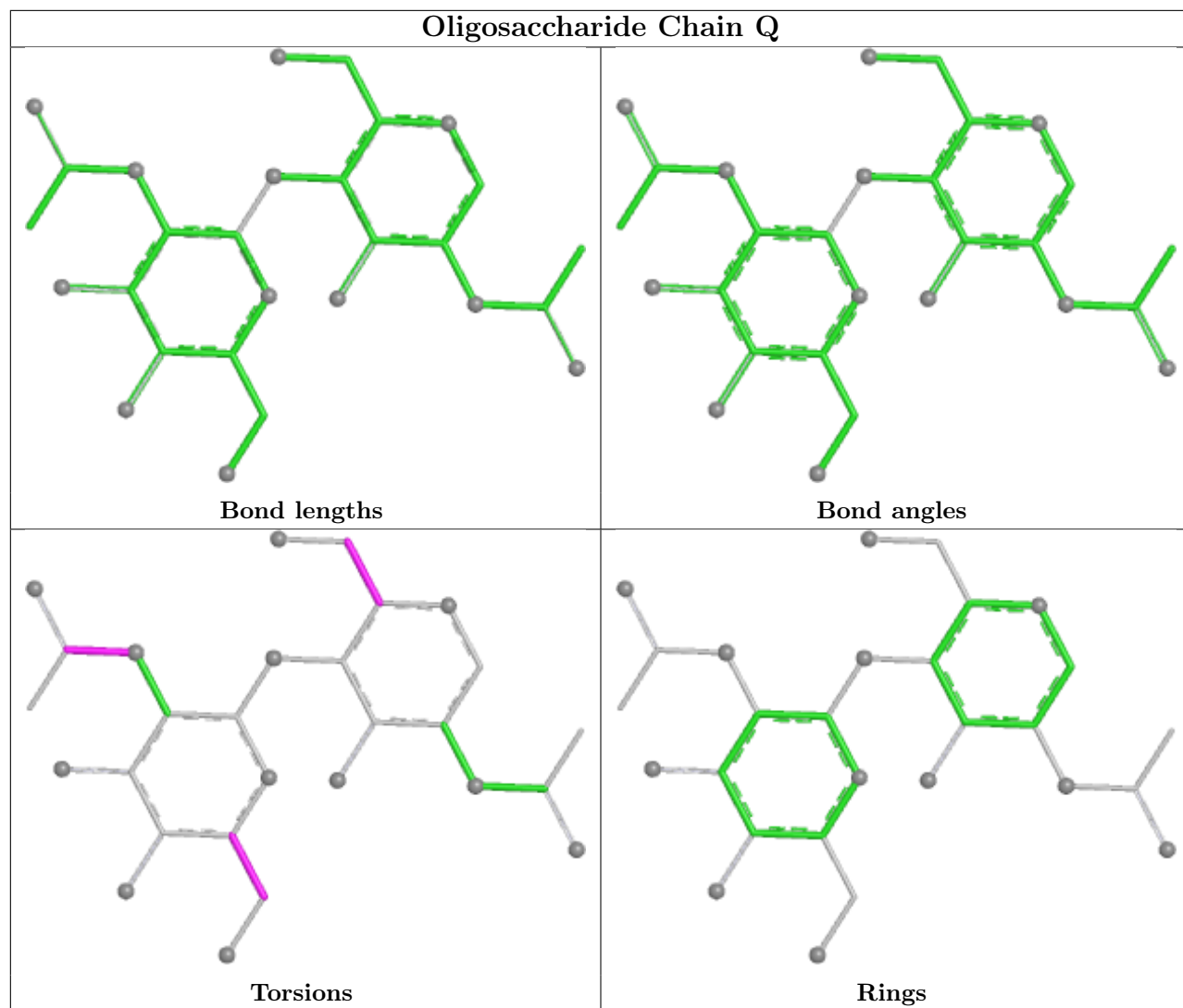
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

