



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 07:23 AM UTC

PDB ID : 9BRZ / pdb_00009brz
EMDB ID : EMD-44846
Title : V0-only V-ATPase and synaptophysin complex in mouse brain isolated synaptic vesicles
Authors : Wang, C.; Jiang, W.; Yang, K.; Wang, X.; Guo, Q.; Brunger, A.T.
Deposited on : 2024-05-12
Resolution : 3.80 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:

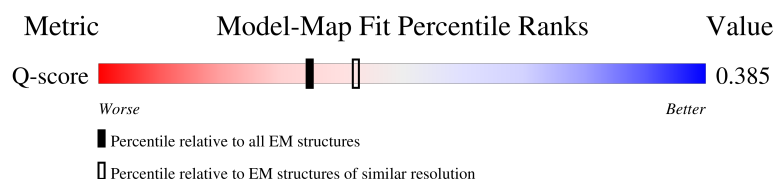
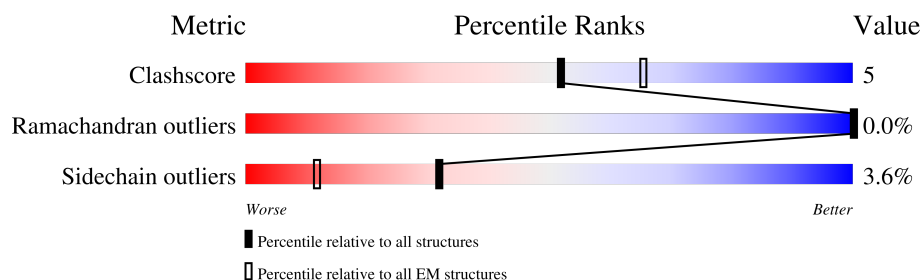
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.80 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.



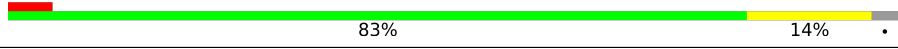
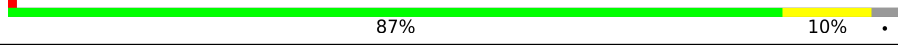
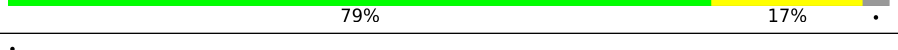
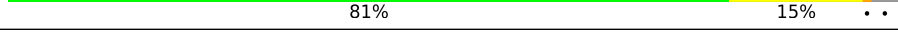
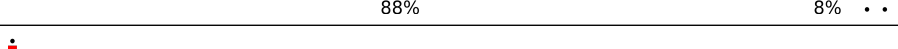
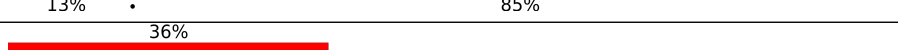
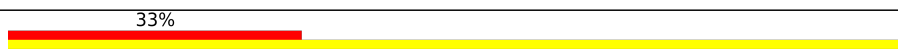
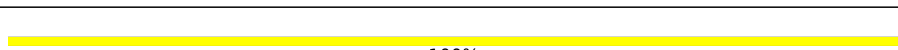
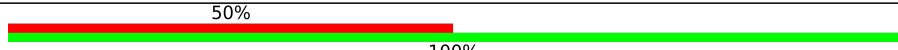
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	c	463	
2	b	205	
3	d	351	
4	f	98	

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Mol	Chain	Length	Quality of chain
5	g	155	
5	h	155	
5	i	155	
5	j	155	
5	k	155	
5	l	155	
5	m	155	
5	n	155	
5	o	155	
6	p	350	
7	s	314	
8	e	81	
9	a	838	
10	A	3	
11	B	2	
11	C	2	
11	D	2	

2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 25204 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 V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	203	Total	C	N	O	S	0	0
			1642	1079	259	295	9		

- Molecule 2 is a protein called V-type proton ATPase 21 kDa proteolipid subunit c''.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	203	Total	C	N	O	S	0	0
			1503	996	237	259	11		

- Molecule 3 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	350	Total	C	N	O	S	0	0
			2833	1829	460	530	14		

- Molecule 4 is a protein called Ribonuclease kappa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	f	86	Total	C	N	O	S	0	0
			666	440	103	116	7		

- Molecule 5 is a protein called V-type proton ATPase 16 kDa proteolipid subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	g	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	h	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	i	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	j	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	k	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	l	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	m	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	n	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		
5	o	150	Total	C	N	O	S	0	0
			1068	699	171	190	8		

- Molecule 6 is a protein called Renin receptor cytoplasmic fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	p	52	Total	C	N	O	S	0	0
			433	292	63	75	3		

- Molecule 7 is a protein called Synaptophysin.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	s	211	Total	C	N	O	S	0	0
			1671	1097	263	299	12		

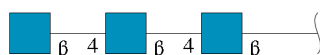
- Molecule 8 is a protein called V-type proton ATPase subunit e 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	e	79	Total	C	N	O	S	0	0
			637	439	99	96	3		

- Molecule 9 is a protein called V-type proton ATPase 116 kDa subunit a 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	743	Total	C	N	O	S	0	0
			6039	3943	1009	1046	41		

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



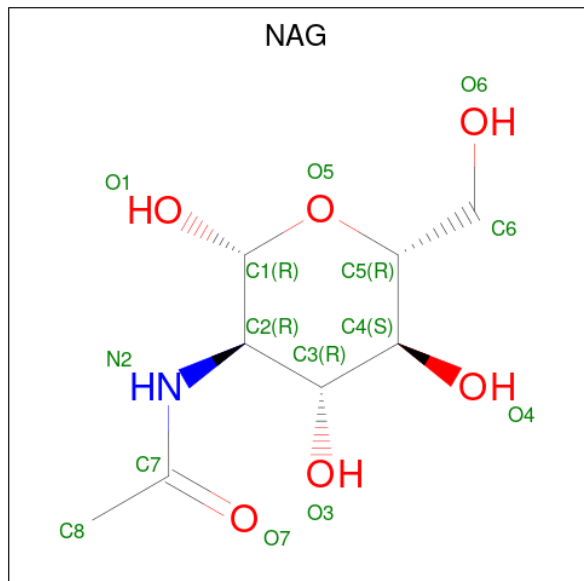
Mol	Chain	Residues	Atoms				AltConf	Trace
10	A	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 11 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
11	B	2	Total	C	N	O	0	0
			28	16	2	10		
11	C	2	Total	C	N	O	0	0
			28	16	2	10		
11	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



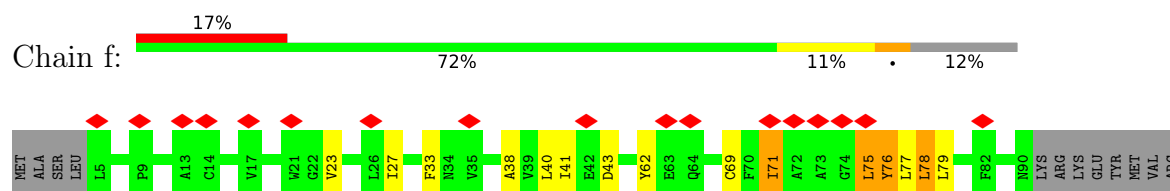
Mol	Chain	Residues	Atoms				AltConf
12	c	1	Total	C	N	O	0
			14	8	1	5	
12	c	1	Total	C	N	O	0
			14	8	1	5	

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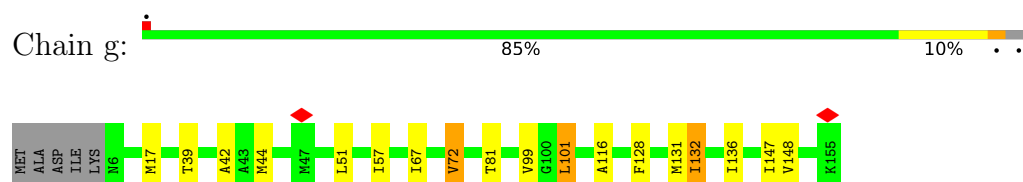
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	c	1	14	8	1	5	0

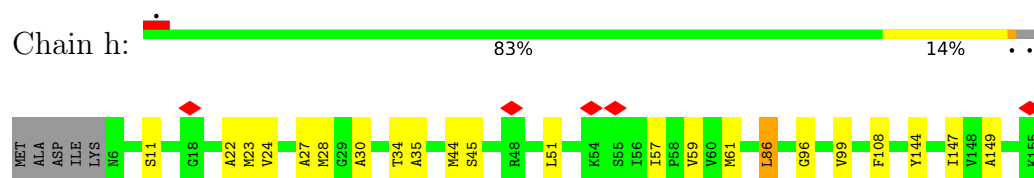
• Molecule 4: Ribonuclease kappa



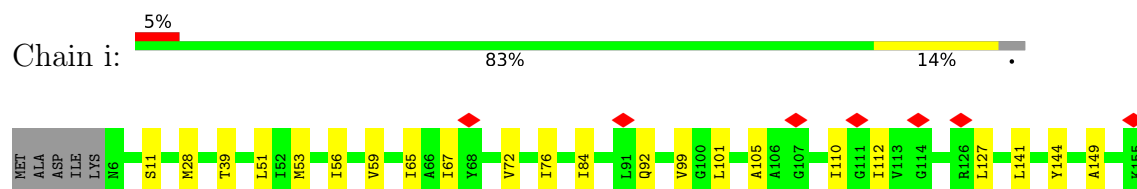
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



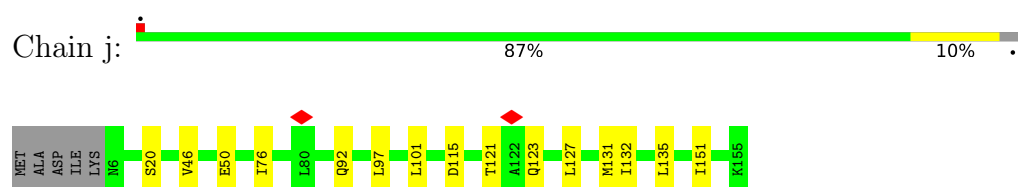
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



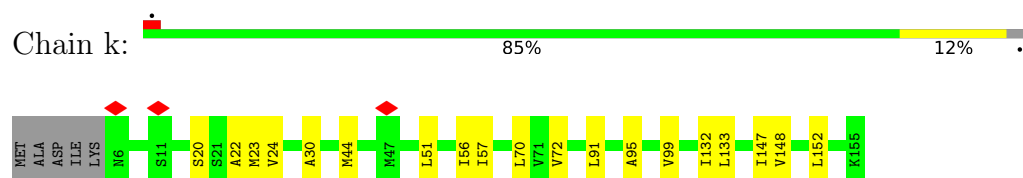
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



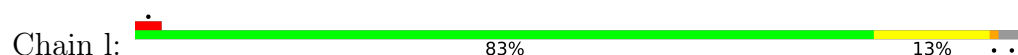
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



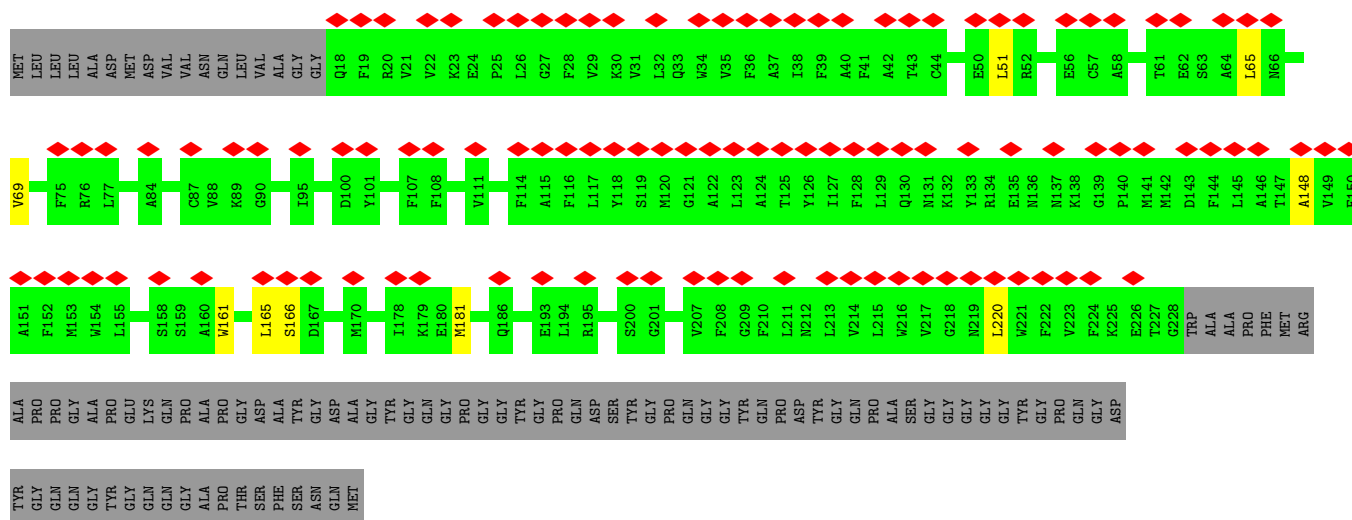
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



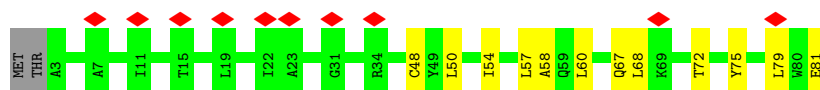
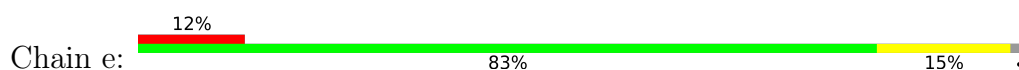
• Molecule 5: V-type proton ATPase 16 kDa proteolipid subunit c



