



Full wwPDB EM Validation Report ⓘ

Jul 21, 2026 – 04:37 pm BST

PDB ID : 9SM2 / pdb_00009sm2
EMDB ID : EMD-55024
Title : Cryo-EM structure of the closed-closed dextran utilisome (BT3087-BT3090), with GHdex D297A E360A catalytic inactivation, with bound IMO4, IMO6 and IMO8
Authors : Feasey, M.; Basle, A.; van den Berg, B.
Deposited on : 2025-09-05
Resolution : 2.50 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:

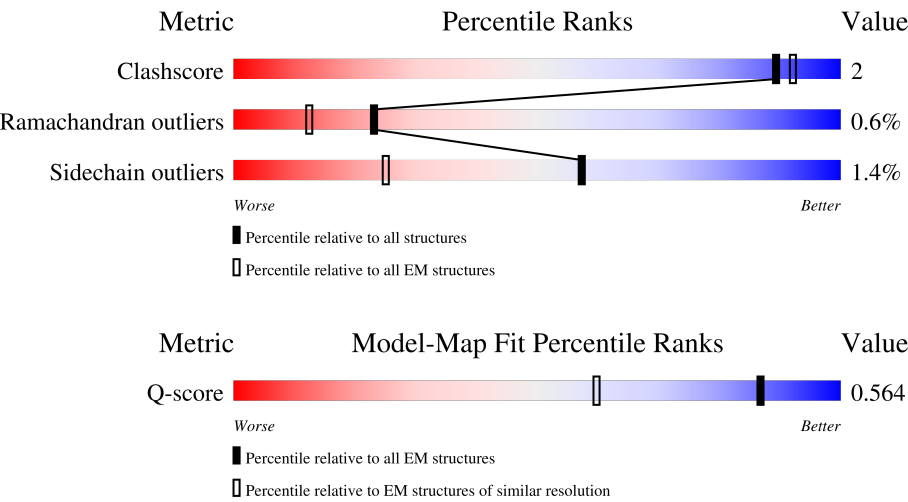
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.50 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.



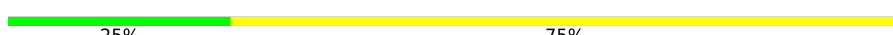
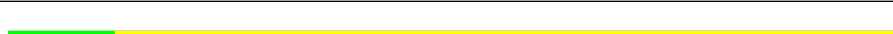
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	999	
1	C	999	
2	B	506	
2	D	506	

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Mol	Chain	Length	Quality of chain
3	E	504	
3	F	504	
4	G	592	
4	H	592	
5	I	4	
5	J	4	
6	K	6	
6	L	6	
7	M	8	
7	N	8	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 32876 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 SusC homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	881	Total	C	N	O	S	0	0
			6913	4358	1183	1345	27		
1	C	881	Total	C	N	O	S	0	0
			6913	4358	1183	1345	27		

- Molecule 2 is a protein called SusD homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	478	Total	C	N	O	S	0	0
			3776	2379	640	734	23		
2	D	478	Total	C	N	O	S	0	0
			3776	2379	640	734	23		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	497	ALA	-	expression tag	UNP Q8A366
B	498	ALA	-	expression tag	UNP Q8A366
B	499	ALA	-	expression tag	UNP Q8A366
B	500	ALA	-	expression tag	UNP Q8A366
B	501	HIS	-	expression tag	UNP Q8A366
B	502	HIS	-	expression tag	UNP Q8A366
B	503	HIS	-	expression tag	UNP Q8A366
B	504	HIS	-	expression tag	UNP Q8A366
B	505	HIS	-	expression tag	UNP Q8A366
B	506	HIS	-	expression tag	UNP Q8A366
D	497	ALA	-	expression tag	UNP Q8A366
D	498	ALA	-	expression tag	UNP Q8A366
D	499	ALA	-	expression tag	UNP Q8A366
D	500	ALA	-	expression tag	UNP Q8A366
D	501	HIS	-	expression tag	UNP Q8A366
D	502	HIS	-	expression tag	UNP Q8A366
D	503	HIS	-	expression tag	UNP Q8A366

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Chain	Residue	Modelled	Actual	Comment	Reference
D	504	HIS	-	expression tag	UNP Q8A366
D	505	HIS	-	expression tag	UNP Q8A366
D	506	HIS	-	expression tag	UNP Q8A366

- Molecule 3 is a protein called BT3088 (SGBPdex).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	134	Total	C	N	O	S	0	0
			1044	647	174	220	3		
3	F	134	Total	C	N	O	S	0	0
			1044	647	174	220	3		

- Molecule 4 is a protein called Cycloisomaltooligosaccharide glucanotransferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	569	Total	C	N	O	S	0	0
			4504	2861	757	864	22		
4	H	569	Total	C	N	O	S	0	0
			4504	2861	757	864	22		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	297	ALA	ASP	engineered mutation	UNP Q8A368
G	360	ALA	GLU	engineered mutation	UNP Q8A368
H	297	ALA	ASP	engineered mutation	UNP Q8A368
H	360	ALA	GLU	engineered mutation	UNP Q8A368

- Molecule 5 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
5	I	4	Total	C	O	0	0
			45	24	21		
5	J	4	Total	C	O	0	0
			45	24	21		

- Molecule 6 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
6	K	6	Total	C	O	0	0
			67	36	31		
6	L	6	Total	C	O	0	0
			67	36	31		

- Molecule 7 is an oligosaccharide called alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose.

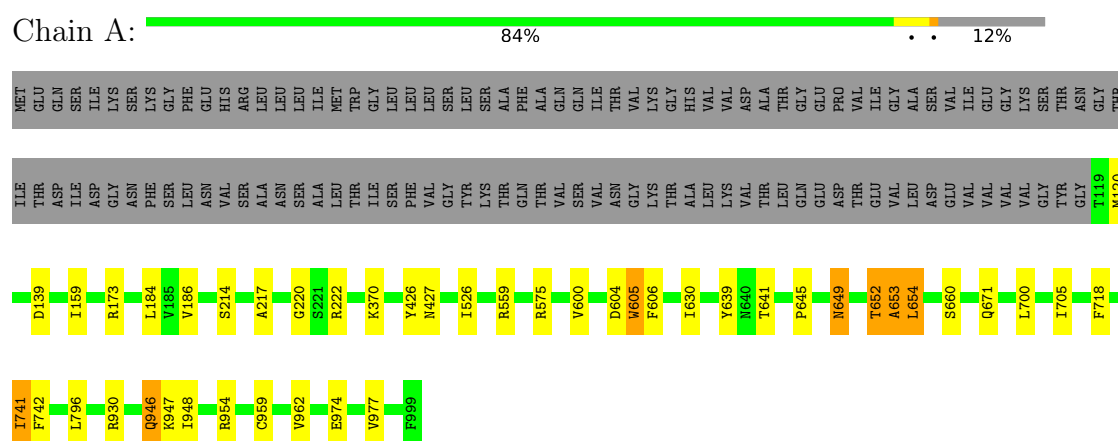


Mol	Chain	Residues	Atoms			AltConf	Trace
7	M	8	Total	C	O	0	0
			89	48	41		
7	N	8	Total	C	O	0	0
			89	48	41		

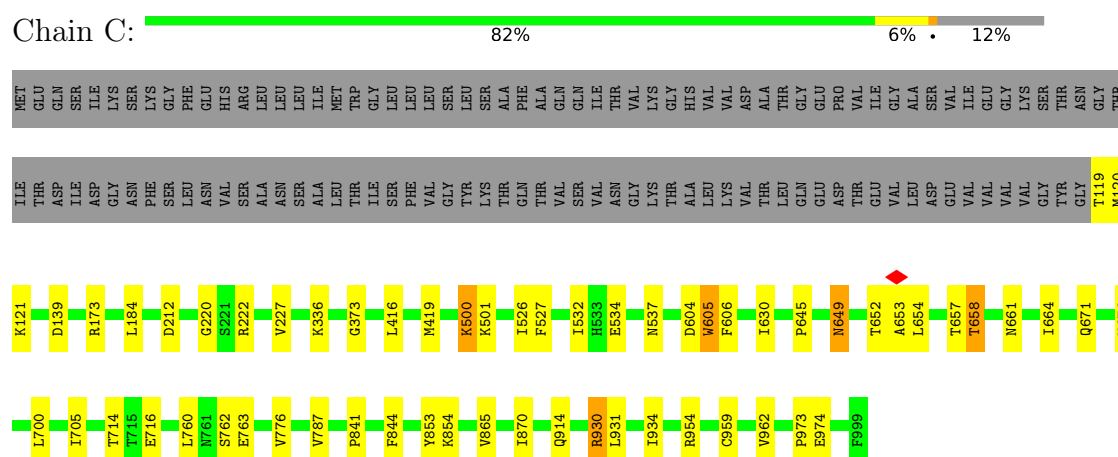
3 Residue-property plots

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.

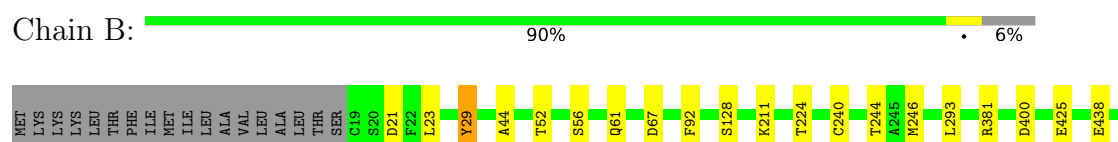
• Molecule 1: SusC homolog

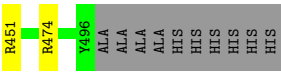


• Molecule 1: SusC homolog

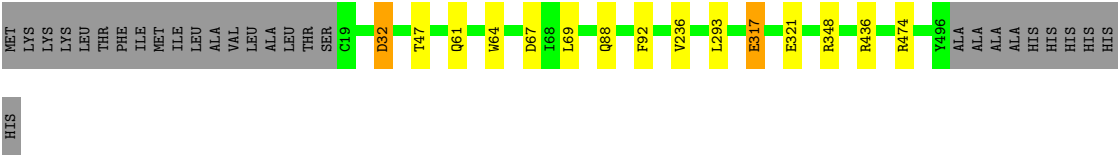
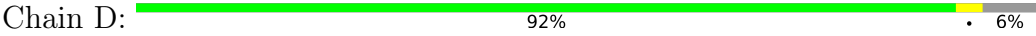


• Molecule 2: SusD homolog

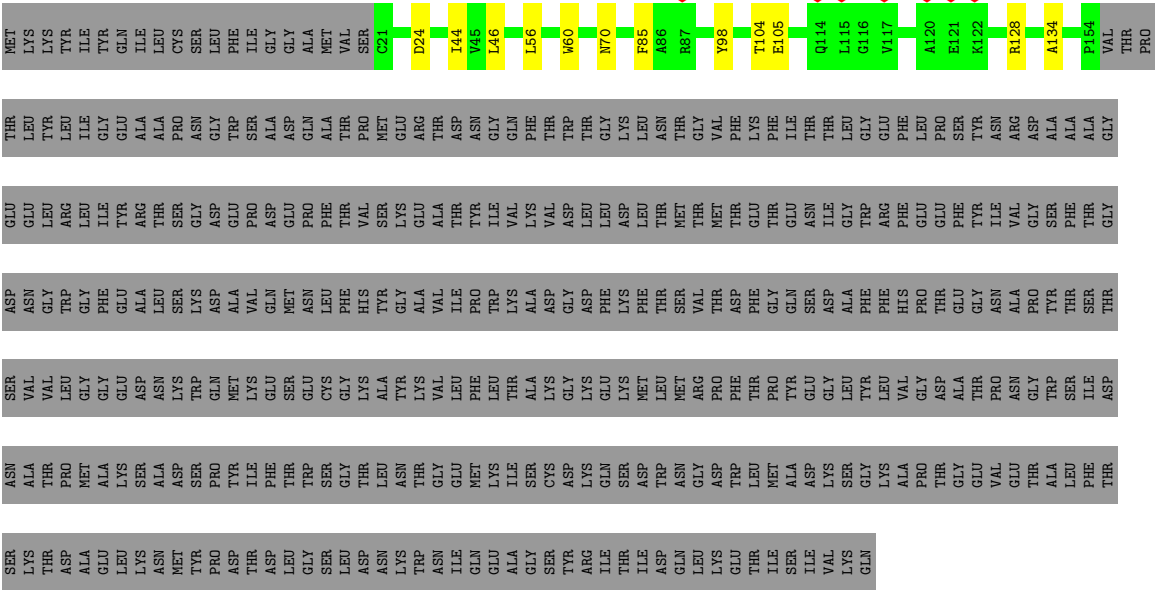




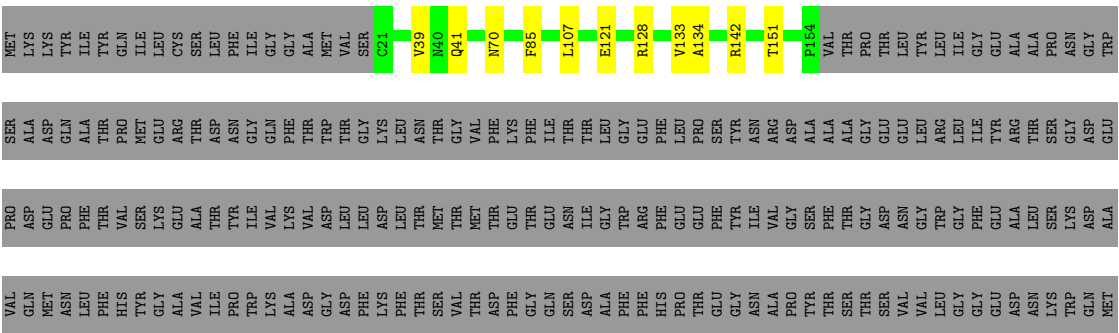
• Molecule 2: SusD homolog

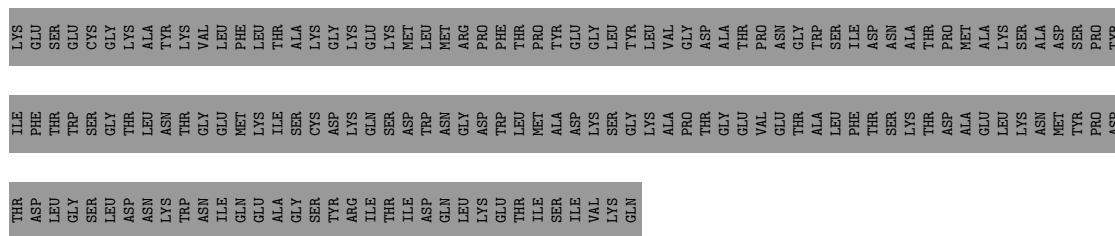


• Molecule 3: BT3088 (SGBPdex)