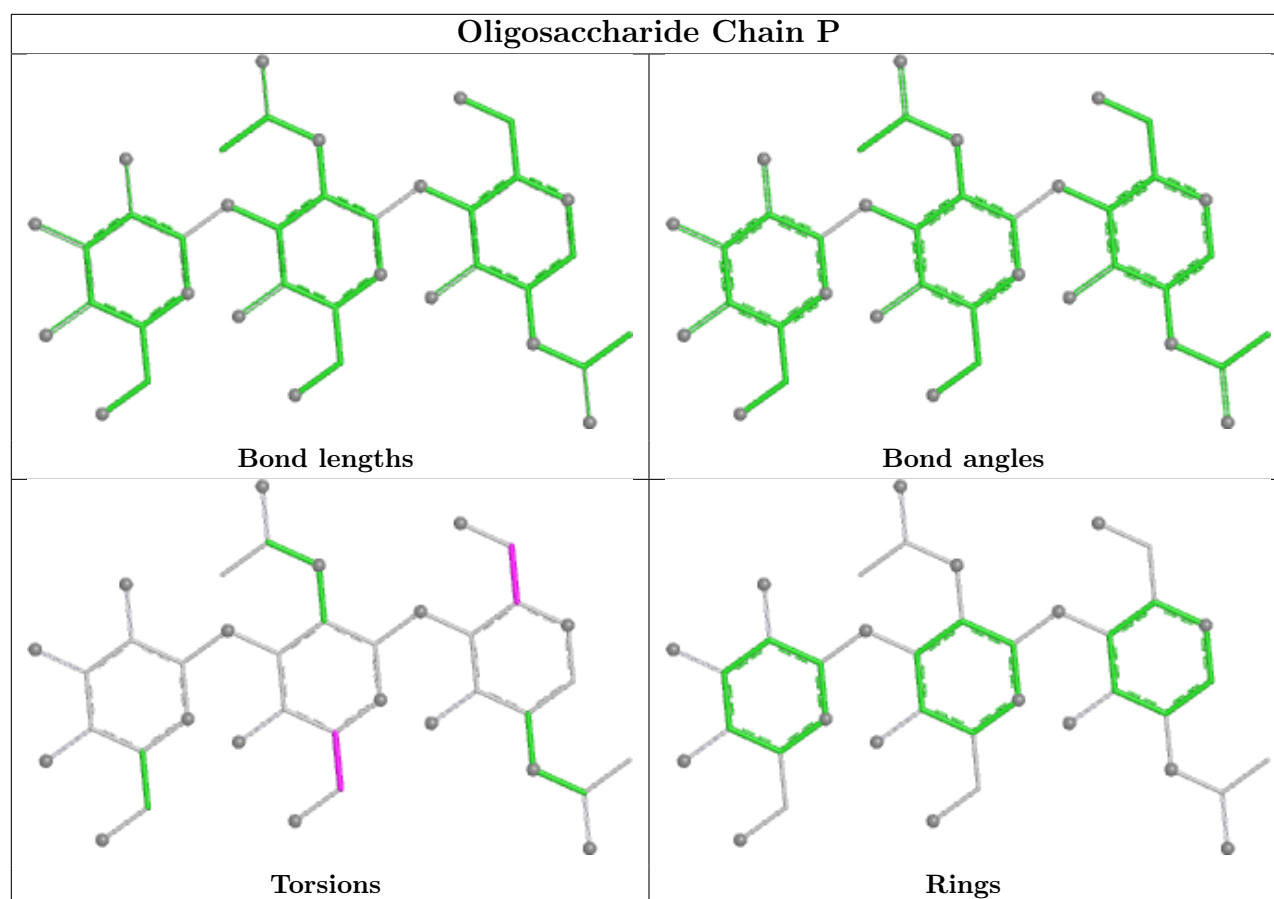












5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
14	NAG	O	801	8	14,14,15	0.21	0	17,19,21	0.38	0
15	CLR	S	301	-	31,31,31	0.40	0	48,48,48	0.74	0
14	NAG	A	401	1	14,14,15	0.40	0	17,19,21	0.45	0
14	NAG	A	402	1	14,14,15	0.23	0	17,19,21	0.40	0
17	P5S	G	301	-	31,32,53	0.52	0	33,39,60	0.41	0
15	CLR	D	302	-	31,31,31	0.38	0	48,48,48	0.50	0
15	CLR	D	301	-	31,31,31	0.37	0	48,48,48	0.48	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
14	NAG	O	801	8	-	1/6/23/26	0/1/1/1
15	CLR	S	301	-	-	5/10/68/68	0/4/4/4
14	NAG	A	401	1	-	2/6/23/26	0/1/1/1
14	NAG	A	402	1	-	2/6/23/26	0/1/1/1
17	P5S	G	301	-	-	20/38/38/59	-
15	CLR	D	302	-	-	4/10/68/68	0/4/4/4
15	CLR	D	301	-	-	5/10/68/68	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	301	P5S	O-C-CA-N
17	G	301	P5S	C-CA-CB-OG
17	G	301	P5S	N-CA-CB-OG
17	G	301	P5S	CB-OG-P12-O15
17	G	301	P5S	C3-O16-P12-OG
17	G	301	P5S	C3-O16-P12-O13
17	G	301	P5S	C3-O16-P12-O15
17	G	301	P5S	C20-C17-O19-C1
17	G	301	P5S	O18-C17-O19-C1
14	A	401	NAG	O5-C5-C6-O6
14	A	402	NAG	O5-C5-C6-O6
14	A	401	NAG	C4-C5-C6-O6
14	A	402	NAG	C4-C5-C6-O6
17	G	301	P5S	OXT-C-CA-N
15	S	301	CLR	C20-C22-C23-C24
15	D	301	CLR	C13-C17-C20-C22
17	G	301	P5S	C42-C43-C44-C45
15	D	301	CLR	C13-C17-C20-C21
17	G	301	P5S	O19-C1-C2-O37
17	G	301	P5S	C41-C42-C43-C44
14	O	801	NAG	O5-C5-C6-O6
15	D	301	CLR	C16-C17-C20-C21

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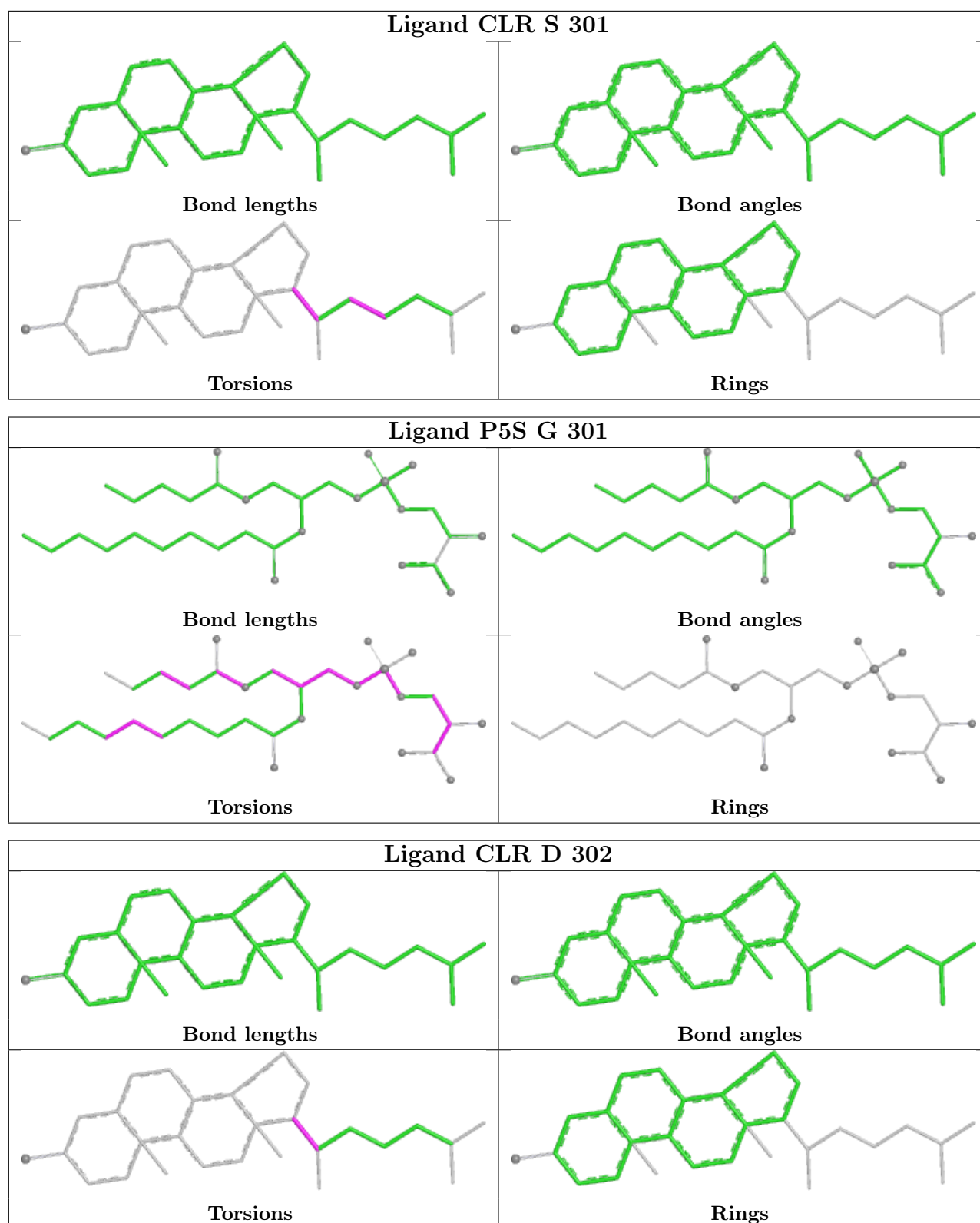
Mol	Chain	Res	Type	Atoms
15	S	301	CLR	C16-C17-C20-C21
15	S	301	CLR	C13-C17-C20-C21
15	S	301	CLR	C13-C17-C20-C22
17	G	301	P5S	O19-C1-C2-C3
15	D	301	CLR	C16-C17-C20-C22
15	D	302	CLR	C13-C17-C20-C22
17	G	301	P5S	C17-C20-C21-C22
15	D	302	CLR	C13-C17-C20-C21
15	S	301	CLR	C16-C17-C20-C22
15	D	301	CLR	C21-C20-C22-C23
15	D	302	CLR	C16-C17-C20-C21
15	D	302	CLR	C16-C17-C20-C22
17	G	301	P5S	O37-C2-C3-O16
17	G	301	P5S	OXT-C-CA-CB
17	G	301	P5S	CB-OG-P12-O16
17	G	301	P5S	C1-C2-C3-O16
17	G	301	P5S	C2-C3-O16-P12

