



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 07:35 PM UTC

PDB ID : 9PD5 / pdb_00009pd5
EMDB ID : EMD-71526
Title : NER dual incision complex - NoF
Authors : Li, C.L.; Kim, J.; Yang, W.
Deposited on : 2025-06-30
Resolution : 5.70 Å(reported)
Based on initial model : 8ebt

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:

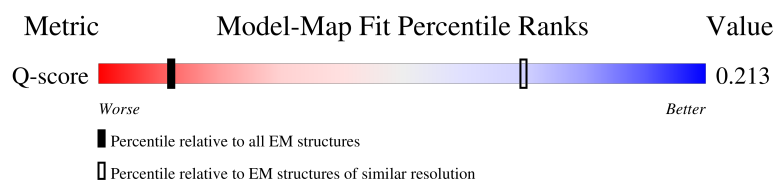
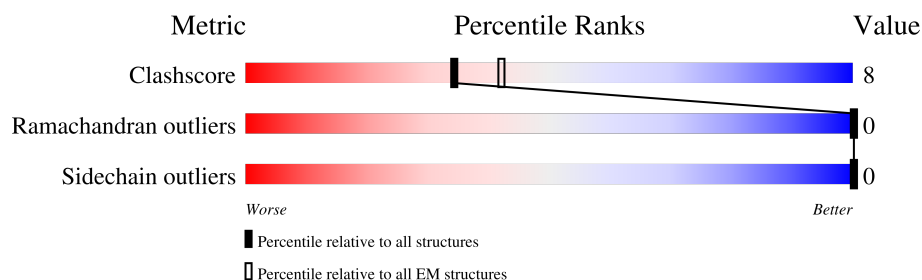
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 5.70 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	503 (5.20 - 6.20)

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	782	
2	B	768	
3	C	548	
4	D	462	

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Mol	Chain	Length	Quality of chain
5	E	395	<div><div></div><div>16%</div><div>77%</div><div>16%</div><div>7%</div></div>
6	F	308	<div><div></div><div>8%</div><div>63%</div><div>21%</div><div>16%</div></div>
7	G	71	<div><div></div><div>20%</div><div>65%</div><div>28%</div><div>7%</div></div>
8	K	273	<div><div></div><div>32%</div><div>48%</div><div>11%</div><div>41%</div></div>
9	L	93	<div><div></div><div>17%</div><div>16%</div><div>67%</div></div>
10	M	94	<div><div></div><div>19%</div><div>77%</div></div>
11	S	1186	<div><div></div><div>5%</div><div>94%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23740 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 TFIIF basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	604	Total	C	N	O	S	0	0
			4882	3119	845	889	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	702	Total	C	N	O	S	0	0
			5659	3622	985	1023	29		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	761	ASP	-	expression tag	UNP P18074
B	762	TYR	-	expression tag	UNP P18074
B	763	LYS	-	expression tag	UNP P18074
B	764	ASP	-	expression tag	UNP P18074
B	765	ASP	-	expression tag	UNP P18074
B	766	ASP	-	expression tag	UNP P18074
B	767	ASP	-	expression tag	UNP P18074
B	768	LYS	-	expression tag	UNP P18074

- Molecule 3 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	154	Total	C	N	O	S	0	0
			1234	779	216	231	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	434	Total	C	N	O	S	0	0
			3483	2245	605	620	13		

- Molecule 5 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	369	Total	C	N	O	S	0	0
			2896	1828	496	545	27		

- Molecule 6 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	258	Total	C	N	O	S	0	0
			2034	1301	337	377	19		

- Molecule 7 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	66	Total	C	N	O	S	0	0
			522	337	82	100	3		

- Molecule 8 is a protein called DNA repair protein complementing XP-A cells.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	160	Total	C	N	O	S	0	0
			1348	843	235	256	14		

- Molecule 9 is a DNA chain called DNA Cy5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	31	Total	C	N	O	P	0	0
			629	301	107	190	31		

- Molecule 10 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	22	Total	C	N	O	P	0	0
			454	216	87	129	22		

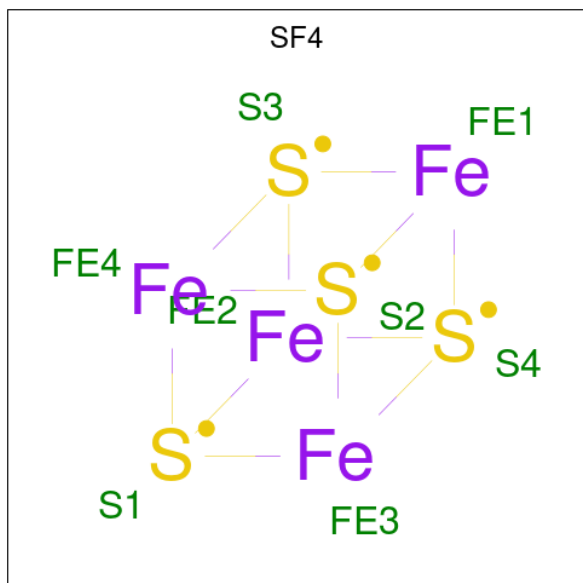
- Molecule 11 is a protein called DNA excision repair protein ERCC-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	69	Total	C	N	O	S	0	0
			585	366	100	116	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1053	ARG	GLY	variant	UNP P28715
S	1080	ARG	GLY	variant	UNP P28715

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

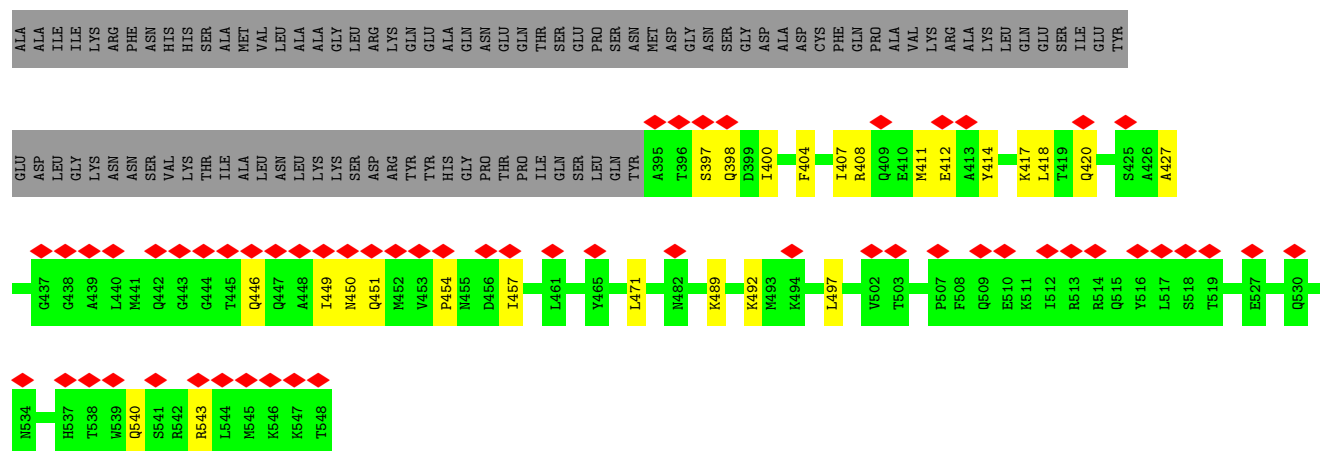


Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	Fe	S	0
			8	4	4	

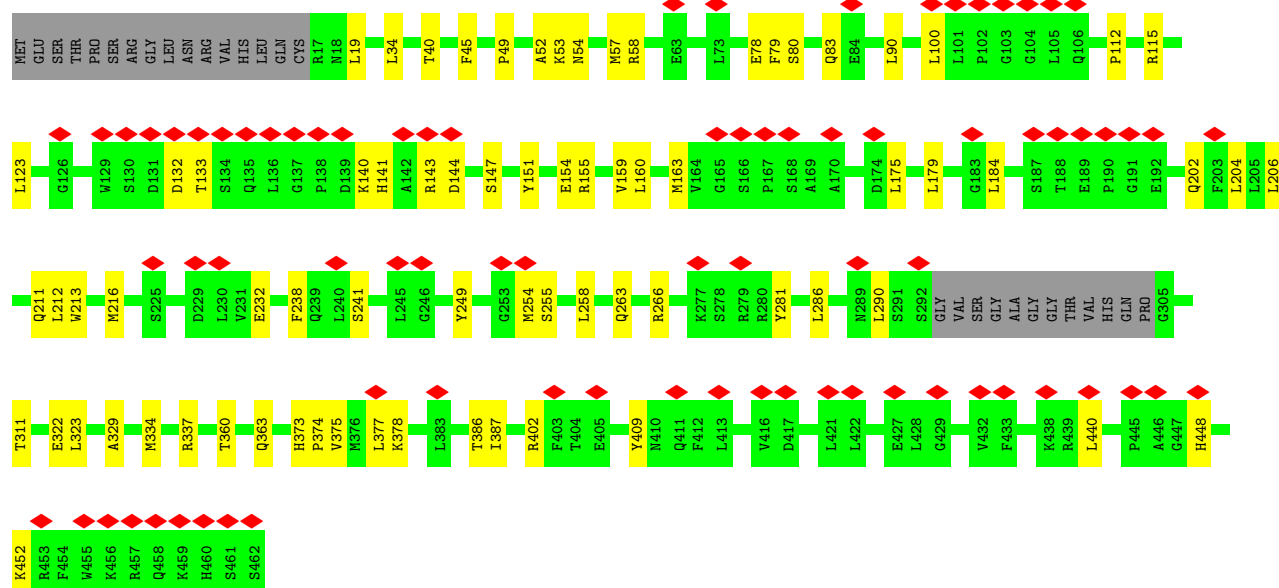
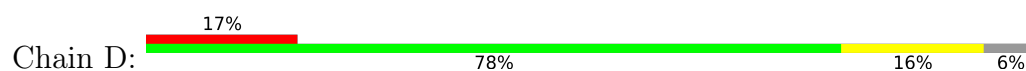
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	E	3	Total	Zn	0
			3	3	
13	F	2	Total	Zn	0
			2	2	
13	K	1	Total	Zn	0
			1	1	

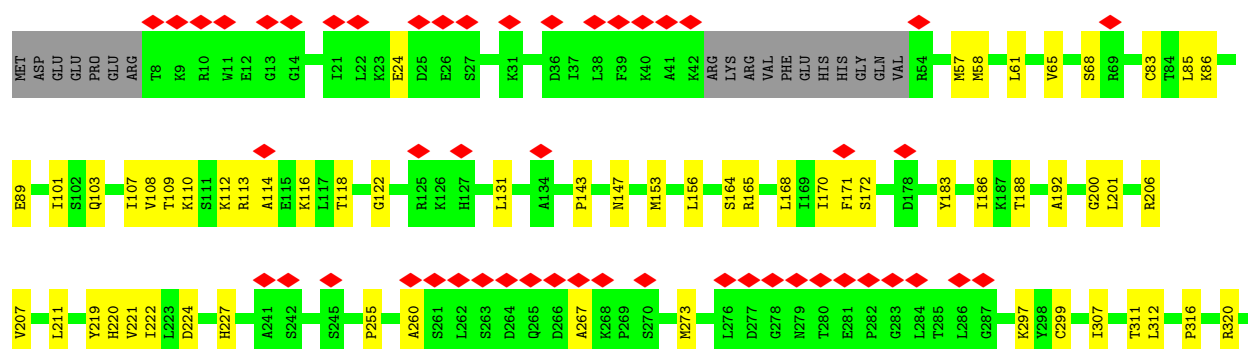
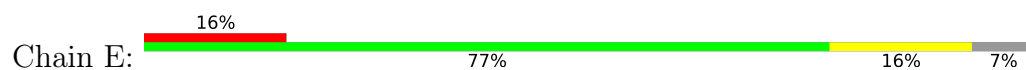


