



## Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 04:45 PM UTC

PDB ID : 9XYU / pdb\_00009xyu  
EMDB ID : EMD-72341  
Title : NER complex - C7CAD.ATP  
Authors : Li, C.L.; Kim, J.; Yang, W.  
Deposited on : 2025-08-26  
Resolution : 3.50 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](mailto: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>.

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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

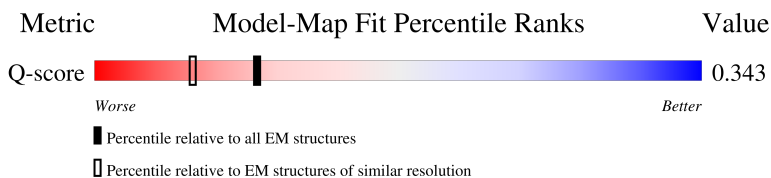
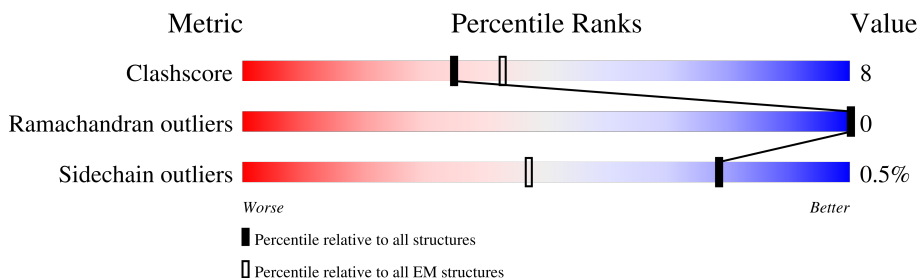
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.



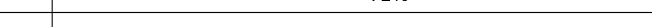

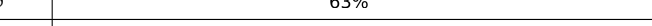

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 ( 3.00 - 4.00 )

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  $\geq 3$ , 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	 61% 16% 23%
2	B	768	 73% 18% 9%
3	C	548	 24% 5% 72%
4	D	462	 73% 21% 6%

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Mol	Chain	Length	Quality of chain
5	E	395	 <div>72%22%7%</div>
6	F	308	 <div>63%21%16%</div>
7	G	71	 <div>68%25%7%</div>
8	H	940	 <div>96%</div>
9	K	273	 <div>45%14%41%</div>
10	L	93	 <div>17%12%71%</div>
11	M	94	 <div>20%77%</div>

## 2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 23406 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-C cells.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	42	Total	C	N	O	0	0
			332	206	60	66		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	939	LYS	GLN	variant	UNP Q01831

- Molecule 9 is a protein called DNA repair protein complementing XP-A cells.

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

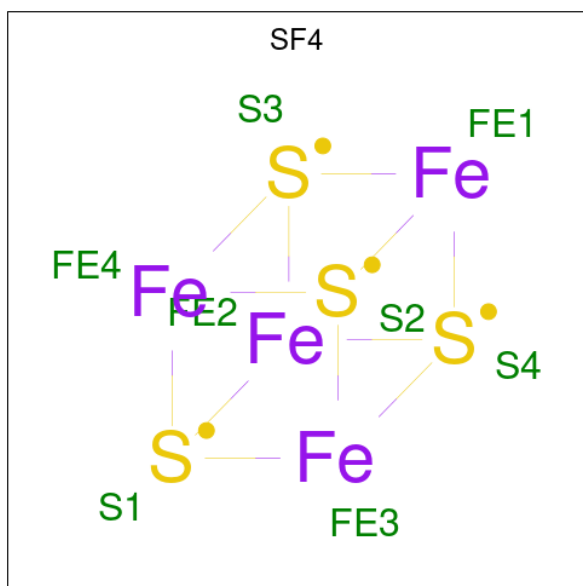
- Molecule 10 is a DNA chain called DNA (CY5).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	27	Total	C	N	O	P	0	0
			548	262	95	164	27		

- Molecule 11 is a DNA chain called DNA.

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

- Molecule 12 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).

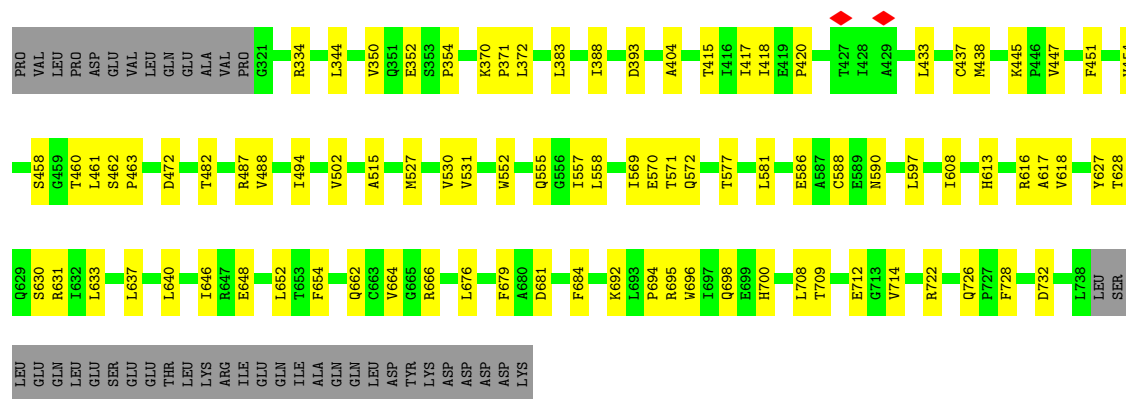


Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	Fe	S	0
			8	4	4	

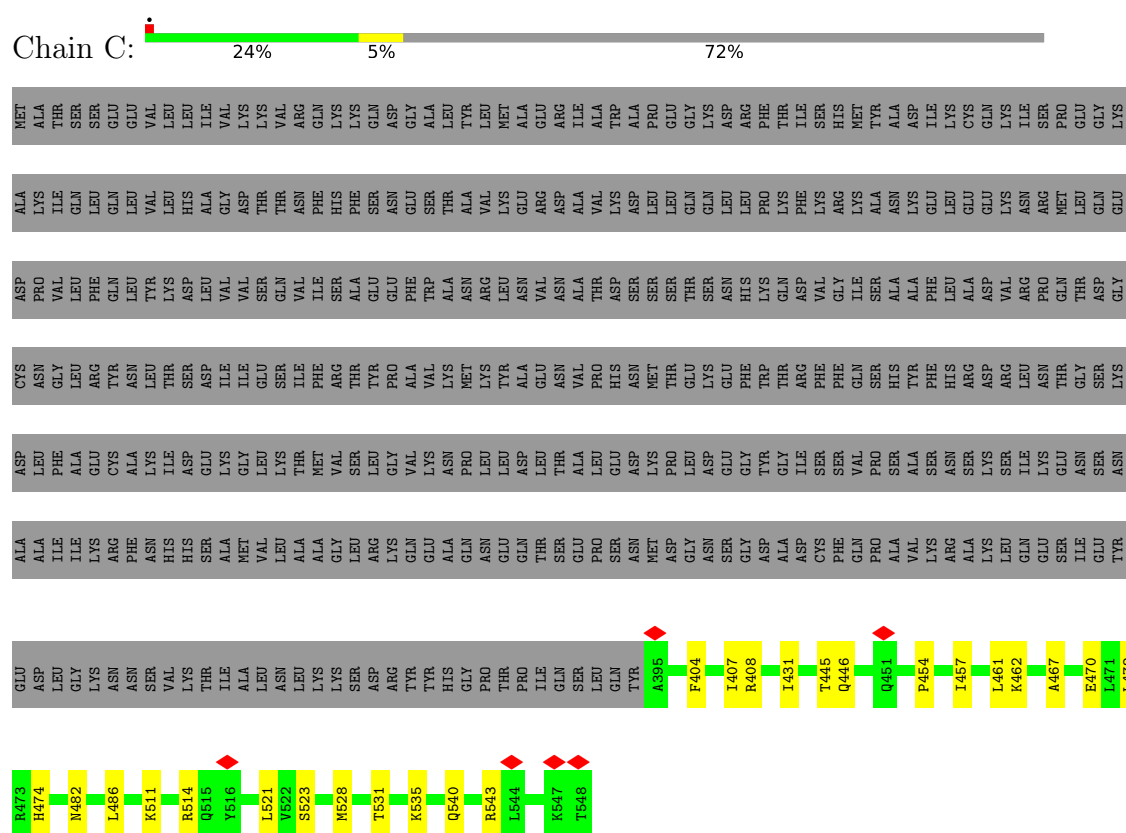
- Molecule 13 is ZINC ION (CCD ID: ZN) (formula:  $\text{Zn}$ ).

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	

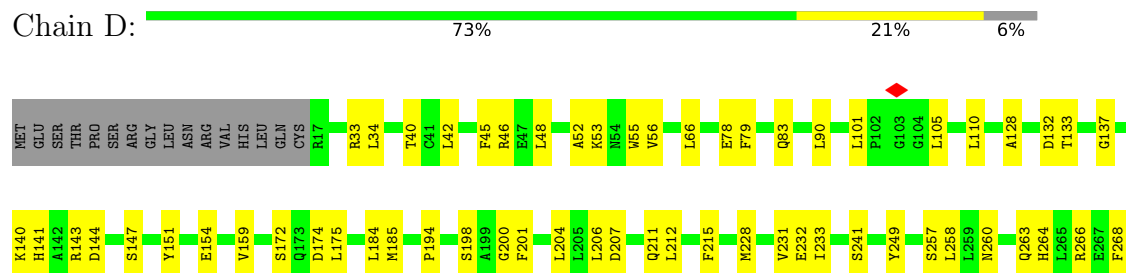




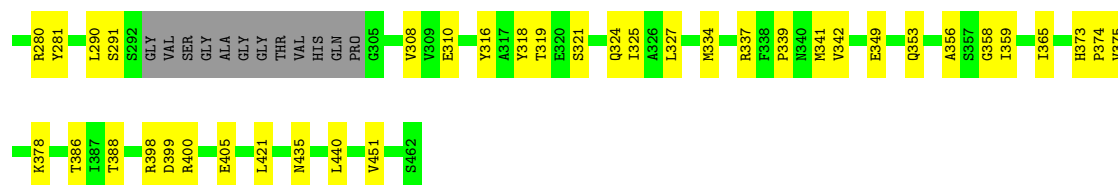
- Molecule 3: General transcription factor IIH subunit 1