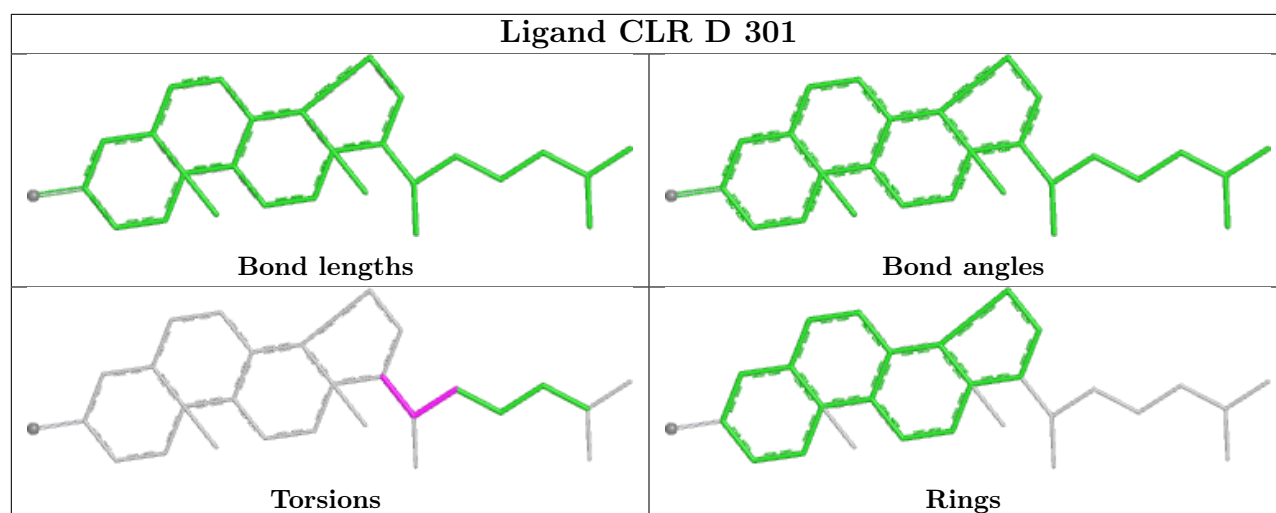
There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	O	801	NAG	1	0
15	S	301	CLR	4	0
14	A	401	NAG	2	0
17	G	301	P5S	3	0
15	D	302	CLR	3	0
15	D	301	CLR	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

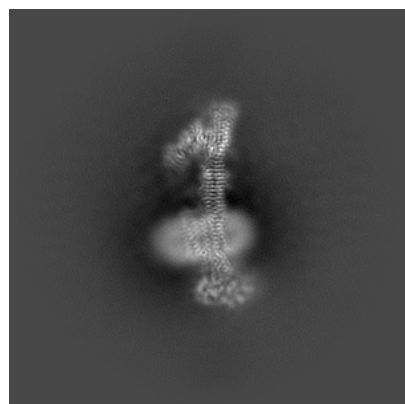
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39568. These allow visual inspection of the internal detail of the map and identification of artifacts.

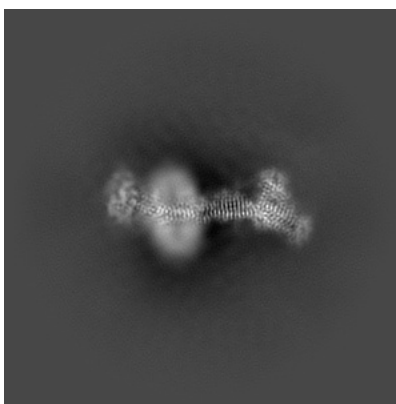
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

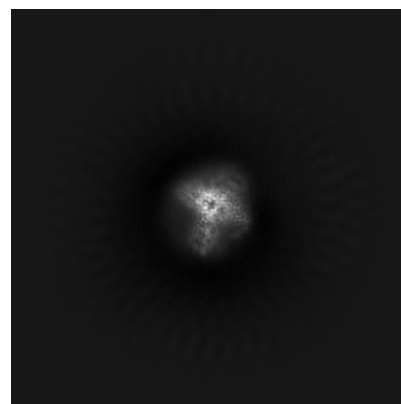
6.1.1 Primary map



X

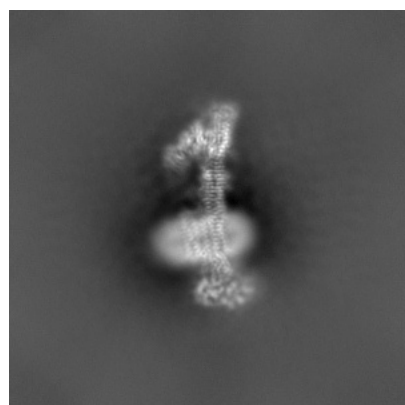


Y

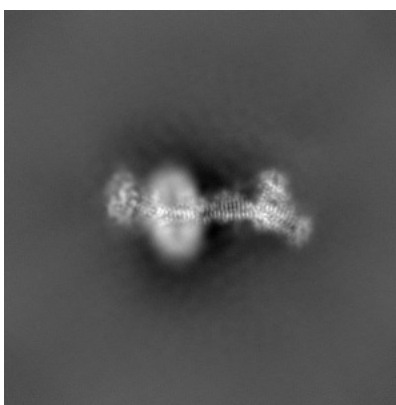


Z

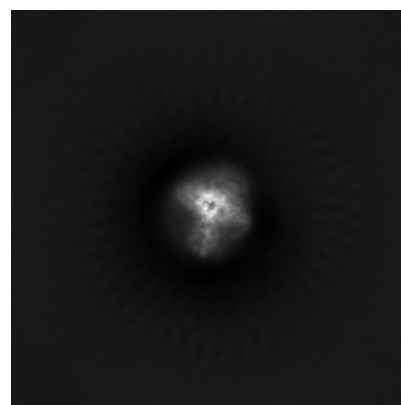
6.1.2 Raw map



X



Y

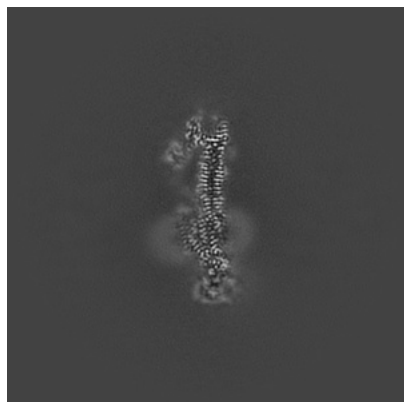


Z

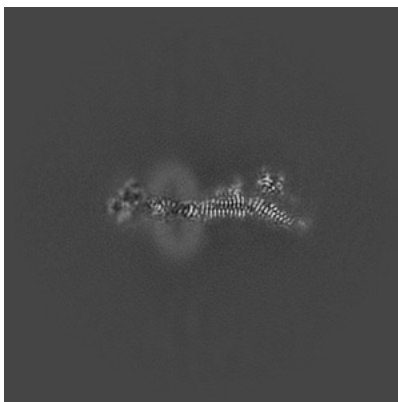
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

