



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 12:28 AM UTC

PDB ID : 8JD9 / pdb_00008jd9
EMDB ID : EMD-36077
Title : Cyro-EM structure of the Na⁺/H⁺ antiporter SOS1 from Arabidopsis thaliana, class1
Authors : Yang, G.H.; Zhang, Y.M.; Zhou, J.Q.; Jia, Y.T.; Xu, X.; Fu, P.; Wu, H.Y.
Deposited on : 2023-05-13
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

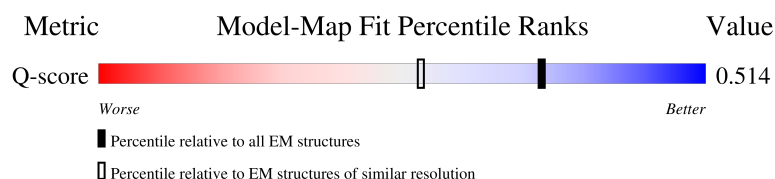
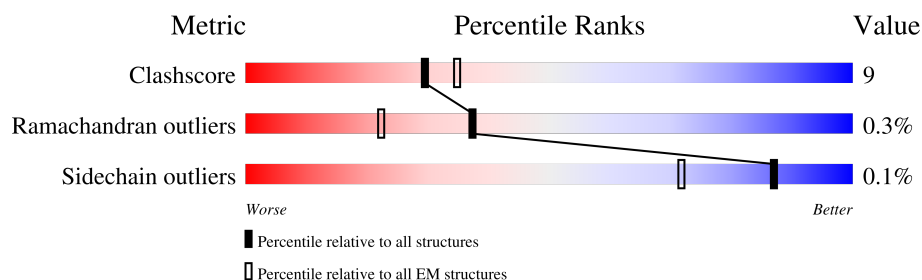
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.87 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	12062 (2.37 - 3.37)

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	1162	12% 61% 19% 20%
1	B	1162	12% 63% 17% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14725 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 Sodium/hydrogen exchanger 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	935	Total	C	N	O	S	0	0
			7318	4769	1194	1325	30		
1	B	935	Total	C	N	O	S	0	0
			7318	4769	1194	1325	30		

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	initiating methionine	UNP Q9LKW9
A	1147	LEU	-	expression tag	UNP Q9LKW9
A	1148	GLU	-	expression tag	UNP Q9LKW9
A	1149	SER	-	expression tag	UNP Q9LKW9
A	1150	ALA	-	expression tag	UNP Q9LKW9
A	1151	TRP	-	expression tag	UNP Q9LKW9
A	1152	SER	-	expression tag	UNP Q9LKW9
A	1153	HIS	-	expression tag	UNP Q9LKW9
A	1154	PRO	-	expression tag	UNP Q9LKW9
A	1155	GLN	-	expression tag	UNP Q9LKW9
A	1156	PHE	-	expression tag	UNP Q9LKW9
A	1157	GLU	-	expression tag	UNP Q9LKW9
A	1158	LYS	-	expression tag	UNP Q9LKW9
A	1159	GLY	-	expression tag	UNP Q9LKW9
A	1160	GLY	-	expression tag	UNP Q9LKW9
A	1161	GLY	-	expression tag	UNP Q9LKW9
A	1162	SER	-	expression tag	UNP Q9LKW9
A	1163	GLY	-	expression tag	UNP Q9LKW9
A	1164	GLY	-	expression tag	UNP Q9LKW9
A	1165	GLY	-	expression tag	UNP Q9LKW9
A	1166	SER	-	expression tag	UNP Q9LKW9
A	1167	GLY	-	expression tag	UNP Q9LKW9
A	1168	GLY	-	expression tag	UNP Q9LKW9
A	1169	SER	-	expression tag	UNP Q9LKW9
A	1170	ALA	-	expression tag	UNP Q9LKW9
A	1171	TRP	-	expression tag	UNP Q9LKW9

Continued on next page...

Continued from previous page...

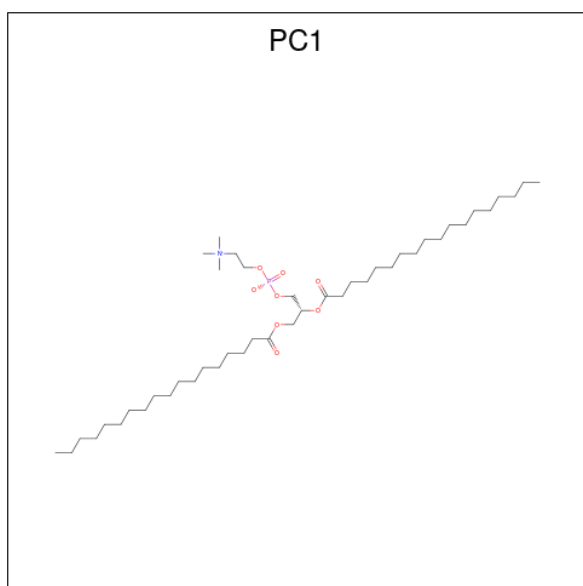
Chain	Residue	Modelled	Actual	Comment	Reference
A	1172	SER	-	expression tag	UNP Q9LKW9
A	1173	HIS	-	expression tag	UNP Q9LKW9
A	1174	PRO	-	expression tag	UNP Q9LKW9
A	1175	GLN	-	expression tag	UNP Q9LKW9
A	1176	PHE	-	expression tag	UNP Q9LKW9
A	1177	GLU	-	expression tag	UNP Q9LKW9
A	1178	LYS	-	expression tag	UNP Q9LKW9
A	1179	GLY	-	expression tag	UNP Q9LKW9
A	1180	SER	-	expression tag	UNP Q9LKW9
A	1181	ASP	-	expression tag	UNP Q9LKW9
A	1182	TYR	-	expression tag	UNP Q9LKW9
A	1183	LYS	-	expression tag	UNP Q9LKW9
A	1184	ASP	-	expression tag	UNP Q9LKW9
A	1185	ASP	-	expression tag	UNP Q9LKW9
A	1186	ASP	-	expression tag	UNP Q9LKW9
A	1187	ASP	-	expression tag	UNP Q9LKW9
A	1188	LYS	-	expression tag	UNP Q9LKW9
B	27	MET	-	initiating methionine	UNP Q9LKW9
B	1147	LEU	-	expression tag	UNP Q9LKW9
B	1148	GLU	-	expression tag	UNP Q9LKW9
B	1149	SER	-	expression tag	UNP Q9LKW9
B	1150	ALA	-	expression tag	UNP Q9LKW9
B	1151	TRP	-	expression tag	UNP Q9LKW9
B	1152	SER	-	expression tag	UNP Q9LKW9
B	1153	HIS	-	expression tag	UNP Q9LKW9
B	1154	PRO	-	expression tag	UNP Q9LKW9
B	1155	GLN	-	expression tag	UNP Q9LKW9
B	1156	PHE	-	expression tag	UNP Q9LKW9
B	1157	GLU	-	expression tag	UNP Q9LKW9
B	1158	LYS	-	expression tag	UNP Q9LKW9
B	1159	GLY	-	expression tag	UNP Q9LKW9
B	1160	GLY	-	expression tag	UNP Q9LKW9
B	1161	GLY	-	expression tag	UNP Q9LKW9
B	1162	SER	-	expression tag	UNP Q9LKW9
B	1163	GLY	-	expression tag	UNP Q9LKW9
B	1164	GLY	-	expression tag	UNP Q9LKW9
B	1165	GLY	-	expression tag	UNP Q9LKW9
B	1166	SER	-	expression tag	UNP Q9LKW9
B	1167	GLY	-	expression tag	UNP Q9LKW9
B	1168	GLY	-	expression tag	UNP Q9LKW9
B	1169	SER	-	expression tag	UNP Q9LKW9
B	1170	ALA	-	expression tag	UNP Q9LKW9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1171	TRP	-	expression tag	UNP Q9LKW9
B	1172	SER	-	expression tag	UNP Q9LKW9
B	1173	HIS	-	expression tag	UNP Q9LKW9
B	1174	PRO	-	expression tag	UNP Q9LKW9
B	1175	GLN	-	expression tag	UNP Q9LKW9
B	1176	PHE	-	expression tag	UNP Q9LKW9
B	1177	GLU	-	expression tag	UNP Q9LKW9
B	1178	LYS	-	expression tag	UNP Q9LKW9
B	1179	GLY	-	expression tag	UNP Q9LKW9
B	1180	SER	-	expression tag	UNP Q9LKW9
B	1181	ASP	-	expression tag	UNP Q9LKW9
B	1182	TYR	-	expression tag	UNP Q9LKW9
B	1183	LYS	-	expression tag	UNP Q9LKW9
B	1184	ASP	-	expression tag	UNP Q9LKW9
B	1185	ASP	-	expression tag	UNP Q9LKW9
B	1186	ASP	-	expression tag	UNP Q9LKW9
B	1187	ASP	-	expression tag	UNP Q9LKW9
B	1188	LYS	-	expression tag	UNP Q9LKW9

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).

