



Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 07:13 am BST

PDB ID : 9I0G / pdb_00009i0g
EMDB ID : EMD-52557
Title : CryoEM structure of holo-GmNifEN
Authors : Paya Tormo, L.; Nguyen, T.Q.; Fyfe, C.; Basbous, H.; Dobrzynska, K.; Echavarri-Erasun, C.; Martin, L.; Caserta, G.; Legrand, P.; Thorn, A.; Amara, P.; Schoehn, G.; Cherrier, M.V.; Rubio, L.M.; Nicolet, Y.
Deposited on : 2025-01-15
Resolution : 2.86 Å(reported)
Based on initial model : .

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 : 1.8.4, CSD as541be (2020)
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

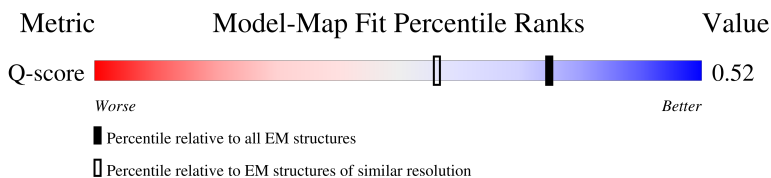
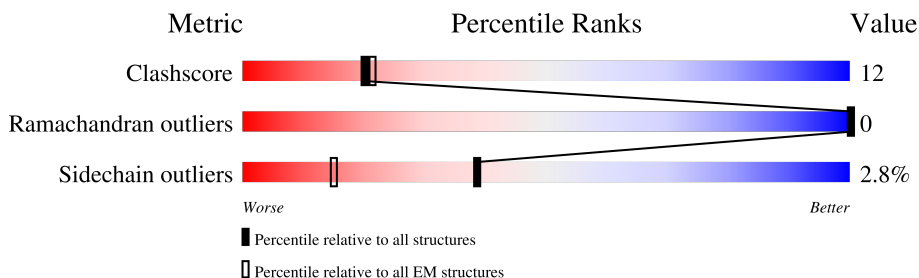
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.86 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	12017 (2.36 - 3.36)

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	919	
1	B	919	

2 Entry composition [i](#)

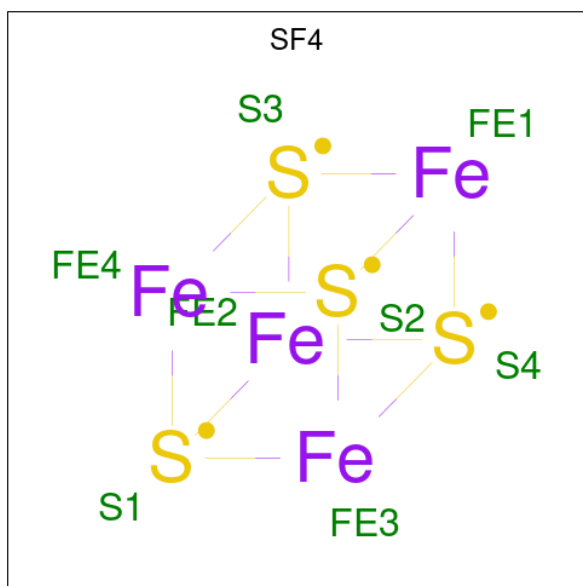
There are 3 unique types of molecules in this entry. The entry contains 13600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE.

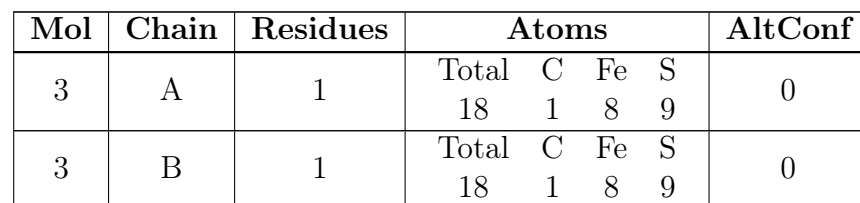
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	887	Total	C	N	O	S	0	0
			6774	4278	1179	1276	41		
1	B	887	Total	C	N	O	S	0	0
			6774	4278	1179	1276	41		

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	Fe	S	0
			8	4	4	
2	B	1	Total	Fe	S	0
			8	4	4	

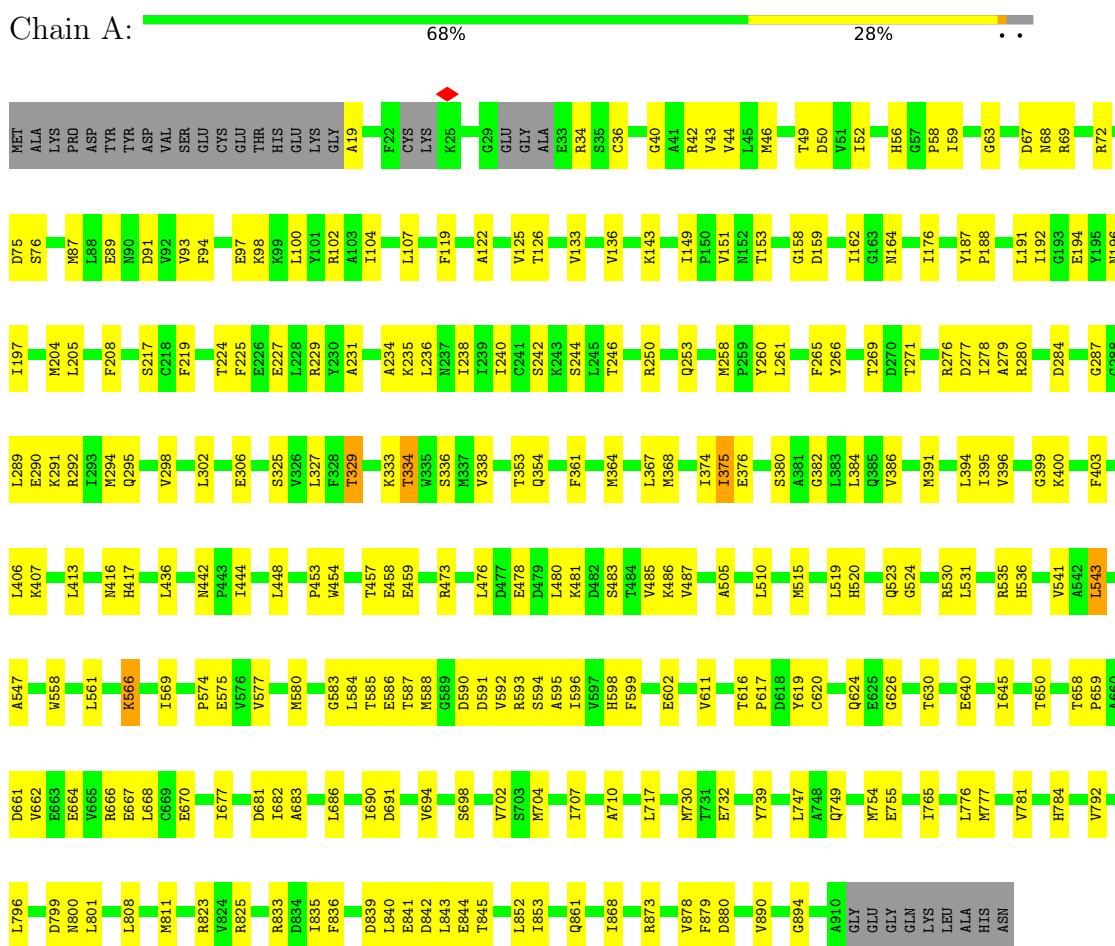
- Molecule 3 is FeFe cofactor (CCD ID: S5Q) (formula: CFe_8S_9).



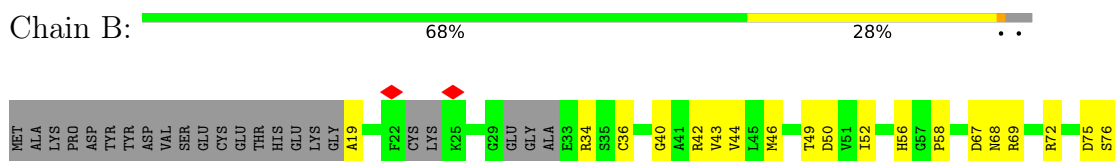
3 Residue-property plots

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: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



- Molecule 1: Nitrogenase iron-molybdenum cofactor biosynthesis protein NifE



L796	E667	K566	H417	I283	M204	M87
D799	L668	I569	L436	M294	L86	L88
N800	C669			Q295	E89	
L801	E670			V298	N90	
	I677	P574	N442	L302	D91	
L808		E575	P443	E306	V92	
	D681	W576	I444		V93	
R823	I682	V577	L448		F94	
W824	A683	G583	K451	R324	E97	
R825		L584		S325	K98	
R833	L686	T585	A452	E226	K99	
D834		E586	P453	E227	L100	
I835	D691	T587	W454	L228		
F836	E692	M588	K455	R229	I104	
	T693	G589	K456	T329	Y230	
	V694	D590	T457	A231	L107	
	S698	D591	E458			
		V592	E459	A234	F119	
V702	S594	R593		K235		
S703	A595	A596	R473	L236	A122	
M704	I596	E602	L476	N237		
	V597	H598	D477	I238	V125	
I707	F599	R600	E478	I239	T126	
A710	Q601	E602	D479	G241	A127	
L717			L480	S242	M128	
	M730	T731	K481	K243	V133	
	E732	E732	D482	S244		
	M736	M736	S483	L245	V136	
	Y739	Y739	T484	T246		
L747	L747	L747	V485	I374	K143	
A748	A748	A748	K486	I375		
Q749	Q749	Q749	V487	E376	I149	
	M754	E755	A505	S380	P150	
E755	T756	L757	L510	A381	V151	
	L757		M515	G382	M152	
	I765	I765	H520	L383	T153	
	M754	E755	H520	Q385	P154	
	T756	L757	H520	V386	I157	
	I765	I765	H520		G158	
	M754	E755	H520		D159	
	T756	L757	H520			
	I765	I765	H520		I162	
	M754	E755	H520		G163	
	T756	L757	H520		M164	
	I765	I765	H520		I176	
	M754	E755	H520		Y187	
	T756	L757	H520		P188	
	I765	I765	H520			
	M754	E755	H520		I192	
	T756	L757	H520		G193	
	I765	I765	H520		E194	
	M754	E755	H520		Y195	
	T756	L757	H520		M196	
	I765	I765	H520		I197	
	M754	E755	H520			
	T756	L757	H520			
	I765	I765	H520			
	M754	E755	H520			
	T756	L757	H520			
	I765	I765	H520			
	M754	E755	H520			
	T756	L757	H520			
	I765	I765	H520			
	M754	E755	H520			
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	I765	I765	H520			
	M754	E755	H520			
	T756	L757	H520			
	I765	I765	H520			
	M754	E755	H520			
	T756	L757	H520			
	I765	I765	H520			
	M7					

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	178282	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	21.309	Depositor
Minimum map value	-0.746	Depositor
Average map value	-0.011	Depositor
Map value standard deviation	0.634	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	280.44, 280.44, 280.44	wwPDB
Map dimensions	246, 246, 246	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	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: SF4, S5Q

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	0.16	0/6900	0.37	0/9341
1	B	0.16	0/6900	0.37	0/9341
All	All	0.16	0/13800	0.37	0/18682

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 [i](#)

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	6774	0	6788	176	0
1	B	6774	0	6788	176	0
2	A	8	0	0	1	0
2	B	8	0	0	1	0
3	A	18	0	0	1	0
3	B	18	0	0	1	0
All	All	13600	0	13576	335	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 12.