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

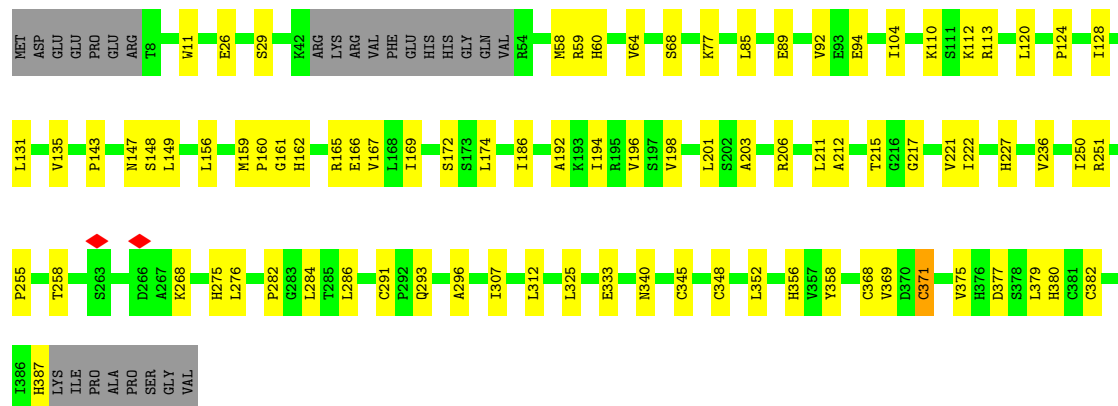






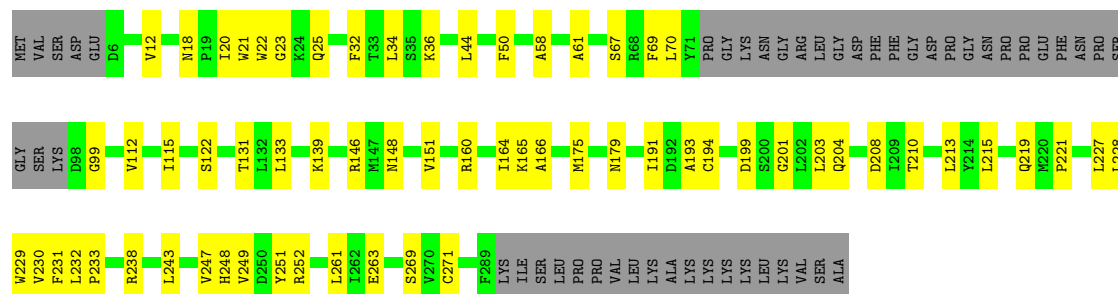
- Molecule 5: General transcription factor IIH subunit 2

Chain E: 72% 22% 7%



- Molecule 6: General transcription factor IIH subunit 3

Chain F: 63% 21% 16%



- Molecule 7: General transcription factor IIH subunit 5

Chain G: 68% 25% 7%

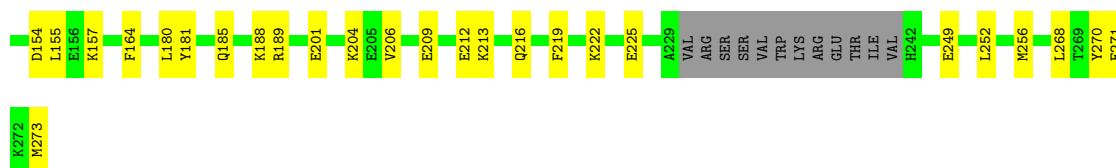


- Molecule 8: DNA repair protein complementing XP-C cells

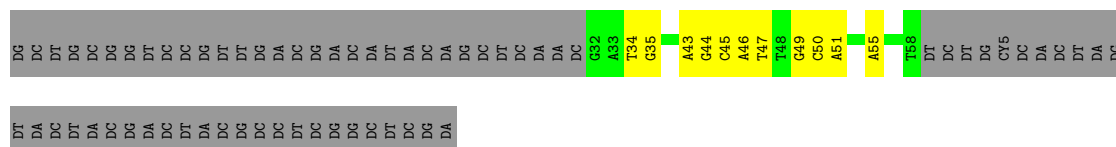
Chain H: 96%



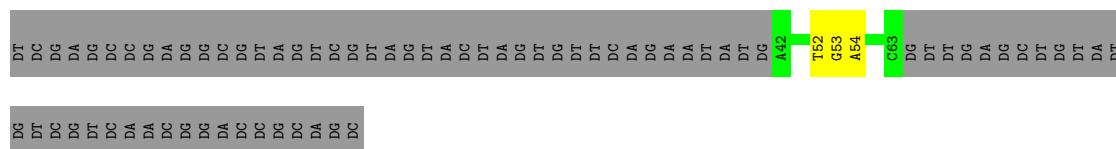
- Molecule 9: DNA repair protein complementing XP-A cells



- Molecule 10: DNA (CY5)



- Molecule 11: DNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	142798	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	0.036	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	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	0.23	0/6734
2	B	0.08	0/5780	0.23	0/7821
3	C	0.09	0/1257	0.25	0/1696
4	D	0.06	0/3564	0.17	0/4827
5	E	0.07	0/2960	0.20	0/4006
6	F	0.07	0/2070	0.19	0/2803
7	G	0.08	0/528	0.24	0/713
8	H	0.08	0/337	0.21	0/448
9	K	0.07	0/1373	0.21	0/1830
10	L	0.18	0/612	0.38	0/941
11	M	0.16	0/510	0.32	0/785
All	All	0.08	0/23976	0.22	0/32604