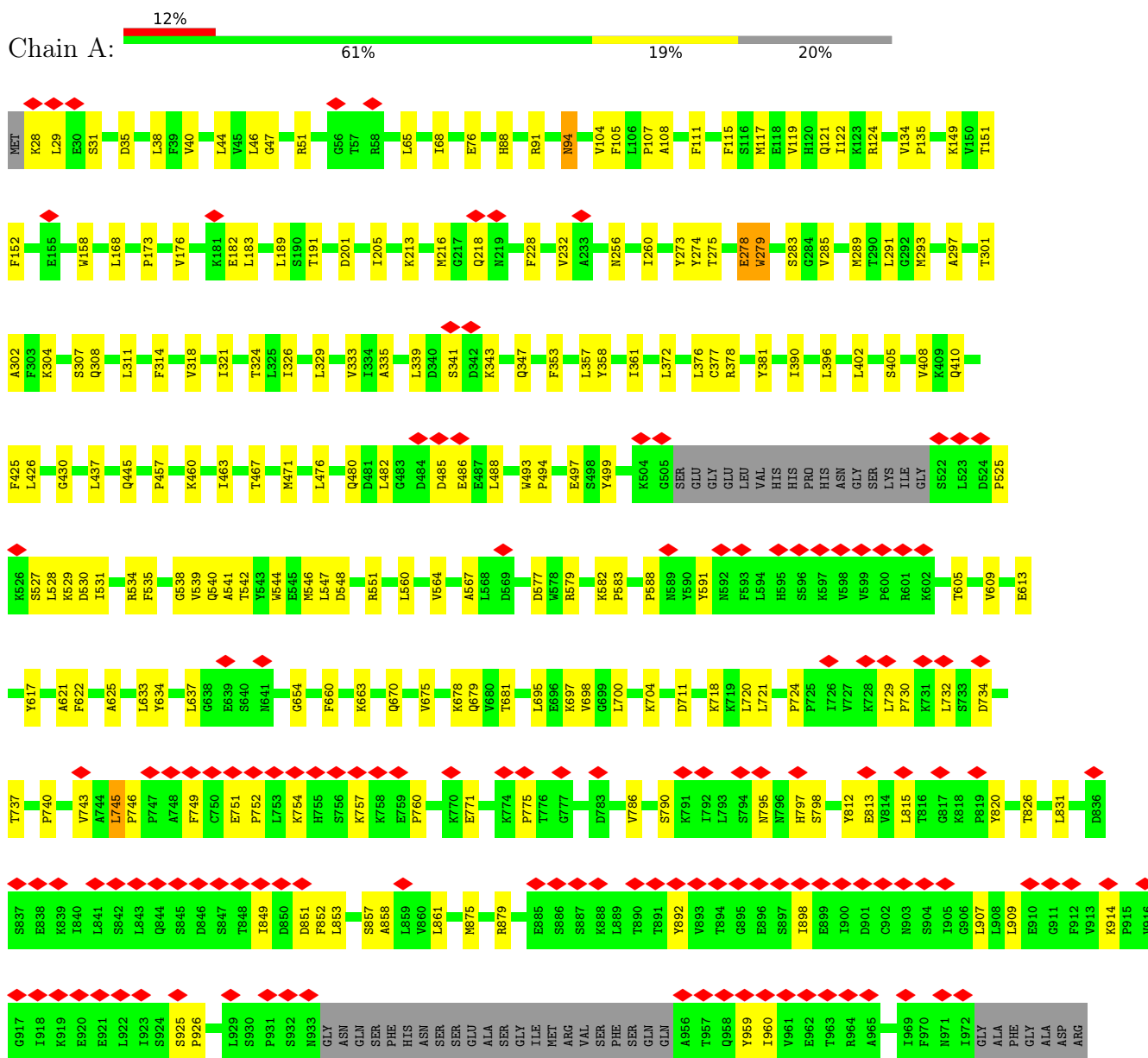


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			41	32	8	1	
2	A	1	Total	C	O	P	0
			48	39	8	1	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Sodium/hydrogen exchanger 7



SER	SER	ASN
ASP	SER	ASN
TYR	LYS	LYS
LYS	LEU	LEU
ASP	GLN	GLN
ASP	ASP	ASP
ASP	LEU	ASN
ASP	GLN	LEU
LYS	PHE	TYR
	ARG	LYS
	LYS	LYS
	GLU	LEU
	H1007	PRO
	R1008	LEU
	G1009	ASN
	L1010	PRO
	M1011	ALA
	S1012	GLN
		GLY
	I1017	LEU
	TYR	VAL
	ALA	SER
	LYS	ALA
	GLN	LYS
	GLN	SER
	GLN	GLU
	ILE	SER
	ASN	ILE
	LYS	VAL
	THR	THR
	THR	LYS
	THR	LYS
	LEU	GLN
	S1031	LEU
	L1032	GLU
	S1033	THR
	F1034	ARG
	M1037	LYS
		HIS
	S1040	ALA
	I1041	CYS
		GLN
	S1044	LEU
	M1045	PRO
	V1046	LEU
		LYS
		GLY
	M1047	GLY
	VAL	GLU
	TYR	SER
	ARG	SER
	ARG	THR
	SER	ARG
	VAL	ASN
	GLN	GLN
	PHE	THR
	GLY	MET
	GLY	LYS
	ILE	VAL
		GLU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	228696	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.606	Depositor
Minimum map value	-2.465	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PC1

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	0.11	0/7472	0.31	2/10129 (0.0%)
1	B	0.11	0/7472	0.30	2/10129 (0.0%)
All	All	0.11	0/14944	0.30	4/20258 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	278	GLU	CA-C-N	5.32	131.71	121.54
1	B	278	GLU	C-N-CA	5.32	131.71	121.54
1	A	278	GLU	CA-C-N	5.31	131.68	121.54
1	A	278	GLU	C-N-CA	5.31	131.68	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	925	SER	Peptide
1	B	925	SER	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7318	0	7542	156	0
1	B	7318	0	7542	135	0
2	A	89	0	130	7	0
All	All	14725	0	15214	274	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 9.

