



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 05:12 PM UTC

PDB ID : 8VI0 / pdb_00008vi0
EMDB ID : EMD-43245
Title : Cryo EM structure of a soybean CesA6 homotrimer
Authors : Ho, R.; Palliniti, P.; Zimmer, J.
Deposited on : 2024-01-02
Resolution : 3.00 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:

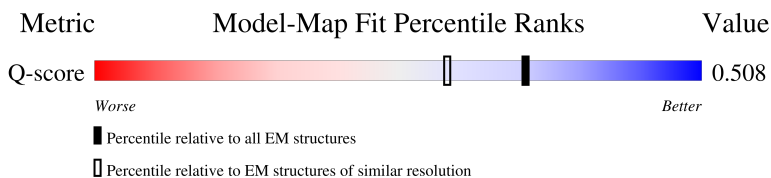
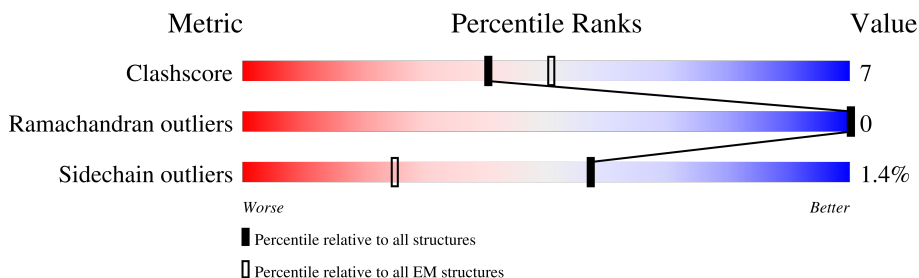
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 3.00 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	14081 (2.50 - 3.50)

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	1078	
1	B	1078	
1	D	1078	
2	C	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	3	 33% 67%
2	F	3	 67% 33%

2 Entry composition [i](#)

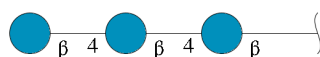
There are 2 unique types of molecules in this entry. The entry contains 17454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cellulose synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	724	Total	C	N	O	S	0	0
			5798	3791	971	1006	30		
1	B	723	Total	C	N	O	S	0	0
			5790	3787	969	1004	30		
1	D	724	Total	C	N	O	S	0	0
			5797	3790	971	1006	30		

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

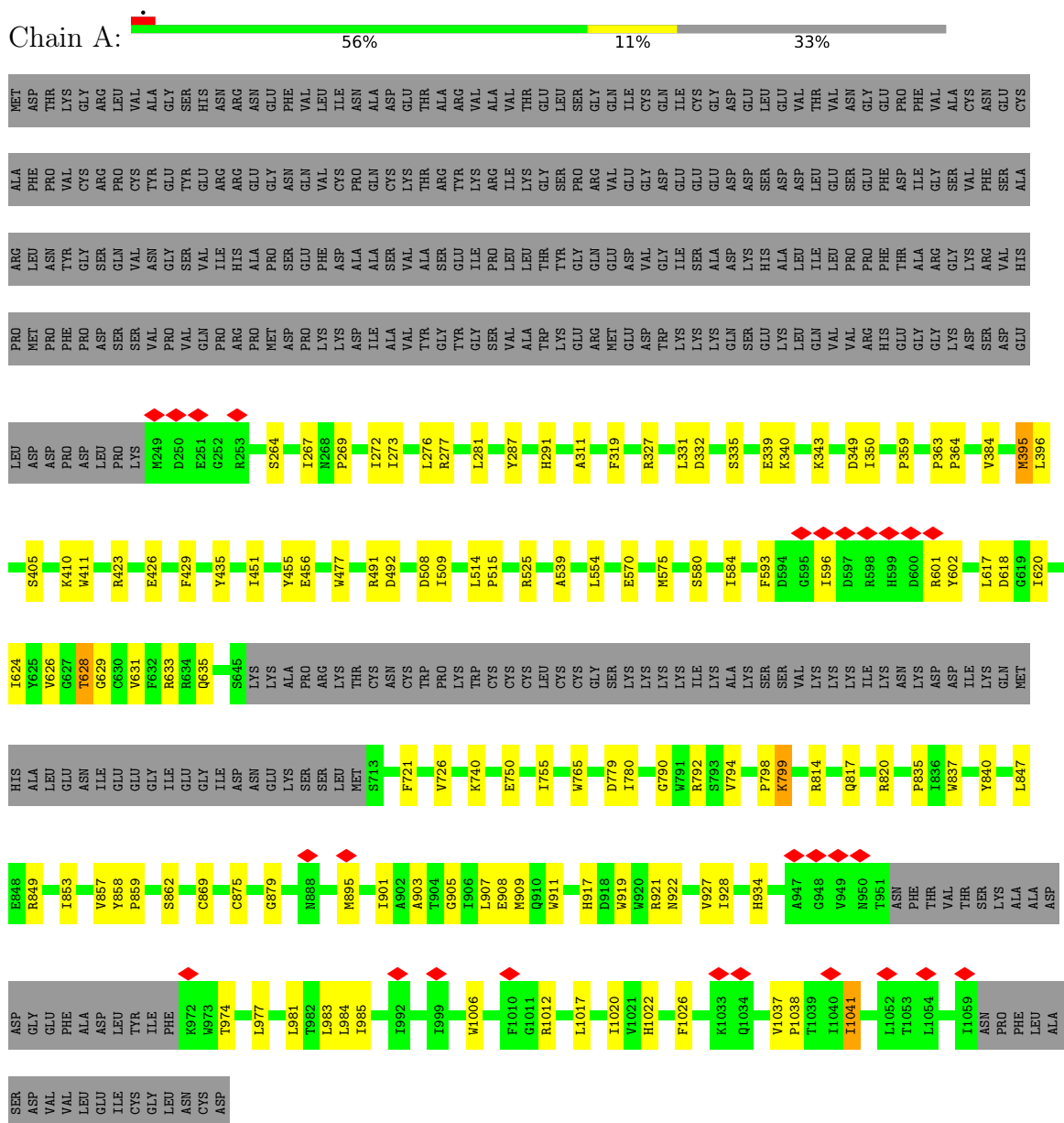


Mol	Chain	Residues	Atoms			AltConf	Trace
2	C	3	Total	C	O	0	1
			23	12	11		
2	E	3	Total	C	O	0	1
			23	12	11		
2	F	3	Total	C	O	0	1
			23	12	11		

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: Cellulose synthase



- Molecule 1: Cellulose synthase

Chain B:

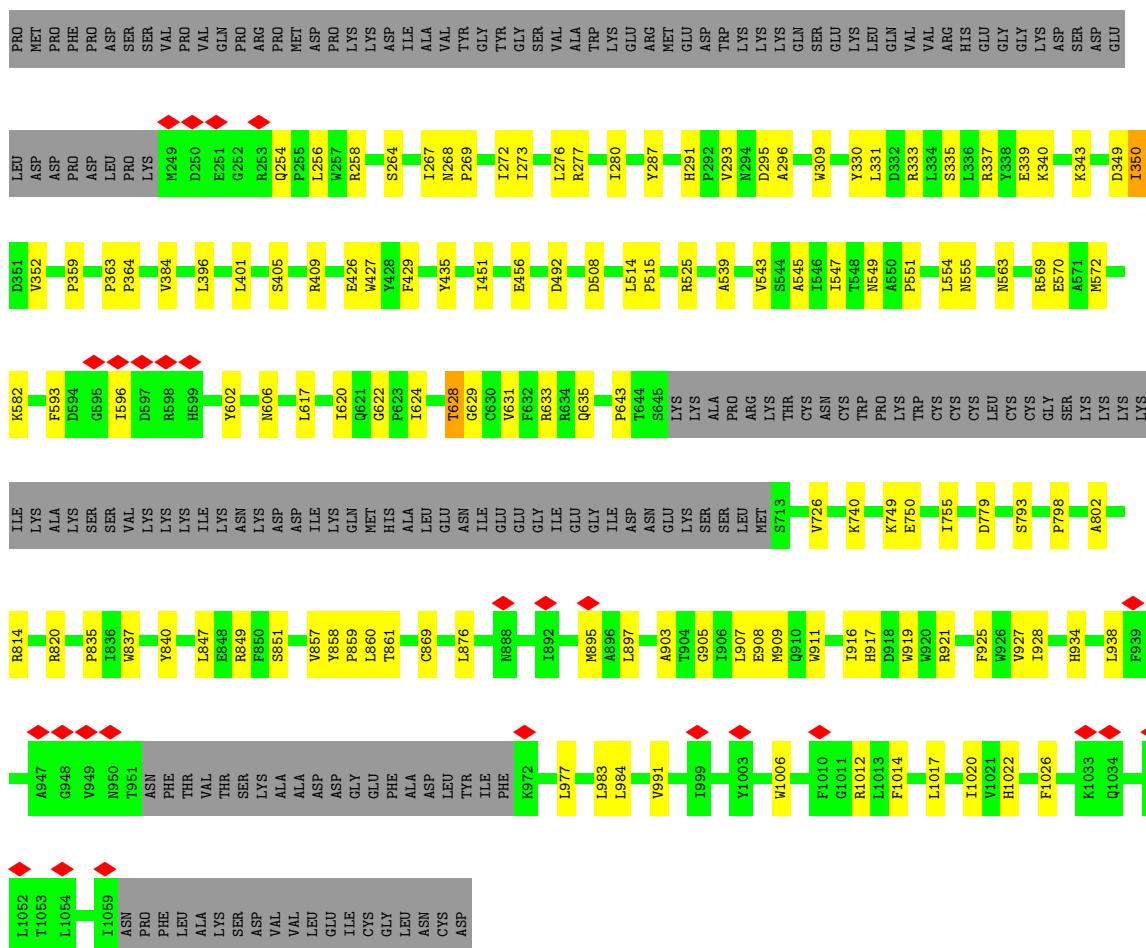


L1017	D918	G790	LYS	D594	A400	LEU	PRO	ARG	ALA	MET
	W919	W791	SER	G595		ASP	LEU	LEU	PHE	ASP
I1020	W920	R792	SER	I596	T404	ASP	PRO	PRO	PRO	THR
W1021	S793	S793	VAL	I596	E406	PRO	PHE	TYR	VAL	TYR
H1022	N922	W794	VAL	D597	E406	ASP	PRO	GLY	CYS	GLY
	E923	W795	LYS	R598		LEU	ASP	SER	ARG	GLY
		G796	LYS	H599	R409	PRO	SER	GLN	PRO	LEU
F1026	V927	W797	ILE	K410	K410	LYS	SER	VAL	CYS	LEU
		P798	LYS	D600	W411		VAL	ASN	TYR	VAL
M1031	H934	R799	ASN	R601			PRO	GLY	GLY	GLY
G1032	L935		LYS	Y602	R423		VAL	VAL	TYR	SER
L1033	F336		ASP				GLN	VAL	GLY	HIS
Q1034	A857	A802	ASP	L617	F429		PRO	ILE	ARG	ASN
		R814	ILE				ARG	HIS	ARG	ASN
P1038	L938	L815	LYS	I620	Y435		PRO	ALA	GLU	ASN
I1040	F939	W821	GLN	Q621	I451		MET	PRO	GLY	ASN
I1041	A947		MET	G622	E456		ASP	PRO	GLN	PHE
	G948	P635	HIS	P623			LYS	GLY	VAL	LEU
	V949		ALA	I624	E456		LYS	PHE	VAL	LEU
L1052	K945		LEU	Y625			LYS	ASP	CYS	ILE
T1053	S846	R945	GLU	V626	D481		ASP	ALA	PRO	ASN
L1054	L947	L847	ILE	G627	G482		ILE	ALA	GLN	ALA
	ASN	T628	GLU	T628	T483		ALA	SER	CYS	ASP
	PHE	F848	GLU	G629			VAL	VAL	CYS	GLY
I1059	R349	R949	GLU	C830	D492		TYR	ALA	THR	THR
ASN	THR		GLY	V631			GLY	SER	ARG	ALA
PRO	VAL	Y852	ILE	F632	V506		TYR	GLU	TYR	ARG
PHE	THR	I853	GLU	R633	R507		GLY	ILE	LYS	VAL
LEU	LYS	ASN	GLY	R634	D508		SER	PRO	ARG	ALA
ALA	ALA	S855	ILE	Q635			VAL	VAL	ILE	VAL
LYS	ALA		ASP		L514		ALA	LEU	LYS	THR
SER	ASP	Y858	ASN	T644			TRP	THR	GLY	GLY
ASP	ASP	P859	GLU	S645	R525		LYS	TYR	SER	LEU
VAL	GLY	L860	LYS	LYS	A539		GLU	GLY	PRO	SER
VAL	GLU		SER	LYS			ARG	GLN	ARG	GLY
LEU	PHE	I663	SER	ALA	A539		MET	GLY	VAL	GLN
GLU	ALA	P864	LEU	PRO	L554		GLU	ASP	GLU	ILE
ILE	ASP		ASP	ARG	N855		VAL	GLY	GLY	CYS
CYS	LEU	L871	MET	THR			TRP	GLY	ASP	GLN
GLY	TYR		S713	THR	N563		LYS	ILE	GLU	ILE
LEU	ILE	C875	CYS	THR			CYS	SER	GLU	CYS
ASN	PHE		F721	ASN	L568		LYS	ALA	GLU	GLY
CYS		G879	W726	CYS	R569		GLN	ASP	ASP	GLY
ASP	K972	K880		TRP	E570		SER	LYS	ASP	GLU
	W973		K740	PRO	M571		GLU	HIS	SER	LEU
	T974			LYS			LYS	ALA	ASP	GLU
		N888	L747	TRP	M572		LEU	ASP	VAL	THR
	L977			TRP			GLN	ILE	LEU	THR
	L984	M895	E750	CYS	M575		VAL	LEU	GLU	VAL
			CYS	CYS			VAL	PRO	SER	ASN
	A903	T904	I755	LEU	S800		ARG	PRO	GLU	ASN
I999	G905		W765	CYS	K583		HIS	PHE	GLY	GLY
	L906		G766	CYS	I584		GLU	THR	ASP	PRO
Y1003	L907			GLY			GLY	ALA	ILE	PHE
	E908		Y773	SER	V587		GLY	ARG	GLY	

- Molecule 1: Cellulose synthase

Chain D:

[illegible]



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



- Molecule 2: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192666	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.495	Depositor
Minimum map value	-1.673	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.2	Depositor
Map size ($\text{\AA}$)	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.10	0/5964	0.27	0/8107
1	B	0.10	0/5955	0.27	0/8093
1	D	0.10	0/5963	0.26	0/8105
All	All	0.10	0/17882	0.27	0/24305

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5798	0	5818	75	0
1	B	5790	0	5811	85	0
1	D	5797	0	5814	86	0
2	C	23	0	19	2	0
2	E	23	0	19	3	0
2	F	23	0	19	1	0
All	All	17454	0	17500	243	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 7.

