



Full wwPDB EM Validation Report ⓘ

Oct 30, 2025 – 06:43 pm GMT

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.dev129
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

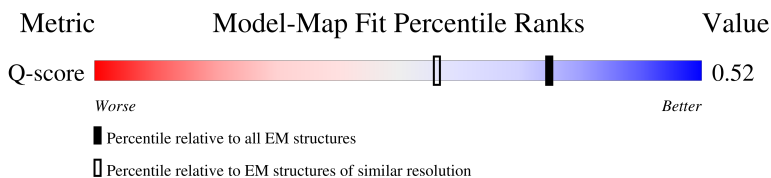
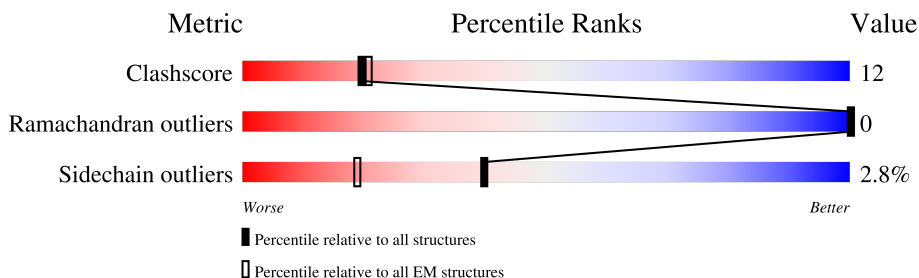
1 Overall quality at a glance

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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
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	 68% 28% ..
1	B	919	 68% 28% ..

2 Entry composition [i](#)

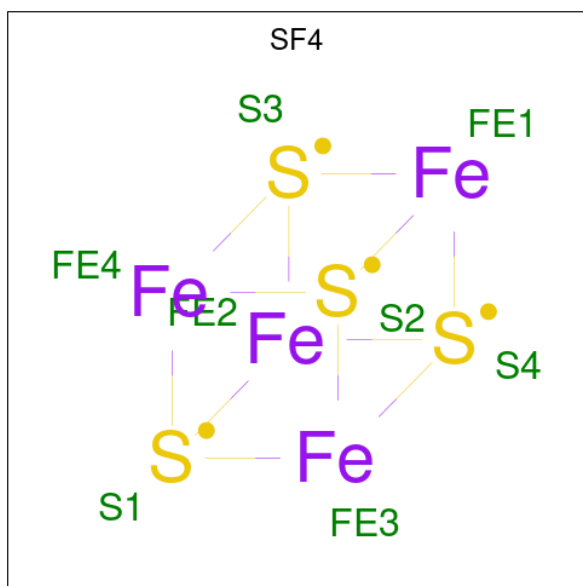
There are 3 unique types of molecules in this entry. The entry contains 13600 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

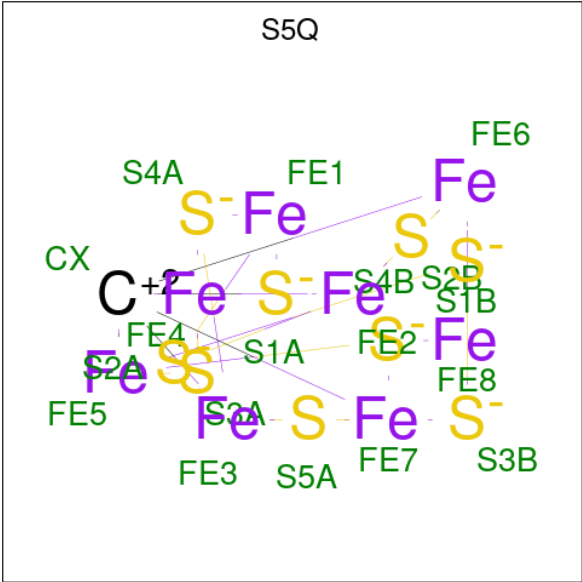
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	887	Total	C	N	O	S	0	0
			6774	4278	1179	1276	41		
1	B	887	Total	C	N	O	S	0	0
			6774	4278	1179	1276	41		

- 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).

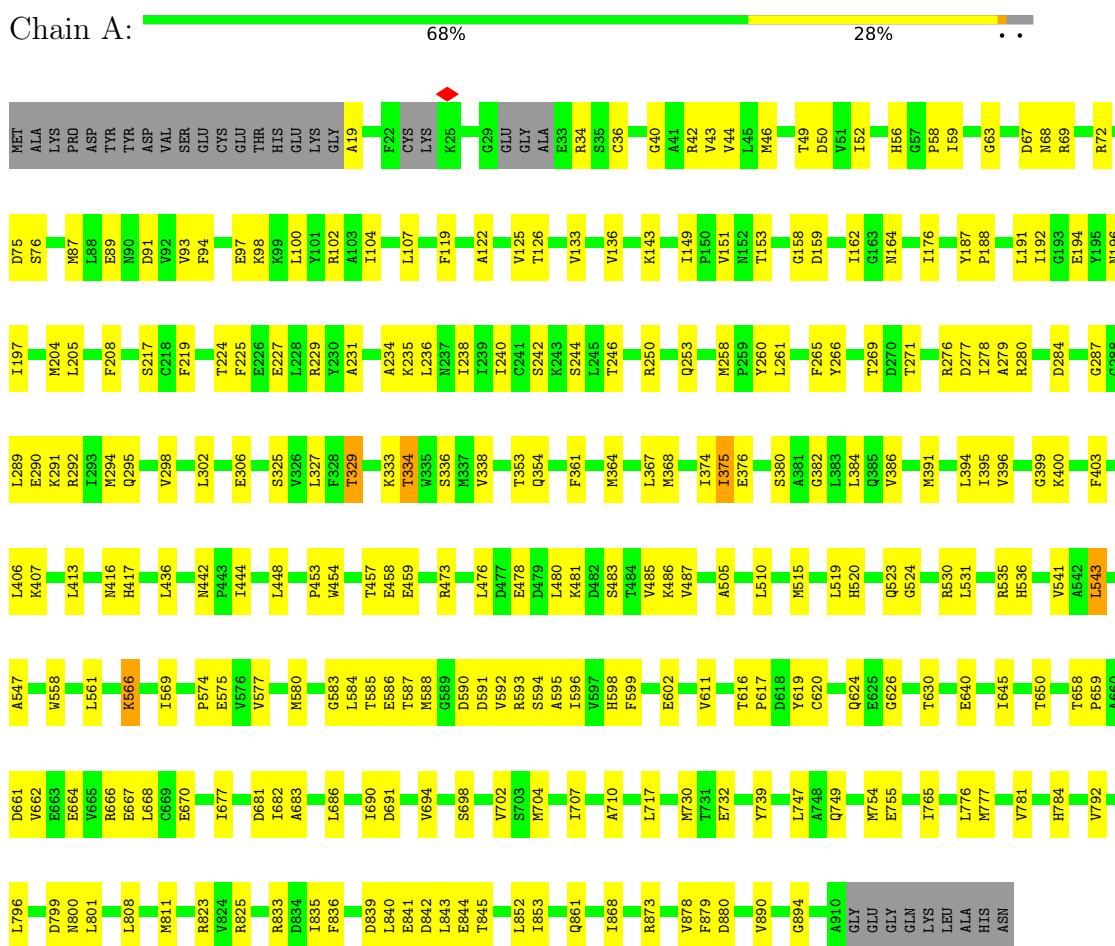


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	Fe	S	0
			18	1	8	9	
3	B	1	Total	C	Fe	S	0
			18	1	8	9	

