



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 11:17 AM UTC

PDB ID : 6NMI / pdb_00006nmi
EMDB ID : EMD-0452
Title : Cryo-EM structure of the human TFIID core complex
Authors : Greber, B.J.; Toso, D.; Fang, J.; Nogales, E.
Deposited on : 2019-01-10
Resolution : 3.70 Å (reported)
Based on initial models : 5OF4, 4ERN, 2JNJ, 5OQJ, 2DII, 5O85, 1G25

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

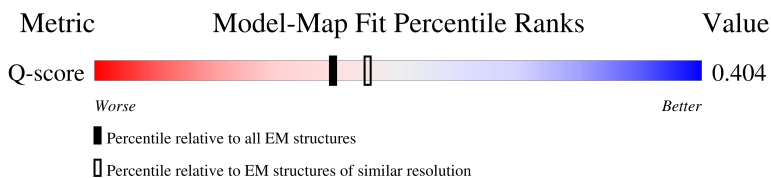
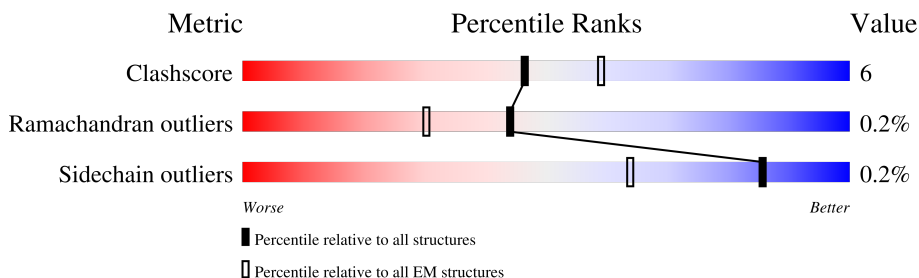
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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.



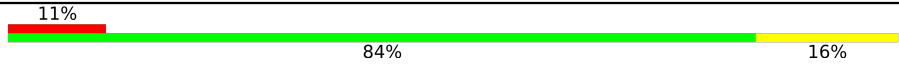

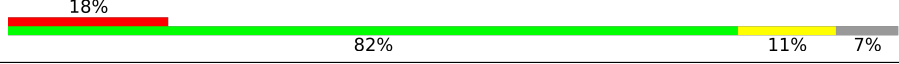
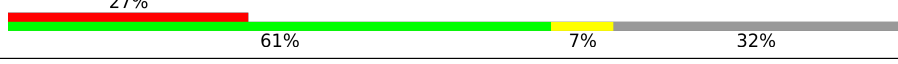
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	653	
2	B	760	
3	C	548	
4	D	462	

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Mol	Chain	Length	Quality of chain
5	E	366	
6	F	308	
7	G	71	
8	H	309	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24379 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 General transcription and DNA repair factor IIIH helicase subunit XPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	653	Total	C	N	O	S	0	0
			5190	3304	899	957	30		

- Molecule 2 is a protein called General transcription and DNA repair factor IIIH helicase subunit XPD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	760	Total	C	N	O	S	0	0
			6040	3856	1056	1099	29		

- Molecule 3 is a protein called General transcription factor IIIH subunit 1, p62.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	408	Total	C	N	O	S	0	0
			2657	1657	489	504	7		

- Molecule 4 is a protein called General transcription factor IIIH subunit 4, p52.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	452	Total	C	N	O	S	0	0
			3589	2307	631	637	14		

- Molecule 5 is a protein called General transcription factor IIIH subunit 2, p44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	366	Total	C	N	O	S	0	0
			2710	1703	476	505	26		

- Molecule 6 is a protein called General transcription factor IIIH subunit 3, p34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	263	2065	1323	344	379	19	0	0

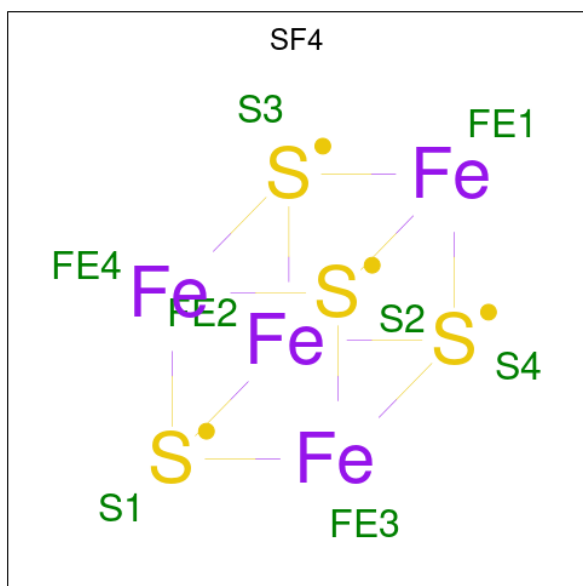
- Molecule 7 is a protein called General transcription factor IIIH subunit 5, p8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	66	522	336	83	100	3	0	0

- Molecule 8 is a protein called CDK-activating kinase assembly factor MAT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	210	1592	986	281	316	9	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

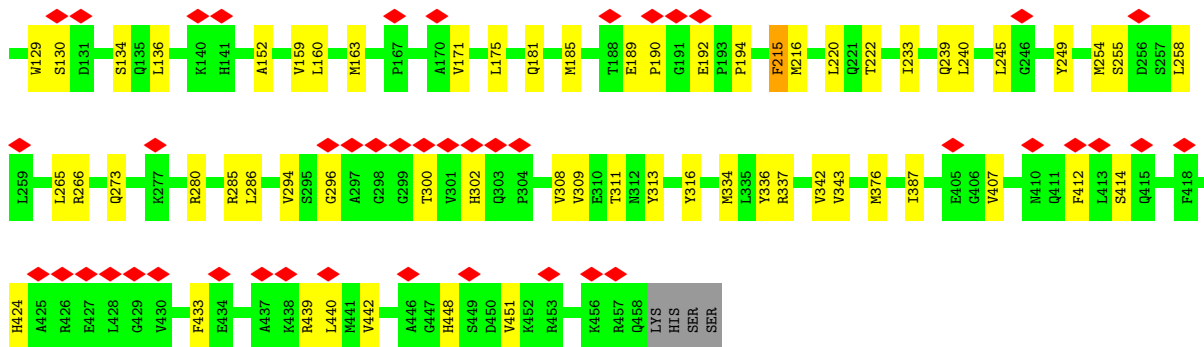
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
10	E	3	3	3	0

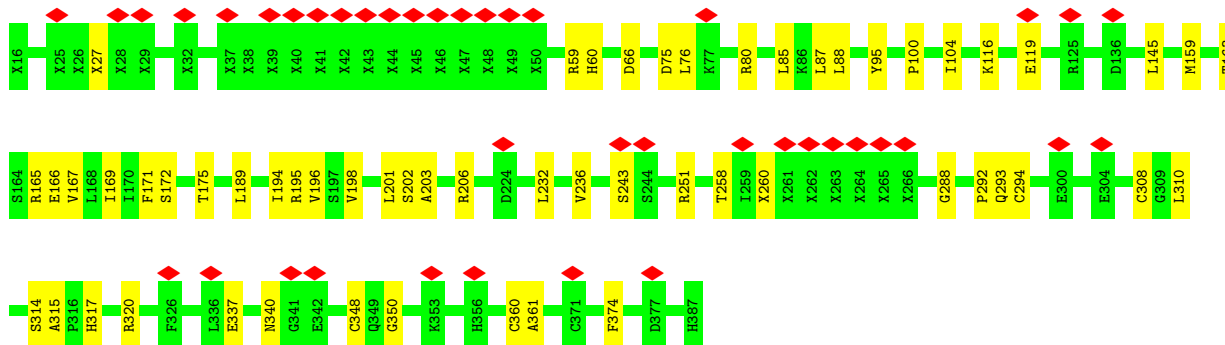
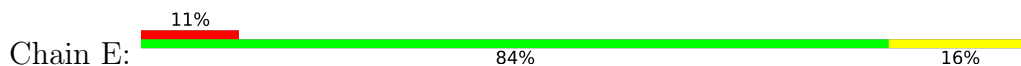
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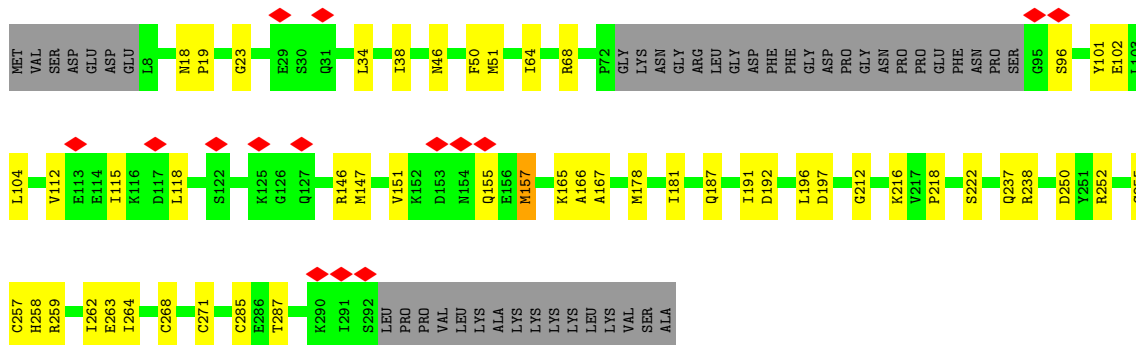
Mol	Chain	Residues	Atoms		AltConf
10	F	1	Total 1	Zn 1	0
10	H	2	Total 2	Zn 2	0



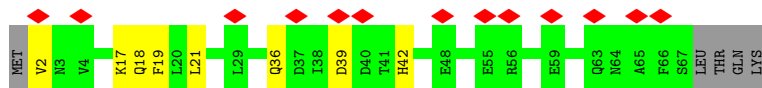
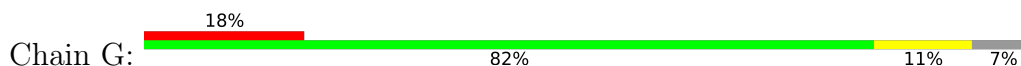
• Molecule 5: General transcription factor IIH subunit 2, p44