All (243) 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:A:984:LEU:HD11	1:A:1020:ILE:HG13	1.69	0.73
1:D:593:PHE:HB2	1:D:596:ILE:HD11	1.71	0.73
1:B:593:PHE:HB2	1:B:596:ILE:HD11	1.72	0.72
1:A:593:PHE:HB2	1:A:596:ILE:HD11	1.72	0.72
1:B:909:MET:HE1	1:B:919:TRP:HB3	1.73	0.71
1:A:909:MET:HE1	1:A:919:TRP:HB3	1.72	0.70
1:A:927:VAL:HG21	1:A:1022:HIS:HD2	1.57	0.69
1:B:934:HIS:O	1:B:938:LEU:HD12	1.94	0.68
1:A:903:ALA:O	1:A:907:LEU:HD12	1.94	0.67
1:B:879:GLY:HA2	1:B:1012:ARG:HH22	1.60	0.67
1:A:273:ILE:HG23	1:A:276:LEU:HD23	1.77	0.67
1:D:258:ARG:NH1	1:D:330:TYR:OH	2.28	0.67
1:D:254:GLN:HB3	1:D:333:ARG:NH1	2.10	0.66
1:B:350:ILE:HD11	1:B:572:MET:HE3	1.77	0.66
1:A:879:GLY:HA2	1:A:1012:ARG:HH22	1.61	0.65
1:B:905:GLY:O	1:B:909:MET:HG2	1.96	0.65
1:D:539:ALA:HB1	1:D:755:ILE:HG22	1.79	0.65
1:A:740:LYS:HE3	1:A:740:LYS:HA	1.79	0.64
1:D:276:LEU:O	1:D:280:ILE:HG23	1.98	0.64
1:A:539:ALA:HB1	1:A:755:ILE:HG22	1.79	0.62
1:A:905:GLY:O	1:A:909:MET:HG2	1.99	0.62
1:A:264:SER:HA	1:A:267:ILE:HG22	1.82	0.62
1:B:539:ALA:HB1	1:B:755:ILE:HG22	1.82	0.62
1:D:934:HIS:O	1:D:938:LEU:HD12	2.00	0.61
1:B:903:ALA:O	1:B:907:LEU:HD12	2.01	0.61
1:B:875:CYS:O	1:B:1012:ARG:NH2	2.34	0.61
1:D:256:LEU:HD21	1:D:337:ARG:HD3	1.82	0.61
1:D:860:LEU:HD13	1:D:938:LEU:HD21	1.82	0.61
1:B:264:SER:HA	1:B:267:ILE:HG22	1.82	0.61
1:B:792:ARG:HH21	1:B:845:LYS:HE3	1.65	0.61
1:A:554:LEU:HD13	1:A:631:VAL:HG22	1.81	0.60
1:B:740:LYS:HA	1:B:740:LYS:HE3	1.83	0.60
1:A:875:CYS:O	1:A:1012:ARG:NH2	2.35	0.60
1:A:281:LEU:HD21	1:A:311:ALA:HB1	1.83	0.60
1:B:350:ILE:HD13	1:B:568:LEU:HD22	1.84	0.59
1:B:1017:LEU:HA	1:B:1020:ILE:HG22	1.85	0.59
1:D:409:ARG:HG3	1:D:508:ASP:HA	1.84	0.58
1:D:876:LEU:HA	1:D:1012:ARG:HH21	1.69	0.58
1:D:905:GLY:O	1:D:909:MET:HG2	2.04	0.58
1:D:984:LEU:HD11	1:D:1020:ILE:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:ARG:HA	1:B:921:ARG:HD3	1.85	0.57
1:A:492:ASP:OD1	1:A:525:ARG:NH1	2.37	0.57
1:D:264:SER:HA	1:D:267:ILE:HG22	1.87	0.57
1:D:628:THR:OG1	1:D:629:GLY:N	2.38	0.57
1:B:352:VAL:HA	1:B:554:LEU:HB3	1.87	0.56
1:A:633:ARG:HE	1:A:635:GLN:HB2	1.68	0.56
1:B:492:ASP:OD1	1:B:525:ARG:NH1	2.36	0.56
1:D:350:ILE:HD11	1:D:572:MET:HE3	1.87	0.56
1:D:582:LYS:HB3	1:D:643:PRO:HG2	1.88	0.56
1:D:633:ARG:HE	1:D:635:GLN:HB2	1.70	0.56
1:A:628:THR:OG1	1:A:629:GLY:N	2.38	0.56
1:A:790:GLY:O	1:A:792:ARG:NH1	2.38	0.56
1:B:273:ILE:HD12	1:B:907:LEU:HD11	1.87	0.56
1:B:977:LEU:HD23	1:B:1026:PHE:HE2	1.71	0.55
1:D:555:ASN:O	1:D:629:GLY:N	2.40	0.55
1:A:456:GLU:OE2	1:B:435:TYR:OH	2.23	0.55
1:B:602:TYR:HB3	1:B:814:ARG:HD3	1.89	0.55
1:A:626:VAL:HB	2:C:3:BGC:H4	1.89	0.55
1:B:281:LEU:HD21	1:B:311:ALA:HB1	1.89	0.55
1:B:628:THR:OG1	1:B:629:GLY:N	2.39	0.55
1:D:620:ILE:HD13	1:D:847:LEU:HB3	1.88	0.55
1:D:1006:TRP:H	1:D:1006:TRP:CD1	2.24	0.55
1:B:481:ASP:OD1	1:B:483:THR:OG1	2.24	0.54
1:D:273:ILE:HD13	1:D:907:LEU:HD21	1.88	0.54
1:D:277:ARG:HA	1:D:280:ILE:HG12	1.89	0.54
1:D:492:ASP:OD1	1:D:525:ARG:NH1	2.38	0.54
1:B:331:LEU:HD21	1:B:570:GLU:HG2	1.90	0.54
1:B:1006:TRP:H	1:B:1006:TRP:CD1	2.25	0.53
1:D:254:GLN:HB3	1:D:333:ARG:HH11	1.72	0.53
1:A:820:ARG:HG2	1:A:820:ARG:HH11	1.73	0.53
1:D:869:CYS:HB3	1:D:983:LEU:HD21	1.90	0.53
1:B:508:ASP:HB3	1:B:514:LEU:HD11	1.91	0.53
1:B:456:GLU:OE2	1:D:435:TYR:OH	2.22	0.52
1:A:1006:TRP:H	1:A:1006:TRP:CD1	2.26	0.52
1:A:435:TYR:OH	1:D:456:GLU:OE2	2.23	0.52
1:B:984:LEU:HD11	1:B:1020:ILE:HG13	1.91	0.52
1:B:269:PRO:O	1:B:273:ILE:HG13	2.09	0.52
1:A:287:TYR:O	1:A:291:HIS:ND1	2.43	0.52
1:B:572:MET:HA	1:B:575:MET:HB2	1.92	0.52
1:A:895:MET:HE2	1:A:895:MET:HA	1.92	0.51
1:B:555:ASN:O	1:B:629:GLY:N	2.43	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PHE:HZ	1:A:451:ILE:HG23	1.76	0.51
1:A:927:VAL:HG11	1:A:1022:HIS:HB3	1.91	0.51
1:D:909:MET:HE1	1:D:919:TRP:HB3	1.92	0.51
1:A:602:TYR:HB3	1:A:814:ARG:HD3	1.93	0.51
1:B:580:SER:O	1:B:584:ILE:HG13	2.11	0.51
1:D:622:GLY:HA3	1:D:793:SER:HB3	1.93	0.51
1:B:590:PRO:HG3	1:B:797:MET:HG3	1.93	0.50
1:D:287:TYR:O	1:D:291:HIS:ND1	2.44	0.50
1:D:352:VAL:HA	1:D:554:LEU:HB3	1.93	0.50
1:B:927:VAL:HG21	1:B:1022:HIS:CD2	2.46	0.50
1:B:622:GLY:HA3	1:B:793:SER:HB3	1.93	0.50
1:D:429:PHE:HZ	1:D:451:ILE:HG23	1.77	0.50
1:B:554:LEU:HD13	1:B:631:VAL:HG22	1.92	0.50
1:D:554:LEU:HD13	1:D:631:VAL:HG22	1.94	0.50
1:D:330:TYR:HB2	1:D:333:ARG:HD2	1.95	0.49
1:A:981:LEU:O	1:A:985:ILE:HG23	2.13	0.49
1:D:858:TYR:CD1	1:D:859:PRO:HD3	2.48	0.49
1:D:927:VAL:HG21	1:D:1022:HIS:CD2	2.47	0.49
1:B:570:GLU:OE1	1:B:798:PRO:HB3	2.13	0.49
1:B:908:GLU:HA	1:B:911:TRP:CD1	2.48	0.49
1:D:269:PRO:O	1:D:273:ILE:HG23	2.13	0.49
1:A:575:MET:HE1	1:A:633:ARG:HB2	1.95	0.48
1:A:340:LYS:HG3	1:A:343:LYS:HB2	1.95	0.48
1:D:602:TYR:O	1:D:814:ARG:NE	2.47	0.48
1:A:335:SER:HA	1:A:339:GLU:HB3	1.94	0.48
1:A:359:PRO:HB2	1:A:396:LEU:HD23	1.95	0.48
1:B:575:MET:HE2	1:B:587:VAL:HG23	1.94	0.48
1:D:908:GLU:HA	1:D:911:TRP:CD1	2.49	0.48
1:B:340:LYS:HG3	1:B:343:LYS:HB2	1.95	0.48
1:D:570:GLU:OE1	1:D:798:PRO:HB3	2.13	0.48
1:B:429:PHE:HZ	1:B:451:ILE:HG23	1.79	0.48
1:B:860:LEU:HA	1:B:938:LEU:HD21	1.95	0.47
1:B:790:GLY:O	1:B:792:ARG:NH1	2.47	0.47
1:D:339:GLU:OE2	1:D:569:ARG:NH2	2.47	0.47
1:D:620:ILE:HG21	1:D:847:LEU:HB2	1.97	0.47
1:A:974:THR:HG21	1:A:1038:PRO:HG2	1.96	0.47
1:B:411:TRP:NE1	1:B:423:ARG:O	2.43	0.47
1:D:820:ARG:HG2	1:D:820:ARG:HH11	1.80	0.47
1:D:857:VAL:O	1:D:860:LEU:HB2	2.15	0.47
1:D:1017:LEU:HA	1:D:1020:ILE:HG22	1.97	0.47
1:A:508:ASP:HB3	1:A:514:LEU:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:LEU:HB2	1:A:1041:ILE:HD11	1.96	0.46
1:D:606:ASN:OD1	2:F:2:BGC:O6	2.17	0.46
1:D:617:LEU:HD13	1:D:624:ILE:HG13	1.96	0.46
1:B:359:PRO:HB2	1:B:396:LEU:HD23	1.98	0.46
1:D:740:LYS:HA	1:D:740:LYS:HE3	1.98	0.46
1:D:917:HIS:O	1:D:921:ARG:HG2	2.16	0.46
1:D:837:TRP:HA	1:D:840:TYR:HE2	1.80	0.46
1:D:602:TYR:HB3	1:D:814:ARG:HD3	1.97	0.46
1:B:602:TYR:O	1:B:814:ARG:NE	2.48	0.45
1:B:974:THR:HG21	1:B:1038:PRO:HG2	1.97	0.45
1:B:977:LEU:HB2	1:B:1041:ILE:HD11	1.98	0.45
1:D:331:LEU:HD21	1:D:570:GLU:HG2	1.98	0.45
1:D:340:LYS:HG3	1:D:343:LYS:HB2	1.96	0.45
1:D:895:MET:HE2	1:D:895:MET:HA	1.98	0.45
1:A:601:ARG:HA	1:A:921:ARG:HD3	1.98	0.45
1:A:837:TRP:HA	1:A:840:TYR:HE2	1.81	0.45
1:A:927:VAL:HG21	1:A:1022:HIS:CD2	2.43	0.45
1:A:853:ILE:O	1:A:857:VAL:HG22	2.17	0.45
1:B:936:PHE:HA	1:B:939:PHE:HB2	1.99	0.45
1:D:814:ARG:HG2	1:D:925:PHE:CZ	2.52	0.45
1:D:876:LEU:HD13	1:D:991:VAL:HA	1.98	0.45
1:A:269:PRO:O	1:A:273:ILE:HG13	2.17	0.45
1:D:309:TRP:HE1	1:D:861:THR:HG22	1.81	0.45
1:B:917:HIS:CE1	1:B:921:ARG:HH12	2.35	0.44
1:D:268:ASN:O	1:D:272:ILE:HG12	2.17	0.44
1:A:602:TYR:O	1:A:814:ARG:NE	2.49	0.44
1:A:928:ILE:HG23	1:A:1026:PHE:HE2	1.82	0.44
1:B:895:MET:HE2	1:B:895:MET:HA	1.98	0.44
1:A:977:LEU:H	1:A:977:LEU:HD12	1.82	0.44
1:B:633:ARG:HE	1:B:635:GLN:HB2	1.82	0.44
1:B:863:ILE:HD11	1:B:938:LEU:HD22	2.00	0.44
1:B:287:TYR:O	1:B:291:HIS:ND1	2.51	0.44
1:D:726:VAL:HB	1:D:750:GLU:HG2	2.00	0.44
1:D:293:VAL:HG12	1:D:296:ALA:H	1.81	0.44
1:A:273:ILE:HA	1:A:276:LEU:HB3	2.00	0.44
1:B:620:ILE:HG21	1:B:847:LEU:HB2	1.98	0.44
1:A:395:MET:HE2	1:A:477:TRP:HB3	2.00	0.44
1:A:617:LEU:HD13	1:A:624:ILE:HG13	1.99	0.44
1:B:293:VAL:HG12	1:B:296:ALA:H	1.83	0.43
1:A:721:PHE:O	1:A:765:TRP:NE1	2.49	0.43
1:B:721:PHE:O	1:B:765:TRP:NE1	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:VAL:HG13	1:D:554:LEU:HB3	2.00	0.43
1:D:330:TYR:CB	1:D:333:ARG:HD2	2.49	0.43
1:A:491:ARG:HG3	1:A:491:ARG:HH11	1.83	0.43
1:B:309:TRP:CG	1:B:864:PRO:HG3	2.54	0.43
1:A:580:SER:O	1:A:584:ILE:HG12	2.19	0.43
1:A:780:ILE:HD11	2:C:3:BGC:H6C2	2.00	0.43
1:B:835:PRO:O	1:B:849:ARG:NH1	2.49	0.43
1:D:349:ASP:HB2	1:D:551:PRO:HD3	2.01	0.43
1:A:277:ARG:CZ	1:A:901:ILE:HG12	2.49	0.43
1:A:384:VAL:HG13	1:A:515:PRO:HB3	2.01	0.43
1:B:623:PRO:HG3	1:B:795:TYR:HB2	2.01	0.43
1:B:780:ILE:HD11	2:E:3:BGC:H6C2	2.00	0.43
1:A:410:LYS:HB2	1:A:410:LYS:HE2	1.84	0.43
1:D:928:ILE:HG23	1:D:1026:PHE:HE1	1.83	0.43
1:D:384:VAL:HG13	1:D:515:PRO:HB3	2.01	0.42
1:D:545:ALA:HA	1:D:549:ASN:HA	2.00	0.42
1:B:821:TRP:CZ3	2:E:2:BGC:H6C2	2.54	0.42
1:D:903:ALA:O	1:D:907:LEU:HD23	2.18	0.42
1:A:869:CYS:HB3	1:A:983:LEU:HD21	2.01	0.42
1:B:400:ALA:O	1:B:404:THR:OG1	2.32	0.42
1:B:871:LEU:HD23	1:B:871:LEU:HA	1.89	0.42
1:A:726:VAL:HB	1:A:750:GLU:HG2	2.00	0.42
1:B:335:SER:HA	1:B:339:GLU:HB3	2.01	0.42
1:B:406:GLU:OE1	1:B:409:ARG:NH2	2.53	0.42
1:B:587:VAL:HG22	1:B:794:VAL:HB	2.01	0.42
1:D:426:GLU:HB3	1:D:427:TRP:CE3	2.55	0.42
1:B:726:VAL:HB	1:B:750:GLU:HG2	2.01	0.42
1:D:359:PRO:HB2	1:D:396:LEU:HD23	2.02	0.42
1:B:287:TYR:HD1	1:B:291:HIS:HD1	1.67	0.42
1:D:543:VAL:O	1:D:547:ILE:HG13	2.20	0.42
1:A:779:ASP:N	1:A:779:ASP:OD1	2.51	0.42
1:B:295:ASP:OD1	1:B:295:ASP:N	2.43	0.42
1:D:835:PRO:O	1:D:849:ARG:NH1	2.53	0.42
1:D:1014:PHE:O	1:D:1017:LEU:HB2	2.20	0.41
1:A:273:ILE:HD12	1:A:907:LEU:HD11	2.02	0.41
1:D:309:TRP:NE1	1:D:861:THR:HG22	2.35	0.41
1:D:909:MET:HE2	1:D:916:ILE:HD13	2.02	0.41
1:A:272:ILE:HD13	1:A:272:ILE:HA	1.89	0.41
1:B:923:GLU:O	1:B:927:VAL:HG23	2.20	0.41
1:A:820:ARG:HG2	1:A:820:ARG:NH1	2.35	0.41
1:B:591:GLN:HE22	1:B:627:GLY:HA3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:ASN:N	1:D:802:ALA:O	2.52	0.41
1:D:779:ASP:OD1	1:D:779:ASP:N	2.50	0.41
1:A:835:PRO:O	1:A:849:ARG:NH1	2.50	0.41
1:A:862:SER:HB3	1:A:934:HIS:HB2	2.02	0.41
1:A:917:HIS:CE1	1:A:921:ARG:HH12	2.38	0.41
1:B:815:LEU:HD23	1:B:815:LEU:HA	1.85	0.41
1:D:409:ARG:HA	1:D:514:LEU:HD11	2.02	0.41
1:D:977:LEU:HD12	1:D:977:LEU:H	1.85	0.41
1:A:411:TRP:NE1	1:A:423:ARG:O	2.48	0.41
1:B:626:VAL:HB	2:E:3:BGC:H4	2.03	0.41
1:A:327:ARG:HH21	1:A:618:ASP:CG	2.27	0.41
1:A:363:PRO:HA	1:A:364:PRO:HD3	1.95	0.41
1:A:620:ILE:HG21	1:A:847:LEU:HB2	2.02	0.41
1:D:280:ILE:CD1	1:D:897:LEU:HA	2.51	0.41
1:A:426:GLU:OE1	1:A:455:TYR:OH	2.33	0.41
1:A:570:GLU:OE1	1:A:798:PRO:HB3	2.21	0.41
1:B:747:LEU:HD23	1:B:747:LEU:HA	1.94	0.41
1:B:779:ASP:OD1	1:B:779:ASP:N	2.52	0.41
1:A:331:LEU:HD21	1:A:570:GLU:HG2	2.03	0.40
1:A:584:ILE:HD12	1:A:794:VAL:HG13	2.01	0.40
1:A:1017:LEU:HA	1:A:1020:ILE:HG22	2.03	0.40
1:B:624:ILE:HG12	1:B:852:TYR:CE1	2.56	0.40
1:A:858:TYR:N	1:A:859:PRO:HD2	2.36	0.40
1:B:266:ARG:HH21	1:B:910:GLN:HG3	1.85	0.40
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.95	0.40
1:B:583:LYS:HB3	1:B:644:THR:O	2.21	0.40
1:B:858:TYR:CD2	1:B:859:PRO:HD3	2.56	0.40
1:B:879:GLY:C	1:B:880:LYS:HD3	2.47	0.40
1:D:280:ILE:HD12	1:D:897:LEU:HA	2.02	0.40
1:D:749:LYS:O	1:D:749:LYS:HD2	2.22	0.40
1:A:799:LYS:H	1:A:799:LYS:HG3	1.59	0.40
1:B:766:GLY:HA3	1:B:773:TYR:CE2	2.57	0.40
1:A:908:GLU:HA	1:A:911:TRP:CD1	2.56	0.40
1:B:267:ILE:HA	1:B:267:ILE:HD12	1.83	0.40
1:B:563:ASN:N	1:B:802:ALA:O	2.55	0.40
1:D:295:ASP:OD1	1:D:295:ASP:N	2.43	0.40
1:D:363:PRO:HA	1:D:364:PRO:HD3	1.97	0.40
1:D:554:LEU:HD12	1:D:554:LEU:HA	1.90	0.40
1:D:984:LEU:HD12	1:D:984:LEU:HA	1.94	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	A	718/1078 (67%)	702 (98%)	16 (2%)	0	100	100
1	B	715/1078 (66%)	701 (98%)	14 (2%)	0	100	100
1	D	718/1078 (67%)	699 (97%)	19 (3%)	0	100	100
All	All	2151/3234 (66%)	2102 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	623/931 (67%)	610 (98%)	13 (2%)	47	75
1	B	622/931 (67%)	613 (99%)	9 (1%)	59	80
1	D	622/931 (67%)	617 (99%)	5 (1%)	73	86
All	All	1867/2793 (67%)	1840 (99%)	27 (1%)	57	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	PHE
1	A	332	ASP
1	A	349	ASP
1	A	350	ILE
1	A	395	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	405	SER
1	A	509	ILE
1	A	628	THR
1	A	799	LYS
1	A	817	GLN
1	A	922	ASN
1	A	1037	VAL
1	A	1041	ILE
1	B	316	PHE
1	B	319	PHE
1	B	332	ASP
1	B	506	VAL
1	B	617	LEU
1	B	628	THR
1	B	799	LYS
1	B	907	LEU
1	B	1041	ILE
1	D	335	SER
1	D	350	ILE
1	D	405	SER
1	D	628	THR
1	D	851	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	463	ASN
1	A	588	GLN
1	A	599	HIS
1	A	635	GLN
1	A	917	HIS
1	A	922	ASN
1	A	924	GLN
1	B	463	ASN
1	B	591	GLN
1	B	599	HIS
1	B	635	GLN
1	B	714	GLN
1	B	924	GLN
1	D	318	GLN
1	D	463	ASN
1	D	588	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	635	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 ⓘ