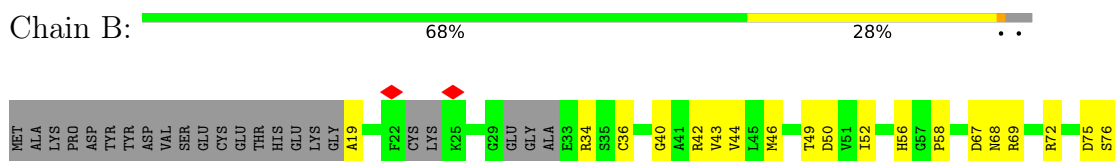
3 Residue-property plots

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	L86	M87	M204	M283	H417	K566	E667	L796
D799	L88	L88	L205	M294	L436	I569	L668	D799
N800	E89	E89	F208	Q295	N442	P574	C669	N800
L801	N90	N90	S217	V298	P443	E575	E670	L801
L808	D91	D91	C918	L302	I444	W576	I677	L808
R823	V92	V92	F219	E306	L448	V577	D681	R823
R825	K98	K98	T224	R324	K451	G583	I682	R825
R833	K99	K99	F225	S325	A452	L584	A683	R833
D834	L100	L100	E226	V326	P453	T585	V824	D834
I835	I104	I104	L228	L327	W454	E586	L686	I835
F836	Y230	Y230	R229	F328	K455	T587	D691	F836
D839	L107	L107	A231	T329	K456	G589	E692	D839
L840	F119	F119	A234	K333	T457	D590	T693	L840
E841	A122	A122	K235	T334	E458	V592	V694	E841
D842	L236	L236	L236	V335	E459	R593	S698	D842
L843	N237	N237	K243	S336	R473	S594	V702	L843
E844	S244	S244	S244	M337	L476	A595	S703	E844
T845	V125	V125	T246	V338	D477	I596	M704	T845
L852	T126	T126	G241	T353	E478	V597	I707	L852
I853	A127	A127	S242	Q354	D479	H598	A710	I853
Q861	V133	V133	K243	F361	L480	F599	L717	Q861
L868	V136	V136	S244	L367	K481	R600	L731	L868
R873	K143	K143	T246	I374	W484	E602	E732	R873
V878	I149	I149	R250	I375	V485	P610	M730	V878
F879	P150	P150	Q253	E376	K486	V611	T731	F879
D880	V151	V151	M258	S380	V487	T616	E732	D880
V890	M152	M152	S264	A381	A505	D618	M736	V890
G894	T153	T153	F265	G382	L510	Y619	Y739	G894
L905	P154	P154	Y266	L383	M515	Q624	L747	L905
A910	I157	I157	T269	Q385	H520	E625	A748	A910
GLY	G158	G158	D270	V386	G523	G626	Q749	GLY
GLU	D159	D159	T271	M391	G524	T630	M754	GLU
GLY	I162	I162	R276	L394	R530	E640	E755	GLY
GLN	N164	N164	D277	I395	L531	I645	L757	GLN
LYS	I176	I176	I278	V396	H535	T650	I765	LYS
LEU	Y187	Y187	A279	G399	H536	T658	R773	LEU
ALA	P188	P188	R280	K400	V541	P659	L776	ALA
HIS	I192	I192	D284	F403	A542	V661	M777	HIS
ASN	G193	G193	G287	L406	W543	D662	V781	ASN
	E194	E194	L289	K407	A547	V663	H784	
	Y195	Y195	K291	L413	L561	E664	V792	
	N196	N196	R292	N416		V665		
	I197	I197				R666		

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 (\AA)	280.44, 280.44, 280.44	wwPDB
Map dimensions	246, 246, 246	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	707/732 (97%)	687 (97%)	20 (3%)	38 64
All	All	1414/1464 (97%)	1374 (97%)	40 (3%)	40 64

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

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

Continued on next page...

Continued from previous page...

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.

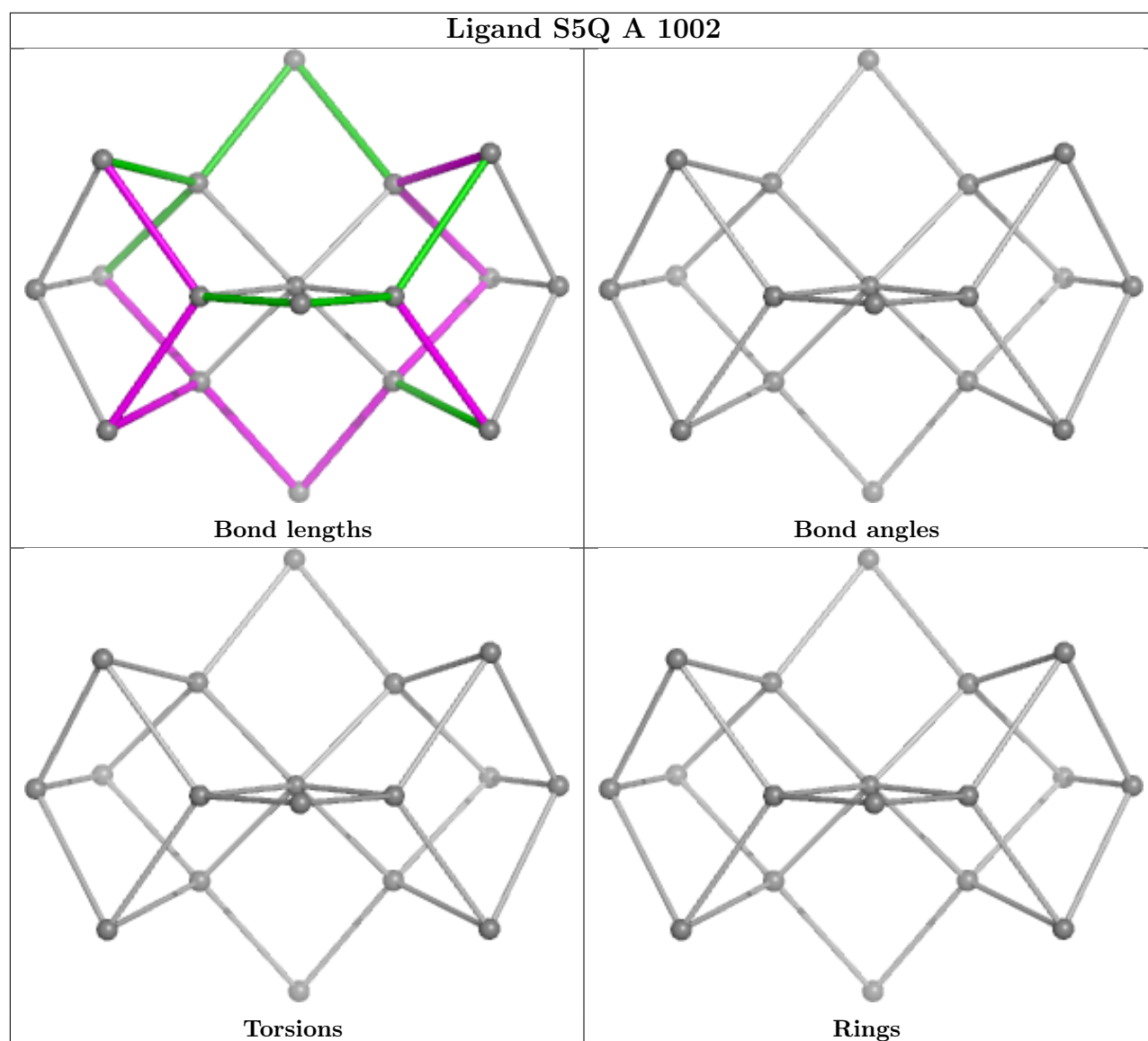
There are no torsion outliers.