All (335) 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:406:LEU:HD12	1:A:781:VAL:HB	1.65	0.77
1:B:406:LEU:HD12	1:B:781:VAL:HB	1.65	0.77
1:A:459:GLU:N	1:A:459:GLU:OE1	2.23	0.71
1:B:459:GLU:OE1	1:B:459:GLU:N	2.23	0.71
1:A:396:VAL:HG12	1:A:413:LEU:HB3	1.73	0.71
1:B:396:VAL:HG12	1:B:413:LEU:HB3	1.73	0.71
1:A:473:ARG:HA	1:A:473:ARG:HH11	1.58	0.69
1:B:458:GLU:N	1:B:458:GLU:OE1	2.27	0.68
1:B:577:VAL:HB	1:B:611:VAL:HG12	1.76	0.68
1:A:34:ARG:HB3	1:A:159:ASP:HB2	1.76	0.67
1:B:473:ARG:HH11	1:B:473:ARG:HA	1.58	0.67
1:A:458:GLU:OE1	1:A:458:GLU:N	2.27	0.67
1:A:481:LYS:HE2	1:A:481:LYS:N	2.10	0.66
1:A:577:VAL:HB	1:A:611:VAL:HG12	1.76	0.65
1:B:481:LYS:N	1:B:481:LYS:HE2	2.10	0.65
1:B:34:ARG:HB3	1:B:159:ASP:HB2	1.76	0.65
1:A:662:VAL:HB	1:A:683:ALA:HB2	1.79	0.63
1:B:662:VAL:HB	1:B:683:ALA:HB2	1.79	0.63
1:B:97:GLU:OE1	1:B:97:GLU:N	2.18	0.62
1:B:72:ARG:O	1:B:196:ASN:ND2	2.33	0.62
1:A:158:GLY:HA3	1:A:162:ILE:HG13	1.82	0.61
1:A:97:GLU:OE1	1:A:97:GLU:N	2.18	0.61
1:A:72:ARG:O	1:A:196:ASN:ND2	2.33	0.61
1:B:391:MET:HE3	1:B:391:MET:HA	1.82	0.61
1:B:194:GLU:HB2	1:B:240:ILE:HD12	1.83	0.60
1:A:391:MET:HE3	1:A:391:MET:HA	1.82	0.60
1:B:158:GLY:HA3	1:B:162:ILE:HG13	1.82	0.60
1:B:302:LEU:O	1:B:306:GLU:HB2	2.01	0.60
1:A:302:LEU:O	1:A:306:GLU:HB2	2.01	0.60
1:A:197:ILE:HD13	1:A:417:HIS:HA	1.84	0.59
1:B:505:ALA:HB2	1:B:616:THR:HG21	1.85	0.59
1:B:197:ILE:HD13	1:B:417:HIS:HA	1.84	0.59
1:A:194:GLU:HB2	1:A:240:ILE:HD12	1.83	0.59
1:A:505:ALA:HB2	1:A:616:THR:HG21	1.85	0.58
1:B:523:GLN:HB2	1:B:547:ALA:HA	1.86	0.58
1:B:234:ALA:HB3	1:B:258:MET:HE1	1.86	0.58
1:B:290:GLU:O	1:B:291:LYS:HG2	2.05	0.57
1:A:234:ALA:HB3	1:A:258:MET:HE1	1.86	0.57
1:A:523:GLN:HB2	1:A:547:ALA:HA	1.86	0.57
1:A:276:ARG:O	1:A:280:ARG:HG3	2.05	0.57
1:A:478:GLU:O	1:A:825:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:LEU:HD13	1:B:800:ASN:HD22	1.70	0.57
1:A:91:ASP:OD1	1:A:91:ASP:N	2.37	0.57
1:A:290:GLU:O	1:A:291:LYS:HG2	2.05	0.57
1:A:796:LEU:HD13	1:A:800:ASN:HD22	1.70	0.57
1:A:873:ARG:NH1	1:A:880:ASP:OD2	2.37	0.57
1:B:873:ARG:NH1	1:B:880:ASP:OD2	2.37	0.57
1:A:593:ARG:HB3	1:A:593:ARG:CZ	2.35	0.56
1:A:67:ASP:OD2	1:B:861:GLN:NE2	2.38	0.56
1:A:448:LEU:HD22	1:A:777:MET:HG2	1.88	0.56
1:B:478:GLU:O	1:B:825:ARG:NH1	2.37	0.56
1:B:276:ARG:O	1:B:280:ARG:HG3	2.05	0.56
1:A:640:GLU:N	1:A:640:GLU:OE1	2.38	0.56
1:A:861:GLN:NE2	1:B:67:ASP:OD2	2.38	0.56
1:B:593:ARG:HB3	1:B:593:ARG:CZ	2.35	0.56
1:A:530:ARG:HH11	1:B:400:LYS:HD2	1.71	0.56
1:B:487:VAL:HG23	1:B:823:ARG:HH21	1.71	0.56
1:B:640:GLU:N	1:B:640:GLU:OE1	2.38	0.56
1:B:34:ARG:NE	1:B:354:GLN:HE22	2.04	0.56
1:B:284:ASP:OD1	1:B:284:ASP:C	2.50	0.55
1:B:717:LEU:HD23	1:B:739:TYR:HB2	1.89	0.55
1:A:34:ARG:NE	1:A:354:GLN:HE22	2.04	0.55
1:B:334:THR:HG21	1:B:353:THR:HG21	1.89	0.55
1:A:284:ASP:C	1:A:284:ASP:OD1	2.50	0.55
1:A:400:LYS:HD2	1:B:530:ARG:HH11	1.71	0.55
1:B:19:ALA:N	1:B:376:GLU:OE1	2.40	0.55
1:B:448:LEU:HD22	1:B:777:MET:HG2	1.88	0.55
1:B:510:LEU:HD11	1:B:541:VAL:HG13	1.90	0.55
1:A:19:ALA:N	1:A:376:GLU:OE1	2.40	0.54
1:A:487:VAL:HG23	1:A:823:ARG:HH21	1.71	0.54
1:B:836:PHE:HE2	1:B:842:ASP:HB3	1.72	0.54
1:A:836:PHE:HE2	1:A:842:ASP:HB3	1.72	0.54
1:B:266:TYR:HB2	1:B:336:SER:HB2	1.89	0.54
1:A:510:LEU:HD11	1:A:541:VAL:HG13	1.90	0.54
1:B:43:VAL:O	1:B:69:ARG:NH2	2.38	0.54
1:A:266:TYR:HB2	1:A:336:SER:HB2	1.89	0.54
1:A:334:THR:HG21	1:A:353:THR:HG21	1.89	0.54
1:B:626:GLY:O	1:B:630:THR:HG22	2.08	0.53
1:A:717:LEU:HD23	1:A:739:TYR:HB2	1.89	0.53
1:A:279:ALA:HB2	1:A:298:VAL:HG21	1.90	0.53
1:A:400:LYS:HD2	1:B:530:ARG:NH1	2.24	0.53
1:B:839:ASP:N	1:B:839:ASP:OD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:GLY:O	1:A:630:THR:HG22	2.08	0.53
1:B:853:ILE:HD11	1:B:868:ILE:HD12	1.90	0.53
1:A:242:SER:O	1:A:246:THR:OG1	2.24	0.53
1:B:279:ALA:HB2	1:B:298:VAL:HG21	1.90	0.53
1:A:853:ILE:HD11	1:A:868:ILE:HD12	1.90	0.53
1:A:505:ALA:HA	1:A:630:THR:HG21	1.91	0.53
1:B:591:ASP:OD2	1:B:594:SER:N	2.37	0.52
1:A:457:THR:HG1	1:A:459:GLU:CD	2.17	0.52
1:A:588:MET:HE1	1:A:590:ASP:HB3	1.90	0.52
1:B:224:THR:HB	1:B:227:GLU:HB3	1.91	0.52
1:B:505:ALA:HA	1:B:630:THR:HG21	1.91	0.52
1:A:43:VAL:O	1:A:69:ARG:NH2	2.38	0.52
1:A:530:ARG:NH1	1:B:400:LYS:HD2	2.24	0.52
1:B:242:SER:O	1:B:246:THR:OG1	2.24	0.52
1:B:575:GLU:N	1:B:575:GLU:OE1	2.42	0.52
1:A:375:ILE:HD13	1:A:386:VAL:HG11	1.92	0.52
1:A:575:GLU:OE1	1:A:575:GLU:N	2.42	0.52
1:B:375:ILE:HD13	1:B:386:VAL:HG11	1.92	0.52
1:A:125:VAL:HG13	1:B:587:THR:HG21	1.90	0.52
1:B:91:ASP:N	1:B:91:ASP:OD1	2.37	0.52
1:A:399:GLY:H	1:A:416:ASN:HD22	1.58	0.52
1:A:587:THR:HG21	1:B:125:VAL:HG13	1.90	0.52
1:B:217:SER:HA	1:B:227:GLU:OE1	2.10	0.52
1:B:583:GLY:O	1:B:587:THR:HG23	2.10	0.52
1:A:217:SER:HA	1:A:227:GLU:OE1	2.10	0.51
1:B:586:GLU:HG3	1:B:617:PRO:HB3	1.91	0.51
1:A:224:THR:HB	1:A:227:GLU:HB3	1.91	0.51
1:A:586:GLU:HG3	1:A:617:PRO:HB3	1.91	0.51
1:A:453:PRO:HB3	1:A:755:GLU:OE2	2.10	0.51
1:A:583:GLY:O	1:A:587:THR:HG23	2.10	0.51
1:B:485:VAL:O	1:B:823:ARG:NH2	2.42	0.51
1:B:588:MET:HE1	1:B:590:ASP:HB3	1.90	0.51
1:B:561:LEU:HD21	1:B:592:VAL:HG13	1.93	0.51
1:A:485:VAL:O	1:A:823:ARG:NH2	2.42	0.51
1:B:399:GLY:H	1:B:416:ASN:HD22	1.58	0.50
1:A:192:ILE:HA	1:A:219:PHE:HB2	1.94	0.50
1:A:840:LEU:O	1:A:843:LEU:HB3	2.12	0.50
1:B:840:LEU:O	1:B:843:LEU:HB3	2.12	0.50
1:A:176:ILE:HD12	1:A:231:ALA:HB3	1.94	0.50
1:A:617:PRO:HG2	1:A:620:CYS:HB2	1.94	0.50
1:A:89:GLU:HG2	1:B:619:TYR:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:THR:OG1	1:A:661:ASP:OD2	2.27	0.50
1:B:842:ASP:HA	1:B:845:THR:HG22	1.93	0.50
1:A:561:LEU:HD21	1:A:592:VAL:HG13	1.93	0.49
1:B:453:PRO:HB3	1:B:755:GLU:OE2	2.10	0.49
1:B:833:ARG:HG3	1:B:833:ARG:HH11	1.77	0.49
1:B:617:PRO:HG2	1:B:620:CYS:HB2	1.94	0.49
1:A:842:ASP:HA	1:A:845:THR:HG22	1.93	0.49
1:B:192:ILE:HA	1:B:219:PHE:HB2	1.94	0.49
1:B:664:GLU:HA	1:B:667:GLU:HB2	1.95	0.49
1:B:87:MET:HA	1:B:87:MET:HE3	1.94	0.49
1:B:287:GLY:HA3	1:B:291:LYS:HZ3	1.78	0.49
1:B:176:ILE:HD12	1:B:231:ALA:HB3	1.94	0.49
1:B:792:VAL:HG22	1:B:852:LEU:HB3	1.95	0.49
1:A:681:ASP:HB2	1:A:702:VAL:HG13	1.95	0.48
1:A:329:THR:O	1:A:334:THR:OG1	2.32	0.48
1:B:480:LEU:O	1:B:483:SER:OG	2.31	0.48
1:A:515:MET:O	1:A:698:SER:OG	2.20	0.48
1:A:619:TYR:CD1	1:B:89:GLU:HG2	2.47	0.48
1:A:833:ARG:HG3	1:A:833:ARG:HH11	1.77	0.48
1:A:238:ILE:HD11	1:A:278:ILE:HG12	1.96	0.48
1:A:591:ASP:OD2	1:A:594:SER:N	2.37	0.48
1:B:403:PHE:O	1:B:407:LYS:HG2	2.14	0.48
1:A:677:ILE:HG21	1:A:710:ALA:HB2	1.96	0.48
1:A:792:VAL:HG22	1:A:852:LEU:HB3	1.95	0.47
1:A:87:MET:HE3	1:A:87:MET:HA	1.94	0.47
1:A:100:LEU:O	1:A:104:ILE:HG12	2.14	0.47
1:B:187:TYR:CE2	1:B:294:MET:HE3	2.49	0.47
1:B:265:PHE:HA	1:B:271:THR:HG22	1.96	0.47
1:A:187:TYR:CE2	1:A:294:MET:HE3	2.49	0.47
1:A:664:GLU:HA	1:A:667:GLU:HB2	1.95	0.47
1:A:682:ILE:HD12	1:A:686:LEU:HD12	1.96	0.47
1:B:238:ILE:HD11	1:B:278:ILE:HG12	1.96	0.47
1:A:747:LEU:HD13	1:A:776:LEU:HD23	1.96	0.47
1:B:681:ASP:HB2	1:B:702:VAL:HG13	1.95	0.47
1:A:265:PHE:HA	1:A:271:THR:HG22	1.96	0.47
1:A:403:PHE:O	1:A:407:LYS:HG2	2.14	0.47
1:A:799:ASP:C	1:A:801:LEU:H	2.22	0.47
1:B:566:LYS:HG2	1:B:599:PHE:HE1	1.80	0.47
1:B:658:THR:OG1	1:B:661:ASP:OD2	2.28	0.47
1:B:451:LYS:NZ	1:B:455:GLU:OE1	2.46	0.47
1:A:566:LYS:HG2	1:A:599:PHE:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:677:ILE:HG21	1:B:710:ALA:HB2	1.96	0.47
1:A:292:ARG:NH1	1:A:295:GLN:HB2	2.30	0.46
1:B:280:ARG:HH11	1:B:280:ARG:HG2	1.80	0.46
1:B:747:LEU:HD13	1:B:776:LEU:HD23	1.96	0.46
1:A:280:ARG:HG2	1:A:295:GLN:HE22	1.81	0.46
1:B:122:ALA:HB2	1:B:133:VAL:HG21	1.97	0.46
1:B:329:THR:O	1:B:334:THR:OG1	2.32	0.46
1:A:98:LYS:HB3	1:A:98:LYS:HZ1	1.80	0.46