Of 9 monosaccharides modelled in this entry, 6 were used for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	C	2	2	11,11,12	0.70	0	15,15,17	0.76	0
2	BGC	C	3	2	11,11,12	0.68	0	15,15,17	0.81	0
2	BGC	E	2	2	11,11,12	0.70	0	15,15,17	0.75	0
2	BGC	E	3	2	11,11,12	0.69	0	15,15,17	0.80	0
2	BGC	F	2	2	11,11,12	0.70	0	15,15,17	0.78	0
2	BGC	F	3	2	11,11,12	0.70	0	15,15,17	0.85	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	C	2	2	-	1/2/19/22	0/1/1/1
2	BGC	C	3	2	-	1/2/19/22	0/1/1/1
2	BGC	E	2	2	-	1/2/19/22	0/1/1/1
2	BGC	E	3	2	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	F	2	2	-	2/2/19/22	0/1/1/1
2	BGC	F	3	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

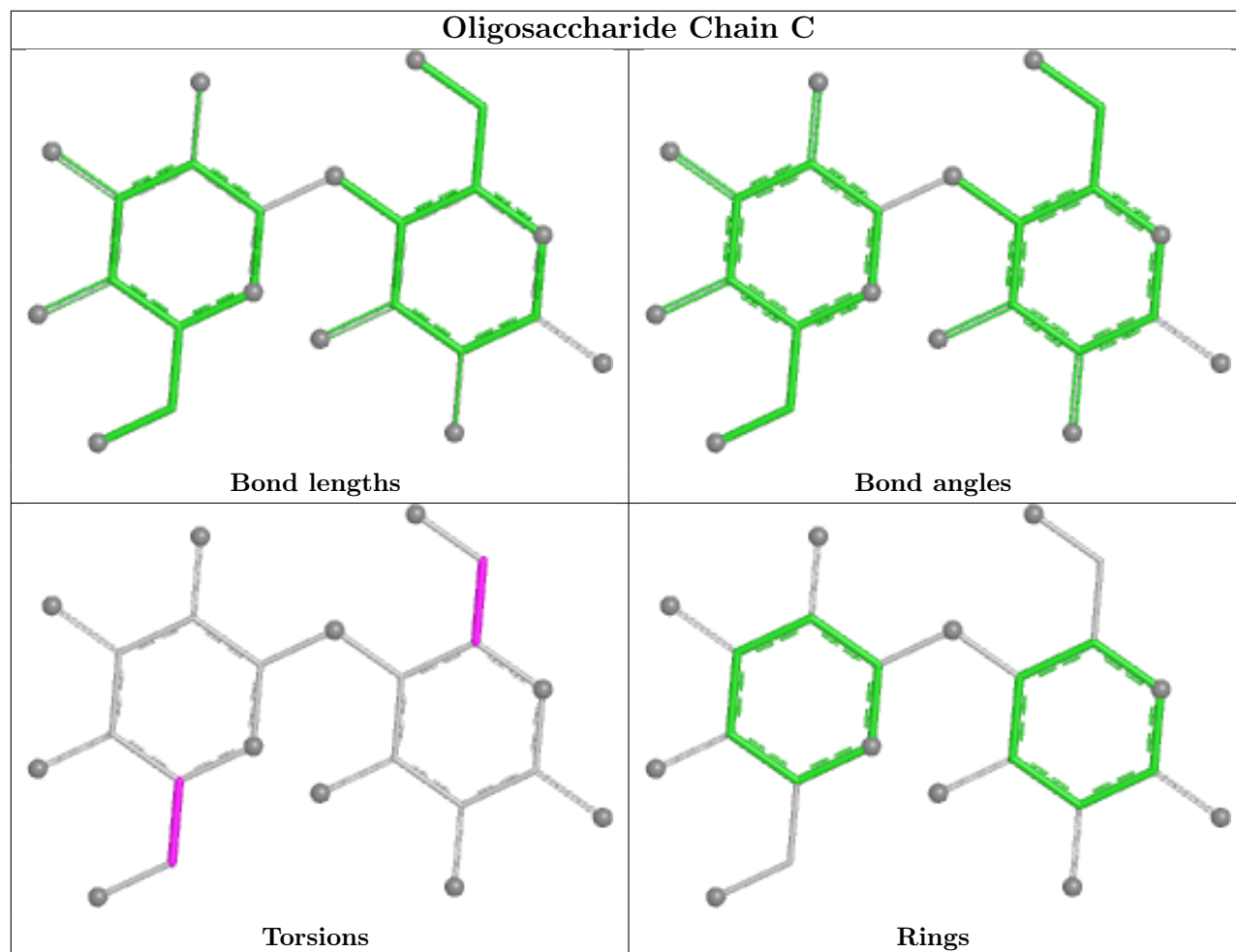
Mol	Chain	Res	Type	Atoms
2	F	2	BGC	O5-C5-C6-O6
2	C	3	BGC	O5-C5-C6-O6
2	E	2	BGC	O5-C5-C6-O6
2	E	3	BGC	O5-C5-C6-O6
2	C	2	BGC	O5-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6

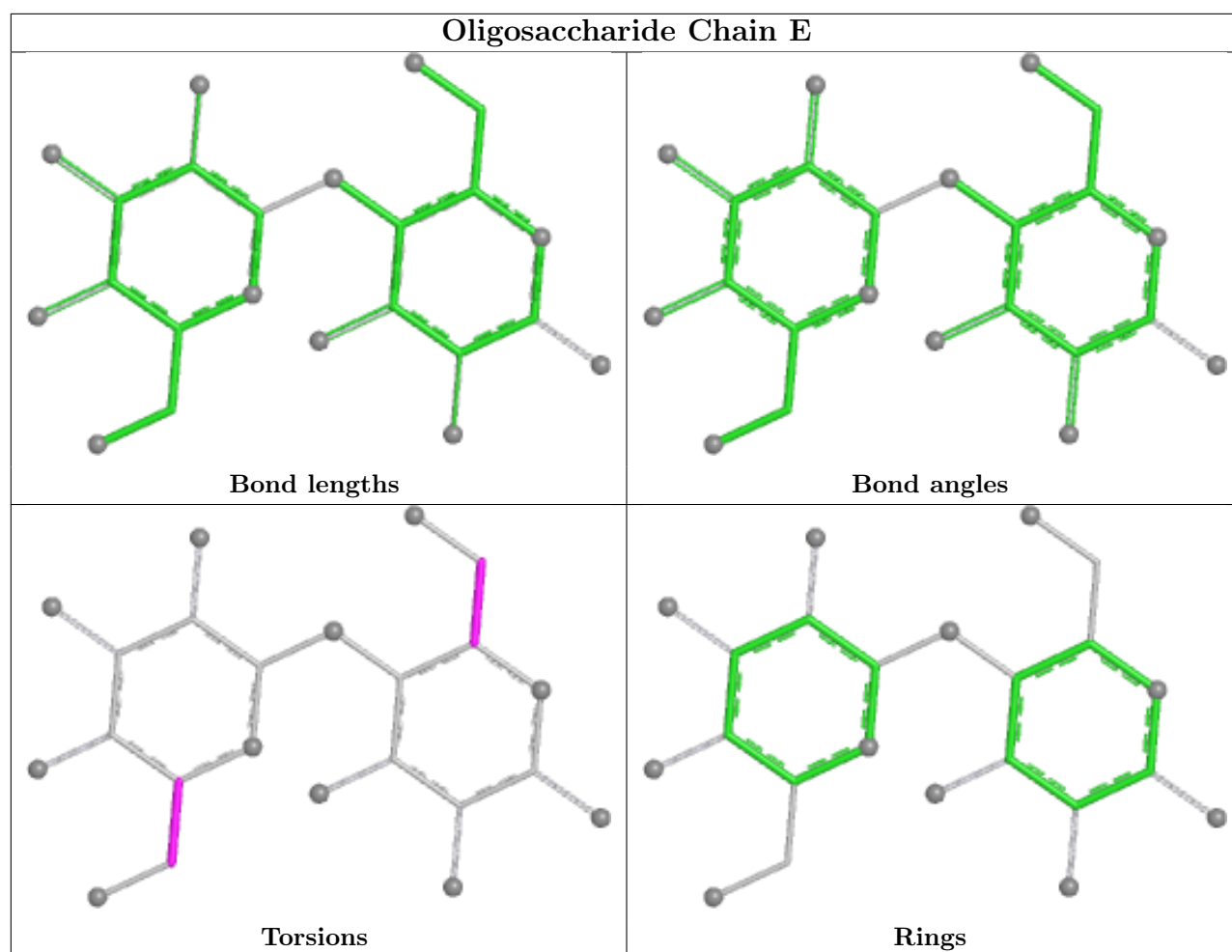
There are no ring outliers.