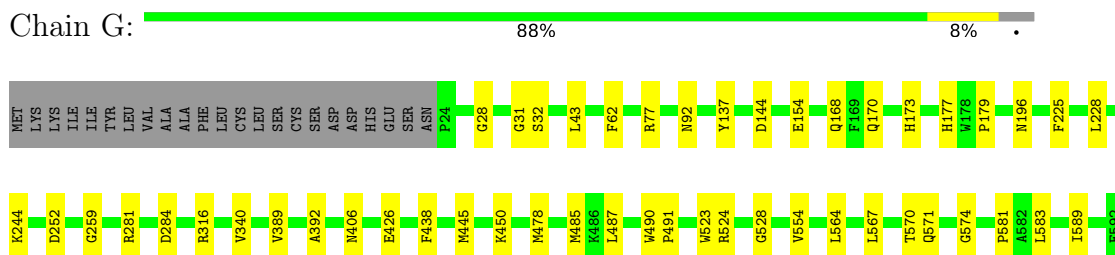


• Molecule 3: BT3088 (SGBPdex)

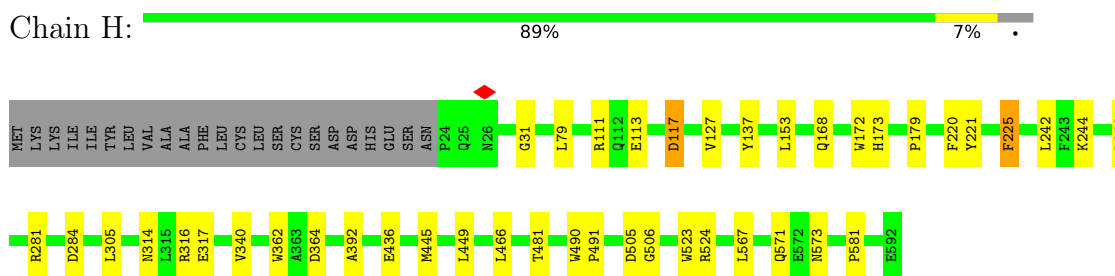




- Molecule 4: Cycloisomaltooligosaccharide glucanotransferase



- Molecule 4: Cycloisomaltooligosaccharide glucanotransferase



- Molecule 5: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose



- Molecule 5: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose



- Molecule 6: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose





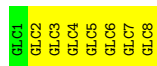
- Molecule 6: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain L:



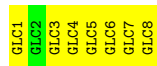
- Molecule 7: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain M:



- Molecule 7: alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose-(1-6)-alpha-D-glucopyranose

Chain N:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116104	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	23.1	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	332.4, 332.4, 332.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.831, 0.831, 0.831	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC

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	0.13	0/7076	0.42	0/9606
1	C	0.17	1/7076 (0.0%)	0.44	0/9606
2	B	0.13	0/3862	0.41	0/5245
2	D	0.13	0/3862	0.42	0/5245
3	E	0.11	0/1059	0.38	0/1439
3	F	0.10	0/1059	0.35	0/1439
4	G	0.11	0/4623	0.41	0/6283
4	H	0.11	0/4623	0.40	0/6283
All	All	0.13	1/33240 (0.0%)	0.41	0/45146

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	LYS	C-N	7.42	1.45	1.33

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	930	ARG	Sidechain

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	6913	0	6636	22	0
1	C	6913	0	6636	25	0
2	B	3776	0	3622	10	0
2	D	3776	0	3622	7	0
3	E	1044	0	1005	4	0
3	F	1044	0	1005	4	0
4	G	4504	0	4295	23	0
4	H	4504	0	4295	23	0
5	I	45	0	39	1	0
5	J	45	0	39	0	0
6	K	67	0	57	1	0
6	L	67	0	57	3	0
7	M	89	0	75	0	0
7	N	89	0	75	1	0
All	All	32876	0	31458	115	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 2.

All (115) 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:C:652:THR:HG22	2:D:47:THR:HG22	1.74	0.68
1:A:639:TYR:HB3	1:A:654:LEU:HA	1.75	0.67
1:A:930:ARG:NH1	1:A:974:GLU:OE2	2.28	0.66
1:C:173:ARG:NH1	1:C:671:GLN:OE1	2.25	0.64
4:G:445:MET:O	4:G:450:LYS:NZ	2.26	0.64
1:A:652:THR:OG1	1:A:653:ALA:N	2.28	0.63
4:G:31:GLY:O	4:G:571:GLN:N	2.31	0.63
4:H:436:GLU:HG3	6:L:2:GLC:H2	1.80	0.63
2:B:21:ASP:O	2:B:23:LEU:N	2.29	0.62
2:B:92:PHE:O	2:B:474:ARG:NH1	2.32	0.59
3:F:70:ASN:ND2	3:F:134:ALA:O	2.33	0.58
3:E:70:ASN:ND2	3:E:134:ALA:O	2.35	0.58
4:H:117:ASP:OD1	4:H:117:ASP:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:O	2:B:44:ALA:HB1	2.04	0.57
1:A:173:ARG:NH1	1:A:671:GLN:OE1	2.31	0.57
4:G:170:GLN:HE22	4:G:438:PHE:H	1.54	0.55
4:H:505:ASP:OD1	4:H:506:GLY:N	2.39	0.55
6:L:2:GLC:H4	6:L:3:GLC:H3	1.88	0.55
2:B:240:CYS:O	2:B:244:THR:HG23	2.05	0.55
1:C:657:THR:O	1:C:658:THR:HG22	2.07	0.54
1:C:630:ILE:HG21	1:C:700:LEU:HD13	1.91	0.53
2:D:317:GLU:OE2	2:D:436:ARG:NH2	2.29	0.53
2:D:61:GLN:HA	2:D:64:TRP:NE1	2.24	0.52
4:H:445:MET:HG3	4:H:449:LEU:HD23	1.90	0.52
4:G:28:GLY:O	4:G:574:GLY:N	2.40	0.52
4:H:314:ASN:ND2	4:H:317:GLU:OE1	2.38	0.52
1:A:741:ILE:HD12	1:A:742:PHE:H	1.74	0.52
1:C:762:SER:OG	1:C:763:GLU:N	2.43	0.52
1:C:714:THR:HG21	7:N:1:GLC:H2	1.91	0.51
4:G:406:ASN:ND2	4:G:528:GLY:O	2.39	0.51
4:H:31:GLY:HA3	4:H:571:GLN:HB3	1.91	0.51
1:A:139:ASP:OD1	1:A:954:ARG:NH1	2.44	0.51
1:A:604:ASP:C	1:A:606:PHE:H	2.18	0.50
1:C:604:ASP:C	1:C:606:PHE:H	2.18	0.50
2:B:29:TYR:HA	1:C:534:GLU:HG3	1.93	0.50
4:H:316:ARG:HG2	4:H:316:ARG:HH11	1.75	0.50
4:H:137:TYR:CZ	4:H:168:GLN:HB2	2.47	0.50
2:B:211:LYS:HD2	2:B:246:MET:HE1	1.95	0.49
4:H:79:LEU:HD22	4:H:466:LEU:HG	1.94	0.49
4:G:43:LEU:H	4:G:43:LEU:HD22	1.77	0.49
4:G:392:ALA:HB1	4:G:523:TRP:CZ3	2.48	0.48
2:B:381:ARG:NH2	2:B:438:GLU:OE2	2.42	0.48
1:C:336:LYS:HB3	1:C:416:LEU:HD21	1.96	0.47
4:G:490:TRP:CG	4:G:491:PRO:HA	2.49	0.47
1:C:661:ASN:HD21	1:C:664:ILE:HG23	1.78	0.47
4:G:137:TYR:CZ	4:G:168:GLN:HB2	2.49	0.47
2:D:321:GLU:OE2	2:D:436:ARG:NH1	2.47	0.47
1:A:639:TYR:CB	1:A:654:LEU:HA	2.45	0.46
4:G:173:HIS:HB2	4:G:179:PRO:HA	1.96	0.46
1:C:959:CYS:SG	1:C:962:VAL:HG22	2.56	0.46
4:H:172:TRP:NE1	4:H:220:PHE:HB2	2.30	0.46
1:C:119:THR:C	1:C:121:LYS:H	2.23	0.46
1:C:139:ASP:OD1	1:C:954:ARG:NH1	2.48	0.46
4:H:567:LEU:HD21	4:H:581:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:62:PHE:O	4:G:92:ASN:ND2	2.33	0.46
1:A:741:ILE:HD12	1:A:742:PHE:N	2.31	0.46
4:G:77:ARG:NH1	4:G:564:LEU:HB3	2.32	0.45
4:G:316:ARG:HH11	4:G:316:ARG:HG2	1.81	0.45
1:A:370:LYS:NZ	5:I:1:GLC:O4	2.40	0.45
1:A:645:PRO:HA	1:A:649:ASN:HA	1.97	0.45
4:H:392:ALA:HB1	4:H:523:TRP:CZ3	2.51	0.45
2:B:224:THR:HA	2:B:451:ARG:HD2	1.98	0.45
1:C:914:GLN:OE1	2:D:88:GLN:NE2	2.50	0.44
4:G:478:MET:HG2	4:G:487:LEU:HD22	1.99	0.44
4:G:524:ARG:HH11	4:G:524:ARG:HG3	1.83	0.44
1:C:931:LEU:HD21	1:C:934:ILE:HD11	2.00	0.44
1:A:946:GLN:O	1:A:948:ILE:N	2.50	0.44
1:A:959:CYS:SG	1:A:962:VAL:HG22	2.58	0.44
4:H:111:ARG:NH1	4:H:113:GLU:OE2	2.47	0.44
3:F:121:GLU:H	3:F:151:THR:HG1	1.63	0.44
4:G:144:ASP:OD1	4:G:144:ASP:N	2.50	0.44
1:A:604:ASP:O	1:A:605:TRP:CG	2.71	0.43
4:G:244:LYS:HE3	4:G:252:ASP:HA	2.00	0.43
1:C:500:LYS:HB3	1:C:500:LYS:HE3	1.72	0.43
1:C:604:ASP:O	1:C:605:TRP:CG	2.71	0.43
4:G:32:SER:HA	4:G:570:THR:HA	2.01	0.43
4:G:554:VAL:HG22	4:G:589:ILE:HG22	2.00	0.43
1:C:373:GLY:HA2	1:C:419:MET:O	2.19	0.43
4:H:490:TRP:CG	4:H:491:PRO:HA	2.54	0.43
1:A:630:ILE:HG21	1:A:700:LEU:HD13	2.00	0.43
4:H:244:LYS:HE3	4:H:252:ASP:HA	1.99	0.42
4:G:196:ASN:ND2	4:G:259:GLY:O	2.51	0.42
1:C:853:TYR:CE2	1:C:854:LYS:HE2	2.55	0.42
1:A:217:ALA:O	1:A:575:ARG:HD2	2.19	0.42
1:C:930:ARG:NH2	1:C:974:GLU:OE1	2.51	0.42
1:A:426:TYR:C	1:A:427:ASN:HD22	2.28	0.42
4:H:173:HIS:HB2	4:H:179:PRO:HA	2.01	0.42
2:B:56:SER:O	2:B:61:GLN:HB3	2.20	0.42
2:D:92:PHE:O	2:D:474:ARG:NH1	2.48	0.41
3:F:128:ARG:HE	3:F:142:ARG:HG2	1.84	0.41
1:C:532:ILE:HG22	1:C:537:ASN:ND2	2.35	0.41
2:D:348:ARG:HD3	4:H:364:ASP:OD1	2.20	0.41
2:B:400:ASP:N	2:B:400:ASP:OD1	2.53	0.41
3:E:85:PHE:CZ	3:E:128:ARG:HB2	2.55	0.41
4:H:281:ARG:NH1	4:H:284:ASP:OD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:505:ASP:CG	4:H:506:GLY:H	2.26	0.41
4:H:524:ARG:HH11	4:H:524:ARG:HG3	1.85	0.41
4:G:281:ARG:NH1	4:G:284:ASP:OD2	2.48	0.41
1:A:184:LEU:HD22	1:A:222:ARG:HB2	2.03	0.41
1:C:645:PRO:HA	1:C:649:ASN:HA	2.03	0.41
3:E:105:GLU:H	3:E:105:GLU:CD	2.29	0.41
1:A:214:SER:O	1:A:559:ARG:NH2	2.48	0.41
1:C:184:LEU:HD22	1:C:222:ARG:HB2	2.03	0.41
1:C:870:ILE:HD11	1:C:973:PRO:O	2.21	0.41
4:G:177:HIS:HE1	4:G:228:LEU:HB2	1.86	0.41
4:G:567:LEU:HD21	4:G:581:PRO:HD3	2.02	0.41
4:H:225:PHE:C	4:H:225:PHE:CD1	2.98	0.41
6:K:3:GLC:O4	6:K:4:GLC:H5	2.21	0.41
1:A:641:THR:HA	1:A:653:ALA:HA	2.02	0.41
4:H:242:LEU:HD23	4:H:305:LEU:HD13	2.03	0.40
1:A:159:ILE:HD12	1:A:977:VAL:HG22	2.03	0.40
3:E:60:TRP:CE2	3:E:98:TYR:HA	2.57	0.40
3:F:85:PHE:CZ	3:F:128:ARG:HB2	2.57	0.40
1:C:841:PRO:HG2	1:C:844:PHE:CZ	2.56	0.40
4:H:362:TRP:CE2	6:L:1:GLC:H61	2.56	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	879/999 (88%)	830 (94%)	39 (4%)	10 (1%)	11	22
1	C	879/999 (88%)	828 (94%)	40 (5%)	11 (1%)	9	18
2	B	476/506 (94%)	456 (96%)	20 (4%)	0	100	100
2	D	476/506 (94%)	460 (97%)	15 (3%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	132/504 (26%)	129 (98%)	2 (2%)	1 (1%)	16	31
3	F	132/504 (26%)	129 (98%)	3 (2%)	0	100	100
4	G	567/592 (96%)	541 (95%)	25 (4%)	1 (0%)	43	63
4	H	567/592 (96%)	546 (96%)	21 (4%)	0	100	100
All	All	4108/5202 (79%)	3919 (95%)	165 (4%)	24 (1%)	23	38