1:B:100:LEU:O	1:B:104:ILE:HG12	2.14	0.46
1:B:250:ARG:HG2	1:B:250:ARG:HH11	1.81	0.46
1:B:799:ASP:C	1:B:801:LEU:H	2.22	0.46
1:A:40:GLY:O	1:A:43:VAL:HG12	2.16	0.46
1:A:280:ARG:HG2	1:A:280:ARG:HH11	1.80	0.46
1:B:287:GLY:HA3	1:B:291:LYS:NZ	2.30	0.46
1:B:736:MET:HE2	1:B:736:MET:HB3	1.79	0.46
1:A:588:MET:HE2	1:A:588:MET:C	2.40	0.46
1:B:143:LYS:NZ	1:B:143:LYS:HB3	2.31	0.46
1:A:250:ARG:HH11	1:A:250:ARG:HG2	1.81	0.46
1:A:289:LEU:O	1:A:292:ARG:HG2	2.16	0.46
1:A:585:THR:HA	1:A:588:MET:SD	2.56	0.46
1:B:289:LEU:O	1:B:292:ARG:HG2	2.16	0.46
1:B:682:ILE:HD12	1:B:686:LEU:HD12	1.96	0.46
1:A:100:LEU:HD23	1:A:136:VAL:HG11	1.98	0.46
1:B:49:THR:OG1	1:B:50:ASP:N	2.49	0.46
1:B:128:MET:HE2	1:B:128:MET:HB2	1.84	0.46
1:A:382:GLY:O	1:A:386:VAL:HG12	2.16	0.46
1:B:382:GLY:O	1:B:386:VAL:HG12	2.16	0.46
1:A:49:THR:OG1	1:A:50:ASP:N	2.49	0.45
1:A:287:GLY:HA3	1:A:291:LYS:NZ	2.30	0.45
1:B:280:ARG:HG2	1:B:295:GLN:HE22	1.81	0.45
1:B:588:MET:C	1:B:588:MET:HE2	2.40	0.45
1:B:650:THR:HG21	1:B:730:MET:HE1	1.98	0.45
1:B:585:THR:HA	1:B:588:MET:SD	2.56	0.45
1:A:841:GLU:HA	1:A:844:GLU:OE2	2.16	0.45
1:B:292:ARG:NH1	1:B:295:GLN:HB2	2.30	0.45
1:A:143:LYS:HB3	1:A:143:LYS:NZ	2.31	0.45
1:A:543:LEU:HD13	1:A:543:LEU:O	2.17	0.45
1:A:569:ILE:HA	1:A:574:PRO:HD2	1.98	0.45
1:B:361:PHE:CZ	1:B:374:ILE:HG21	2.52	0.45
1:B:841:GLU:HA	1:B:844:GLU:OE2	2.16	0.45
1:A:98:LYS:HB3	1:A:98:LYS:NZ	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:HB2	1:A:133:VAL:HG21	1.97	0.45
1:A:624:GLN:OE1	1:A:799:ASP:N	2.50	0.45
1:B:98:LYS:NZ	1:B:98:LYS:HB3	2.32	0.45
1:B:624:GLN:OE1	1:B:799:ASP:N	2.50	0.45
1:A:666:ARG:O	1:A:670:GLU:HG3	2.17	0.45
1:A:668:LEU:HD13	1:A:754:MET:HE1	1.98	0.45
1:B:93:VAL:HG23	1:B:94:PHE:CD1	2.52	0.45
1:B:100:LEU:HD23	1:B:136:VAL:HG11	1.98	0.45
1:A:93:VAL:HG23	1:A:94:PHE:CD1	2.52	0.45
1:B:600:ARG:HD3	1:B:600:ARG:HA	1.70	0.45
1:B:668:LEU:HD13	1:B:754:MET:HE1	1.98	0.45
1:A:361:PHE:CZ	1:A:374:ILE:HG21	2.52	0.45
1:B:543:LEU:HD13	1:B:543:LEU:O	2.17	0.45
1:B:520:HIS:O	1:B:585:THR:HG21	2.17	0.44
1:B:536:HIS:CD2	1:B:878:VAL:H	2.36	0.44
1:B:569:ILE:HA	1:B:574:PRO:HD2	1.98	0.44
1:B:749:GLN:N	1:B:749:GLN:OE1	2.50	0.44
1:A:42:ARG:HB2	1:A:46:MET:HE3	2.00	0.44
1:A:44:VAL:HG21	1:A:164:ASN:HA	1.99	0.44
1:A:704:MET:HA	1:A:707:ILE:HG22	1.99	0.44
1:B:40:GLY:O	1:B:43:VAL:HG12	2.16	0.44
1:B:50:ASP:N	1:B:50:ASP:OD1	2.46	0.44
1:B:333:LYS:HE2	3:B:1002:S5Q:S2B	2.57	0.44
1:B:792:VAL:HG11	1:B:808:LEU:HD13	1.99	0.44
1:A:650:THR:HG21	1:A:730:MET:HE1	1.98	0.44
1:B:42:ARG:HB2	1:B:46:MET:HE3	2.00	0.44
1:A:56:HIS:ND1	1:A:126:THR:OG1	2.37	0.44
1:A:59:ILE:O	1:A:63:GLY:N	2.40	0.44
1:A:333:LYS:HE2	3:A:1002:S5Q:S2B	2.57	0.44
1:B:666:ARG:O	1:B:670:GLU:HG3	2.17	0.44
1:B:704:MET:HA	1:B:707:ILE:HG22	1.99	0.44
1:A:596:ILE:HD12	1:A:611:VAL:HG21	2.00	0.44
1:A:50:ASP:N	1:A:50:ASP:OD1	2.46	0.44
1:A:520:HIS:O	1:A:585:THR:HG21	2.17	0.44
1:A:749:GLN:OE1	1:A:749:GLN:N	2.50	0.44
1:A:792:VAL:HG11	1:A:808:LEU:HD13	1.99	0.44
1:A:536:HIS:CD2	1:A:878:VAL:H	2.36	0.44
1:A:659:PRO:HG3	1:A:682:ILE:HG22	2.00	0.44
1:B:486:LYS:HD2	1:B:487:VAL:O	2.18	0.44
1:B:598:HIS:O	1:B:602:GLU:HG2	2.17	0.44
1:B:659:PRO:HG3	1:B:682:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:ILE:HD12	1:B:611:VAL:HG21	2.00	0.44
1:A:598:HIS:O	1:A:602:GLU:HG2	2.17	0.43
1:B:36:CYS:HB3	2:B:1001:SF4:S2	2.58	0.43
1:B:44:VAL:HG21	1:B:164:ASN:HA	1.99	0.43
1:A:58:PRO:HG2	1:A:125:VAL:HG21	2.01	0.43
1:A:486:LYS:HD2	1:A:487:VAL:O	2.18	0.43
1:B:487:VAL:CG2	1:B:823:ARG:HH21	2.31	0.43
1:B:58:PRO:HG2	1:B:125:VAL:HG21	2.01	0.43
1:B:204:MET:HB2	1:B:204:MET:HE2	1.76	0.43
1:A:46:MET:HE3	1:A:46:MET:HB2	1.87	0.43
1:A:68:ASN:ND2	1:B:531:LEU:HD21	2.34	0.43
1:A:839:ASP:OD1	1:A:839:ASP:N	2.39	0.43
1:A:98:LYS:HZ3	1:A:102:ARG:HH12	1.66	0.43
1:A:204:MET:HB2	1:A:204:MET:HE2	1.76	0.43
1:A:664:GLU:O	1:A:668:LEU:HG	2.18	0.43
1:B:457:THR:HG1	1:B:459:GLU:CD	2.27	0.43
1:A:52:ILE:HG21	1:A:107:LEU:HD13	2.01	0.43
1:A:294:MET:HE2	1:A:294:MET:HA	2.01	0.43
1:A:327:LEU:HD21	1:A:338:VAL:HG22	2.01	0.43
1:B:176:ILE:HD11	1:B:219:PHE:CZ	2.53	0.43
1:A:487:VAL:CG2	1:A:823:ARG:HH21	2.31	0.43
1:A:36:CYS:HB3	2:A:1001:SF4:S2	2.58	0.42
1:A:754:MET:HB3	1:A:765:ILE:HD13	2.01	0.42
1:B:515:MET:O	1:B:698:SER:OG	2.20	0.42
1:A:524:GLY:HA3	1:B:36:CYS:HB3	2.01	0.42
1:B:119:PHE:CE2	1:B:149:ILE:HD12	2.55	0.42
1:A:176:ILE:HD11	1:A:219:PHE:CZ	2.53	0.42
1:A:531:LEU:HD21	1:B:68:ASN:ND2	2.34	0.42
1:B:52:ILE:HG21	1:B:107:LEU:HD13	2.01	0.42
1:B:327:LEU:HD21	1:B:338:VAL:HG22	2.01	0.42
1:A:535:ARG:HG3	1:A:879:PHE:HB3	2.01	0.42
1:B:485:VAL:HG23	1:B:835:ILE:O	2.20	0.42
1:B:905:LEU:HD23	1:B:905:LEU:HA	1.87	0.42
1:B:225:PHE:HE2	1:B:229:ARG:HH11	1.67	0.42
1:B:664:GLU:O	1:B:668:LEU:HG	2.18	0.42
1:A:225:PHE:HE2	1:A:229:ARG:HH11	1.67	0.42
1:A:485:VAL:HG23	1:A:835:ILE:O	2.20	0.42
1:B:253:GLN:HA	1:B:258:MET:H	1.84	0.42
1:B:413:LEU:HD22	1:B:436:LEU:HD13	2.02	0.42
1:A:119:PHE:CE2	1:A:149:ILE:HD12	2.55	0.42
1:A:253:GLN:HA	1:A:258:MET:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:ARG:HG3	1:B:879:PHE:HB3	2.01	0.42
1:B:56:HIS:ND1	1:B:126:THR:OG1	2.37	0.41
1:B:294:MET:HE2	1:B:294:MET:HA	2.01	0.41
1:B:754:MET:HB3	1:B:765:ILE:HD13	2.01	0.41
1:A:364:MET:O	1:A:368:MET:N	2.50	0.41
1:A:413:LEU:HD22	1:A:436:LEU:HD13	2.02	0.41
1:B:264:SER:OG	1:B:270:ASP:OD2	2.35	0.41
1:B:324:ARG:H	1:B:324:ARG:HG2	1.64	0.41
1:A:36:CYS:HB3	1:B:524:GLY:HA3	2.01	0.41
1:A:325:SER:HA	1:A:394:LEU:O	2.21	0.41
1:A:188:PRO:HD2	1:A:235:LYS:HG3	2.02	0.41
1:A:384:LEU:HD11	1:B:694:VAL:HB	2.03	0.41
1:A:811:MET:HE2	1:A:811:MET:HB3	1.71	0.41
1:A:151:VAL:HG12	1:A:153:THR:HG23	2.02	0.41
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.93	0.41
1:A:442:ASN:ND2	1:A:784:HIS:HB2	2.36	0.41
1:A:558:TRP:HB2	1:A:595:ALA:HB2	2.03	0.41
1:A:566:LYS:HE2	1:A:566:LYS:HB3	1.91	0.41
1:A:890:VAL:N	1:A:894:GLY:HA3	2.36	0.41
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.89	0.41
1:B:454:TRP:CZ2	1:B:773:ARG:HD3	2.56	0.41
1:A:280:ARG:HG2	1:A:295:GLN:NE2	2.35	0.41
1:B:75:ASP:CG	1:B:76:SER:H	2.28	0.41
1:B:154:PRO:HD2	1:B:157:ILE:HD13	2.03	0.41
1:B:280:ARG:HG2	1:B:295:GLN:NE2	2.35	0.41
1:B:442:ASN:ND2	1:B:784:HIS:HB2	2.36	0.41
1:B:575:GLU:O	1:B:610:PRO:HD2	2.22	0.40
1:B:890:VAL:N	1:B:894:GLY:HA3	2.36	0.40
1:A:34:ARG:HG3	1:A:354:GLN:NE2	2.37	0.40
1:A:260:TYR:CD1	1:A:260:TYR:C	2.99	0.40
1:B:151:VAL:HG12	1:B:153:THR:HG23	2.02	0.40
1:B:188:PRO:HD2	1:B:235:LYS:HG3	2.02	0.40
1:A:176:ILE:HD11	1:A:219:PHE:HZ	1.86	0.40
1:A:191:LEU:HD13	1:A:191:LEU:HA	1.99	0.40
1:A:584:LEU:H	1:A:584:LEU:HD23	1.86	0.40
1:A:666:ARG:HH22	1:A:681:ASP:CG	2.30	0.40
1:B:325:SER:HA	1:B:394:LEU:O	2.21	0.40
1:B:692:GLU:OE1	1:B:693:THR:N	2.55	0.40
1:B:757:LEU:HD23	1:B:757:LEU:HA	1.90	0.40
1:A:75:ASP:CG	1:A:76:SER:H	2.28	0.40
1:A:596:ILE:HD13	1:A:596:ILE:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ILE:HD12	1:B:777:MET:HB3	2.03	0.40
1:A:694:VAL:HB	1:B:384:LEU:HD11	2.03	0.40
1:A:480:LEU:O	1:A:483:SER:OG	2.31	0.40
1:A:519:LEU:HB2	1:A:580:MET:HE3	2.04	0.40
1:B:480:LEU:HB2	1:B:481:LYS:HE2	2.04	0.40
1:B:584:LEU:HD23	1:B:584:LEU:H	1.86	0.40
1:B:666:ARG:HH22	1:B:681:ASP:CG	2.30	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	881/919 (96%)	844 (96%)	37 (4%)	0	100	100
1	B	881/919 (96%)	844 (96%)	37 (4%)	0	100	100
All	All	1762/1838 (96%)	1688 (96%)	74 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	707/732 (97%)	687 (97%)	20 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	707/732 (97%)	687 (97%)	20 (3%)	38 62
All	All	1414/1464 (97%)	1374 (97%)	40 (3%)	38 62