All (274) 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:551:ARG:O	1:A:679:GLN:NE2	2.16	0.78
1:A:547:LEU:HD23	1:B:698:VAL:HG22	1.67	0.76
1:B:745:LEU:HD13	1:B:852:PHE:HD2	1.53	0.72
1:A:745:LEU:HD11	1:A:849:ILE:HG23	1.71	0.72
1:A:698:VAL:HG22	1:B:547:LEU:HD23	1.72	0.71
1:A:678:LYS:HG3	1:A:720:LEU:HD21	1.75	0.69
1:A:301:THR:HB	1:A:721:LEU:HB3	1.75	0.69
1:B:745:LEU:HD11	1:B:849:ILE:HG23	1.74	0.68
1:A:104:VAL:HG13	2:A:1202:PC1:H3C1	1.77	0.67
1:A:463:ILE:HG21	1:B:700:LEU:HD11	1.77	0.66
1:B:813:GLU:HG2	1:B:820:TYR:HA	1.78	0.66
1:B:480:GLN:HE22	1:B:1041:ILE:HB	1.60	0.65
1:A:567:ALA:HB2	1:A:577:ASP:HB3	1.78	0.65
1:B:678:LYS:HG3	1:B:720:LEU:HD21	1.80	0.63
1:A:302:ALA:O	1:A:718:LYS:NZ	2.32	0.62
1:A:745:LEU:HD12	1:A:849:ILE:HD12	1.82	0.62
1:A:813:GLU:HG2	1:A:820:TYR:HA	1.81	0.62
1:A:745:LEU:HB3	1:A:746:PRO:HD3	1.82	0.62
1:A:205:ILE:HG21	1:A:285:VAL:HB	1.83	0.61
1:A:304:LYS:HG3	1:A:307:SER:H	1.66	0.61
1:A:121:GLN:HG2	1:A:191:THR:HG21	1.82	0.61
1:A:795:ASN:OD1	1:A:798:SER:OG	2.19	0.61
1:A:274:TYR:OH	1:B:35:ASP:OD1	2.20	0.59
1:A:35:ASP:OD1	1:B:274:TYR:OH	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:HA	1:B:482:LEU:HD21	1.84	0.59
1:B:1031:SER:OG	1:B:1032:LEU:N	2.35	0.59
1:A:1031:SER:OG	1:A:1032:LEU:N	2.31	0.59
1:A:745:LEU:HD13	1:A:852:PHE:HD2	1.67	0.59
2:A:1201:PC1:H362	2:A:1202:PC1:H2A2	1.84	0.58
1:A:256:ASN:ND2	1:A:711:ASP:OD1	2.36	0.58
1:A:582:LYS:HG3	1:A:583:PRO:HD3	1.84	0.58
1:B:861:LEU:HB3	1:B:907:LEU:HD11	1.85	0.58
1:B:105:PHE:HB3	1:B:326:ILE:HD11	1.85	0.58
1:B:730:PRO:HB3	1:B:734:ASP:HB2	1.86	0.58
1:B:122:ILE:HD12	1:B:129:MET:HE1	1.85	0.58
1:A:38:LEU:HD12	1:B:274:TYR:CE1	2.39	0.57
1:B:457:PRO:HG2	1:B:460:LYS:HD3	1.87	0.57
1:A:740:PRO:HG3	1:B:1040:SER:HB2	1.87	0.57
1:A:189:LEU:HD21	1:A:390:ILE:HG21	1.87	0.57
1:A:542:THR:HG21	1:A:625:ALA:HA	1.87	0.57
1:A:737:THR:HG23	1:A:743:VAL:HG21	1.86	0.56
1:A:289:MET:O	1:A:293:MET:HG2	2.05	0.56
1:A:695:LEU:HD11	1:A:700:LEU:HD22	1.87	0.56
1:A:697:LYS:HE3	1:B:547:LEU:HD11	1.87	0.56
1:B:121:GLN:HG2	1:B:191:THR:HG21	1.88	0.56
2:A:1201:PC1:H3E1	2:A:1202:PC1:H2H2	1.88	0.56
1:B:861:LEU:HD23	1:B:907:LEU:HD21	1.87	0.56
1:A:134:VAL:HB	1:A:135:PRO:HD3	1.87	0.56
1:B:47:GLY:HA2	1:B:65:LEU:HD21	1.88	0.56
1:B:134:VAL:HB	1:B:135:PRO:HD3	1.87	0.56
1:B:582:LYS:HG3	1:B:583:PRO:HD3	1.87	0.56
1:B:189:LEU:HD21	1:B:390:ILE:HG21	1.87	0.55
1:B:538:GLY:HA3	1:B:1011:MET:HE3	1.86	0.55
1:B:542:THR:HG21	1:B:625:ALA:HA	1.88	0.55
1:B:289:MET:O	1:B:293:MET:HG2	2.06	0.55
1:A:609:VAL:HG11	1:A:724:PRO:HB3	1.87	0.55
1:A:730:PRO:HB3	1:A:734:ASP:HB2	1.87	0.55
1:A:858:ALA:HA	1:A:861:LEU:HB2	1.89	0.55
1:A:482:LEU:HD21	1:B:551:ARG:HA	1.88	0.55
1:B:232:VAL:HG13	1:B:283:SER:HB2	1.88	0.55
1:A:76:GLU:OE2	1:A:91:ARG:NH1	2.38	0.54
1:A:44:LEU:HD21	1:A:321:ILE:HG23	1.89	0.54
1:B:745:LEU:HB3	1:B:746:PRO:HD3	1.89	0.54
1:B:76:GLU:OE2	1:B:91:ARG:NH1	2.35	0.54
1:A:377:CYS:SG	1:A:378:ARG:NH1	2.80	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:PHE:HE1	1:B:291:LEU:HD23	1.72	0.54
1:B:732:LEU:HD23	1:B:757:LYS:HB3	1.89	0.54
1:B:737:THR:HG23	1:B:743:VAL:HG21	1.90	0.54
1:A:861:LEU:HB3	1:A:907:LEU:HD11	1.89	0.54
1:A:47:GLY:HA2	1:A:65:LEU:HD21	1.89	0.54
1:A:467:THR:O	1:A:471:MET:HE2	2.08	0.53
1:A:732:LEU:HD23	1:A:757:LYS:HB3	1.89	0.53
1:B:205:ILE:HG21	1:B:285:VAL:HB	1.89	0.53
2:A:1201:PC1:H3I3	2:A:1202:PC1:H2D1	1.90	0.53
1:B:751:GLU:HA	1:B:754:LYS:HG3	1.91	0.53
1:A:579:ARG:HA	1:A:582:LYS:HE3	1.91	0.53
1:A:111:PHE:HE1	1:A:291:LEU:HD23	1.74	0.53
1:A:408:VAL:HG11	1:A:425:PHE:HD2	1.73	0.53
1:A:105:PHE:HB3	1:A:326:ILE:HD11	1.91	0.53
1:A:697:LYS:HG2	1:B:547:LEU:HD21	1.90	0.53
1:B:732:LEU:HD13	1:B:760:PRO:HG3	1.89	0.53
1:B:821:LEU:HD21	1:B:926:PRO:HG3	1.90	0.53
1:A:31:SER:HA	1:A:88:HIS:HB3	1.91	0.52
1:B:579:ARG:HA	1:B:582:LYS:HE3	1.92	0.52
1:A:378:ARG:HG3	1:A:378:ARG:HH11	1.75	0.52
1:A:605:THR:O	1:A:609:VAL:HG23	2.09	0.52
1:B:302:ALA:O	1:B:718:LYS:NZ	2.40	0.52
1:A:861:LEU:HD23	1:A:907:LEU:HD21	1.91	0.52
1:B:408:VAL:HG11	1:B:425:PHE:HD2	1.75	0.52
1:A:457:PRO:HG2	1:A:460:LYS:HD3	1.91	0.52
1:A:634:TYR:HE2	1:A:797:HIS:HB3	1.75	0.52
1:B:812:TYR:HB2	1:B:857:SER:HB2	1.92	0.52
1:A:232:VAL:HG13	1:A:283:SER:HB2	1.92	0.52
1:A:538:GLY:HA3	1:A:1011:MET:HE3	1.92	0.52
1:B:31:SER:HA	1:B:88:HIS:HB3	1.91	0.52
1:A:256:ASN:OD1	1:A:304:LYS:NZ	2.42	0.51
1:A:698:VAL:HG21	1:B:544:TRP:CD1	2.46	0.51
1:A:732:LEU:HD13	1:A:760:PRO:HG3	1.93	0.51
1:A:746:PRO:HB2	1:A:749:PHE:HB3	1.93	0.51
1:B:541:ALA:HB2	1:B:1010:LEU:HB3	1.92	0.51
1:A:548:ASP:OD2	1:A:1008:ARG:NH2	2.44	0.51
1:A:335:ALA:O	1:A:339:LEU:HB2	2.11	0.51
1:A:851:ASP:OD1	1:A:852:PHE:N	2.44	0.51
1:B:335:ALA:O	1:B:339:LEU:HB2	2.12	0.50
1:A:541:ALA:HB2	1:A:1010:LEU:HB3	1.94	0.50
1:A:546:MET:HE1	1:A:621:ALA:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:ILE:HG21	1:B:799:LEU:HD22	1.93	0.50
1:A:704:LYS:NZ	1:B:182:GLU:O	2.44	0.50
1:B:546:MET:HE1	1:B:621:ALA:HA	1.94	0.50
1:B:898:ILE:HB	1:B:959:TYR:HB2	1.94	0.50
1:B:560:LEU:O	1:B:564:VAL:HG23	2.12	0.49
1:A:485:ASP:OD1	1:A:488:LEU:HB2	2.12	0.49
1:A:914:LYS:HB3	1:A:960:ILE:HB	1.94	0.49
1:A:812:TYR:HB2	1:A:857:SER:HB2	1.92	0.49
1:B:535:PHE:HD2	1:B:633:LEU:HD22	1.77	0.49
1:B:128:GLN:HG3	1:B:376:LEU:HD22	1.94	0.49
1:B:531:ILE:HD12	1:B:637:LEU:HD11	1.94	0.49
1:A:124:ARG:HH21	1:A:381:TYR:HE1	1.59	0.49
1:A:107:PRO:HG3	1:A:273:TYR:CD2	2.48	0.49
1:A:560:LEU:O	1:A:564:VAL:HG23	2.12	0.49
1:A:670:GLN:HB3	1:A:729:LEU:HD21	1.95	0.49
1:B:745:LEU:HD13	1:B:852:PHE:CD2	2.42	0.49
1:B:760:PRO:HG2	1:B:831:LEU:HD22	1.95	0.49
1:A:28:LYS:NZ	1:A:29:LEU:O	2.44	0.49
1:A:617:TYR:OH	1:A:675:VAL:O	2.28	0.48
1:A:751:GLU:HA	1:A:754:LYS:HG3	1.94	0.48
1:A:588:PRO:HD2	1:A:591:TYR:CE2	2.48	0.48
1:B:588:PRO:HD2	1:B:591:TYR:CE2	2.48	0.48
1:A:1040:SER:HB2	1:B:740:PRO:HG3	1.95	0.48
1:B:107:PRO:HG3	1:B:273:TYR:CD2	2.48	0.48
1:B:532:ARG:NH2	1:B:649:GLU:OE2	2.38	0.48
1:A:343:LYS:O	1:A:347:GLN:HG3	2.14	0.48
1:A:914:LYS:O	1:A:960:ILE:N	2.40	0.48
1:B:525:PRO:HA	1:B:531:ILE:HD11	1.96	0.48
1:B:535:PHE:O	1:B:539:VAL:HG23	2.14	0.48
1:A:609:VAL:O	1:A:613:GLU:HB2	2.13	0.48
1:B:183:LEU:HD22	1:B:445:GLN:OE1	2.14	0.48
1:A:698:VAL:HG12	1:A:700:LEU:HB2	1.95	0.47
1:B:173:PRO:HD3	1:B:201:ASP:OD2	2.14	0.47
1:A:124:ARG:HH11	1:A:583:PRO:HG2	1.78	0.47
1:B:1037:MET:O	1:B:1041:ILE:HG12	2.15	0.47
1:A:544:TRP:CD1	1:B:698:VAL:HG21	2.49	0.47
1:A:94:ASN:O	1:A:410:GLN:NE2	2.47	0.47
1:A:182:GLU:O	1:B:704:LYS:NZ	2.47	0.47
1:A:622:PHE:HE2	1:A:654:GLY:HA2	1.80	0.47
1:A:775:PRO:HG3	1:A:813:GLU:HB3	1.97	0.47
1:A:898:ILE:HB	1:A:959:TYR:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:HD3	1:A:201:ASP:OD2	2.15	0.47
1:B:622:PHE:HE2	1:B:654:GLY:HA2	1.79	0.47
1:A:117:MET:SD	1:A:122:ILE:HG13	2.55	0.47
1:A:535:PHE:O	1:A:539:VAL:HG23	2.14	0.47
1:A:605:THR:OG1	1:A:670:GLN:NE2	2.43	0.47
2:A:1202:PC1:H241	2:A:1202:PC1:H321	1.97	0.47
1:B:38:LEU:HD21	1:B:86:ILE:HA	1.96	0.46
1:A:213:LYS:HE2	1:A:228:PHE:CG	2.50	0.46
1:A:760:PRO:HG2	1:A:831:LEU:HD22	1.97	0.46
1:B:551:ARG:O	1:B:679:GLN:NE2	2.49	0.46
1:B:661:LEU:O	1:B:665:ARG:HG3	2.15	0.46
1:A:493:TRP:HE1	1:A:1046:VAL:HG11	1.80	0.46
1:A:786:VAL:HG12	1:A:826:THR:HG22	1.97	0.46
1:A:875:MET:O	1:A:879:ARG:HG2	2.16	0.46
1:B:343:LYS:O	1:B:347:GLN:HG3	2.15	0.46
1:A:771:GLU:OE2	1:A:790:SER:HA	2.16	0.45
1:B:775:PRO:HG3	1:B:813:GLU:HB3	1.98	0.45
1:B:278:GLU:O	1:B:279:TRP:CG	2.70	0.45
1:A:341:SER:O	1:A:343:LYS:HG2	2.17	0.45
1:A:372:LEU:HB3	1:A:376:LEU:HG	1.98	0.45
1:B:875:MET:O	1:B:879:ARG:HG2	2.15	0.45
1:A:115:PHE:HE2	1:A:311:LEU:HG	1.80	0.45
1:A:278:GLU:O	1:A:279:TRP:CG	2.69	0.45
1:A:499:TYR:CE2	1:B:720:LEU:HD12	2.52	0.45
1:B:541:ALA:HB1	1:B:1008:ARG:HB2	1.98	0.45
1:B:548:ASP:OD2	1:B:1008:ARG:NH2	2.49	0.45
1:A:535:PHE:HD2	1:A:633:LEU:HD22	1.81	0.44
1:B:374:PRO:O	1:B:378:ARG:NH1	2.50	0.44
1:A:213:LYS:HG2	1:A:218:GLN:HG3	1.99	0.44
1:B:341:SER:O	1:B:343:LYS:HG2	2.16	0.44
1:A:525:PRO:HA	1:A:531:ILE:HD11	1.99	0.44
1:B:540:GLN:HG3	1:B:564:VAL:HG11	1.99	0.44
1:B:570:GLN:HG3	1:B:579:ARG:HH22	1.83	0.44
1:A:260:ILE:HD11	1:B:51:ARG:HD3	1.99	0.44
1:A:304:LYS:O	1:A:308:GLN:HG3	2.18	0.44
1:B:124:ARG:HH11	1:B:583:PRO:HG2	1.82	0.44
1:B:129:MET:O	1:B:133:ALA:N	2.51	0.44
1:B:494:PRO:HA	1:B:497:GLU:HG2	2.00	0.44
1:A:530:ASP:O	1:A:534:ARG:HG2	2.18	0.44
1:B:396:LEU:HD22	1:B:437:LEU:HD23	1.99	0.44
1:A:476:LEU:O	1:A:480:GLN:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:VAL:HG12	1:B:826:THR:HG22	1.99	0.43
1:A:51:ARG:HD3	1:B:260:ILE:HD11	1.99	0.43
1:A:260:ILE:HD12	1:B:55:ARG:HH22	1.83	0.43
1:B:65:LEU:HD13	1:B:324:THR:HA	2.00	0.43
1:B:94:ASN:O	1:B:410:GLN:NE2	2.52	0.43
1:B:784:GLY:HA3	1:B:830:VAL:HG22	2.01	0.43
1:A:151:THR:HG22	1:A:353:PHE:HE2	1.83	0.43
1:A:540:GLN:HG3	1:A:564:VAL:HG11	1.99	0.43
1:B:670:GLN:HB3	1:B:729:LEU:HD21	1.99	0.43
1:A:396:LEU:HD22	1:A:437:LEU:HD23	2.01	0.43
1:A:745:LEU:CD1	1:A:849:ILE:HG23	2.46	0.43
1:B:213:LYS:HE2	1:B:228:PHE:CG	2.52	0.43
1:B:751:GLU:HB2	1:B:752:PRO:HD3	2.01	0.43
1:A:65:LEU:HD13	1:A:324:THR:HA	2.00	0.43
1:A:149:LYS:HG2	1:A:158:TRP:CE2	2.54	0.43
1:A:256:ASN:HA	1:A:304:LYS:NZ	2.33	0.43
1:B:609:VAL:HG11	1:B:724:PRO:HB3	2.00	0.43
1:A:314:PHE:O	1:A:318:VAL:HG23	2.18	0.43
1:A:745:LEU:HD13	1:A:852:PHE:CD2	2.48	0.43
1:B:858:ALA:HA	1:B:861:LEU:HB2	2.00	0.43
1:A:168:LEU:HD23	1:A:168:LEU:HA	1.90	0.43
1:B:149:LYS:HG2	1:B:158:TRP:CE2	2.54	0.43
1:A:660:PHE:HA	1:A:663:LYS:HE3	2.01	0.42
1:A:201:ASP:O	1:A:205:ILE:HG12	2.18	0.42
1:A:751:GLU:HB2	1:A:752:PRO:HD3	2.00	0.42
1:A:812:TYR:OH	1:A:909:LEU:O	2.34	0.42
1:B:846:ASP:HB2	1:B:849:ILE:HG12	2.01	0.42
1:B:740:PRO:HG2	1:B:879:ARG:HH22	1.84	0.42
1:A:108:ALA:HB1	1:A:318:VAL:HG12	2.00	0.42
1:A:402:LEU:HD21	1:A:430:GLY:HA2	2.01	0.42
1:B:634:TYR:CE1	1:B:797:HIS:HB3	2.55	0.42
1:A:751:GLU:HA	1:A:754:LYS:HE2	2.01	0.42
1:B:256:ASN:ND2	1:B:711:ASP:OD1	2.41	0.42
1:B:474:LYS:HB3	1:B:474:LYS:HE3	1.85	0.42
1:B:694:ASN:O	1:B:698:VAL:HG23	2.19	0.42
1:A:405:SER:HB2	1:A:426:LEU:HA	2.01	0.42
1:B:275:THR:HG23	1:B:279:TRP:HE3	1.84	0.42
1:A:119:VAL:HG21	1:A:297:ALA:HB2	2.02	0.42
1:A:358:TYR:O	1:A:361:ILE:HG22	2.20	0.42
1:A:541:ALA:HB1	1:A:1008:ARG:HB2	2.01	0.42
1:B:117:MET:HE3	1:B:122:ILE:HG13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:PRO:HA	1:A:176:VAL:HG22	2.02	0.42
1:B:251:LEU:HG	1:B:264:LEU:HD23	2.02	0.42
1:A:527:SER:C	1:A:529:LYS:H	2.28	0.42
1:A:40:VAL:HG11	2:A:1201:PC1:H3A1	2.02	0.41
1:A:275:THR:HG23	1:A:279:TRP:HE3	1.85	0.41
1:A:749:PHE:HE2	1:A:754:LYS:HD3	1.84	0.41
2:A:1202:PC1:H392	2:A:1202:PC1:H2E2	2.02	0.41
1:B:109:LEU:HD11	1:B:326:ILE:HD12	2.02	0.41
1:B:168:LEU:HD23	1:B:168:LEU:HA	1.93	0.41
1:B:173:PRO:HA	1:B:176:VAL:HG22	2.02	0.41
1:A:534:ARG:NH1	1:A:1012:SER:HA	2.35	0.41
1:B:213:LYS:HD3	1:B:228:PHE:CE1	2.56	0.41
1:B:329:LEU:O	1:B:333:VAL:HG23	2.20	0.41
1:A:183:LEU:HD22	1:A:445:GLN:OE1	2.21	0.41
1:A:329:LEU:O	1:A:333:VAL:HG23	2.20	0.41
1:B:44:LEU:HD21	1:B:321:ILE:HG23	2.03	0.41
1:A:486:GLU:OE1	1:B:804:SER:OG	2.36	0.41
1:B:314:PHE:O	1:B:318:VAL:HG23	2.20	0.41
1:B:790:SER:HB2	1:B:822:CYS:HB3	2.02	0.41
1:B:803:PHE:CE2	1:B:809:LEU:HD11	2.55	0.41
1:A:152:PHE:HZ	1:A:357:LEU:HB2	1.86	0.41
1:A:531:ILE:HD12	1:A:637:LEU:HD11	2.02	0.41
1:A:1032:LEU:HD23	1:A:1032:LEU:HA	1.88	0.41
1:A:46:LEU:HD13	1:A:68:ILE:HG21	2.03	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.86	0.41
1:A:494:PRO:HA	1:A:497:GLU:HG2	2.02	0.41
1:B:117:MET:HE2	1:B:119:VAL:HG22	2.02	0.41
1:B:152:PHE:HZ	1:B:357:LEU:HB2	1.86	0.41
1:B:402:LEU:HD21	1:B:430:GLY:HA2	2.03	0.41
1:B:530:ASP:O	1:B:534:ARG:HG2	2.20	0.41
1:B:216:MET:HE2	1:B:216:MET:HA	2.02	0.41
1:B:258:THR:O	1:B:262:ILE:HG13	2.21	0.40
1:B:660:PHE:HA	1:B:663:LYS:HE3	2.02	0.40
1:A:815:LEU:HD21	1:A:853:LEU:HD13	2.03	0.40
1:B:213:LYS:HG2	1:B:218:GLN:HG3	2.02	0.40
1:B:364:SER:O	1:B:368:VAL:HG23	2.21	0.40
1:A:681:THR:OG1	1:B:496:VAL:HG22	2.21	0.40
1:A:892:TYR:CZ	1:A:898:ILE:HG12	2.57	0.40
1:B:108:ALA:HB1	1:B:318:VAL:HG12	2.04	0.40
1:B:210:LEU:HD11	1:B:225:ILE:HG23	2.04	0.40
1:A:216:MET:HA	1:A:216:MET:HE2	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:O	1:A:528:LEU:HD23	2.22	0.40
1:A:745:LEU:HD21	1:A:853:LEU:HD21	2.03	0.40
1:B:534:ARG:NH1	1:B:1012:SER:HA	2.37	0.40
1:B:892:TYR:CZ	1:B:898:ILE:HG12	2.57	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	925/1162 (80%)	870 (94%)	52 (6%)	3 (0%)	36	62
1	B	925/1162 (80%)	877 (95%)	45 (5%)	3 (0%)	36	62
All	All	1850/2324 (80%)	1747 (94%)	97 (5%)	6 (0%)	37	62