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	654	LEU
1	A	220	GLY
1	A	649	ASN
1	C	220	GLY
1	C	658	THR
1	A	605	TRP
1	A	653	ALA
1	A	718	PHE
1	A	947	LYS
1	C	527	PHE
1	C	653	ALA
1	C	716	GLU
3	E	24	ASP
1	A	946	GLN
1	C	526	ILE
1	C	605	TRP
1	C	649	ASN
1	A	526	ILE
1	A	660	SER
1	C	120	MET
1	C	705	ILE
1	A	705	ILE
4	G	426	GLU
2	D	32	ASP

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	747/846 (88%)	740 (99%)	7 (1%)	70	87
1	C	747/846 (88%)	739 (99%)	8 (1%)	65	84
2	B	403/425 (95%)	397 (98%)	6 (2%)	57	80
2	D	403/425 (95%)	397 (98%)	6 (2%)	57	80
3	E	112/423 (26%)	108 (96%)	4 (4%)	31	58
3	F	112/423 (26%)	108 (96%)	4 (4%)	31	58
4	G	477/498 (96%)	471 (99%)	6 (1%)	61	82
4	H	477/498 (96%)	469 (98%)	8 (2%)	53	78
All	All	3478/4384 (79%)	3429 (99%)	49 (1%)	57	81

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	MET
1	A	186	VAL
1	A	600	VAL
1	A	652	THR
1	A	654	LEU
1	A	741	ILE
1	A	796	LEU
2	B	29	TYR
2	B	52	THR
2	B	67	ASP
2	B	128	SER
2	B	293	LEU
2	B	425	GLU
1	C	212	ASP
1	C	227	VAL
1	C	500	LYS
1	C	676	VAL
1	C	760	LEU
1	C	776	VAL
1	C	787	VAL
1	C	865	VAL
2	D	32	ASP
2	D	67	ASP
2	D	69	LEU
2	D	236	VAL

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Mol	Chain	Res	Type
2	D	293	LEU
2	D	317	GLU
3	E	44	ILE
3	E	46	LEU
3	E	56	LEU
3	E	104	THR
3	F	39	VAL
3	F	41	GLN
3	F	107	LEU
3	F	133	VAL
4	G	154	GLU
4	G	225	PHE
4	G	340	VAL
4	G	389	VAL
4	G	485	MET
4	G	583	LEU
4	H	117	ASP
4	H	127	VAL
4	H	153	LEU
4	H	221	TYR
4	H	225	PHE
4	H	340	VAL
4	H	481	THR
4	H	573	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	225	ASN
1	A	245	ASN
1	A	251	GLN
1	A	331	GLN
1	A	362	ASN
1	A	427	ASN
1	A	459	ASN
1	A	515	ASN
1	A	650	ASN
1	A	761	ASN
1	A	770	GLN
1	A	773	ASN
2	B	242	GLN

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Mol	Chain	Res	Type
2	B	401	GLN
1	C	251	GLN
1	C	331	GLN
1	C	362	ASN
1	C	459	ASN
1	C	481	ASN
1	C	515	ASN
1	C	516	ASN
1	C	650	ASN
1	C	661	ASN
1	C	755	ASN
1	C	809	GLN
1	C	913	ASN
1	C	996	ASN
2	D	242	GLN
2	D	352	ASN
3	E	114	GLN
3	F	114	GLN
3	F	153	GLN
4	G	330	HIS
4	G	384	ASN
4	G	488	ASN
4	H	114	ASN
4	H	160	ASN
4	H	295	GLN
4	H	330	HIS
4	H	395	ASN
4	H	440	ASN
4	H	474	ASN
4	H	488	ASN
4	H	508	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 ⓘ

36 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	$\# Z > 2$
5	GLC	I	1	5	12,12,12	0.43	0	17,17,17	1.36	3 (17%)
5	GLC	I	2	5	11,11,12	0.49	0	15,15,17	1.11	1 (6%)
5	GLC	I	3	5	11,11,12	0.58	0	15,15,17	0.88	0
5	GLC	I	4	5	11,11,12	0.37	0	15,15,17	0.78	0
5	GLC	J	1	5	12,12,12	0.48	0	17,17,17	1.04	1 (5%)
5	GLC	J	2	5	11,11,12	0.24	0	15,15,17	0.68	0
5	GLC	J	3	5	11,11,12	0.56	0	15,15,17	1.34	1 (6%)
5	GLC	J	4	5	11,11,12	0.59	0	15,15,17	0.92	1 (6%)
6	GLC	K	1	6	12,12,12	0.48	0	17,17,17	0.63	0
6	GLC	K	2	6	11,11,12	0.20	0	15,15,17	0.70	0
6	GLC	K	3	6	11,11,12	0.21	0	15,15,17	0.76	1 (6%)
6	GLC	K	4	6	11,11,12	0.42	0	15,15,17	0.88	1 (6%)
6	GLC	K	5	6	11,11,12	0.66	0	15,15,17	1.05	1 (6%)
6	GLC	K	6	6	11,11,12	0.55	0	15,15,17	1.07	1 (6%)
6	GLC	L	1	6	12,12,12	0.45	0	17,17,17	0.64	0
6	GLC	L	2	6	11,11,12	0.28	0	15,15,17	0.75	0
6	GLC	L	3	6	11,11,12	0.30	0	15,15,17	1.31	1 (6%)
6	GLC	L	4	6	11,11,12	0.19	0	15,15,17	0.85	1 (6%)
6	GLC	L	5	6	11,11,12	0.62	0	15,15,17	1.37	2 (13%)
6	GLC	L	6	6	11,11,12	0.59	0	15,15,17	1.05	1 (6%)
7	GLC	M	1	7	12,12,12	0.11	0	17,17,17	0.28	0
7	GLC	M	2	7	11,11,12	0.31	0	15,15,17	0.74	1 (6%)
7	GLC	M	3	7	11,11,12	0.57	0	15,15,17	1.37	1 (6%)
7	GLC	M	4	7	11,11,12	0.59	0	15,15,17	1.14	2 (13%)
7	GLC	M	5	7	11,11,12	0.62	0	15,15,17	0.97	1 (6%)
7	GLC	M	6	7	11,11,12	0.57	0	15,15,17	1.08	1 (6%)
7	GLC	M	7	7	11,11,12	0.61	0	15,15,17	1.14	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GLC	M	8	7	11,11,12	0.62	0	15,15,17	0.85	1 (6%)
7	GLC	N	1	7	12,12,12	0.44	0	17,17,17	0.60	0
7	GLC	N	2	7	11,11,12	0.18	0	15,15,17	0.81	0
7	GLC	N	3	7	11,11,12	0.57	0	15,15,17	1.25	1 (6%)
7	GLC	N	4	7	11,11,12	0.59	0	15,15,17	1.00	1 (6%)
7	GLC	N	5	7	11,11,12	0.62	0	15,15,17	0.86	1 (6%)
7	GLC	N	6	7	11,11,12	0.54	0	15,15,17	1.27	1 (6%)
7	GLC	N	7	7	11,11,12	0.61	0	15,15,17	1.01	1 (6%)
7	GLC	N	8	7	11,11,12	0.60	0	15,15,17	0.90	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GLC	I	1	5	-	2/2/22/22	0/1/1/1
5	GLC	I	2	5	-	2/2/19/22	0/1/1/1
5	GLC	I	3	5	-	0/2/19/22	0/1/1/1
5	GLC	I	4	5	-	2/2/19/22	0/1/1/1
5	GLC	J	1	5	-	2/2/22/22	0/1/1/1
5	GLC	J	2	5	-	2/2/19/22	0/1/1/1
5	GLC	J	3	5	-	0/2/19/22	0/1/1/1
5	GLC	J	4	5	-	0/2/19/22	0/1/1/1
6	GLC	K	1	6	-	0/2/22/22	0/1/1/1
6	GLC	K	2	6	-	0/2/19/22	0/1/1/1
6	GLC	K	3	6	-	1/2/19/22	0/1/1/1
6	GLC	K	4	6	-	2/2/19/22	0/1/1/1
6	GLC	K	5	6	-	2/2/19/22	0/1/1/1
6	GLC	K	6	6	-	0/2/19/22	0/1/1/1
6	GLC	L	1	6	-	0/2/22/22	0/1/1/1
6	GLC	L	2	6	-	2/2/19/22	0/1/1/1
6	GLC	L	3	6	-	1/2/19/22	0/1/1/1
6	GLC	L	4	6	-	0/2/19/22	0/1/1/1
6	GLC	L	5	6	-	1/2/19/22	0/1/1/1
6	GLC	L	6	6	-	1/2/19/22	0/1/1/1
7	GLC	M	1	7	-	0/2/22/22	0/1/1/1
7	GLC	M	2	7	-	0/2/19/22	0/1/1/1
7	GLC	M	3	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLC	M	4	7	-	0/2/19/22	0/1/1/1
7	GLC	M	5	7	-	2/2/19/22	0/1/1/1
7	GLC	M	6	7	-	0/2/19/22	0/1/1/1
7	GLC	M	7	7	-	0/2/19/22	0/1/1/1
7	GLC	M	8	7	-	0/2/19/22	0/1/1/1
7	GLC	N	1	7	-	0/2/22/22	0/1/1/1
7	GLC	N	2	7	-	0/2/19/22	0/1/1/1
7	GLC	N	3	7	-	0/2/19/22	0/1/1/1
7	GLC	N	4	7	-	0/2/19/22	0/1/1/1
7	GLC	N	5	7	-	2/2/19/22	0/1/1/1
7	GLC	N	6	7	-	0/2/19/22	0/1/1/1
7	GLC	N	7	7	-	0/2/19/22	0/1/1/1
7	GLC	N	8	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	N	6	GLC	C1-O5-C5	4.52	118.31	112.19
5	J	3	GLC	C1-O5-C5	4.47	118.24	112.19
7	M	3	GLC	C1-O5-C5	4.09	117.73	112.19
6	L	3	GLC	O5-C1-C2	-3.96	104.66	110.77
7	M	7	GLC	C1-O5-C5	3.78	117.32	112.19
6	K	6	GLC	C1-O5-C5	3.66	117.16	112.19
7	M	6	GLC	C1-O5-C5	3.66	117.15	112.19
6	L	5	GLC	C1-O5-C5	3.62	117.09	112.19
7	N	3	GLC	C1-O5-C5	3.53	116.98	112.19
5	I	1	GLC	O6-C6-C5	-3.40	99.64	111.29
7	N	7	GLC	C1-O5-C5	3.34	116.72	112.19
7	M	4	GLC	C1-O5-C5	3.28	116.64	112.19
6	L	5	GLC	C1-C2-C3	3.23	113.64	109.67
7	M	5	GLC	C1-O5-C5	3.14	116.45	112.19
5	I	2	GLC	C1-O5-C5	3.03	116.29	112.19
5	J	4	GLC	C1-O5-C5	2.99	116.25	112.19
7	N	4	GLC	C1-O5-C5	2.85	116.05	112.19
7	N	8	GLC	C1-O5-C5	2.79	115.97	112.19
5	J	1	GLC	C1-O5-C5	-2.64	108.67	113.66
7	M	8	GLC	C1-O5-C5	2.59	115.70	112.19
7	N	5	GLC	C1-O5-C5	2.57	115.68	112.19
6	K	5	GLC	C1-C2-C3	2.51	112.75	109.67
6	K	3	GLC	C1-C2-C3	2.49	112.72	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	M	4	GLC	O5-C5-C6	2.38	110.93	107.20
6	L	6	GLC	C1-O5-C5	2.30	115.31	112.19
6	K	4	GLC	O5-C1-C2	-2.24	107.31	110.77
5	I	1	GLC	C1-O5-C5	-2.24	109.44	113.66
5	I	1	GLC	O5-C5-C6	2.24	112.00	106.44
7	M	2	GLC	C1-C2-C3	2.04	112.18	109.67
6	L	4	GLC	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (24) torsion outliers are listed below:

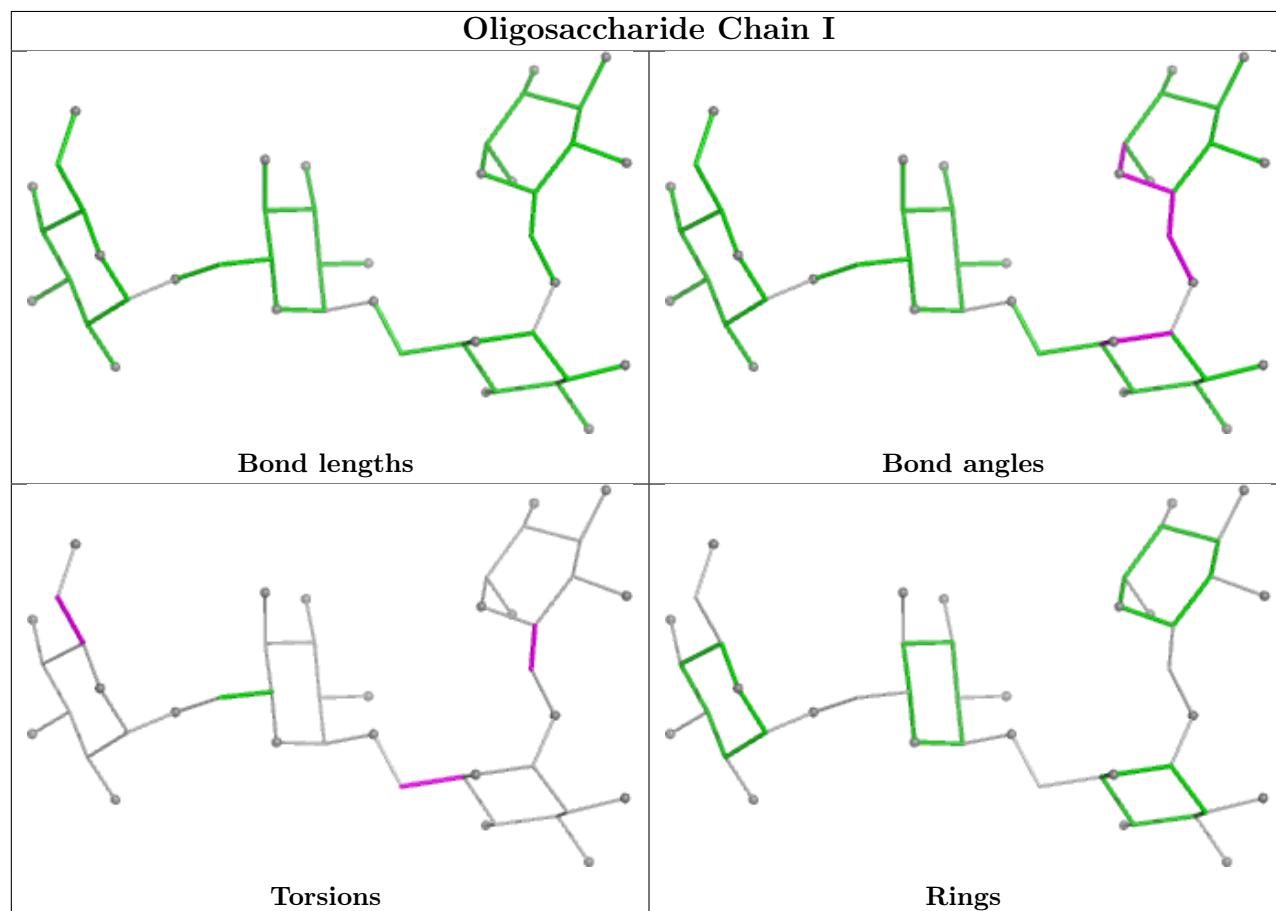
Mol	Chain	Res	Type	Atoms
6	K	5	GLC	C4-C5-C6-O6
5	I	1	GLC	O5-C5-C6-O6
5	J	1	GLC	O5-C5-C6-O6
5	J	1	GLC	C4-C5-C6-O6
6	K	5	GLC	O5-C5-C6-O6
7	N	5	GLC	O5-C5-C6-O6
5	I	1	GLC	C4-C5-C6-O6
7	M	5	GLC	O5-C5-C6-O6
5	J	2	GLC	C4-C5-C6-O6
5	I	4	GLC	O5-C5-C6-O6
5	I	4	GLC	C4-C5-C6-O6
5	J	2	GLC	O5-C5-C6-O6
7	M	5	GLC	C4-C5-C6-O6
5	I	2	GLC	C4-C5-C6-O6
6	L	2	GLC	C4-C5-C6-O6
7	N	5	GLC	C4-C5-C6-O6
5	I	2	GLC	O5-C5-C6-O6
6	K	4	GLC	O5-C5-C6-O6
6	L	3	GLC	C4-C5-C6-O6
6	L	2	GLC	O5-C5-C6-O6
6	L	5	GLC	C4-C5-C6-O6
6	K	3	GLC	C4-C5-C6-O6
6	L	6	GLC	C4-C5-C6-O6
6	K	4	GLC	C4-C5-C6-O6

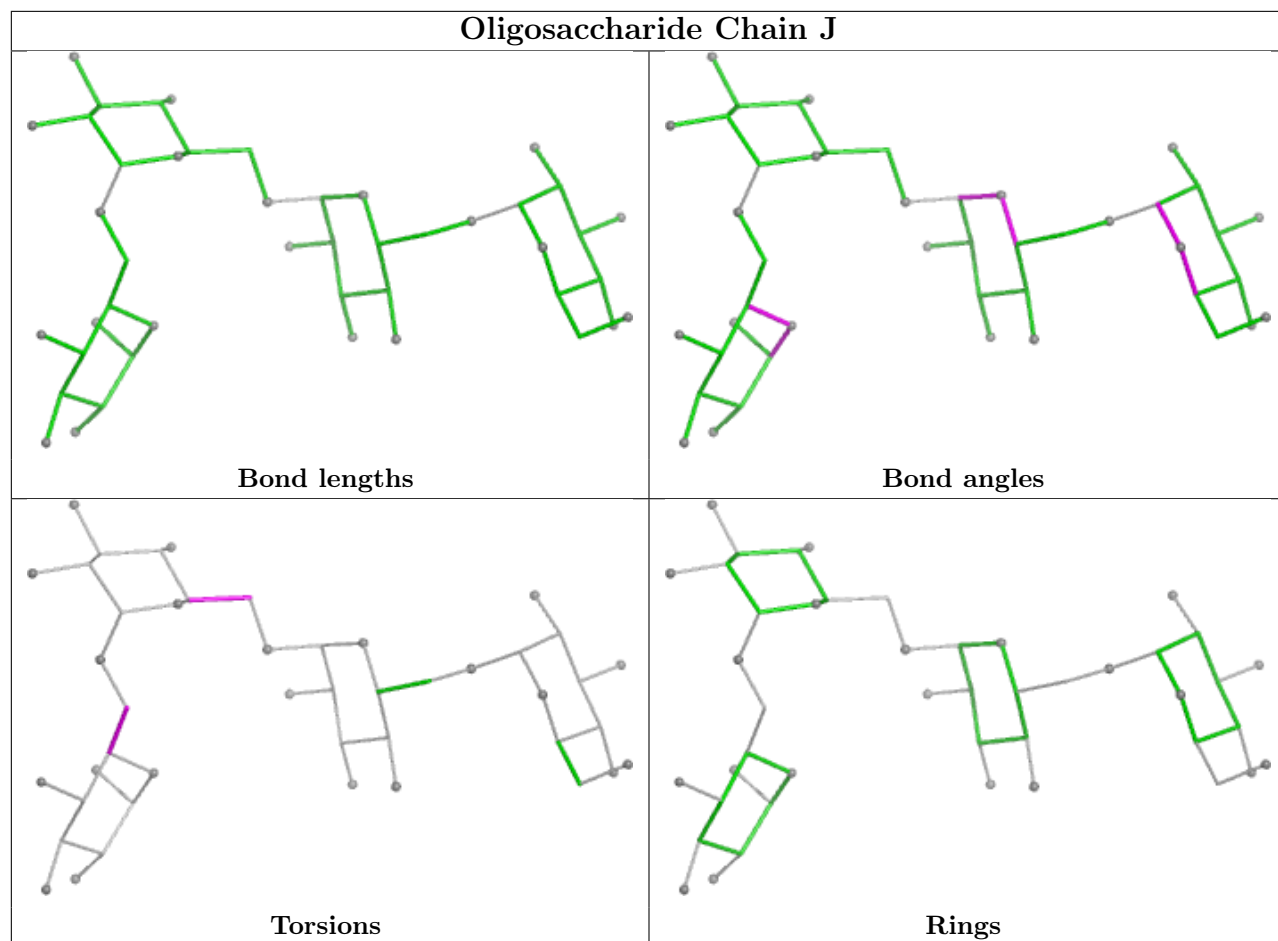
There are no ring outliers.

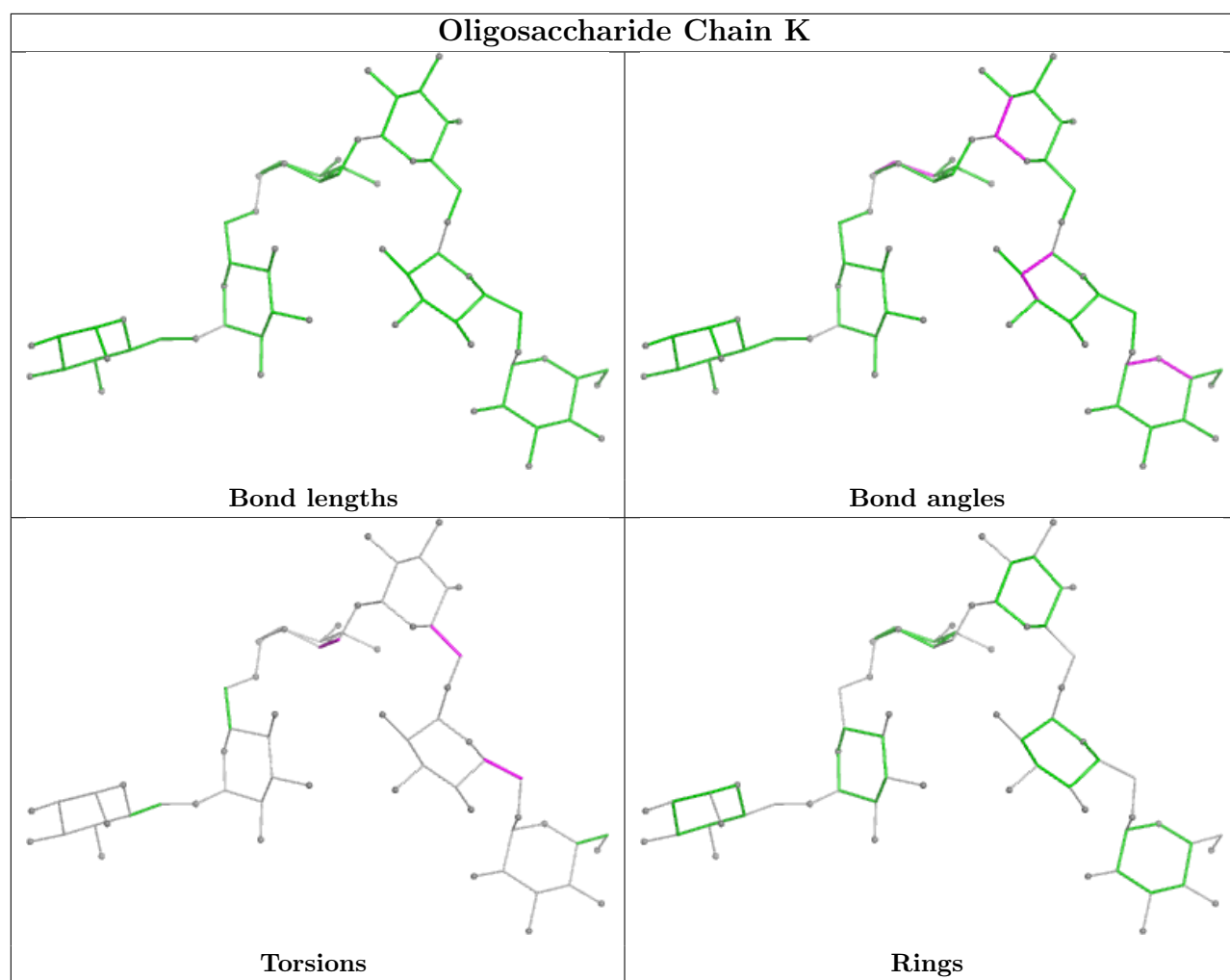
7 monomers are involved in 6 short contacts:

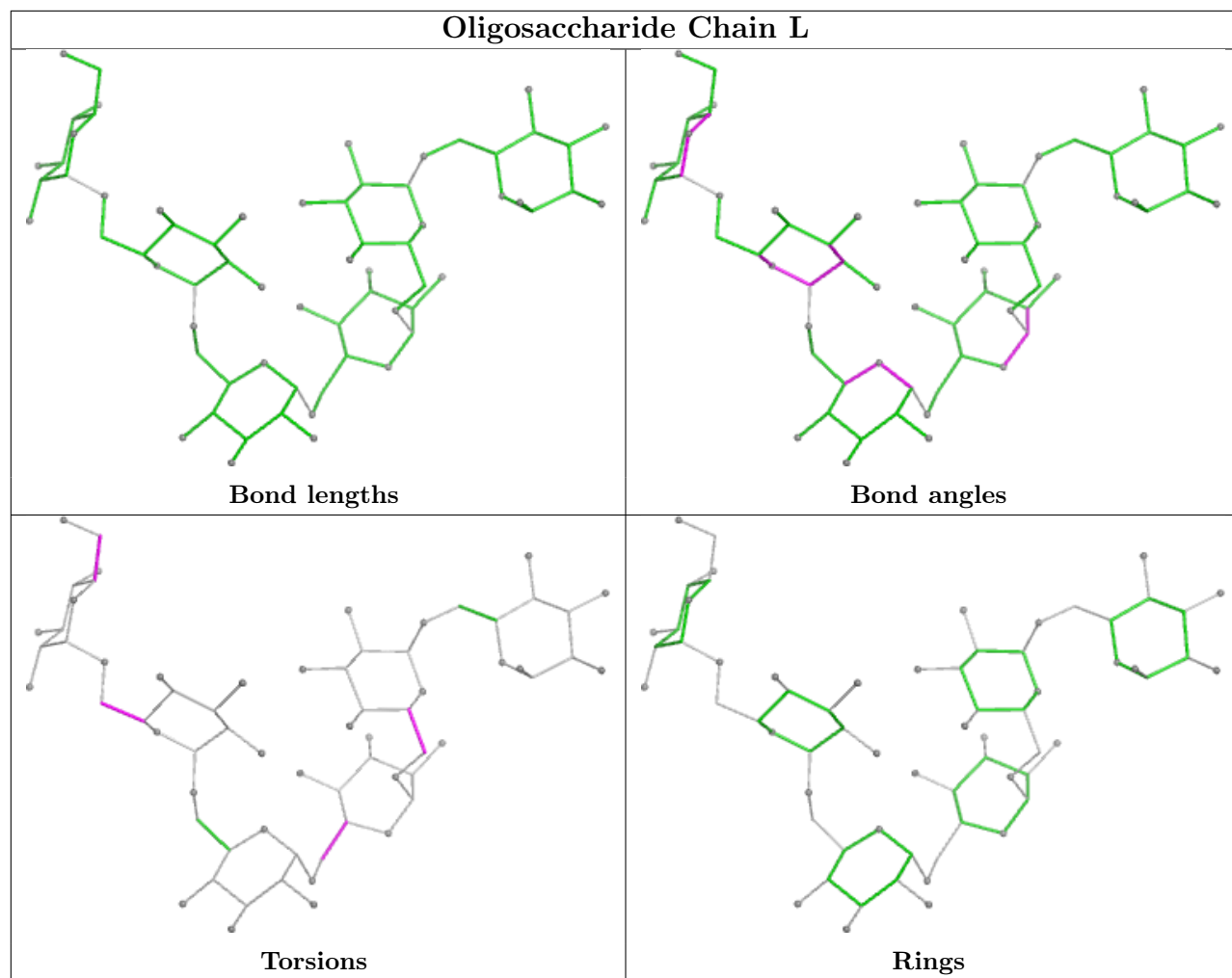
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	K	3	GLC	1	0
6	L	1	GLC	1	0
6	L	3	GLC	1	0
5	I	1	GLC	1	0
6	L	2	GLC	2	0
7	N	1	GLC	1	0
6	K	4	GLC	1	0

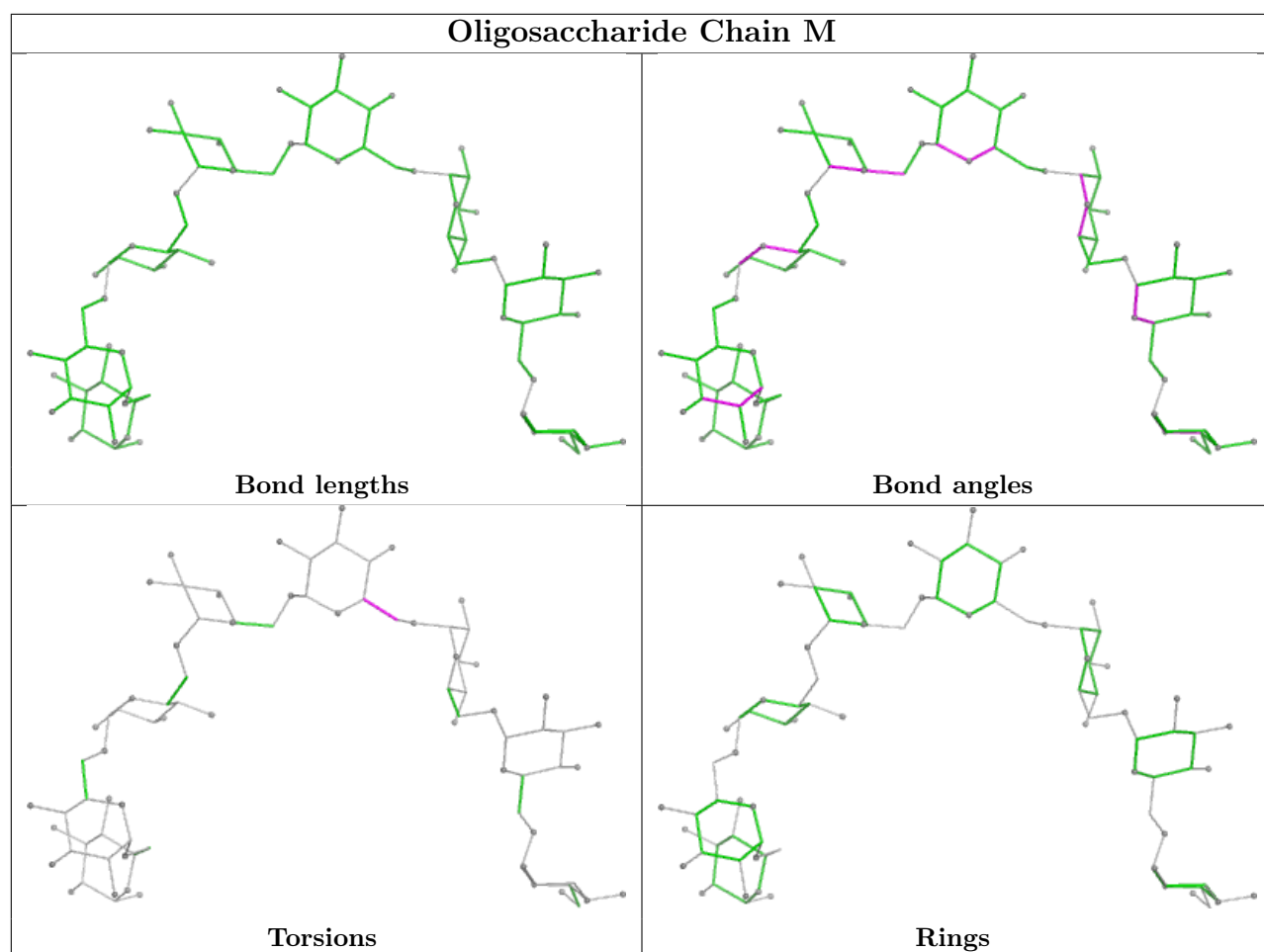
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

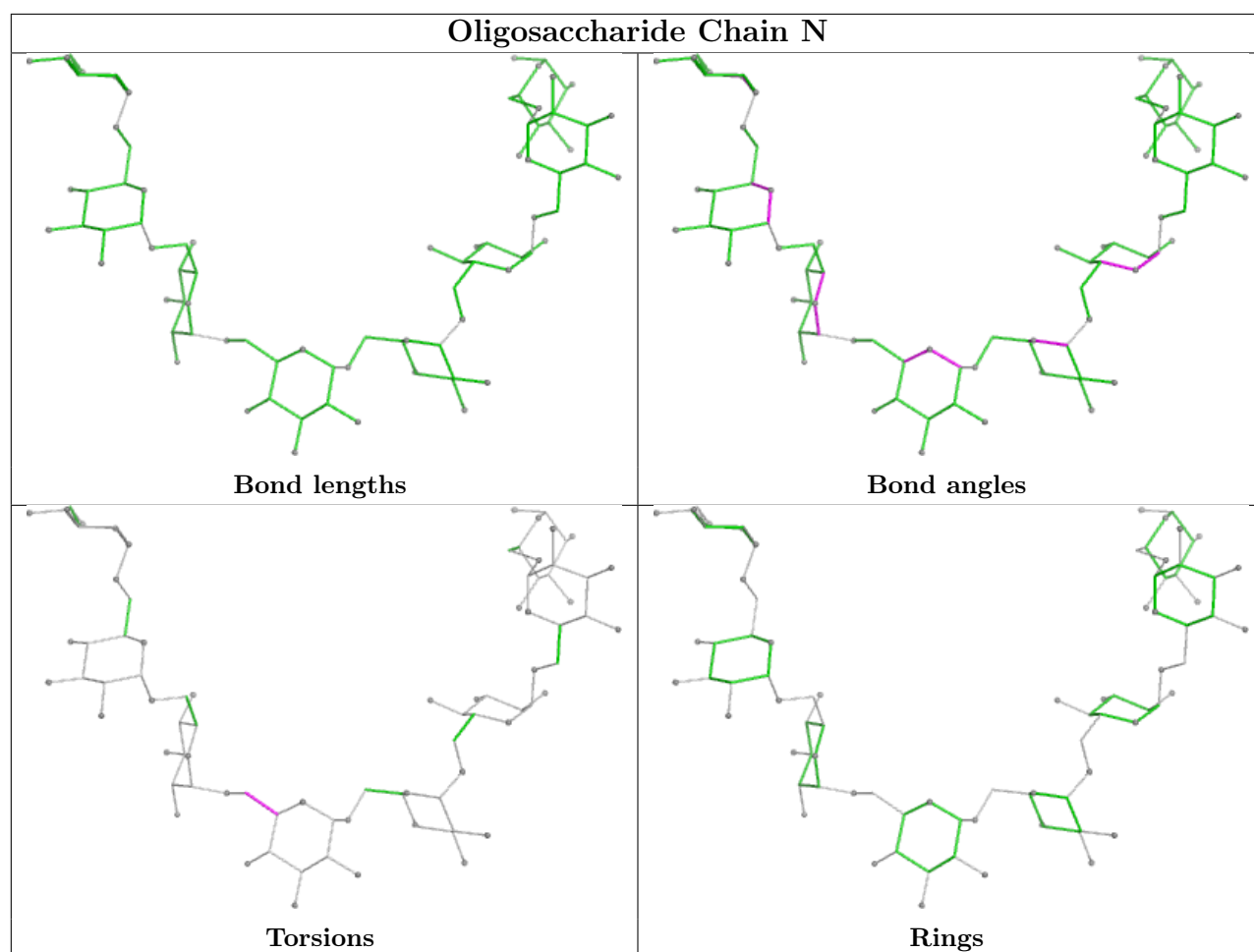












5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

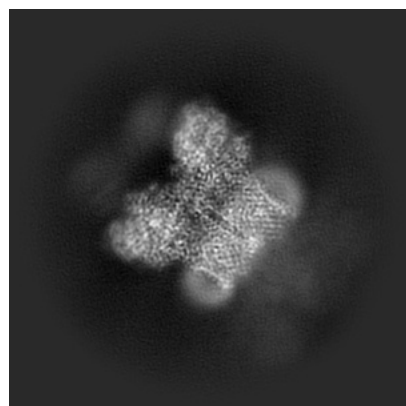
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55024. These allow visual inspection of the internal detail of the map and identification of artifacts.