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	81	0
2	B	5659	0	5699	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1234	0	1250	19	0
4	D	3483	0	3526	61	0
5	E	2896	0	2857	60	0
6	F	2034	0	2050	41	0
7	G	522	0	531	11	0
8	H	332	0	322	4	0
9	K	1348	0	1323	26	0
10	L	548	0	306	8	0
11	M	454	0	248	3	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	23406	0	23035	370	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 (370) 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)
6:F:219:GLN:HG3	6:F:221:PRO:HD2	1.69	0.74
1:A:168:LEU:HD11	1:A:277:ILE:HD11	1.71	0.72
6:F:175:MET:SD	6:F:179:ASN:ND2	2.64	0.69
1:A:551:HIS:HB2	1:A:558:ILE:HD11	1.76	0.68
8:H:903:SER:O	8:H:907:ASN:ND2	2.24	0.68
2:B:487:ARG:HH12	2:B:728:PHE:HA	1.60	0.67
2:B:637:LEU:HB3	2:B:648:GLU:HG2	1.77	0.67
5:E:258:THR:HA	6:F:248:HIS:HB2	1.75	0.67
1:A:375:LYS:HE2	1:A:391:ARG:HE	1.60	0.67
4:D:34:LEU:HB3	4:D:40:THR:HG21	1.77	0.67
5:E:68:SER:HB3	5:E:143:PRO:HD3	1.77	0.67
1:A:60:ASP:HA	4:D:337:ARG:HB3	1.77	0.66
6:F:32:PHE:HA	6:F:36:LYS:HD2	1.76	0.66
1:A:84:ILE:HB	1:A:116:TYR:HB2	1.79	0.65
2:B:460:THR:HG21	2:B:662:GLN:HA	1.79	0.65
4:D:33:ARG:HG2	4:D:231:VAL:HG21	1.78	0.65
4:D:263:GLN:HG2	4:D:266:ARG:HH22	1.61	0.64
5:E:382:CYS:HB3	5:E:385:CYS:SG	2.38	0.64
7:G:4:VAL:N	9:K:271:GLU:O	2.32	0.63
5:E:222:ILE:HA	5:E:227:HIS:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:53:DG:HE2'	11:M:54:DA:H8	1.64	0.63
5:E:162:HIS:HE1	5:E:250:ILE:HD11	1.63	0.62
2:B:488:VAL:HG13	2:B:700:HIS:HD2	1.65	0.62
5:E:368:CYS:SG	5:E:371:CYS:HB2	2.38	0.61
1:A:581:TYR:HD1	1:A:583:PRO:HD2	1.64	0.61
1:A:591:GLN:O	1:A:595:ASN:ND2	2.33	0.61
2:B:354:PRO:HG3	2:B:415:THR:HA	1.83	0.61
1:A:104:ALA:HA	1:A:122:SER:HB2	1.82	0.61
2:B:695:ARG:NH1	2:B:698:GLN:OE1	2.34	0.61
4:D:399:ASP:O	8:H:908:ARG:NH1	2.33	0.60
1:A:623:LEU:HB3	1:A:659:PHE:HB2	1.81	0.60
6:F:191:ILE:H	6:F:210:THR:HG21	1.67	0.60
1:A:601:LYS:HG3	1:A:602:ILE:HG13	1.83	0.60
3:C:431:ILE:HD13	4:D:66:LEU:HD21	1.84	0.60
2:B:109:LEU:HB2	2:B:207:TYR:HB3	1.84	0.60
9:K:132:ALA:HA	9:K:136:HIS:HB2	1.83	0.60
1:A:472:ARG:H	1:A:477:ILE:HD11	1.66	0.59
6:F:12:VAL:HG12	6:F:58:ALA:HB3	1.84	0.59
2:B:586:GLU:O	2:B:590:ASN:ND2	2.35	0.59
1:A:547:LEU:O	1:A:551:HIS:ND1	2.36	0.59
1:A:82:GLY:O	1:A:83:HIS:ND1	2.36	0.58
5:E:165:ARG:NH2	5:E:192:ALA:O	2.36	0.58
5:E:194:ILE:O	5:E:215:THR:OG1	2.22	0.58
1:A:274:GLN:NE2	1:A:456:THR:O	2.36	0.58
1:A:525:ILE:HD12	1:A:529:LYS:HB3	1.86	0.58
4:D:206:LEU:O	4:D:211:GLN:NE2	2.37	0.58
4:D:45:PHE:HE2	6:F:50:PHE:HB3	1.68	0.58
2:B:57:MET:SD	2:B:60:GLN:NE2	2.77	0.58
2:B:5:VAL:HG12	2:B:6:ASP:H	1.69	0.57
4:D:228:MET:HG3	4:D:257:SER:HB2	1.86	0.57
4:D:349:GLU:OE2	4:D:353:GLN:NE2	2.37	0.57
5:E:89:GLU:HG3	5:E:128:ILE:HD12	1.86	0.57
5:E:110:LYS:O	5:E:113:ARG:NH1	2.37	0.57
2:B:350:VAL:HG11	2:B:631:ARG:HG3	1.85	0.57
2:B:458:SER:HB3	2:B:461:LEU:HG	1.87	0.57
1:A:548:ILE:HG21	1:A:577:LYS:HE3	1.86	0.57
1:A:580:ILE:HD12	1:A:607:ILE:HG12	1.87	0.56
4:D:241:SER:HB2	4:D:291:SER:HB3	1.87	0.56
1:A:304:PRO:HG2	1:A:360:ARG:HD2	1.86	0.56
1:A:568:LEU:HD11	1:A:606:PHE:HB3	1.88	0.56
4:D:308:VAL:HB	4:D:316:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:OE2	1:A:325:ARG:NH2	2.39	0.56
2:B:117:ILE:HG23	2:B:181:LYS:HE2	1.87	0.56
2:B:170:LEU:HD11	2:B:194:LEU:HD21	1.87	0.56
2:B:569:ILE:HG13	2:B:597:LEU:HD11	1.88	0.56
6:F:160:ARG:NH1	6:F:233:PRO:O	2.39	0.56
6:F:194:CYS:HB2	6:F:231:PHE:HE2	1.70	0.56
4:D:128:ALA:HA	6:F:99:GLY:H	1.71	0.56
2:B:372:LEU:HD11	2:B:404:ALA:HB1	1.87	0.55
2:B:637:LEU:HD13	2:B:648:GLU:HB3	1.88	0.55
5:E:156:LEU:HG	5:E:165:ARG:HD2	1.89	0.55
2:B:664:VAL:HG21	2:B:679:PHE:HE1	1.72	0.55
9:K:117:LEU:O	9:K:122:ASP:N	2.39	0.55
5:E:160:PRO:HB2	5:E:162:HIS:HD2	1.71	0.55
1:A:706:LYS:NZ	8:H:895:GLU:OE2	2.37	0.55
6:F:238:ARG:HB3	6:F:243:LEU:HD11	1.89	0.55
1:A:173:ASN:ND2	1:A:432:THR:O	2.40	0.55
5:E:174:LEU:HD21	5:E:203:ALA:HB3	1.89	0.55
6:F:204:GLN:HB3	6:F:249:VAL:HG12	1.87	0.55
6:F:208:ASP:OD2	6:F:251:TYR:OH	2.25	0.55
3:C:482:ASN:H	3:C:486:LEU:HD12	1.71	0.54
5:E:186:ILE:HG12	5:E:211:LEU:HD12	1.90	0.54
7:G:9:LEU:HD11	7:G:42:HIS:HB3	1.89	0.54
2:B:71:ILE:HB	2:B:231:VAL:HA	1.90	0.54
9:K:154:ASP:O	9:K:189:ARG:NH1	2.40	0.54
2:B:76:THR:OG1	2:B:77:VAL:N	2.35	0.54
4:D:33:ARG:HE	4:D:231:VAL:HG11	1.73	0.53
5:E:58:MET:H	6:F:269:SER:HB3	1.72	0.53
2:B:531:VAL:HG21	2:B:617:ALA:HB2	1.90	0.53
4:D:159:VAL:HG23	4:D:175:LEU:HD21	1.91	0.53
9:K:117:LEU:HD13	9:K:123:LEU:HD23	1.90	0.53
5:E:156:LEU:HD21	5:E:165:ARG:HB3	1.89	0.53
1:A:89:PHE:CG	4:D:375:VAL:HG21	2.43	0.53
5:E:375:VAL:HG12	5:E:379:LEU:HD12	1.90	0.53
2:B:25:MET:HG3	2:B:55:LEU:HD22	1.91	0.53
4:D:375:VAL:O	4:D:378:LYS:NZ	2.40	0.53
9:K:138:LEU:HB3	9:K:180:LEU:HB3	1.91	0.53
4:D:232:GLU:HB3	4:D:258:LEU:HD21	1.90	0.53
9:K:273:MET:SD	9:K:273:MET:N	2.83	0.53
6:F:164:ILE:HG22	6:F:194:CYS:HB3	1.91	0.52
4:D:175:LEU:HD13	4:D:268:PHE:HE1	1.74	0.52
2:B:56:ILE:HG21	2:B:70:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:421:LEU:HD11	4:D:451:VAL:HG13	1.90	0.52
1:A:277:ILE:HD12	1:A:280:LEU:HD21	1.92	0.52
1:A:568:LEU:HD22	1:A:608:SER:HB2	1.91	0.52
2:B:76:THR:HG23	2:B:78:PRO:HD2	1.91	0.52
2:B:722:ARG:NH1	5:E:201:LEU:O	2.42	0.52
9:K:123:LEU:HD12	9:K:124:PRO:HD2	1.90	0.52
2:B:383:LEU:HD22	2:B:388:ILE:HD13	1.91	0.52
4:D:132:ASP:OD1	4:D:133:THR:N	2.43	0.52
6:F:201:GLY:HA2	6:F:204:GLN:HE21	1.75	0.51
4:D:228:MET:HG2	4:D:233:ILE:HD11	1.92	0.51
4:D:325:ILE:HD12	4:D:342:VAL:HG11	1.92	0.51
2:B:640:LEU:HB3	2:B:646:ILE:HB	1.93	0.51
1:A:469:THR:HG21	1:A:638:GLN:HG3	1.93	0.51
4:D:172:SER:OG	4:D:174:ASP:OD1	2.28	0.51
11:M:52:DT:C2	11:M:53:DG:C8	2.98	0.51
4:D:321:SER:OG	4:D:324:GLN:OE1	2.28	0.51
11:M:53:DG:H2'	11:M:54:DA:C8	2.44	0.51
4:D:198:SER:HB2	4:D:358:GLY:HA3	1.93	0.51
4:D:56:VAL:HG23	4:D:110:LEU:HD21	1.93	0.51
1:A:110:PRO:HD2	1:A:114:HIS:HA	1.93	0.50
1:A:558:ILE:HB	1:A:604:THR:HG22	1.93	0.50
2:B:261:GLY:O	2:B:264:GLU:HG3	2.12	0.50
4:D:185:MET:HB3	4:D:194:PRO:HB2	1.93	0.50
10:L:44:DG:H2'	10:L:45:DC:C6	2.46	0.50
2:B:726:GLN:NE2	5:E:221:VAL:O	2.37	0.50
5:E:377:ASP:O	5:E:380:HIS:NE2	2.44	0.50
2:B:588:CYS:O	2:B:613:HIS:NE2	2.43	0.50
6:F:21:TRP:NE1	6:F:25:GLN:HE21	2.09	0.50
4:D:356:ALA:HB2	4:D:398:ARG:HH12	1.76	0.50
2:B:118:HIS:HB3	2:B:121:VAL:HG12	1.93	0.50
2:B:627:TYR:HD2	2:B:630:SER:HB2	1.76	0.50
1:A:168:LEU:HD12	1:A:291:LEU:HD22	1.92	0.50
5:E:255:PRO:HG3	5:E:312:LEU:HB3	1.94	0.50
2:B:502:VAL:HG11	2:B:515:ALA:HB1	1.94	0.50
1:A:313:THR:HG21	2:B:732:ASP:HA	1.92	0.49
5:E:85:LEU:HD22	5:E:131:LEU:HD22	1.94	0.49
5:E:333:GLU:OE2	5:E:356:HIS:ND1	2.38	0.49
1:A:626:ILE:HG22	1:A:662:LEU:HB2	1.95	0.49
3:C:404:PHE:HZ	6:F:20:ILE:HG12	1.76	0.49
1:A:440:LEU:HD22	1:A:484:ILE:HD11	1.95	0.49
1:A:628:SER:OG	1:A:676:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:GLY:O	4:D:280:ARG:NH2	2.39	0.49
1:A:308:ILE:HG22	1:A:384:ILE:HD13	1.94	0.49
2:B:42:MET:HB3	2:B:48:LYS:HD3	1.95	0.49
1:A:385:ASP:OD2	1:A:387:SER:OG	2.30	0.49
4:D:365:ILE:HD13	4:D:388:THR:HG23	1.94	0.49
1:A:574:ARG:HG2	1:A:703:PHE:HE1	1.78	0.49
2:B:617:ALA:HA	2:B:676:LEU:HB3	1.95	0.49
2:B:628:THR:HA	2:B:633:LEU:HD23	1.95	0.49
2:B:25:MET:HE1	2:B:51:SER:HB2	1.95	0.48
4:D:319:THR:HG21	4:D:324:GLN:HG2	1.95	0.48
1:A:580:ILE:HG23	1:A:589:ARG:HG2	1.93	0.48
1:A:125:ALA:O	1:A:128:SER:OG	2.27	0.48
2:B:637:LEU:HD22	2:B:648:GLU:HA	1.94	0.48
4:D:260:ASN:O	4:D:264:HIS:ND1	2.34	0.48
4:D:373:HIS:CG	4:D:374:PRO:HD2	2.49	0.48
5:E:201:LEU:HA	5:E:222:ILE:HG12	1.95	0.48
1:A:599:ASN:HD21	1:A:601:LYS:HE2	1.78	0.48
2:B:552:TRP:HB3	2:B:558:LEU:HB2	1.94	0.48
5:E:161:GLY:HA2	5:E:165:ARG:HH12	1.77	0.48
9:K:213:LYS:HG2	9:K:216:GLN:HE21	1.79	0.48
4:D:52:ALA:HB1	4:D:90:LEU:HD21	1.95	0.48
1:A:447:PRO:HD3	1:A:480:LEU:HD21	1.95	0.48
1:A:666:ASP:OD2	4:D:400:ARG:NH2	2.39	0.48
4:D:204:LEU:HG	4:D:327:LEU:HD21	1.95	0.48
6:F:193:ALA:HB1	6:F:203:LEU:HD13	1.96	0.48
2:B:122:THR:N	2:B:123:PRO:HD2	2.28	0.48
5:E:284:LEU:HD23	5:E:284:LEU:H	1.79	0.48
6:F:61:ALA:HB2	6:F:70:LEU:HD11	1.94	0.48
1:A:472:ARG:HH12	1:A:474:ASP:HB2	1.79	0.47
2:B:69:LYS:NZ	2:B:199:ILE:O	2.41	0.47
5:E:345:CYS:HB2	5:E:352:LEU:HD21	1.96	0.47
2:B:207:TYR:HE1	2:B:212:LEU:HB2	1.79	0.47
7:G:13:ASP:OD1	7:G:13:ASP:N	2.46	0.47
1:A:516:PRO:HG3	7:G:14:PRO:HB2	1.96	0.47
2:B:708:LEU:HB3	2:B:712:GLU:HG3	1.95	0.47
4:D:184:LEU:HD22	4:D:200:GLY:HA2	1.96	0.47
4:D:435:ASN:N	4:D:440:LEU:O	2.46	0.47
5:E:26:GLU:HG3	5:E:29:SER:HB3	1.97	0.47
9:K:185:GLN:O	9:K:188:LYS:HG3	2.15	0.47
2:B:530:VAL:HG21	2:B:714:VAL:HG13	1.96	0.47
1:A:75:PRO:HD2	1:A:143:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:H	1:A:292:LEU:HD23	1.79	0.47
5:E:60:HIS:HB3	5:E:120:LEU:HD21	1.97	0.47
10:L:46:DA:H2'	10:L:47:DT:C6	2.48	0.47
2:B:494:ILE:HG13	2:B:679:PHE:HB2	1.97	0.47
2:B:262:ASN:ND2	2:B:393:ASP:O	2.44	0.47
3:C:454:PRO:HD2	3:C:457:ILE:HD13	1.97	0.47
6:F:21:TRP:HE1	6:F:25:GLN:HE21	1.62	0.47