• Molecule 6: General transcription factor IIH subunit 3, p34



• Molecule 7: General transcription factor IIH subunit 5, p8



• Molecule 8: CDK-activating kinase assembly factor MAT1

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	138659	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction during 3D reconstruction in RELION 3.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	700	Depositor
Magnification	43478	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.069	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0172	Depositor
Map size (\AA)	294.4, 294.4, 294.4	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.15, 1.15, 1.15	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: ZN, SF4

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	0.33	0/5206	0.65	1/7035 (0.0%)
2	B	0.38	0/6028	0.72	0/8157
3	C	0.31	0/1847	0.71	5/2499 (0.2%)
4	D	0.32	0/3672	0.63	0/4979
5	E	0.35	0/2484	0.62	0/3364
6	F	0.33	0/2102	0.56	0/2844
7	G	0.29	0/528	0.66	0/713
8	H	0.27	0/1609	0.63	0/2170
All	All	0.34	0/23476	0.66	6/31761 (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	5
2	B	0	3
3	C	0	3
4	D	0	3
5	E	0	2
8	H	0	1
All	All	0	17

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	VAL	N-CA-C	-6.36	105.16	111.77
3	C	414	TYR	CA-C-N	5.70	135.70	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	414	TYR	C-N-CA	5.70	135.70	121.80
3	C	442	GLN	CA-C-O	-5.48	111.48	120.80
3	C	227	SER	CA-C-N	5.21	131.48	121.54
3	C	227	SER	C-N-CA	5.21	131.48	121.54

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	400	PRO	Peptide
1	A	475	ASP	Peptide
1	A	476	LYS	Peptide
1	A	503	ALA	Peptide
1	A	55	GLU	Peptide
2	B	102	LEU	Peptide
2	B	425	THR	Peptide
2	B	532	PRO	Peptide
3	C	211	VAL	Peptide
3	C	212	PRO	Peptide
3	C	415	THR	Peptide
4	D	134	SER	Peptide
4	D	189	GLU	Peptide
4	D	192	GLU	Peptide
5	E	260	UNK	Peptide
5	E	315	ALA	Peptide
8	H	56	SER	Peptide

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	5190	0	5150	68	0
2	B	6040	0	5970	90	0
3	C	2657	0	1864	21	0
4	D	3589	0	3621	48	0
5	E	2710	0	2472	41	0
6	F	2065	0	2098	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	522	0	528	6	0
8	H	1592	0	1461	14	0
9	B	8	0	0	0	0
10	E	3	0	0	0	0
10	F	1	0	0	0	0
10	H	2	0	0	0	0
All	All	24379	0	23164	291	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 6.