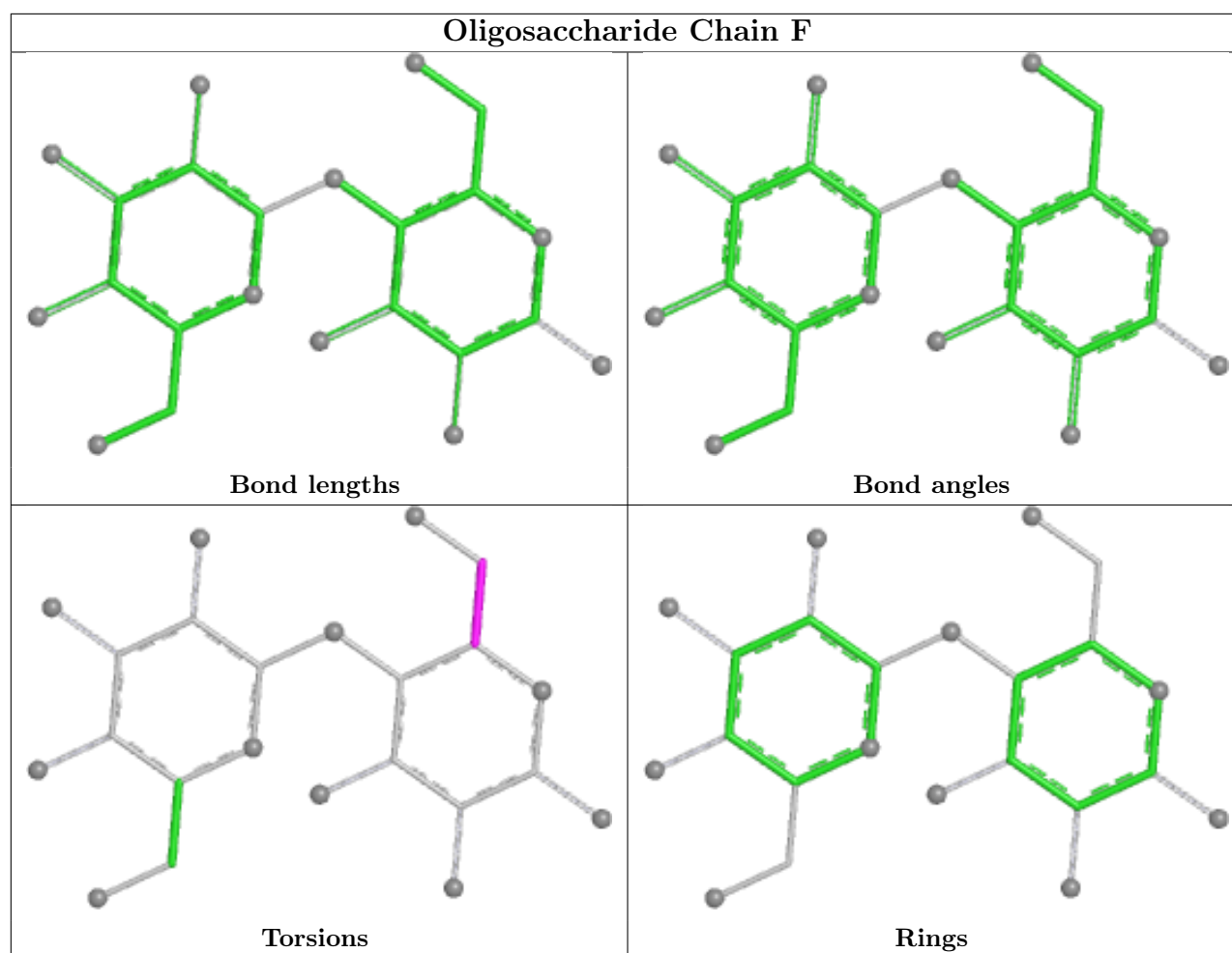
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	BGC	1	0
2	E	3	BGC	2	0
2	C	3	BGC	2	0
2	F	2	BGC	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.

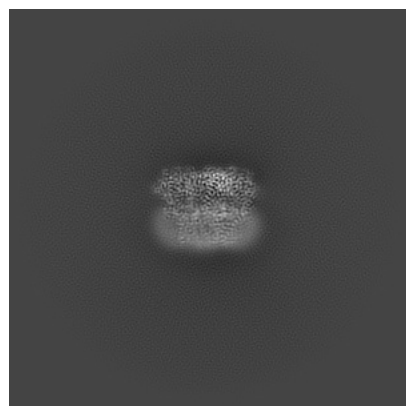
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43245. These allow visual inspection of the internal detail of the map and identification of artifacts.

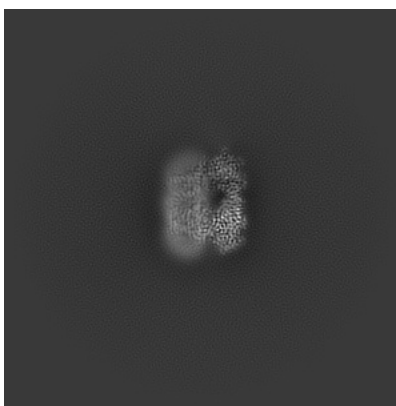
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

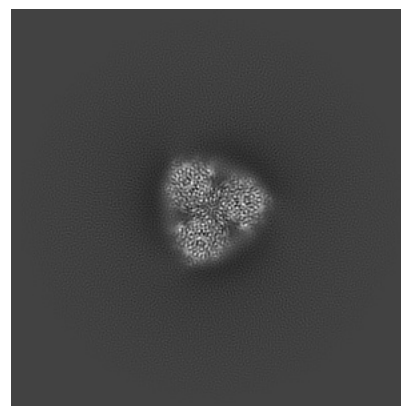
6.1.1 Primary map



X

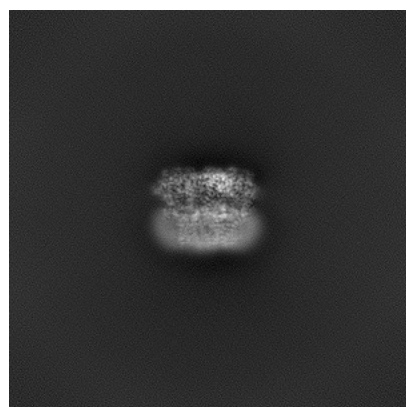


Y

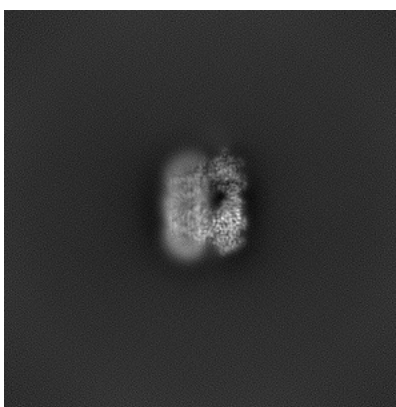


Z

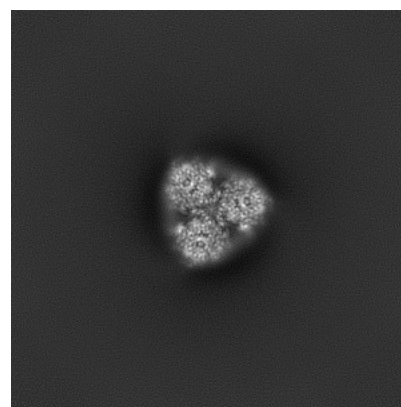
6.1.2 Raw map



X



Y

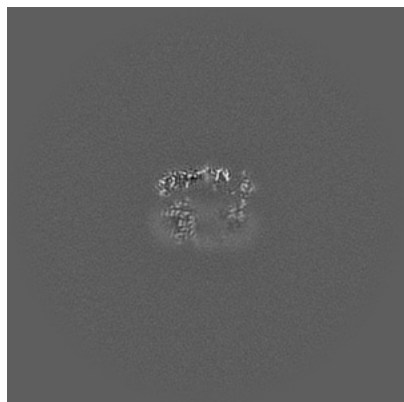


Z

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

6.2 Central slices [i](#)

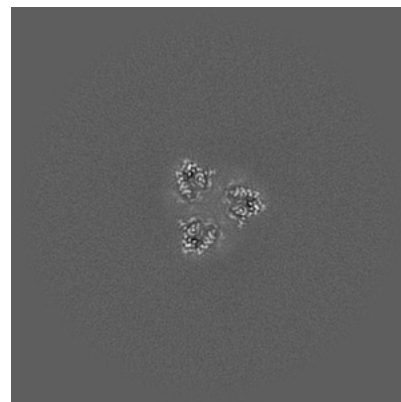
6.2.1 Primary map



X Index: 200

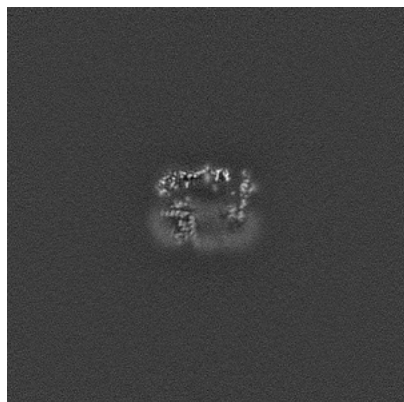


Y Index: 200

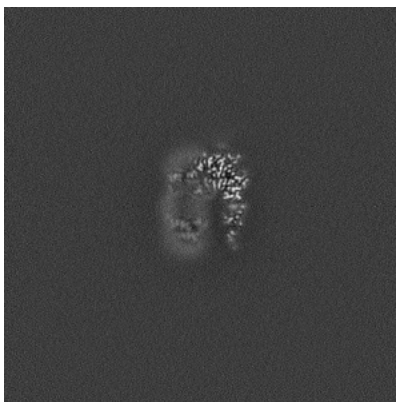


Z Index: 200

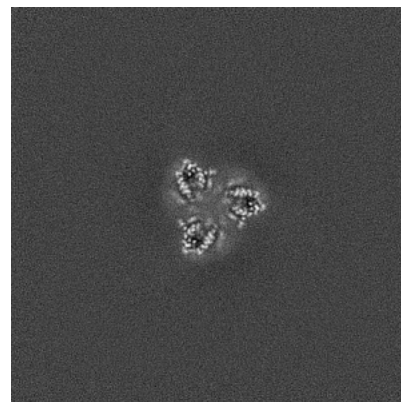
6.2.2 Raw map



X Index: 200



Y Index: 200

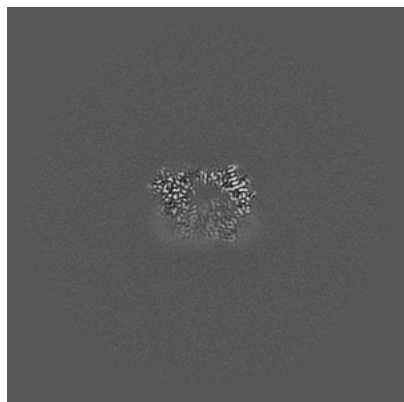


Z Index: 200

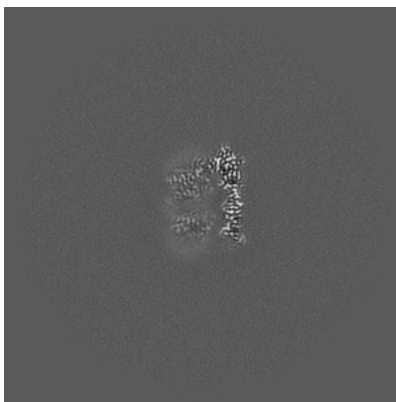
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