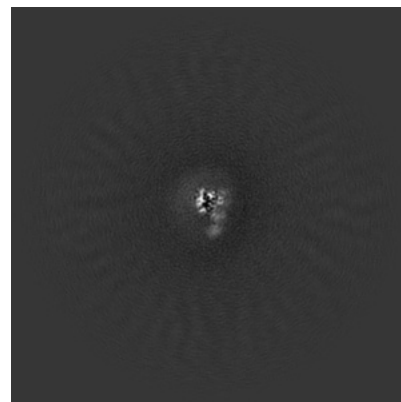
6.2.1 Primary map



X Index: 216

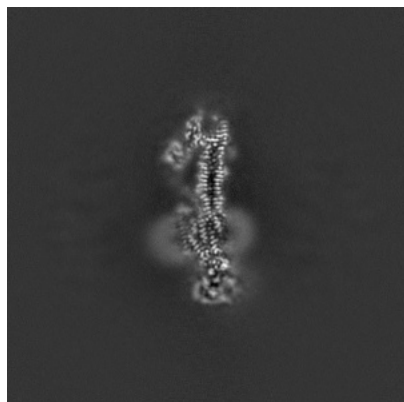


Y Index: 216

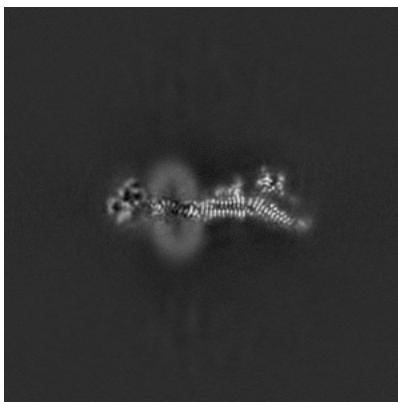


Z Index: 216

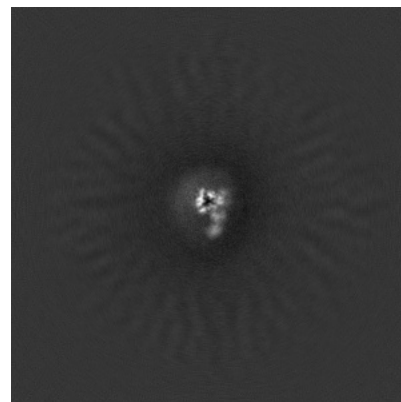
6.2.2 Raw map



X Index: 216



Y Index: 216



Z Index: 216

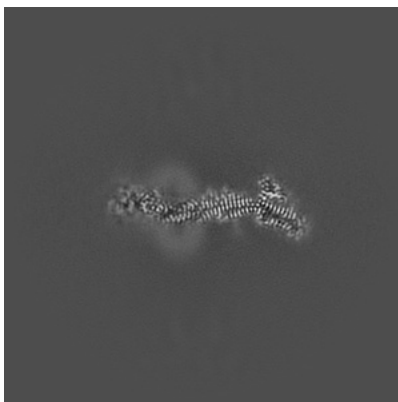
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

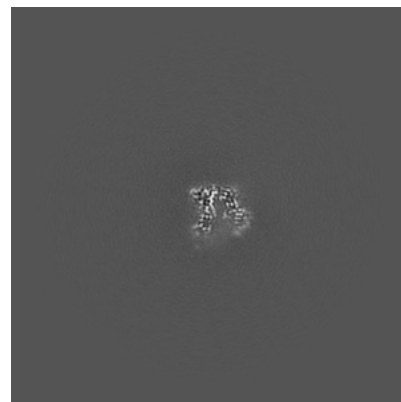
6.3.1 Primary map



X Index: 211

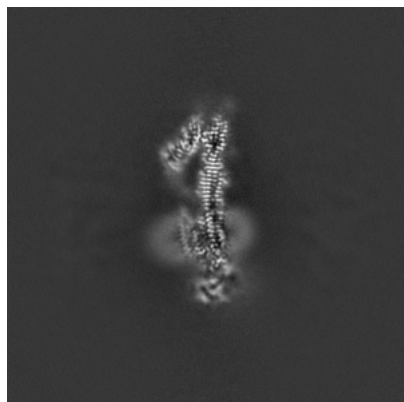


Y Index: 226

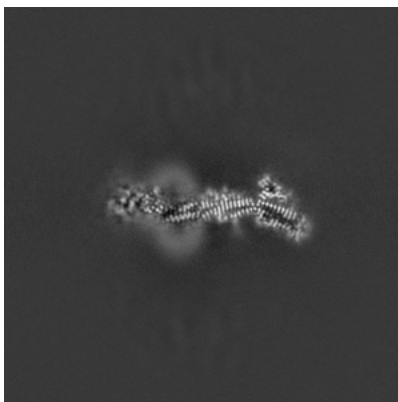


Z Index: 288

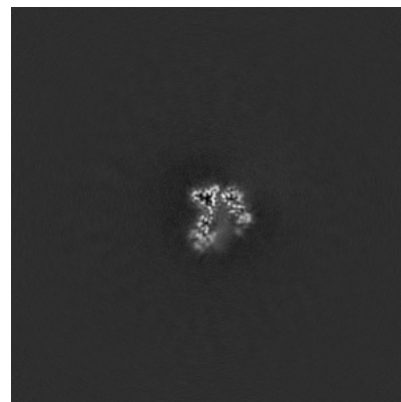
6.3.2 Raw map



X Index: 211



Y Index: 227

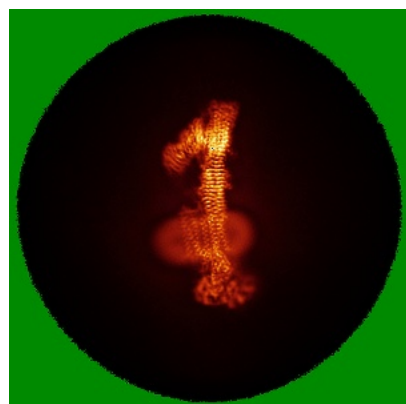


Z Index: 284

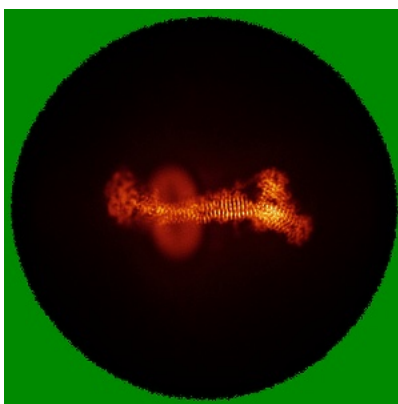
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