All (291) 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)
5:E:294:CYS:HB3	5:E:308:CYS:SG	1.93	1.09
2:B:534:GLY:HA2	2:B:594:ALA:O	1.62	0.98
6:F:191:ILE:O	6:F:212:GLY:HA3	1.67	0.94
6:F:268:CYS:HB3	6:F:271:CYS:SG	2.14	0.87
1:A:374:TRP:O	1:A:378:PHE:HB2	1.83	0.77
6:F:46:ASN:O	6:F:50:PHE:HB2	1.85	0.76
4:D:130:SER:HB2	4:D:239:GLN:HE22	1.55	0.72
8:H:125:TYR:O	8:H:129:ASN:HB2	1.91	0.70
2:B:487:ARG:HE	2:B:724:MET:HG2	1.59	0.67
2:B:468:PRO:HA	2:B:473:PHE:HB3	1.78	0.66
7:G:39:ASP:HB3	7:G:42:HIS:H	1.63	0.64
5:E:116:LYS:HE2	5:E:119:GLU:HG2	1.80	0.64
7:G:17:LYS:NZ	7:G:39:ASP:O	2.32	0.62
2:B:16:TYR:HE2	2:B:730:ARG:HE	1.48	0.62
5:E:350:GLY:HA3	6:F:146:ARG:HH22	1.65	0.62
1:A:74:ARG:NH2	5:E:27:UNK:O	2.33	0.61
1:A:455:LEU:HD22	1:A:483:LEU:HG	1.81	0.61
4:D:334:MET:HE2	4:D:342:VAL:HG11	1.81	0.61
1:A:182:PRO:HB3	1:A:268:VAL:HG21	1.83	0.60
2:B:23:SER:HB2	2:B:757:ALA:HB2	1.82	0.60
2:B:231:VAL:HB	2:B:454:VAL:HG12	1.83	0.60
2:B:617:ALA:HA	2:B:676:LEU:O	2.01	0.60
1:A:325:ARG:NH1	2:B:712:GLU:OE2	2.34	0.59
2:B:333:LEU:HD13	2:B:397:LEU:HD11	1.83	0.59
4:D:60:LEU:O	4:D:119:ARG:NH2	2.35	0.59
2:B:728:PHE:HE2	2:B:733:GLN:HE21	1.51	0.59
1:A:105:GLU:HG3	1:A:122:SER:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:337:GLU:O	5:E:340:ASN:ND2	2.37	0.58
8:H:108:ASN:OD1	8:H:112:ASN:ND2	2.36	0.58
5:E:360:CYS:SG	5:E:361:ALA:N	2.77	0.58
6:F:38:ILE:HG21	6:F:115:ILE:HD13	1.86	0.58
2:B:338:GLU:HG3	8:H:68:VAL:HG21	1.85	0.57
2:B:143:ARG:NH2	2:B:162:ASP:OD2	2.37	0.57
5:E:292:PRO:HB3	6:F:263:GLU:HG3	1.85	0.57
2:B:284:GLU:OE2	2:B:287:ARG:NH2	2.37	0.57
1:A:109:ARG:NH1	1:A:492:ASN:OD1	2.37	0.57
2:B:84:ILE:HG13	2:B:108:ALA:HB2	1.87	0.57
4:D:35:TYR:O	4:D:117:ASN:ND2	2.38	0.57
2:B:532:PRO:HG3	5:E:203:ALA:HB1	1.85	0.57
6:F:166:ALA:HB2	6:F:196:LEU:HD12	1.86	0.57
2:B:192:TYR:OH	2:B:196:ARG:NH2	2.37	0.56
4:D:69:ALA:O	4:D:73:LEU:HB2	2.04	0.56
3:C:470:GLU:OE2	3:C:474:HIS:NE2	2.38	0.56
2:B:339:TYR:OH	2:B:343:ARG:NH2	2.35	0.56
2:B:71:ILE:HB	2:B:231:VAL:HG22	1.88	0.56
2:B:396:PRO:O	2:B:399:LEU:HB3	2.06	0.56
4:D:336:TYR:HB2	4:D:343:VAL:HB	1.88	0.56
5:E:145:LEU:HD11	5:E:169:ILE:HD13	1.87	0.56
6:F:197:ASP:O	6:F:216:LYS:NZ	2.39	0.56
2:B:322:SER:HB3	8:H:99:LEU:HB3	1.88	0.56
1:A:677:GLN:NE2	4:D:313:TYR:OH	2.35	0.56
2:B:17:ILE:HD11	2:B:744:LEU:HD21	1.87	0.56
3:C:407:ILE:HD11	6:F:34:LEU:HD22	1.88	0.56
3:C:475:PHE:O	3:C:479:PHE:HB2	2.06	0.55
4:D:129:TRP:O	4:D:239:GLN:NE2	2.39	0.55
4:D:255:SER:H	4:D:258:LEU:HD12	1.71	0.55
1:A:374:TRP:NE1	1:A:441:ASP:OD2	2.39	0.55
2:B:325:THR:HB	2:B:328:HIS:HD2	1.71	0.55
1:A:344:ALA:HB2	1:A:502:ILE:HD11	1.88	0.55
4:D:53:LYS:NZ	6:F:51:MET:O	2.38	0.55
2:B:237:HIS:CE1	2:B:460:THR:HB	2.42	0.54
6:F:165:LYS:NZ	6:F:167:ALA:O	2.37	0.54
1:A:365:GLY:HA2	1:A:441:ASP:HB2	1.89	0.54
2:B:690:ARG:O	2:B:698:GLN:NE2	2.41	0.54
2:B:39:VAL:HG22	2:B:456:ILE:HB	1.88	0.54
2:B:238:ASN:HB3	2:B:241:ASN:HB2	1.88	0.54
1:A:306:ILE:HD13	1:A:404:SER:HA	1.90	0.54
3:C:436:PRO:HA	3:C:441:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:424:HIS:HD2	4:D:451:VAL:HG22	1.73	0.54
4:D:433:PHE:HB3	4:D:442:VAL:HB	1.90	0.54
2:B:56:ILE:HG21	2:B:70:LEU:HD13	1.89	0.53
1:A:54:ASP:OD2	4:D:337:ARG:NH1	2.38	0.53
1:A:480:LEU:HD22	1:A:483:LEU:HD22	1.89	0.53
5:E:80:ARG:NH2	5:E:202:SER:OG	2.41	0.53
5:E:100:PRO:HG3	5:E:320:ARG:HD2	1.91	0.53
3:C:470:GLU:OE1	3:C:473:ARG:NH1	2.41	0.53
4:D:294:VAL:HG12	4:D:296:GLY:H	1.73	0.53
5:E:348:CYS:SG	6:F:146:ARG:NH1	2.81	0.53
1:A:510:VAL:HG22	1:A:690:ILE:HB	1.90	0.53
2:B:61:ARG:NH2	2:B:98:GLU:OE2	2.42	0.53
5:E:169:ILE:HG22	5:E:171:PHE:HB2	1.91	0.53
6:F:151:VAL:HG13	6:F:155:GLN:HG3	1.91	0.53
2:B:609:ASP:OD1	2:B:666:ARG:NH1	2.42	0.52
6:F:101:TYR:HD2	6:F:104:LEU:HG	1.74	0.52
6:F:192:ASP:OD2	6:F:238:ARG:NH2	2.42	0.52
6:F:255:CYS:SG	6:F:258:HIS:N	2.70	0.52
1:A:530:ARG:HA	1:A:533:LEU:HD12	1.90	0.52
2:B:35:LYS:HG2	2:B:452:GLN:HE21	1.74	0.52
2:B:658:ARG:O	2:B:662:GLN:HB2	2.09	0.52
5:E:159:MET:HB2	5:E:165:ARG:HD3	1.91	0.52
2:B:458:SER:HB2	2:B:461:LEU:HG	1.90	0.52
6:F:285:CYS:SG	6:F:287:THR:OG1	2.64	0.52
3:C:387:THR:O	6:F:259:ARG:NH2	2.42	0.52
2:B:343:ARG:HG2	2:B:357:PHE:HE1	1.74	0.52
1:A:76:LEU:HB2	1:A:144:SER:HA	1.92	0.52
1:A:566:PHE:HZ	1:A:715:LYS:HG2	1.74	0.51
4:D:245:LEU:HD11	4:D:285:ARG:HD3	1.92	0.51
1:A:374:TRP:O	1:A:378:PHE:CB	2.57	0.51
1:A:388:GLN:HB3	1:A:404:SER:HB3	1.93	0.51
8:H:113:VAL:O	8:H:117:ASN:ND2	2.42	0.51
2:B:618:VAL:HG11	2:B:664:VAL:HA	1.91	0.51
2:B:280:ARG:NH2	2:B:387:GLU:OE1	2.29	0.51
5:E:258:THR:O	5:E:288:GLY:N	2.44	0.51
6:F:257:CYS:SG	6:F:258:HIS:ND1	2.81	0.51
1:A:363:VAL:HB	1:A:407:ILE:HG12	1.93	0.51
2:B:695:ARG:HH12	2:B:758:GLN:HB2	1.76	0.51
1:A:366:ASN:ND2	1:A:442:GLU:OE1	2.44	0.50
5:E:172:SER:HA	5:E:201:LEU:HB2	1.92	0.50
1:A:361:CYS:SG	1:A:362:LEU:N	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:63:GLU:OE2	4:D:115:ARG:NH2	2.45	0.50
4:D:309:VAL:H	4:D:376:MET:HE3	1.77	0.50
4:D:160:LEU:HA	4:D:163:MET:HE3	1.94	0.50
1:A:308:ILE:HG12	1:A:384:ILE:HG12	1.94	0.50
2:B:417:ILE:HG23	2:B:434:HIS:HB2	1.94	0.50
1:A:472:ARG:HH21	1:A:480:LEU:HB2	1.77	0.49
1:A:688:LYS:HE3	1:A:690:ILE:HD11	1.94	0.49
2:B:722:ARG:HE	5:E:202:SER:HA	1.77	0.49
8:H:22:MET:HA	8:H:59:ARG:O	2.12	0.49
2:B:17:ILE:HB	2:B:21:GLN:HG2	1.94	0.49
4:D:266:ARG:HE	4:D:273:GLN:HB2	1.77	0.49
6:F:178:MET:HA	6:F:181:ILE:HD12	1.94	0.49
2:B:220:LEU:HD12	2:B:221:VAL:HG23	1.94	0.49
2:B:650:ASP:OD1	2:B:692:LYS:NZ	2.35	0.49
4:D:181:GLN:NE2	4:D:222:THR:OG1	2.45	0.49
2:B:461:LEU:HD22	2:B:467:TYR:HE2	1.77	0.49
6:F:46:ASN:HD22	6:F:104:LEU:HD22	1.77	0.49
8:H:120:LYS:HE3	8:H:124:ILE:HD11	1.94	0.49
2:B:235:GLU:OE2	2:B:666:ARG:NH2	2.33	0.49
1:A:472:ARG:HD2	1:A:474:ASP:H	1.78	0.49
5:E:59:ARG:NH1	5:E:236:VAL:O	2.42	0.49
2:B:180:LEU:HD21	2:B:195:ALA:HB2	1.95	0.49
2:B:27:GLU:OE2	2:B:30:ARG:NH1	2.46	0.49
2:B:425:THR:HG23	2:B:428:ILE:HB	1.95	0.49
3:C:414:TYR:HE2	6:F:112:VAL:HG22	1.77	0.48
4:D:100:LEU:HD23	4:D:106:GLN:HA	1.94	0.48
8:H:44:GLY:HA2	8:H:53:LEU:HD22	1.94	0.48
1:A:640:LEU:HG	1:A:644:LEU:HD12	1.94	0.48
2:B:237:HIS:HE1	2:B:460:THR:HB	1.78	0.48
4:D:185:MET:HE2	4:D:194:PRO:HB2	1.96	0.48
4:D:19:LEU:HD23	4:D:47:GLU:HG3	1.96	0.48
1:A:591:GLN:OE1	1:A:595:ASN:ND2	2.47	0.48
5:E:374:PHE:HE1	6:F:187:GLN:HE21	1.62	0.48
2:B:494:ILE:HD12	2:B:706:LEU:HD12	1.96	0.48
2:B:25:MET:HE3	2:B:51:SER:HB2	1.96	0.47
4:D:152:ALA:HB1	4:D:286:LEU:HG	1.96	0.47
1:A:276:MET:O	1:A:280:LEU:N	2.33	0.47
4:D:56:VAL:HG13	4:D:110:LEU:HD21	1.96	0.47
5:E:167:VAL:HB	5:E:196:VAL:HG22	1.95	0.47
1:A:351:VAL:HG22	1:A:378:PHE:HD1	1.78	0.47
3:C:417:LYS:HB3	4:D:123:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:430:THR:OG1	6:F:222:SER:OG	2.24	0.47
5:E:76:LEU:HD23	5:E:80:ARG:HG2	1.96	0.47
1:A:519:TYR:HE2	7:G:19:PHE:HB2	1.79	0.47
2:B:567:LEU:HA	2:B:595:ILE:HG23	1.97	0.47
2:B:403:PHE:HE1	2:B:435:PHE:HB2	1.80	0.47
4:D:50:SER:HB2	6:F:237:GLN:HE21	1.79	0.47
1:A:48:GLU:O	1:A:51:THR:OG1	2.26	0.47
1:A:187:HIS:HD2	1:A:289:TYR:HE2	1.63	0.47
2:B:486:ALA:HB2	2:B:736:LEU:HB2	1.97	0.47
4:D:240:LEU:HD11	4:D:265:LEU:HD21	1.97	0.47
8:H:125:TYR:O	8:H:129:ASN:CB	2.61	0.47
1:A:438:MET:HE2	1:A:440:LEU:HD21	1.96	0.47
1:A:521:GLU:HG3	1:A:713:LEU:HD11	1.96	0.47
2:B:530:VAL:HG21	2:B:714:VAL:HG13	1.96	0.47
1:A:497:GLN:HB3	1:A:504:LYS:HG2	1.97	0.46
2:B:53:LEU:HD11	2:B:83:VAL:HG13	1.97	0.46
2:B:191:PRO:HA	2:B:194:LEU:HB3	1.96	0.46
4:D:159:VAL:HG12	4:D:163:MET:HE2	1.96	0.46
2:B:273:ILE:HG21	2:B:386:LEU:HD22	1.96	0.46
5:E:60:HIS:HD2	5:E:163:THR:HG21	1.80	0.46
2:B:85:GLU:HG3	3:C:354:LEU:HD13	1.97	0.46
2:B:335:ARG:HH22	8:H:75:ARG:HD3	1.79	0.46
6:F:250:ASP:HB2	6:F:252:ARG:HG2	1.97	0.46
1:A:165:LYS:HD2	1:A:181:HIS:CE1	2.51	0.46
1:A:364:LEU:HD21	1:A:413:LEU:HD22	1.97	0.46
2:B:619:ILE:HA	2:B:678:VAL:HG22	1.97	0.46
2:B:669:ARG:HD2	3:C:360:TYR:HE1	1.80	0.46
5:E:80:ARG:HD3	5:E:201:LEU:HD13	1.97	0.46
5:E:314:SER:HB3	5:E:317:HIS:HD2	1.81	0.46
1:A:613:THR:HB	1:A:614:SER:HB3	1.98	0.46
4:D:412:PHE:HA	7:G:2:VAL:HG21	1.98	0.46
6:F:255:CYS:HB3	6:F:262:ILE:HD11	1.98	0.45
1:A:369:VAL:HG21	1:A:615:PHE:HA	1.97	0.45
3:C:154:UNK:C	3:C:156:UNK:H	2.29	0.45
3:C:440:LEU:HD11	6:F:218:PRO:HD3	1.98	0.45
2:B:493:MET:HE3	2:B:676:LEU:HD11	1.98	0.45
4:D:171:VAL:HG13	4:D:175:LEU:HB3	1.98	0.45
4:D:215:PHE:HB3	4:D:216:MET:HE2	1.99	0.45
4:D:308:VAL:HB	4:D:316:TYR:HB2	1.98	0.45
1:A:177:VAL:O	1:A:269:SER:HA	2.16	0.45
5:E:75:ASP:OD2	5:E:80:ARG:NH2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD23	1:A:454:VAL:HG22	1.99	0.45
1:A:612:ASP:HA	1:A:613:THR:HA	1.68	0.45
2:B:500:ASP:HB2	2:B:502:VAL:HG23	1.99	0.45
6:F:68:ARG:HD2	6:F:118:LEU:HD13	1.98	0.45
1:A:624:ILE:HG12	1:A:660:TYR:HB2	1.99	0.45
6:F:18:ASN:HD22	6:F:19:PRO:HD2	1.82	0.45
2:B:48:LYS:O	2:B:52:LEU:HB2	2.17	0.44
2:B:118:HIS:CD2	2:B:121:VAL:HG23	2.52	0.44
4:D:407:VAL:HG11	4:D:448:HIS:HB2	1.98	0.44
3:C:360:TYR:HD2	3:C:363:LEU:HD12	1.82	0.44
4:D:249:TYR:OH	6:F:102:GLU:OE2	2.30	0.44
4:D:440:LEU:HD22	7:G:36:GLN:HE22	1.81	0.44
8:H:114:ASP:HA	8:H:117:ASN:HD22	1.82	0.44
5:E:87:LEU:HD23	5:E:87:LEU:HA	1.78	0.44
1:A:134:SER:O	1:A:138:GLU:HB2	2.18	0.44
2:B:75:ARG:NH2	2:B:235:GLU:OE2	2.51	0.44
1:A:52:LYS:HZ2	1:A:63:LEU:HB2	1.83	0.44
2:B:616:ARG:O	2:B:676:LEU:N	2.51	0.44
3:C:372:ILE:HD11	5:E:243:SER:HA	1.99	0.44
4:D:65:PRO:HB2	4:D:107:GLY:HA3	1.99	0.44
6:F:19:PRO:HD2	6:F:64:ILE:HG23	2.00	0.44
2:B:424:ARG:NH2	3:C:286:UNK:O	2.51	0.43
8:H:193:PRO:HG2	8:H:196:LEU:HD12	1.99	0.43
6:F:268:CYS:CB	6:F:271:CYS:SG	2.90	0.43
1:A:336:GLY:HA3	1:A:488:LEU:HD13	1.99	0.43
2:B:573:ASP:HB2	2:B:576:GLU:HB2	2.00	0.43
6:F:96:SER:HB3	6:F:102:GLU:HG2	1.99	0.43
5:E:169:ILE:HB	5:E:198:VAL:HG22	2.00	0.43
1:A:361:CYS:HB3	1:A:405:VAL:HG22	2.00	0.43
2:B:319:VAL:HG11	2:B:324:ARG:HH21	1.84	0.43
2:B:562:GLN:HE21	2:B:567:LEU:HD12	1.84	0.43
6:F:147:MET:HB3	6:F:157:MET:HE1	1.99	0.43
4:D:220:LEU:HD21	4:D:233:ILE:HG21	2.01	0.43
1:A:339:VAL:HG21	1:A:470:LEU:HG	2.01	0.43
1:A:522:TYR:HE1	1:A:534:TYR:HD1	1.67	0.43
2:B:251:LEU:HD22	2:B:433:LEU:HD23	2.00	0.43
4:D:101:LEU:HB2	4:D:105:LEU:HB2	2.00	0.43
1:A:300:ASP:OD2	1:A:303:ASN:ND2	2.45	0.43
1:A:612:ASP:OD1	1:A:612:ASP:N	2.52	0.43
7:G:18:GLN:HG3	7:G:21:LEU:HD12	2.00	0.43
1:A:51:THR:HG22	1:A:53:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:OD1	1:A:398:ASP:N	2.51	0.42
5:E:189:LEU:HD22	5:E:194:ILE:HG21	2.01	0.42
1:A:556:ASP:OD1	1:A:647:LYS:NZ	2.48	0.42
1:A:562:ALA:HB3	1:A:568:LEU:HD13	2.01	0.42
2:B:365:VAL:O	2:B:367:ILE:N	2.52	0.42
4:D:87:THR:HG23	4:D:96:TRP:HZ3	1.84	0.42
8:H:113:VAL:HG12	8:H:115:LEU:H	1.84	0.42
2:B:613:HIS:CE1	5:E:206:ARG:HG2	2.54	0.42
4:D:311:THR:HA	4:D:387:ILE:HD11	2.02	0.42
2:B:641:ARG:NH2	2:B:648:GLU:OE1	2.53	0.42
2:B:653:THR:HG22	2:B:692:LYS:HD2	2.02	0.42
5:E:60:HIS:CD2	5:E:163:THR:HG21	2.54	0.42
5:E:66:ASP:OD2	5:E:172:SER:N	2.36	0.42
2:B:118:HIS:HD2	2:B:121:VAL:HG23	1.83	0.42
2:B:542:TYR:O	2:B:546:GLU:HB2	2.18	0.42
4:D:254:MET:HE2	4:D:258:LEU:HB3	2.00	0.42
1:A:134:SER:O	1:A:138:GLU:CB	2.67	0.42
2:B:524:LEU:HD11	2:B:595:ILE:HD11	2.02	0.42
2:B:611:VAL:HG12	2:B:612:HIS:H	1.85	0.42
4:D:99:GLN:O	4:D:107:GLY:N	2.53	0.42
1:A:87:GLU:OE2	1:A:145:LYS:NZ	2.44	0.42
2:B:564:ASN:O	5:E:175:THR:OG1	2.38	0.42
3:C:140:GLU:O	3:C:144:ALA:HB2	2.19	0.42
5:E:232:LEU:HD23	5:E:232:LEU:HA	1.89	0.42
2:B:25:MET:SD	2:B:55:LEU:HB2	2.59	0.42
5:E:293:GLN:HB2	5:E:310:LEU:HD22	2.02	0.41
4:D:136:LEU:HD12	4:D:280:ARG:HH21	1.85	0.41
6:F:255:CYS:SG	6:F:257:CYS:N	2.88	0.41
1:A:178:GLU:HG2	1:A:269:SER:HB3	2.01	0.41
1:A:184:VAL:O	1:A:188:LEU:HB2	2.20	0.41
2:B:170:LEU:HD21	2:B:194:LEU:HD21	2.01	0.41
4:D:300:THR:HG22	4:D:302:HIS:H	1.84	0.41
2:B:145:GLN:HA	2:B:148:HIS:CE1	2.55	0.41
5:E:88:LEU:HA	5:E:88:LEU:HD23	1.88	0.41
5:E:251:ARG:HE	6:F:264:ILE:HG21	1.86	0.41
3:C:172:UNK:N	3:C:186:UNK:O	2.54	0.41
5:E:166:GLU:HA	5:E:195:ARG:O	2.20	0.41
5:E:314:SER:HB3	5:E:317:HIS:CD2	2.55	0.41
4:D:53:LYS:HE3	4:D:53:LYS:HB2	1.91	0.41
2:B:117:ILE:HG23	2:B:185:ARG:HE	1.84	0.41
2:B:497:ARG:HB3	2:B:709:THR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:505:SER:HA	2:B:681:ASP:HB2	2.03	0.41
5:E:95:TYR:HD2	5:E:104:ILE:HD11	1.85	0.41
1:A:103:ILE:HD13	1:A:136:ILE:HG23	2.03	0.41
1:A:280:LEU:HG	1:A:291:LEU:HD11	2.02	0.41
2:B:464:LEU:HB2	2:B:760:LEU:HD12	2.03	0.41
2:B:537:ALA:HB1	2:B:621:PHE:HE2	1.86	0.41
3:C:403:SER:HB2	6:F:23:GLY:HA3	2.03	0.41
4:D:414:SER:O	4:D:439:ARG:NH1	2.45	0.41
1:A:568:LEU:HD11	1:A:606:PHE:HB3	2.02	0.41
2:B:672:THR:OG1	3:C:362:ASP:OD1	2.33	0.41
1:A:203:GLU:OE2	8:H:177:ARG:NH1	2.54	0.40
2:B:517:ILE:HG23	2:B:548:THR:HG23	2.04	0.40
5:E:85:LEU:HD12	5:E:85:LEU:HA	1.94	0.40
3:C:389:ILE:HG13	6:F:259:ARG:HE	1.86	0.40
1:A:476:LYS:O	1:A:478:VAL:N	2.54	0.40
1:A:531:ILE:O	1:A:535:THR:OG1	2.28	0.40
1:A:505:VAL:HA	1:A:657:ALA:HB3	2.03	0.40
4:D:424:HIS:CD2	4:D:451:VAL:HG22	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/653 (97%)	569 (90%)	62 (10%)	1 (0%)	43	72
2	B	731/760 (96%)	641 (88%)	90 (12%)	0	100	100
3	C	236/548 (43%)	200 (85%)	34 (14%)	2 (1%)	16	48
4	D	450/462 (97%)	406 (90%)	43 (10%)	1 (0%)	43	72
5	E	309/366 (84%)	276 (89%)	33 (11%)	0	100	100
6	F	259/308 (84%)	244 (94%)	15 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	64/71 (90%)	59 (92%)	5 (8%)	0	100	100
8	H	208/309 (67%)	181 (87%)	25 (12%)	2 (1%)	12	43
All	All	2889/3477 (83%)	2576 (89%)	307 (11%)	6 (0%)	44	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	213	HIS
8	H	57	ASN
8	H	7	PRO
3	C	212	PRO
4	D	190	PRO
1	A	477	ILE