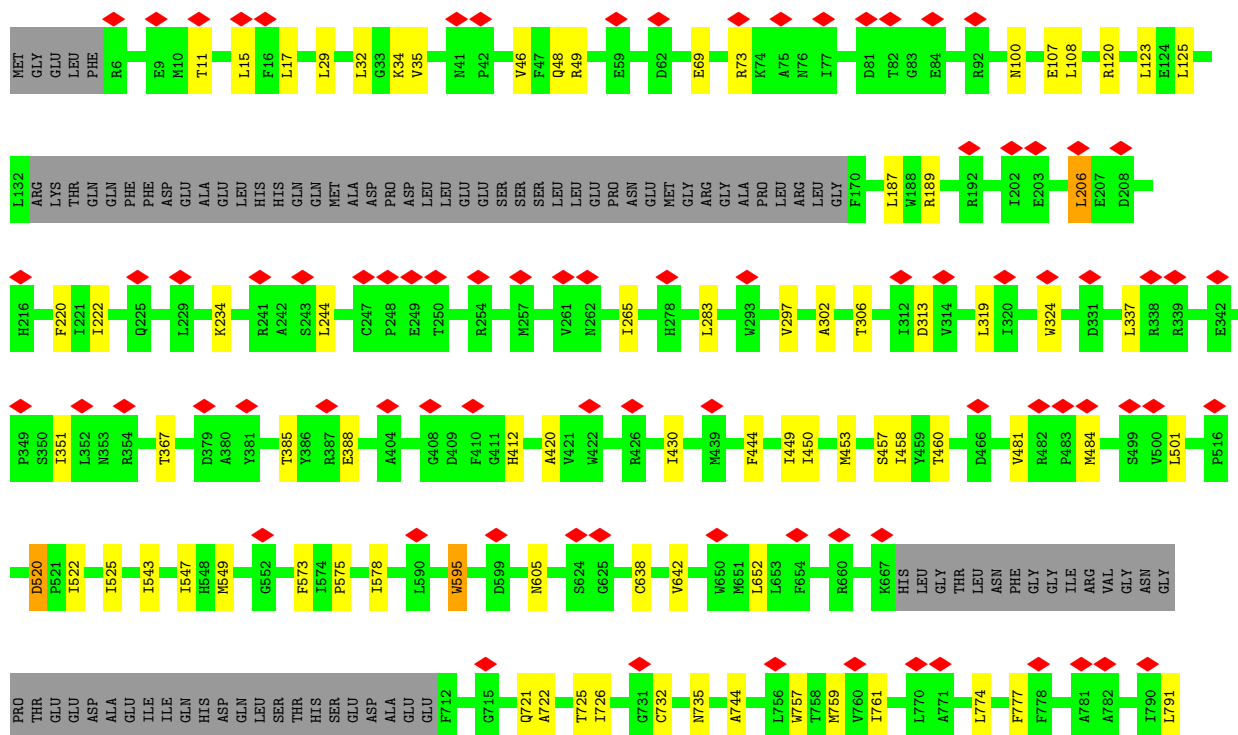
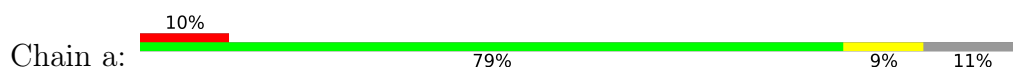




• Molecule 8: V-type proton ATPase subunit e 2



• Molecule 9: V-type proton ATPase 116 kDa subunit a 1





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



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 11: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42137	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.960	Depositor
Minimum map value	-1.514	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	319.968, 319.968, 319.968	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.111, 1.111, 1.111	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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	c	0.29	0/1697	0.56	0/2311
2	b	0.23	0/1537	0.47	0/2088
3	d	0.23	0/2899	0.45	0/3927
4	f	0.63	3/682 (0.4%)	0.85	3/926 (0.3%)
5	g	0.28	0/1083	0.53	0/1466
5	h	0.27	0/1083	0.53	0/1466
5	i	0.29	0/1083	0.53	0/1466
5	j	0.26	0/1083	0.50	0/1466
5	k	0.26	0/1083	0.54	0/1466
5	l	0.27	0/1083	0.56	0/1466
5	m	0.26	0/1083	0.55	0/1466
5	n	0.27	0/1083	0.55	0/1466
5	o	0.26	0/1083	0.56	0/1466
6	p	0.59	0/446	0.71	0/610
7	s	0.20	0/1716	0.45	0/2327
8	e	0.23	0/662	0.44	0/910
9	a	0.25	0/6195	0.52	0/8382
All	All	0.28	3/25581 (0.0%)	0.53	3/34675 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	f	76	TYR	CA-C	-8.39	1.41	1.52
4	f	78	LEU	C-O	-7.68	1.15	1.24
4	f	76	TYR	C-O	-5.75	1.16	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	69	CYS	N-CA-C	-6.96	104.67	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	75	LEU	N-CA-C	-6.61	104.08	111.28
4	f	76	TYR	N-CA-C	-6.23	103.79	112.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	c	1642	0	1561	35	0
2	b	1503	0	1551	18	0
3	d	2833	0	2770	31	0
4	f	666	0	663	20	0
5	g	1068	0	1136	20	0
5	h	1068	0	1136	21	0
5	i	1068	0	1136	18	0
5	j	1068	0	1136	8	0
5	k	1068	0	1136	21	0
5	l	1068	0	1136	11	0
5	m	1068	0	1136	17	0
5	n	1068	0	1136	14	0
5	o	1068	0	1136	11	0
6	p	433	0	432	7	0
7	s	1671	0	1649	5	0
8	e	637	0	652	14	0
9	a	6039	0	6068	70	0
10	A	42	0	37	0	0
11	B	28	0	25	0	0
11	C	28	0	25	0	0
11	D	28	0	25	1	0
12	c	42	0	39	0	0
All	All	25204	0	25721	277	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 5.