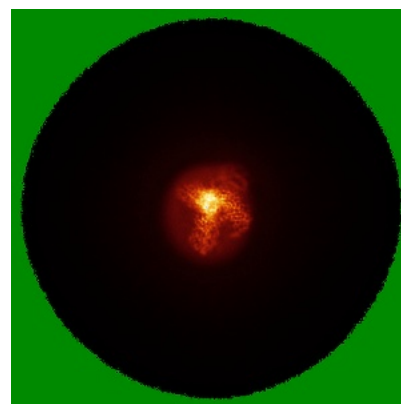
6.4.1 Primary map



X

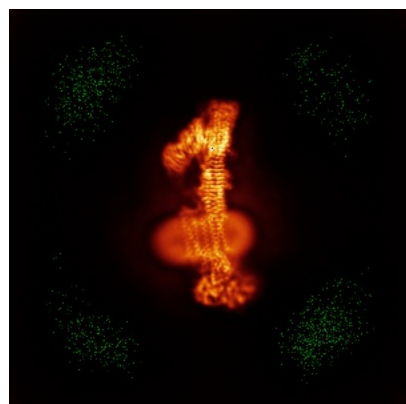


Y

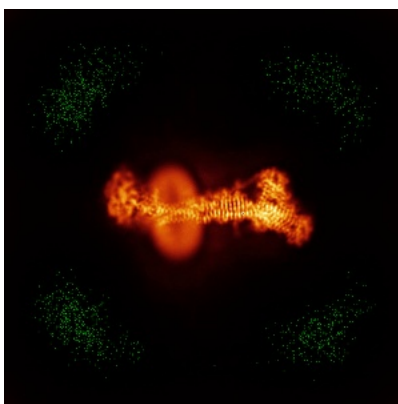


Z

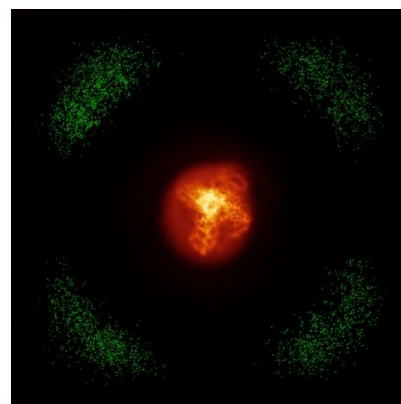
6.4.2 Raw map



X



Y

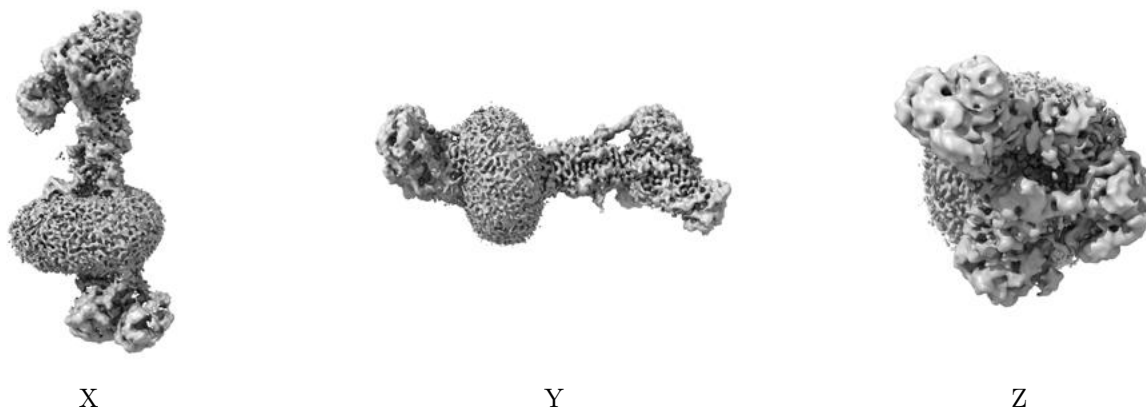


Z

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.

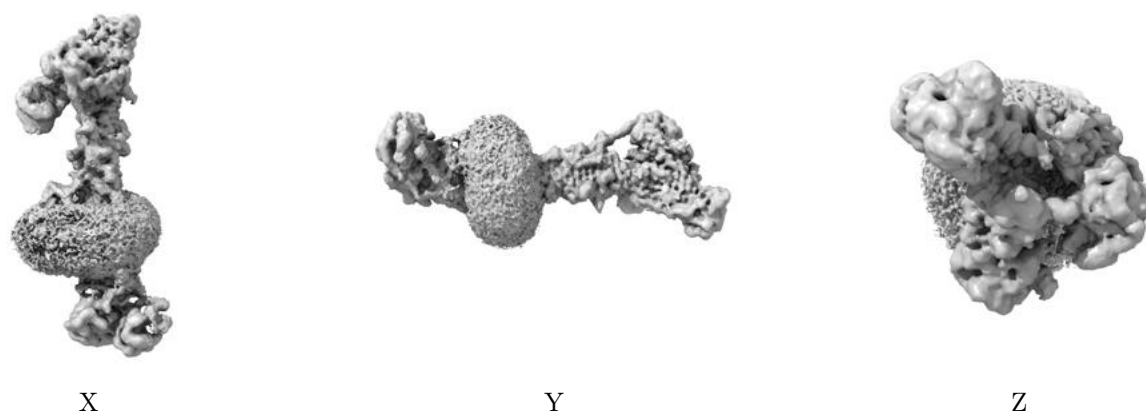
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

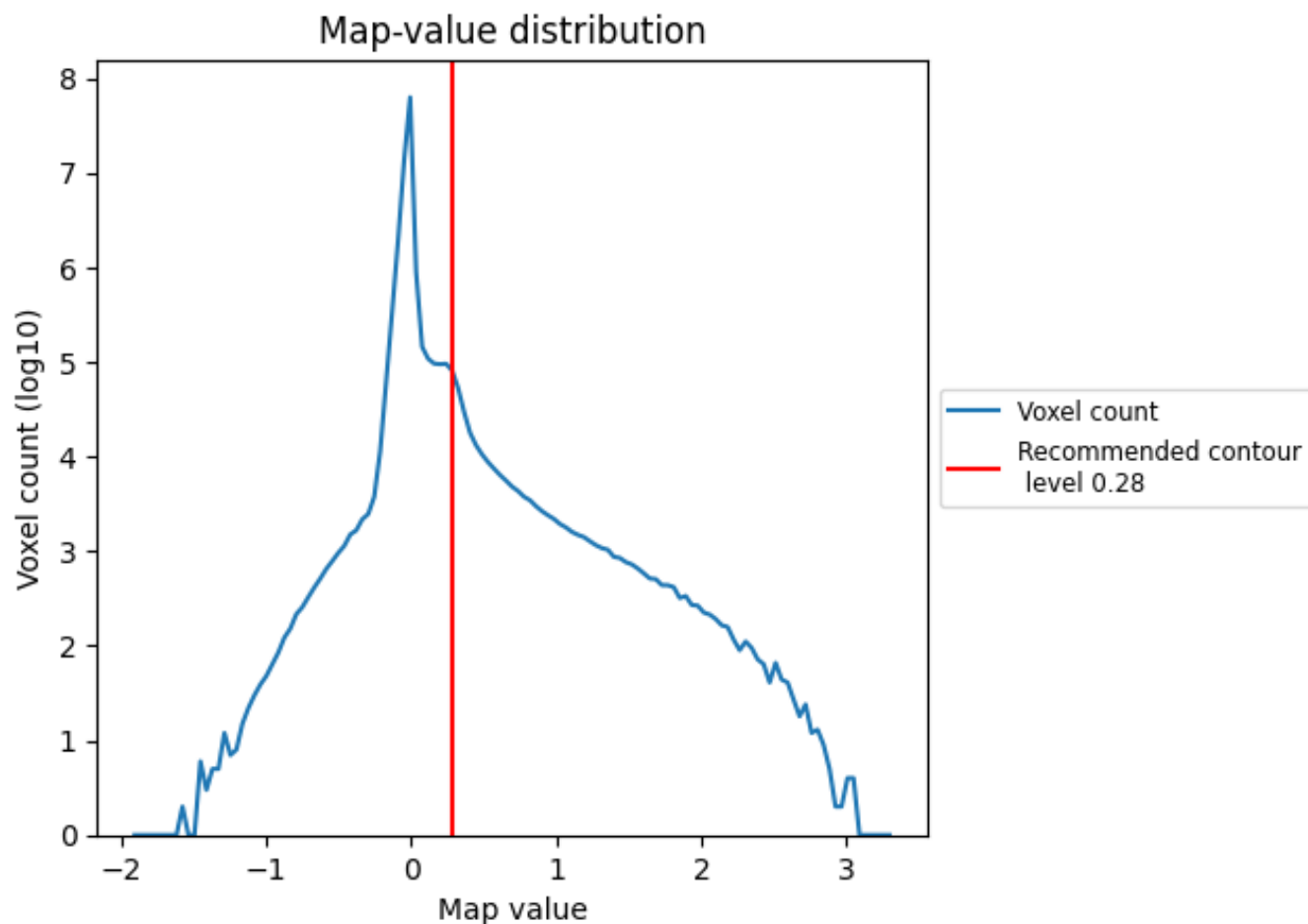
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