9:K:249:GLU:OE1	9:K:270:TYR:OH	2.33	0.47
1:A:668:GLN:NE2	1:A:672:TYR:OH	2.47	0.47
2:B:231:VAL:HB	2:B:454:VAL:HG22	1.97	0.47
3:C:445:THR:O	3:C:446:GLN:HG3	2.15	0.47
5:E:291:CYS:HB3	5:E:296:ALA:H	1.80	0.46
1:A:74:ARG:HB2	1:A:145:LYS:HB2	1.95	0.46
6:F:112:VAL:HA	6:F:115:ILE:HG22	1.97	0.46
6:F:228:LEU:HD22	6:F:232:LEU:HD22	1.97	0.46
1:A:635:GLN:OE1	1:A:676:ARG:NH2	2.48	0.46
4:D:249:TYR:HB2	4:D:281:TYR:CZ	2.51	0.46
8:H:907:ASN:OD1	8:H:908:ARG:NE	2.48	0.46
6:F:18:ASN:HB2	6:F:131:THR:HG22	1.98	0.46
1:A:325:ARG:HG2	5:E:11:TRP:HA	1.97	0.46
2:B:616:ARG:O	2:B:676:LEU:N	2.43	0.46
5:E:149:LEU:HD21	5:E:169:ILE:HD11	1.98	0.46
5:E:64:VAL:HB	5:E:169:ILE:HA	1.97	0.46
5:E:325:LEU:HD21	6:F:271:CYS:HB2	1.97	0.46
10:L:49:DG:H4'	10:L:50:DC:OP1	2.14	0.46
1:A:129:VAL:HG12	1:A:130:GLY:H	1.81	0.46
1:A:424:GLU:O	1:A:427:MET:HG3	2.16	0.46
1:A:703:PHE:HE2	1:A:712:LEU:HD22	1.81	0.46
2:B:570:GLU:HG2	2:B:577:THR:HG22	1.98	0.46
5:E:59:ARG:NH2	5:E:166:GLU:OE1	2.44	0.46
4:D:201:PHE:HB3	4:D:359:ILE:HD11	1.98	0.46
1:A:431:LYS:HE2	1:A:457:ILE:HG23	1.98	0.45
3:C:470:GLU:O	3:C:474:HIS:ND1	2.38	0.45
4:D:34:LEU:HD23	4:D:231:VAL:HG23	1.98	0.45
5:E:124:PRO:O	5:E:128:ILE:HG12	2.14	0.45
4:D:212:LEU:HG	4:D:290:LEU:HD13	1.99	0.45
4:D:318:TYR:HE1	4:D:341:MET:HE2	1.81	0.45
1:A:615:PHE:H	1:A:642:ARG:HH22	1.64	0.45
10:L:43:DA:H2'	10:L:44:DG:H8	1.80	0.45
1:A:316:LEU:H	1:A:316:LEU:HD23	1.82	0.45
4:D:405:GLU:HA	7:G:8:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:133:LEU:HD22	6:F:165:LYS:HD2	1.99	0.45
2:B:527:MET:O	2:B:531:VAL:HG12	2.17	0.45
4:D:151:TYR:O	4:D:154:GLU:HG3	2.17	0.45
2:B:152:LEU:HD12	2:B:153:PRO:HD2	1.99	0.45
3:C:511:LYS:HG3	3:C:514:ARG:HH21	1.82	0.45
9:K:155:LEU:HD13	9:K:181:TYR:HE2	1.81	0.45
1:A:86:LEU:HB3	1:A:114:HIS:HB2	1.99	0.45
2:B:370:LYS:HB3	2:B:371:PRO:HD3	2.00	0.45
3:C:407:ILE:HG21	6:F:23:GLY:HA2	1.99	0.45
4:D:48:LEU:O	4:D:53:LYS:NZ	2.49	0.45
1:A:58:ALA:HB2	4:D:334:MET:HB3	1.99	0.44
5:E:77:LYS:HE2	5:E:77:LYS:HB2	1.88	0.44
6:F:21:TRP:CD1	6:F:166:ALA:HB1	2.52	0.44
9:K:107:GLU:OE2	9:K:135:LYS:NZ	2.50	0.44
9:K:209:GLU:HA	9:K:212:GLU:HG2	1.99	0.44
10:L:34:DT:H2"	10:L:35:DG:C8	2.51	0.44
2:B:352:GLU:HG2	2:B:417:ILE:HG12	1.99	0.44
3:C:540:GLN:O	3:C:543:ARG:HG3	2.17	0.44
5:E:251:ARG:HH22	5:E:293:GLN:HG3	1.82	0.44
2:B:79:GLU:N	2:B:79:GLU:OE1	2.50	0.44
2:B:268:LYS:O	2:B:271:LEU:HG	2.18	0.44
5:E:375:VAL:HA	5:E:379:LEU:HB2	2.00	0.44
1:A:613:THR:O	1:A:642:ARG:NH2	2.50	0.44
5:E:387:HIS:HE1	6:F:67:SER:H	1.66	0.44
2:B:156:ARG:H	2:B:156:ARG:HD3	1.83	0.44
6:F:44:LEU:HD12	6:F:227:LEU:HD13	1.99	0.44
6:F:252:ARG:NH1	6:F:263:GLU:OE2	2.51	0.44
4:D:399:ASP:OD1	4:D:399:ASP:N	2.51	0.44
9:K:201:GLU:HA	9:K:204:LYS:HG2	1.99	0.44
6:F:252:ARG:HD3	6:F:261:LEU:HD13	2.00	0.43
2:B:124:LEU:HD23	2:B:129:ASP:HB3	1.99	0.43
2:B:344:LEU:HD11	2:B:433:LEU:HD22	2.00	0.43
2:B:437:CYS:SG	2:B:438:MET:N	2.91	0.43
7:G:54:GLN:HA	7:G:57:VAL:HG12	1.99	0.43
9:K:164:PHE:HB3	9:K:181:TYR:CE1	2.53	0.43
9:K:219:PHE:HD1	9:K:222:LYS:HZ3	1.64	0.43
2:B:445:LYS:HD3	2:B:472:ASP:HB3	1.99	0.43
2:B:447:VAL:HG12	2:B:454:VAL:HG21	2.00	0.43
10:L:50:DC:H2"	10:L:51:DA:C8	2.53	0.43
1:A:393:THR:O	1:A:393:THR:OG1	2.36	0.43
2:B:709:THR:HG22	2:B:712:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:LEU:HD11	2:B:608:ILE:HG21	1.99	0.43
1:A:588:GLU:O	1:A:591:GLN:HG3	2.18	0.43
2:B:571:THR:OG1	2:B:572:GLN:N	2.52	0.43
1:A:199:LEU:HG	1:A:200:ARG:HG2	2.00	0.43
5:E:340:ASN:OD1	5:E:340:ASN:N	2.52	0.43
3:C:462:LYS:HG3	5:E:276:LEU:HD22	1.99	0.43
5:E:131:LEU:O	5:E:135:VAL:HG23	2.18	0.43
5:E:275:HIS:HB3	5:E:282:PRO:HA	2.00	0.43
2:B:53:LEU:HD12	2:B:87:LEU:HD13	2.00	0.43
2:B:555:GLN:HB2	2:B:557:ILE:HG22	2.00	0.43
5:E:112:LYS:O	5:E:147:ASN:ND2	2.52	0.43
5:E:348:CYS:HB3	6:F:146:ARG:HD3	2.00	0.43
1:A:88:ALA:HB2	1:A:114:HIS:CD2	2.54	0.42
2:B:42:MET:HG2	2:B:48:LYS:HB2	1.99	0.42
3:C:461:LEU:HD22	3:C:521:LEU:HD13	2.00	0.42
5:E:92:VAL:HG23	5:E:104:ILE:HG13	2.00	0.42
9:K:141:LYS:HE2	9:K:141:LYS:HB3	1.88	0.42
9:K:252:LEU:HB2	9:K:256:MET:HB3	2.01	0.42
1:A:633:ARG:HG2	1:A:676:ARG:HA	2.01	0.42
2:B:463:PRO:HG3	2:B:654:PHE:HD1	1.83	0.42
3:C:523:SER:HB3	5:E:268:LYS:HG3	2.01	0.42
6:F:22:TRP:CD1	6:F:34:LEU:HD12	2.54	0.42
1:A:114:HIS:HE1	1:A:492:ASN:HD21	1.66	0.42
1:A:678:ARG:HD3	7:G:66:PHE:HE2	1.84	0.42
5:E:212:ALA:O	5:E:217:GLY:N	2.52	0.42
2:B:263:LEU:HB3	2:B:334:ARG:NH1	2.34	0.42
3:C:446:GLN:HG2	5:E:286:LEU:HG	2.02	0.42
4:D:101:LEU:HD23	4:D:105:LEU:HB2	2.01	0.42
9:K:157:LYS:HE3	9:K:157:LYS:HB2	1.90	0.42
5:E:169:ILE:HD12	5:E:198:VAL:HG22	2.01	0.42
1:A:375:LYS:HE3	1:A:375:LYS:HB3	1.83	0.42
1:A:446:ILE:O	1:A:448:ALA:N	2.49	0.42
2:B:627:TYR:HA	10:L:55:DA:H2"	2.00	0.42
4:D:42:LEU:HD11	4:D:46:ARG:HH21	1.85	0.42
1:A:418:LYS:HE3	1:A:418:LYS:HB3	1.94	0.42
5:E:147:ASN:OD1	5:E:148:SER:N	2.53	0.42
1:A:448:ALA:O	1:A:452:ARG:N	2.51	0.42
2:B:633:LEU:HD21	2:B:652:LEU:HD21	2.02	0.42
3:C:431:ILE:HG12	6:F:229:TRP:HZ3	1.84	0.42
4:D:55:TRP:HH2	4:D:83:GLN:HE21	1.68	0.42
1:A:384:ILE:HD11	1:A:388:GLN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:HIS:CE1	2:B:120:GLU:HB2	2.54	0.41
2:B:76:THR:O	2:B:80:ILE:HG12	2.20	0.41
6:F:69:PHE:HE1	6:F:139:LYS:HE2	1.84	0.41
6:F:199:ASP:OD1	6:F:199:ASP:N	2.52	0.41
1:A:119:THR:O	1:A:122:SER:OG	2.28	0.41
3:C:467:ALA:O	3:C:470:GLU:HG3	2.20	0.41
4:D:144:ASP:O	4:D:147:SER:OG	2.32	0.41
5:E:94:GLU:HG3	5:E:236:VAL:HG11	2.01	0.41
9:K:222:LYS:O	9:K:225:GLU:HG3	2.21	0.41
1:A:439:ILE:HG23	1:A:466:LEU:HD13	2.03	0.41
1:A:165:LYS:HB3	1:A:184:VAL:HG11	2.01	0.41
2:B:20:GLU:HG3	2:B:482:THR:O	2.20	0.41
1:A:326:LYS:O	1:A:334:ARG:NH2	2.53	0.41
1:A:510:VAL:HG23	1:A:690:ILE:O	2.20	0.41
1:A:537:ASN:O	1:A:540:LYS:HG2	2.21	0.41
2:B:216:LYS:HE3	2:B:216:LYS:HB3	1.87	0.41
6:F:148:ASN:O	6:F:151:VAL:HG12	2.21	0.41
7:G:5:LEU:HD21	9:K:268:LEU:HD21	2.03	0.41
7:G:22:TYR:HA	7:G:25:GLU:HG2	2.02	0.41
1:A:112:HIS:HB2	4:D:310:GLU:OE1	2.21	0.41
1:A:511:TRP:HE1	1:A:691:THR:HB	1.85	0.41
2:B:263:LEU:HD13	2:B:334:ARG:HD3	2.03	0.41
2:B:418:ILE:HG22	2:B:420:PRO:HD3	2.02	0.41
7:G:34:ILE:HG23	7:G:45:VAL:HG12	2.02	0.41
9:K:206:VAL:HA	9:K:209:GLU:HG2	2.02	0.41
2:B:462:SER:HB3	2:B:692:LYS:O	2.21	0.41
2:B:662:GLN:O	2:B:666:ARG:HG2	2.20	0.41
2:B:681:ASP:HB3	2:B:684:PHE:HD2	1.85	0.41
3:C:408:ARG:NH2	6:F:122:SER:O	2.54	0.41
4:D:78:GLU:HG3	4:D:79:PHE:CD2	2.55	0.41
4:D:143:ARG:NH2	4:D:147:SER:HB2	2.35	0.41
4:D:207:ASP:OD1	4:D:207:ASP:N	2.52	0.41
5:E:60:HIS:CD2	5:E:159:MET:HE1	2.56	0.41
5:E:167:VAL:HB	5:E:196:VAL:HG22	2.01	0.41
9:K:213:LYS:O	9:K:216:GLN:HG3	2.21	0.41
1:A:686:SER:HB2	4:D:386:THR:HG21	2.03	0.41
2:B:195:ALA:O	2:B:199:ILE:HG23	2.21	0.41
2:B:229:ALA:HB3	2:B:451:PHE:HD1	1.86	0.41
2:B:640:LEU:HD22	2:B:646:ILE:HD12	2.03	0.41
3:C:535:LYS:HE2	3:C:535:LYS:HB2	1.88	0.41
10:L:43:DA:H2'	10:L:44:DG:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:MET:HE2	2:B:25:MET:HB2	1.97	0.40
2:B:618:VAL:HG11	2:B:664:VAL:HA	2.03	0.40
3:C:528:MET:HA	3:C:531:THR:HG22	2.02	0.40
6:F:215:LEU:HD22	6:F:230:VAL:HG11	2.03	0.40
9:K:117:LEU:HD12	9:K:125:THR:HB	2.03	0.40
1:A:62:ARG:HA	4:D:339:PRO:HG3	2.02	0.40
2:B:494:ILE:HG12	2:B:684:PHE:HB3	2.02	0.40
2:B:681:ASP:HB3	2:B:684:PHE:CD2	2.56	0.40
2:B:694:PRO:HB2	2:B:696:TRP:CD1	2.56	0.40
5:E:172:SER:HA	5:E:201:LEU:HB2	2.03	0.40
5:E:255:PRO:HD3	5:E:312:LEU:HD22	2.02	0.40
7:G:14:PRO:HA	7:G:17:LYS:HB3	2.03	0.40
1:A:363:VAL:HG22	1:A:439:ILE:HD12	2.02	0.40
2:B:613:HIS:CD2	5:E:206:ARG:HB2	2.56	0.40
5:E:358:TYR:HE2	5:E:369:VAL:HG22	1.85	0.40
9:K:164:PHE:HB3	9:K:181:TYR:HE1	1.86	0.40
2:B:52:LEU:HD22	2:B:72:TYR:HE1	1.87	0.40
2:B:161:PHE:O	2:B:165:GLY:N	2.52	0.40
6:F:213:LEU:HB3	6:F:231:PHE:HE1	1.86	0.40
3:C:472:LEU:HB3	5:E:307:ILE:HG23	2.03	0.40
4:D:140:LYS:HG3	4:D:141:HIS:ND1	2.35	0.40
4:D:204:LEU:O	4:D:211:GLN:NE2	2.54	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	598/782 (76%)	563 (94%)	35 (6%)	0	100	100
2	B	698/768 (91%)	675 (97%)	23 (3%)	0	100	100
3	C	152/548 (28%)	148 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	430/462 (93%)	428 (100%)	2 (0%)	0	100	100
5	E	365/395 (92%)	360 (99%)	5 (1%)	0	100	100
6	F	254/308 (82%)	251 (99%)	3 (1%)	0	100	100
7	G	64/71 (90%)	61 (95%)	3 (5%)	0	100	100
8	H	38/940 (4%)	37 (97%)	1 (3%)	0	100	100
9	K	156/273 (57%)	153 (98%)	3 (2%)	0	100	100
All	All	2755/4547 (61%)	2676 (97%)	79 (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%)	531 (99%)	5 (1%)	70	76
2	B	614/672 (91%)	613 (100%)	1 (0%)	87	85
3	C	140/484 (29%)	140 (100%)	0	100	100
4	D	377/399 (94%)	376 (100%)	1 (0%)	86	83
5	E	329/352 (94%)	328 (100%)	1 (0%)	86	83
6	F	230/272 (85%)	229 (100%)	1 (0%)	84	81
7	G	59/64 (92%)	56 (95%)	3 (5%)	21	48
8	H	33/804 (4%)	32 (97%)	1 (3%)	36	60
9	K	150/233 (64%)	150 (100%)	0	100	100
All	All	2468/3968 (62%)	2455 (100%)	13 (0%)	78	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	VAL
1	A	415	HIS