All (277) 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:308:GLU:CG	1:c:309:PRO:HD2	1.72	1.17
1:c:308:GLU:CD	1:c:309:PRO:HD2	1.71	1.14
1:c:308:GLU:HG2	1:c:309:PRO:HD2	1.28	1.13
5:k:95:ALA:HB2	5:k:152:LEU:HD22	1.18	1.11
1:c:308:GLU:OE2	1:c:309:PRO:HG2	1.50	1.11
9:a:123:LEU:CD1	9:a:244:LEU:HD22	1.83	1.07
5:h:44:MET:HE2	5:h:51:LEU:HB2	1.35	1.04
3:d:323:LEU:HD11	3:d:352:ILE:CD1	1.89	1.02
5:h:44:MET:CE	5:h:51:LEU:HB2	1.90	1.01
3:d:323:LEU:HD11	3:d:352:ILE:HD12	1.36	1.00
1:c:308:GLU:CD	1:c:309:PRO:CD	2.35	0.99
5:k:51:LEU:HD12	5:k:51:LEU:O	1.63	0.98
5:k:95:ALA:HB2	5:k:152:LEU:CD2	1.94	0.97
1:c:308:GLU:OE2	1:c:309:PRO:CG	2.12	0.97
9:a:123:LEU:HD13	9:a:244:LEU:HD22	1.44	0.97
5:k:95:ALA:CB	5:k:152:LEU:HD22	1.96	0.95
9:a:800:PHE:CD2	9:a:801:LEU:HD12	2.02	0.93
9:a:125:LEU:HD21	9:a:206:LEU:HD11	1.54	0.88
3:d:323:LEU:CD1	3:d:352:ILE:HD12	2.04	0.87
1:c:308:GLU:OE2	1:c:309:PRO:HD2	1.75	0.86
1:c:308:GLU:OE2	1:c:309:PRO:CD	2.22	0.86
4:f:76:TYR:O	4:f:77:LEU:C	2.16	0.85
3:d:23:ARG:O	3:d:26:LYS:HG2	1.76	0.85
4:f:75:LEU:HD12	9:a:777:PHE:HB2	1.59	0.83
4:f:75:LEU:HD11	9:a:774:LEU:HA	1.61	0.83
5:g:128:PHE:O	5:g:131:MET:HG2	1.80	0.81
1:c:308:GLU:CG	1:c:309:PRO:CD	2.59	0.79
4:f:71:ILE:O	4:f:75:LEU:HG	1.82	0.78
8:e:50:LEU:HD21	9:a:547:ILE:HD13	1.66	0.77
5:j:123:GLN:HG2	6:p:639:ARG:HH22	1.49	0.77
8:e:54:ILE:HD11	9:a:543:ILE:HG21	1.65	0.76
5:j:123:GLN:HG2	6:p:639:ARG:NH2	2.01	0.75
5:n:131:MET:SD	5:n:135:LEU:HD11	2.29	0.73
1:c:446:MET:HE1	5:g:42:ALA:HB3	1.70	0.72
1:c:308:GLU:HG2	1:c:309:PRO:CD	2.14	0.72
5:j:121:THR:HG23	5:j:127:LEU:HD22	1.70	0.72
5:m:19:ALA:HB2	5:m:76:ILE:HG21	1.72	0.71
5:h:44:MET:CE	5:h:51:LEU:CB	2.68	0.70
3:d:142:ALA:O	3:d:145:ILE:HG22	1.92	0.69
5:h:45:SER:OG	5:i:127:LEU:HD13	1.93	0.68
9:a:123:LEU:HD12	9:a:244:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:721:GLN:O	9:a:725:THR:HG23	1.94	0.68
2:b:195:ALA:O	2:b:199:THR:HG22	1.94	0.67
1:c:320:ILE:N	1:c:320:ILE:HD13	2.10	0.66
5:i:72:VAL:O	5:i:76:ILE:HD12	1.96	0.66
5:m:86:LEU:HD12	5:m:90:PHE:CZ	2.30	0.66
8:e:68:LEU:HD12	8:e:72:THR:HG21	1.78	0.66
5:k:51:LEU:O	5:k:51:LEU:CD1	2.39	0.66
5:m:20:SER:O	5:m:24:VAL:HG23	1.96	0.65
5:h:23:MET:HE1	5:i:144:TYR:HB3	1.79	0.64
1:c:432:ILE:HD12	5:g:101:LEU:HD21	1.78	0.64
5:k:22:ALA:HB1	5:k:72:VAL:HG13	1.79	0.63
2:b:60:SER:OG	5:g:101:LEU:HD23	1.98	0.63
5:k:91:LEU:O	5:k:152:LEU:HD21	1.99	0.63
3:d:323:LEU:CD1	3:d:352:ILE:CD1	2.68	0.62
5:h:61:MET:N	5:h:61:MET:HE2	2.14	0.62
5:k:44:MET:HE1	5:k:51:LEU:CD1	2.30	0.62
3:d:114:LEU:HB3	3:d:143:VAL:HG21	1.82	0.61
9:a:123:LEU:HD13	9:a:244:LEU:CD2	2.25	0.61
5:h:44:MET:HE2	5:h:51:LEU:CB	2.22	0.61
4:f:40:LEU:HD13	8:e:75:TYR:CD2	2.36	0.61
1:c:385:VAL:HG23	1:c:385:VAL:O	1.98	0.61
6:p:632:GLY:O	6:p:633:TYR:C	2.42	0.61
3:d:323:LEU:HD11	3:d:352:ILE:HD11	1.78	0.60
5:n:131:MET:SD	5:n:135:LEU:CD1	2.90	0.60
5:j:121:THR:CG2	5:j:127:LEU:HD22	2.31	0.60
9:a:549:MET:HE1	9:a:735:ASN:CB	2.32	0.59
5:g:136:ILE:HG13	9:a:801:LEU:HD22	1.84	0.59
5:g:136:ILE:CG1	9:a:801:LEU:HD22	2.32	0.59
5:k:23:MET:HE1	5:k:70:LEU:CD1	2.33	0.58
9:a:800:PHE:CE2	9:a:801:LEU:HD12	2.38	0.58
3:d:178:MET:HE2	3:d:178:MET:HA	1.85	0.58
5:h:57:ILE:HD12	5:h:57:ILE:H	1.68	0.58
4:f:75:LEU:CD1	9:a:777:PHE:HB2	2.33	0.58
5:k:95:ALA:CA	5:k:152:LEU:HD22	2.33	0.58
2:b:59:ILE:HD11	5:g:148:VAL:HG21	1.84	0.57
9:a:481:VAL:CG1	9:a:484:MET:HE2	2.34	0.57
5:l:99:VAL:HG23	5:l:149:ALA:HB2	1.86	0.57
9:a:759:MET:HE2	9:a:759:MET:HA	1.86	0.57
3:d:26:LYS:HD3	3:d:308:PHE:CZ	2.41	0.56
8:e:54:ILE:HD11	9:a:543:ILE:CG2	2.32	0.56
4:f:38:ALA:HB3	4:f:62:TYR:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:l:28:MET:SD	5:m:105:ALA:HB2	2.45	0.56
3:d:23:ARG:HD3	3:d:26:LYS:CE	2.35	0.56
1:c:301:ALA:HB3	1:c:321:LEU:HD11	1.88	0.56
1:c:308:GLU:CD	1:c:309:PRO:N	2.63	0.56
1:c:446:MET:HE2	5:g:39:THR:HG23	1.87	0.56
9:a:757:TRP:CZ3	9:a:761:ILE:HG23	2.40	0.56
3:d:23:ARG:HD3	3:d:26:LYS:HE2	1.89	0.55
9:a:306:THR:HG21	9:a:826:PHE:CZ	2.41	0.55
2:b:59:ILE:CD1	5:g:148:VAL:HG21	2.36	0.55
5:k:44:MET:CE	5:k:51:LEU:HD11	2.37	0.55
5:k:72:VAL:HG11	5:k:99:VAL:HG11	1.88	0.55
7:s:161:TRP:CD1	7:s:165:LEU:HD23	2.41	0.55
3:d:23:ARG:CD	3:d:26:LYS:CE	2.85	0.55
2:b:79:GLY:O	2:b:82:VAL:HG12	2.07	0.55
5:o:51:LEU:O	5:o:51:LEU:HD12	2.07	0.55
1:c:321:LEU:C	1:c:321:LEU:HD12	2.31	0.55
5:i:76:ILE:HG23	5:i:92:GLN:HB3	1.88	0.55
5:h:28:MET:SD	5:i:105:ALA:HB2	2.47	0.55
5:m:59:VAL:HG21	5:n:134:ILE:HD13	1.89	0.55
2:b:190:PHE:CE1	5:o:70:LEU:HD22	2.42	0.54
5:o:127:LEU:O	5:o:127:LEU:HD23	2.07	0.54
6:p:635:SER:O	6:p:639:ARG:HG2	2.08	0.54
9:a:481:VAL:HG11	9:a:484:MET:HE2	1.88	0.54
5:j:76:ILE:HD11	5:j:92:GLN:HG3	1.88	0.54
5:k:51:LEU:HD12	5:k:51:LEU:C	2.31	0.54
5:g:72:VAL:HG11	5:g:99:VAL:HG11	1.90	0.53
5:g:147:ILE:HD11	9:a:744:ALA:CB	2.38	0.53
8:e:67:GLN:HG2	9:a:501:LEU:HD11	1.90	0.53
9:a:302:ALA:O	9:a:306:THR:HG23	2.08	0.53
9:a:549:MET:HE1	9:a:735:ASN:HB2	1.90	0.53
9:a:123:LEU:HD11	9:a:244:LEU:HD22	1.86	0.53
9:a:800:PHE:HD2	9:a:801:LEU:HD12	1.63	0.53
9:a:125:LEU:HD21	9:a:206:LEU:CD1	2.33	0.53
4:f:38:ALA:HB3	4:f:62:TYR:CD1	2.43	0.53
1:c:301:ALA:HB3	1:c:321:LEU:CD1	2.40	0.52
5:i:99:VAL:HG21	5:i:149:ALA:HB2	1.89	0.52
5:k:57:ILE:HD13	5:k:132:ILE:HD11	1.92	0.52
3:d:112:ILE:HA	3:d:115:ILE:HG22	1.91	0.52
2:b:78:ILE:HG21	5:g:116:ALA:HB1	1.92	0.52
7:s:148:ALA:HA	7:s:220:LEU:HD11	1.91	0.52
9:a:520:ASP:OD2	9:a:522:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:d:23:ARG:CD	3:d:26:LYS:HE2	2.40	0.52
9:a:120:ARG:O	9:a:123:LEU:HB3	2.10	0.52
5:m:45:SER:OG	5:m:52:ILE:HD11	2.10	0.52
7:s:65:LEU:O	7:s:65:LEU:HD23	2.09	0.52
1:c:310:LEU:C	1:c:310:LEU:HD12	2.35	0.52
1:c:446:MET:CE	5:g:42:ALA:HB3	2.38	0.52
5:m:106:ALA:O	5:m:110:ILE:HD12	2.09	0.52
9:a:722:ALA:O	9:a:726:ILE:HG23	2.09	0.52
5:m:56:ILE:HD11	5:n:134:ILE:HG12	1.92	0.51
5:n:59:VAL:HG12	5:o:137:PHE:HD2	1.74	0.51
3:d:81:VAL:HG11	3:d:133:PRO:HG2	1.92	0.51
8:e:57:LEU:HD12	8:e:60:LEU:HD23	1.91	0.51
5:j:123:GLN:CG	6:p:639:ARG:HH22	2.21	0.51
4:f:79:LEU:HD22	9:a:777:PHE:HZ	1.76	0.51
5:l:68:TYR:O	5:l:72:VAL:HG23	2.11	0.51
5:i:99:VAL:CG2	5:i:149:ALA:HB2	2.40	0.51
5:h:44:MET:HE3	5:h:51:LEU:HB2	1.90	0.50
5:m:44:MET:HG2	5:m:122:ALA:HB2	1.93	0.50
9:a:549:MET:HE1	9:a:735:ASN:HB3	1.94	0.50
5:j:101:LEU:HD22	6:p:619:VAL:HG21	1.93	0.50
9:a:123:LEU:CD1	9:a:244:LEU:CD2	2.75	0.50
3:d:23:ARG:CD	3:d:26:LYS:HE3	2.42	0.50
8:e:57:LEU:CD1	8:e:60:LEU:HD23	2.42	0.50
3:d:88:ARG:NH2	3:d:96:ALA:HB1	2.26	0.49
9:a:385:THR:HG22	9:a:388:GLU:OE1	2.12	0.49
5:o:44:MET:CE	5:o:51:LEU:HD11	2.42	0.49
5:h:35:ALA:HB1	5:i:112:ILE:HG21	1.94	0.49
7:s:148:ALA:HA	7:s:220:LEU:CD1	2.42	0.49
2:b:82:VAL:HG11	3:d:21:LEU:HD13	1.94	0.49
4:f:40:LEU:HD13	8:e:75:TYR:CE2	2.48	0.48
4:f:76:TYR:C	4:f:78:LEU:N	2.66	0.48
3:d:112:ILE:HD13	3:d:184:ARG:HB2	1.95	0.48
9:a:107:GLU:CD	9:a:283:LEU:HD22	2.37	0.48
1:c:432:ILE:CD1	5:g:101:LEU:HD21	2.43	0.48
5:g:132:ILE:CG2	9:a:801:LEU:HD21	2.43	0.48
5:l:36:LYS:O	5:l:39:THR:HG22	2.13	0.48
5:m:60:VAL:HG22	5:n:137:PHE:HE2	1.77	0.48
5:i:76:ILE:HD12	5:i:76:ILE:H	1.79	0.48
2:b:163:ALA:HB1	2:b:177:ILE:HD12	1.95	0.48
5:g:44:MET:HE1	5:g:51:LEU:O	2.14	0.48
2:b:165:LEU:O	2:b:165:LEU:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:169:GLN:HE21	3:d:26:LYS:HZ2	1.62	0.48
9:a:449:ILE:HG13	9:a:453:MET:HE3	1.96	0.48
1:c:336:MET:SD	1:c:352:VAL:HG21	2.54	0.47
5:k:30:ALA:HB3	5:l:141:LEU:HD21	1.96	0.47
2:b:95:ILE:HD12	2:b:95:ILE:H	1.78	0.47
5:m:70:LEU:HD13	5:n:144:TYR:HB3	1.97	0.47
2:b:190:PHE:CD1	5:o:70:LEU:HD22	2.49	0.47
5:k:44:MET:CE	5:k:51:LEU:CD1	2.93	0.47
5:n:27:ALA:HB1	5:o:141:LEU:HD11	1.95	0.47
9:a:501:LEU:HD12	9:a:501:LEU:O	2.14	0.47
5:j:97:LEU:HD23	5:j:101:LEU:HD12	1.96	0.47
5:k:24:VAL:HG21	5:l:101:LEU:HD23	1.97	0.47
5:o:76:ILE:HD11	5:o:92:GLN:CG	2.45	0.47
1:c:310:LEU:CD1	1:c:311:PHE:HD2	2.28	0.46
7:s:165:LEU:HD12	7:s:166:SER:N	2.31	0.46
9:a:757:TRP:CE3	9:a:761:ILE:HG23	2.51	0.46
9:a:32:LEU:HD11	9:a:34:LYS:HG3	1.98	0.46
5:m:69:GLY:O	5:m:72:VAL:HG12	2.16	0.46
9:a:638:CYS:O	9:a:642:VAL:HG12	2.15	0.46
8:e:58:ALA:HB2	9:a:595:TRP:CH2	2.50	0.46
1:c:321:LEU:CD1	1:c:398:PHE:CE1	2.99	0.45
1:c:323:SER:HA	1:c:334:PHE:HA	1.97	0.45
5:h:34:THR:HG23	5:h:59:VAL:HG13	1.98	0.45
1:c:267:ASN:OD1	11:D:1:NAG:N2	2.50	0.45
5:n:45:SER:HB2	5:n:52:ILE:HD11	1.98	0.45
2:b:174:PHE:CE1	2:b:178:LEU:HD21	2.52	0.45
4:f:75:LEU:HD13	9:a:777:PHE:CD2	2.52	0.45
5:i:65:ILE:HD11	5:i:110:ILE:HD12	1.98	0.45
5:k:44:MET:SD	5:k:51:LEU:HD11	2.57	0.45
5:m:72:VAL:HG11	5:m:99:VAL:HG11	1.99	0.45
8:e:68:LEU:O	9:a:501:LEU:HD12	2.18	0.44
1:c:322:ALA:HA	1:c:398:PHE:CZ	2.52	0.44
5:m:137:PHE:O	5:m:140:VAL:HG22	2.17	0.44
8:e:67:GLN:CD	9:a:501:LEU:HD21	2.42	0.44
9:a:430:ILE:HG21	9:a:444:PHE:CE2	2.53	0.44
5:l:80:LEU:HD23	5:m:87:TYR:OH	2.17	0.44
9:a:800:PHE:CD2	9:a:801:LEU:CD1	2.89	0.44
1:c:379:VAL:HG22	1:c:380:THR:H	1.83	0.44
4:f:75:LEU:HD13	9:a:777:PHE:HD2	1.83	0.44
9:a:107:GLU:OE2	9:a:283:LEU:HD22	2.18	0.44
5:h:24:VAL:HG11	5:i:101:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:321:LEU:HD12	1:c:321:LEU:O	2.18	0.43
9:a:108:LEU:O	9:a:108:LEU:HD23	2.17	0.43
4:f:23:VAL:HG22	4:f:27:ILE:HD11	2.01	0.43
9:a:575:PRO:HA	9:a:578:ILE:HG22	1.99	0.43
5:n:70:LEU:HD22	5:o:144:TYR:CG	2.53	0.43
2:b:108:MET:HA	2:b:108:MET:HE2	2.01	0.43
3:d:158:VAL:HG22	9:a:189:ARG:CZ	2.48	0.43
4:f:76:TYR:O	4:f:78:LEU:N	2.51	0.43
5:h:99:VAL:HG21	5:h:149:ALA:HB2	2.01	0.43
9:a:313:ASP:O	9:a:319:LEU:HD12	2.18	0.43
5:g:67:ILE:HD13	5:h:144:TYR:HE2	1.84	0.43
5:h:27:ALA:HA	5:i:141:LEU:HD11	2.01	0.43
2:b:59:ILE:HD13	5:g:148:VAL:HG11	2.01	0.42
2:b:163:ALA:CB	2:b:177:ILE:HD12	2.49	0.42
5:m:44:MET:CG	5:m:122:ALA:HB2	2.48	0.42
5:n:131:MET:O	5:n:135:LEU:HD13	2.19	0.42
1:c:368:VAL:O	1:c:368:VAL:HG23	2.18	0.42
3:d:23:ARG:HB3	3:d:26:LYS:HE3	2.00	0.42
1:c:323:SER:H	1:c:398:PHE:HE2	1.66	0.42
5:i:28:MET:HE3	5:i:28:MET:HA	2.02	0.42
9:a:457:SER:HA	9:a:460:THR:HG22	2.02	0.42
1:c:322:ALA:HA	1:c:398:PHE:HZ	1.83	0.42
5:n:80:LEU:HD23	5:n:84:ILE:HD12	2.01	0.42
5:n:81:THR:HG22	5:n:82:ASP:N	2.34	0.42
9:a:234:LYS:HA	9:a:234:LYS:HE3	2.01	0.42
5:k:152:LEU:HD23	5:k:152:LEU:O	2.20	0.42
3:d:139:GLN:OE1	3:d:139:GLN:N	2.53	0.42
3:d:201:LEU:O	3:d:201:LEU:HD23	2.19	0.42
4:f:41:ILE:HA	9:a:525:ILE:HG21	2.01	0.42
5:i:51:LEU:HD12	5:i:51:LEU:N	2.34	0.42
5:l:62:ALA:O	5:l:65:ILE:HG22	2.19	0.42
5:h:23:MET:HE1	5:i:144:TYR:CB	2.49	0.42
5:l:64:ILE:O	5:l:67:ILE:HG22	2.19	0.42
5:l:72:VAL:HG21	5:l:99:VAL:HG11	2.02	0.42
5:g:136:ILE:HG13	9:a:801:LEU:CD2	2.49	0.42
5:k:56:ILE:O	5:k:56:ILE:HG22	2.20	0.41
9:a:220:PHE:HE2	9:a:222:ILE:HD12	1.84	0.41
3:d:23:ARG:CB	3:d:26:LYS:HE3	2.50	0.41
3:d:209:ALA:HB3	3:d:313:HIS:ND1	2.35	0.41
6:p:632:GLY:C	6:p:634:ASP:N	2.77	0.41
5:h:22:ALA:HB2	5:h:96:GLY:HA2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:e:75:TYR:C	8:e:79:LEU:HD12	2.45	0.41
9:a:11:THR:HG1	9:a:324:TRP:HB3	1.85	0.41
5:k:44:MET:HE1	5:k:51:LEU:HD12	2.02	0.41
9:a:420:ALA:HB2	9:a:450:ILE:HG22	2.01	0.41
4:f:71:ILE:HG22	4:f:75:LEU:CD2	2.51	0.41
9:a:46:VAL:HA	9:a:49:ARG:HE	1.85	0.41
5:h:35:ALA:HB1	5:i:112:ILE:CG2	2.50	0.41
5:m:123:GLN:OE1	5:m:123:GLN:HA	2.21	0.41
9:a:48:GLN:O	9:a:48:GLN:HG2	2.21	0.41
5:h:11:SER:HB3	5:h:86:LEU:HD22	2.02	0.41
5:i:56:ILE:O	5:i:59:VAL:HG12	2.21	0.41
9:a:69:GLU:O	9:a:73:ARG:HG3	2.21	0.41
3:d:26:LYS:HD3	3:d:308:PHE:CE1	2.55	0.41
8:e:81:GLU:HG3	9:a:481:VAL:HG22	2.03	0.41
2:b:169:GLN:NE2	3:d:26:LYS:NZ	2.68	0.41
5:o:17:MET:HA	5:o:17:MET:HE3	2.02	0.41
9:a:29:LEU:HG	9:a:35:VAL:HG21	2.03	0.41
4:f:33:PHE:HA	4:f:38:ALA:HB2	2.02	0.40
9:a:337:LEU:HD23	9:a:337:LEU:C	2.46	0.40
9:a:412:HIS:NE2	9:a:791:LEU:HD23	2.36	0.40
5:n:145:GLY:O	5:n:148:VAL:HG12	2.22	0.40
1:c:320:ILE:N	1:c:320:ILE:CD1	2.77	0.40
1:c:432:ILE:HD12	5:g:101:LEU:CD2	2.49	0.40
3:d:291:THR:HG22	3:d:294:ASP:OD2	2.22	0.40
4:f:71:ILE:O	4:f:75:LEU:N	2.53	0.40
3:d:36:LEU:HD23	3:d:36:LEU:O	2.21	0.40
4:f:71:ILE:HG22	4:f:75:LEU:HD21	2.03	0.40
5:h:30:ALA:HB3	5:i:141:LEU:HD22	2.04	0.40
5:l:76:ILE:HD11	5:l:92:GLN:HB3	2.03	0.40
5:o:76:ILE:HD11	5:o:92:GLN:CD	2.46	0.40
9:a:17:LEU:HD11	9:a:351:ILE:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c	201/463 (43%)	174 (87%)	27 (13%)	0	100	100
2	b	201/205 (98%)	195 (97%)	6 (3%)	0	100	100
3	d	348/351 (99%)	330 (95%)	18 (5%)	0	100	100
4	f	84/98 (86%)	73 (87%)	11 (13%)	0	100	100
5	g	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
5	h	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
5	i	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
5	j	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
5	k	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
5	l	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
5	m	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
5	n	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
5	o	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
6	p	50/350 (14%)	44 (88%)	5 (10%)	1 (2%)	6	32
7	s	209/314 (67%)	203 (97%)	6 (3%)	0	100	100
8	e	77/81 (95%)	76 (99%)	1 (1%)	0	100	100
9	a	737/838 (88%)	689 (94%)	48 (6%)	0	100	100
All	All	3239/4095 (79%)	3086 (95%)	152 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	p	631	PRO