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LEU
1	A	208	PHE
1	A	236	LEU
1	A	244	SER
1	A	269	THR
1	A	277	ASP
1	A	329	THR
1	A	334	THR
1	A	367	LEU
1	A	375	ILE
1	A	380	SER
1	A	395	ILE
1	A	444	ILE
1	A	454	TRP
1	A	476	LEU
1	A	543	LEU
1	A	566	LYS
1	A	645	ILE
1	A	691	ASP
1	A	732	GLU
1	B	205	LEU
1	B	208	PHE
1	B	236	LEU
1	B	244	SER
1	B	269	THR
1	B	277	ASP
1	B	329	THR
1	B	334	THR
1	B	367	LEU
1	B	375	ILE
1	B	380	SER
1	B	395	ILE
1	B	444	ILE
1	B	454	TRP
1	B	476	LEU
1	B	543	LEU

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Mol	Chain	Res	Type
1	B	566	LYS
1	B	645	ILE
1	B	691	ASP
1	B	732	GLU

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	68	ASN
1	A	164	ASN
1	A	295	GLN
1	A	354	GLN
1	A	499	ASN
1	A	532	GLN
1	A	897	ASN
1	B	68	ASN
1	B	164	ASN
1	B	295	GLN
1	B	354	GLN
1	B	897	ASN
1	B	904	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
3	S5Q	A	1002	1	18,30,30	2.13	10 (55%)	-		
3	S5Q	B	1002	1	18,30,30	2.13	10 (55%)	-		
2	SF4	B	1001	1	0,12,12	-	-	-		
2	SF4	A	1001	1	0,12,12	-	-	-		

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	SF4	B	1001	1	-	-	0/6/5/5
2	SF4	A	1001	1	-	-	0/6/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	S5Q	S4A-FE4	-3.44	2.23	2.32
3	B	1002	S5Q	S4A-FE4	-3.44	2.23	2.32
3	A	1002	S5Q	S1B-FE5	-2.97	2.25	2.32
3	B	1002	S5Q	S1B-FE5	-2.97	2.25	2.32
3	A	1002	S5Q	S2A-FE3	-2.86	2.25	2.32
3	B	1002	S5Q	S2A-FE3	-2.86	2.25	2.32
3	A	1002	S5Q	S3A-FE4	-2.85	2.18	2.24
3	B	1002	S5Q	S3A-FE4	-2.85	2.18	2.24
3	A	1002	S5Q	S3B-FE6	-2.80	2.25	2.32
3	B	1002	S5Q	S3B-FE6	-2.80	2.25	2.32
3	A	1002	S5Q	S1A-FE2	-2.62	2.25	2.32
3	B	1002	S5Q	S1A-FE2	-2.62	2.25	2.32
3	A	1002	S5Q	S4A-FE3	-2.36	2.26	2.32
3	B	1002	S5Q	S4A-FE3	-2.36	2.26	2.32
3	A	1002	S5Q	S4B-FE5	-2.27	2.26	2.32
3	B	1002	S5Q	S4B-FE5	-2.27	2.26	2.32
3	A	1002	S5Q	S1B-FE6	-2.15	2.27	2.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	S5Q	S1B-FE6	-2.15	2.27	2.32
3	A	1002	S5Q	S3A-FE5	-2.05	2.20	2.24
3	B	1002	S5Q	S3A-FE5	-2.05	2.20	2.24

There are no bond angle outliers.

There are no chirality outliers.

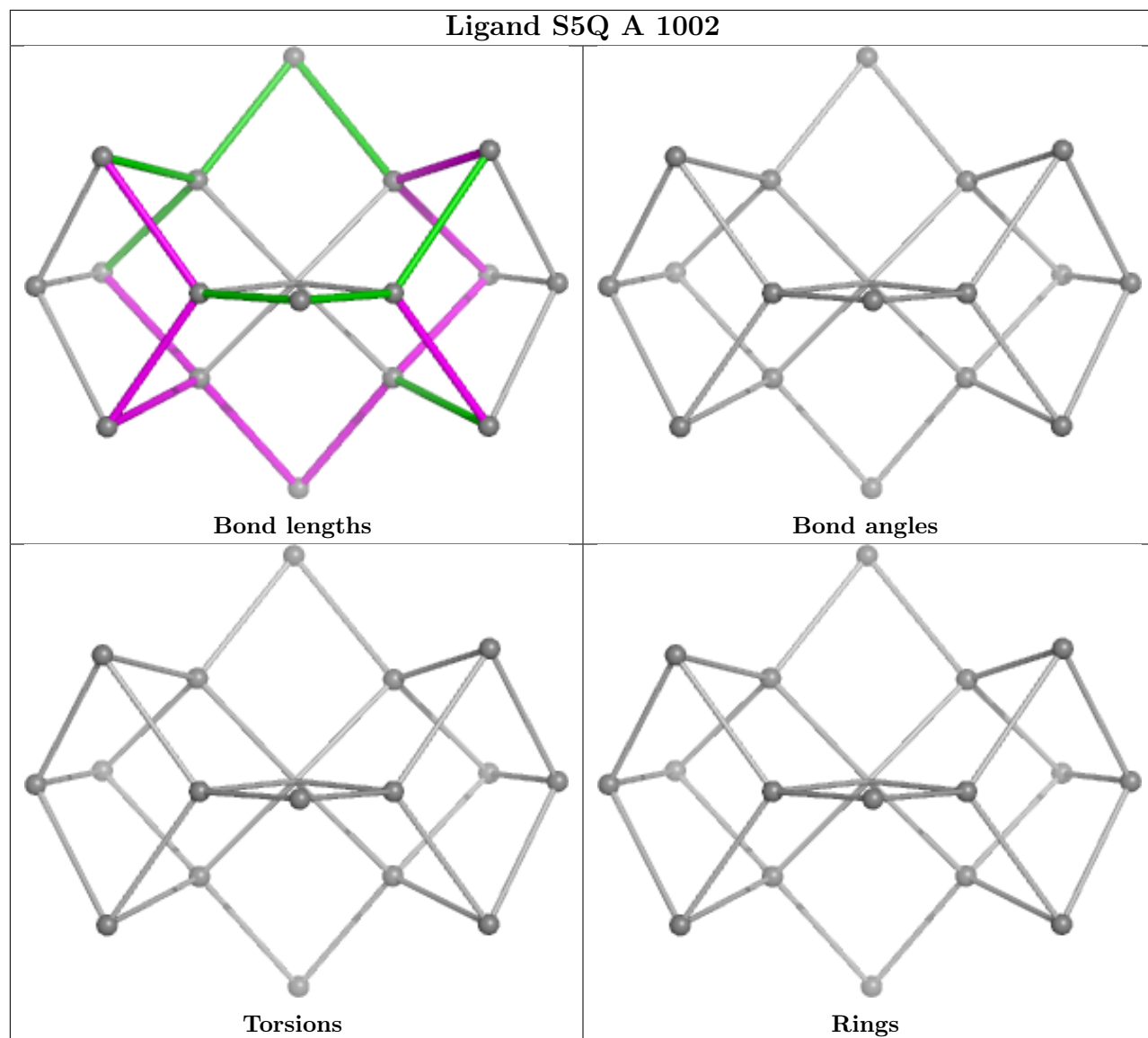
There are no torsion outliers.