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Mol	Chain	Res	Type
1	A	502	ILE
1	A	510	VAL
1	A	523	VAL
2	B	5	VAL
4	D	215	PHE
5	E	371	CYS
6	F	247	VAL
7	G	21	LEU
7	G	48	GLU
7	G	60	LEU
8	H	904	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	ASN
1	A	307	ASN
1	A	492	ASN
1	A	497	GLN
1	A	506	GLN
1	A	595	ASN
1	A	599	ASN
1	A	656	ASN
1	A	668	GLN
2	B	118	HIS
2	B	154	HIS
2	B	187	GLN
2	B	203	ASN
2	B	260	GLN
2	B	262	ASN
2	B	543	GLN
2	B	555	GLN
2	B	700	HIS
3	C	405	GLN
3	C	458	GLN
4	D	54	ASN
4	D	97	HIS
4	D	211	GLN
4	D	260	ASN
4	D	273	GLN
4	D	353	GLN
4	D	390	GLN

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Mol	Chain	Res	Type
5	E	99	ASN
5	E	154	GLN
5	E	162	HIS
5	E	220	HIS
5	E	227	HIS
5	E	257	HIS
6	F	9	ASN
6	F	25	GLN
6	F	185	GLN
6	F	204	GLN
6	F	248	HIS
9	K	169	ASN
9	K	208	GLN
9	K	244	HIS

### 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.

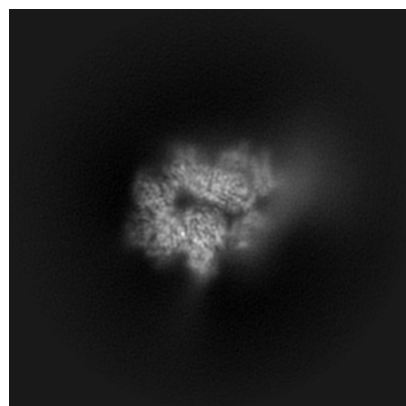
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72341. These allow visual inspection of the internal detail of the map and identification of artifacts.

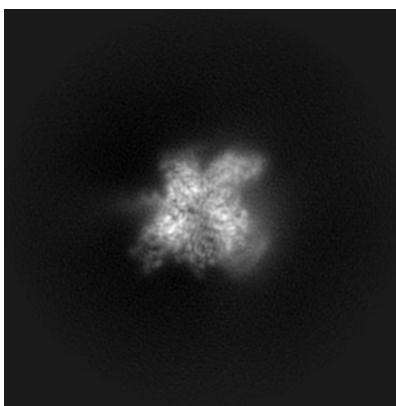
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

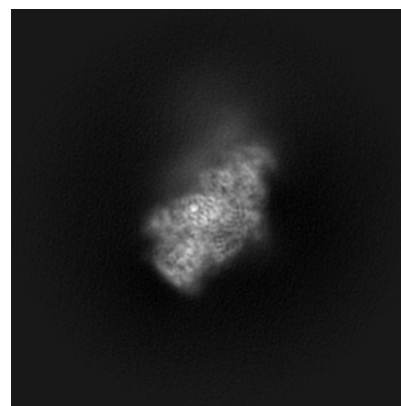
#### 6.1.1 Primary map



X

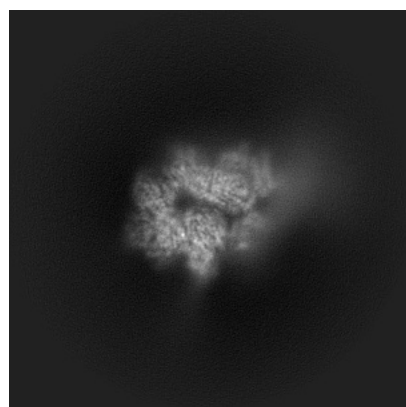


Y

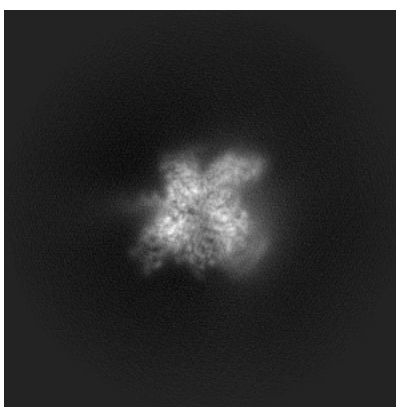


Z

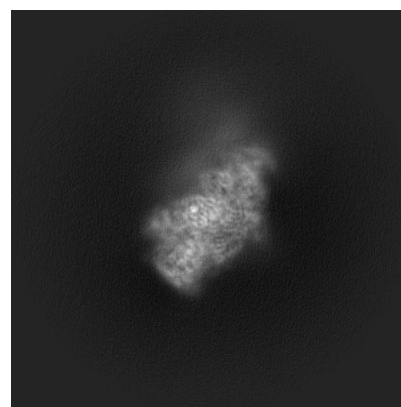
#### 6.1.2 Raw map



X



Y

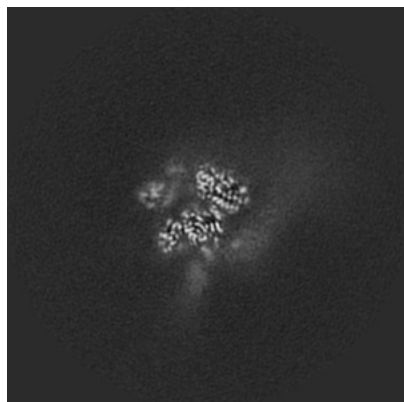


Z

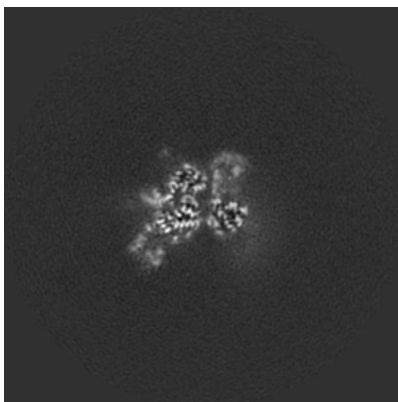
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