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	TRP
1	A	926	PRO
1	B	279	TRP
1	B	926	PRO
1	A	745	LEU
1	B	745	LEU

5.3.2 Protein sidechains [i](#)

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	809/1006 (80%)	808 (100%)	1 (0%)	88	97
1	B	809/1006 (80%)	809 (100%)	0	100	100
All	All	1618/2012 (80%)	1617 (100%)	1 (0%)	87	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	414	ASN
1	A	631	GLN
1	A	844	GLN
1	A	971	ASN
1	B	120	HIS
1	B	414	ASN
1	B	480	GLN
1	B	595	HIS
1	B	631	GLN
1	B	795	ASN
1	B	844	GLN
1	B	1038	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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$
2	PC1	A	1201	-	40,40,53	0.66	1 (2%)	43,45,61	0.74	2 (4%)
2	PC1	A	1202	-	47,47,53	0.62	1 (2%)	50,52,61	0.74	2 (4%)

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	PC1	A	1201	-	-	13/42/42/57	-
2	PC1	A	1202	-	-	23/49/49/57	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	PC1	P-O13	2.93	1.65	1.54
2	A	1202	PC1	P-O13	2.90	1.65	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1202	PC1	O12-P-O14	3.28	123.62	110.83
2	A	1201	PC1	O12-P-O14	3.21	123.34	110.83
2	A	1201	PC1	O13-P-O11	-2.32	100.62	106.67
2	A	1202	PC1	O13-P-O11	-2.24	100.83	106.67

There are no chirality outliers.

All (36) torsion outliers are listed below:

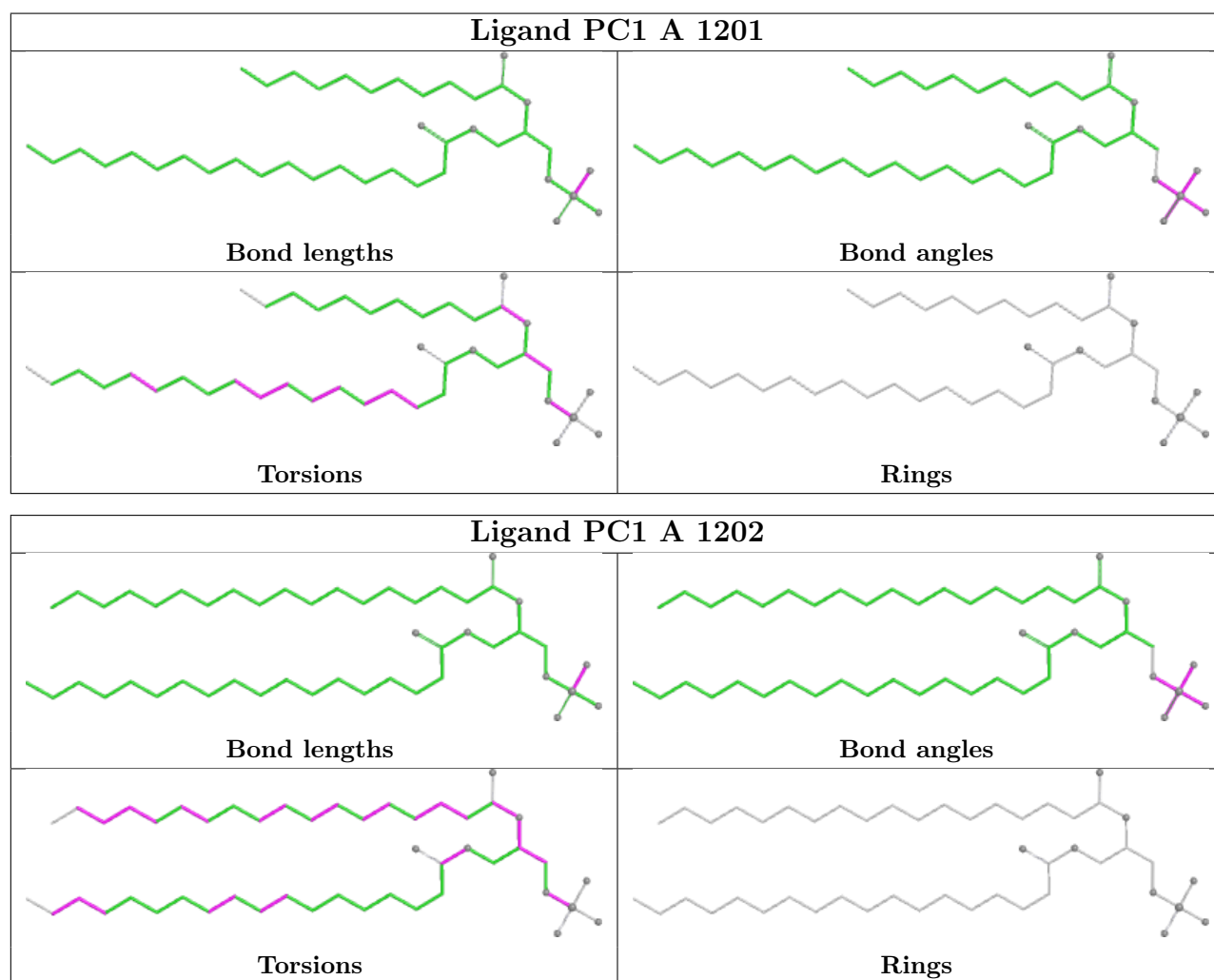
Mol	Chain	Res	Type	Atoms
2	A	1201	PC1	C1-O11-P-O12
2	A	1201	PC1	C1-O11-P-O14
2	A	1201	PC1	C1-O11-P-O13
2	A	1202	PC1	C1-O11-P-O12
2	A	1202	PC1	C1-O11-P-O14
2	A	1202	PC1	C1-O11-P-O13
2	A	1202	PC1	O11-C1-C2-O21
2	A	1202	PC1	C32-C31-O31-C3
2	A	1202	PC1	O32-C31-O31-C3
2	A	1202	PC1	C22-C21-O21-C2
2	A	1202	PC1	O22-C21-O21-C2
2	A	1202	PC1	C2D-C2E-C2F-C2G
2	A	1201	PC1	C37-C38-C39-C3A
2	A	1201	PC1	C22-C21-O21-C2
2	A	1201	PC1	O22-C21-O21-C2
2	A	1202	PC1	C39-C3A-C3B-C3C
2	A	1201	PC1	C33-C34-C35-C36
2	A	1202	PC1	C3-C2-O21-C21
2	A	1201	PC1	O11-C1-C2-O21
2	A	1202	PC1	C2F-C2G-C2H-C2I
2	A	1202	PC1	C3F-C3G-C3H-C3I
2	A	1201	PC1	C38-C39-C3A-C3B
2	A	1202	PC1	C28-C29-C2A-C2B
2	A	1202	PC1	O11-C1-C2-C3
2	A	1202	PC1	C37-C38-C39-C3A
2	A	1202	PC1	C3E-C3F-C3G-C3H
2	A	1201	PC1	O11-C1-C2-C3
2	A	1202	PC1	C22-C23-C24-C25
2	A	1202	PC1	C24-C25-C26-C27
2	A	1202	PC1	C2B-C2C-C2D-C2E
2	A	1202	PC1	C21-C22-C23-C24
2	A	1202	PC1	C26-C27-C28-C29
2	A	1201	PC1	C3C-C3D-C3E-C3F
2	A	1202	PC1	C2E-C2F-C2G-C2H
2	A	1201	PC1	C35-C36-C37-C38
2	A	1201	PC1	C32-C33-C34-C35