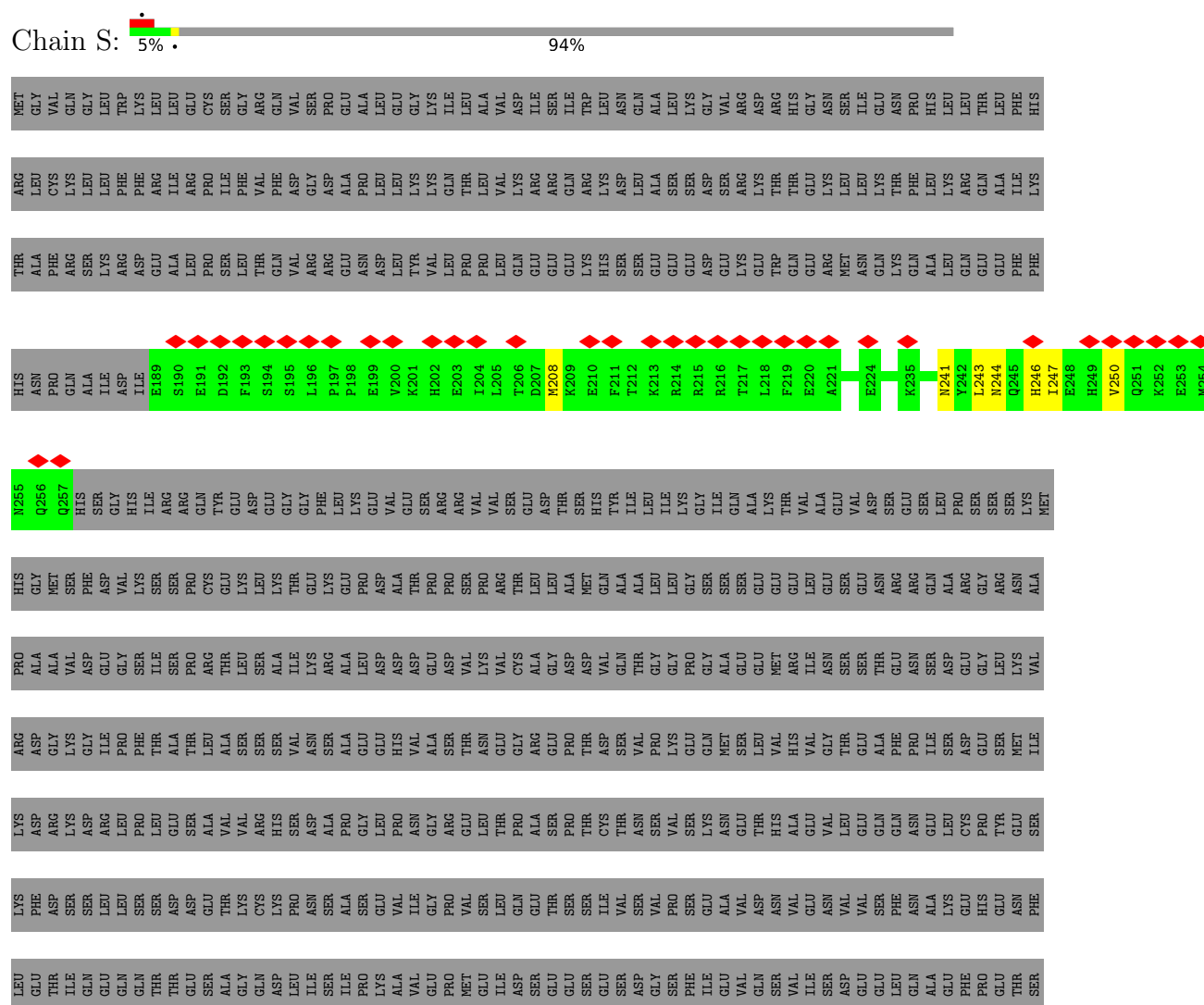


• Molecule 4: General transcription factor IIH subunit 4, p52



• Molecule 5: General transcription factor IIH subunit 2







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64352	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.007	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.005	Depositor
Map size (Å)	378.72003, 378.72003, 378.72003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	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, ZN

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	0.08	0/4985	0.26	0/6734
2	B	0.13	0/5780	0.26	0/7821
3	C	0.09	0/1257	0.24	0/1696
4	D	0.07	0/3564	0.20	0/4827
5	E	0.08	0/2960	0.22	0/4006
6	F	0.08	0/2070	0.22	0/2803
7	G	0.09	0/528	0.26	0/713
8	K	0.07	0/1373	0.22	0/1830
9	L	0.19	0/702	0.40	0/1080
10	M	0.17	0/510	0.33	0/785
11	S	0.09	0/596	0.21	0/797
All	All	0.10	0/24325	0.25	0/33092

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	4882	0	4923	106	0
2	B	5659	0	5699	95	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1234	0	1250	17	0
4	D	3483	0	3526	52	0
5	E	2896	0	2857	40	0
6	F	2034	0	2050	44	0
7	G	522	0	531	18	0
8	K	1348	0	1323	19	0
9	L	629	0	352	15	0
10	M	454	0	248	3	0
11	S	585	0	565	4	0
12	B	8	0	0	0	0
13	E	3	0	0	0	0
13	F	2	0	0	0	0
13	K	1	0	0	0	0
All	All	23740	0	23324	382	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 8.