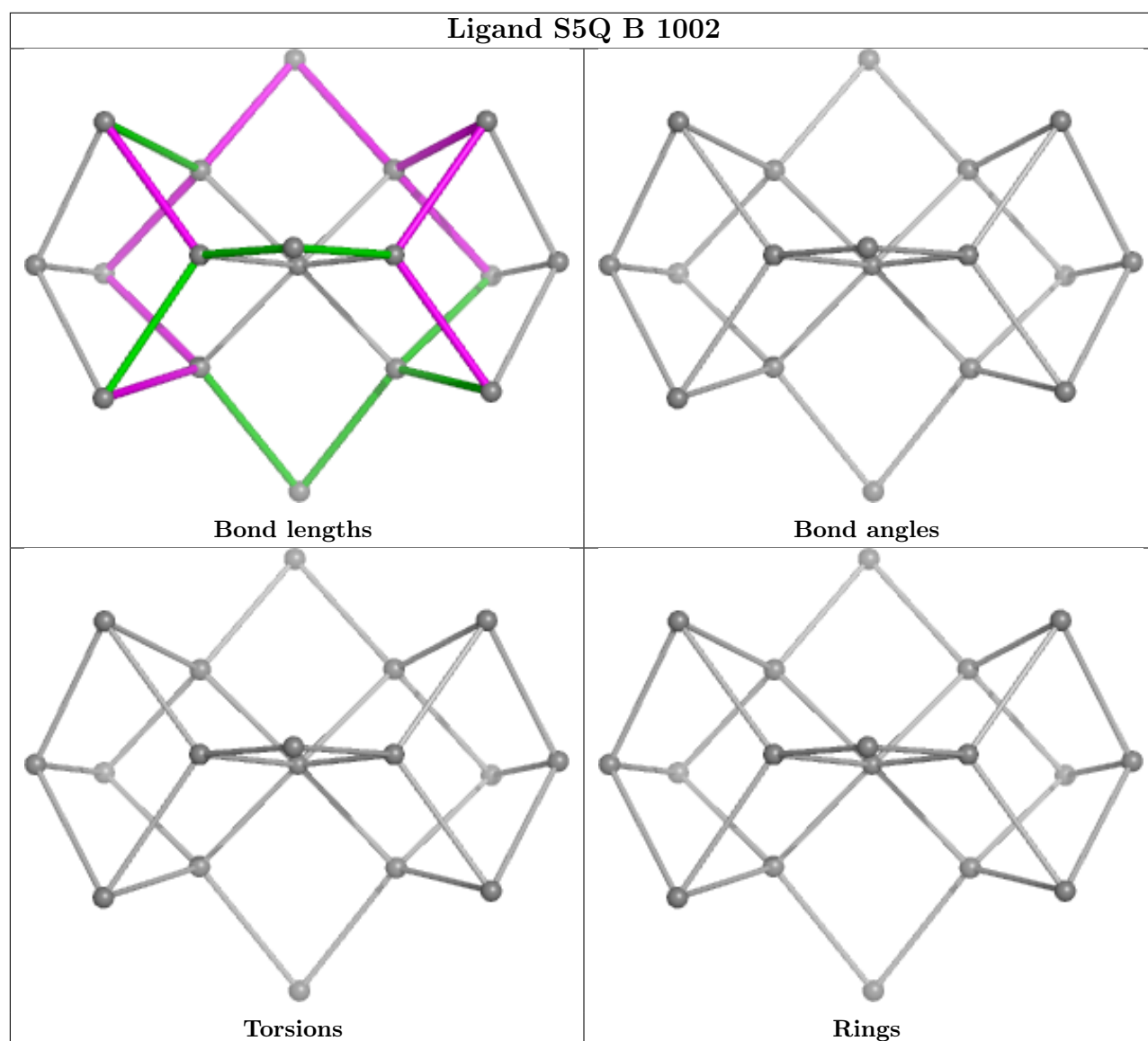
There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

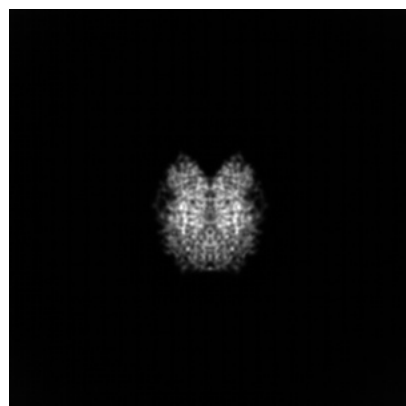
6 Map visualisation [i](#)

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.

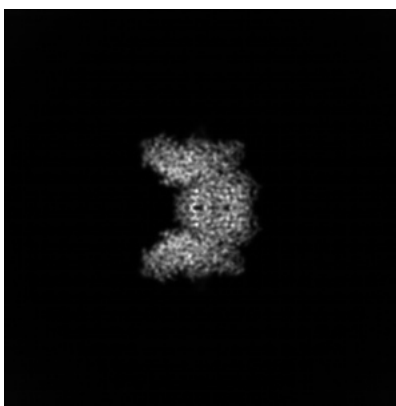
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