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	PC1	4	0
2	A	1202	PC1	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

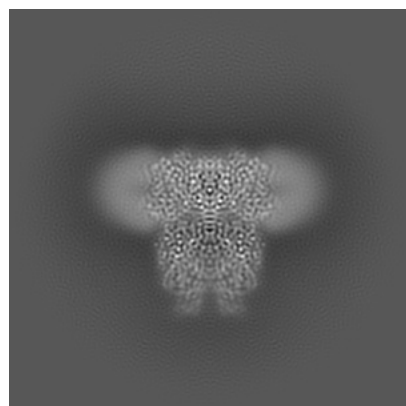
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36077. These allow visual inspection of the internal detail of the map and identification of artifacts.

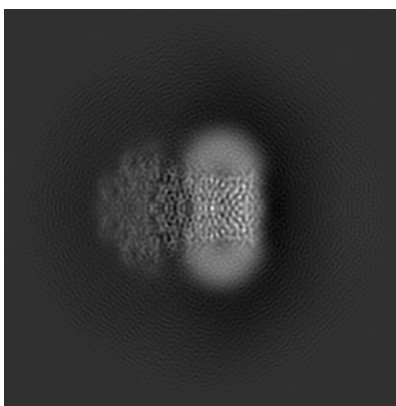
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

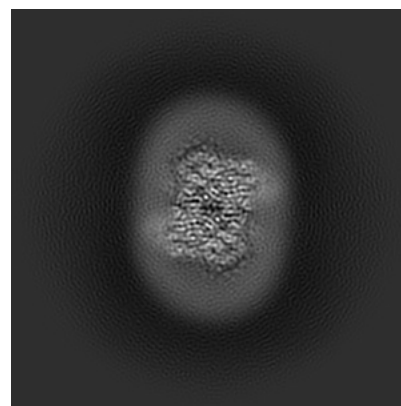
6.1.1 Primary map



X

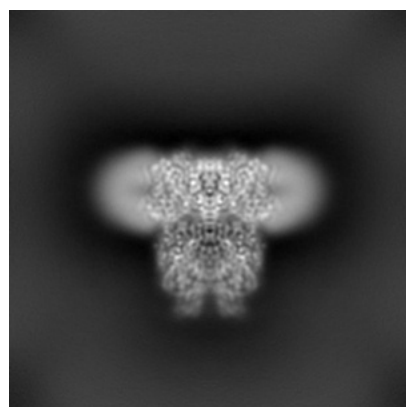


Y

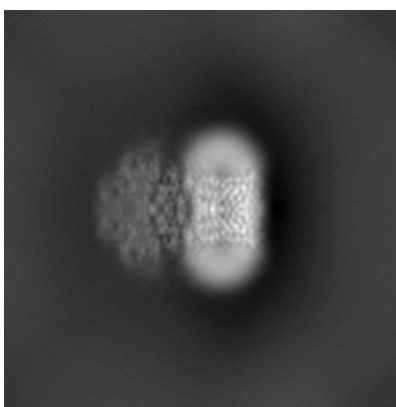


Z

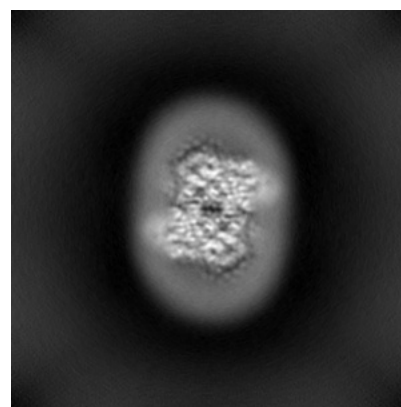
6.1.2 Raw map



X



Y

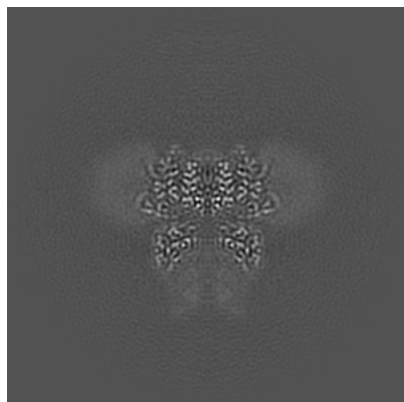


Z

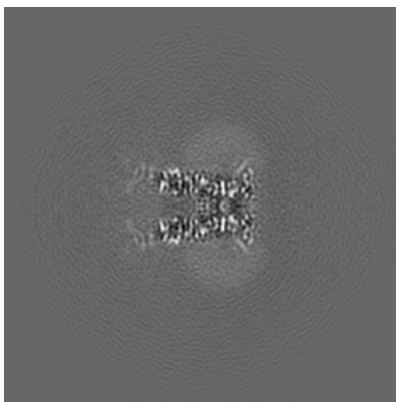
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

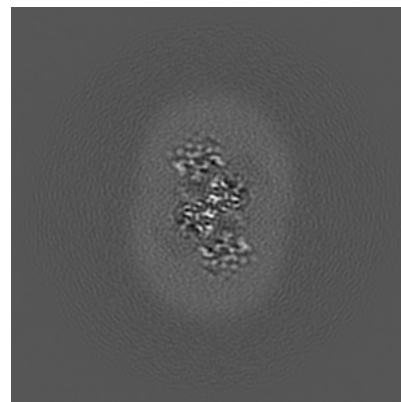
6.2.1 Primary map



X Index: 128

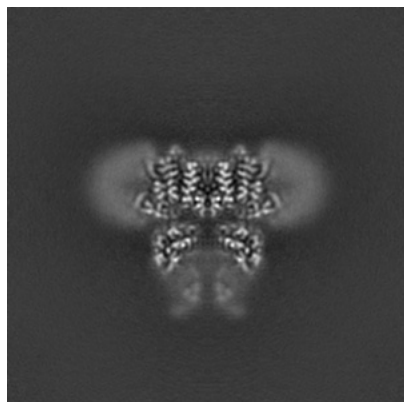


Y Index: 128

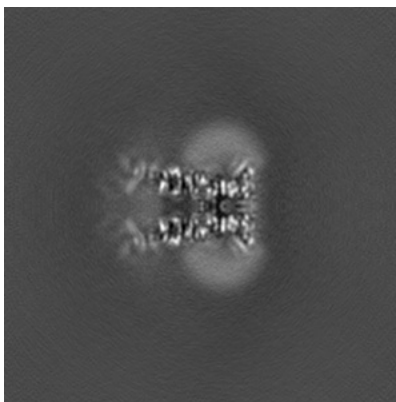


Z Index: 128

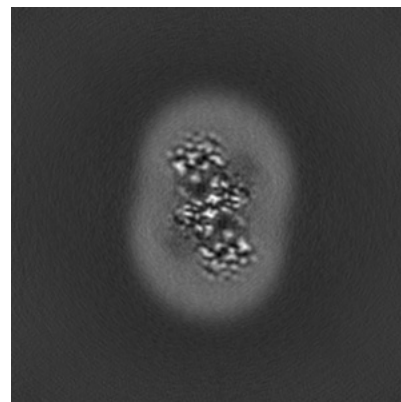
6.2.2 Raw map



X Index: 128



Y Index: 128

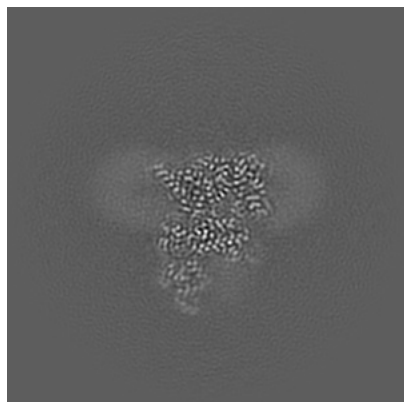


Z Index: 128

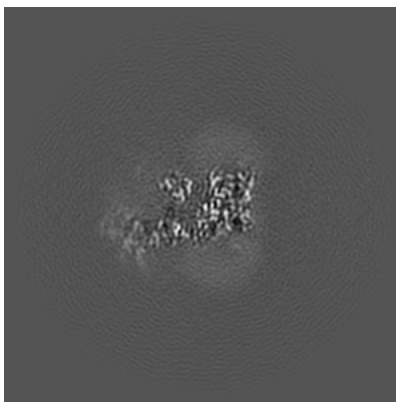
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