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	558/559 (100%)	558 (100%)	0	100	100
2	B	640/643 (100%)	638 (100%)	2 (0%)	86	83
3	C	176/334 (53%)	176 (100%)	0	100	100
4	D	384/399 (96%)	383 (100%)	1 (0%)	86	83
5	E	279/279 (100%)	279 (100%)	0	100	100
6	F	234/272 (86%)	233 (100%)	1 (0%)	84	81
7	G	59/64 (92%)	59 (100%)	0	100	100
8	H	158/283 (56%)	158 (100%)	0	100	100
All	All	2488/2833 (88%)	2484 (100%)	4 (0%)	85	86

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	444	ILE

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Mol	Chain	Res	Type
2	B	678	VAL
4	D	215	PHE
6	F	157	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	HIS
1	A	187	HIS
1	A	591	GLN
1	A	595	ASN
1	A	598	HIS
1	A	677	GLN
2	B	37	HIS
2	B	118	HIS
2	B	201	HIS
2	B	210	HIS
2	B	237	HIS
2	B	238	ASN
2	B	260	GLN
2	B	328	HIS
2	B	348	HIS
2	B	452	GLN
2	B	499	ASN
2	B	562	GLN
2	B	733	GLN
3	C	524	HIS
4	D	18	ASN
4	D	54	ASN
4	D	97	HIS
4	D	181	GLN
4	D	239	GLN
4	D	390	GLN
4	D	424	HIS
5	E	220	HIS
5	E	256	GLN
5	E	257	HIS
5	E	317	HIS
5	E	356	HIS
6	F	18	ASN
6	F	108	ASN
6	F	187	GLN

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Mol	Chain	Res	Type
6	F	204	GLN
6	F	225	GLN
6	F	248	HIS
8	H	117	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](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SF4	B	1000	2	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SF4	B	1000	2	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	203:GLU	C	248:UNK	N	29.49
1	E	274:UNK	C	281:UNK	N	8.01

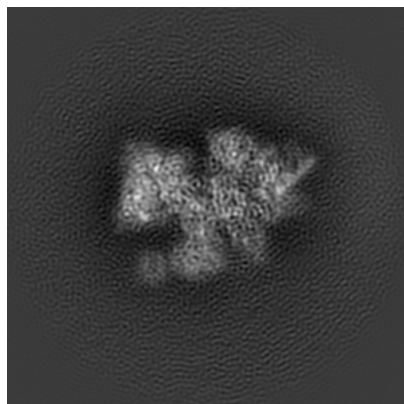
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0452. These allow visual inspection of the internal detail of the map and identification of artifacts.