All (382) 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:375:LYS:HE2	1:A:391:ARG:CG	2.14	0.77
1:A:375:LYS:HE2	1:A:391:ARG:HG3	1.65	0.76
1:A:393:THR:O	1:A:393:THR:HG22	1.82	0.76
2:B:5:VAL:HG12	2:B:6:ASP:N	1.97	0.75
2:B:5:VAL:HG12	2:B:6:ASP:H	1.51	0.74
2:B:56:ILE:HG12	2:B:70:LEU:HD13	1.68	0.74
7:G:46:ILE:HG23	7:G:48:GLU:OE1	1.88	0.74
6:F:59:VAL:HG23	6:F:70:LEU:HB2	1.71	0.72
2:B:591:GLY:N	5:E:207:VAL:HG21	2.05	0.71
2:B:107:LEU:HD13	2:B:109:LEU:CD2	2.20	0.71
4:D:34:LEU:HB3	4:D:40:THR:HG21	1.72	0.70
2:B:70:LEU:HD23	2:B:204:VAL:HG23	1.74	0.70
2:B:5:VAL:CG1	2:B:6:ASP:H	2.07	0.68
4:D:202:GLN:O	4:D:363:GLN:NE2	2.27	0.67
3:C:407:ILE:HG21	6:F:23:GLY:HA2	1.77	0.66
1:A:313:THR:HG21	2:B:732:ASP:HA	1.79	0.65
5:E:112:LYS:O	5:E:147:ASN:ND2	2.30	0.65
7:G:46:ILE:HG23	7:G:48:GLU:CD	2.22	0.64
4:D:311:THR:HA	4:D:387:ILE:HD11	1.80	0.64
7:G:4:VAL:N	8:K:271:GLU:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:110:LYS:O	5:E:113:ARG:NH1	2.31	0.63
7:G:17:LYS:HE3	7:G:43:VAL:HG22	1.79	0.63
2:B:641:ARG:NH1	8:K:177:ASP:OD2	2.30	0.63
6:F:238:ARG:HB3	6:F:243:LEU:HD11	1.80	0.63
2:B:5:VAL:CG1	2:B:6:ASP:N	2.61	0.62
2:B:40:LEU:HD23	2:B:455:ILE:HD11	1.81	0.62
1:A:84:ILE:HB	1:A:116:TYR:HB2	1.82	0.61
4:D:112:PRO:HA	4:D:115:ARG:HE	1.65	0.61
4:D:212:LEU:HB3	4:D:290:LEU:HD13	1.82	0.61
2:B:418:ILE:HG13	2:B:420:PRO:HD3	1.82	0.60
4:D:206:LEU:O	4:D:211:GLN:NE2	2.34	0.60
1:A:317:ARG:HD2	1:A:319:TYR:HE2	1.67	0.60
1:A:375:LYS:HD2	1:A:389:ILE:CG2	2.32	0.59
5:E:297:LYS:NZ	5:E:299:CYS:SG	2.74	0.59
7:G:46:ILE:HG12	7:G:48:GLU:OE1	2.02	0.59
8:K:132:ALA:HA	8:K:136:HIS:HB2	1.84	0.59
8:K:138:LEU:HB3	8:K:180:LEU:HB3	1.84	0.59
3:C:454:PRO:HD2	3:C:457:ILE:HD12	1.85	0.59
6:F:175:MET:SD	6:F:175:MET:N	2.76	0.59
6:F:68:ARG:HD3	6:F:118:LEU:HD13	1.83	0.59
5:E:116:LYS:NZ	5:E:118:THR:O	2.35	0.59
6:F:61:ALA:HB2	6:F:70:LEU:HD11	1.85	0.59
6:F:67:SER:O	6:F:139:LYS:NZ	2.35	0.59
2:B:460:THR:HG21	2:B:662:GLN:HA	1.85	0.59
8:K:273:MET:SD	8:K:273:MET:N	2.76	0.58
3:C:397:SER:OG	3:C:398:GLN:OE1	2.18	0.58
1:A:106:PRO:HG3	1:A:109:ARG:HH11	1.68	0.58
2:B:57:MET:SD	2:B:60:GLN:NE2	2.76	0.58
6:F:208:ASP:HB2	6:F:249:VAL:HG21	1.85	0.58
3:C:450:ASN:OD1	3:C:451:GLN:NE2	2.36	0.58
2:B:586:GLU:O	2:B:590:ASN:ND2	2.37	0.58
1:A:74:ARG:HB2	1:A:145:LYS:HB3	1.87	0.57
1:A:76:LEU:HD11	1:A:100:LEU:HD21	1.85	0.57
1:A:82:GLY:O	1:A:83:HIS:ND1	2.37	0.57
2:B:43:PRO:HG2	2:B:483:MET:HG2	1.87	0.57
7:G:46:ILE:CG2	7:G:48:GLU:OE1	2.53	0.57
1:A:375:LYS:HE2	1:A:391:ARG:HG2	1.85	0.57
1:A:562:ALA:HB3	1:A:568:LEU:HD13	1.87	0.57
5:E:57:MET:SD	5:E:57:MET:N	2.78	0.57
2:B:458:SER:HB3	2:B:461:LEU:HG	1.87	0.56
1:A:705:THR:N	1:A:708:GLU:OE2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:LEU:O	1:A:551:HIS:ND1	2.30	0.56
1:A:77:TRP:HB2	1:A:85:PHE:HB2	1.87	0.56
4:D:255:SER:H	4:D:258:LEU:HD12	1.70	0.55
5:E:224:ASP:OD1	5:E:227:HIS:ND1	2.28	0.55
1:A:472:ARG:H	1:A:477:ILE:HD11	1.71	0.55
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.89	0.55
1:A:375:LYS:HE3	1:A:390:CYS:O	2.07	0.55
1:A:629:HIS:O	1:A:676:ARG:NH1	2.40	0.55
1:A:185:ILE:HD13	1:A:188:LEU:HD21	1.89	0.55
2:B:559:GLU:OE2	2:B:560:ASN:ND2	2.40	0.55
8:K:154:ASP:O	8:K:189:ARG:NH1	2.40	0.54
1:A:439:ILE:HG23	1:A:466:LEU:HD13	1.89	0.54
4:D:409:TYR:OH	4:D:448:HIS:ND1	2.37	0.54
3:C:408:ARG:NH1	3:C:412:GLU:OE1	2.32	0.54
8:K:107:GLU:OE2	8:K:135:LYS:NZ	2.41	0.54
4:D:19:LEU:HB2	4:D:213:TRP:HZ2	1.73	0.54
5:E:103:GLN:OE1	5:E:122:GLY:N	2.41	0.54
5:E:186:ILE:HD11	5:E:211:LEU:HA	1.87	0.54
2:B:441:SER:OG	2:B:470:ILE:O	2.25	0.54
6:F:235:GLN:HA	6:F:238:ARG:HB2	1.88	0.54
1:A:168:LEU:HB2	1:A:291:LEU:HD23	1.89	0.53
4:D:132:ASP:OD1	4:D:133:THR:N	2.41	0.53
7:G:29:LEU:HD12	7:G:31:LYS:H	1.73	0.53
4:D:45:PHE:HZ	4:D:57:MET:HE3	1.73	0.53
1:A:274:GLN:NE2	1:A:456:THR:O	2.42	0.53
10:M:48:DA:H2'	10:M:49:DT:H71	1.90	0.53
2:B:117:ILE:HG23	2:B:181:LYS:HE2	1.90	0.53
6:F:8:LEU:HD23	6:F:54:SER:HB2	1.91	0.53
2:B:686:ARG:NH1	9:L:54:DC:OP1	2.42	0.53
3:C:404:PHE:HE1	6:F:20:ILE:HA	1.74	0.53
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.91	0.53
8:K:139:ILE:HG23	8:K:183:LYS:HZ2	1.74	0.53
1:A:568:LEU:HD22	1:A:608:SER:HB3	1.91	0.52
2:B:50:VAL:HG12	2:B:86:GLU:HB3	1.91	0.52
6:F:191:ILE:H	6:F:210:THR:HG21	1.73	0.52
2:B:637:LEU:HB3	2:B:648:GLU:HG2	1.91	0.52
1:A:664:SER:O	1:A:667:THR:OG1	2.27	0.52
4:D:360:THR:HG23	4:D:363:GLN:H	1.73	0.52
1:A:525:ILE:HG12	1:A:529:LYS:HB2	1.91	0.52
1:A:415:HIS:HB2	1:A:419:ARG:HH21	1.75	0.52
1:A:633:ARG:HD3	1:A:678:ARG:HE	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:201:LEU:HG	5:E:222:ILE:HD12	1.91	0.52
6:F:21:TRP:NE1	6:F:25:GLN:OE1	2.43	0.52
1:A:448:ALA:HB1	10:M:54:DA:H5''	1.91	0.52
1:A:368:ALA:HB2	1:A:393:THR:HG21	1.92	0.51
2:B:496:GLY:N	2:B:708:LEU:O	2.38	0.51
2:B:647:ARG:HE	2:B:649:ASN:HB3	1.75	0.51
4:D:402:ARG:HE	7:G:11:GLU:HB3	1.75	0.51
5:E:333:GLU:OE2	5:E:356:HIS:ND1	2.43	0.51
8:K:123:LEU:HD12	8:K:124:PRO:HD2	1.92	0.51
4:D:100:LEU:HD23	4:D:100:LEU:H	1.75	0.51
4:D:329:ALA:HA	4:D:334:MET:HE3	1.93	0.51
5:E:382:CYS:HB3	5:E:385:CYS:SG	2.50	0.51
2:B:627:TYR:HA	9:L:55:DA:H2''	1.93	0.51
2:B:70:LEU:HD23	2:B:204:VAL:CG2	2.40	0.51
2:B:122:THR:N	2:B:123:PRO:HD2	2.26	0.51
3:C:418:LEU:HD22	4:D:123:LEU:HB3	1.93	0.51
1:A:304:PRO:HG2	1:A:360:ARG:HD2	1.92	0.50
2:B:438:MET:HE1	2:B:635:ALA:HB1	1.93	0.50
4:D:440:LEU:HD13	7:G:38:ILE:HG22	1.92	0.50
4:D:377:LEU:HD22	6:F:154:ASN:HB3	1.94	0.50
5:E:58:MET:HE1	5:E:103:GLN:HG2	1.92	0.50
5:E:219:TYR:O	5:E:220:HIS:ND1	2.44	0.50
9:L:42:DC:H2'	9:L:43:DA:H8	1.77	0.50
1:A:375:LYS:HZ1	1:A:407:ILE:HB	1.76	0.50
2:B:354:PRO:HG3	2:B:415:THR:HA	1.92	0.50
3:C:417:LYS:HD2	3:C:420:GLN:HB2	1.93	0.50
1:A:74:ARG:NH2	5:E:24:GLU:OE2	2.44	0.50
1:A:375:LYS:CE	1:A:390:CYS:O	2.60	0.50
2:B:107:LEU:C	2:B:107:LEU:HD12	2.36	0.50
5:E:101:ILE:HD11	5:E:311:THR:HG21	1.94	0.50
1:A:393:THR:O	1:A:393:THR:CG2	2.54	0.50
2:B:437:CYS:SG	2:B:438:MET:N	2.85	0.50
2:B:462:SER:HB2	2:B:463:PRO:HD3	1.94	0.50
5:E:61:LEU:HD11	5:E:168:LEU:HD23	1.93	0.50
4:D:232:GLU:HB3	4:D:258:LEU:HD21	1.94	0.49
8:K:185:GLN:O	8:K:188:LYS:HG3	2.12	0.49
4:D:249:TYR:HB2	4:D:281:TYR:CZ	2.48	0.49
9:L:45:DC:H2''	9:L:46:DA:C8	2.48	0.49
4:D:160:LEU:HD22	4:D:323:LEU:HD13	1.94	0.49
7:G:46:ILE:CG2	7:G:48:GLU:OE2	2.60	0.49
1:A:173:ASN:OD1	1:A:459:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:LEU:HD23	2:B:55:LEU:HD23	1.94	0.49
6:F:226:TYR:O	6:F:230:VAL:HG22	2.14	0.48
1:A:535:THR:O	1:A:571:TYR:OH	2.29	0.48
1:A:613:THR:O	1:A:642:ARG:NH2	2.46	0.48
2:B:508:PHE:HZ	9:L:55:DA:H3'	1.79	0.48
1:A:306:ILE:HG23	1:A:308:ILE:HG22	1.95	0.48
1:A:340:LEU:HB2	1:A:346:LYS:HG2	1.95	0.48
6:F:213:LEU:HD11	6:F:243:LEU:HD13	1.96	0.48
5:E:377:ASP:O	5:E:380:HIS:NE2	2.47	0.48
3:C:427:ALA:HA	6:F:225:GLN:OE1	2.13	0.48
8:K:202:GLU:O	8:K:205:GLU:HG3	2.13	0.48
9:L:49:DG:H4'	9:L:50:DC:OP1	2.13	0.48
1:A:357:VAL:HG12	1:A:359:LYS:H	1.77	0.48
5:E:65:VAL:N	5:E:107:ILE:O	2.46	0.48
1:A:156:ILE:O	1:A:160:THR:HG22	2.14	0.48
1:A:418:LYS:NZ	9:L:46:DA:O3'	2.41	0.48
2:B:107:LEU:CD1	2:B:109:LEU:HD23	2.44	0.48
2:B:488:VAL:HG13	2:B:700:HIS:CD2	2.49	0.48
6:F:228:LEU:HG	6:F:232:LEU:HD22	1.96	0.48
6:F:160:ARG:NH1	6:F:233:PRO:O	2.46	0.48
9:L:44:DG:H2'	9:L:45:DC:C6	2.49	0.48
1:A:591:GLN:O	1:A:595:ASN:ND2	2.46	0.47
1:A:704:SER:N	1:A:708:GLU:OE2	2.46	0.47
2:B:664:VAL:HG12	2:B:677:MET:HE2	1.96	0.47
5:E:65:VAL:HB	5:E:108:VAL:HG22	1.96	0.47
1:A:412:MET:HA	1:A:415:HIS:CE1	2.49	0.47
8:K:117:LEU:HD12	8:K:125:THR:HB	1.96	0.47
9:L:37:DC:H2''	9:L:38:DA:H8	1.79	0.47
1:A:104:ALA:HA	1:A:122:SER:HB2	1.96	0.47
1:A:375:LYS:NZ	1:A:407:ILE:HB	2.29	0.47
6:F:215:LEU:HD11	6:F:244:PRO:HG2	1.97	0.47
7:G:10:ILE:HG22	7:G:17:LYS:HZ2	1.79	0.47
2:B:107:LEU:CD1	2:B:109:LEU:CD2	2.92	0.47
2:B:383:LEU:HD22	2:B:388:ILE:HD13	1.96	0.47
2:B:609:ASP:OD1	2:B:609:ASP:N	2.47	0.47
2:B:725:ALA:HB1	5:E:221:VAL:HG21	1.97	0.47
3:C:489:LYS:HD3	3:C:492:LYS:HD2	1.97	0.47
6:F:15:VAL:HG12	6:F:164:ILE:HD11	1.97	0.47
9:L:44:DG:H2'	9:L:45:DC:H6	1.78	0.47
1:A:575:LEU:HD22	1:A:606:PHE:HZ	1.79	0.47
2:B:170:LEU:HD11	2:B:194:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:86:LYS:O	5:E:89:GLU:HG2	2.14	0.47
5:E:165:ARG:NH2	5:E:192:ALA:O	2.47	0.47
2:B:588:CYS:O	2:B:613:HIS:NE2	2.45	0.47
1:A:65:MET:HE3	1:A:146:THR:HG21	1.97	0.46
2:B:709:THR:OG1	2:B:710:VAL:N	2.48	0.46
2:B:627:TYR:HD2	2:B:630:SER:HB3	1.80	0.46
4:D:45:PHE:CZ	4:D:57:MET:HE3	2.50	0.46
5:E:273:MET:HE3	5:E:307:ILE:HD11	1.97	0.46
6:F:143:TYR:O	6:F:147:MET:HG2	2.16	0.46
1:A:198:ARG:HG3	1:A:202:SER:HB3	1.98	0.46
6:F:271:CYS:SG	6:F:273:SER:OG	2.70	0.46
2:B:32:LEU:HD11	2:B:67:VAL:HG11	1.97	0.46
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.97	0.46
2:B:139:ALA:HB3	2:B:142:VAL:HG23	1.98	0.46
5:E:85:LEU:HD11	5:E:131:LEU:HD22	1.97	0.46
7:G:52:VAL:O	7:G:55:GLU:HG3	2.16	0.46
1:A:338:ILE:HD11	1:A:488:LEU:HD12	1.96	0.46
4:D:144:ASP:O	4:D:147:SER:OG	2.33	0.46
1:A:279:GLU:HA	1:A:282:LYS:HE3	1.97	0.46
1:A:446:ILE:O	1:A:448:ALA:N	2.46	0.46
5:E:65:VAL:HG13	5:E:170:ILE:HD11	1.97	0.46
2:B:372:LEU:HD11	2:B:404:ALA:HB1	1.98	0.46
2:B:463:PRO:HD2	2:B:467:TYR:HE2	1.80	0.46