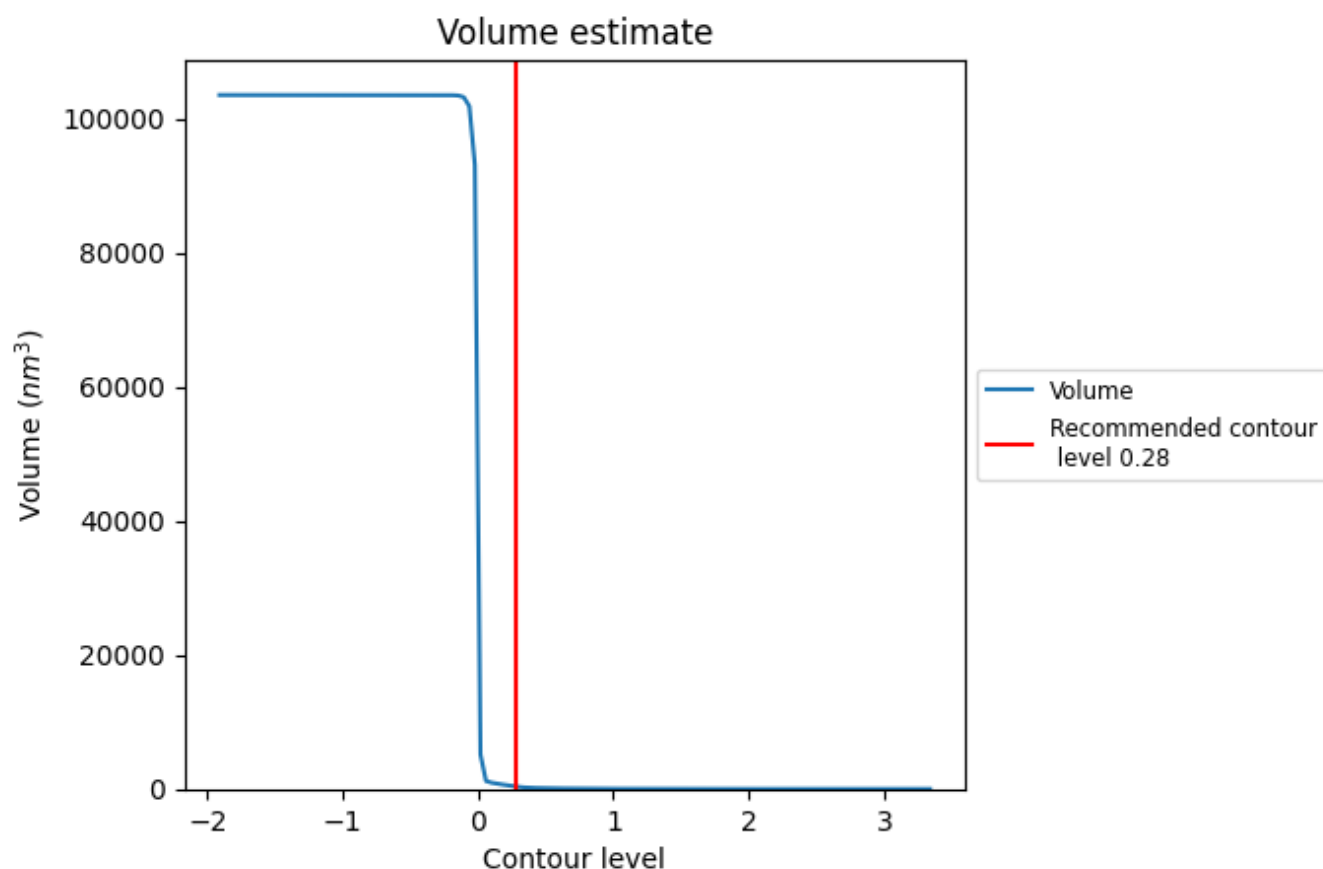
This section contains the results of statistical analysis of the map.

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.