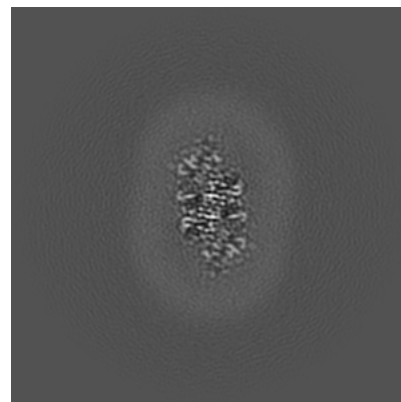
6.3.1 Primary map



X Index: 115

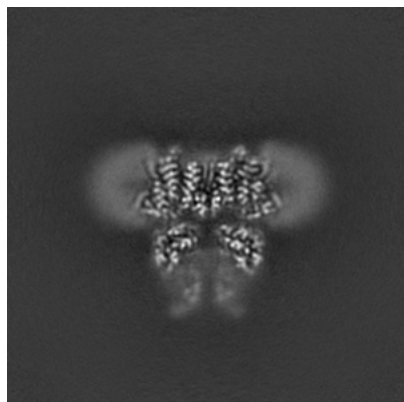


Y Index: 122

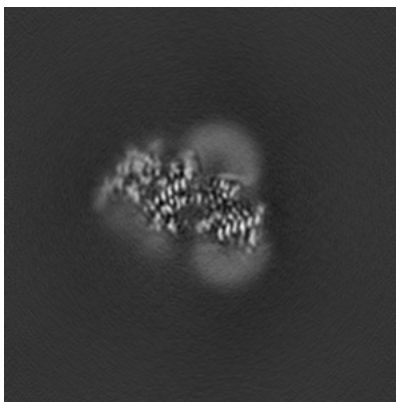


Z Index: 133

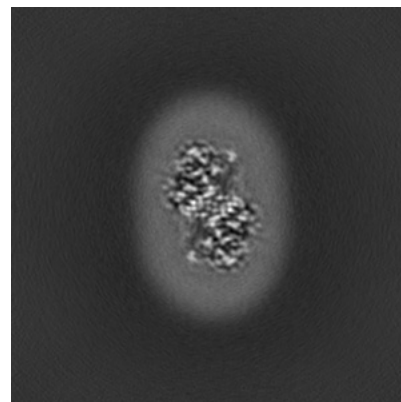
6.3.2 Raw map



X Index: 127



Y Index: 147

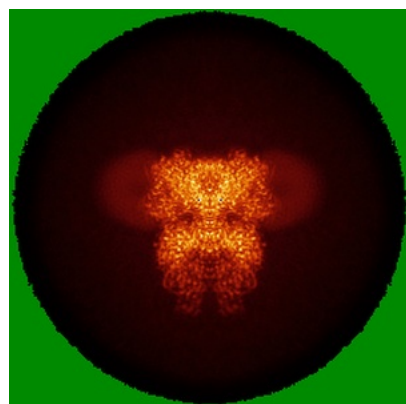


Z Index: 154

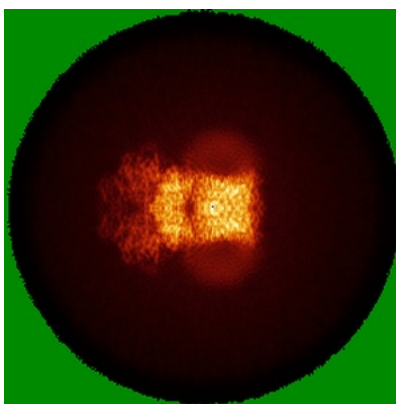
The images above show the largest variance slices of the map in three orthogonal directions.

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

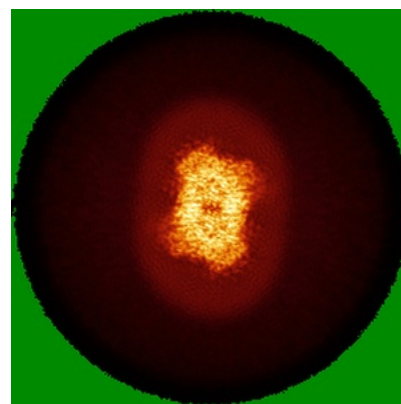
6.4.1 Primary map



X

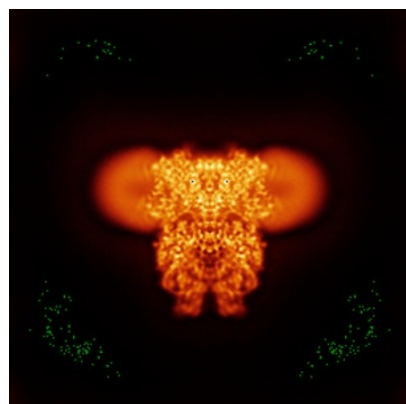


Y

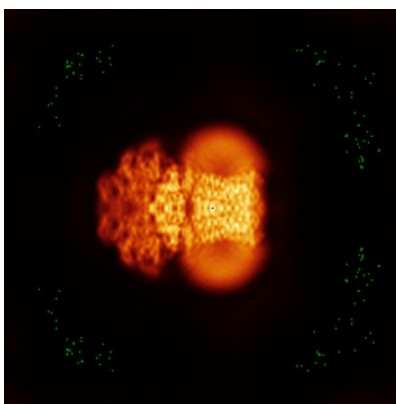


Z

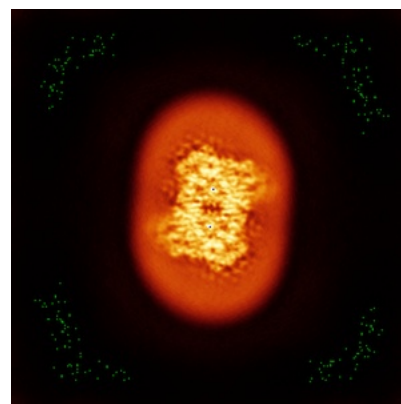
6.4.2 Raw map



X



Y

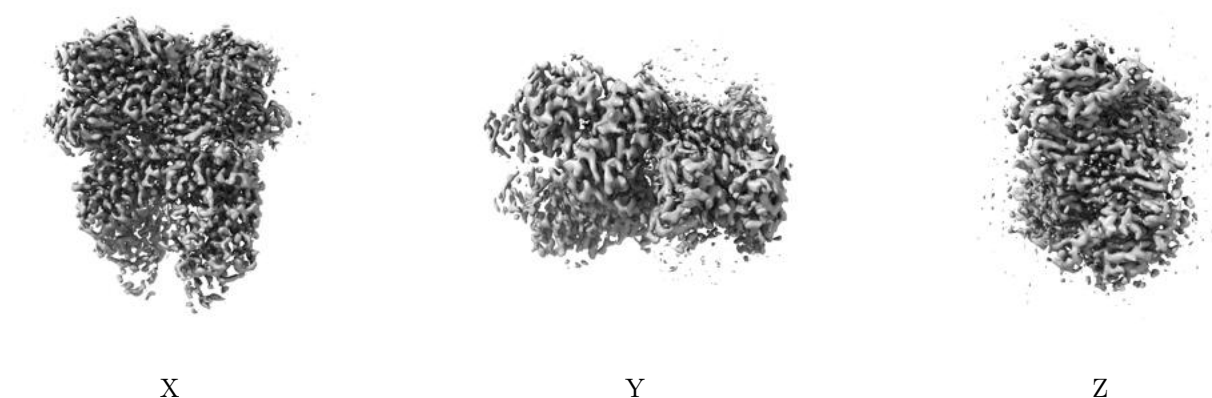


Z

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 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

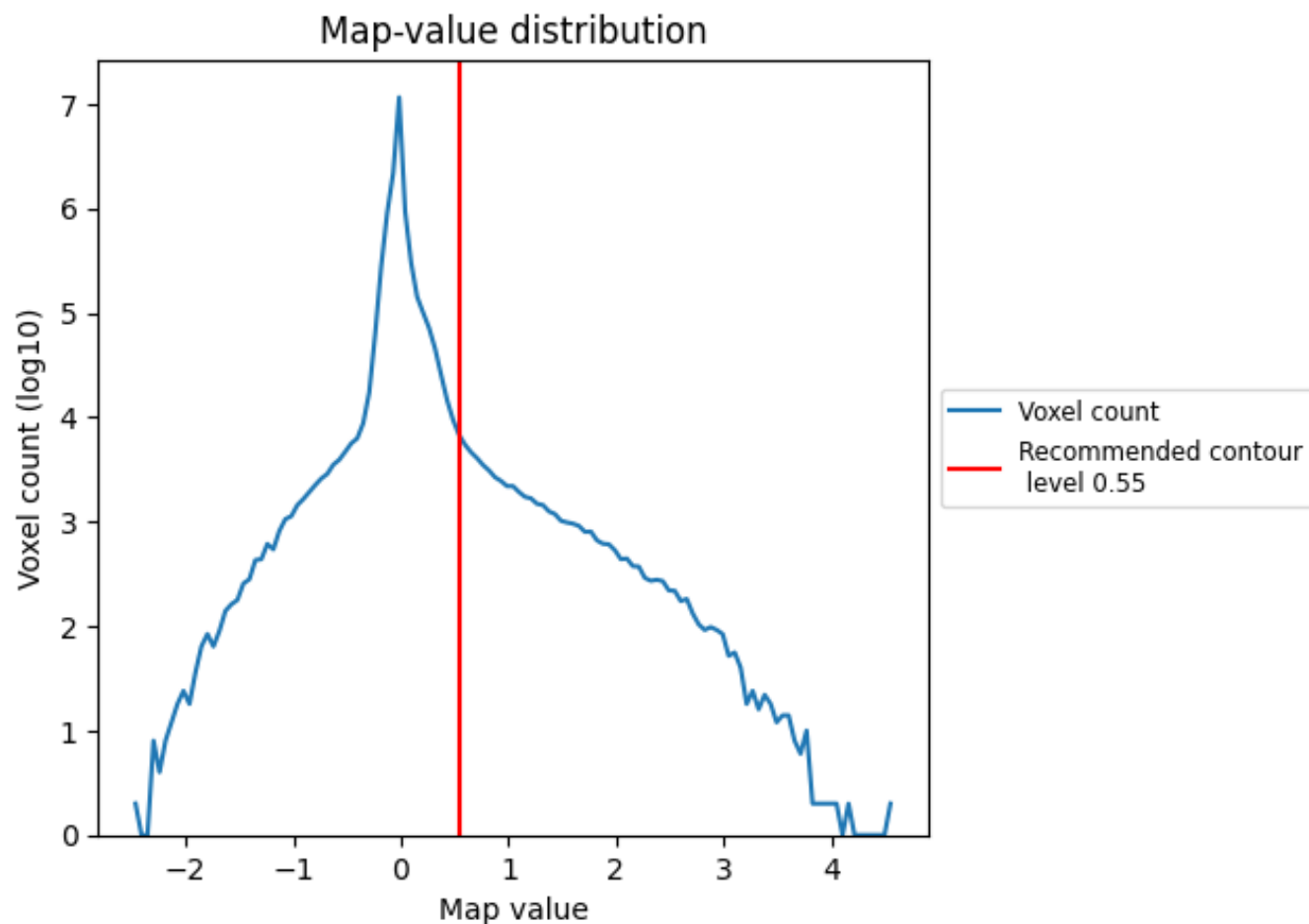
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