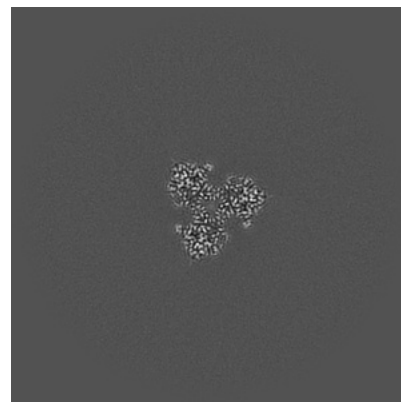
6.3.1 Primary map



X Index: 181

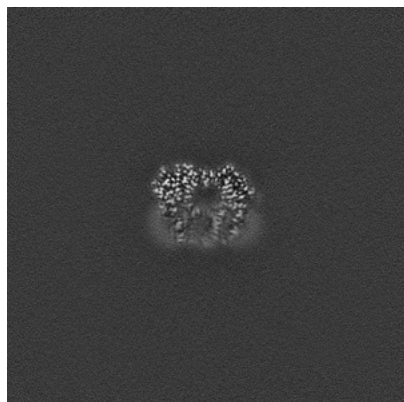


Y Index: 209

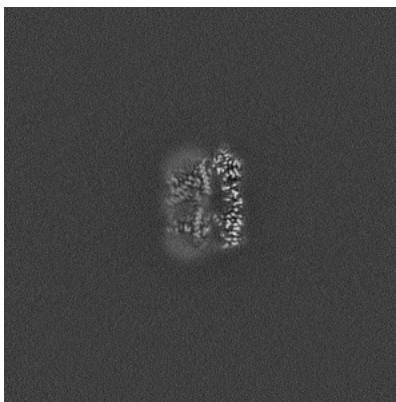


Z Index: 226

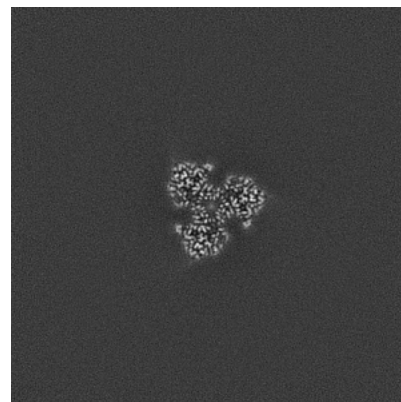
6.3.2 Raw map



X Index: 188



Y Index: 214

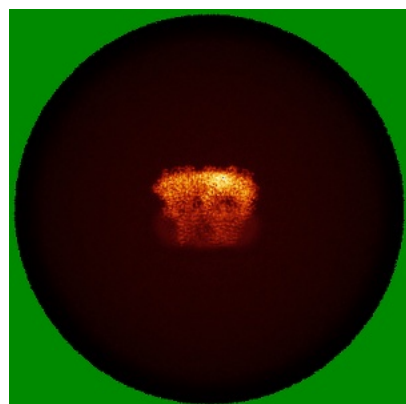


Z Index: 226

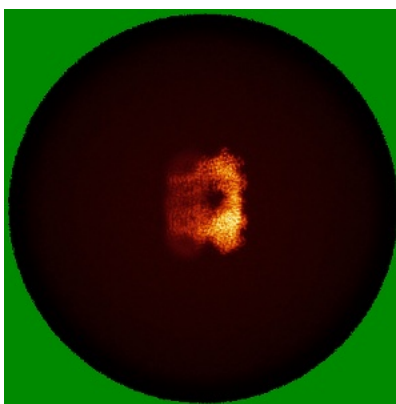
The images above show the largest variance slices of the map in three orthogonal directions.

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

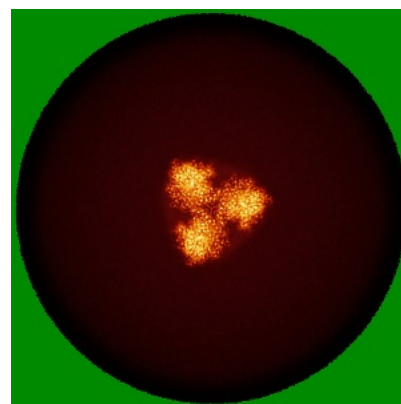
6.4.1 Primary map



X

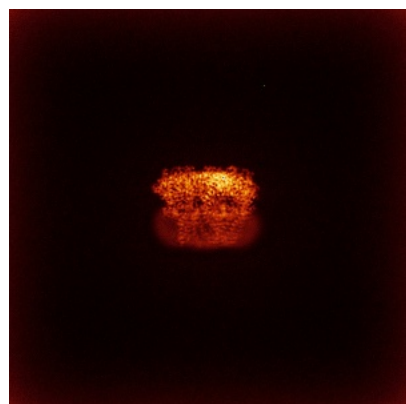


Y

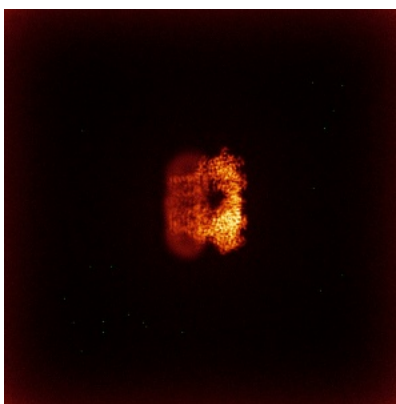


Z

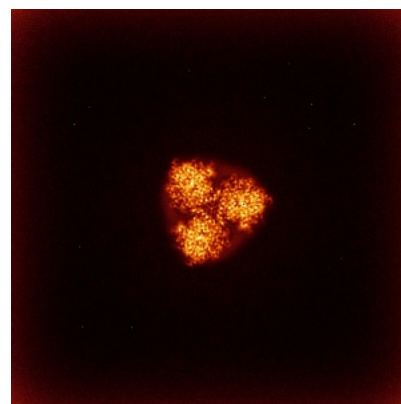
6.4.2 Raw map



X



Y

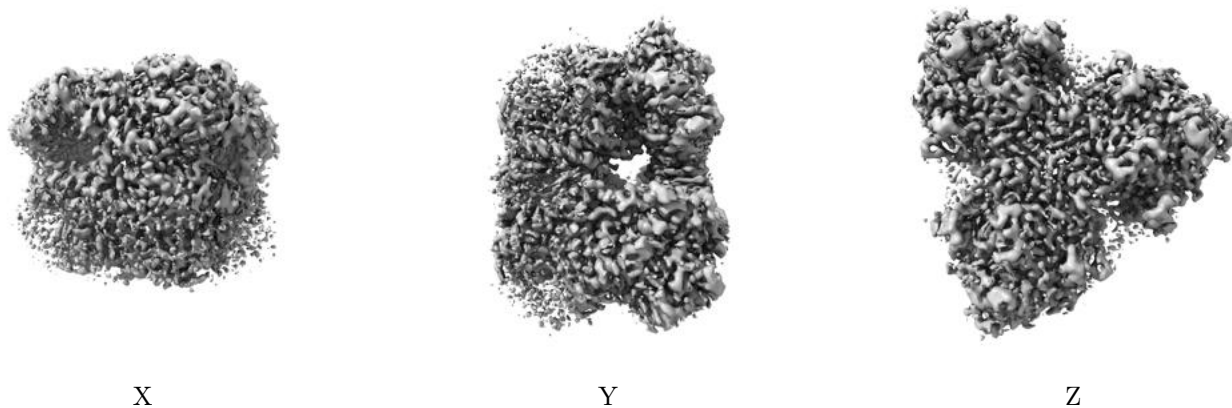


Z

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.

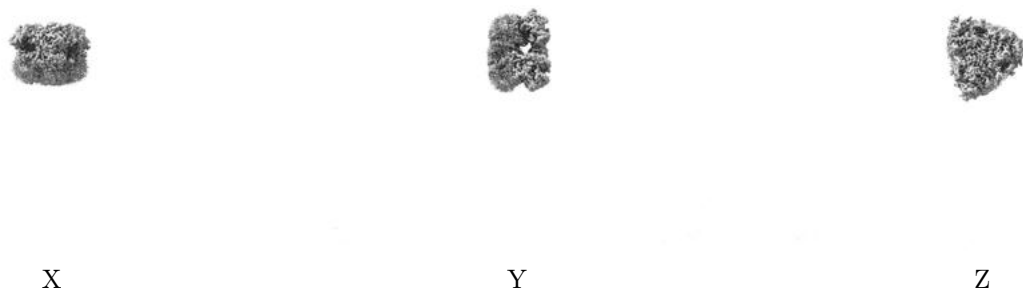
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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.

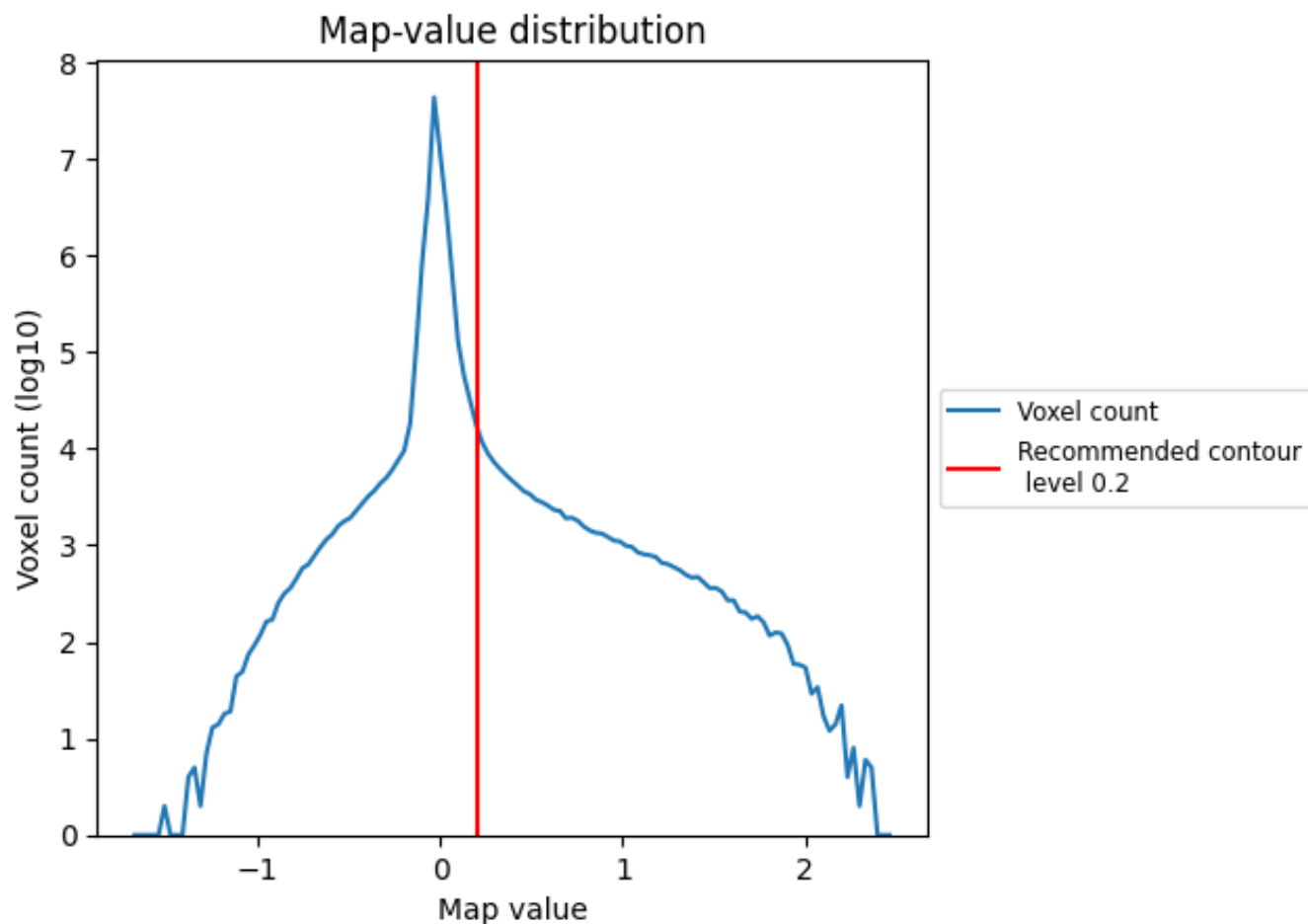
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