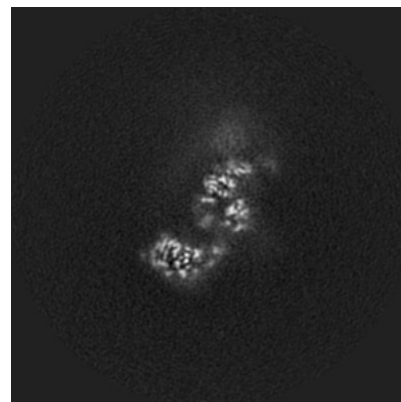
### 6.2.1 Primary map



X Index: 180

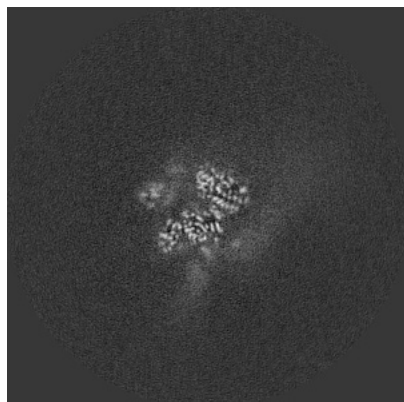


Y Index: 180

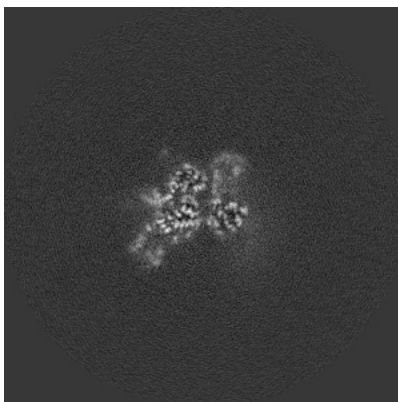


Z Index: 180

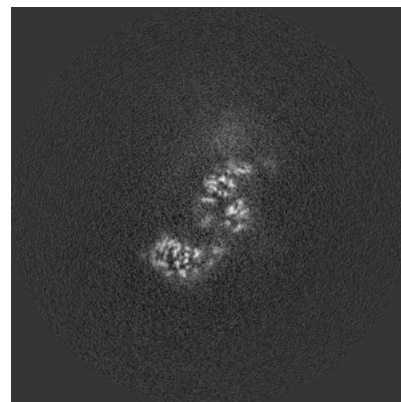
### 6.2.2 Raw map



X Index: 180



Y Index: 180

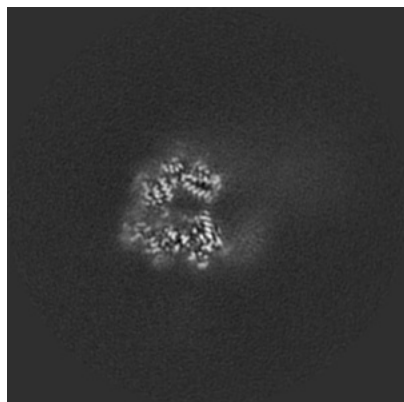


Z Index: 180

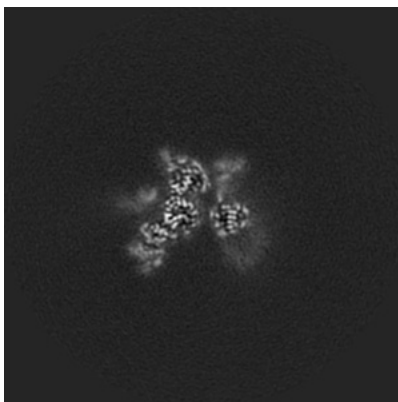
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

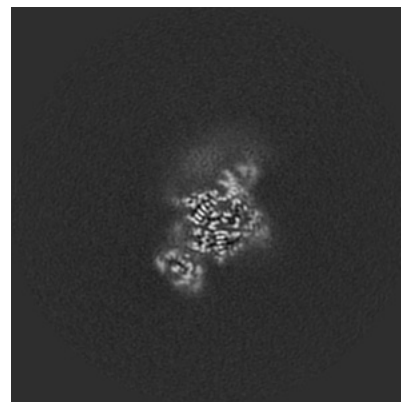
### 6.3.1 Primary map



X Index: 163

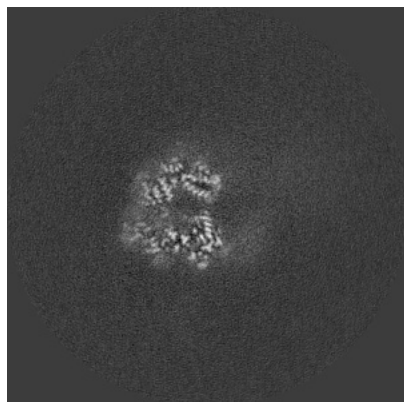


Y Index: 174

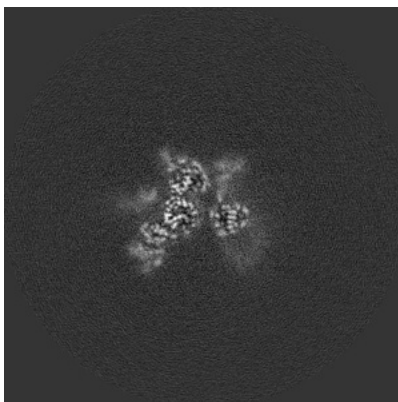


Z Index: 158

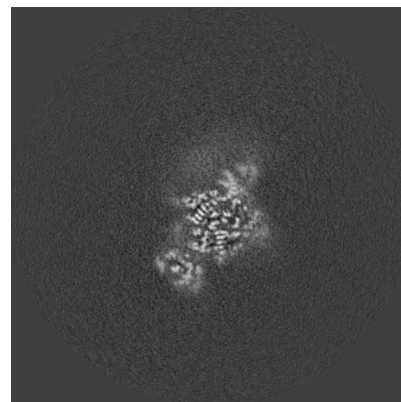
### 6.3.2 Raw map



X Index: 163



Y Index: 174



Z Index: 158

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

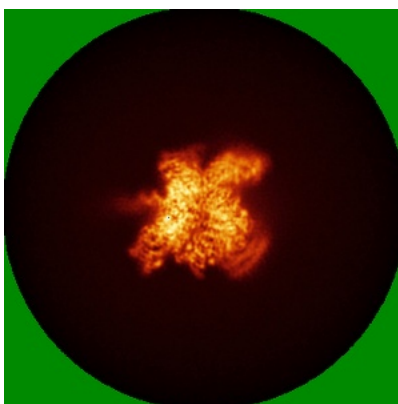


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

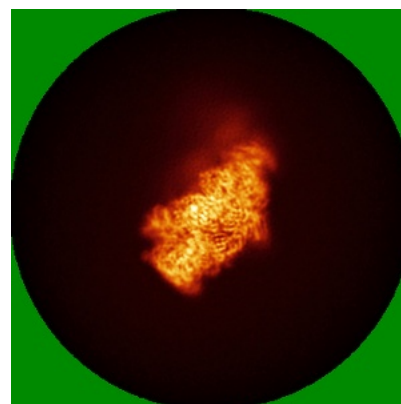
### 6.4.1 Primary map



X

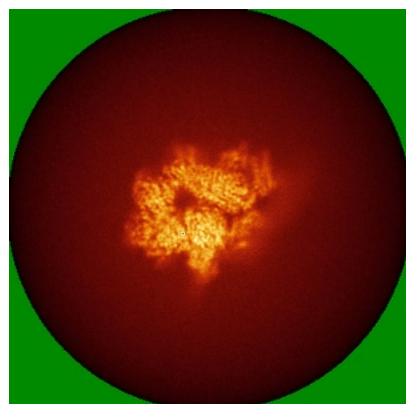


Y

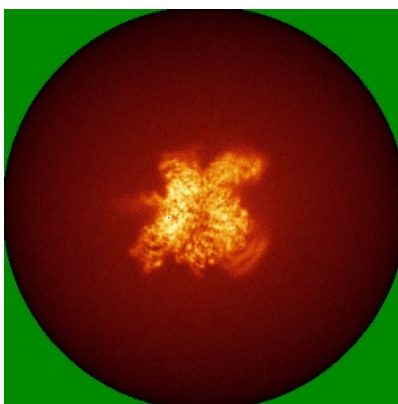


Z

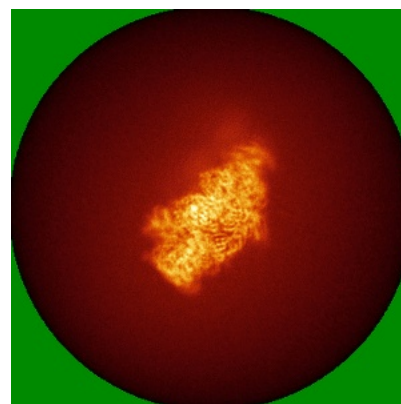
### 6.4.2 Raw map



X



Y

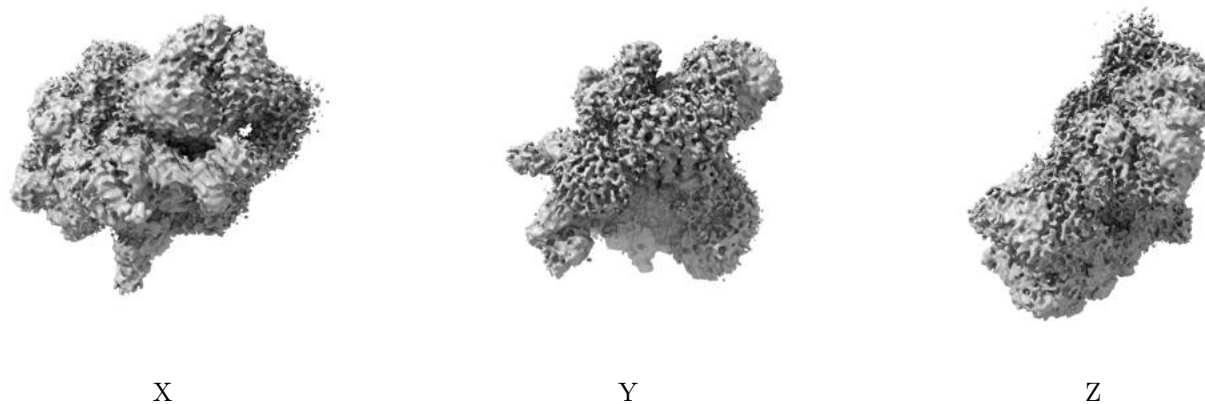


Z

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.