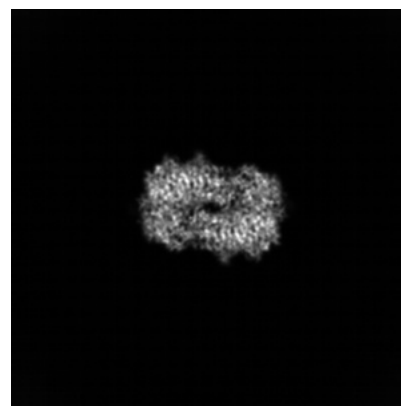
6.1.1 Primary map



X

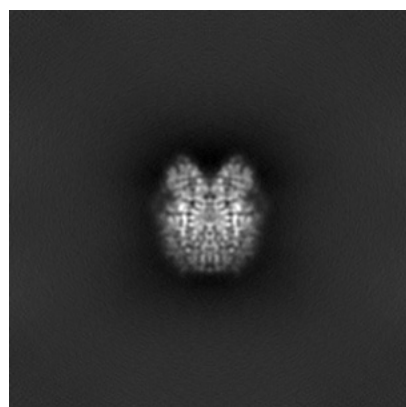


Y

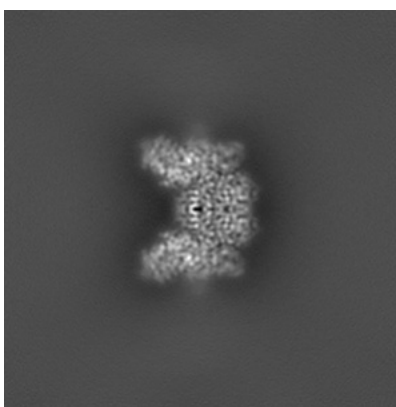


Z

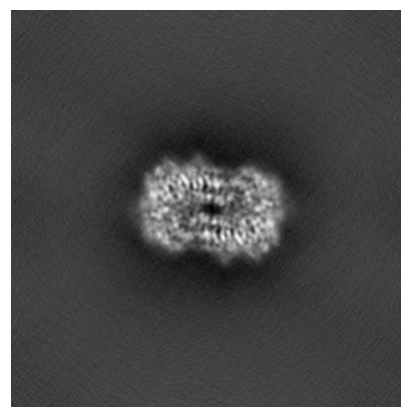
6.1.2 Raw map



X



Y

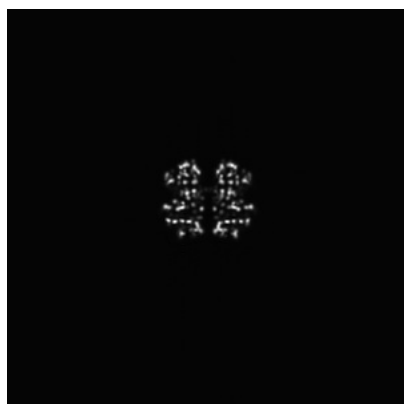


Z

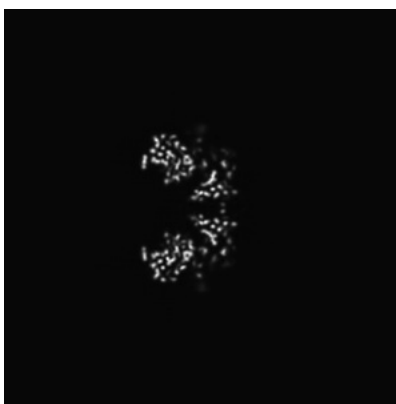
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

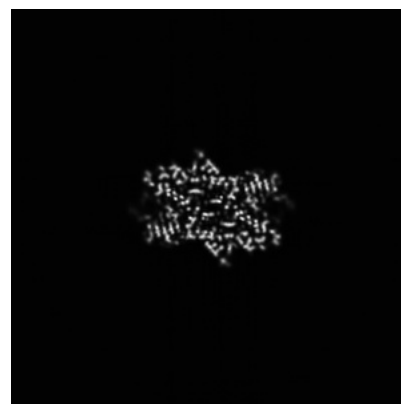
6.2.1 Primary map



X Index: 123

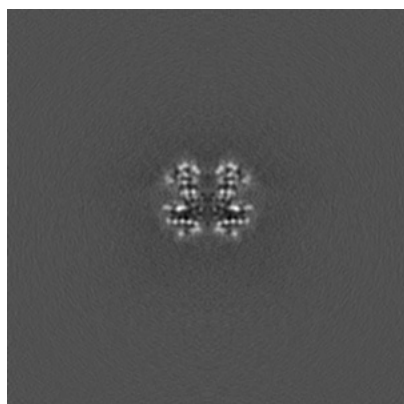


Y Index: 123

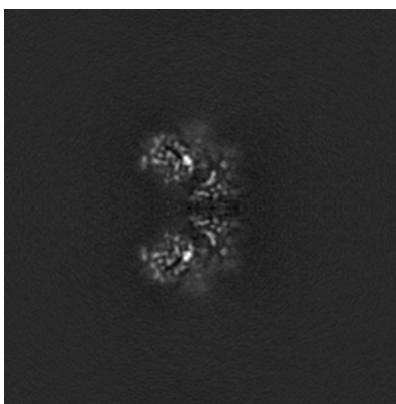


Z Index: 123

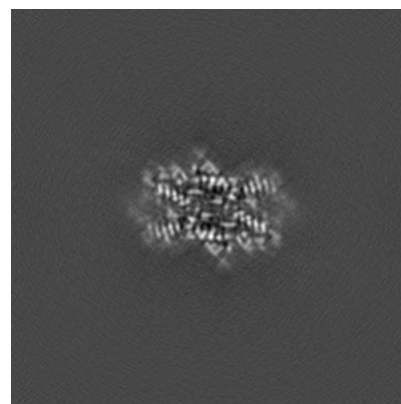
6.2.2 Raw map



X Index: 123



Y Index: 123

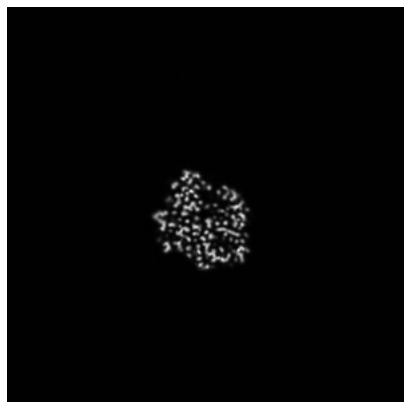


Z Index: 123

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

6.3 Largest variance slices [i](#)

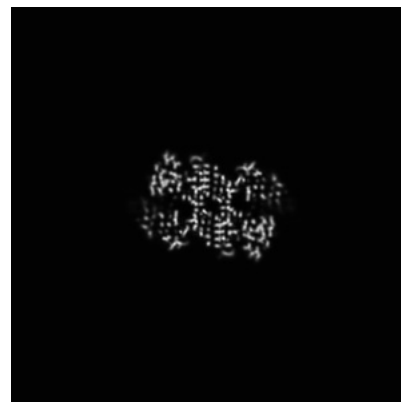
6.3.1 Primary map



X Index: 151

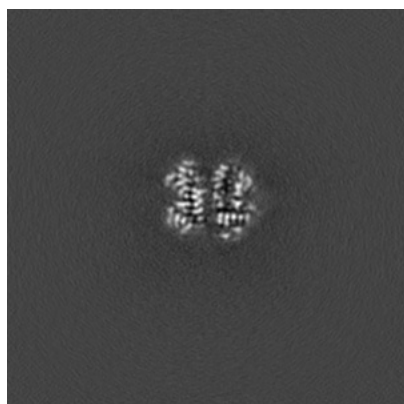


Y Index: 107

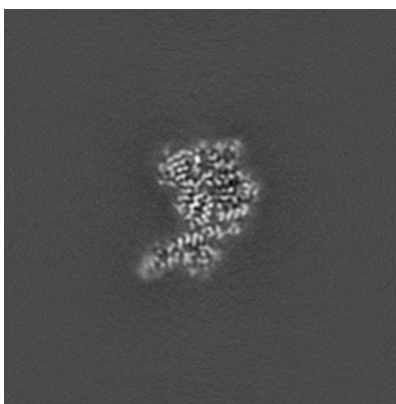


Z Index: 118

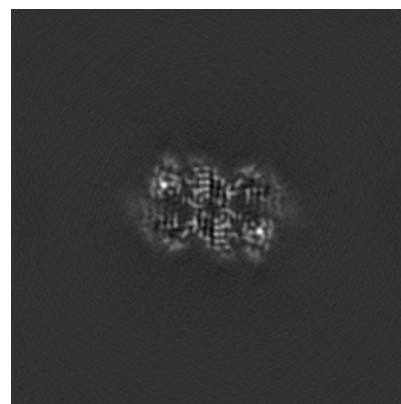
6.3.2 Raw map



X Index: 120



Y Index: 107

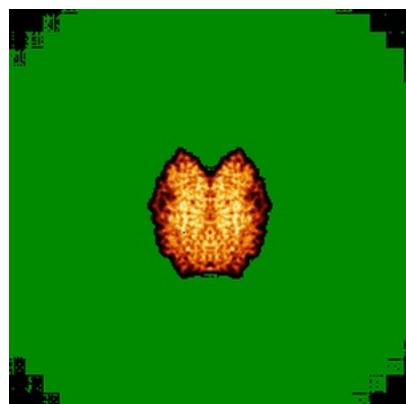


Z Index: 118

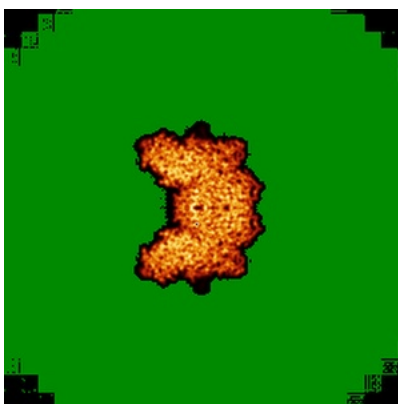
The images above show the largest variance slices of the map in three orthogonal directions.