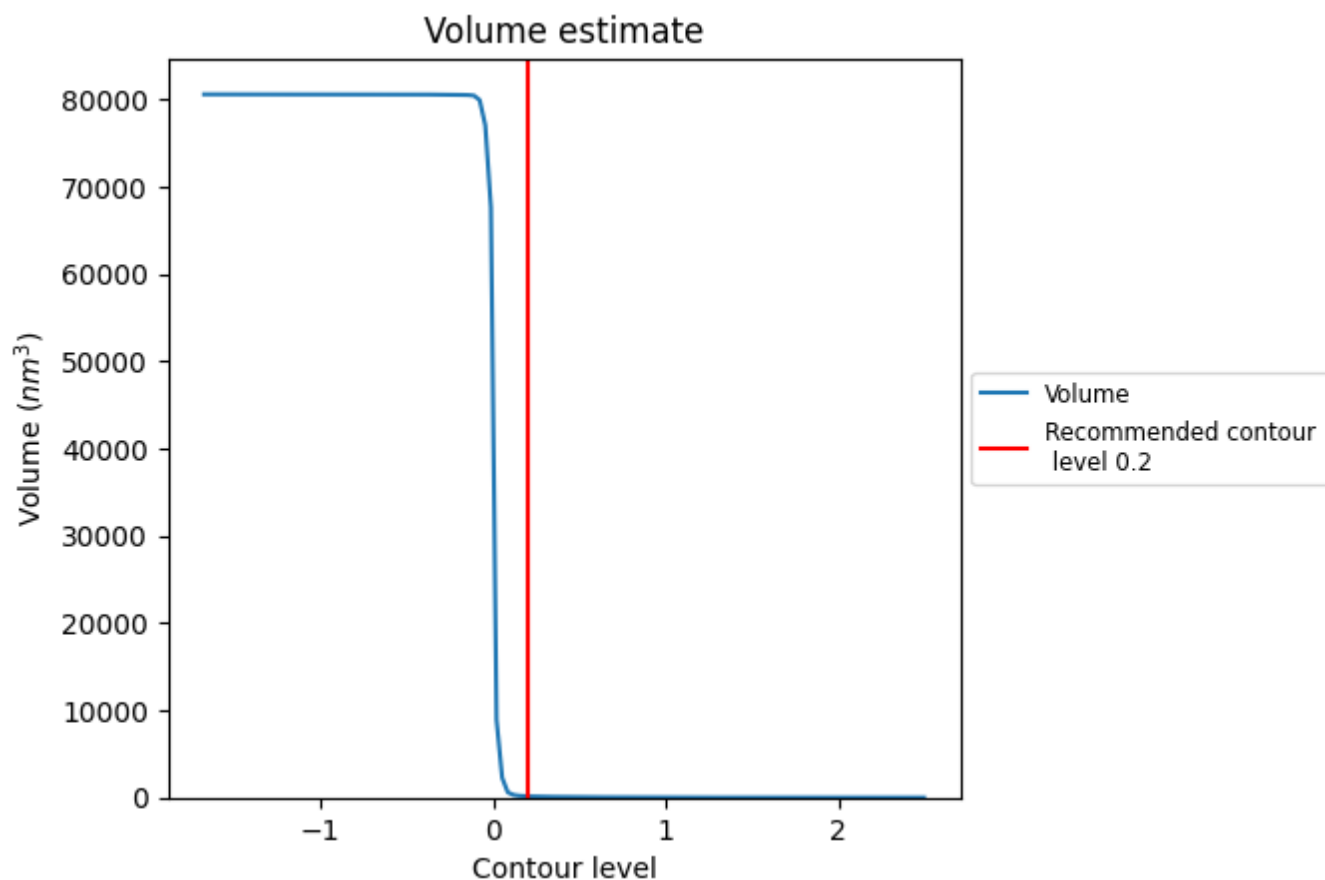
This section contains the results of statistical analysis of the map.

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.

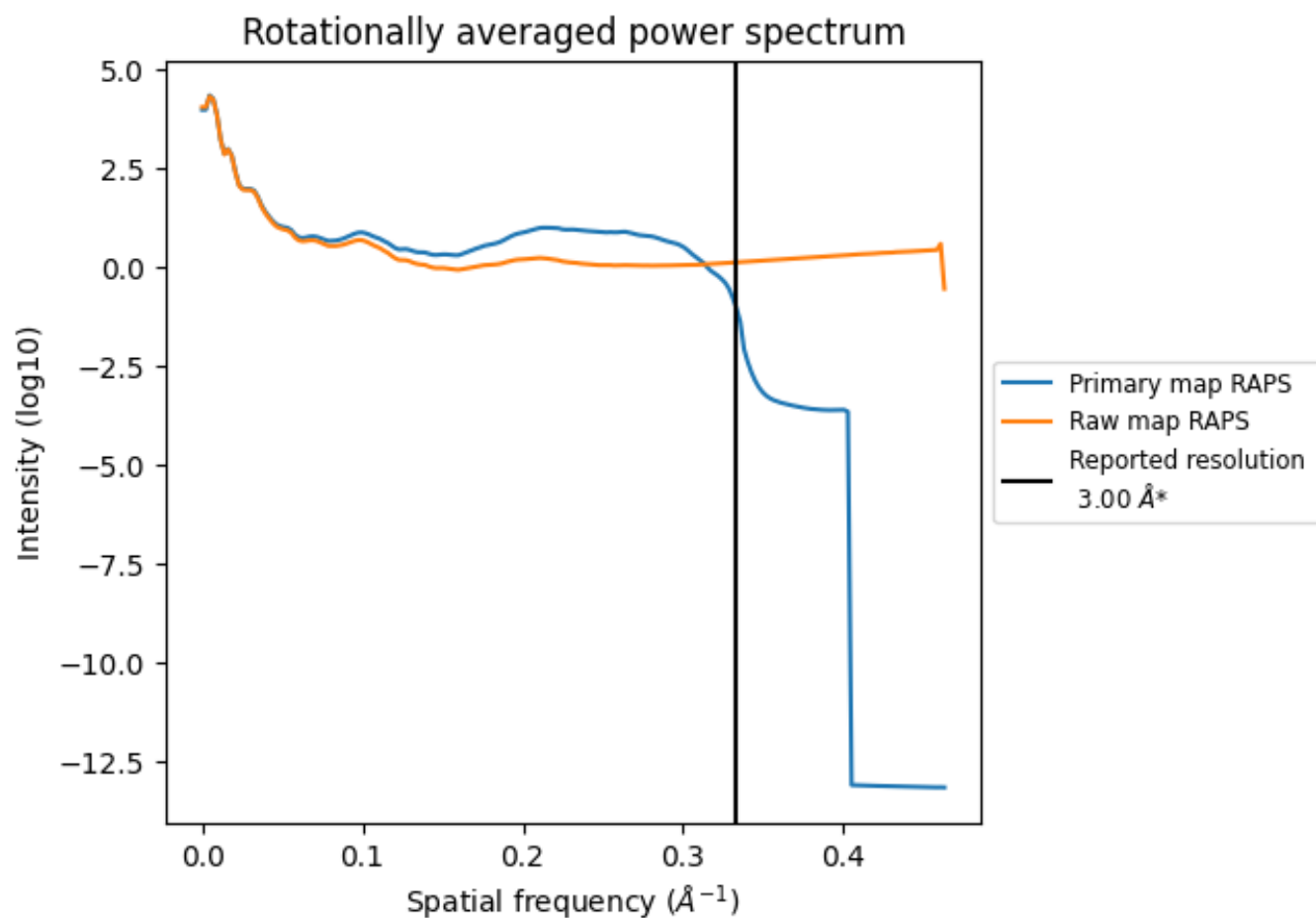
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 142 nm³; this corresponds to an approximate mass of 128 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 ⓘ