3:C:471:LEU:HD13	3:C:497:LEU:HD23	1.97	0.46
2:B:546:GLU:OE2	11:S:241:ASN:N	2.49	0.46
4:D:286:LEU:O	4:D:290:LEU:N	2.48	0.46
1:A:202:SER:HB2	1:A:271:GLU:HG3	1.97	0.46
4:D:159:VAL:HG23	4:D:175:LEU:HD21	1.98	0.46
6:F:52:ASN:ND2	6:F:54:SER:OG	2.49	0.46
1:A:341:PRO:HB3	1:A:644:LEU:HD11	1.98	0.45
2:B:662:GLN:O	2:B:666:ARG:HG2	2.16	0.45
1:A:551:HIS:HB2	1:A:558:ILE:HD11	1.99	0.45
2:B:88:ARG:HG2	2:B:174:ILE:HB	1.98	0.45
2:B:370:LYS:HB3	2:B:371:PRO:HD3	1.97	0.45
2:B:637:LEU:O	2:B:641:ARG:HG3	2.17	0.45
3:C:540:GLN:O	3:C:543:ARG:HG3	2.16	0.45
1:A:371:VAL:HG13	1:A:407:ILE:CG2	2.47	0.45
6:F:112:VAL:HA	6:F:115:ILE:HG12	1.97	0.45
6:F:240:GLN:OE1	6:F:240:GLN:N	2.49	0.45
9:L:42:DC:H2'	9:L:43:DA:C8	2.51	0.45
2:B:666:ARG:NH1	2:B:666:ARG:HA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:ASP:OD1	6:F:204:GLN:NE2	2.45	0.45
7:G:46:ILE:CG2	7:G:48:GLU:CD	2.88	0.45
1:A:375:LYS:NZ	1:A:407:ILE:HD13	2.32	0.45
1:A:385:ASP:OD2	1:A:387:SER:OG	2.35	0.45
3:C:414:TYR:OH	6:F:39:ASP:OD1	2.34	0.45
4:D:179:LEU:HD11	4:D:184:LEU:HD12	1.99	0.45
1:A:92:VAL:HG22	1:A:95:TYR:HB2	1.98	0.45
1:A:117:LYS:NZ	1:A:118:LEU:O	2.50	0.45
1:A:149:PRO:HG2	1:A:152:ILE:HG12	1.99	0.45
2:B:372:LEU:HD23	2:B:408:SER:HB3	1.99	0.45
3:C:400:ILE:HD11	6:F:20:ILE:HG23	1.97	0.45
8:K:205:GLU:O	8:K:208:GLN:HG3	2.17	0.45
4:D:216:MET:HG3	4:D:290:LEU:HD11	1.99	0.45
1:A:680:LEU:HD12	1:A:687:PHE:HZ	1.82	0.45
4:D:452:LYS:HE3	8:K:273:MET:HG3	1.98	0.45
5:E:156:LEU:HD21	5:E:165:ARG:HB3	1.99	0.45
5:E:171:PHE:HB3	5:E:200:GLY:HA2	1.99	0.45
6:F:167:ALA:O	6:F:198:SER:OG	2.34	0.45
2:B:268:LYS:HE3	2:B:272:ARG:HE	1.82	0.44
4:D:254:MET:HE2	4:D:258:LEU:HB3	2.00	0.44
1:A:610:VAL:HG12	1:A:615:PHE:HE2	1.82	0.44
2:B:268:LYS:O	2:B:271:LEU:HG	2.18	0.44
6:F:21:TRP:CD1	6:F:166:ALA:HB1	2.52	0.44
1:A:129:VAL:HG13	1:A:131:LEU:H	1.83	0.44
2:B:476:VAL:HG23	2:B:477:THR:HG23	1.99	0.44
4:D:78:GLU:HG3	4:D:79:PHE:CD2	2.53	0.44
1:A:76:LEU:HB3	1:A:143:LEU:O	2.18	0.44
8:K:213:LYS:HG2	8:K:216:GLN:HE21	1.83	0.44
1:A:273:LYS:HG2	1:A:275:GLU:HG3	2.00	0.44
1:A:506:GLN:HB3	1:A:658:PHE:HB3	1.99	0.44
1:A:686:SER:HB2	4:D:386:THR:HG21	1.99	0.44
2:B:217:ILE:O	2:B:221:VAL:HG12	2.18	0.44
4:D:79:PHE:CG	6:F:240:GLN:HG3	2.52	0.44
6:F:39:ASP:O	6:F:42:MET:HG3	2.18	0.44
8:K:224:LYS:HA	8:K:227:ARG:HD2	2.00	0.44
1:A:628:SER:HB3	1:A:676:ARG:NH1	2.33	0.44
2:B:487:ARG:HD3	2:B:726:GLN:HE21	1.83	0.44
2:B:664:VAL:HG21	2:B:679:PHE:HE1	1.82	0.44
2:B:711:ASP:O	2:B:715:GLN:HG2	2.18	0.44
2:B:42:MET:HB3	2:B:48:LYS:HD3	2.00	0.44
2:B:263:LEU:HD13	2:B:334:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:263:GLN:HB2	4:D:266:ARG:HH12	1.83	0.44
5:E:109:THR:OG1	5:E:114:ALA:HB2	2.18	0.44
8:K:117:LEU:HD13	8:K:123:LEU:HD23	2.00	0.44
11:S:208:MET:HG3	11:S:243:LEU:HD21	2.00	0.44
2:B:277:ASP:HA	2:B:280:ARG:HG2	2.00	0.43
4:D:373:HIS:CG	4:D:374:PRO:HD2	2.53	0.43
4:D:54:ASN:HB3	4:D:58:ARG:HH21	1.82	0.43
1:A:628:SER:OG	1:A:635:GLN:NE2	2.47	0.43
2:B:87:LEU:HD21	2:B:204:VAL:HG11	1.98	0.43
5:E:260:ALA:HB1	5:E:267:ALA:HA	2.00	0.43
7:G:34:ILE:HD11	7:G:53:LEU:HD11	2.00	0.43
1:A:671:ALA:HB2	7:G:64:ASN:HA	2.01	0.43
4:D:322:GLU:OE1	4:D:337:ARG:NH2	2.51	0.43
2:B:600:ALA:O	2:B:659:HIS:NE2	2.35	0.43
2:B:613:HIS:CD2	5:E:206:ARG:HB2	2.54	0.43
1:A:110:PRO:HD2	1:A:114:HIS:HA	2.00	0.43
1:A:277:ILE:O	1:A:280:LEU:HG	2.19	0.43
1:A:570:GLU:HA	1:A:573:ILE:HG12	2.01	0.43
4:D:45:PHE:O	4:D:53:LYS:NZ	2.51	0.43
4:D:163:MET:HE3	4:D:163:MET:HB3	1.85	0.43
4:D:375:VAL:O	4:D:378:LYS:NZ	2.47	0.43
2:B:195:ALA:O	2:B:199:ILE:HG23	2.18	0.43
4:D:374:PRO:HA	4:D:377:LEU:HG	2.00	0.43
10:M:54:DA:H2''	10:M:55:DA:H5'	2.00	0.43
1:A:447:PRO:HD3	1:A:480:LEU:HD21	2.01	0.43
2:B:416:ILE:HD11	2:B:433:LEU:HD12	2.00	0.43
2:B:628:THR:HA	2:B:633:LEU:HD23	2.01	0.43
1:A:185:ILE:HD12	1:A:270:PHE:HE1	1.84	0.43
5:E:172:SER:HB2	5:E:201:LEU:HD22	2.01	0.43
2:B:107:LEU:HD11	2:B:205:VAL:HG23	2.00	0.42
2:B:603:LYS:O	2:B:607:GLY:N	2.47	0.42
2:B:679:PHE:HB3	2:B:684:PHE:CD2	2.53	0.42
6:F:9:ASN:HB2	6:F:55:ASN:ND2	2.34	0.42
1:A:375:LYS:HD2	1:A:389:ILE:HG21	2.00	0.42
9:L:48:DT:H2''	9:L:49:DG:C8	2.54	0.42
1:A:588:GLU:O	1:A:591:GLN:HG3	2.20	0.42
4:D:143:ARG:NH2	4:D:147:SER:HB2	2.34	0.42
6:F:68:ARG:NH2	6:F:117:ASP:OD2	2.53	0.42
7:G:13:ASP:OD1	7:G:16:MET:HG2	2.18	0.42
1:A:412:MET:HE3	1:A:412:MET:HB3	1.86	0.42
6:F:216:LYS:HE3	6:F:216:LYS:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:CD	1:A:276:MET:HG3	2.45	0.42
1:A:521:GLU:HG2	1:A:717:LEU:HD11	2.01	0.42
1:A:340:LEU:HD23	1:A:491:ALA:HB2	2.02	0.42
1:A:634:ARG:H	1:A:634:ARG:HD3	1.85	0.42
6:F:131:THR:HG23	6:F:133:LEU:HG	2.01	0.42
1:A:84:ILE:HG21	1:A:100:LEU:HD22	2.02	0.42
1:A:528:LYS:HA	1:A:528:LYS:HD3	1.85	0.42
2:B:505:SER:HB3	2:B:682:LYS:HB2	2.02	0.42
3:C:411:MET:O	6:F:116:LYS:NZ	2.44	0.42
5:E:153:MET:HE1	5:E:188:THR:HB	2.01	0.42
5:E:183:TYR:HA	5:E:186:ILE:HG22	2.02	0.42
6:F:236:ASP:OD1	6:F:237:GLN:N	2.53	0.42
1:A:561:PHE:HB3	1:A:639:ARG:CZ	2.49	0.42
4:D:238:PHE:O	4:D:241:SER:OG	2.30	0.42
1:A:282:LYS:HB3	1:A:482:PHE:CE1	2.55	0.42
1:A:549:LYS:HZ1	1:A:701:LEU:HD21	1.84	0.42
1:A:60:ASP:OD1	1:A:62:ARG:HG3	2.20	0.41
1:A:86:LEU:HB3	1:A:114:HIS:HB2	2.01	0.41
1:A:296:ASP:OD1	1:A:296:ASP:N	2.48	0.41
4:D:52:ALA:HB1	4:D:90:LEU:HD21	2.02	0.41
4:D:151:TYR:O	4:D:154:GLU:HG3	2.20	0.41
5:E:255:PRO:HD3	5:E:312:LEU:HD22	2.02	0.41
1:A:129:VAL:HG22	1:A:130:GLY:H	1.85	0.41
1:A:530:ARG:HA	1:A:533:LEU:HD22	2.01	0.41
7:G:31:LYS:HD2	7:G:33:PHE:CE2	2.55	0.41
2:B:72:TYR:O	2:B:206:VAL:HA	2.21	0.41
1:A:549:LYS:HZ2	1:A:701:LEU:HD11	1.85	0.41
1:A:668:GLN:OE1	1:A:668:GLN:N	2.46	0.41
2:B:261:GLY:O	2:B:264:GLU:HG3	2.21	0.41
2:B:263:LEU:HB3	2:B:334:ARG:NH1	2.35	0.41
2:B:590:ASN:HA	5:E:207:VAL:CG2	2.50	0.41
4:D:140:LYS:HG3	4:D:141:HIS:CD2	2.56	0.41
1:A:569:LYS:NZ	1:A:579:TYR:OH	2.48	0.41
1:A:585:SER:O	1:A:589:ARG:NE	2.53	0.41
2:B:196:ARG:O	2:B:199:ILE:HG12	2.20	0.41
4:D:373:HIS:ND1	4:D:374:PRO:HD2	2.35	0.41
9:L:43:DA:H2'	9:L:44:DG:C8	2.55	0.41
2:B:115:LEU:HD11	2:B:177:LEU:HD22	2.02	0.41
2:B:464:LEU:HD21	2:B:478:MET:O	2.21	0.41
4:D:19:LEU:HB2	4:D:213:TRP:CZ2	2.53	0.41
6:F:13:ILE:HA	6:F:162:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:206:VAL:HA	8:K:209:GLU:HG2	2.03	0.41
1:A:550:PHE:HD1	1:A:553:ARG:HH21	1.67	0.41
2:B:77:VAL:O	2:B:78:PRO:C	2.64	0.41
2:B:641:ARG:HH21	8:K:167:LYS:C	2.29	0.41
3:C:446:GLN:HG2	3:C:449:ILE:HB	2.02	0.41
4:D:204:LEU:O	4:D:211:GLN:NE2	2.54	0.41
6:F:32:PHE:HA	6:F:36:LYS:HD2	2.02	0.41
7:G:22:TYR:HA	7:G:25:GLU:HG2	2.03	0.41
9:L:51:DA:H4'	9:L:52:DC:OP2	2.20	0.41
1:A:424:GLU:O	1:A:427:MET:HG3	2.21	0.41
2:B:211:TYR:OH	9:L:62:DG:OP1	2.26	0.41
4:D:80:SER:HA	4:D:83:GLN:HG2	2.03	0.41
4:D:151:TYR:O	4:D:155:ARG:HG2	2.21	0.41
6:F:106:SER:HA	6:F:109:GLU:HG2	2.03	0.41
1:A:154:GLN:OE1	1:A:154:GLN:N	2.50	0.40
5:E:316:PRO:O	5:E:320:ARG:HG2	2.21	0.40
11:S:244:ASN:HA	11:S:247:ILE:HG12	2.03	0.40
1:A:446:ILE:HD13	1:A:446:ILE:HA	1.94	0.40
2:B:71:ILE:HD11	2:B:225:LEU:HD11	2.03	0.40
2:B:121:VAL:HG22	2:B:130:VAL:HG23	2.03	0.40
2:B:598:SER:OG	2:B:599:VAL:N	2.55	0.40
1:A:580:ILE:HD11	1:A:592:ILE:HG21	2.03	0.40
2:B:75:ARG:HD2	2:B:209:TYR:HE2	1.85	0.40
2:B:156:ARG:H	2:B:156:ARG:HD3	1.86	0.40
2:B:531:VAL:HG12	2:B:721:LEU:HD11	2.02	0.40
5:E:58:MET:O	5:E:164:SER:N	2.55	0.40
1:A:378:PHE:O	1:A:382:SER:HB3	2.21	0.40
1:A:591:GLN:OE1	1:A:595:ASN:ND2	2.55	0.40
3:C:404:PHE:CZ	6:F:20:ILE:HG12	2.57	0.40
4:D:49:PRO:O	4:D:53:LYS:HG3	2.22	0.40
2:B:579:VAL:O	2:B:583:LYS:HG2	2.21	0.40
4:D:144:ASP:OD1	4:D:144:ASP:N	2.54	0.40
5:E:83:CYS:O	5:E:86:LYS:HG3	2.21	0.40
11:S:246:HIS:O	11:S:250:VAL:HG23	2.22	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	598/782 (76%)	566 (95%)	32 (5%)	0	100	100
2	B	698/768 (91%)	675 (97%)	23 (3%)	0	100	100
3	C	152/548 (28%)	147 (97%)	5 (3%)	0	100	100
4	D	430/462 (93%)	428 (100%)	2 (0%)	0	100	100
5	E	365/395 (92%)	357 (98%)	8 (2%)	0	100	100
6	F	254/308 (82%)	252 (99%)	2 (1%)	0	100	100
7	G	64/71 (90%)	62 (97%)	2 (3%)	0	100	100
8	K	156/273 (57%)	153 (98%)	3 (2%)	0	100	100
11	S	67/1186 (6%)	66 (98%)	1 (2%)	0	100	100
All	All	2784/4793 (58%)	2706 (97%)	78 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	536/688 (78%)	536 (100%)	0	100	100
2	B	614/672 (91%)	614 (100%)	0	100	100
3	C	140/484 (29%)	140 (100%)	0	100	100
4	D	377/399 (94%)	377 (100%)	0	100	100
5	E	329/352 (94%)	329 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	230/272 (85%)	230 (100%)	0	100	100
7	G	59/64 (92%)	59 (100%)	0	100	100
8	K	150/233 (64%)	150 (100%)	0	100	100
11	S	67/1050 (6%)	67 (100%)	0	100	100
All	All	2502/4214 (59%)	2502 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	ASN
1	A	492	ASN
1	A	498	ASN
1	A	564	ASN
1	A	586	GLN
1	A	594	GLN
1	A	595	ASN
1	A	603	ASN
2	B	97	GLN
2	B	187	GLN
2	B	203	ASN
2	B	519	ASN
2	B	522	ASN
2	B	645	GLN
2	B	700	HIS
3	C	446	GLN
3	C	451	GLN
4	D	390	GLN
5	E	60	HIS
5	E	140	HIS
6	F	52	ASN
6	F	179	ASN
7	G	18	GLN
8	K	172	HIS
8	K	244	HIS
11	S	241	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	$\# Z > 2$
12	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	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](#)