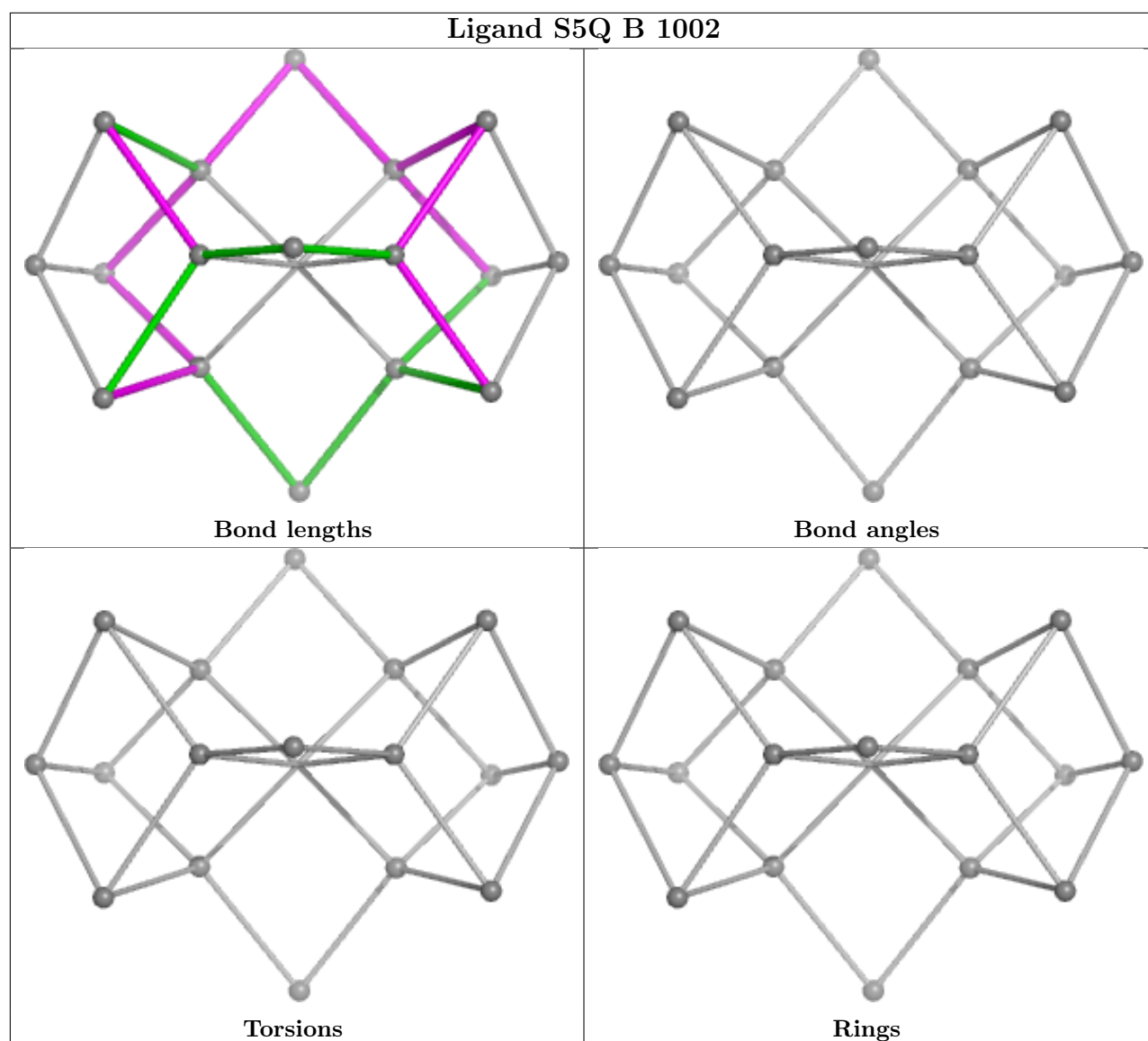
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	S5Q	1	0
3	B	1002	S5Q	1	0
2	B	1001	SF4	1	0
2	A	1001	SF4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

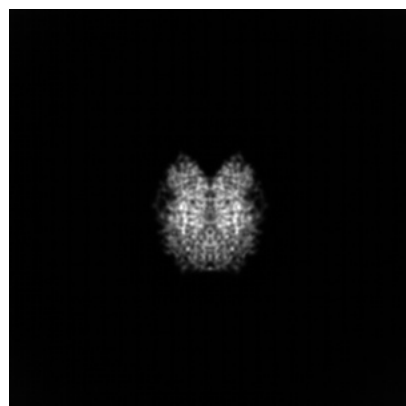
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52557. These allow visual inspection of the internal detail of the map and identification of artifacts.

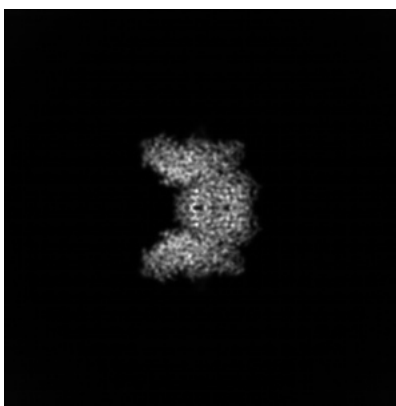
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

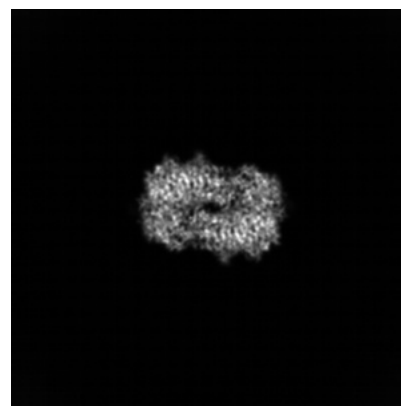
6.1.1 Primary map



X

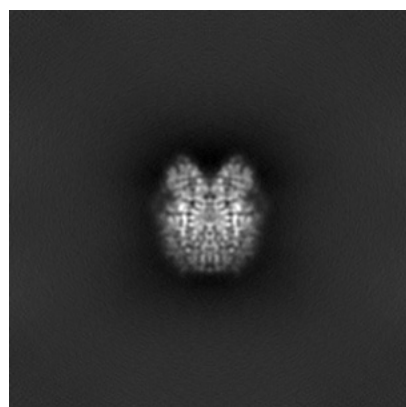


Y

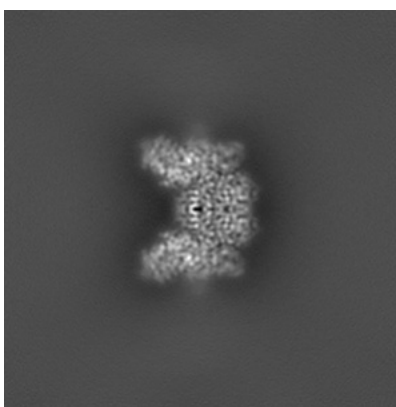


Z

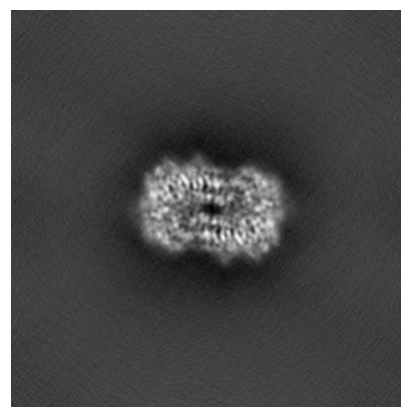
6.1.2 Raw map



X



Y

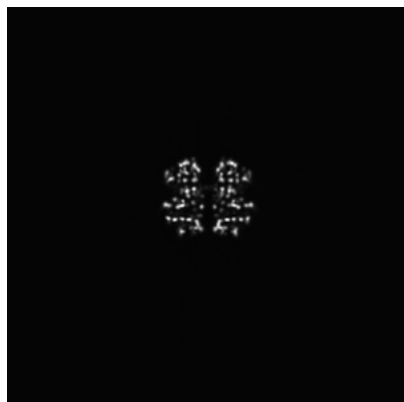


Z

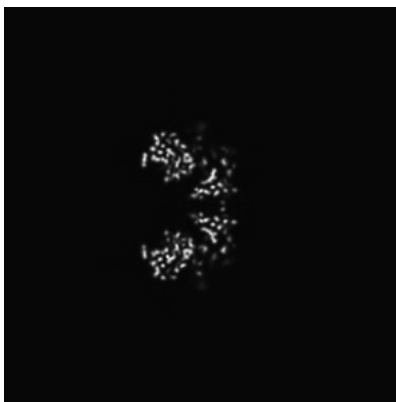
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