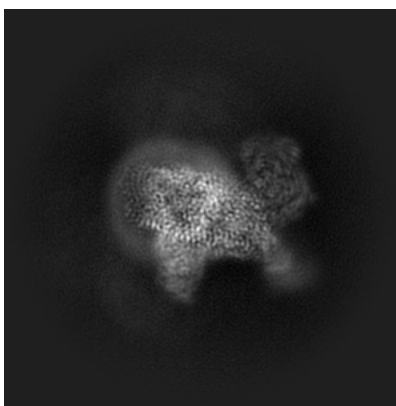
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

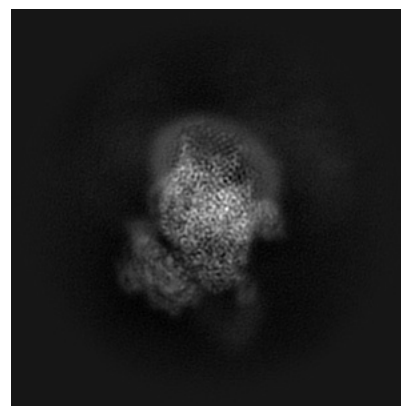
6.1.1 Primary map



X

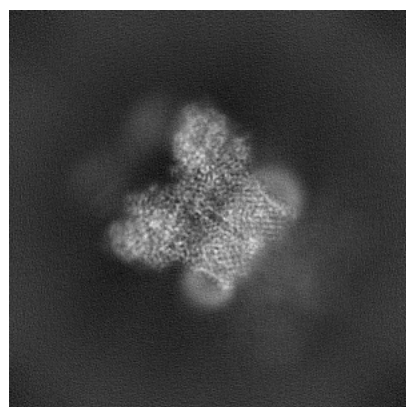


Y

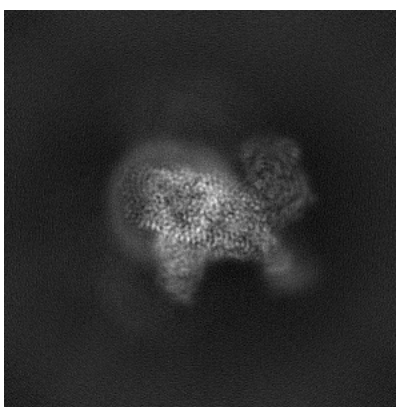


Z

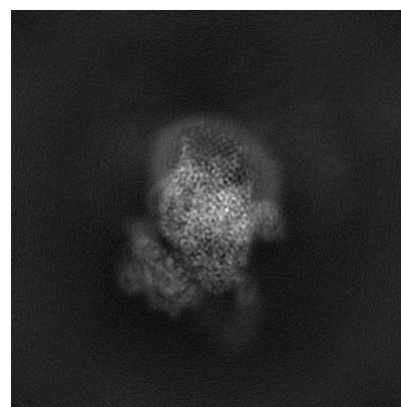
6.1.2 Raw map



X



Y

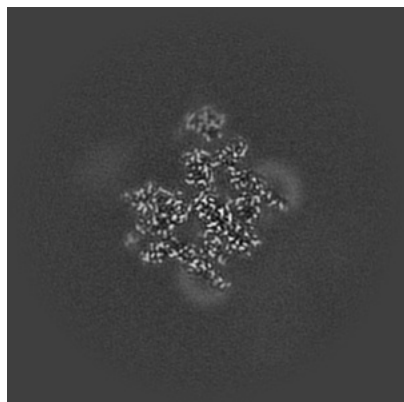


Z

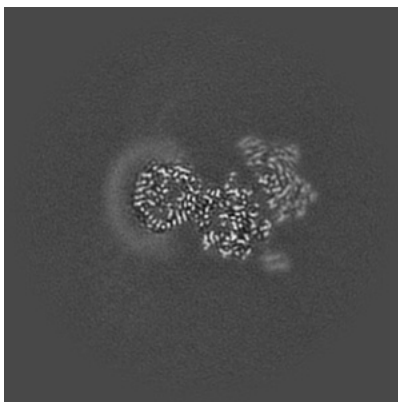
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

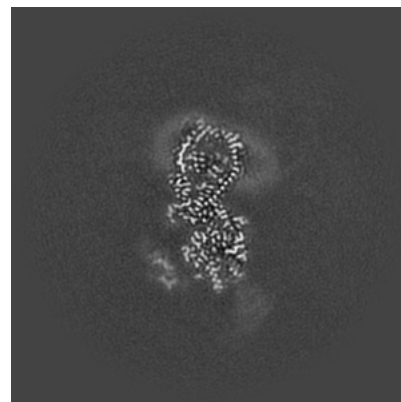
6.2.1 Primary map



X Index: 200

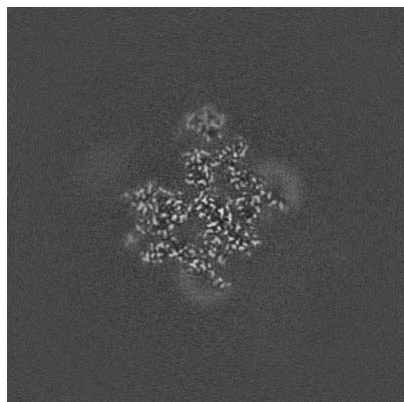


Y Index: 200

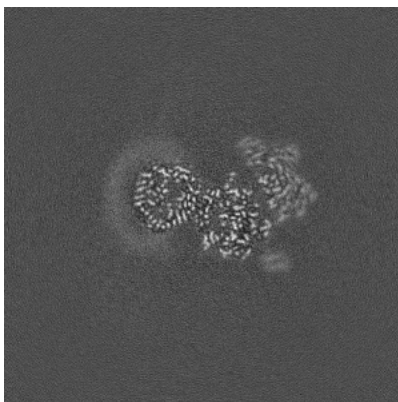


Z Index: 200

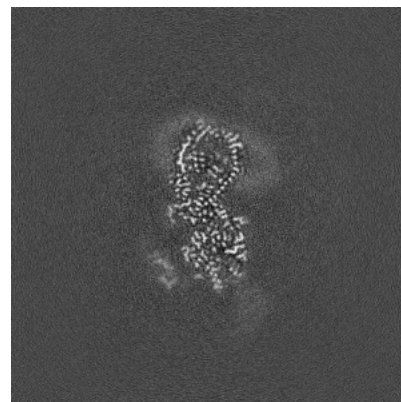
6.2.2 Raw map



X Index: 200



Y Index: 200

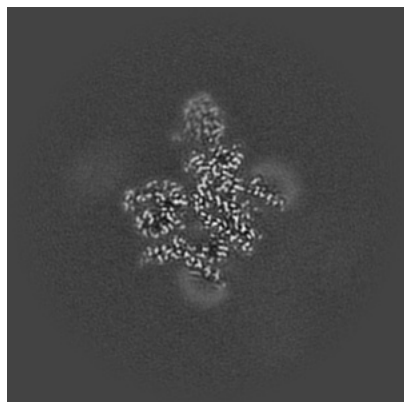


Z Index: 200

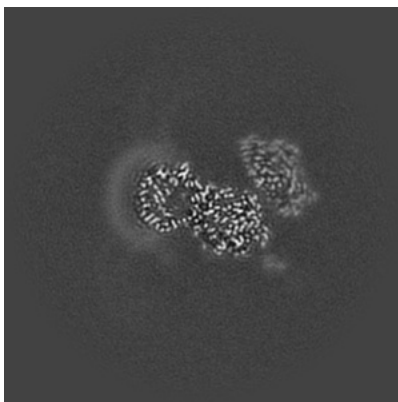
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

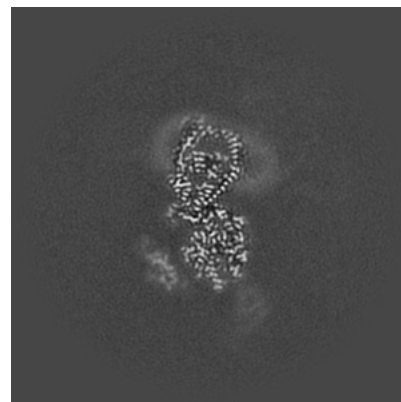
6.3.1 Primary map



X Index: 210

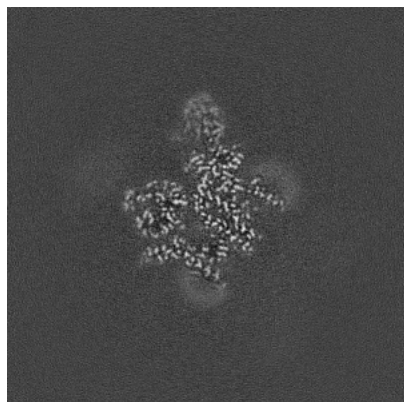


Y Index: 195

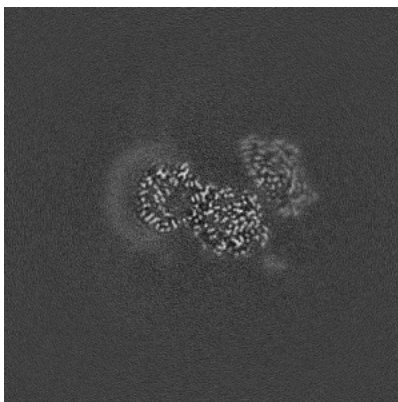


Z Index: 199

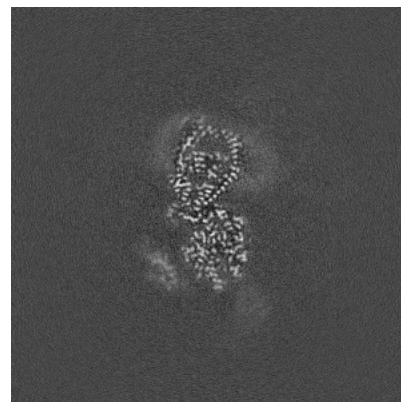
6.3.2 Raw map



X Index: 210



Y Index: 195

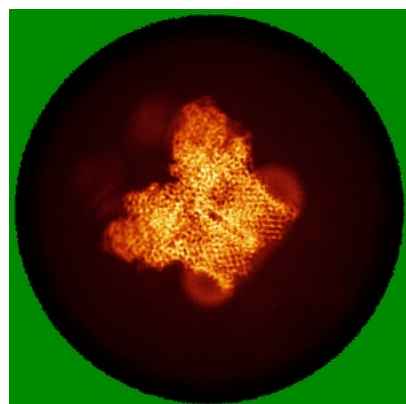


Z Index: 199

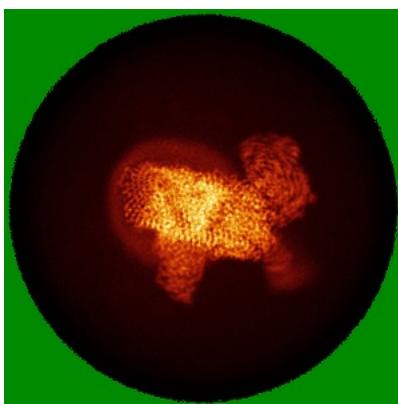
The images above show the largest variance slices of the map in three orthogonal directions.

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

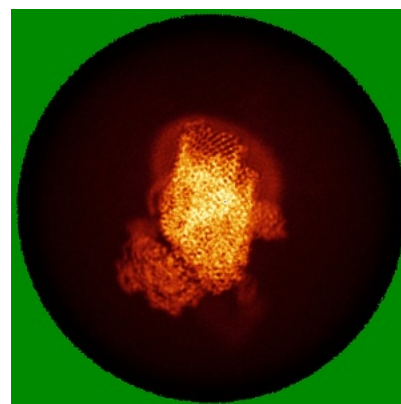
6.4.1 Primary map



X

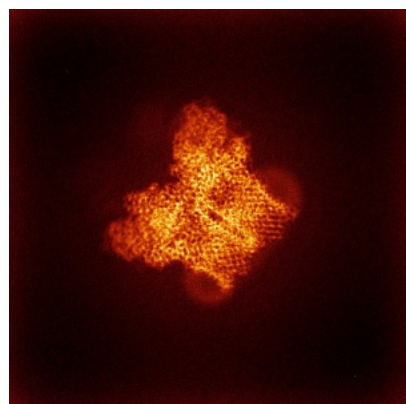


Y

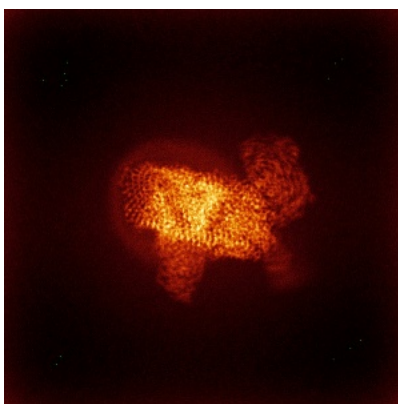


Z

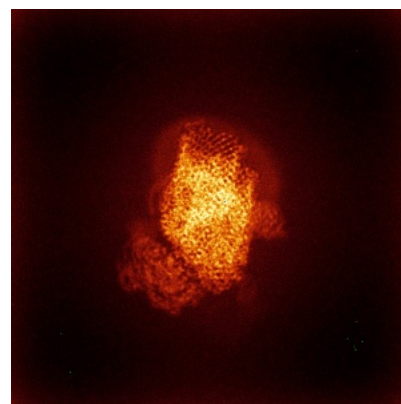
6.4.2 Raw map



X



Y

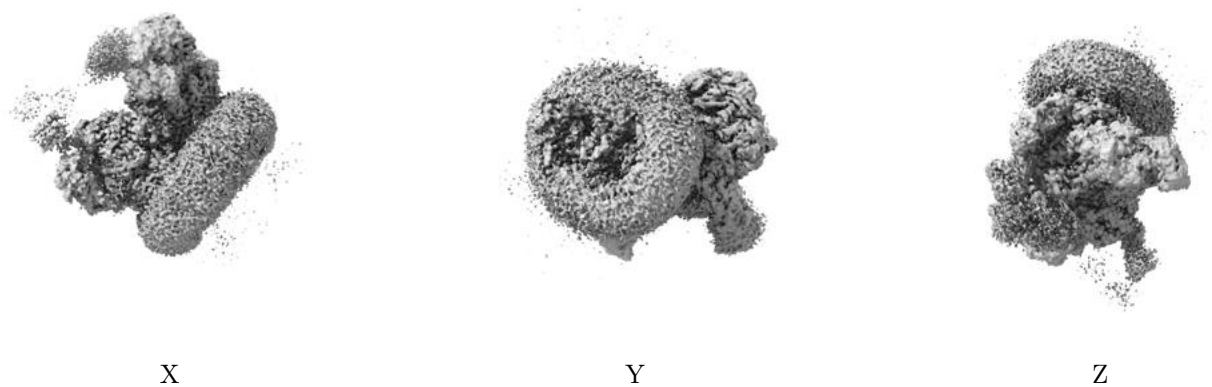


Z

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.