There are no chain breaks in this entry.

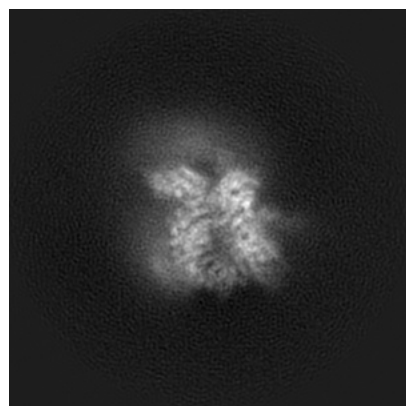
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71526. These allow visual inspection of the internal detail of the map and identification of artifacts.

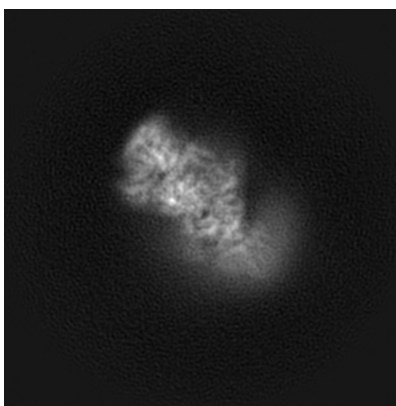
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

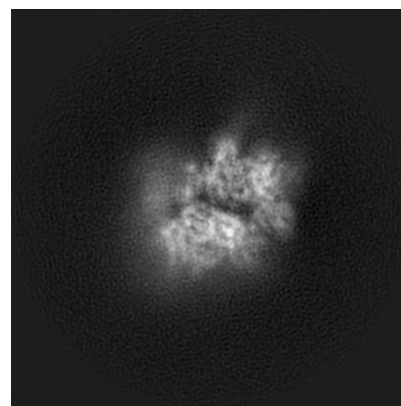
6.1.1 Primary map



X

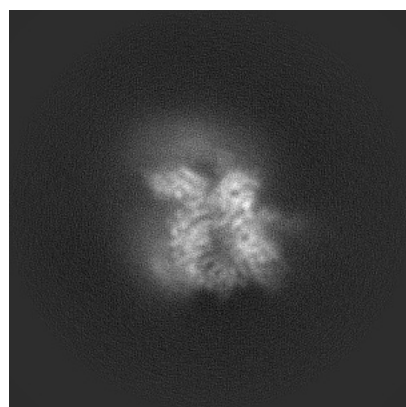


Y

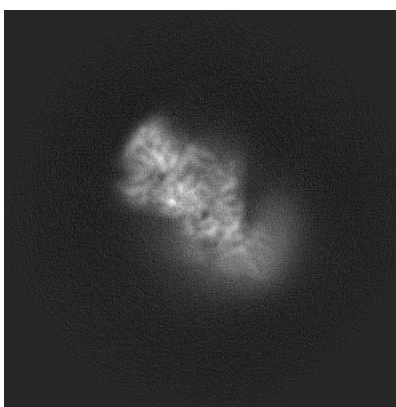


Z

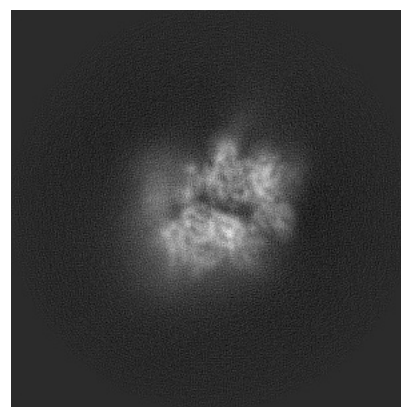
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

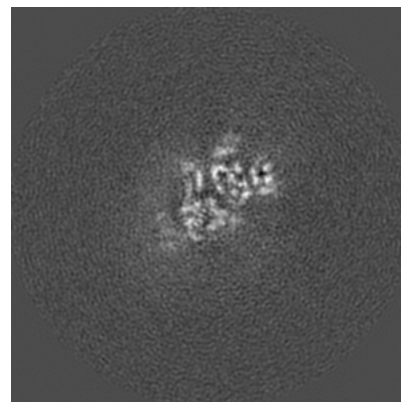
6.2.1 Primary map



X Index: 180

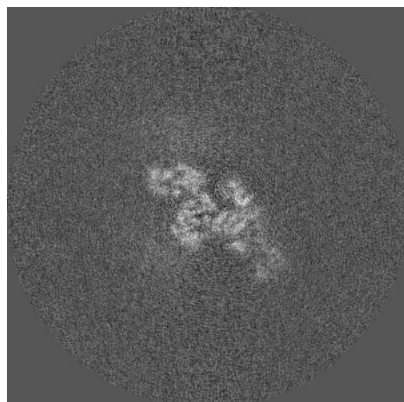


Y Index: 180

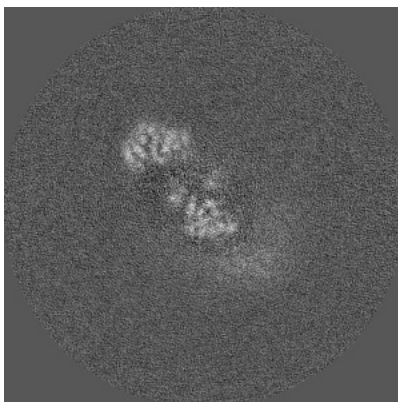


Z Index: 180

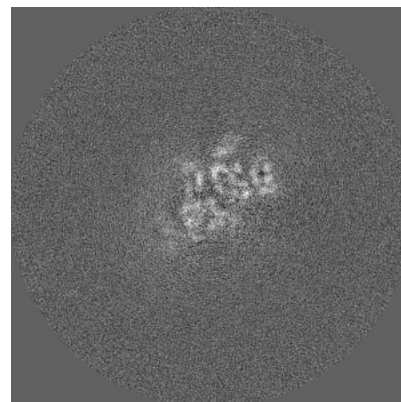
6.2.2 Raw map



X Index: 180



Y Index: 180

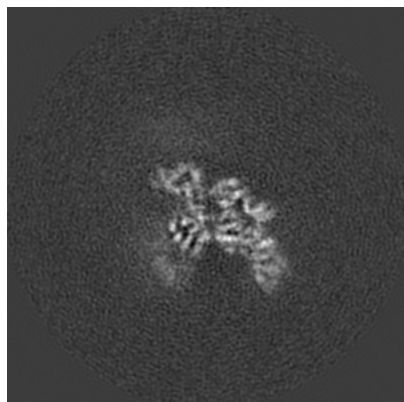


Z Index: 180

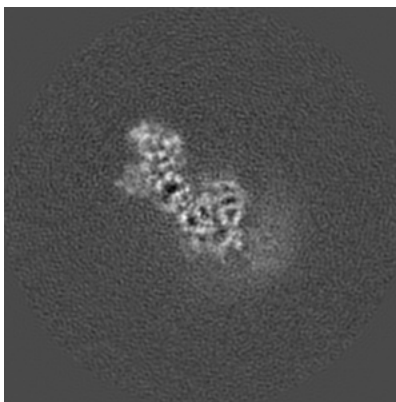
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