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	c	180/395 (46%)	173 (96%)	7 (4%)	28	52
2	b	156/158 (99%)	148 (95%)	8 (5%)	21	46
3	d	305/306 (100%)	296 (97%)	9 (3%)	36	57
4	f	72/83 (87%)	70 (97%)	2 (3%)	38	58
5	g	109/113 (96%)	103 (94%)	6 (6%)	19	45
5	h	109/113 (96%)	106 (97%)	3 (3%)	38	58
5	i	109/113 (96%)	104 (95%)	5 (5%)	24	48
5	j	109/113 (96%)	101 (93%)	8 (7%)	13	39
5	k	109/113 (96%)	105 (96%)	4 (4%)	30	54
5	l	109/113 (96%)	103 (94%)	6 (6%)	19	45
5	m	109/113 (96%)	106 (97%)	3 (3%)	38	58
5	n	109/113 (96%)	99 (91%)	10 (9%)	8	31
5	o	109/113 (96%)	105 (96%)	4 (4%)	30	54
6	p	47/309 (15%)	46 (98%)	1 (2%)	47	64
7	s	180/246 (73%)	177 (98%)	3 (2%)	53	67
8	e	66/68 (97%)	65 (98%)	1 (2%)	57	69
9	a	661/741 (89%)	646 (98%)	15 (2%)	44	63
All	All	2648/3323 (80%)	2553 (96%)	95 (4%)	32	54

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	294	SER
1	c	316	THR
1	c	320	ILE
1	c	328	VAL
1	c	334	PHE
1	c	365	CYS
1	c	442	SER
2	b	7	LEU
2	b	31	ASP
2	b	71	TYR
2	b	96	ILE
2	b	172	SER
2	b	173	LEU
2	b	181	GLU
2	b	194	VAL

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Mol	Chain	Res	Type
3	d	30	LEU
3	d	112	ILE
3	d	123	SER
3	d	197	LYS
3	d	200	THR
3	d	225	ILE
3	d	308	PHE
3	d	350	ILE
3	d	352	ILE
4	f	43	ASP
4	f	71	ILE
5	g	17	MET
5	g	57	ILE
5	g	72	VAL
5	g	81	THR
5	g	101	LEU
5	g	132	ILE
5	h	86	LEU
5	h	108	PHE
5	h	147	ILE
5	i	11	SER
5	i	39	THR
5	i	53	MET
5	i	67	ILE
5	i	84	ILE
5	j	20	SER
5	j	46	VAL
5	j	50	GLU
5	j	115	ASP
5	j	131	MET
5	j	132	ILE
5	j	135	LEU
5	j	151	ILE
5	k	20	SER
5	k	133	LEU
5	k	147	ILE
5	k	148	VAL
5	l	16	VAL
5	l	20	SER
5	l	64	ILE
5	l	74	VAL
5	l	112	ILE

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Mol	Chain	Res	Type
5	l	132	ILE
5	m	64	ILE
5	m	67	ILE
5	m	74	VAL
5	n	9	GLU
5	n	12	SER
5	n	16	VAL
5	n	20	SER
5	n	37	SER
5	n	74	VAL
5	n	115	ASP
5	n	132	ILE
5	n	134	ILE
5	n	140	VAL
5	o	84	ILE
5	o	118	VAL
5	o	132	ILE
5	o	141	LEU
6	p	619	VAL
7	s	51	LEU
7	s	69	VAL
7	s	181	MET
8	e	48	CYS
9	a	15	LEU
9	a	100	ASN
9	a	187	LEU
9	a	206	LEU
9	a	265	ILE
9	a	297	VAL
9	a	367	THR
9	a	458	ILE
9	a	520	ASP
9	a	573	PHE
9	a	595	TRP
9	a	605	ASN
9	a	652	LEU
9	a	732	CYS
9	a	822	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	c	394	GLN
2	b	169	GLN
3	d	147	GLN
5	j	92	GLN
7	s	130	GLN
8	e	4	HIS
9	a	502	GLN
9	a	524	ASN
9	a	735	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

9 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	A	1	1,10	14,14,15	1.03	1 (7%)	17,19,21	2.28	9 (52%)
10	NAG	A	2	10	14,14,15	0.65	0	17,19,21	1.53	3 (17%)
10	NAG	A	3	10	14,14,15	0.72	0	17,19,21	1.45	2 (11%)
11	NAG	B	1	1,11	14,14,15	0.74	0	17,19,21	2.03	3 (17%)
11	NAG	B	2	11	14,14,15	0.80	0	17,19,21	1.04	1 (5%)
11	NAG	C	1	1,11	14,14,15	0.71	0	17,19,21	0.96	0
11	NAG	C	2	11	14,14,15	0.75	0	17,19,21	0.85	0
11	NAG	D	1	1,11	14,14,15	1.32	1 (7%)	17,19,21	2.27	7 (41%)
11	NAG	D	2	11	14,14,15	0.73	0	17,19,21	1.12	1 (5%)

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	A	1	1,10	-	1/6/23/26	0/1/1/1
10	NAG	A	2	10	-	0/6/23/26	0/1/1/1
10	NAG	A	3	10	-	3/6/23/26	0/1/1/1
11	NAG	B	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	B	2	11	-	2/6/23/26	0/1/1/1
11	NAG	C	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	C	2	11	-	0/6/23/26	0/1/1/1
11	NAG	D	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	D	2	11	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1	NAG	C1-C2	4.36	1.58	1.52
10	A	1	NAG	C1-C2	3.37	1.56	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1	NAG	C1-C2-N2	5.54	119.16	110.43
11	B	1	NAG	C2-N2-C7	4.55	129.00	122.90
11	B	1	NAG	O5-C1-C2	-4.47	104.38	111.29
10	A	2	NAG	C1-O5-C5	4.16	117.76	112.19
10	A	3	NAG	C2-N2-C7	4.13	128.44	122.90
11	D	1	NAG	O5-C1-C2	-4.00	105.11	111.29
10	A	1	NAG	C1-C2-N2	3.76	116.35	110.43
11	B	1	NAG	C1-O5-C5	-3.68	107.26	112.19
10	A	1	NAG	C2-N2-C7	3.66	127.81	122.90
11	D	1	NAG	O5-C5-C6	3.10	113.70	107.66
10	A	1	NAG	O5-C1-C2	-3.07	106.54	111.29
11	D	1	NAG	O4-C4-C3	-3.06	103.16	110.38
10	A	1	NAG	C1-O5-C5	2.99	116.19	112.19
10	A	1	NAG	O5-C5-C6	2.94	113.39	107.66
10	A	1	NAG	O7-C7-N2	2.92	127.14	121.98
11	B	2	NAG	O5-C1-C2	-2.91	106.79	111.29
10	A	1	NAG	O4-C4-C5	2.79	116.19	109.32
10	A	3	NAG	O5-C1-C2	-2.66	107.18	111.29
10	A	2	NAG	O5-C1-C2	-2.51	107.40	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1	NAG	C8-C7-N2	-2.37	112.19	116.12
10	A	1	NAG	C8-C7-N2	-2.34	112.24	116.12
11	D	1	NAG	C1-O5-C5	2.33	115.31	112.19
11	D	1	NAG	O7-C7-N2	2.24	125.94	121.98
11	D	2	NAG	O5-C1-C2	-2.21	107.88	111.29
10	A	1	NAG	O5-C5-C4	-2.11	105.70	110.83
10	A	2	NAG	C3-C4-C5	-2.09	106.44	110.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

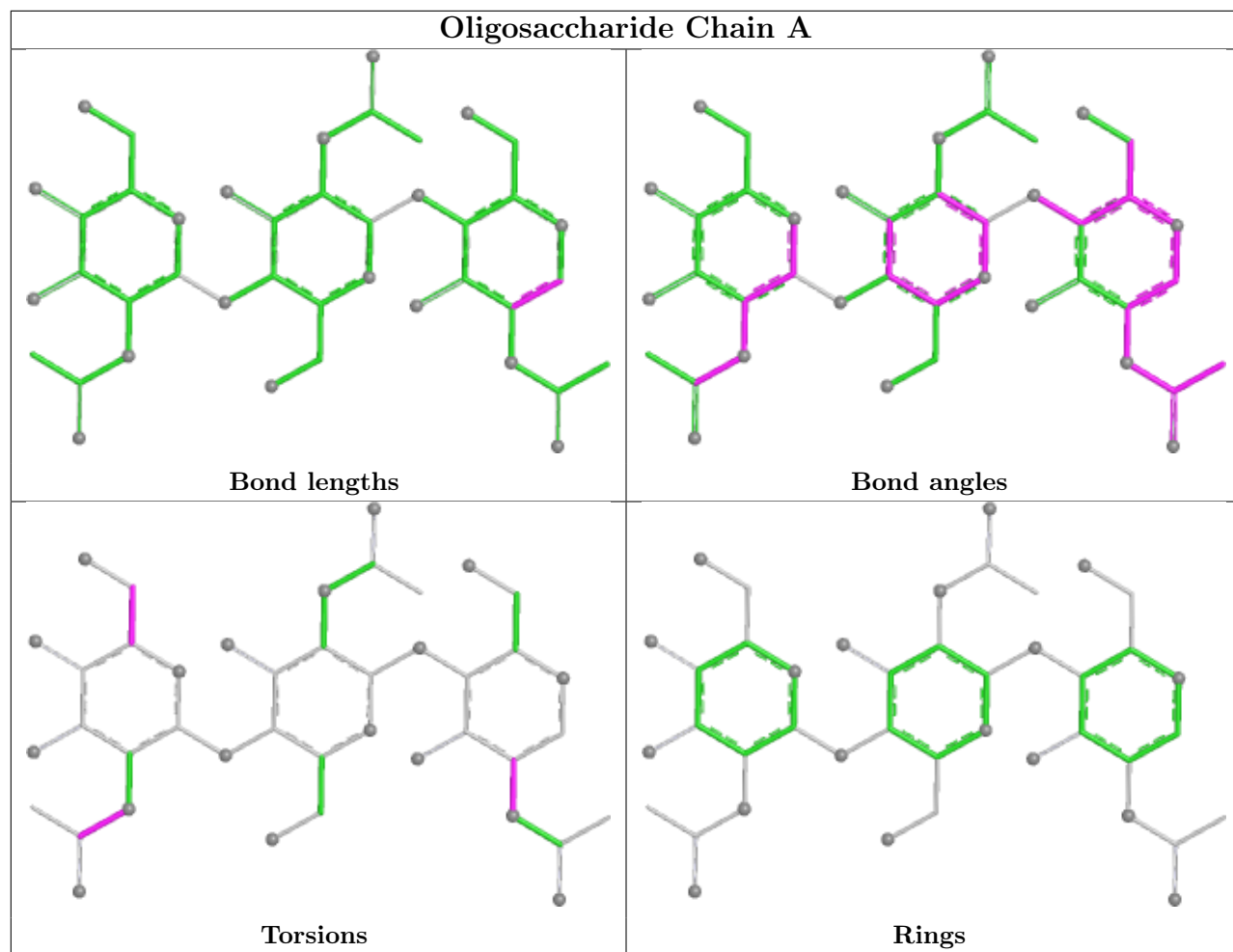
Mol	Chain	Res	Type	Atoms
11	B	2	NAG	C1-C2-N2-C7
10	A	3	NAG	C8-C7-N2-C2
10	A	3	NAG	O7-C7-N2-C2
11	B	1	NAG	C8-C7-N2-C2
11	B	1	NAG	O7-C7-N2-C2
10	A	3	NAG	O5-C5-C6-O6
10	A	1	NAG	C3-C2-N2-C7
11	B	2	NAG	C3-C2-N2-C7