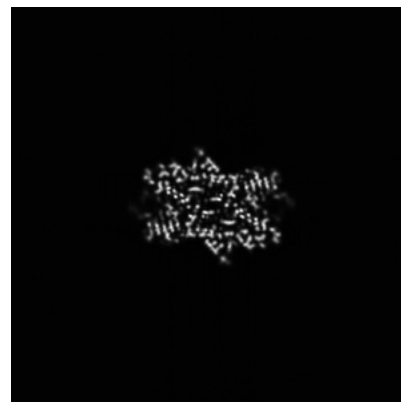
6.2.1 Primary map



X Index: 123

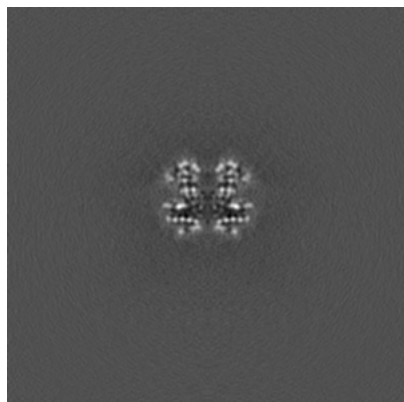


Y Index: 123

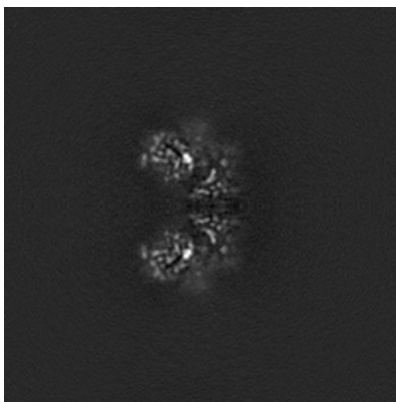


Z Index: 123

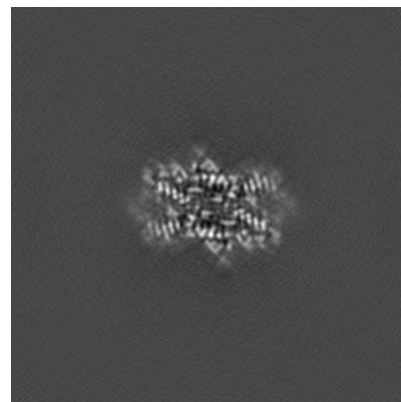
6.2.2 Raw map



X Index: 123



Y Index: 123

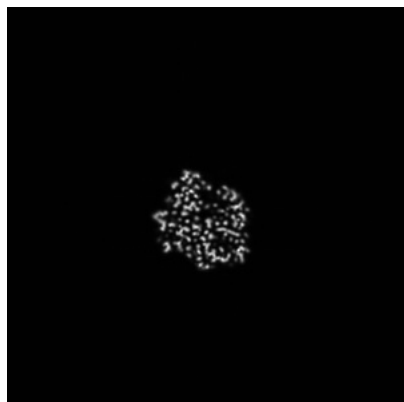


Z Index: 123

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

6.3 Largest variance slices [i](#)

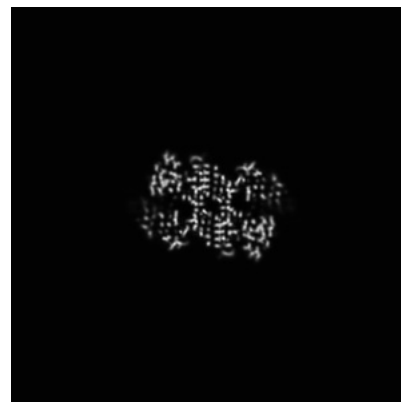
6.3.1 Primary map



X Index: 151

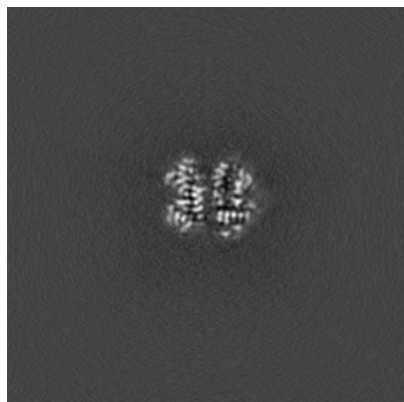


Y Index: 107

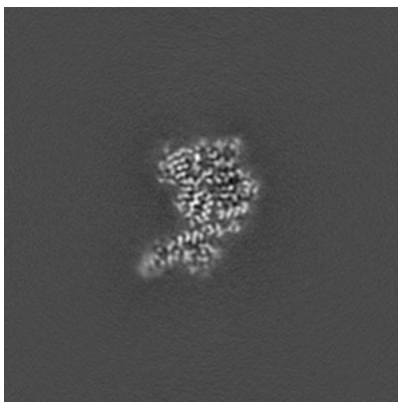


Z Index: 118

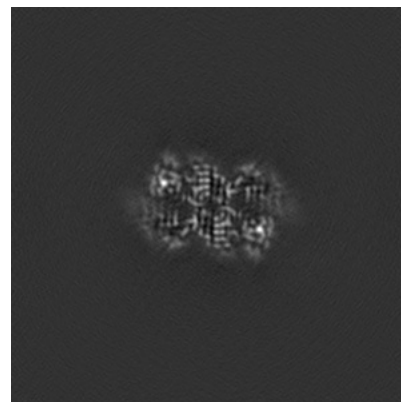
6.3.2 Raw map



X Index: 120



Y Index: 107

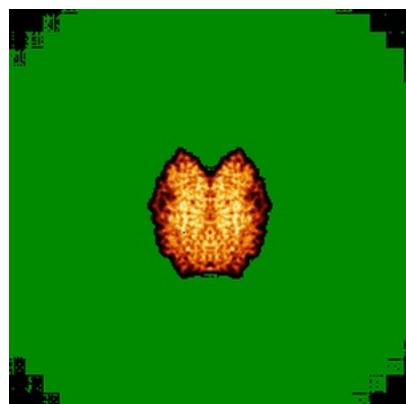


Z Index: 118

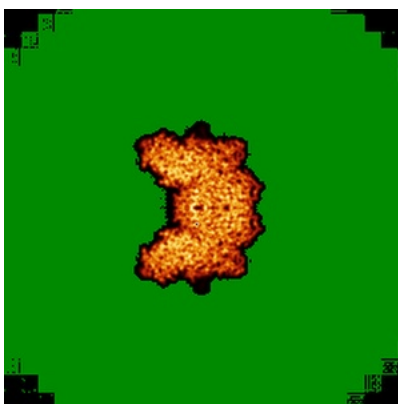
The images above show the largest variance slices of the map in three orthogonal directions.

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

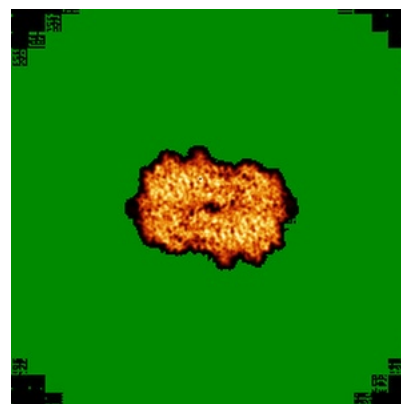
6.4.1 Primary map



X

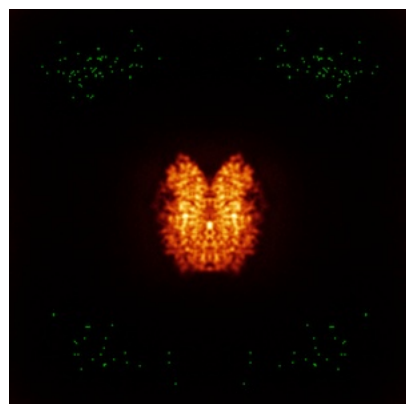


Y

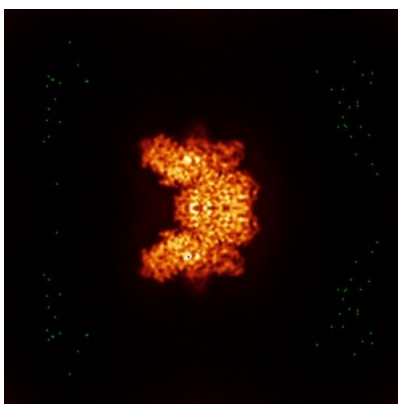


Z

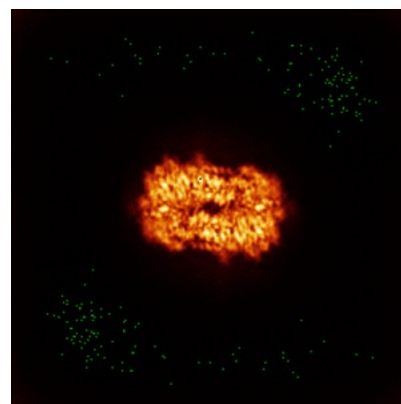
6.4.2 Raw map



X



Y

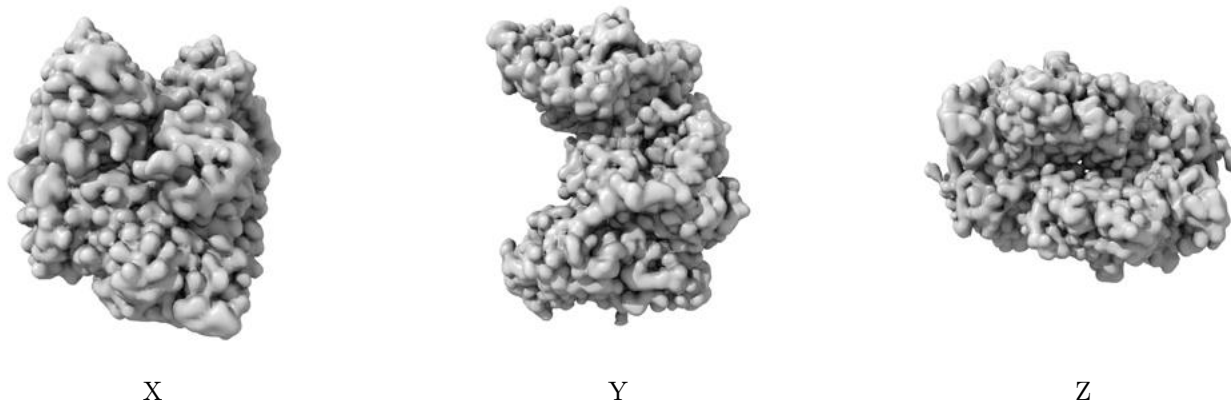


Z

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.

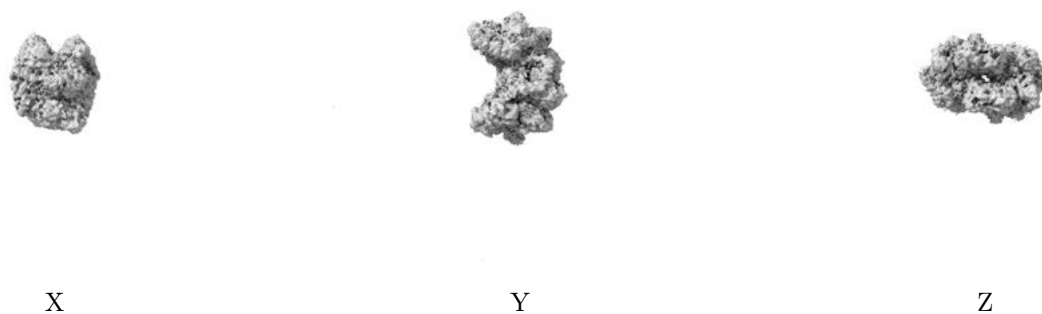
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.9. 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.