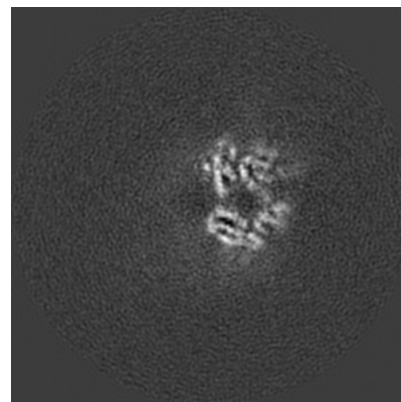
6.3.1 Primary map



X Index: 188

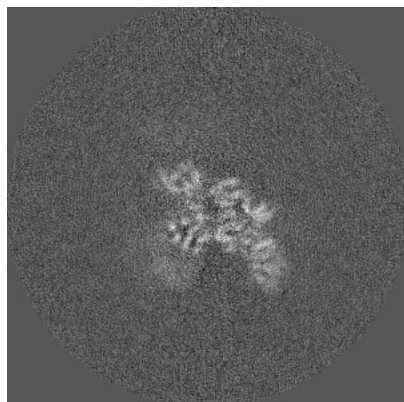


Y Index: 165

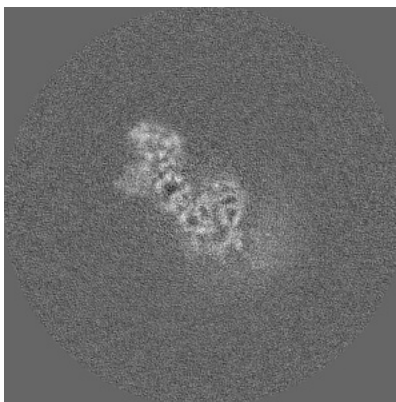


Z Index: 150

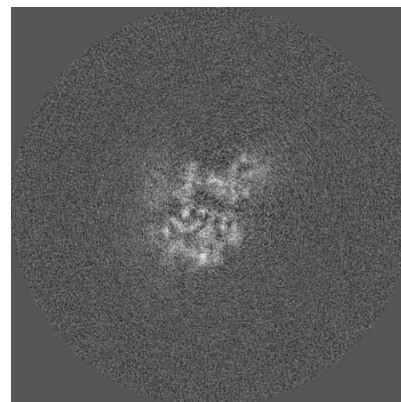
6.3.2 Raw map



X Index: 189



Y Index: 165

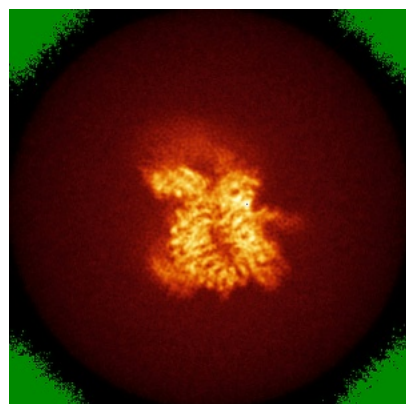


Z Index: 200

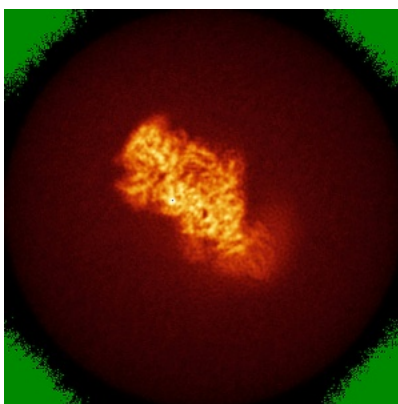
The images above show the largest variance slices of the map in three orthogonal directions.

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

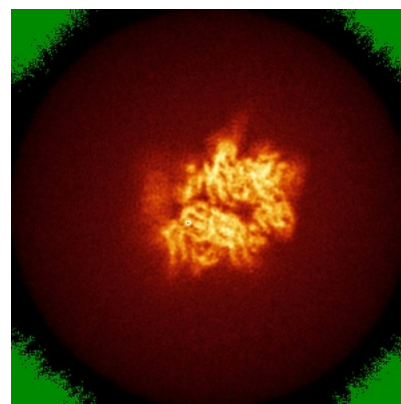
6.4.1 Primary map



X

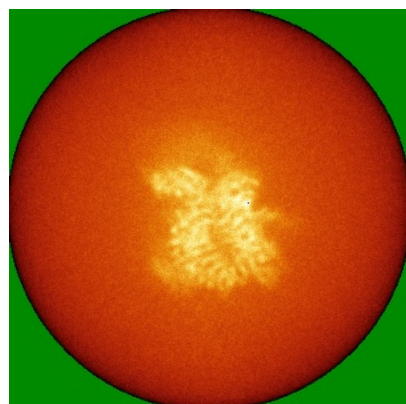


Y

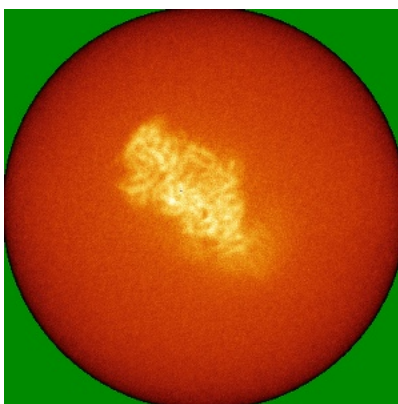


Z

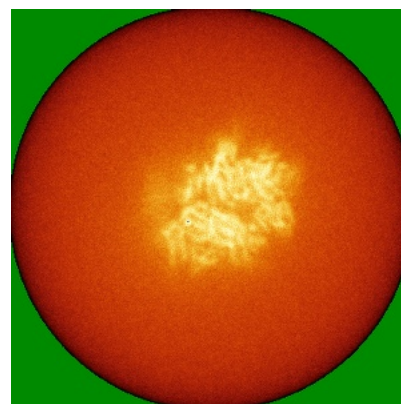
6.4.2 Raw map



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.

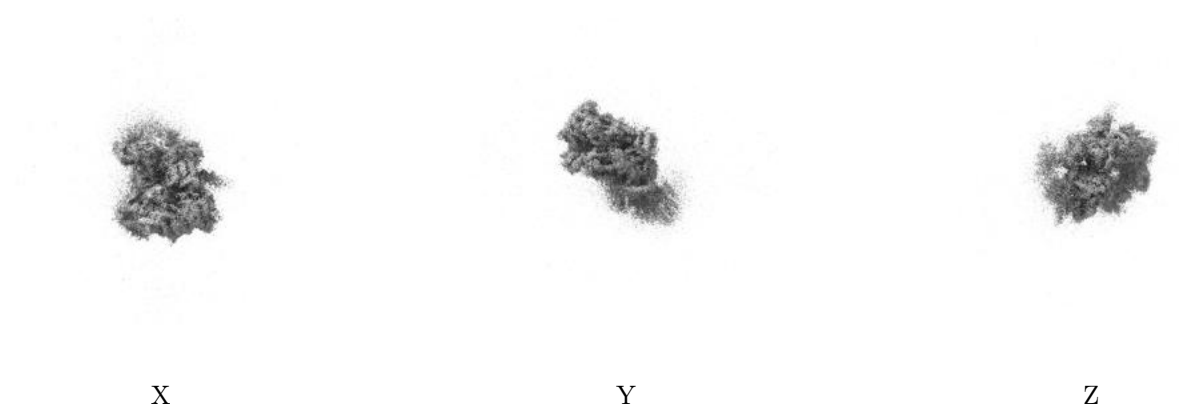
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.005. 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.

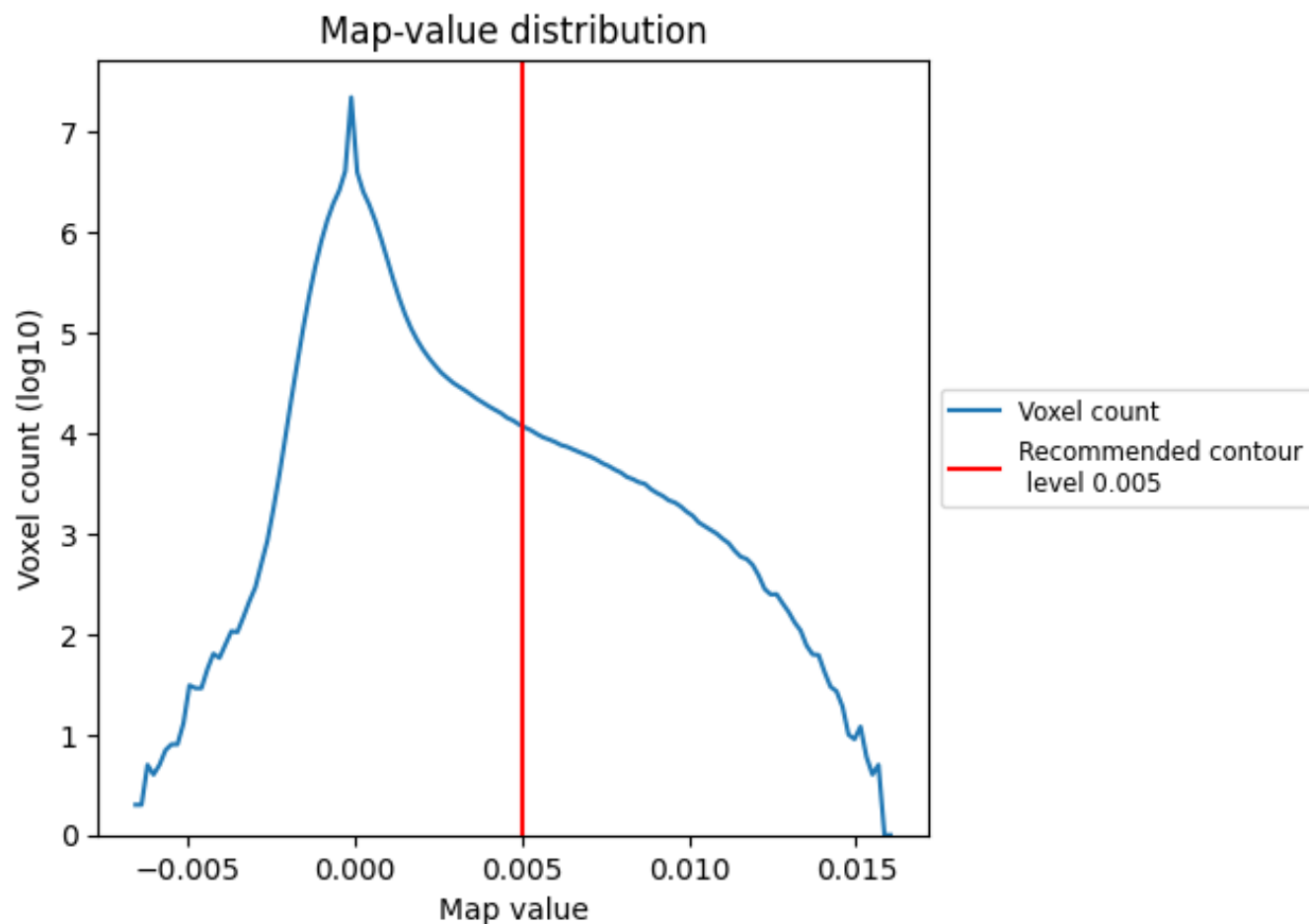
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