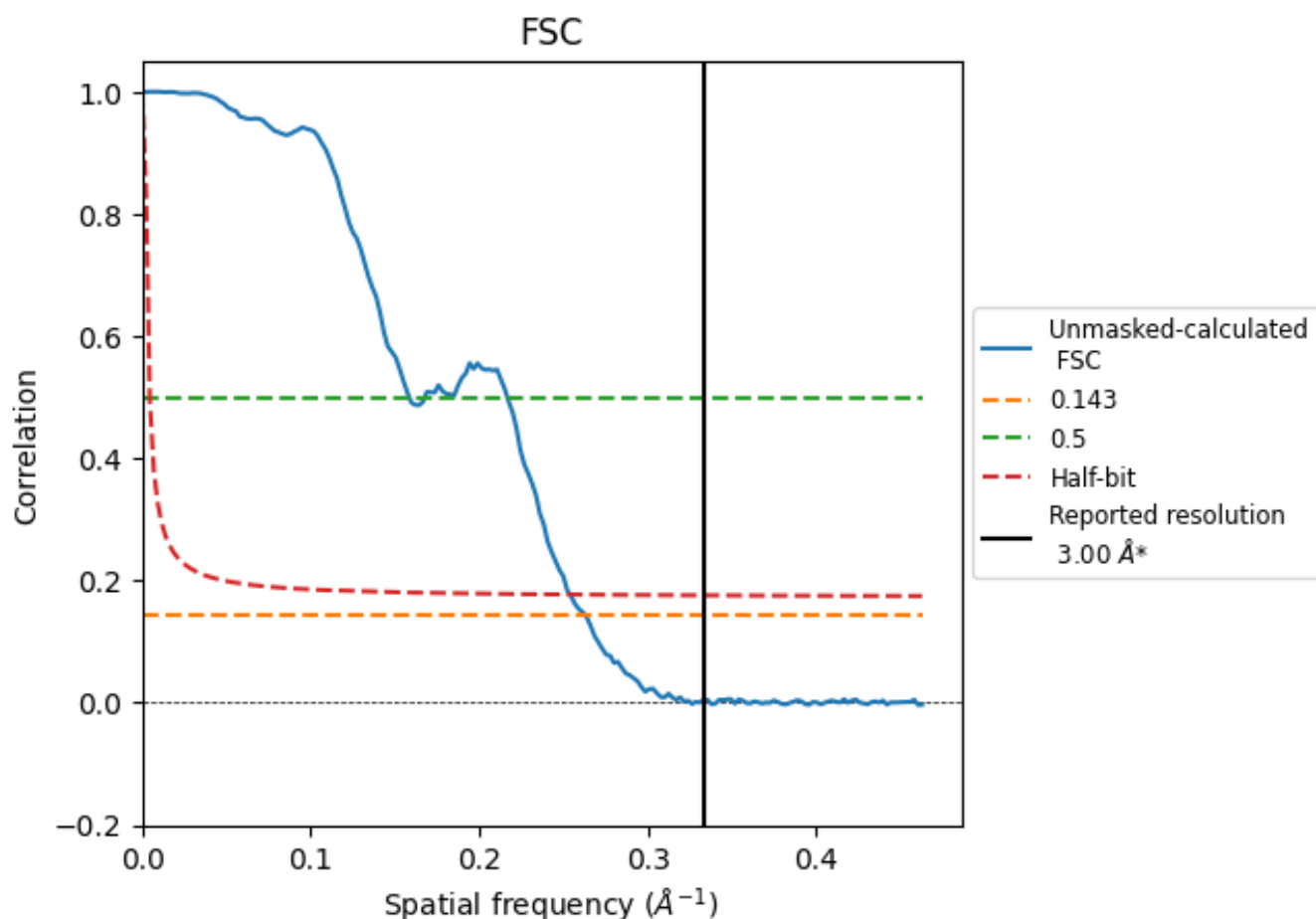


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

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 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

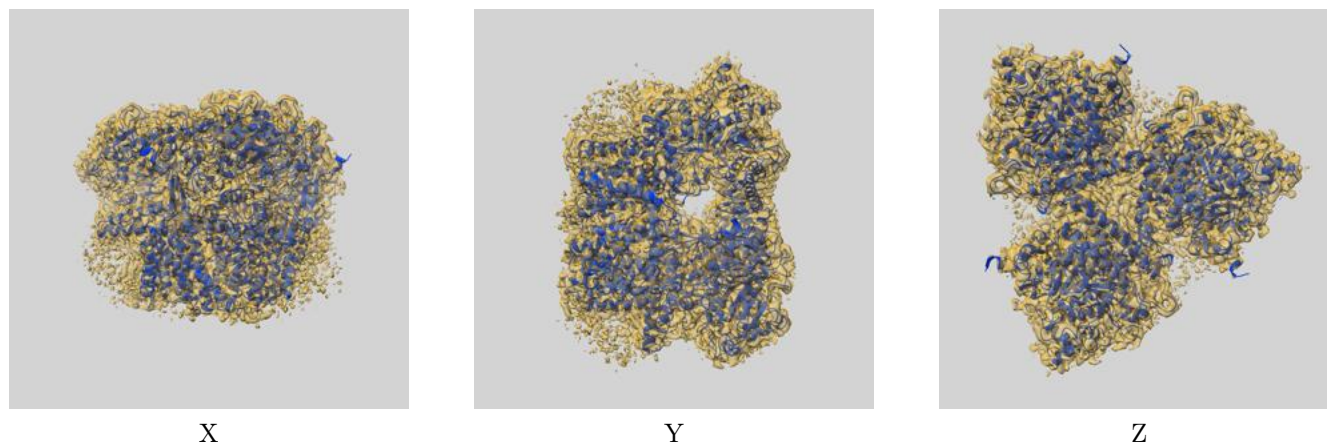
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	6.31	3.94

*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 3.80 differs from the reported value 3.0 by more than 10 %

9 Map-model fit [i](#)

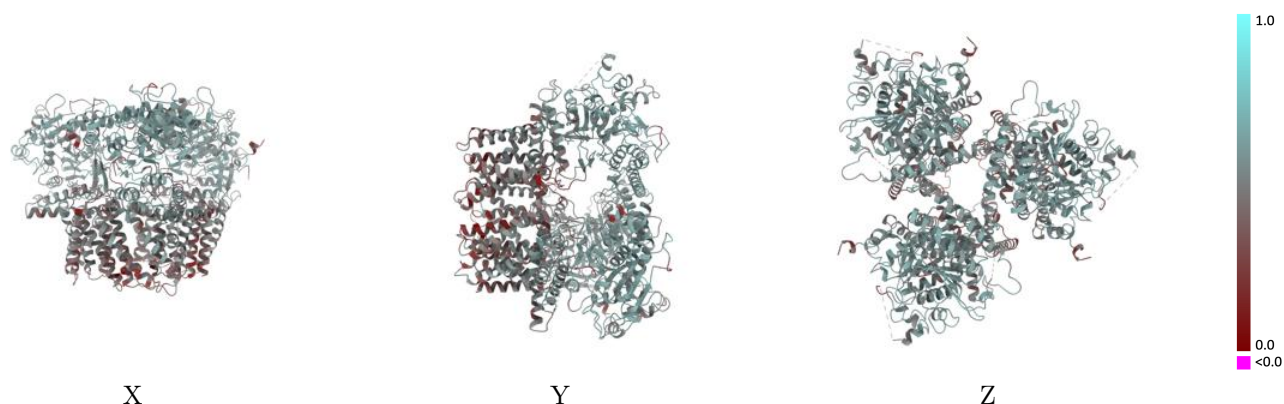
This section contains information regarding the fit between EMDB map EMD-43245 and PDB model 8VI0. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



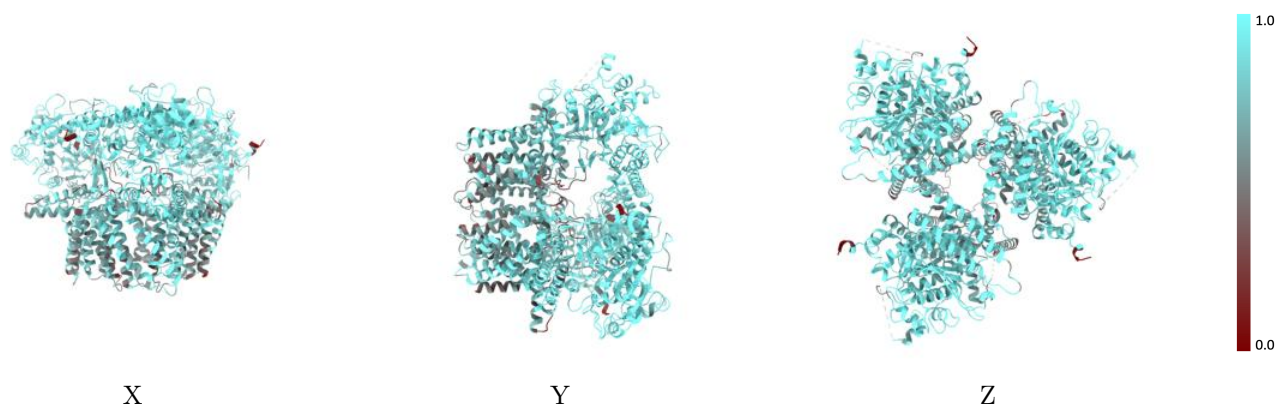
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



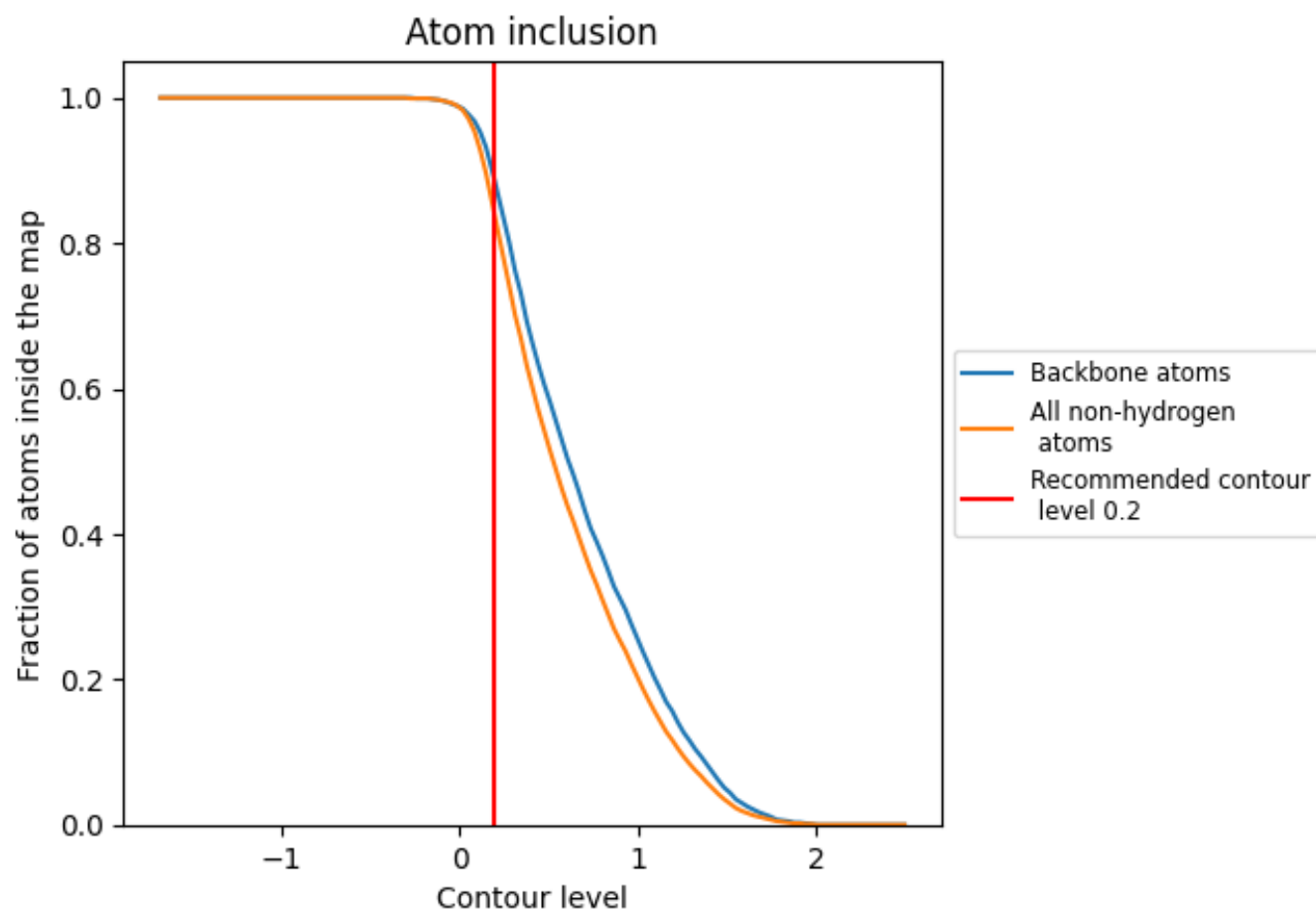
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8370	0.5080
A	0.8370	0.5070
B	0.8390	0.5090
C	0.7390	0.5100
D	0.8360	0.5060
E	0.8260	0.5510
F	0.8260	0.5350

1.0

0.0

<0.0