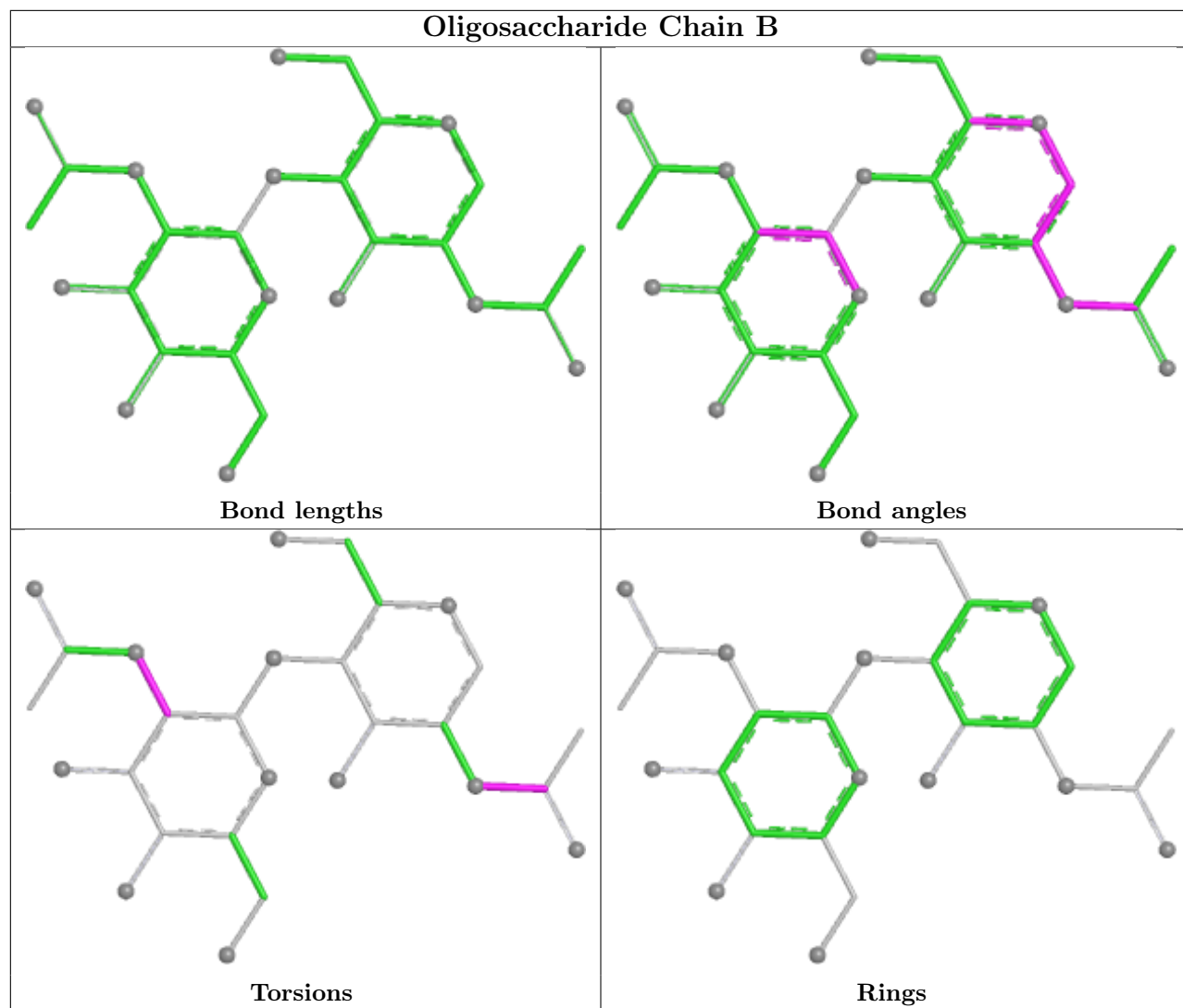
There are no ring outliers.

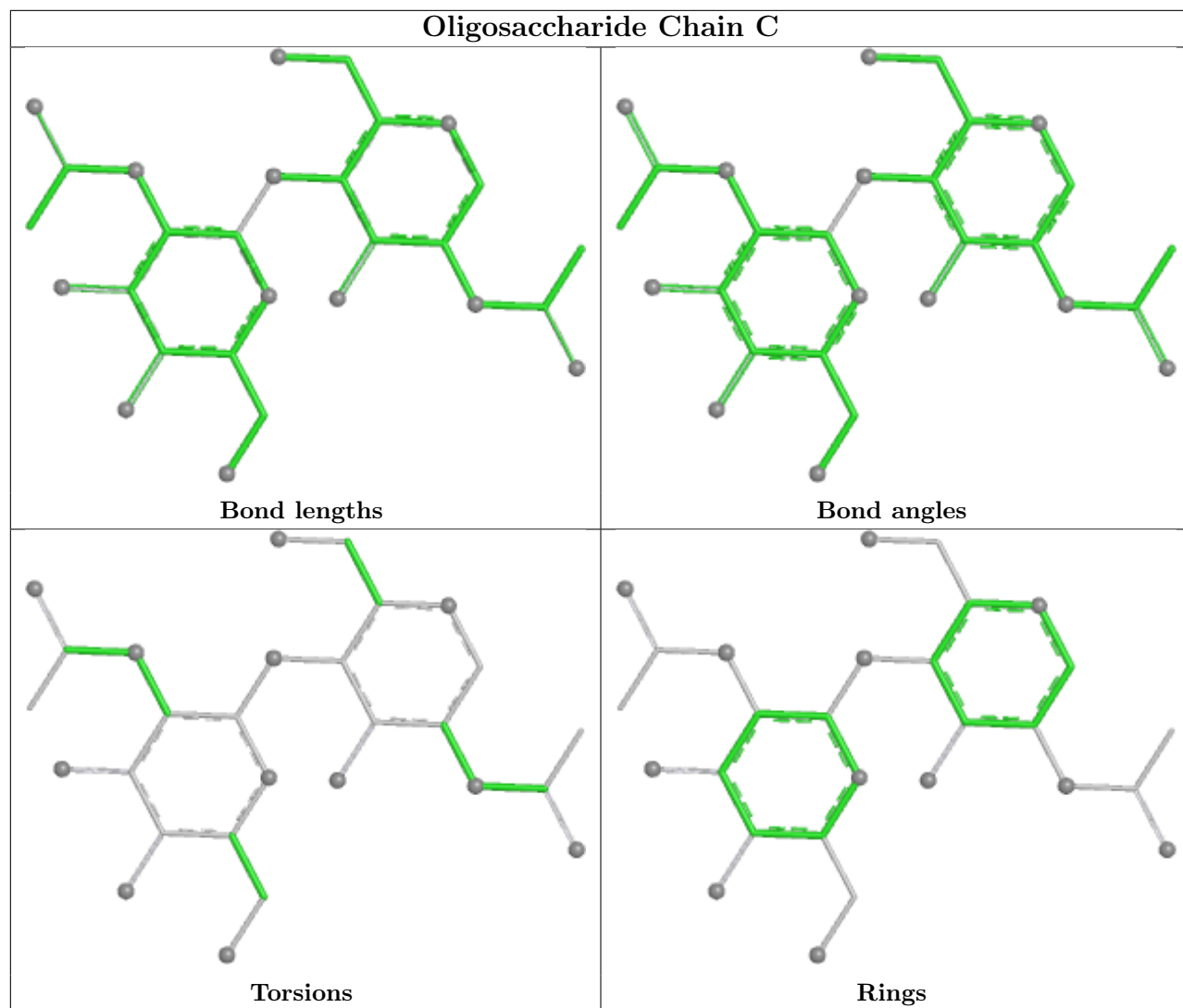
1 monomer is involved in 1 short contact:

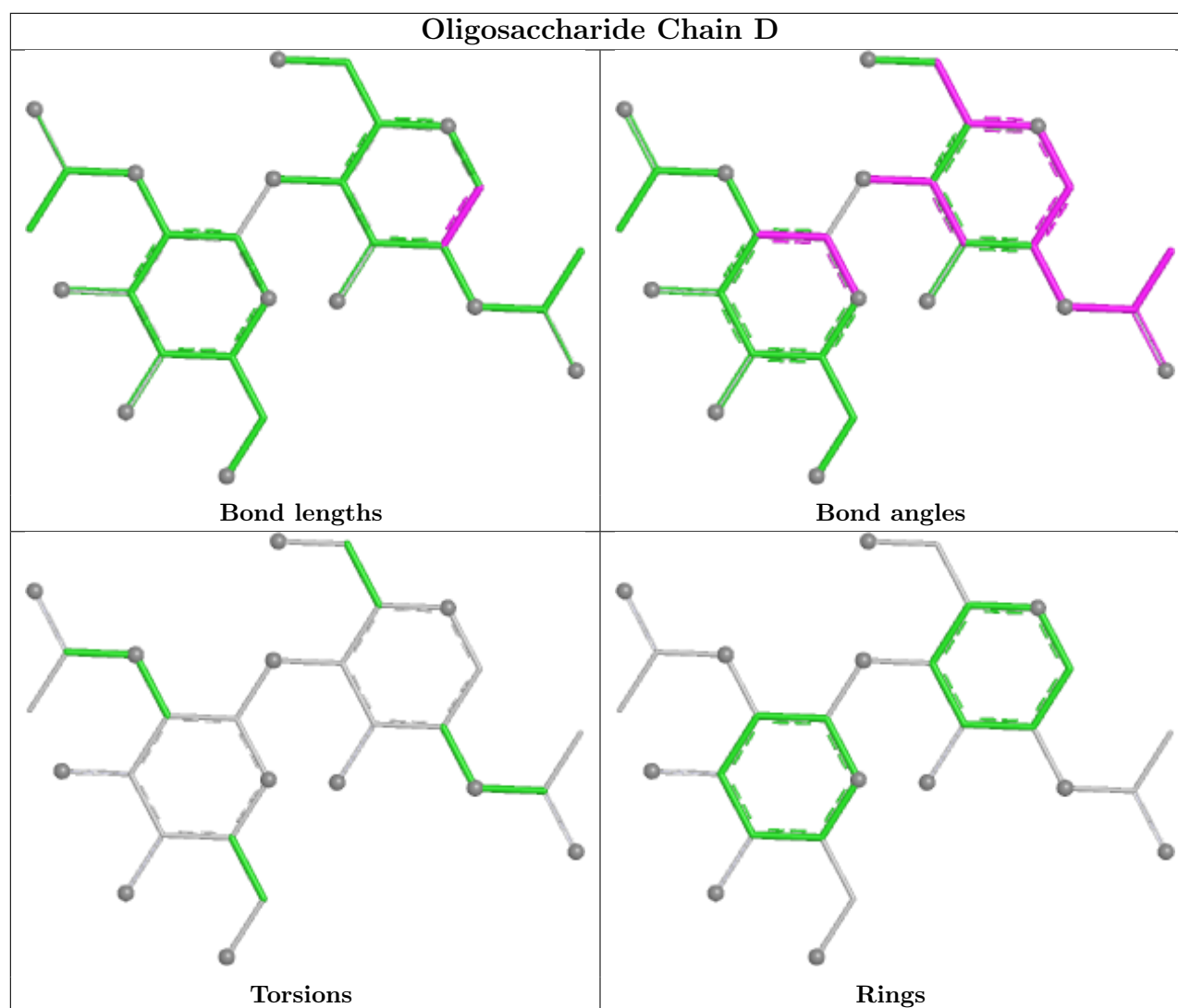
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1	NAG	1	0

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









5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	NAG	c	501	1	14,14,15	0.74	0	17,19,21	0.98	0
12	NAG	c	502	1	14,14,15	0.92	1 (7%)	17,19,21	1.51	2 (11%)
12	NAG	c	503	1	14,14,15	0.76	0	17,19,21	1.22	1 (5%)

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
12	NAG	c	501	1	-	0/6/23/26	0/1/1/1
12	NAG	c	502	1	-	0/6/23/26	0/1/1/1
12	NAG	c	503	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	c	502	NAG	C1-C2	2.40	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	c	502	NAG	C1-O5-C5	4.79	118.61	112.19
12	c	503	NAG	O5-C1-C2	-3.21	106.32	111.29
12	c	502	NAG	O5-C1-C2	-2.42	107.54	111.29

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	c	503	NAG	C1-C2-N2-C7
12	c	503	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.

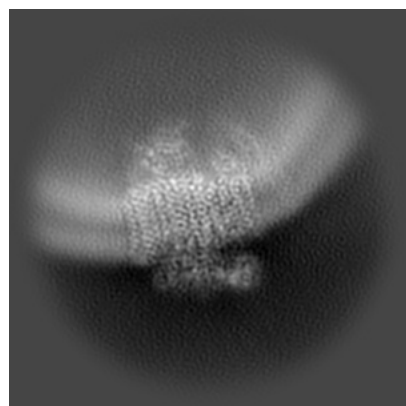
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44846. These allow visual inspection of the internal detail of the map and identification of artifacts.