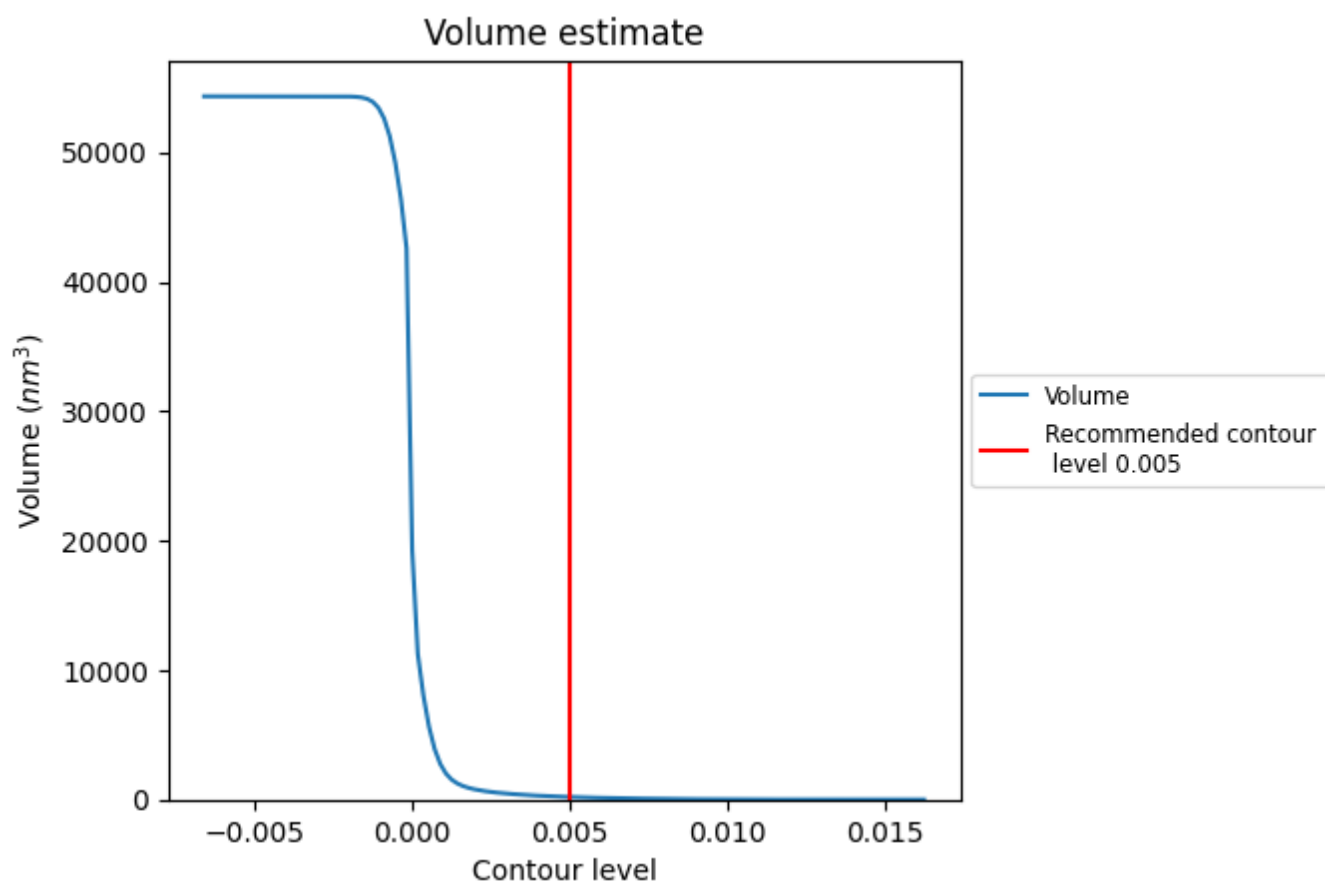
This section contains the results of statistical analysis of the map.

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.

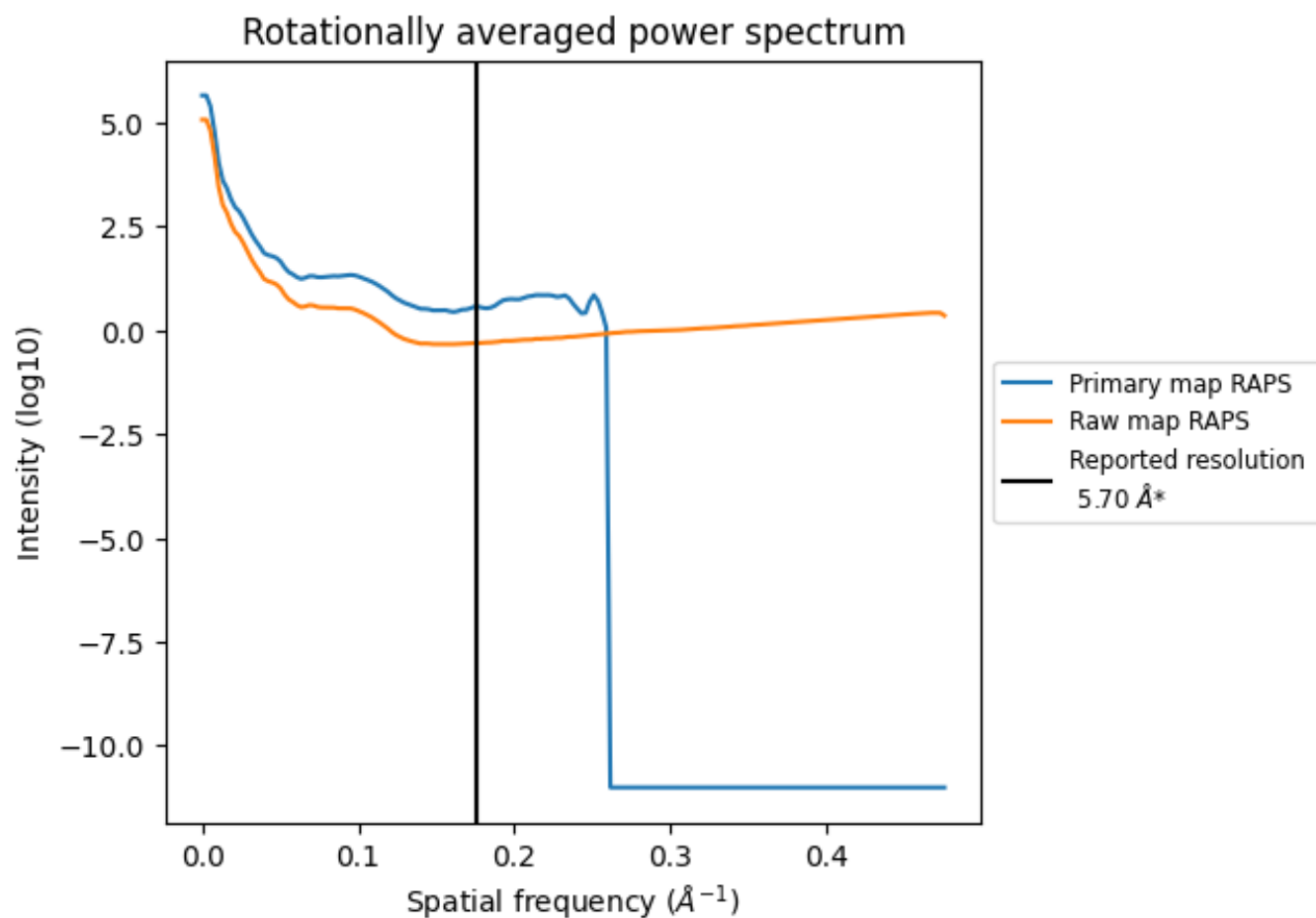
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 198 nm³; this corresponds to an approximate mass of 178 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 ⓘ