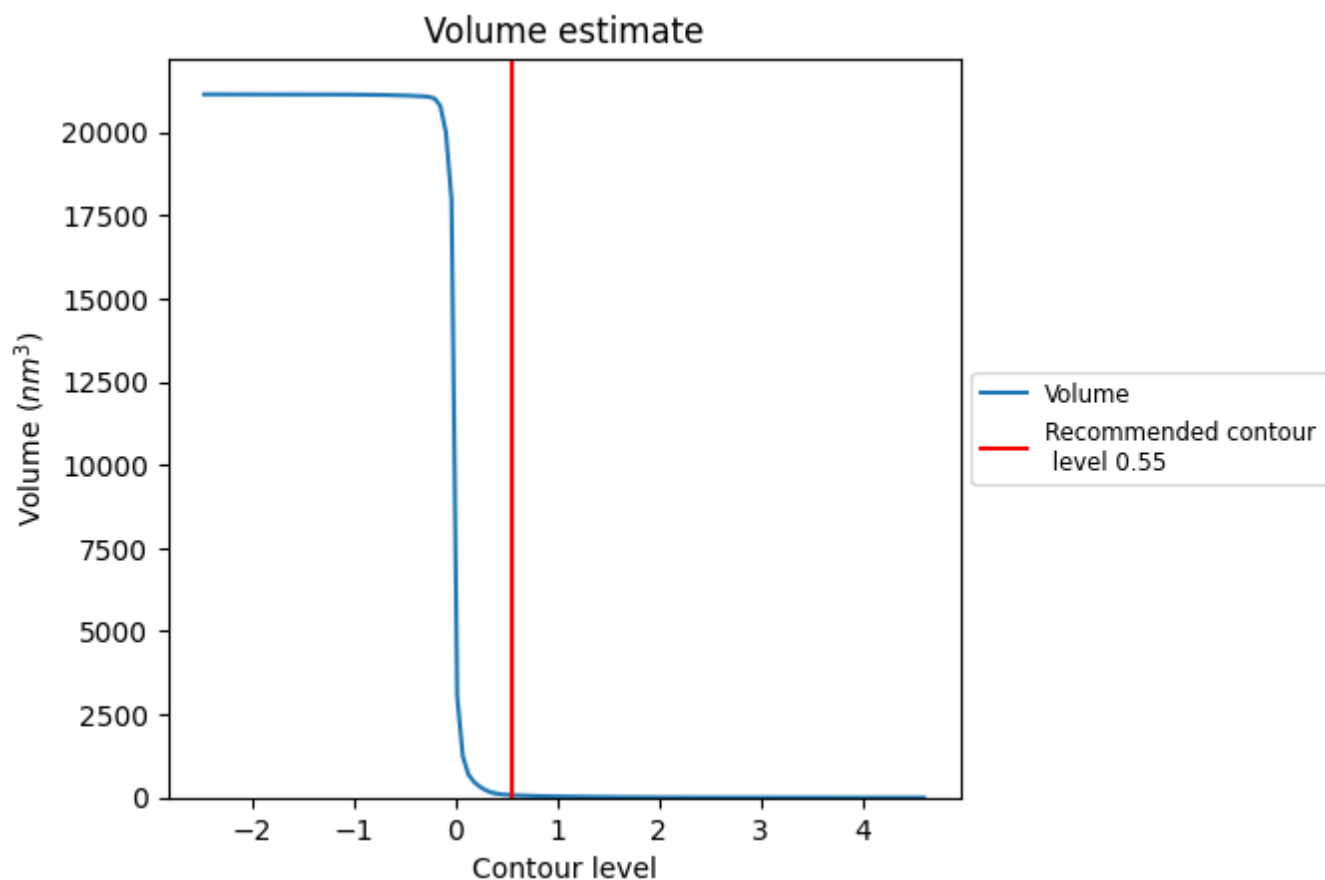
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

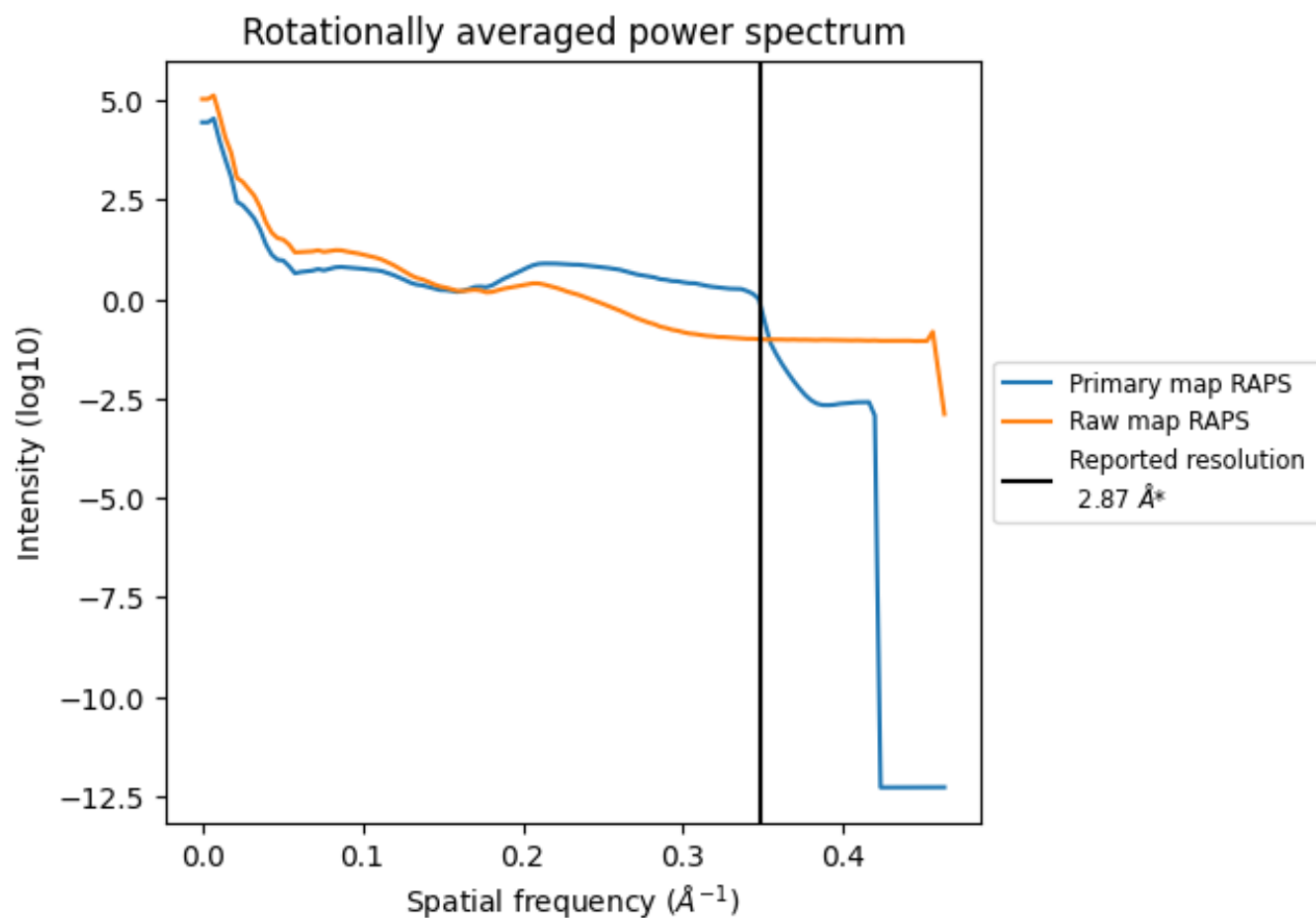
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 67 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 ⓘ

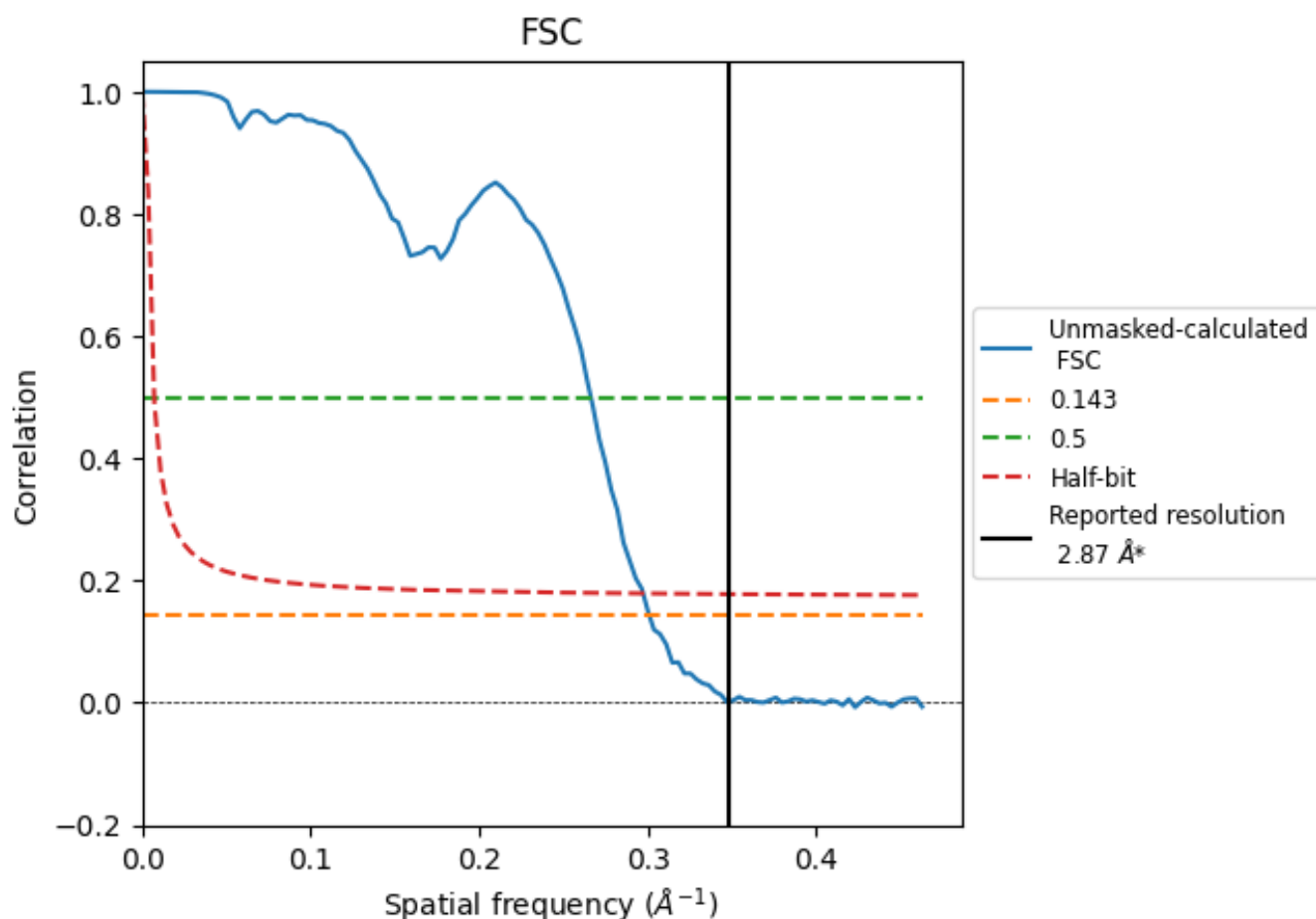


*Reported resolution corresponds to spatial frequency of 0.348 Å⁻¹

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 $0.348 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