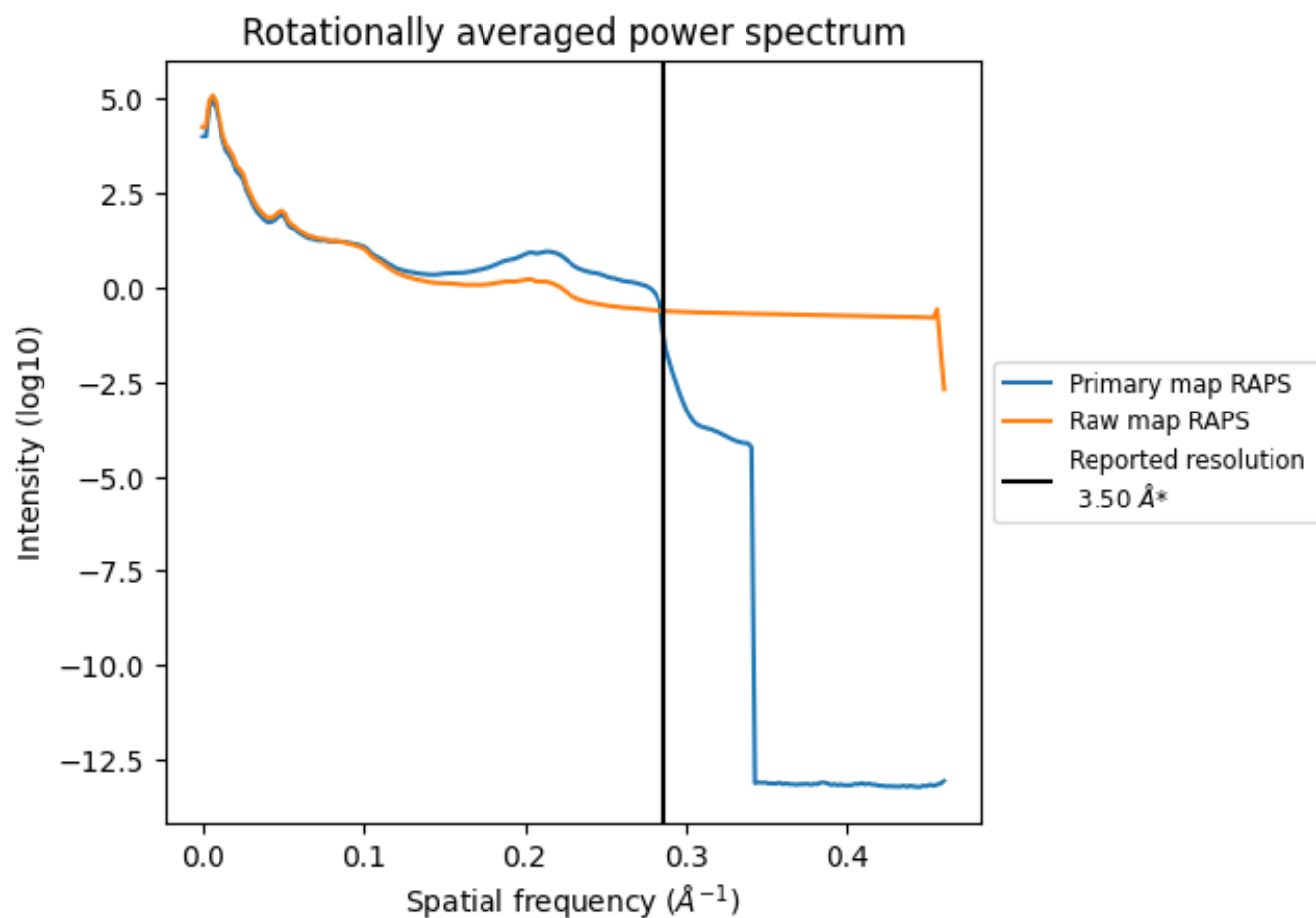
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 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 ⓘ

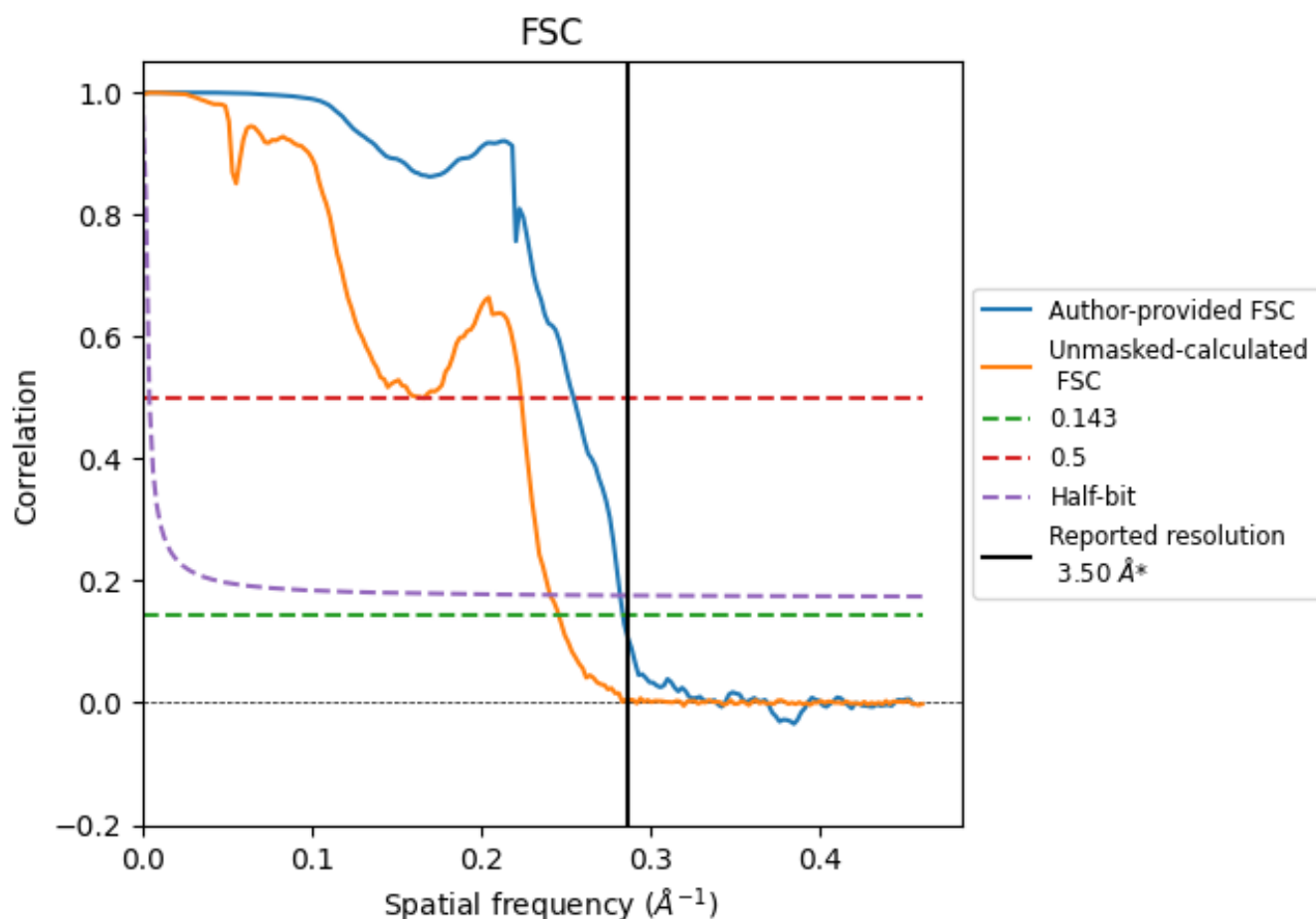


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.53	3.93	3.55
Unmasked-calculated*	4.07	6.06	4.16