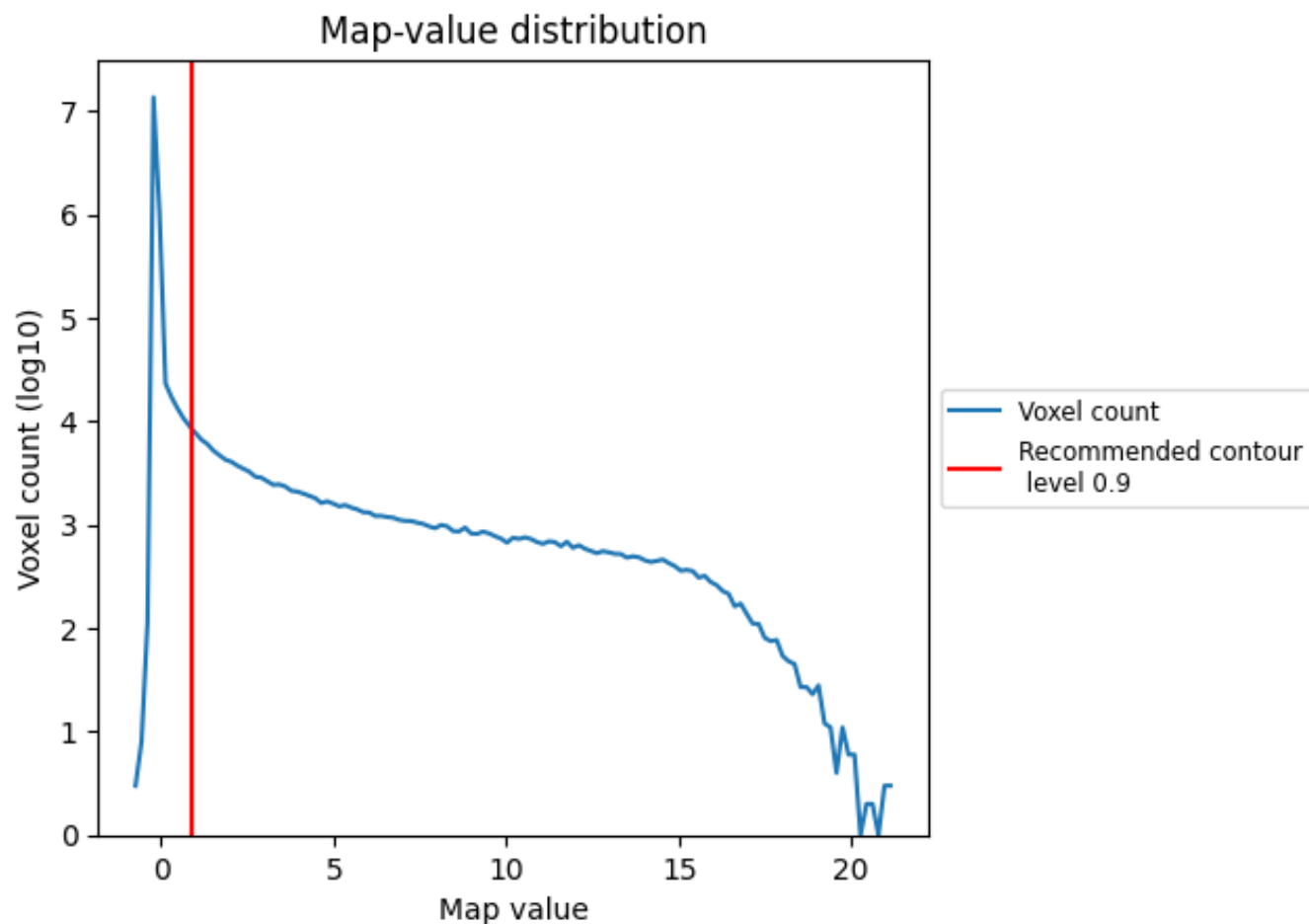
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

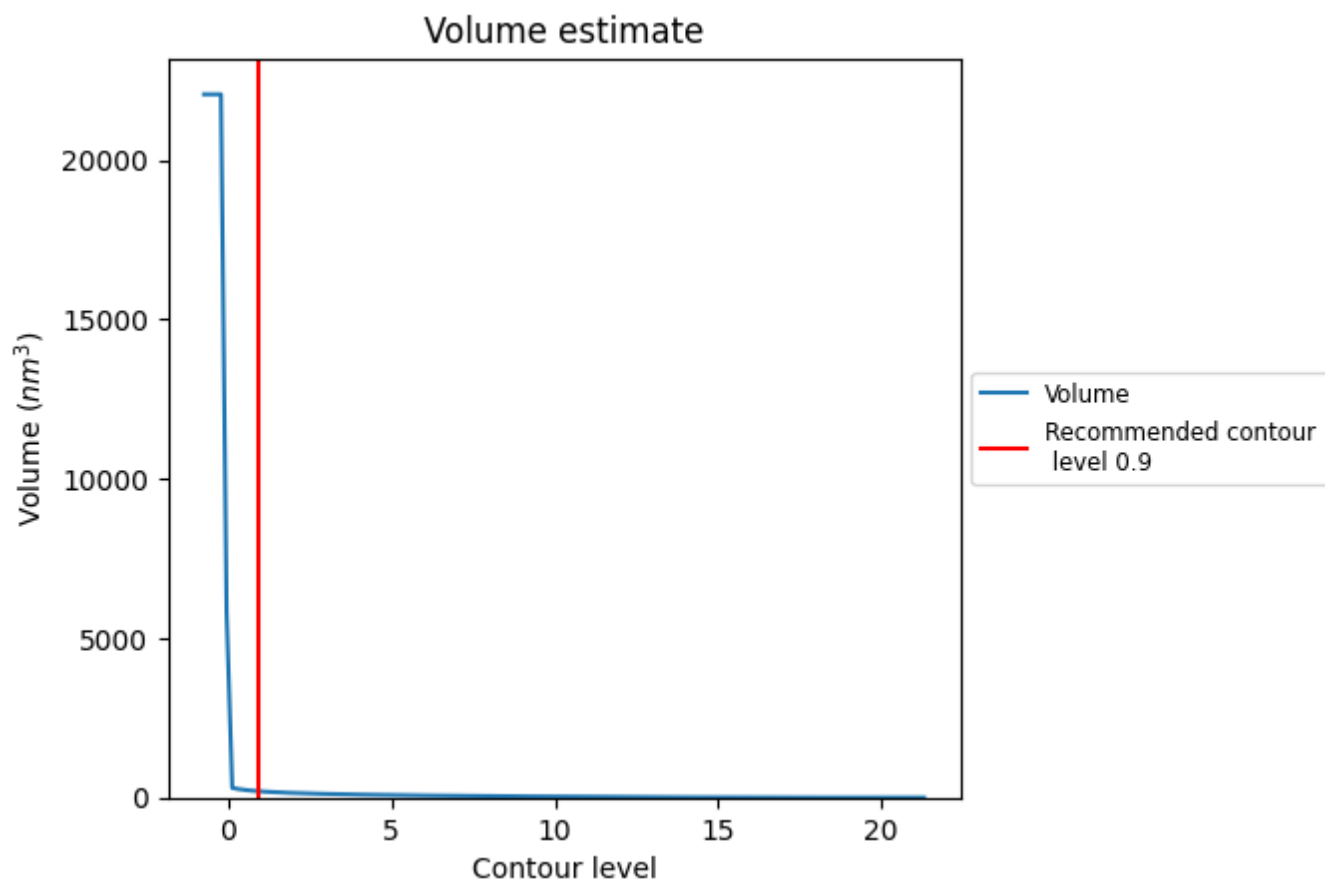
This section contains the results of statistical analysis of the map.

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.

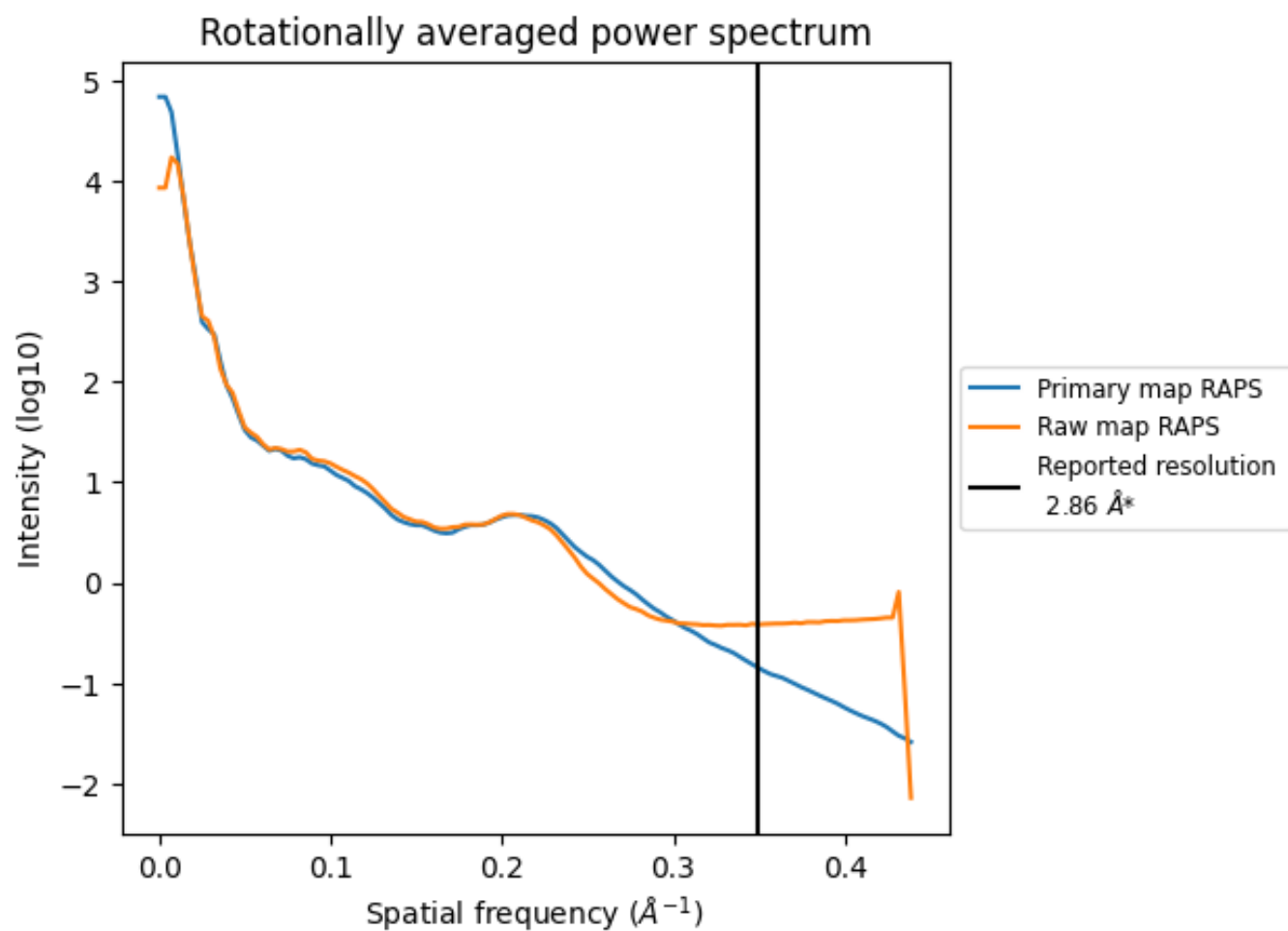
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 181 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 ⓘ