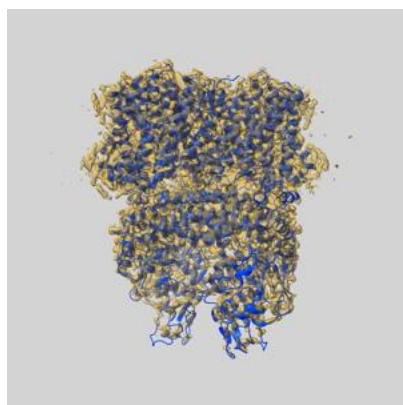
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.87	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.32	3.76	3.36

*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 3.32 differs from the reported value 2.87 by more than 10 %

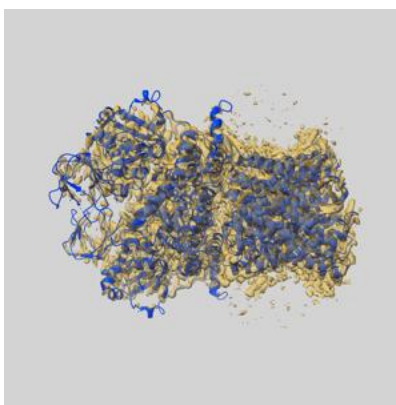
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36077 and PDB model 8JD9. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

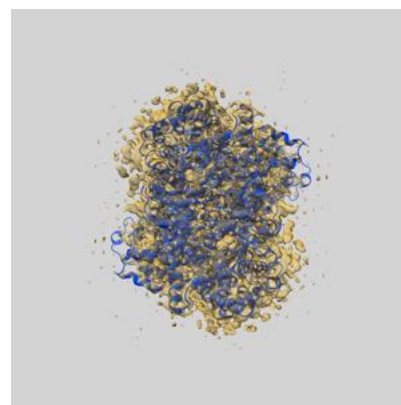
9.1 Map-model overlay [i](#)



X



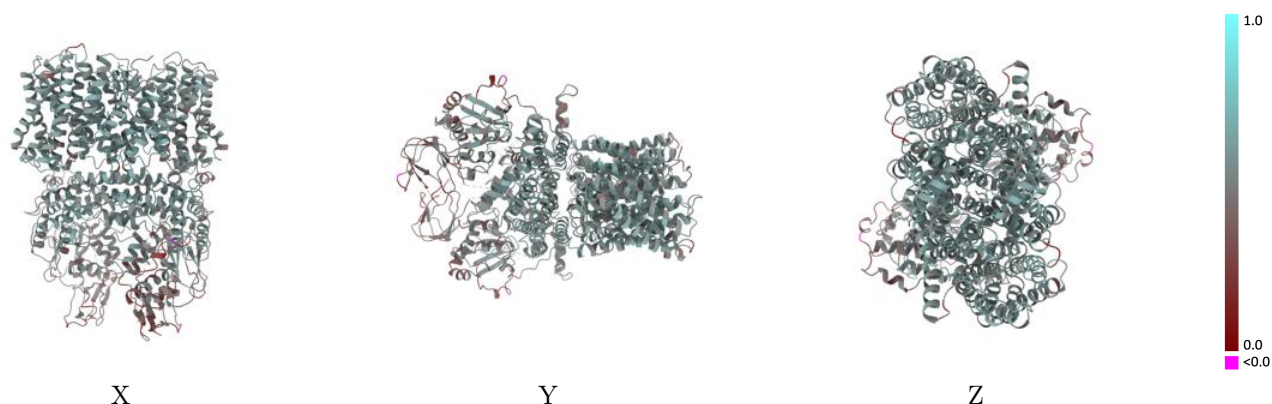
Y



Z

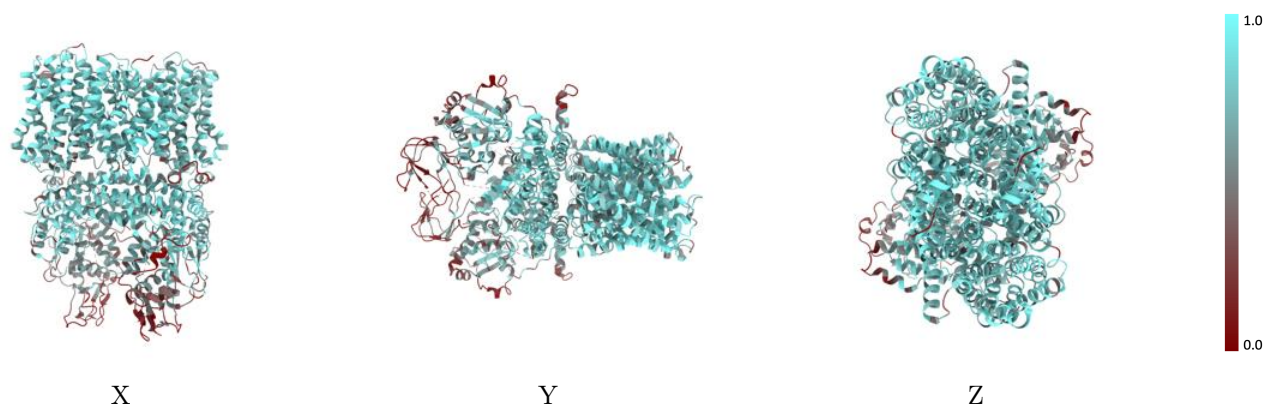
The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



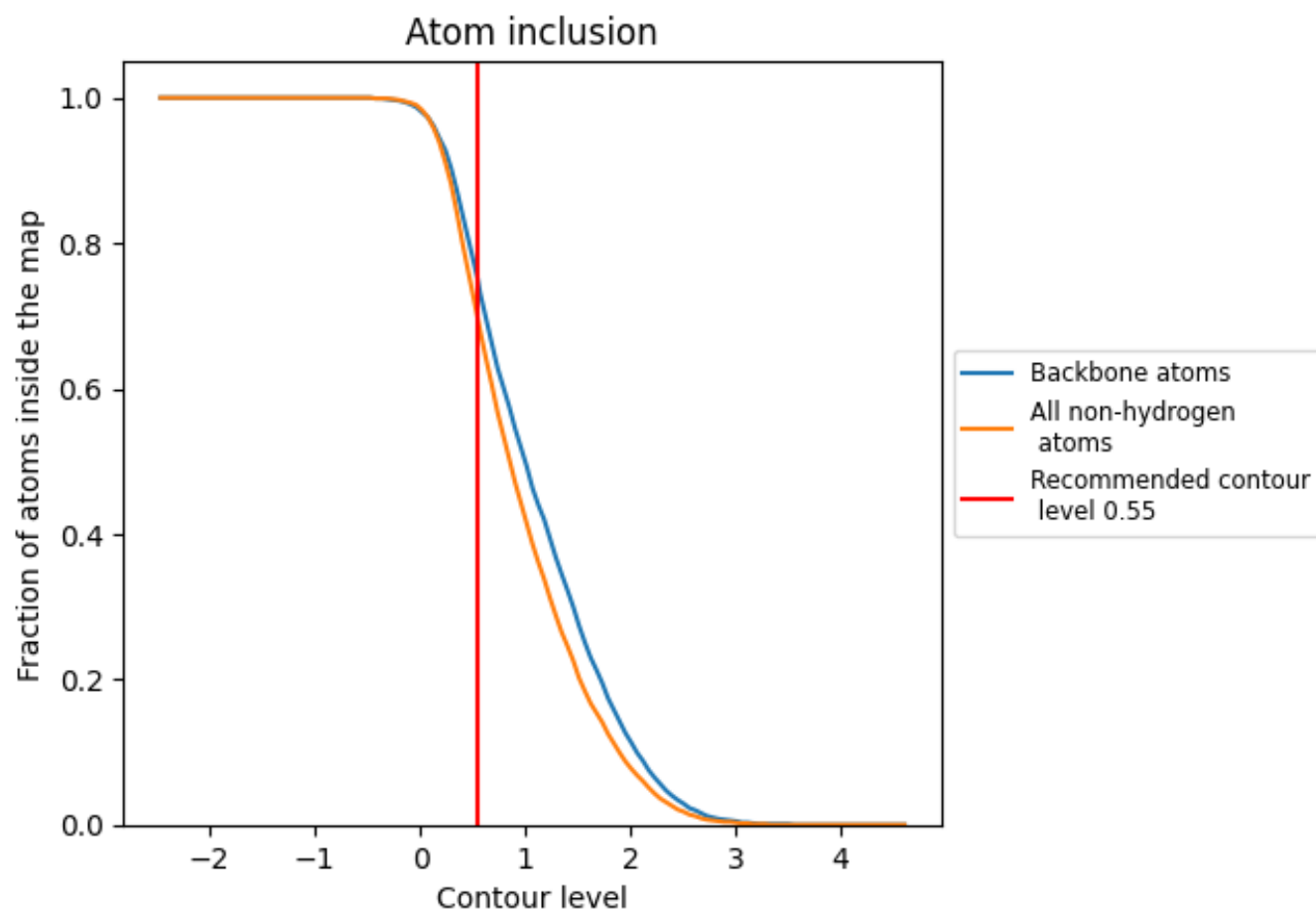
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.55).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 70% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.5140
A	0.6970	0.5130
B	0.6960	0.5150