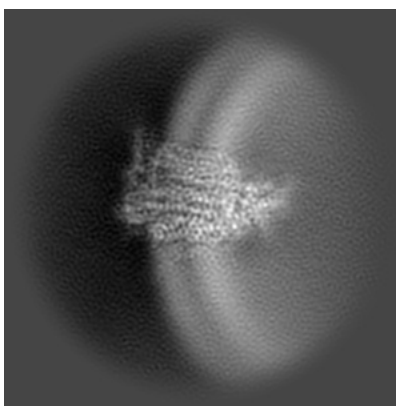
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

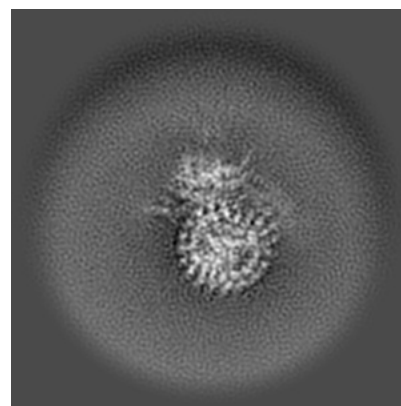
6.1.1 Primary map



X

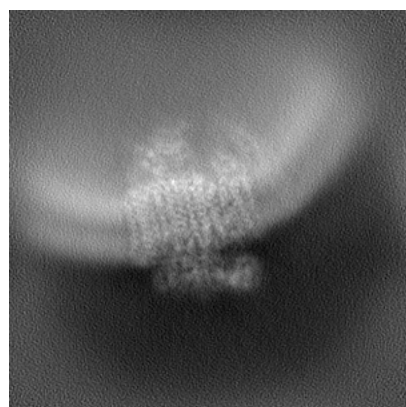


Y

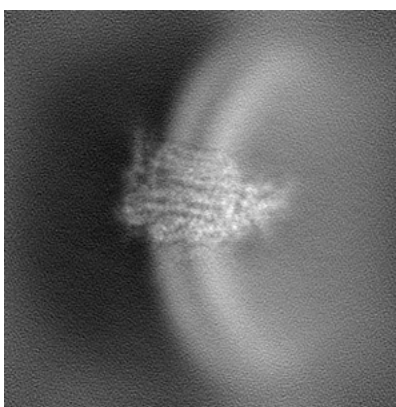


Z

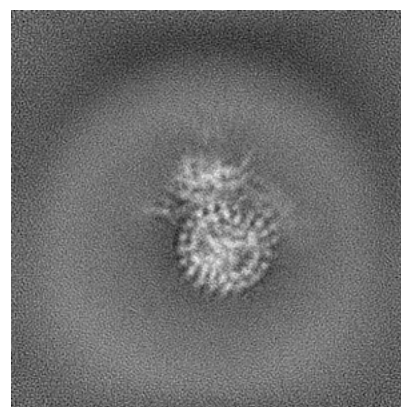
6.1.2 Raw map



X



Y

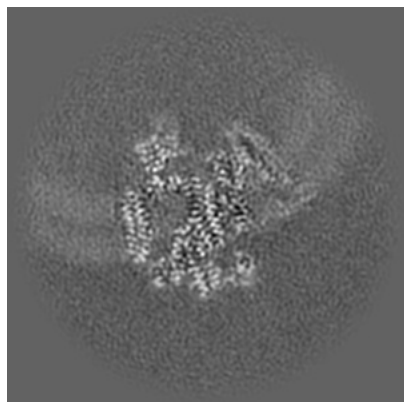


Z

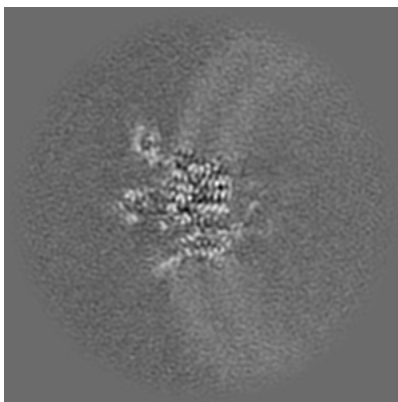
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

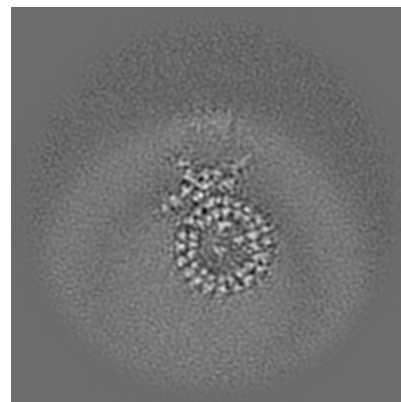
6.2.1 Primary map



X Index: 144

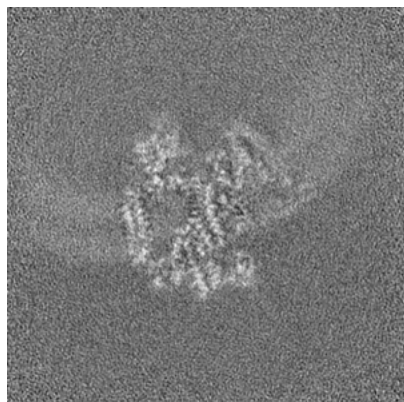


Y Index: 144

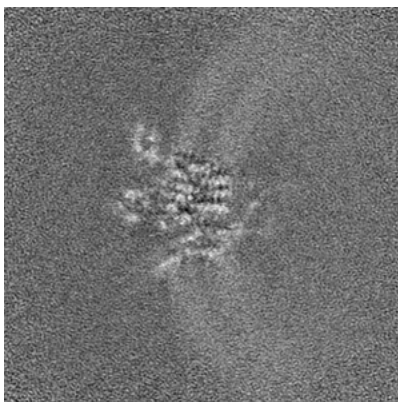


Z Index: 144

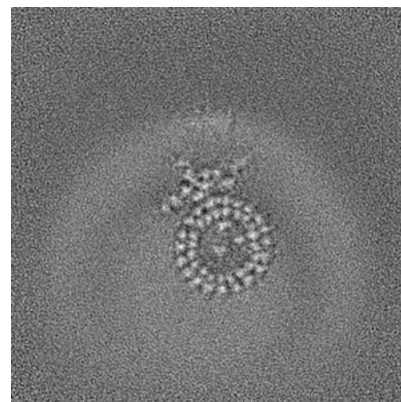
6.2.2 Raw map



X Index: 144



Y Index: 144

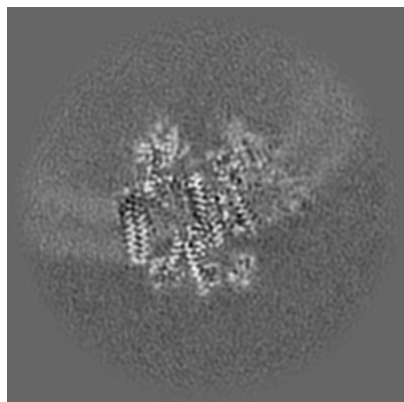


Z Index: 144

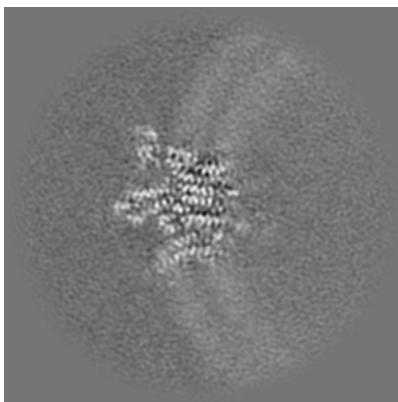
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

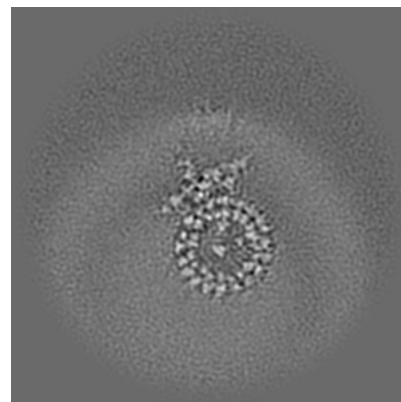
6.3.1 Primary map



X Index: 146

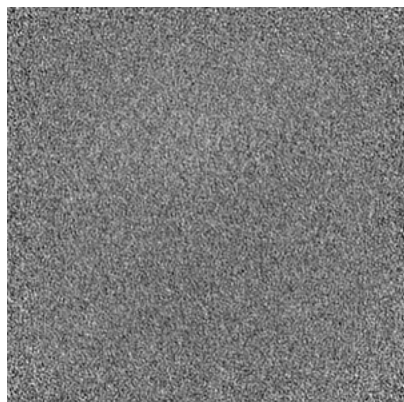


Y Index: 141

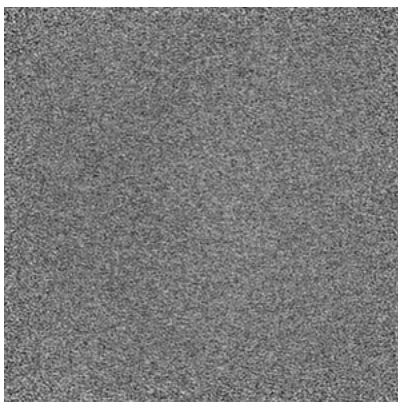


Z Index: 145

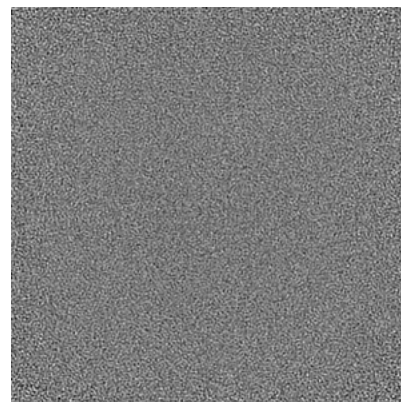
6.3.2 Raw map



X Index: 0



Y Index: 0

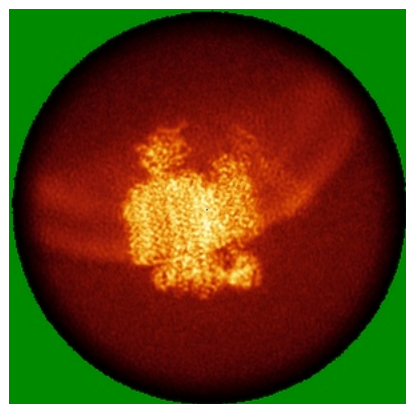


Z Index: 0

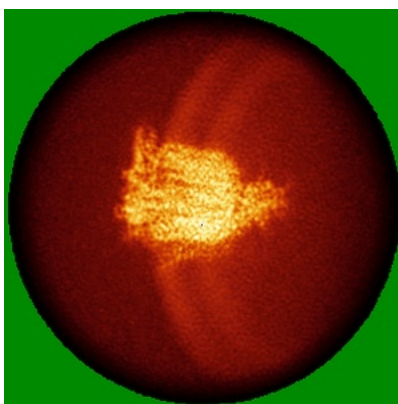
The images above show the largest variance slices of the map in three orthogonal directions.

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

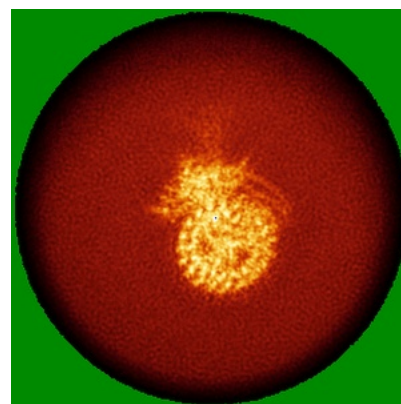
6.4.1 Primary map



X

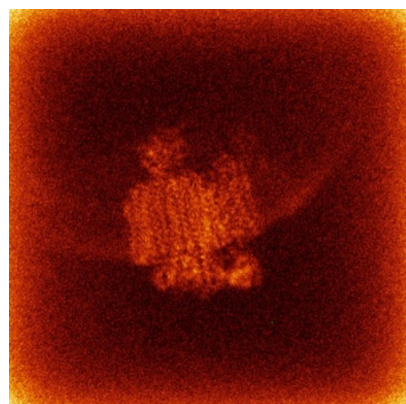


Y

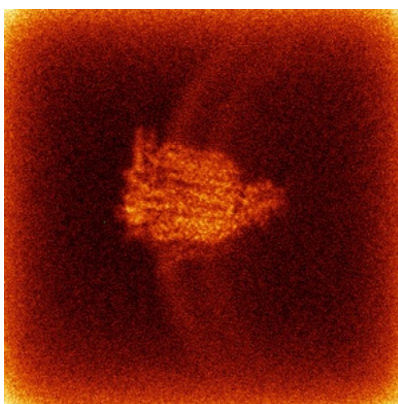


Z

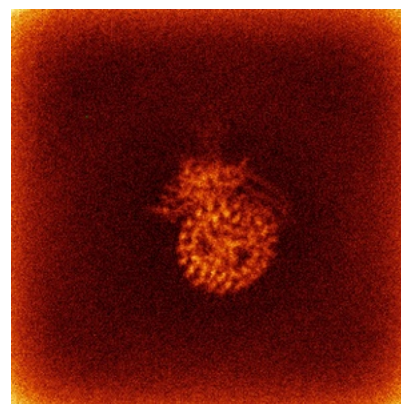
6.4.2 Raw map



X



Y

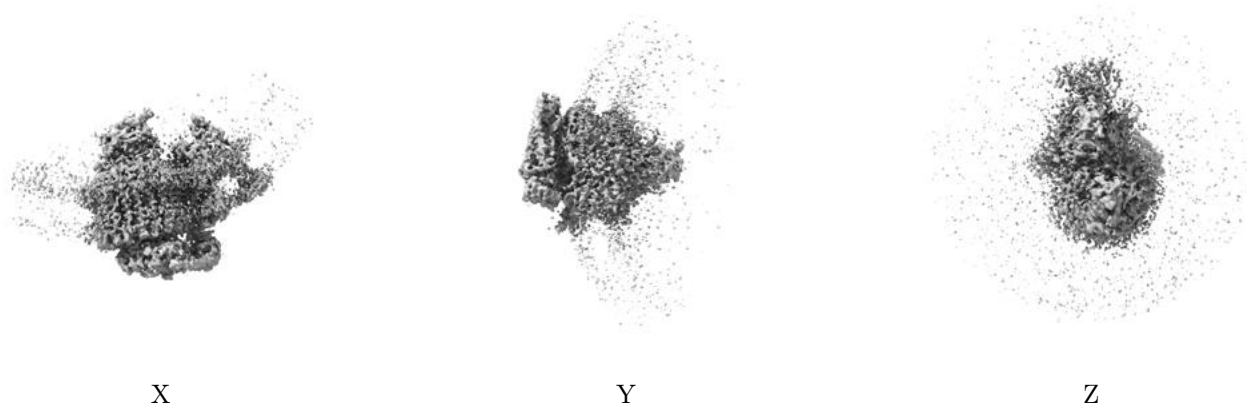


Z

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.