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

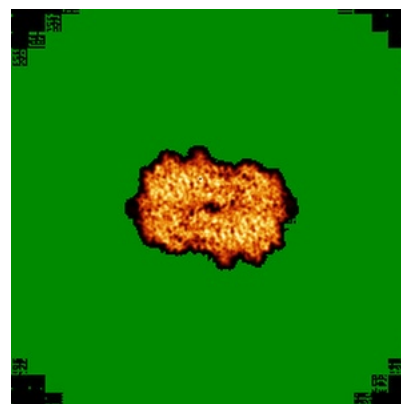
6.4.1 Primary map



X

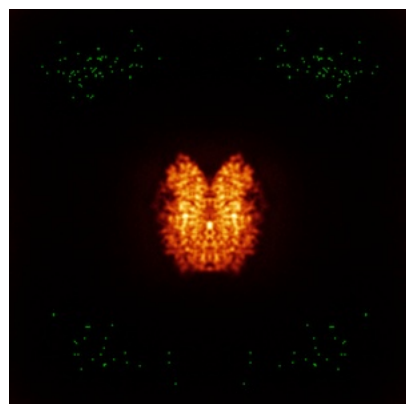


Y

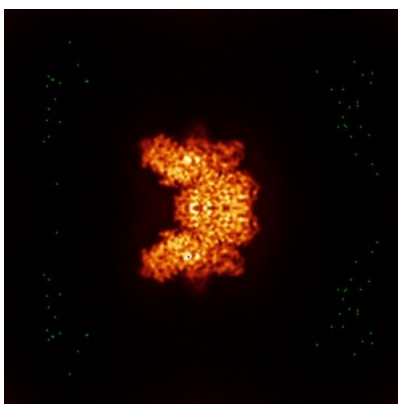


Z

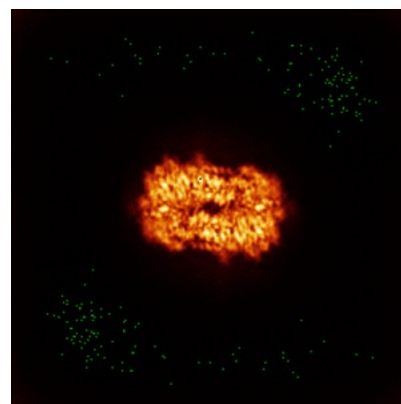
6.4.2 Raw map



X



Y

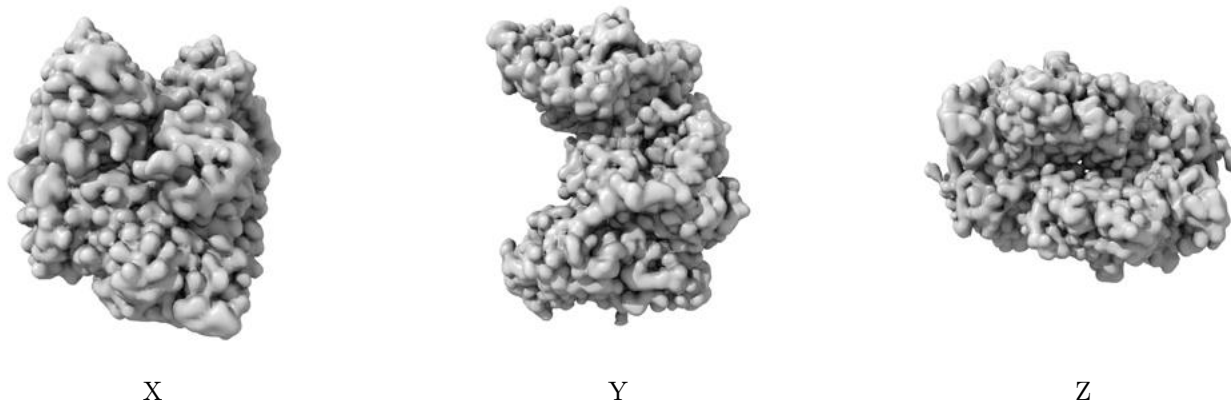


Z

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.

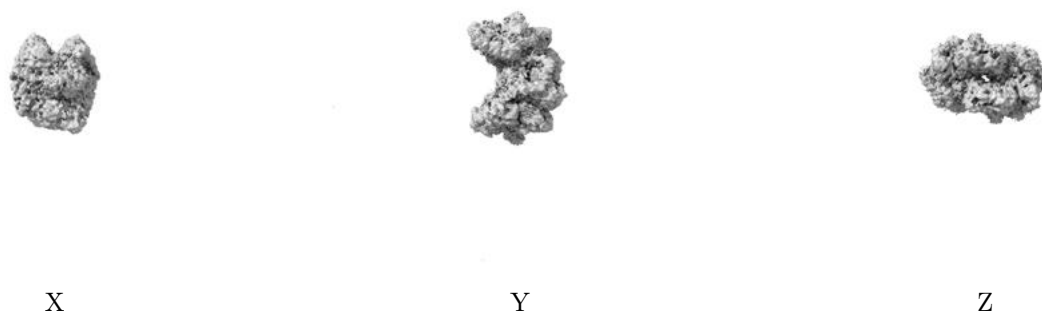
6.5 Orthogonal surface views [i](#)

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.