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.5 by more than 10 %

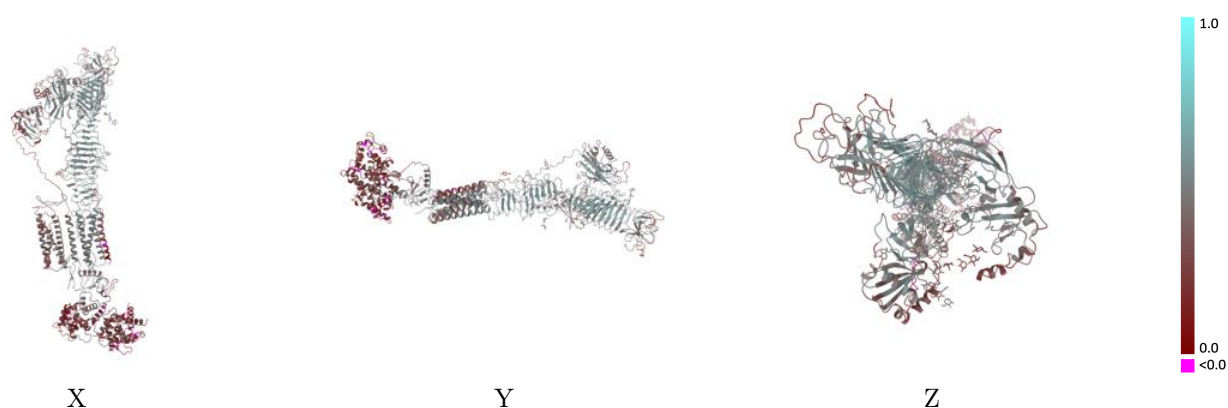
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-39568 and PDB model 8YT8. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

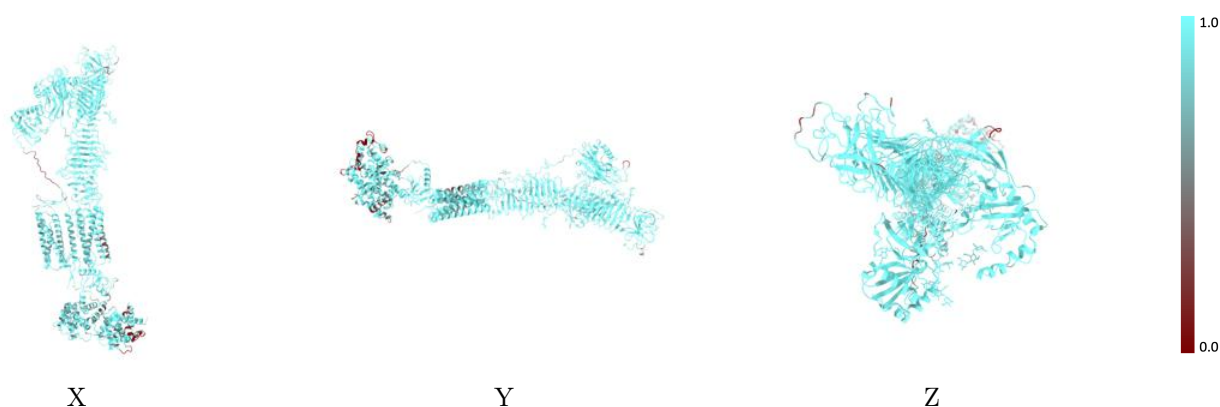
This section was not generated.

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



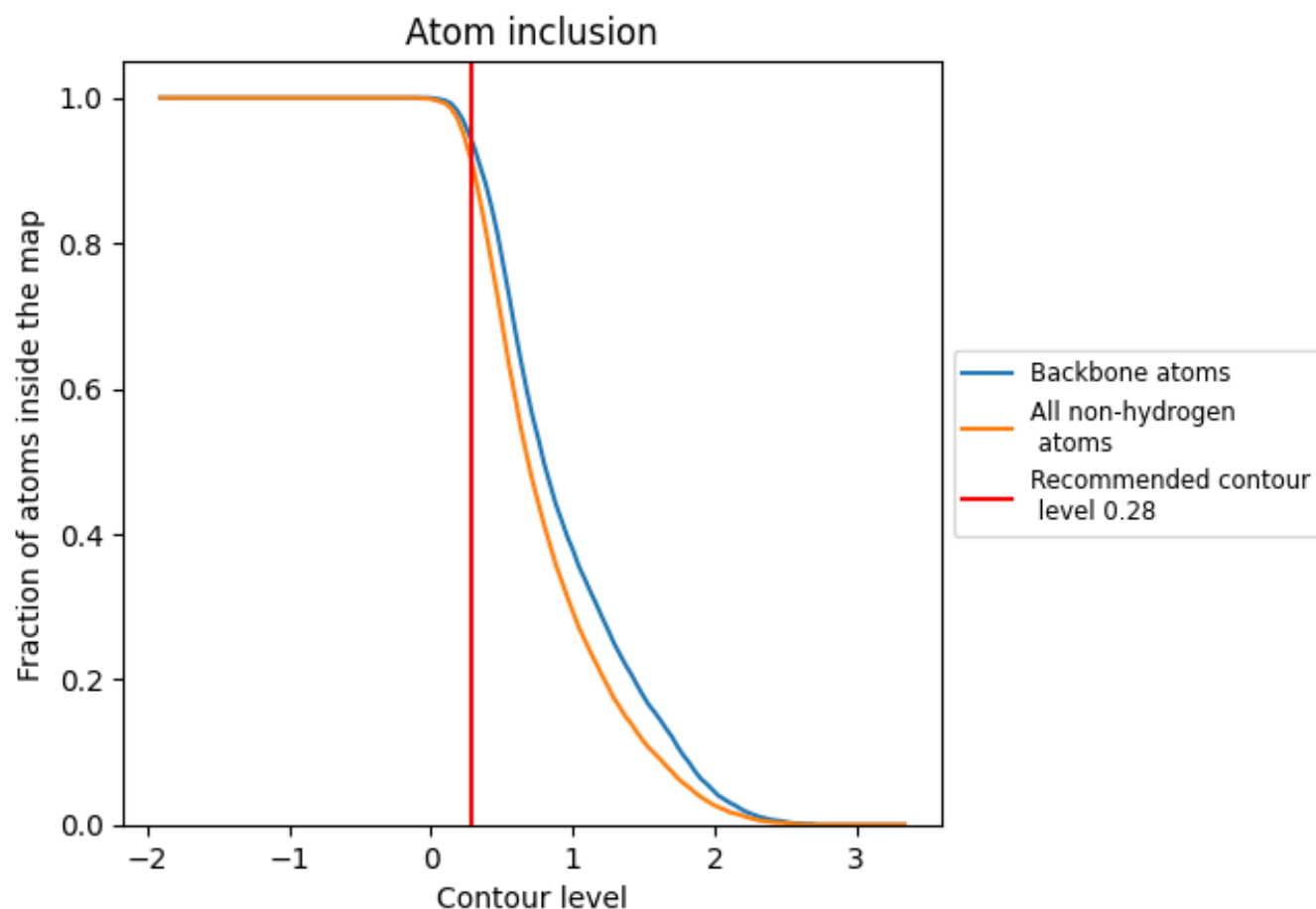
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.4120
A	 0.9380	 0.4330
B	 0.9690	 0.4960
C	 0.7730	 0.2360
D	 0.9660	 0.4920
E	 0.8370	 0.2830
F	 1.0000	 0.4390
G	 0.9650	 0.5020
H	 0.7950	 0.2110
I	 0.9730	 0.5040
J	 0.9640	 0.4210
K	 0.9490	 0.4240
L	 0.9490	 0.4370
M	 1.0000	 0.4610
N	 0.9490	 0.3410
O	 0.9280	 0.4240
P	 0.9490	 0.3670
Q	 0.9290	 0.2650
S	 0.8950	 0.3670