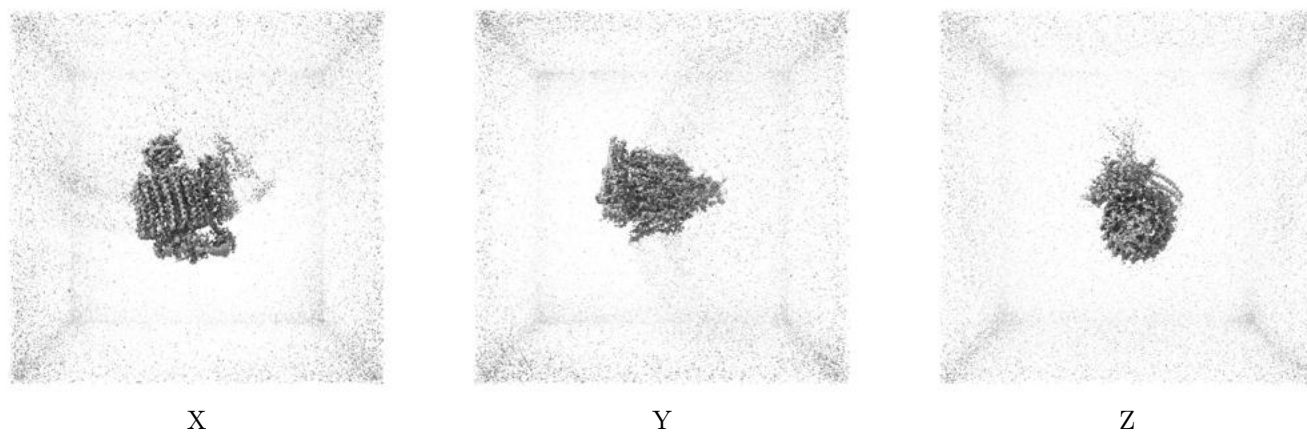
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

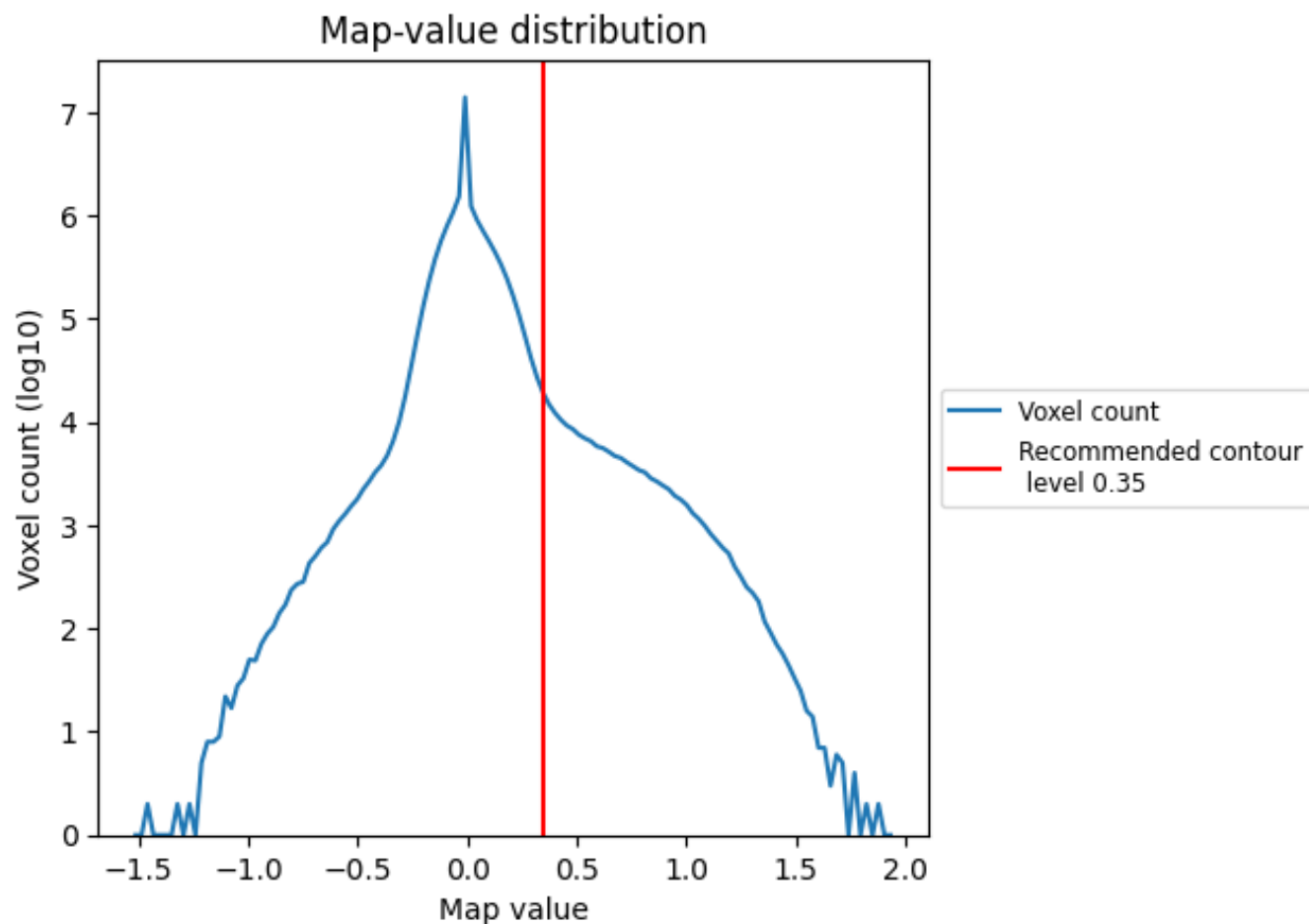
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

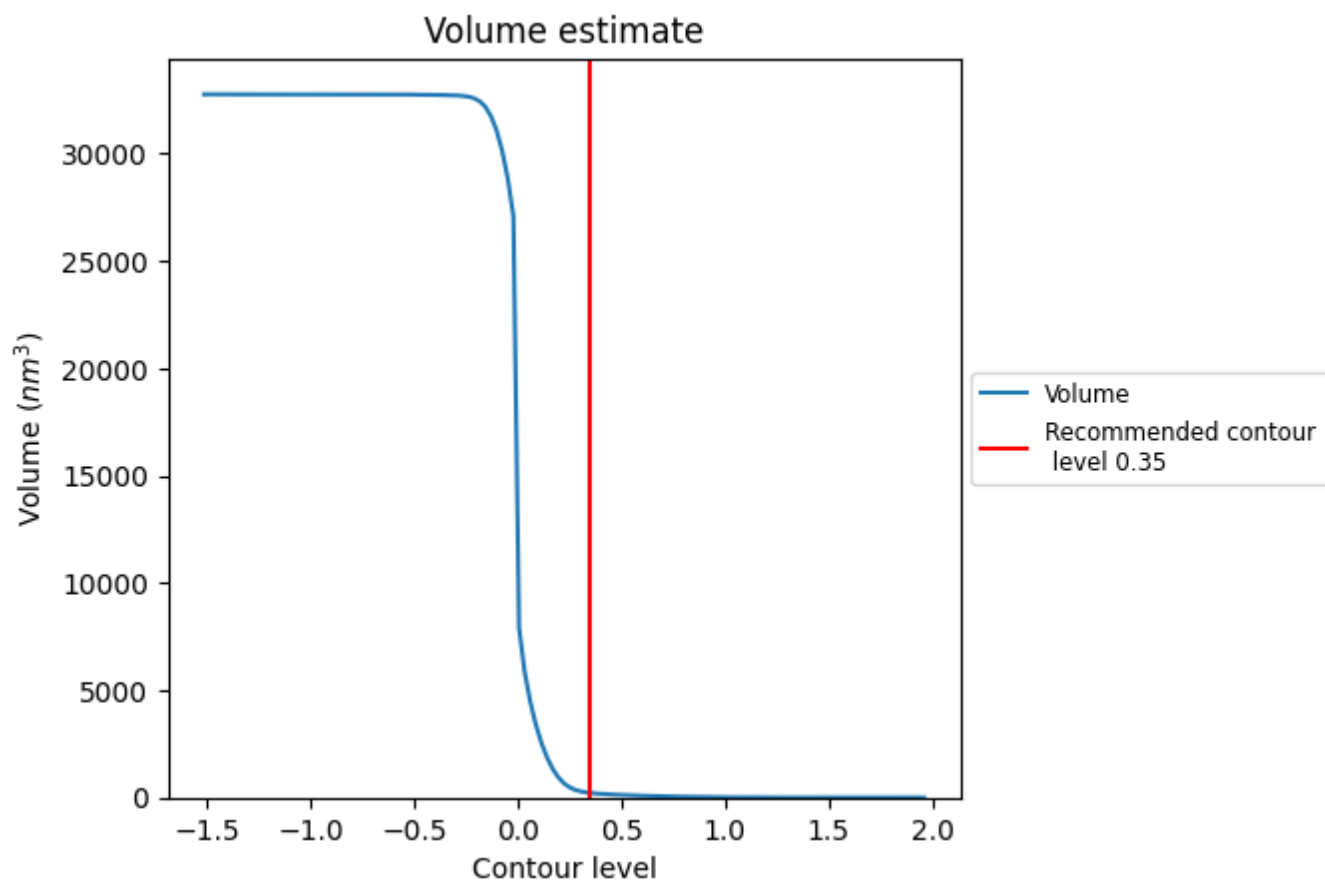
This section contains the results of statistical analysis of the map.

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.

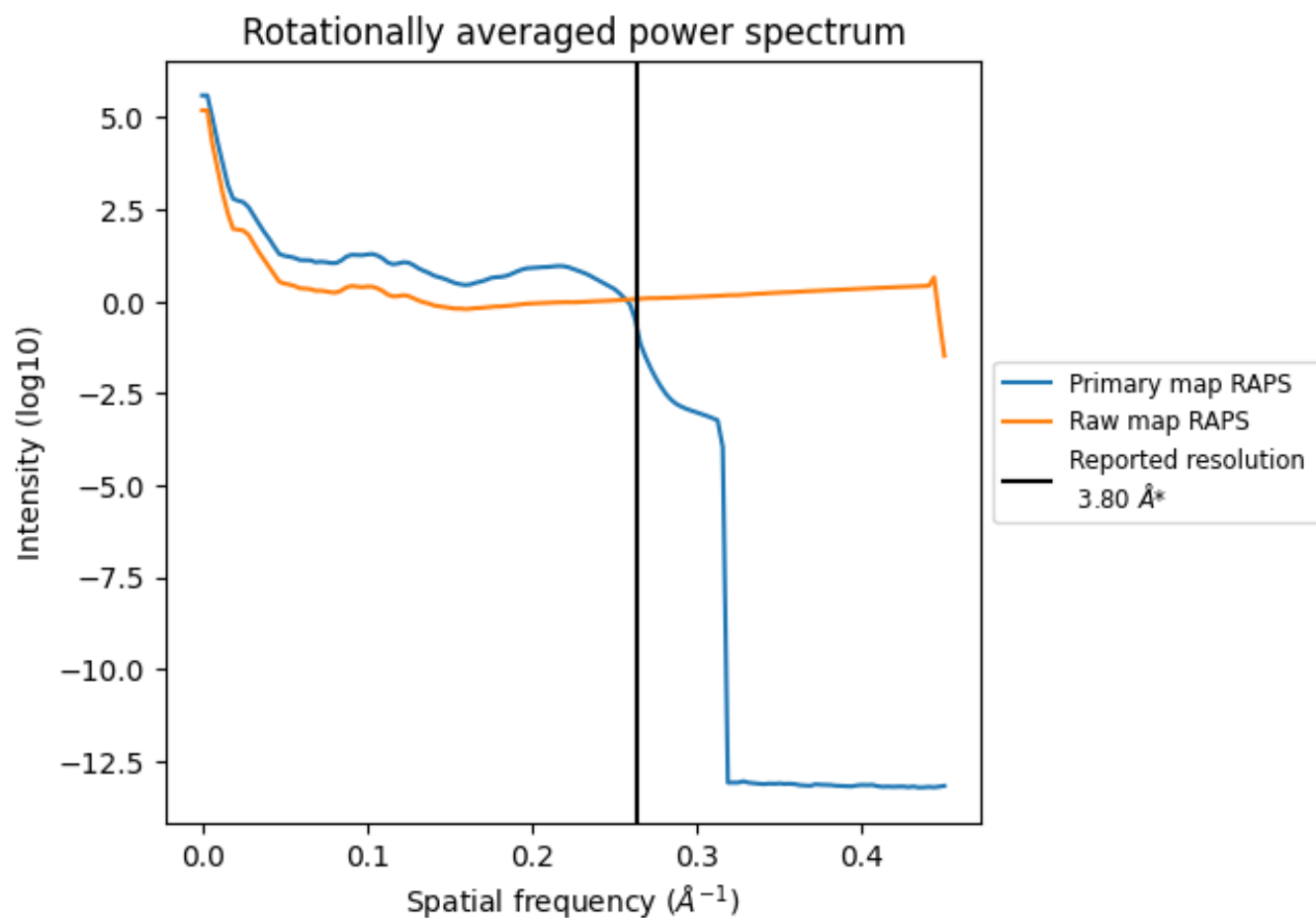
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 216 nm³; this corresponds to an approximate mass of 195 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 ⓘ