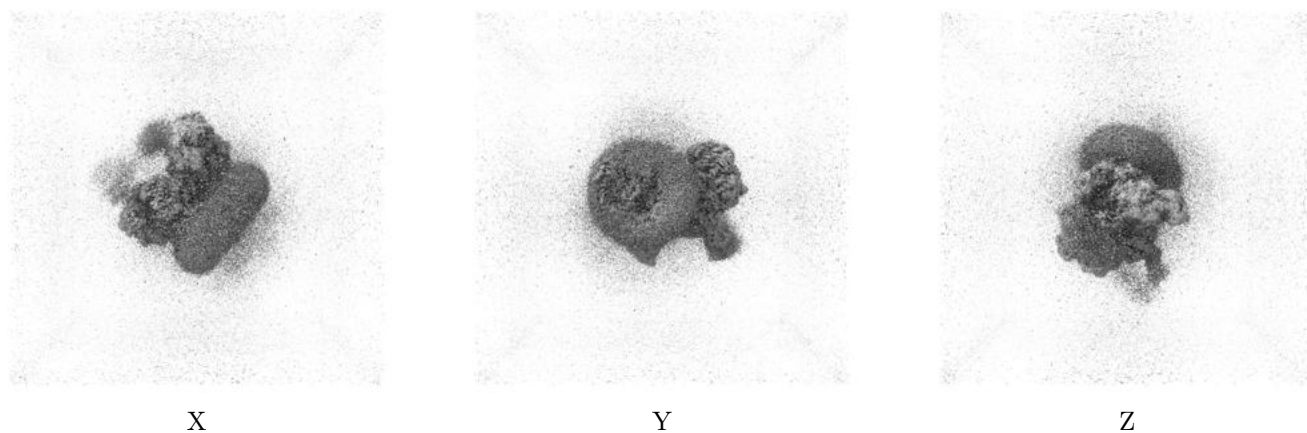
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

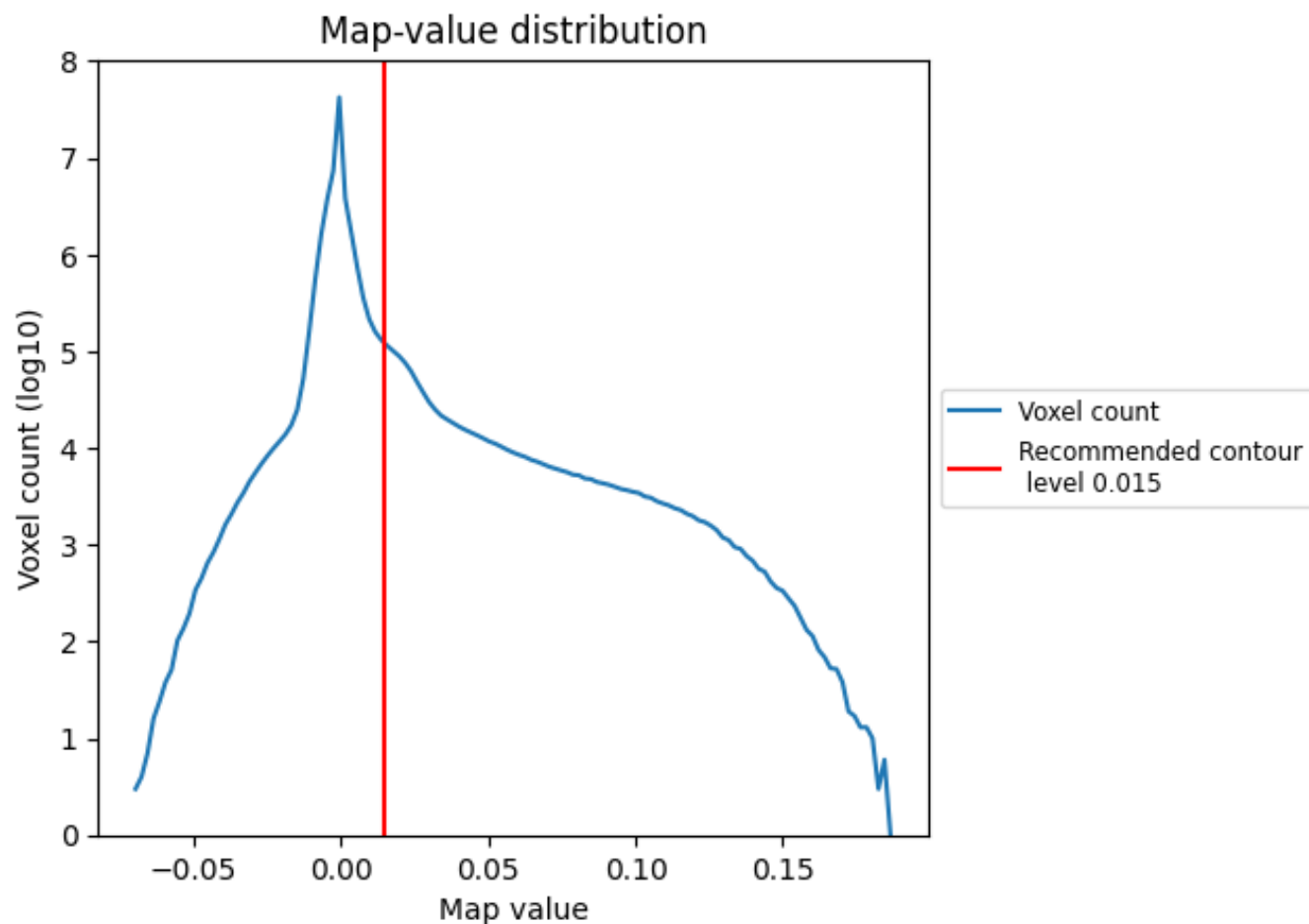
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

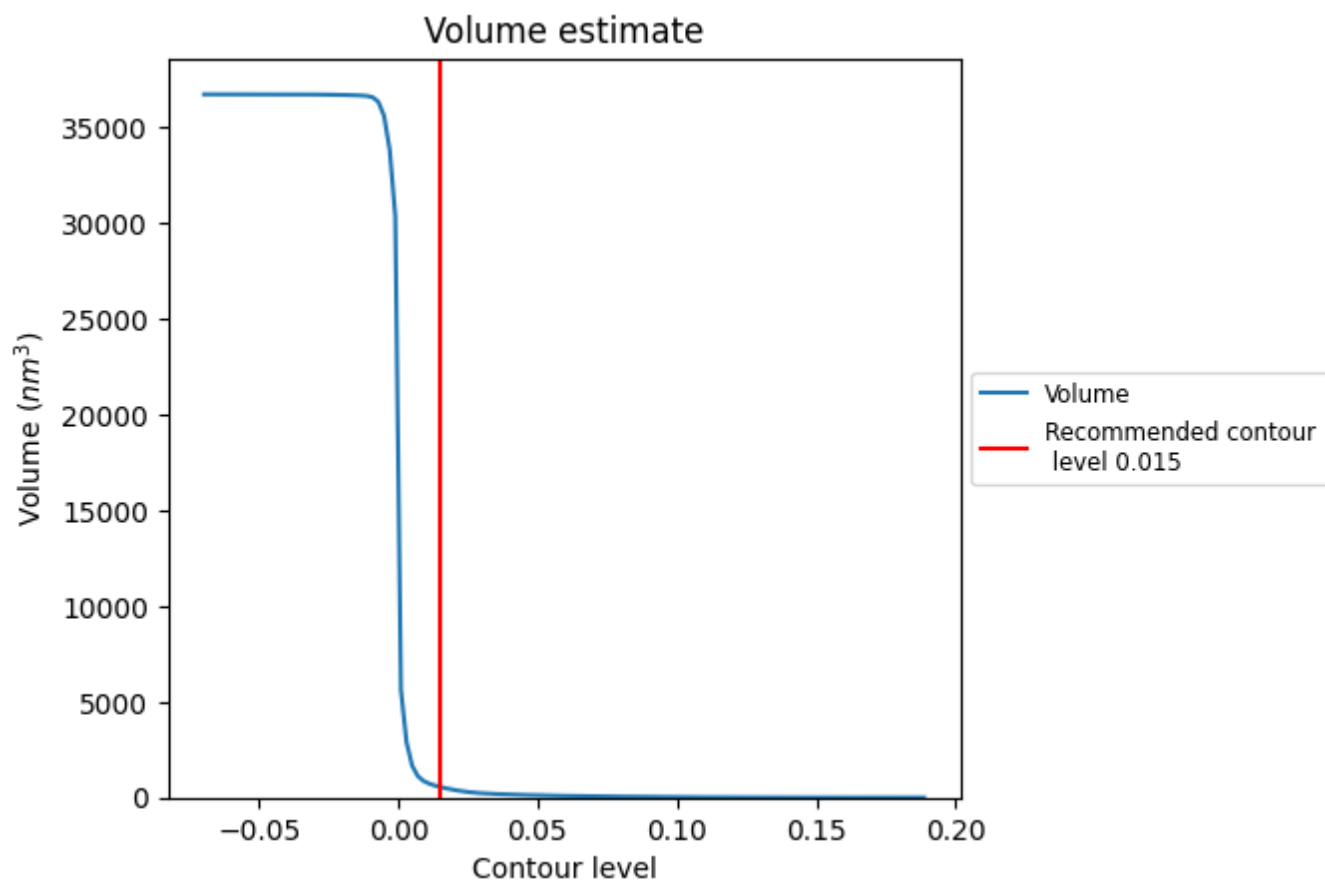
This section contains the results of statistical analysis of the map.

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.

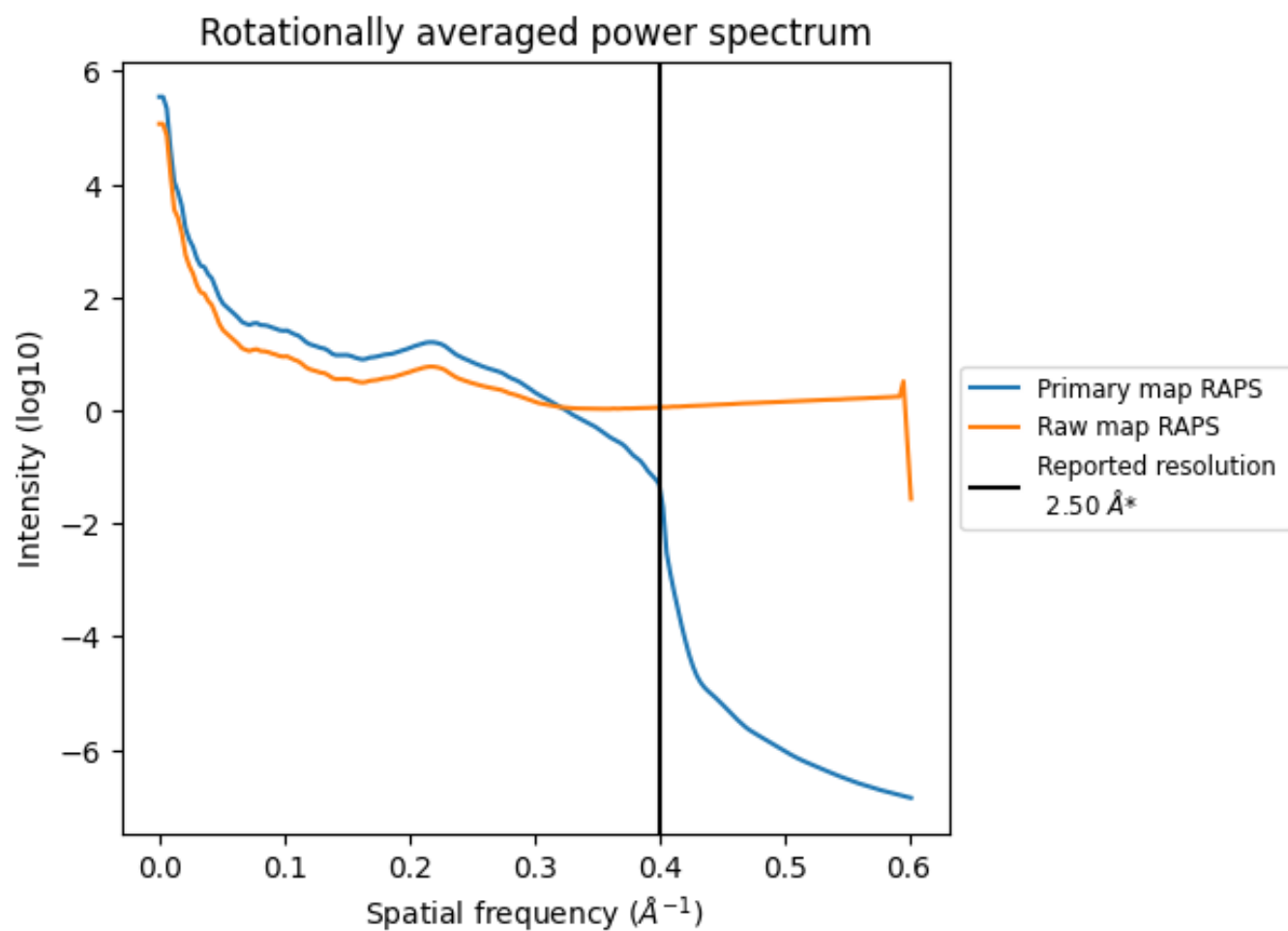
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 555 nm³; this corresponds to an approximate mass of 502 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 ⓘ