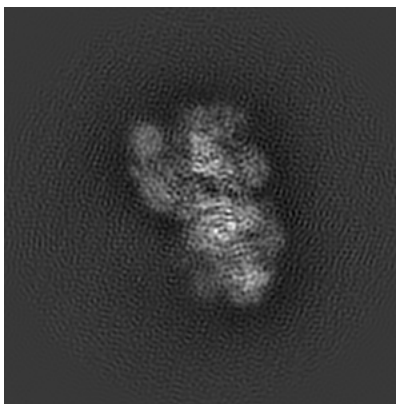
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

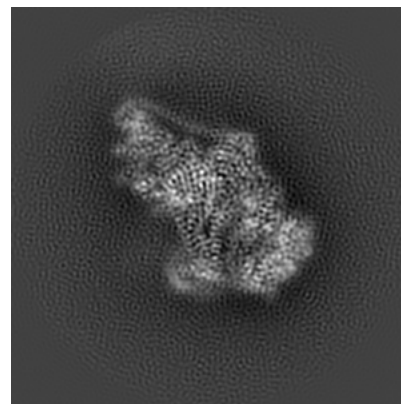
6.1.1 Primary map



X

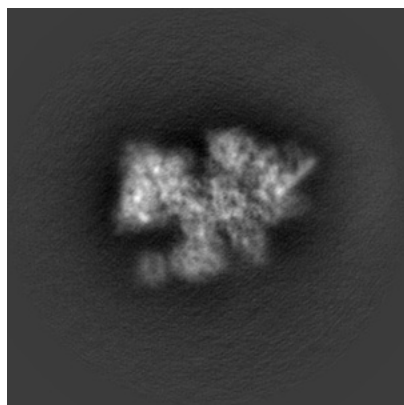


Y

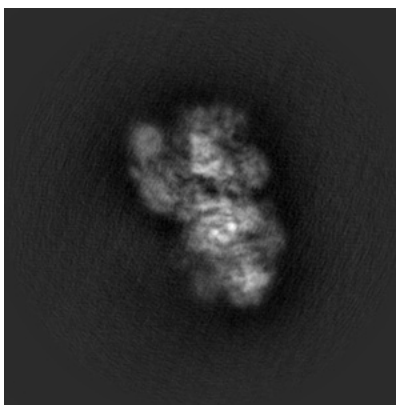


Z

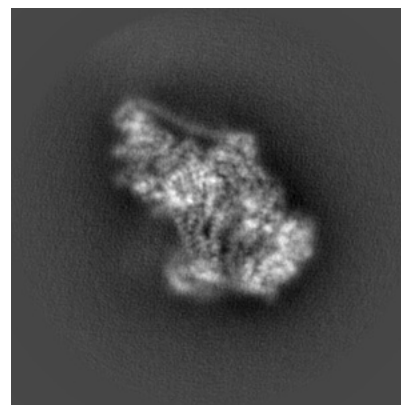
6.1.2 Raw map



X



Y

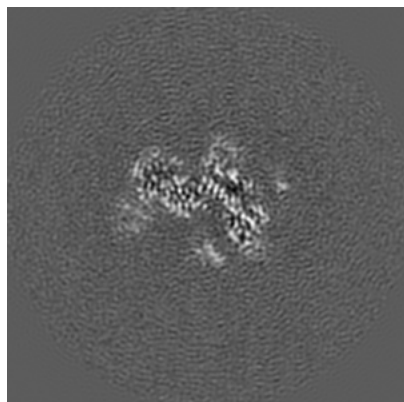


Z

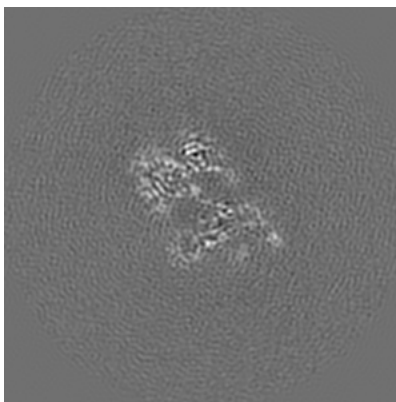
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

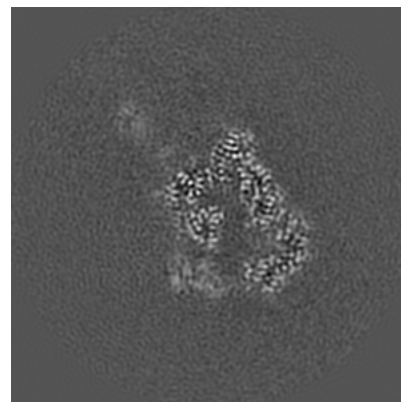
6.2.1 Primary map



X Index: 128

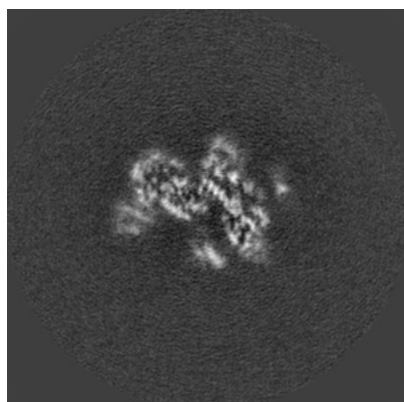


Y Index: 128

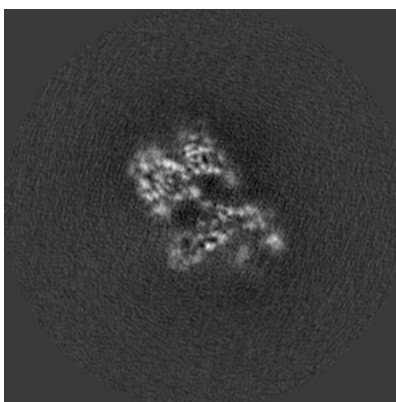


Z Index: 128

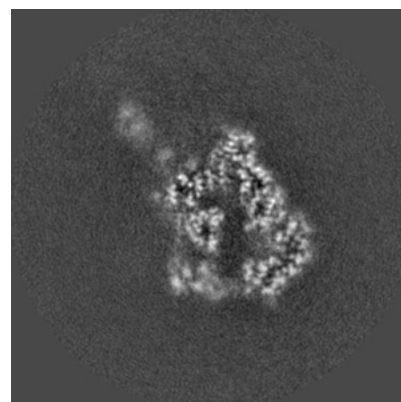
6.2.2 Raw map



X Index: 128



Y Index: 128

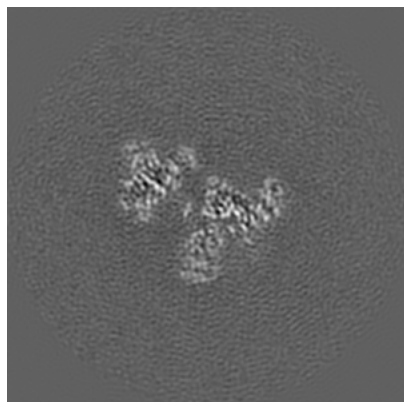


Z Index: 128

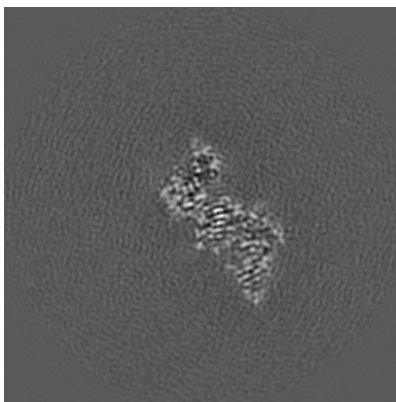
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