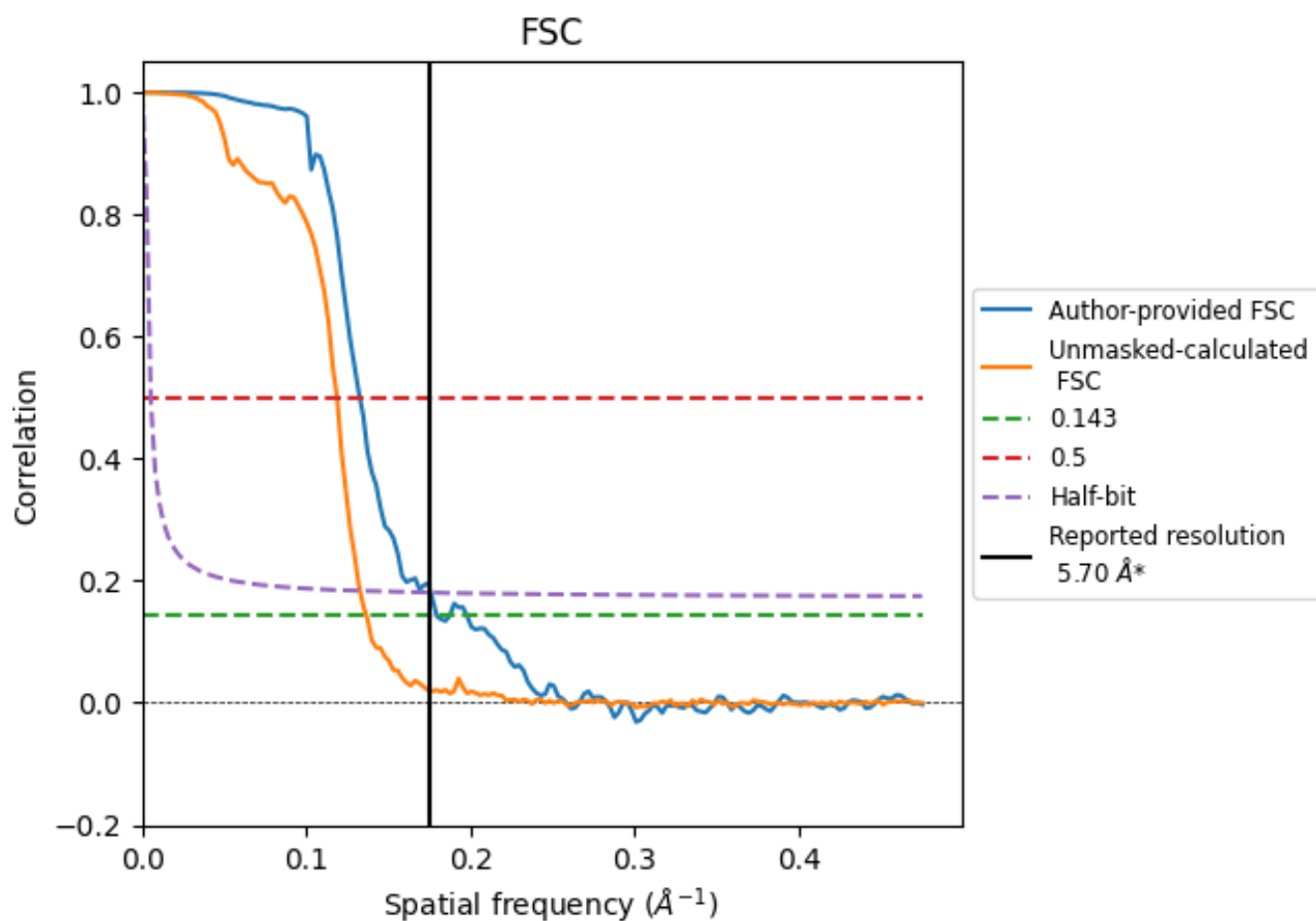


*Reported resolution corresponds to spatial frequency of 0.175 \AA^{-1}

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 0.175 \AA^{-1}

8.2 Resolution estimates [i](#)

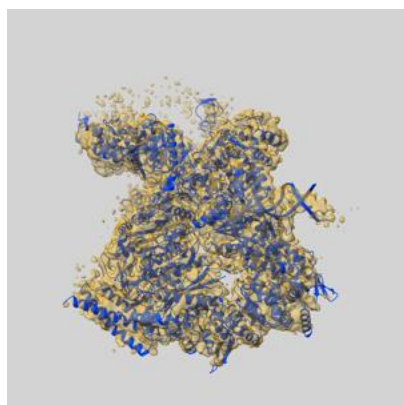
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.70	-	-
Author-provided FSC curve	5.57	7.54	5.69
Unmasked-calculated*	7.33	8.42	7.53

*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 7.33 differs from the reported value 5.7 by more than 10 %

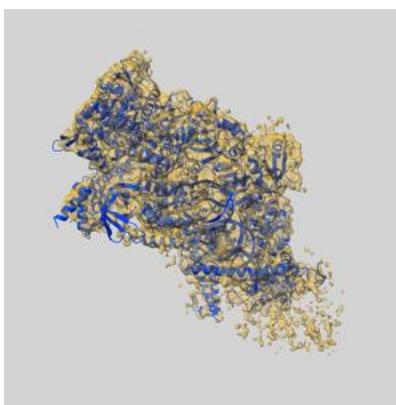
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71526 and PDB model 9PD5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

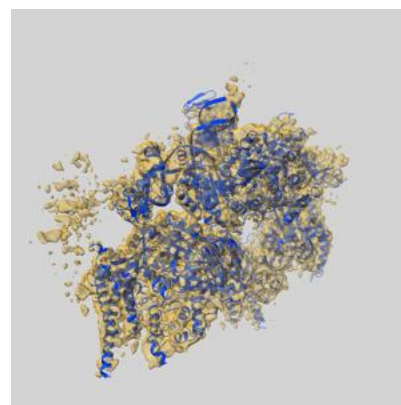
9.1 Map-model overlay [i](#)



X



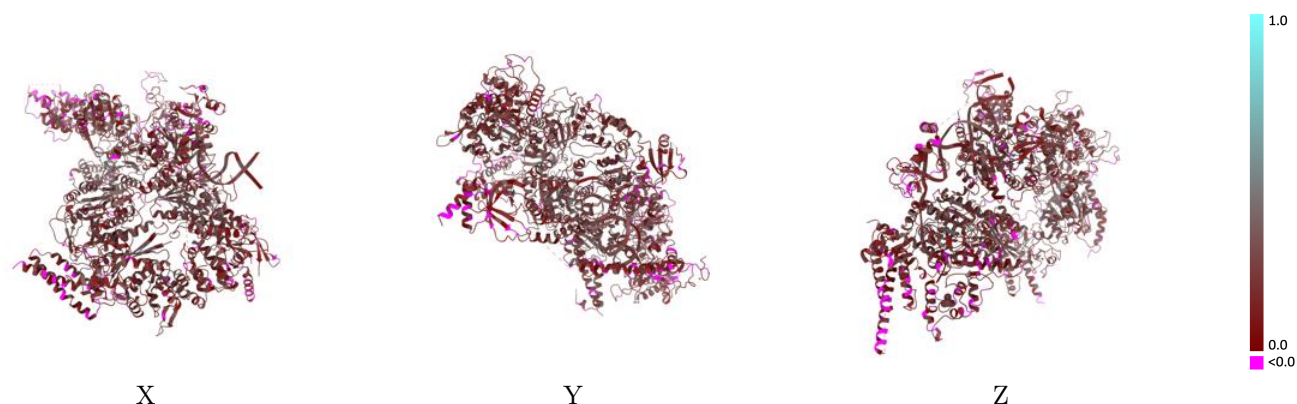
Y



Z

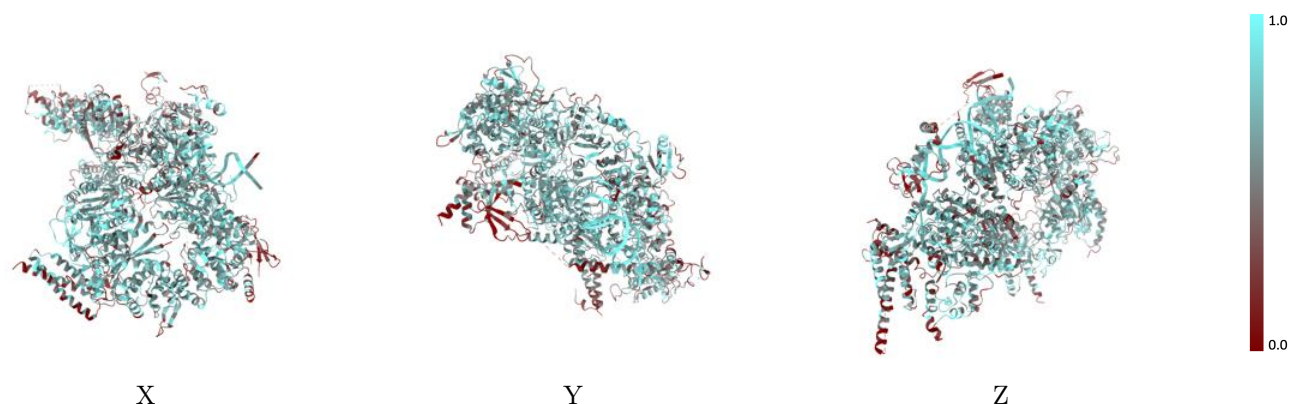
The images above show the 3D surface view of the map at the recommended contour level 0.005 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



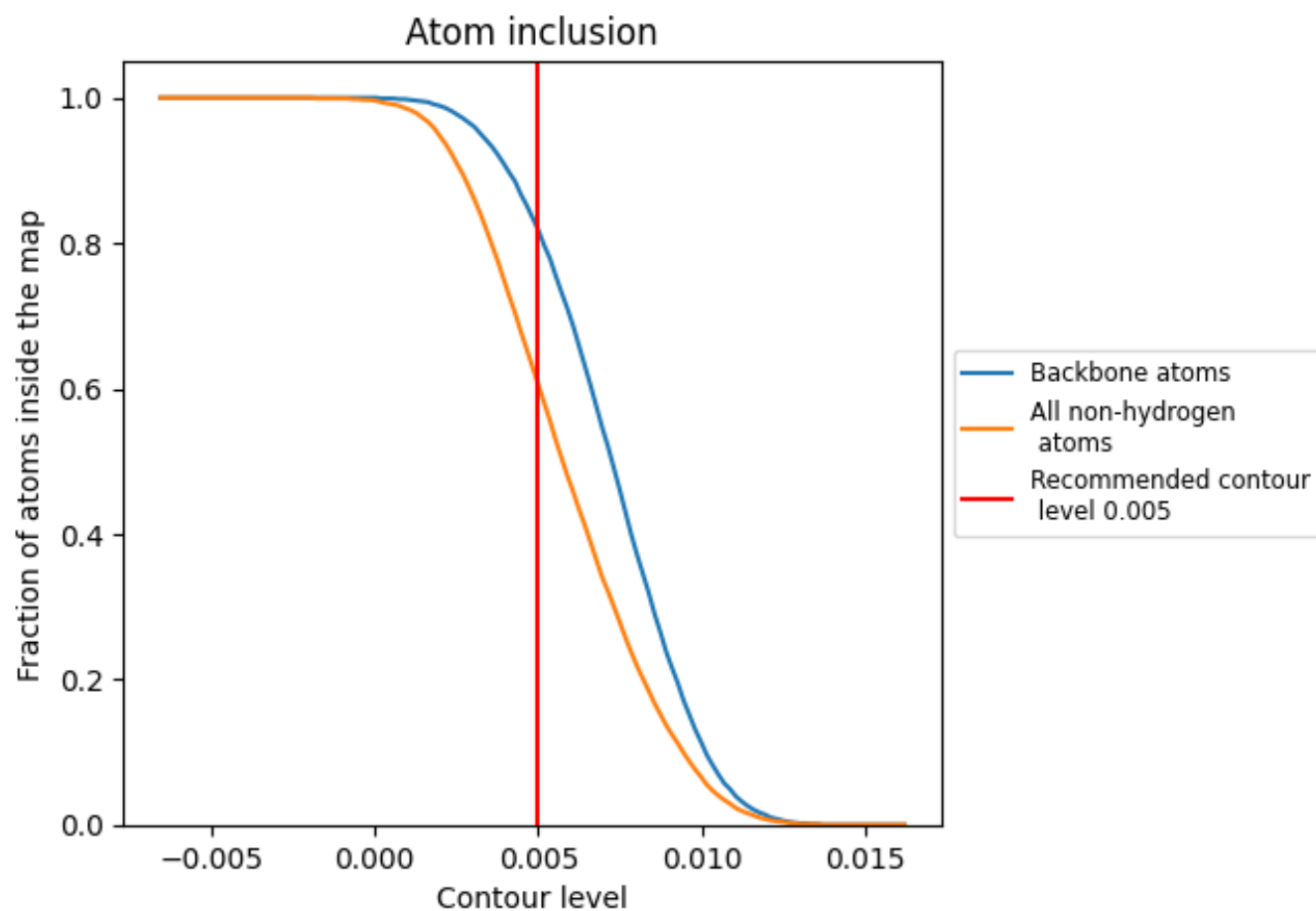
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.005).

























9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 60% 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 (0.005) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6050	 0.2130
A	 0.6450	 0.2290
B	 0.6010	 0.1920
C	 0.5020	 0.1430
D	 0.6080	 0.2220
E	 0.6500	 0.2550
F	 0.6620	 0.2490
G	 0.5880	 0.2190
K	 0.3470	 0.1310
L	 0.7890	 0.2250
M	 0.8170	 0.2570
S	 0.3500	 0.1900