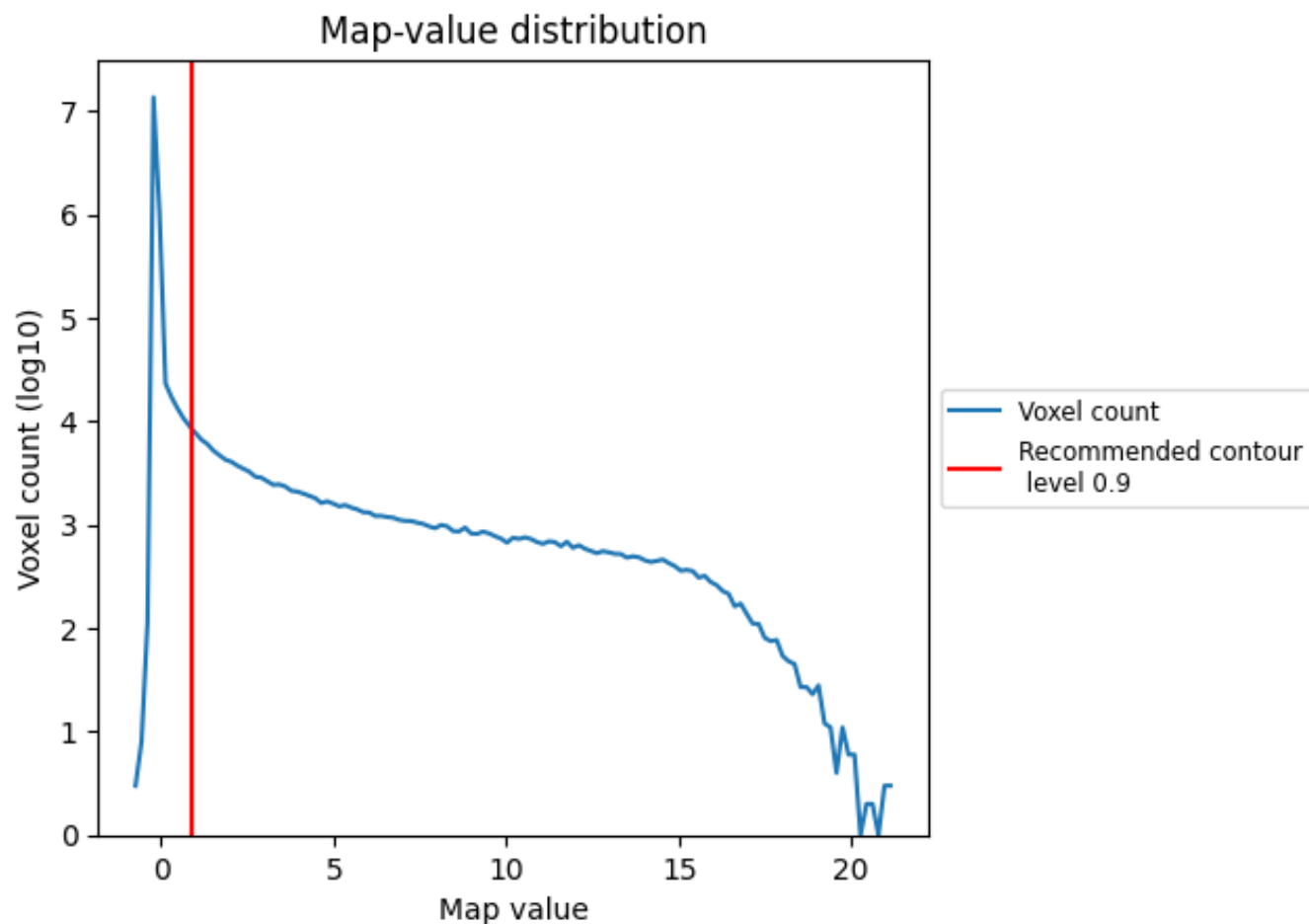
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

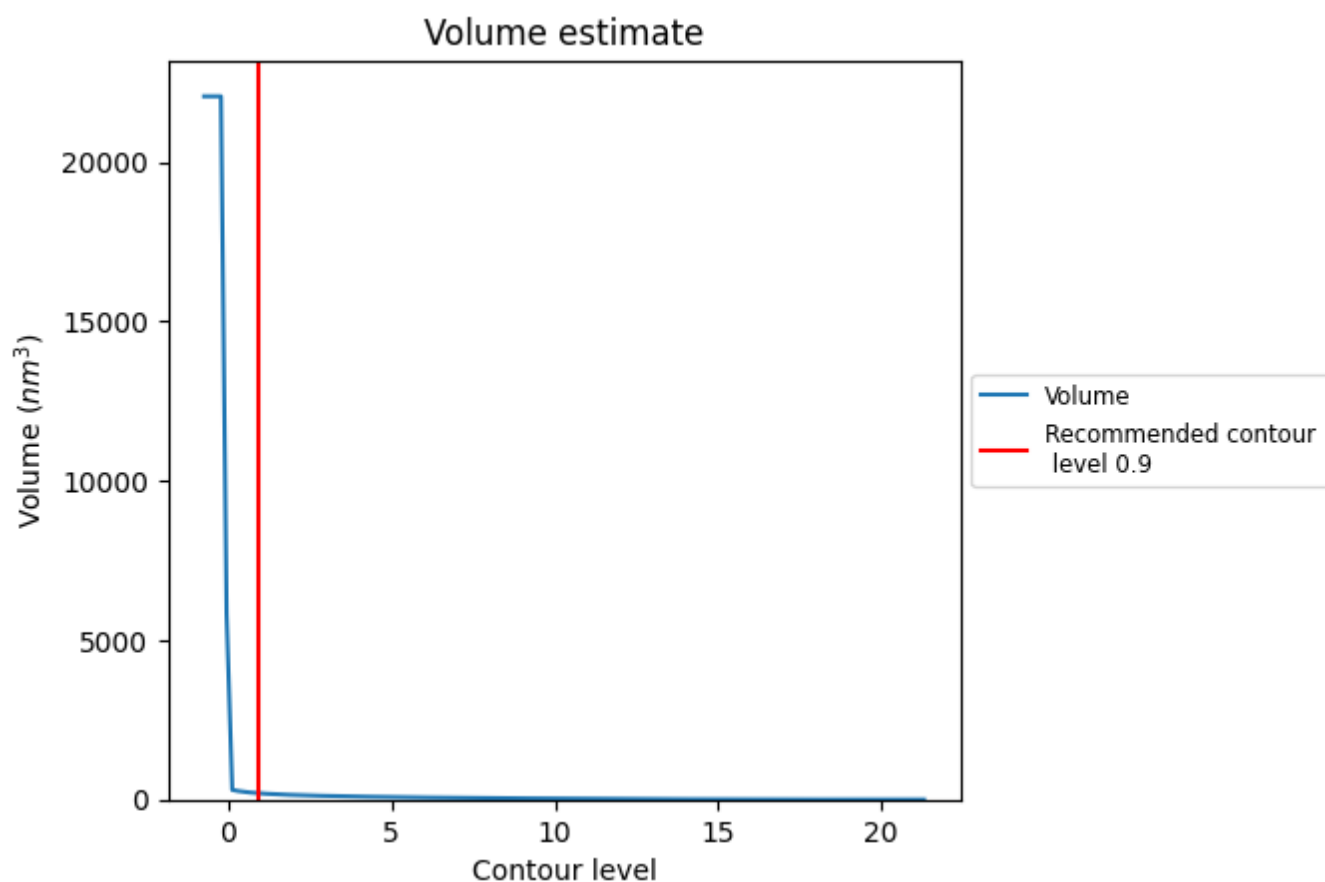
This section contains the results of statistical analysis of the map.

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.