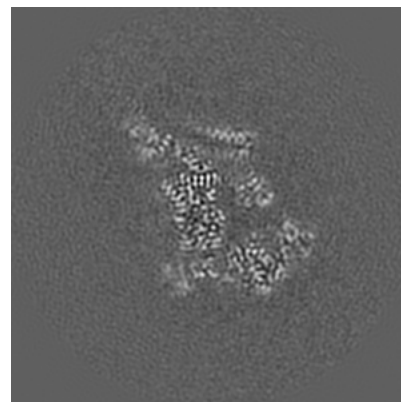
6.3.1 Primary map



X Index: 151

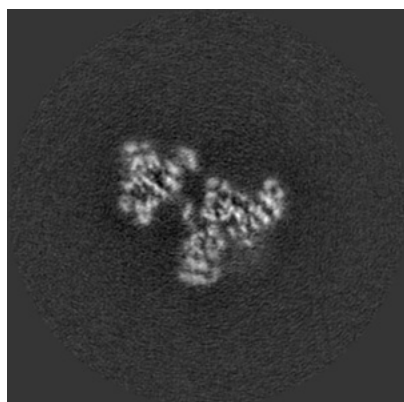


Y Index: 146

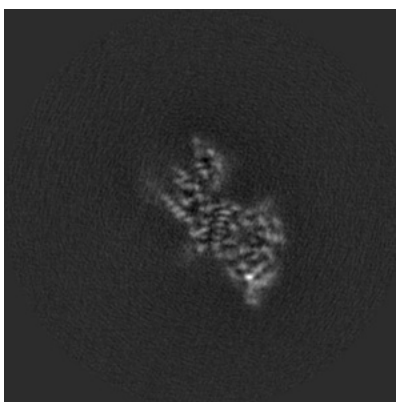


Z Index: 138

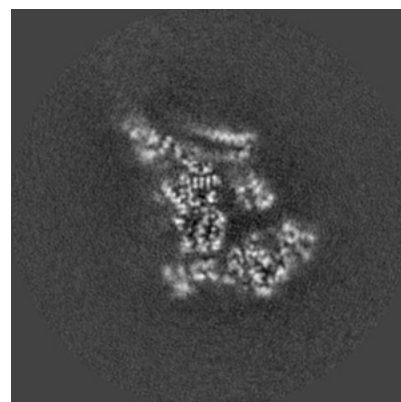
6.3.2 Raw map



X Index: 151



Y Index: 143

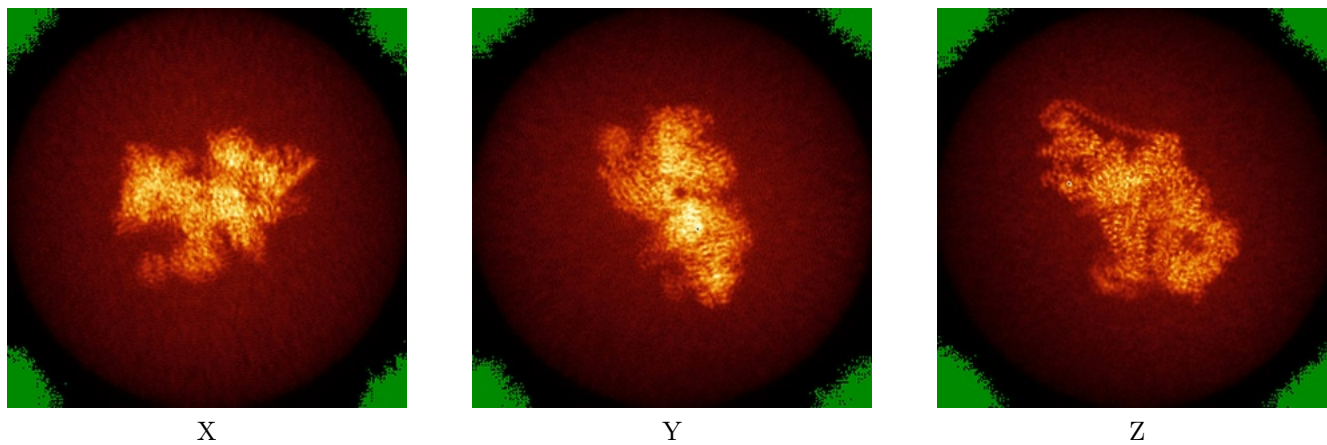


Z Index: 138

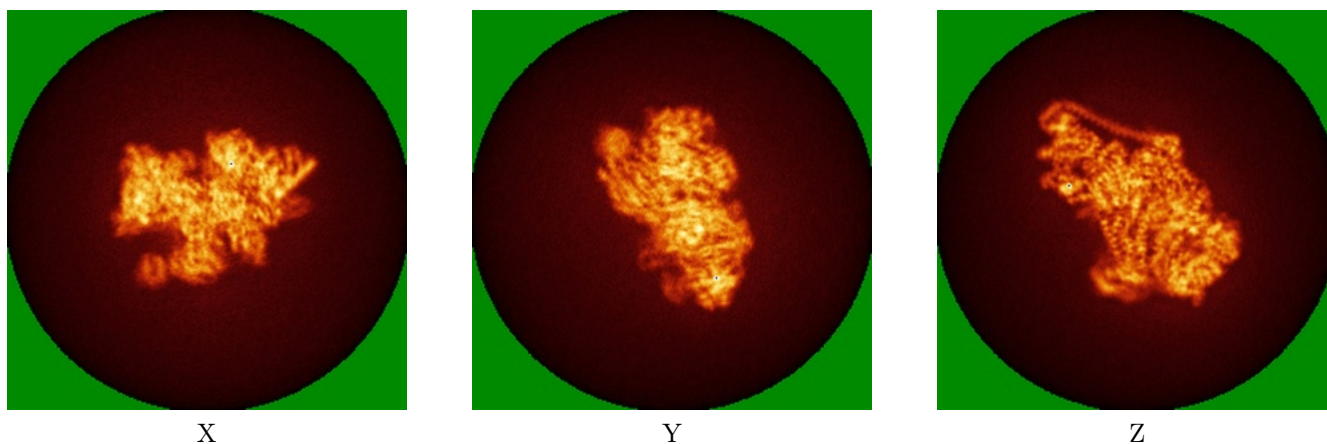
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

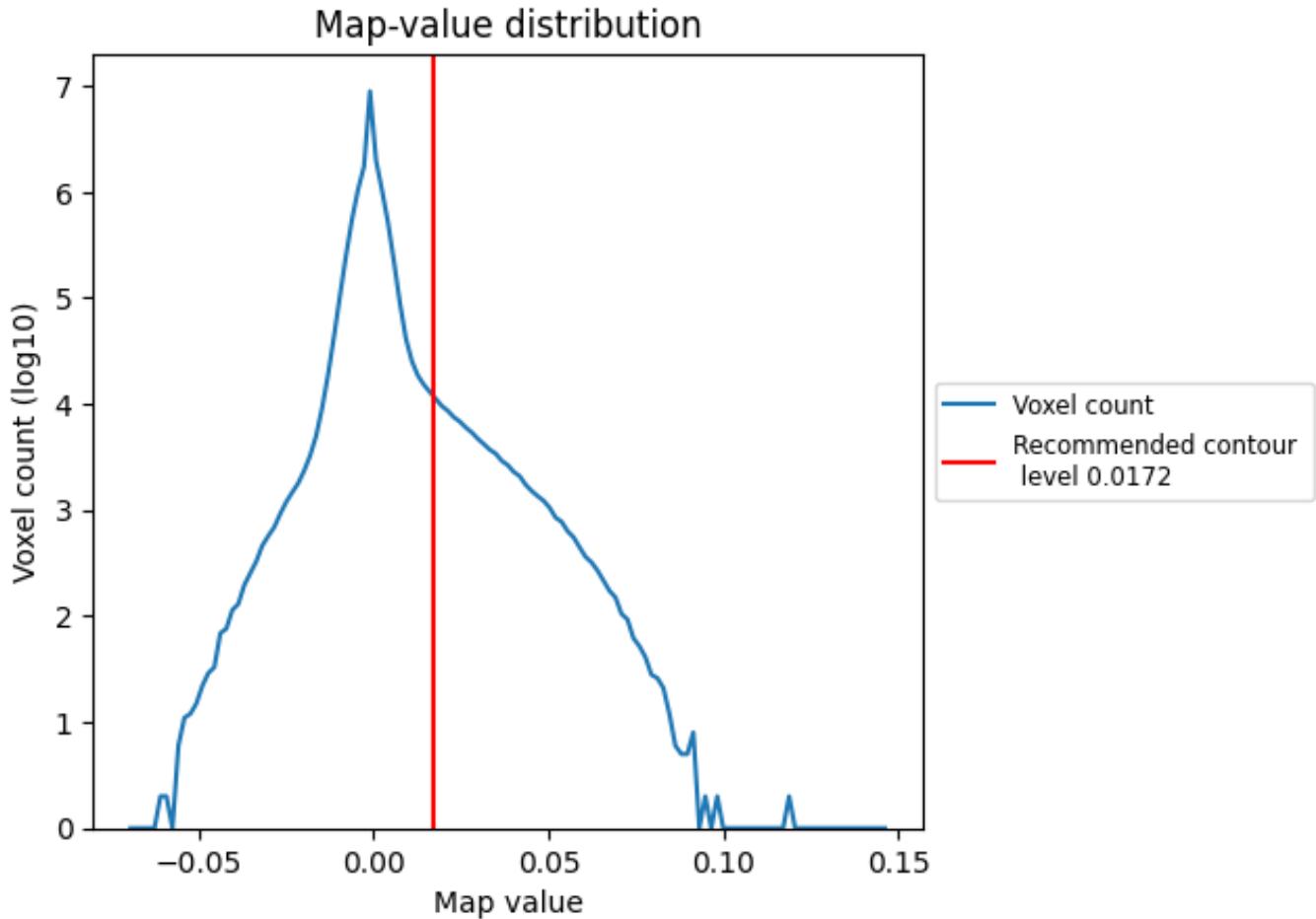
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