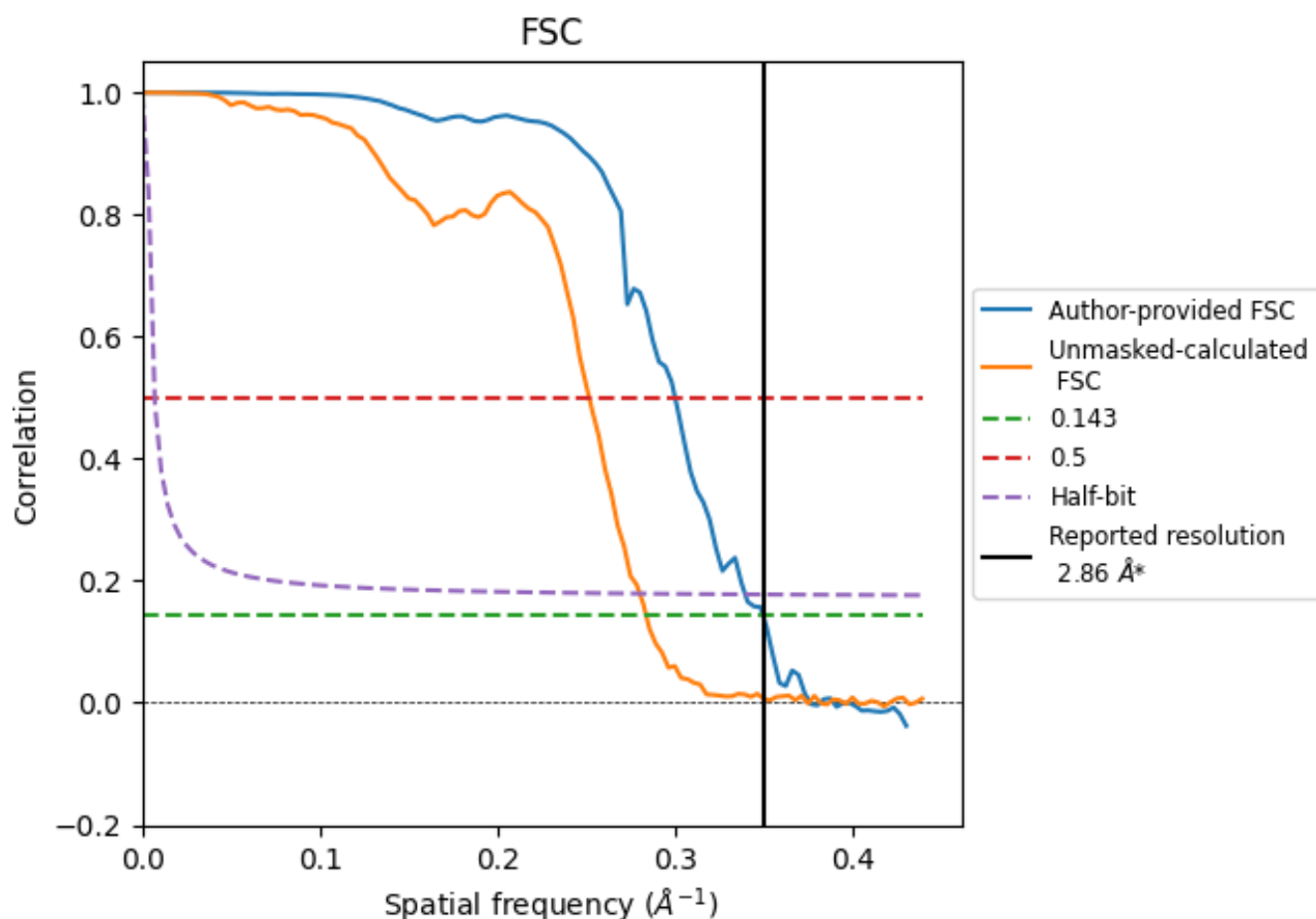


*Reported resolution corresponds to spatial frequency of 0.350 Å⁻¹

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 0.350 \AA^{-1}

8.2 Resolution estimates [i](#)

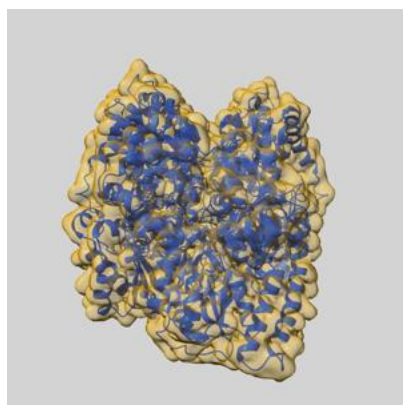
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.34	2.95
Unmasked-calculated*	3.53	3.98	3.57

*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 3.53 differs from the reported value 2.86 by more than 10 %

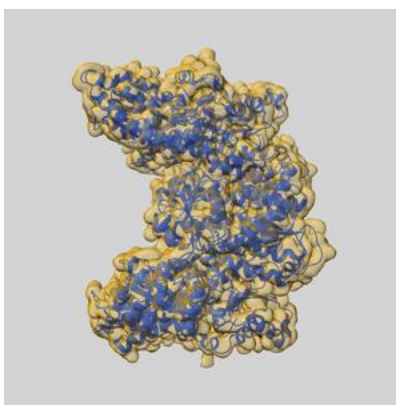
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-52557 and PDB model 9I0G. Per-residue inclusion information can be found in section 3 on page 5.

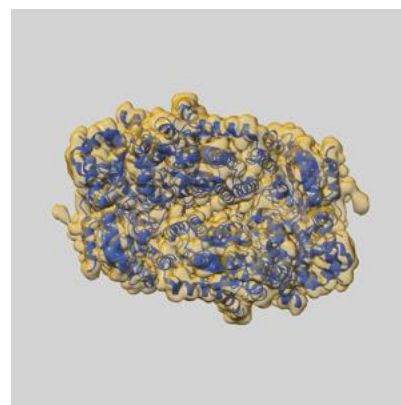
9.1 Map-model overlay [i](#)



X



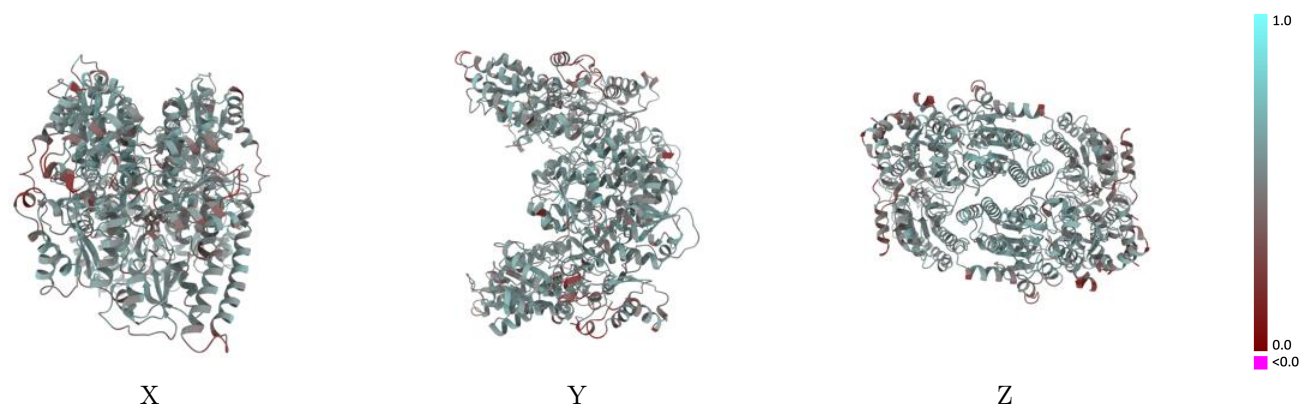
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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](#)



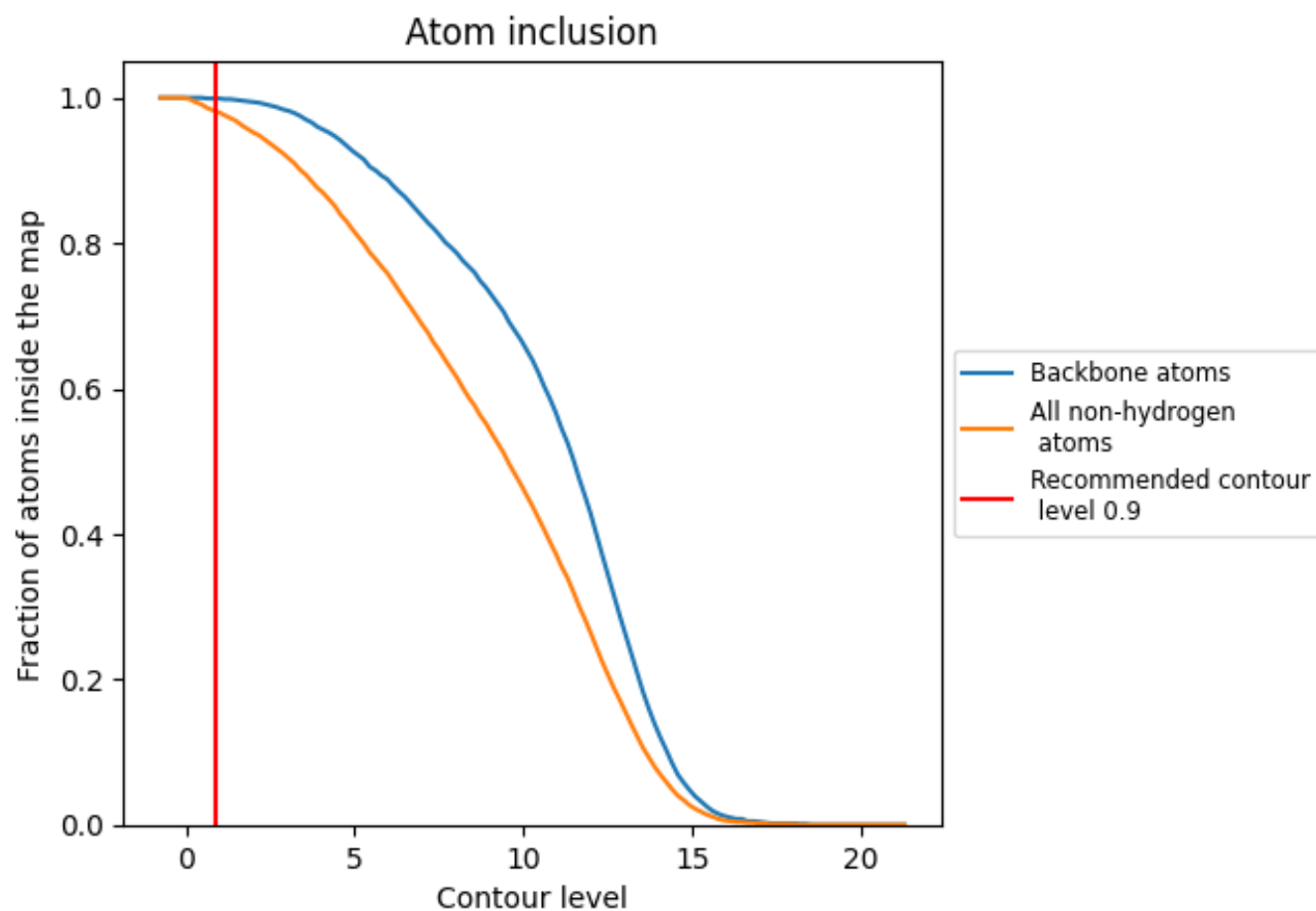
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.9).

9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 98% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9810	<div><div></div></div> 0.5200
A	<div><div></div></div> 0.9820	<div><div></div></div> 0.5240
B	<div><div></div></div> 0.9810	<div><div></div></div> 0.5160