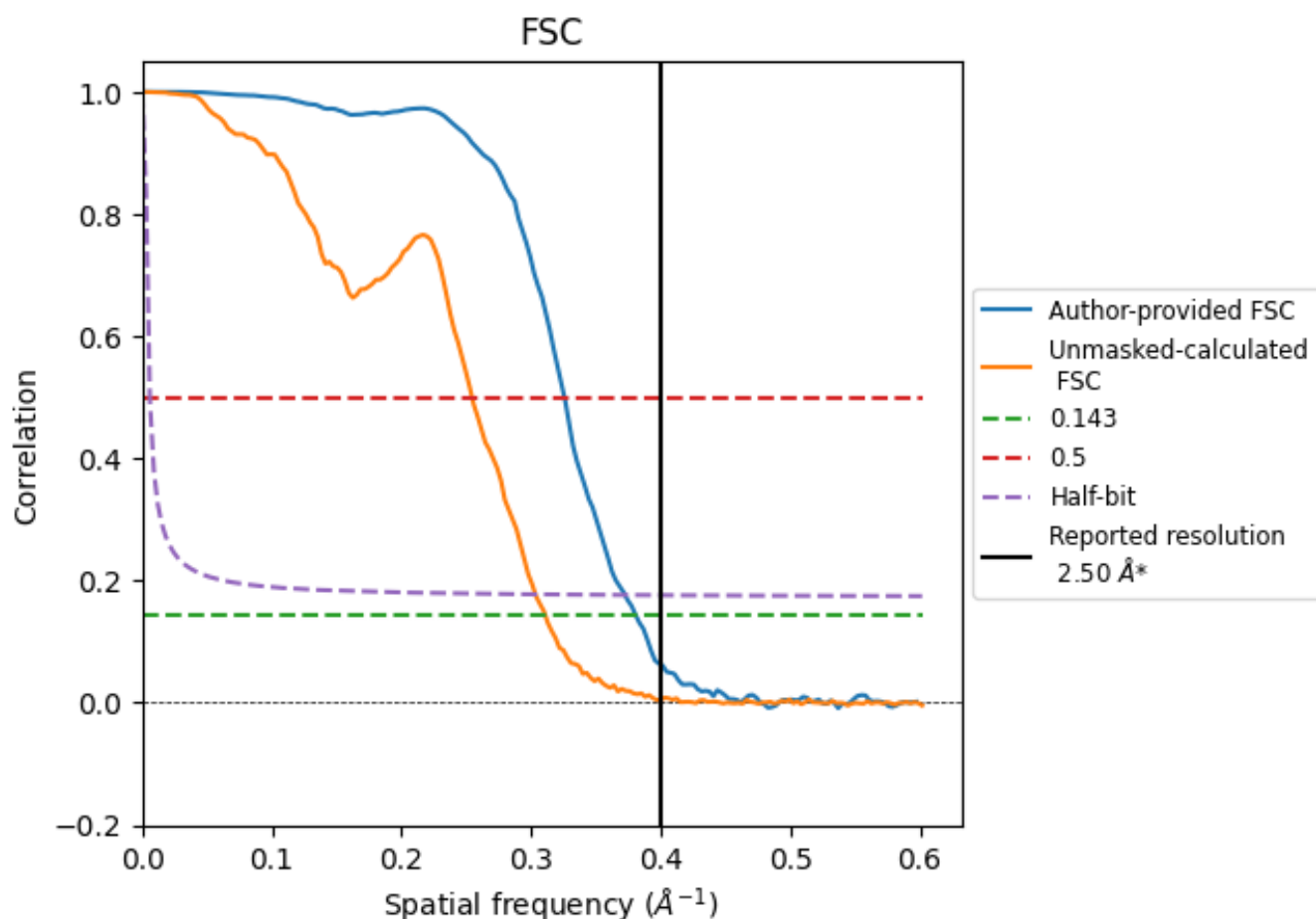


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

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 0.400 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.63	3.07	2.68
Unmasked-calculated*	3.22	3.93	3.30

*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 3.22 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

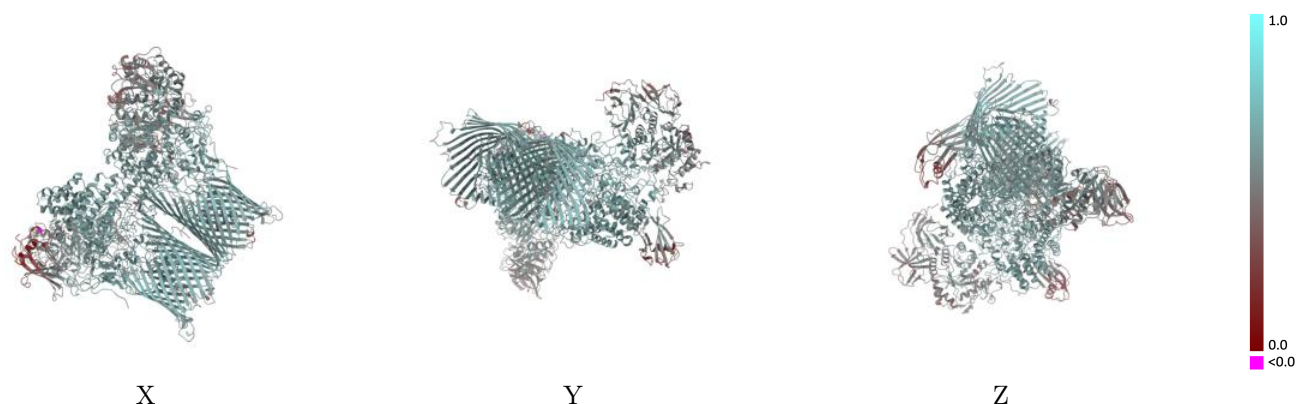
This section contains information regarding the fit between EMDB map EMD-55024 and PDB model 9SM2. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



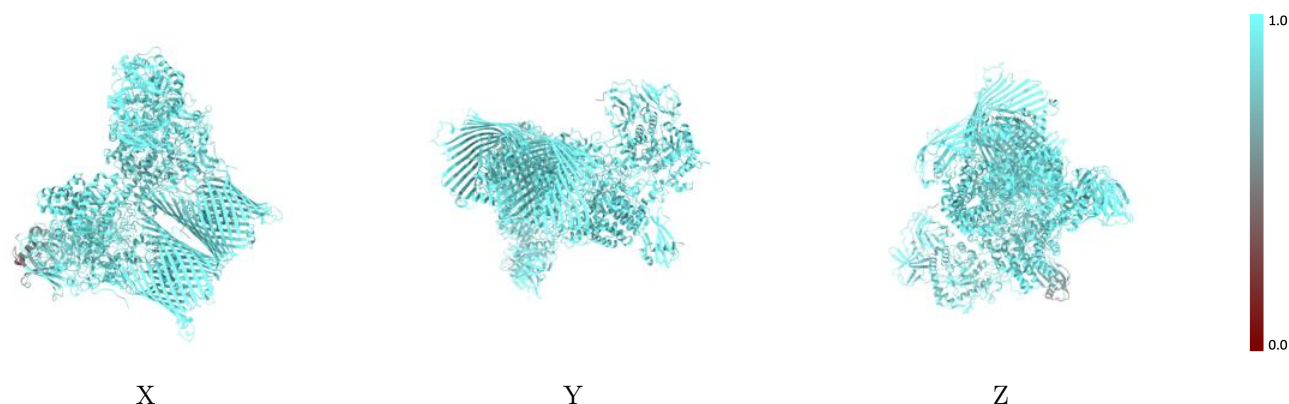
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



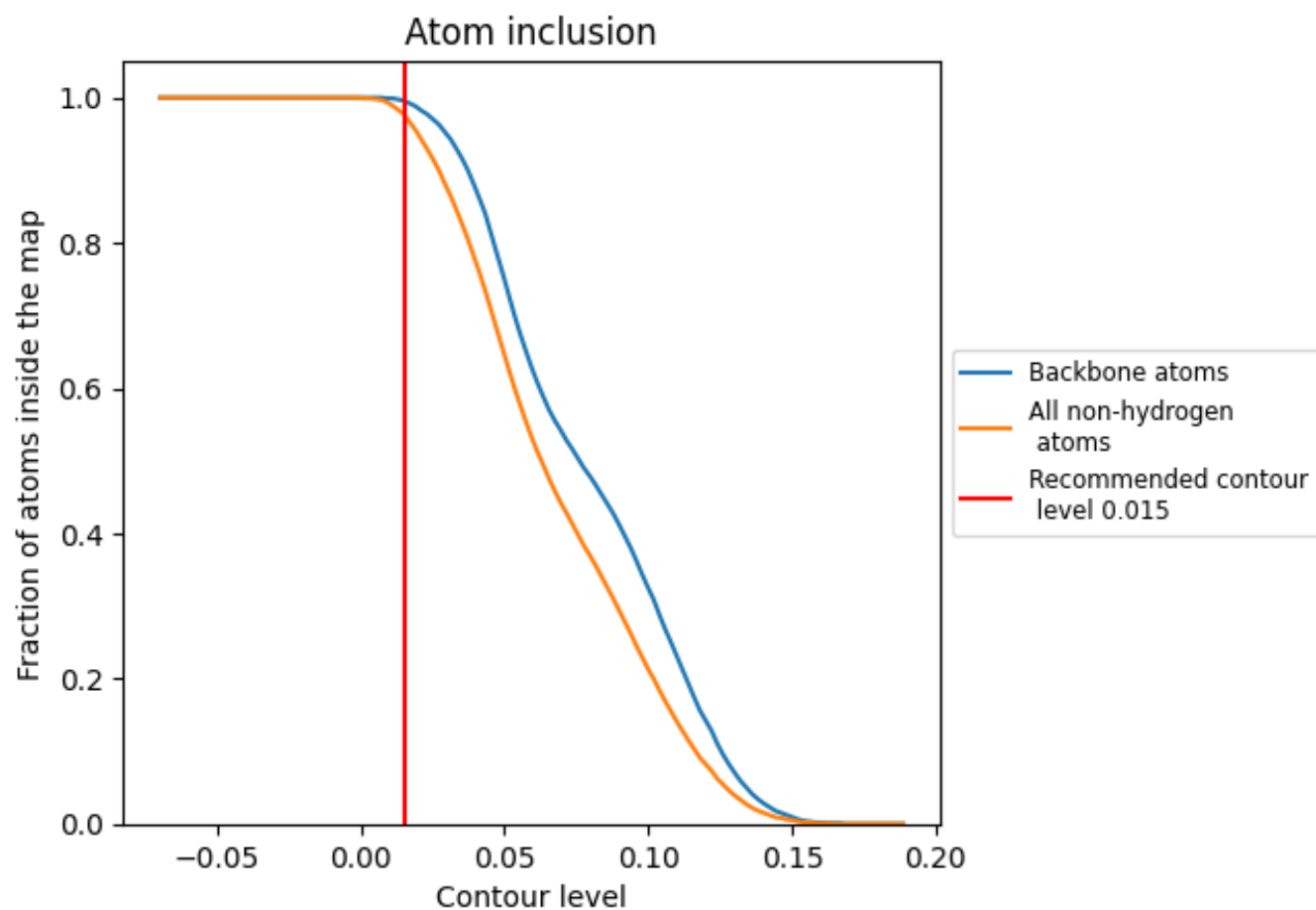
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 98% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.5640
A	 0.9870	 0.6070
B	 0.9910	 0.6080
C	 0.9880	 0.6050
D	 0.9920	 0.6080
E	 0.7490	 0.3920
F	 0.9450	 0.4320
G	 0.9810	 0.5060
H	 0.9790	 0.4930
I	 1.0000	 0.5920
J	 0.9560	 0.5660
K	 0.8660	 0.4610
L	 0.8660	 0.3710
M	 0.9890	 0.5940
N	 1.0000	 0.5830