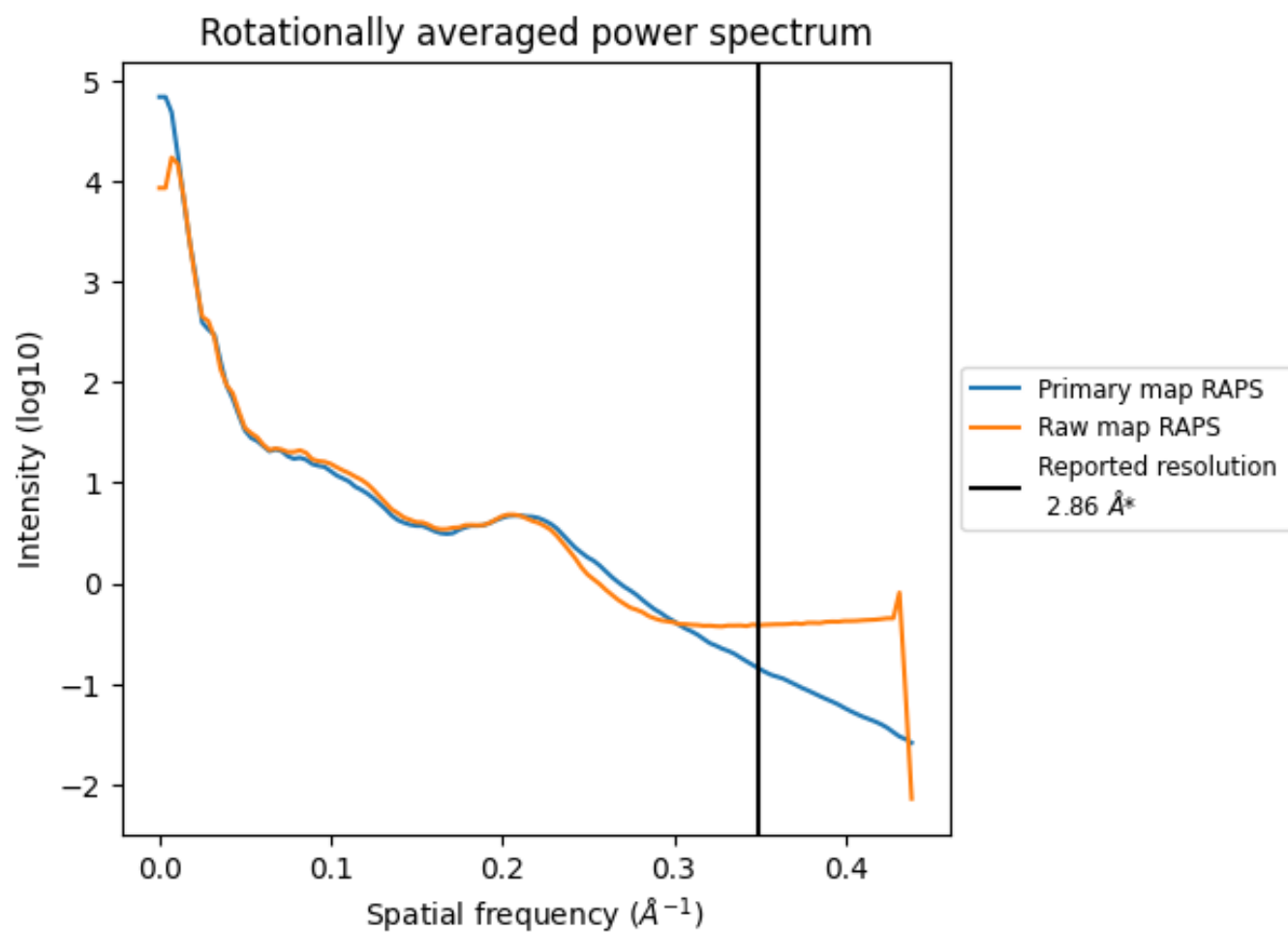
7.2 Volume estimate [i](#)



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 ⓘ

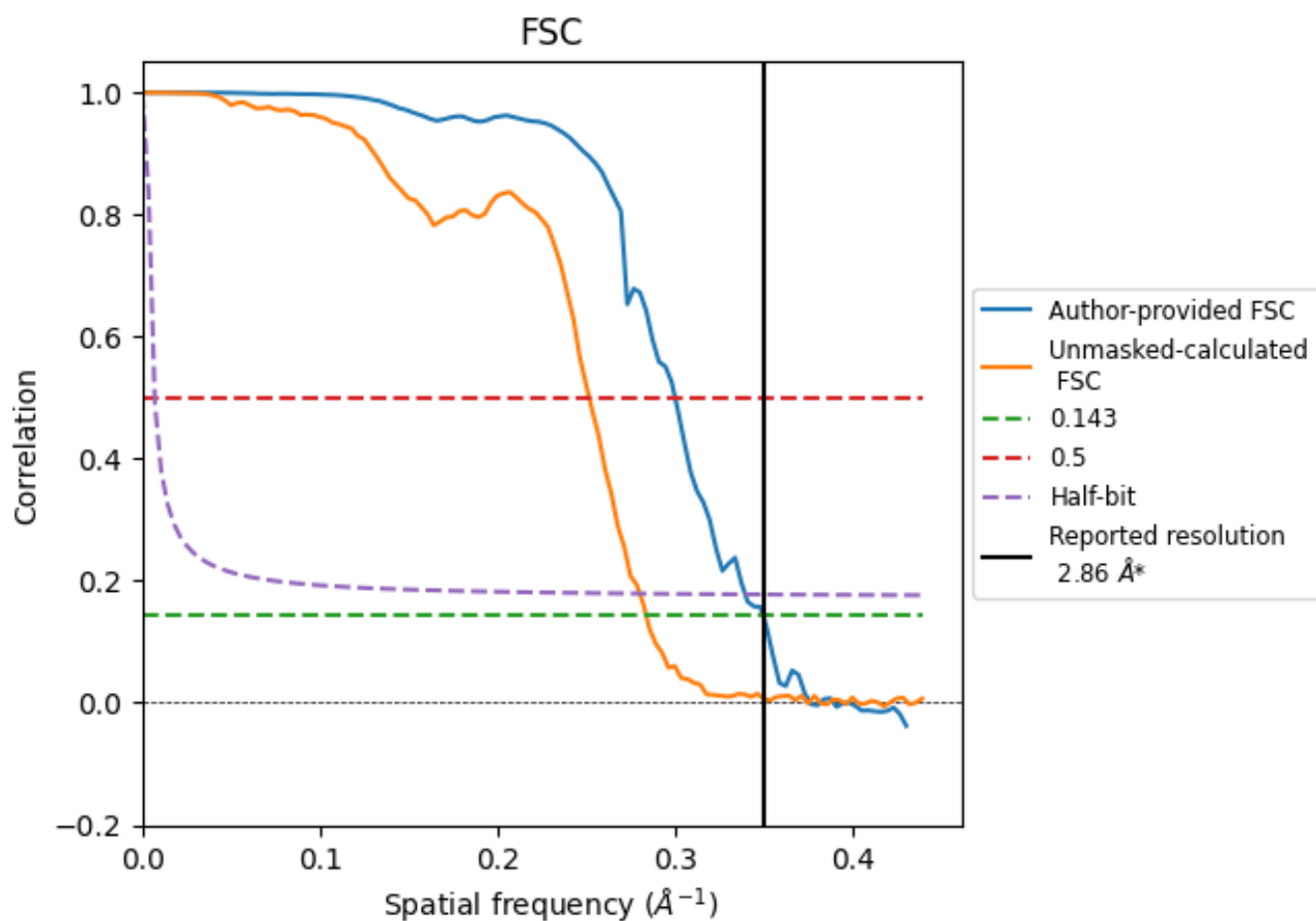


*Reported resolution corresponds to spatial frequency of 0.350 \AA^{-1}

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](#)