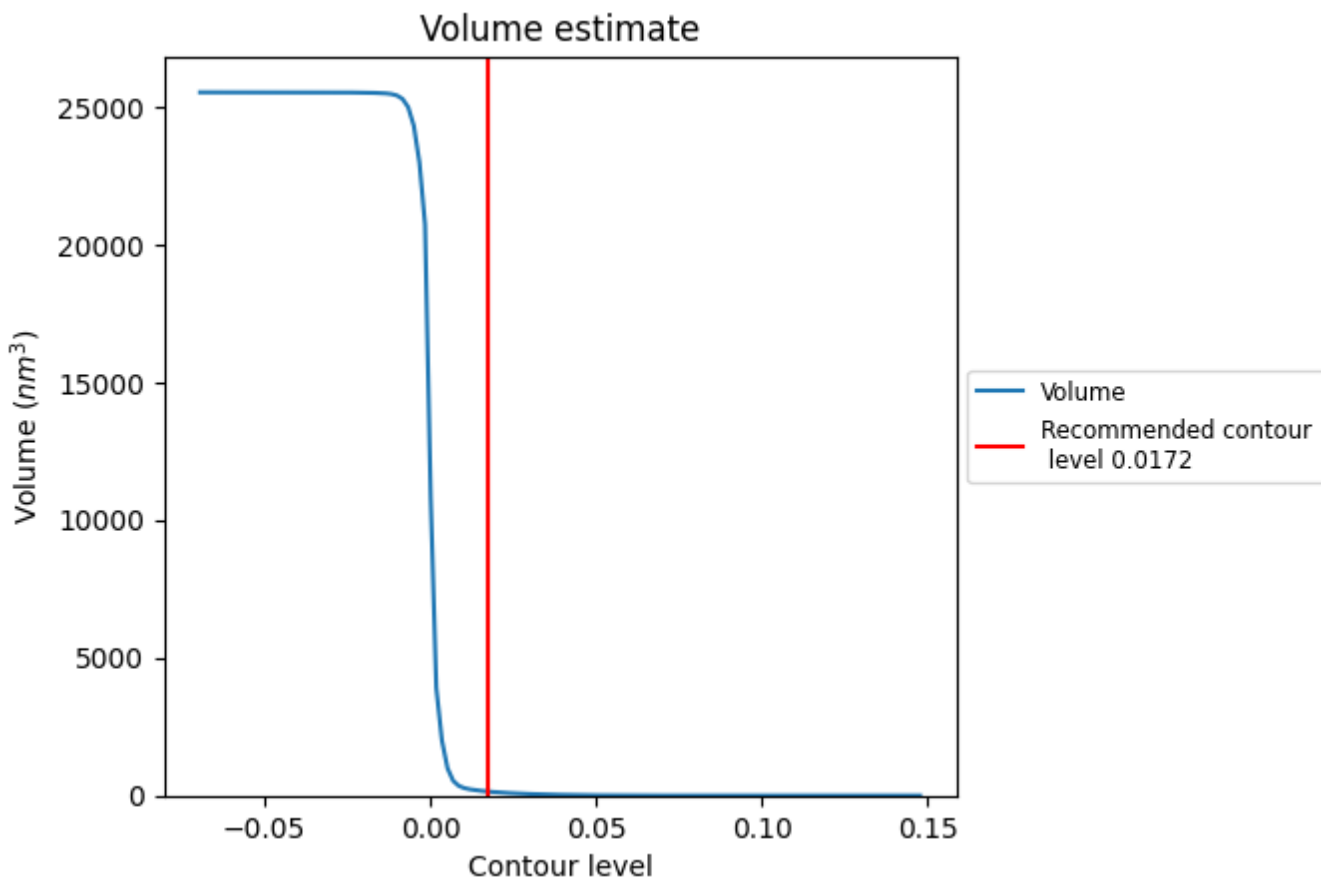
This section contains the results of statistical analysis of the map.

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.

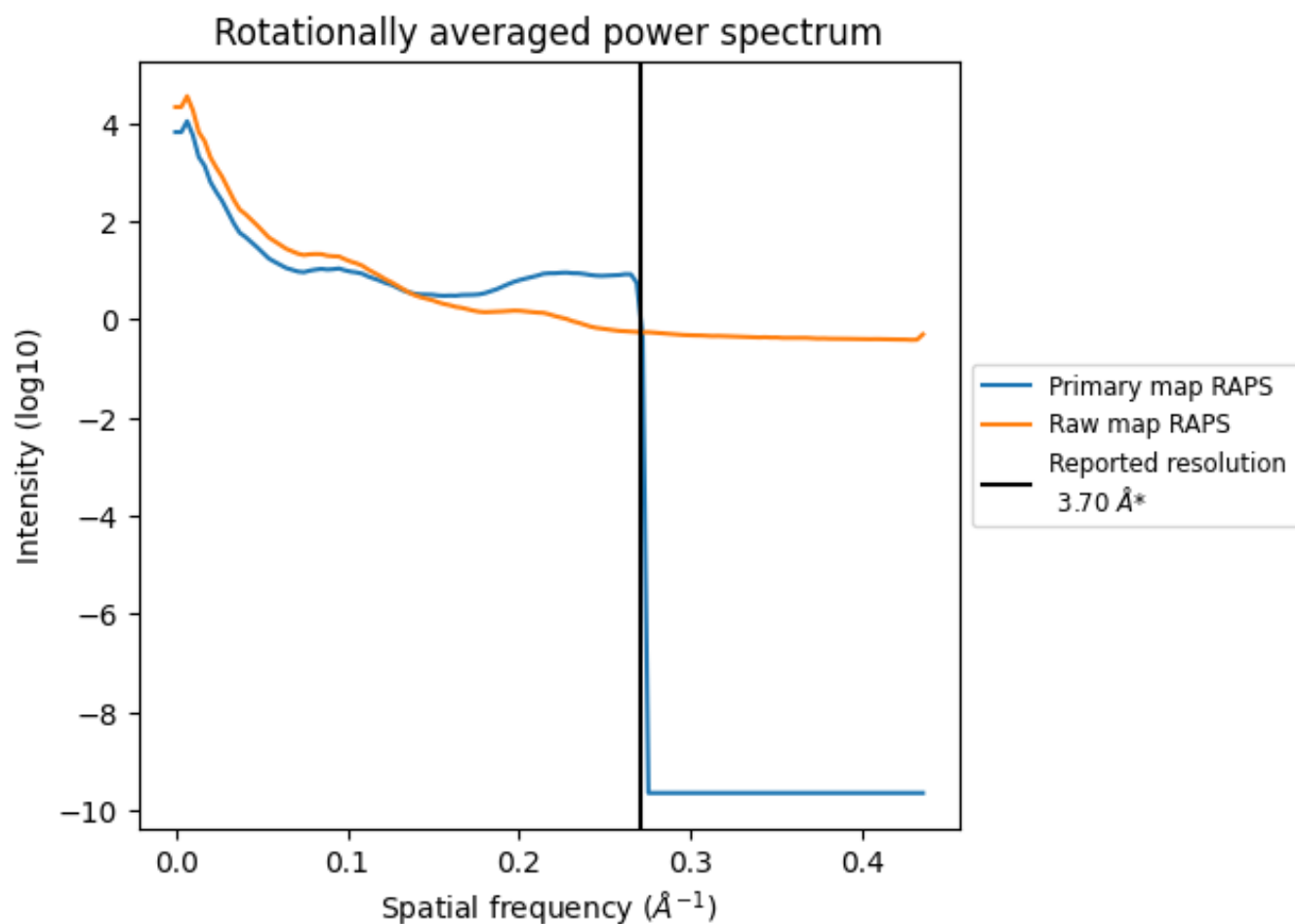
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 149 nm^3 ; this corresponds to an approximate mass of 135 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 i