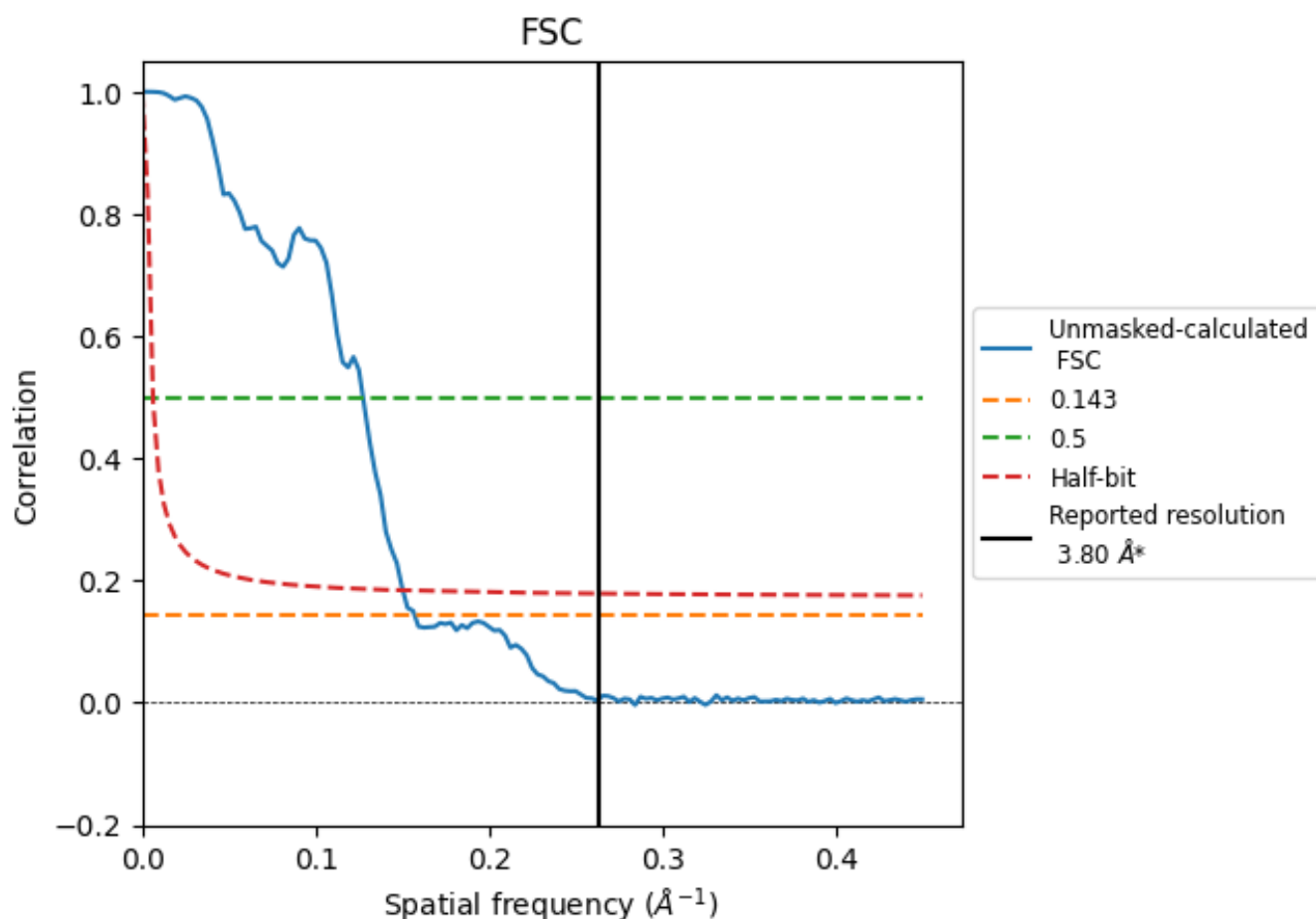


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

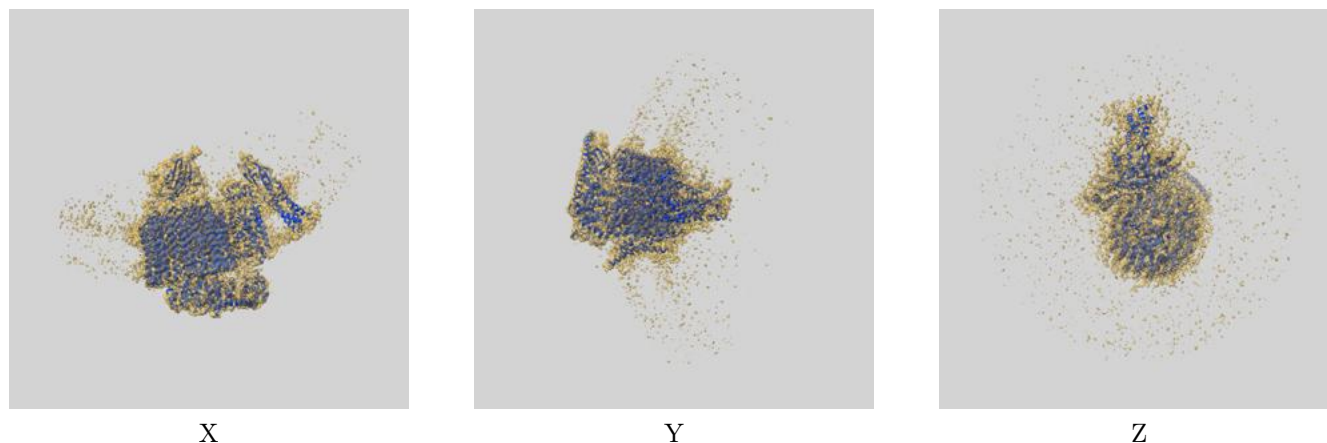
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.37	7.85	6.65

*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 6.37 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

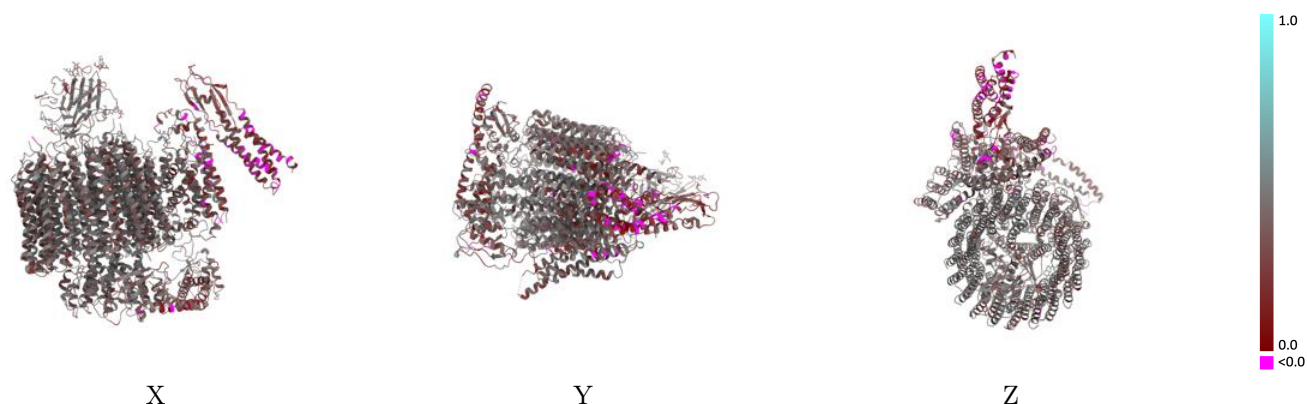
This section contains information regarding the fit between EMDB map EMD-44846 and PDB model 9BRZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



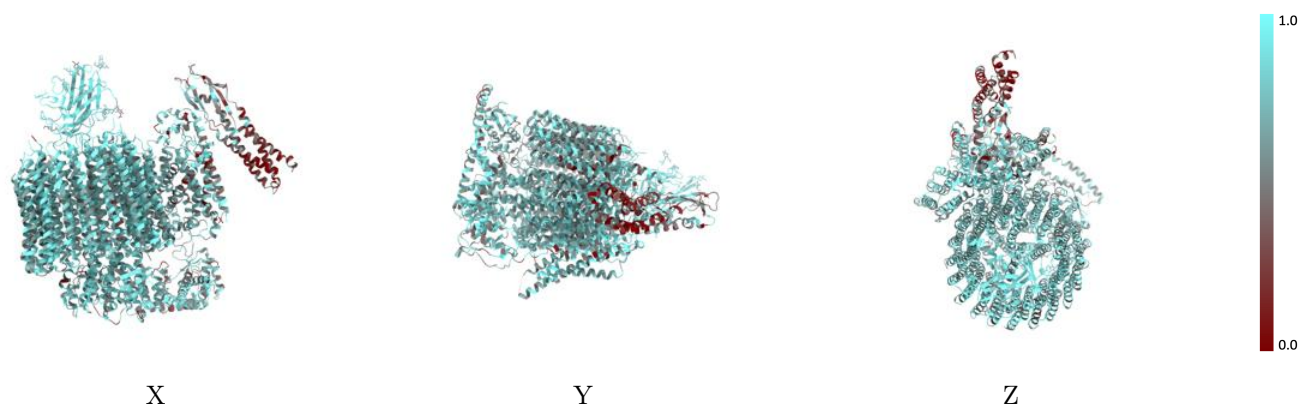
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



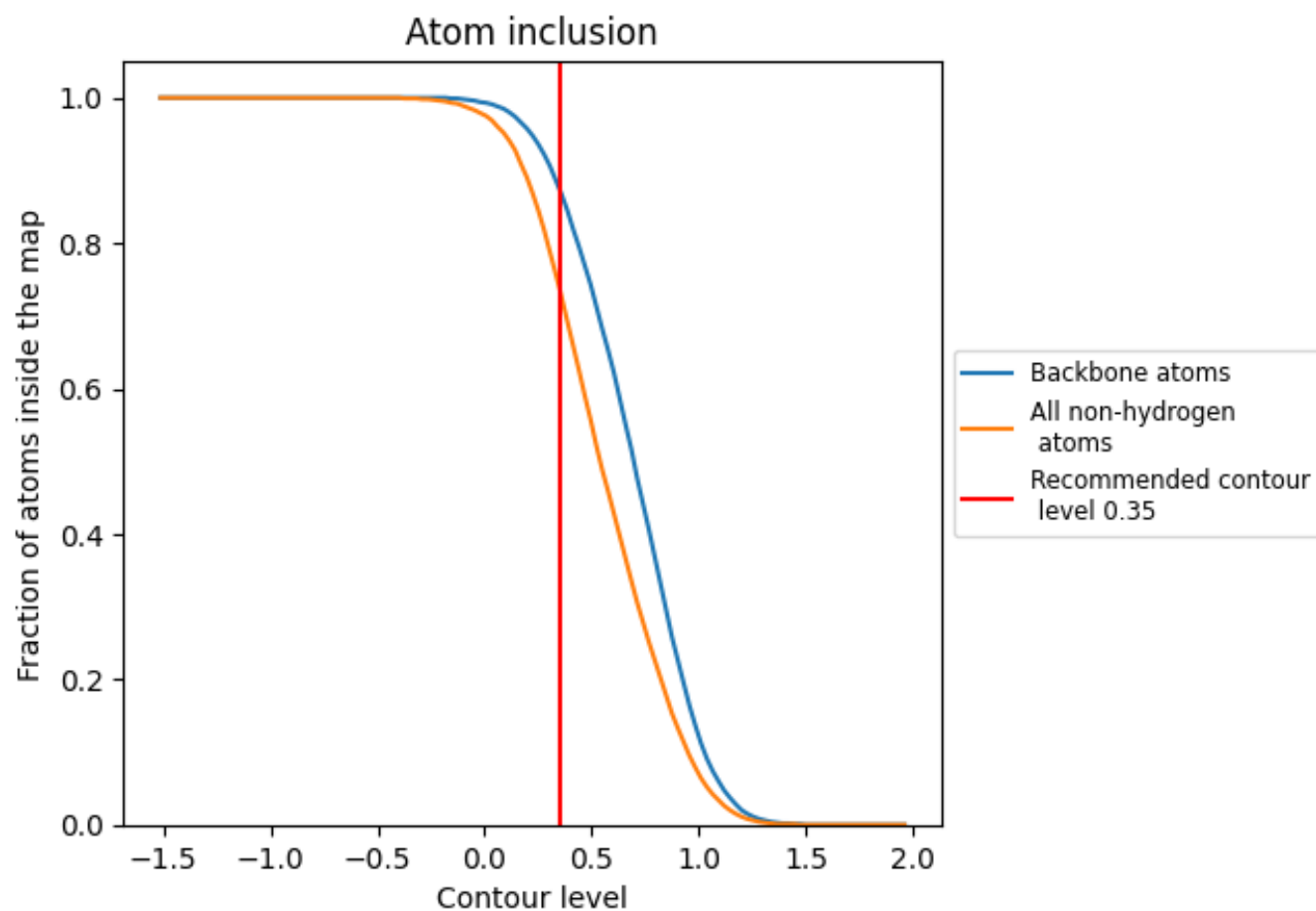
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.3850
A	 0.6430	 0.3300
B	 0.6790	 0.3030
C	 0.6070	 0.3510
D	 0.7860	 0.4750
a	 0.6970	 0.3490
b	 0.8190	 0.4520
c	 0.8630	 0.4330
d	 0.7700	 0.4290
e	 0.7110	 0.3430
f	 0.6480	 0.2990
g	 0.8030	 0.4380
h	 0.7740	 0.3950
i	 0.7540	 0.3980
j	 0.7770	 0.3970
k	 0.7900	 0.4150
l	 0.7550	 0.4080
m	 0.7700	 0.4250
n	 0.8190	 0.4440
o	 0.8050	 0.4510
p	 0.8030	 0.4370
s	 0.3860	 0.1760