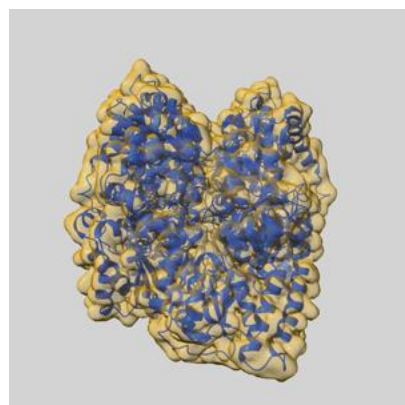
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.34	2.95
Unmasked-calculated*	3.53	3.98	3.57

*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 %

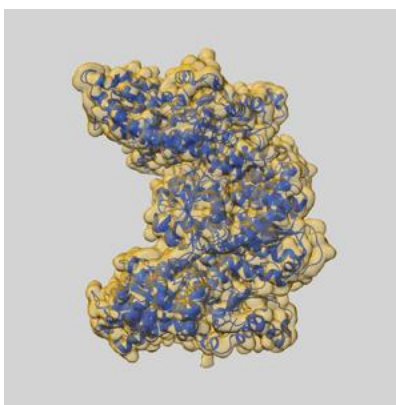
9 Map-model fit [i](#)

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

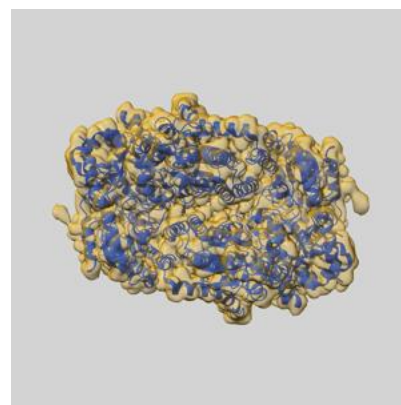
9.1 Map-model overlay [i](#)



X



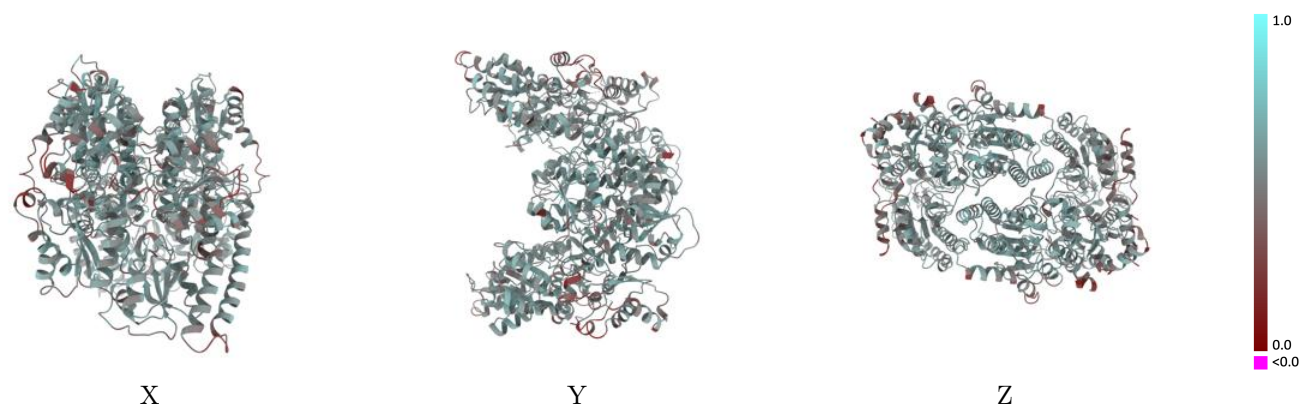
Y



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](#)



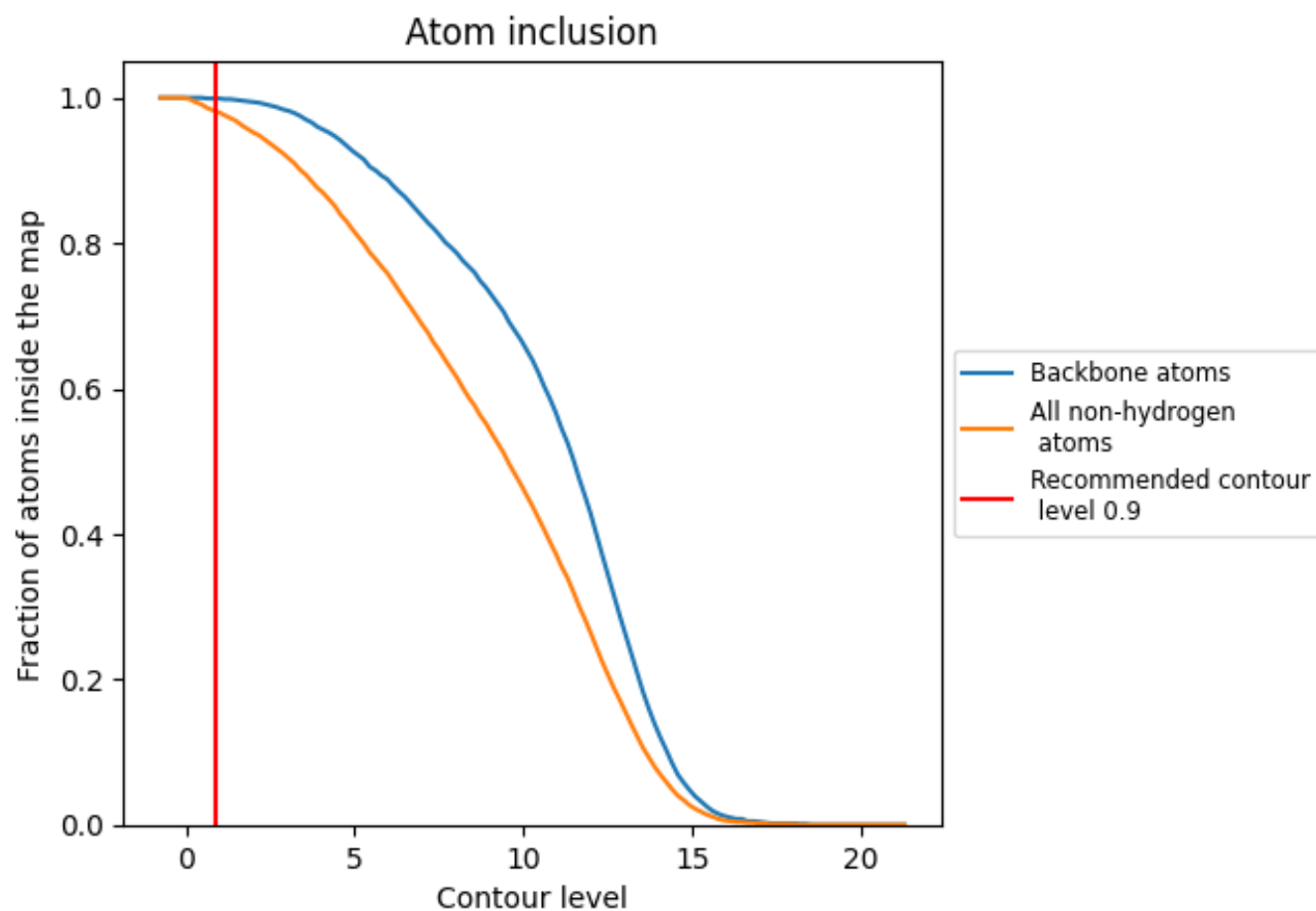
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.9) 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