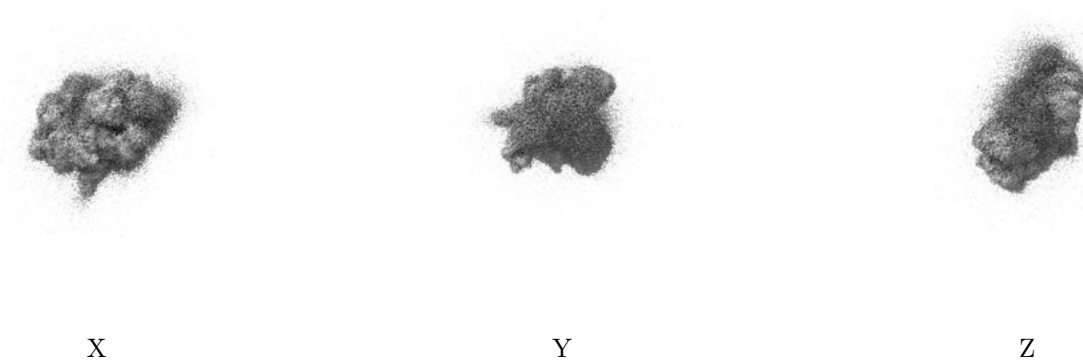
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.004. 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](#)

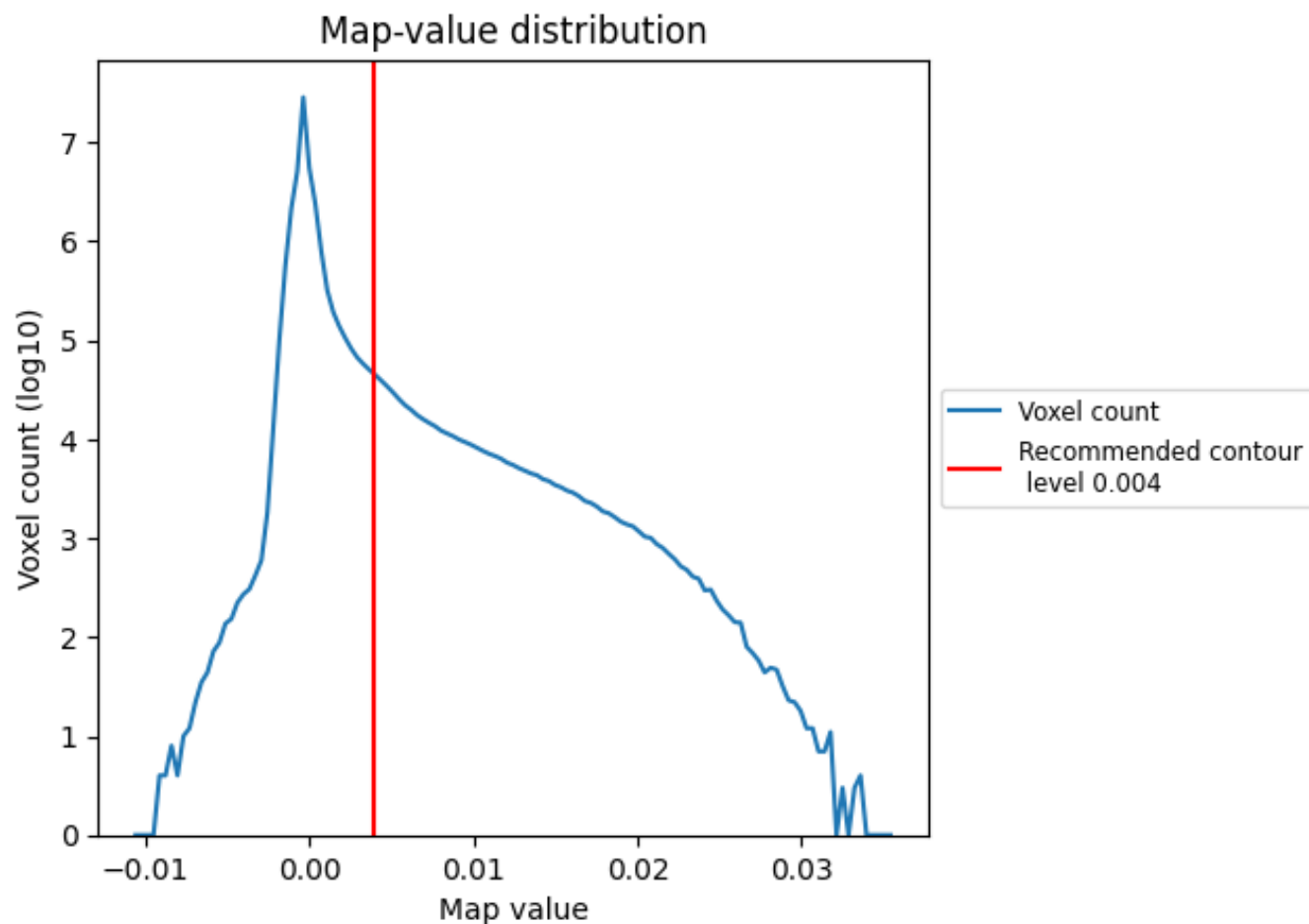
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

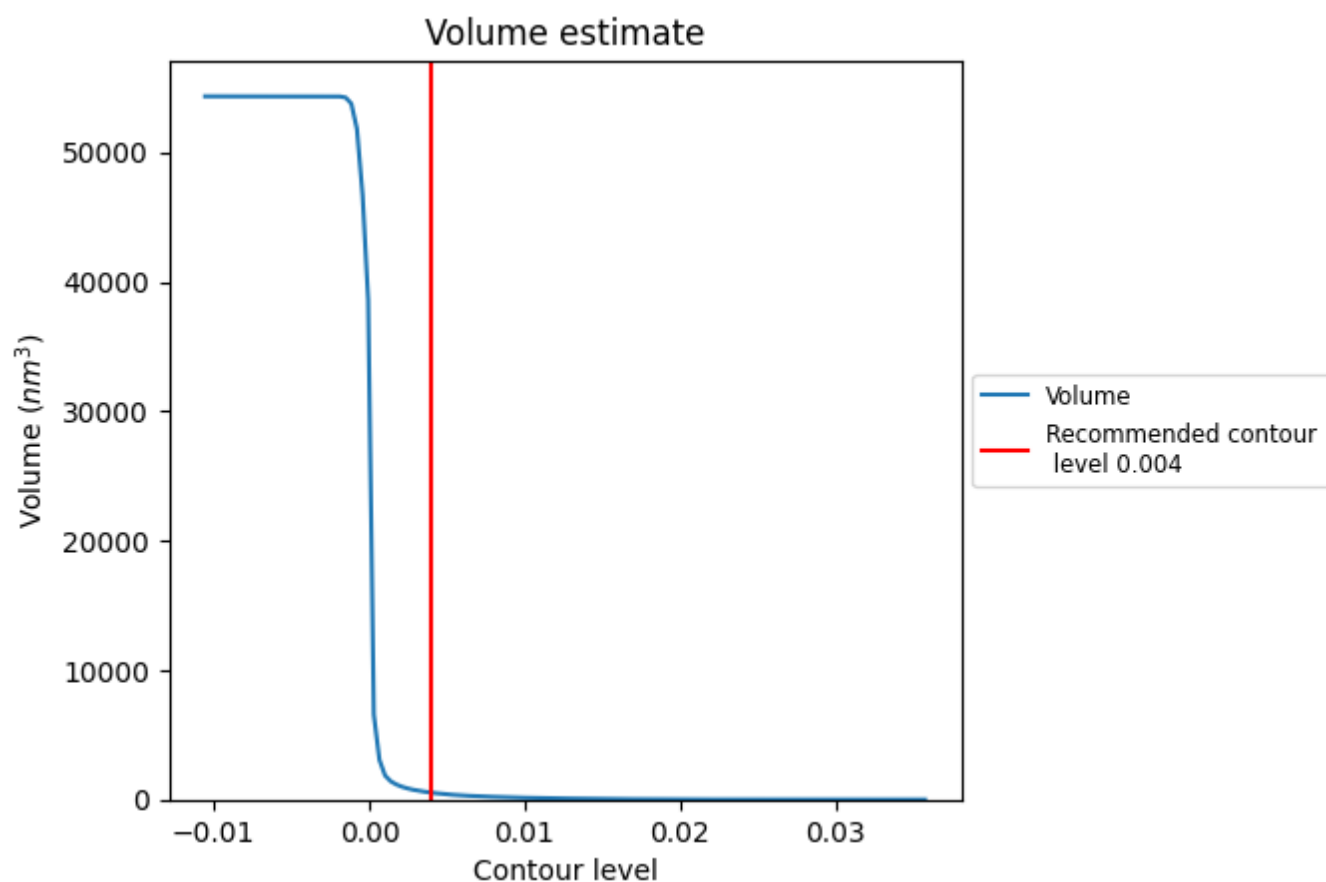
This section contains the results of statistical analysis of the map.

### 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.

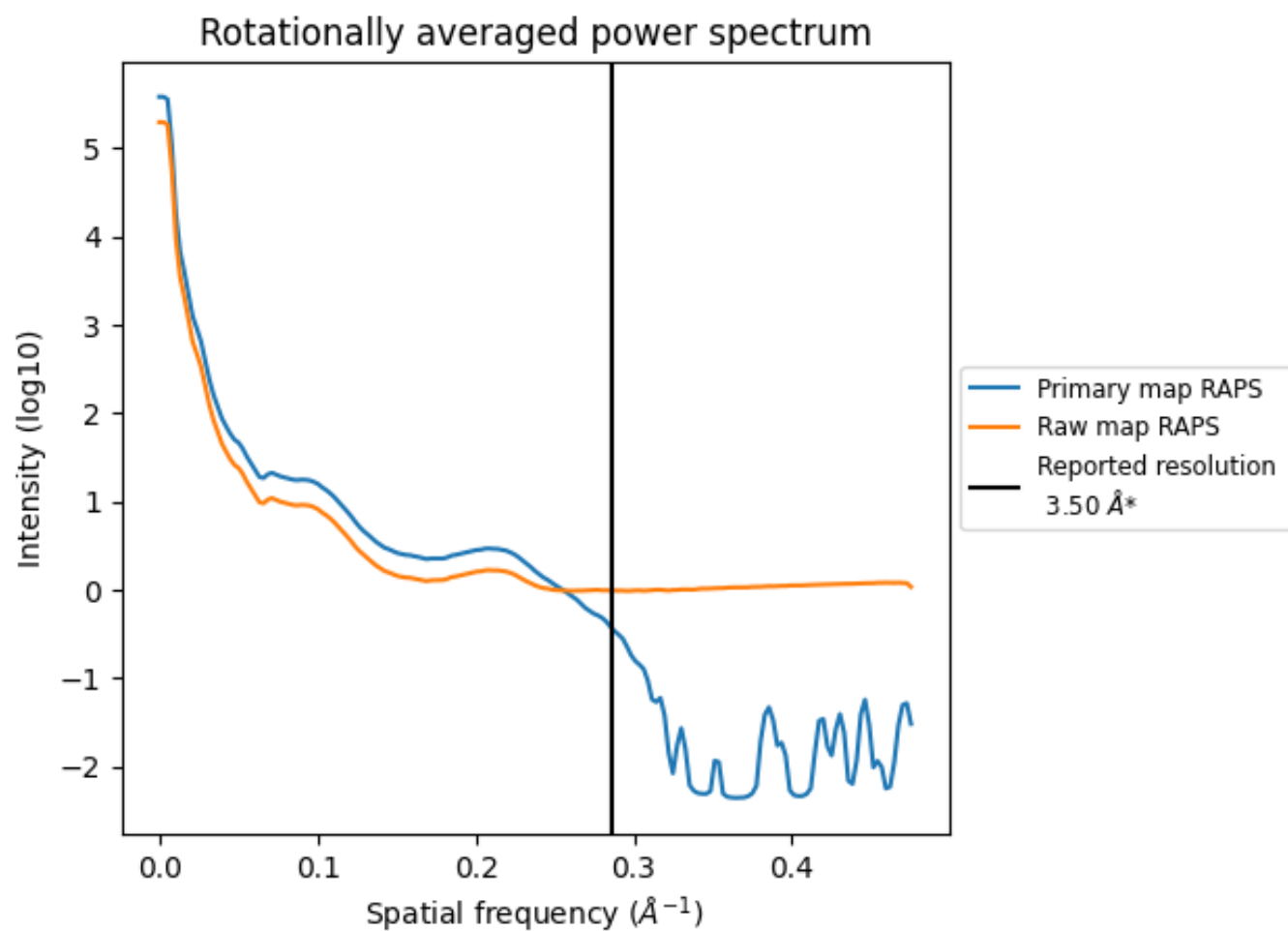
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 535  $\text{nm}^3$ ; this corresponds to an approximate mass of 483 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 ⓘ