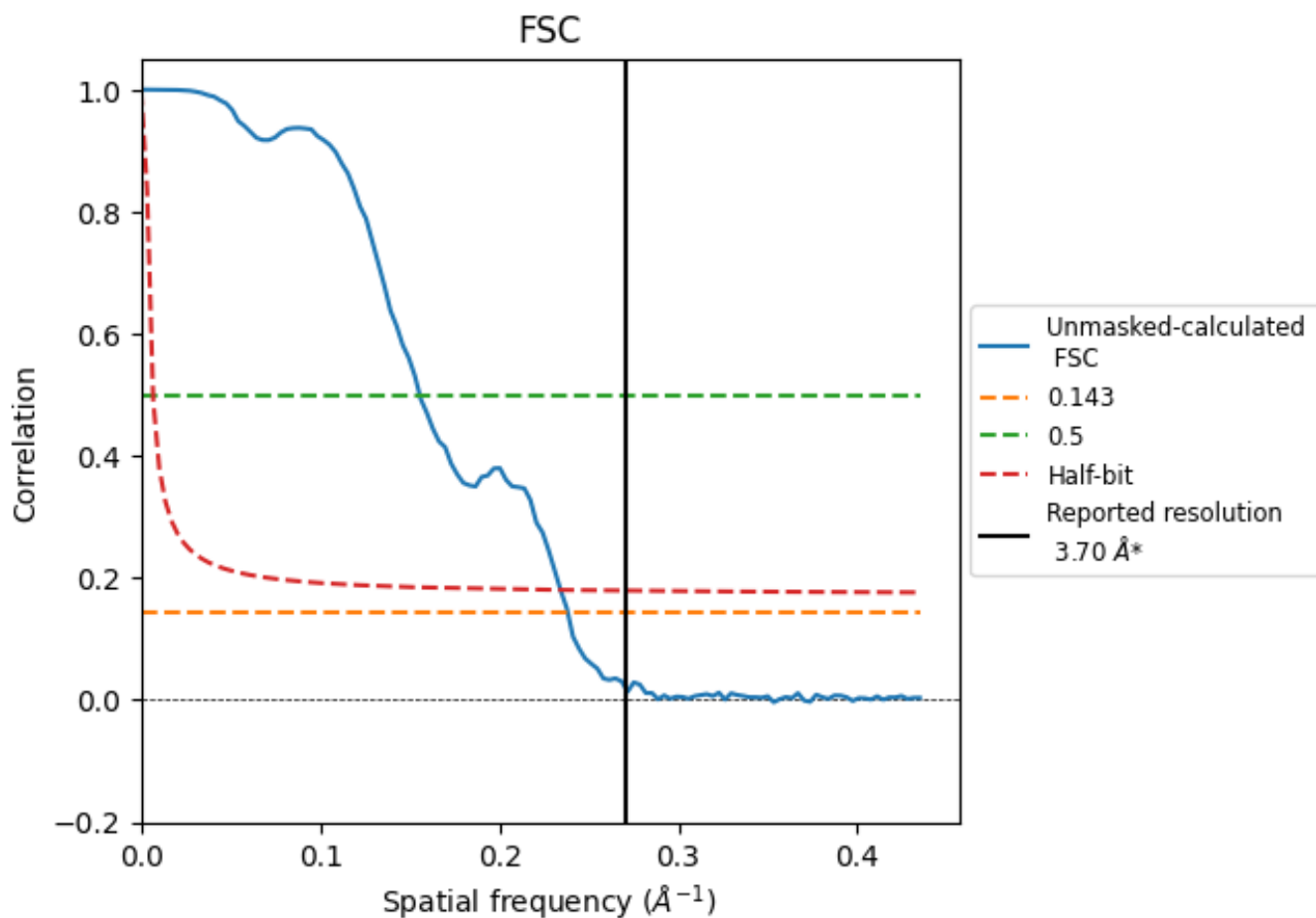


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270\AA^{-1}

8.2 Resolution estimates [i](#)

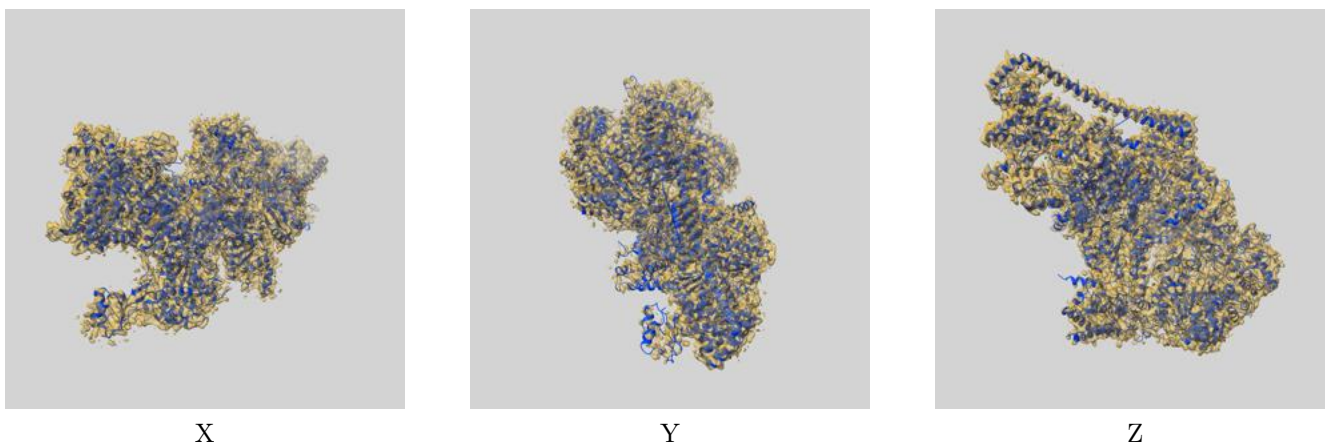
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.20	6.43	4.27

*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 4.20 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

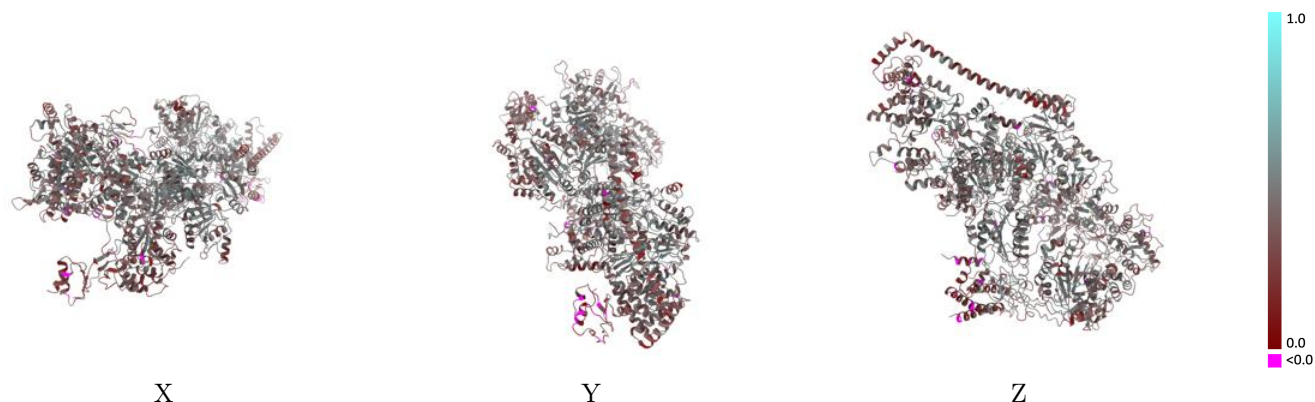
This section contains information regarding the fit between EMDB map EMD-0452 and PDB model 6NMI. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



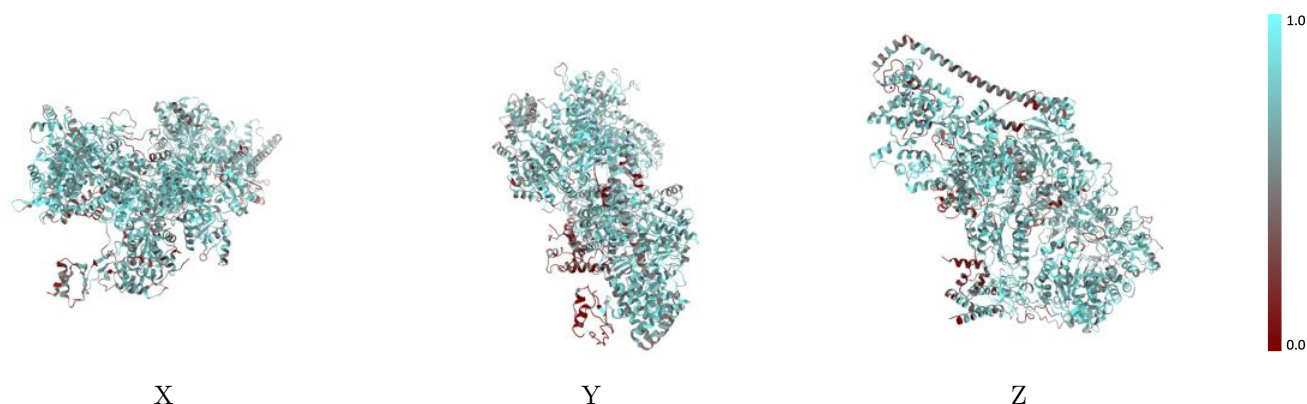
The images above show the 3D surface view of the map at the recommended contour level 0.0172 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



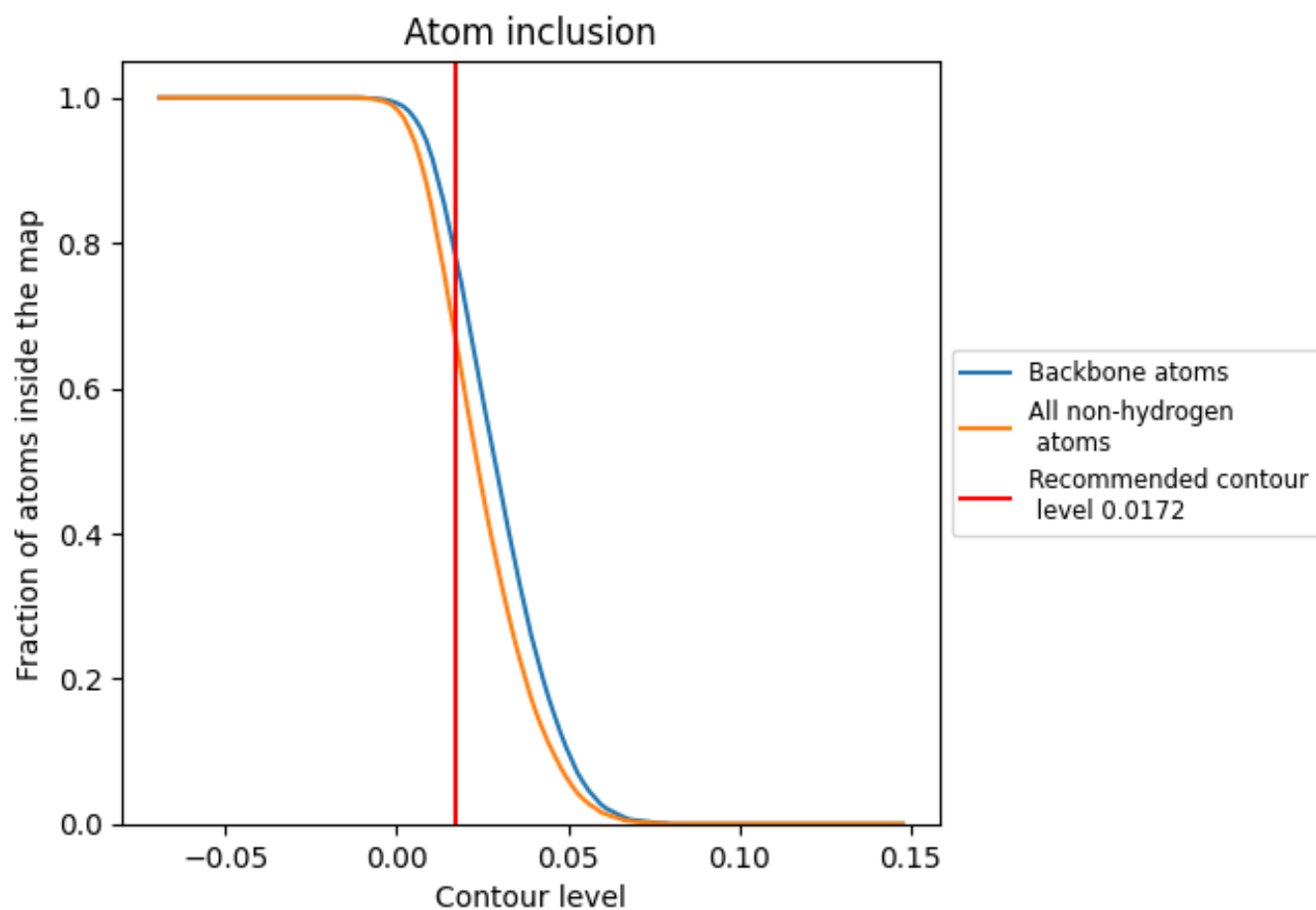
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0172).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 67% 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 (0.0172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6680	 0.4040
A	 0.6830	 0.4120
B	 0.7420	 0.4390
C	 0.4600	 0.3290
D	 0.6940	 0.4080
E	 0.7090	 0.4370
F	 0.7390	 0.4360
G	 0.5650	 0.3200
H	 0.5000	 0.2960