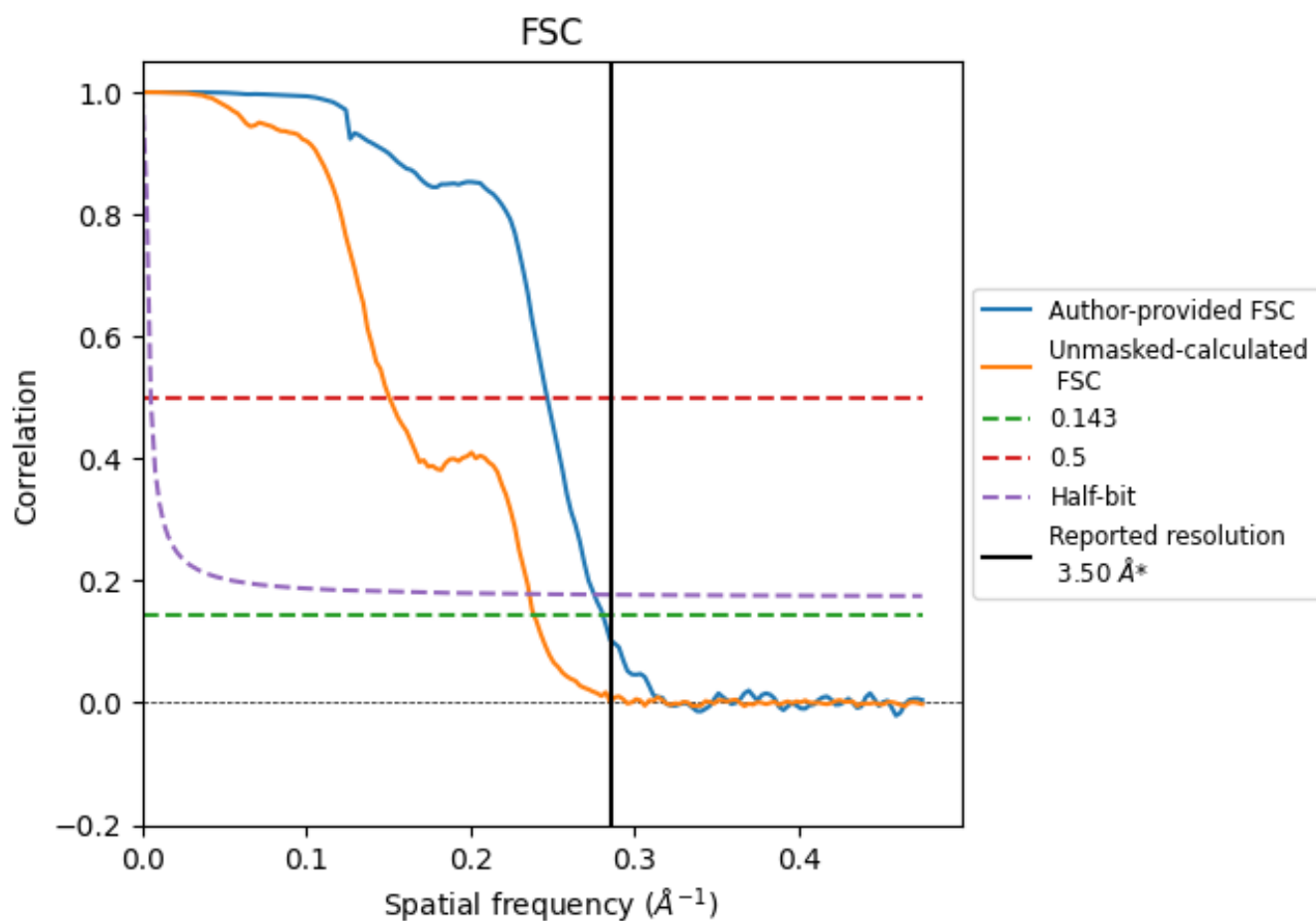


\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 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 0.286  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

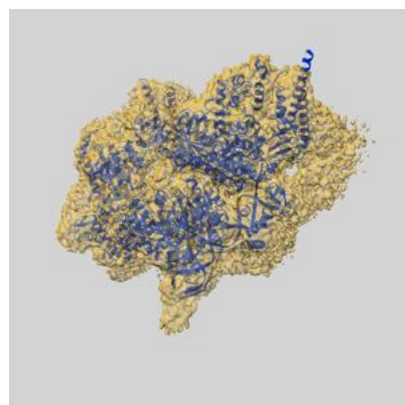
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.56	4.05	3.63
Unmasked-calculated*	4.19	6.64	4.24

\*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 4.19 differs from the reported value 3.5 by more than 10 %

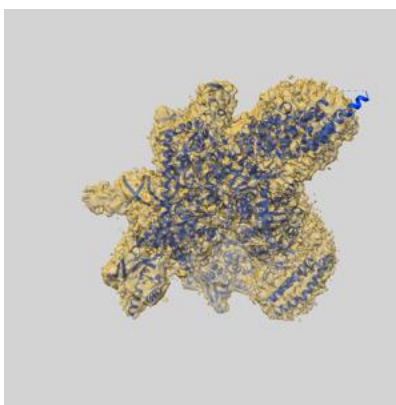
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-72341 and PDB model 9XYU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

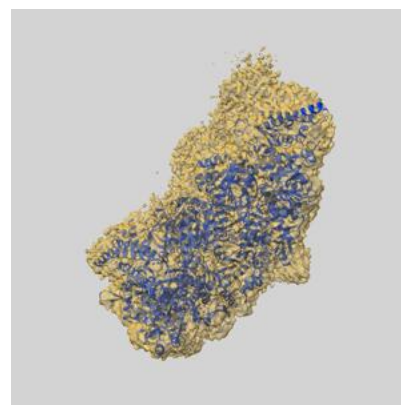
### 9.1 Map-model overlay [i](#)



X



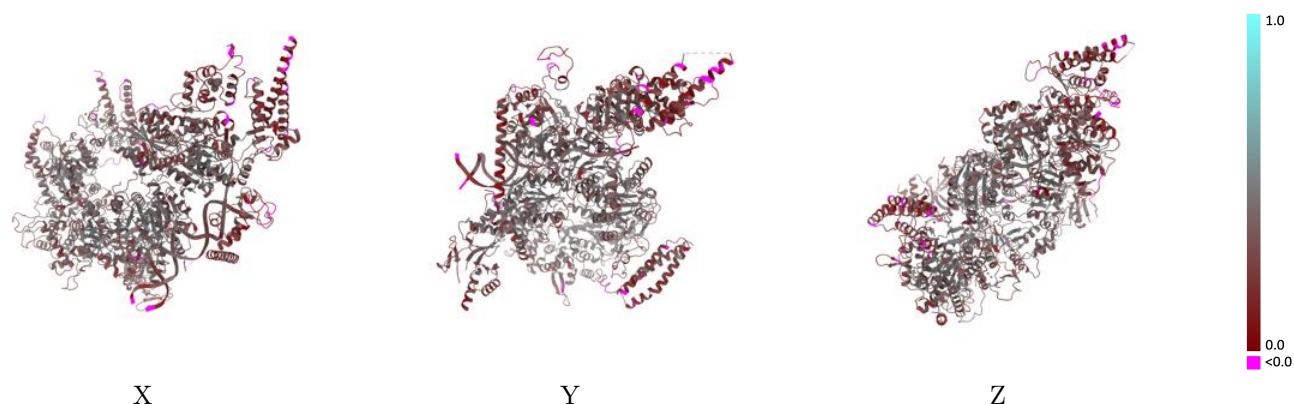
Y



Z

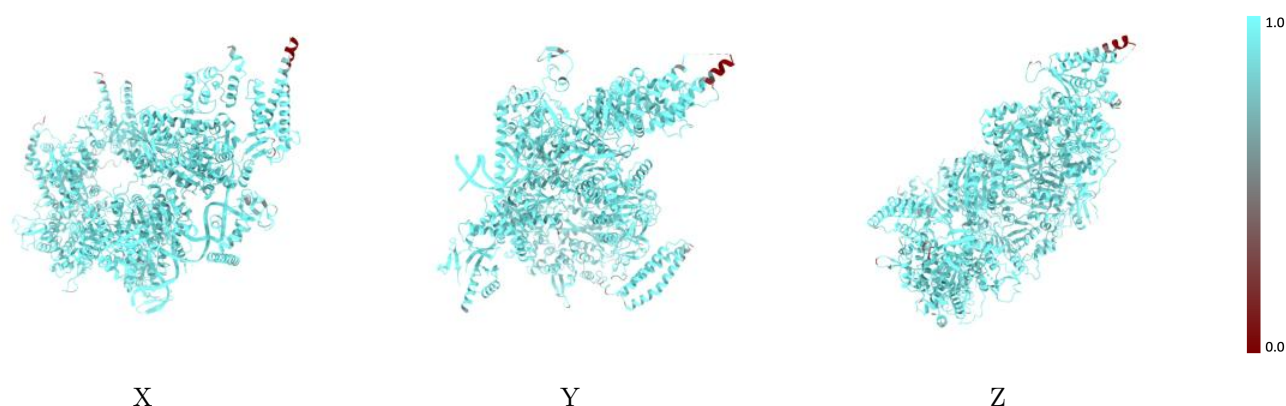
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



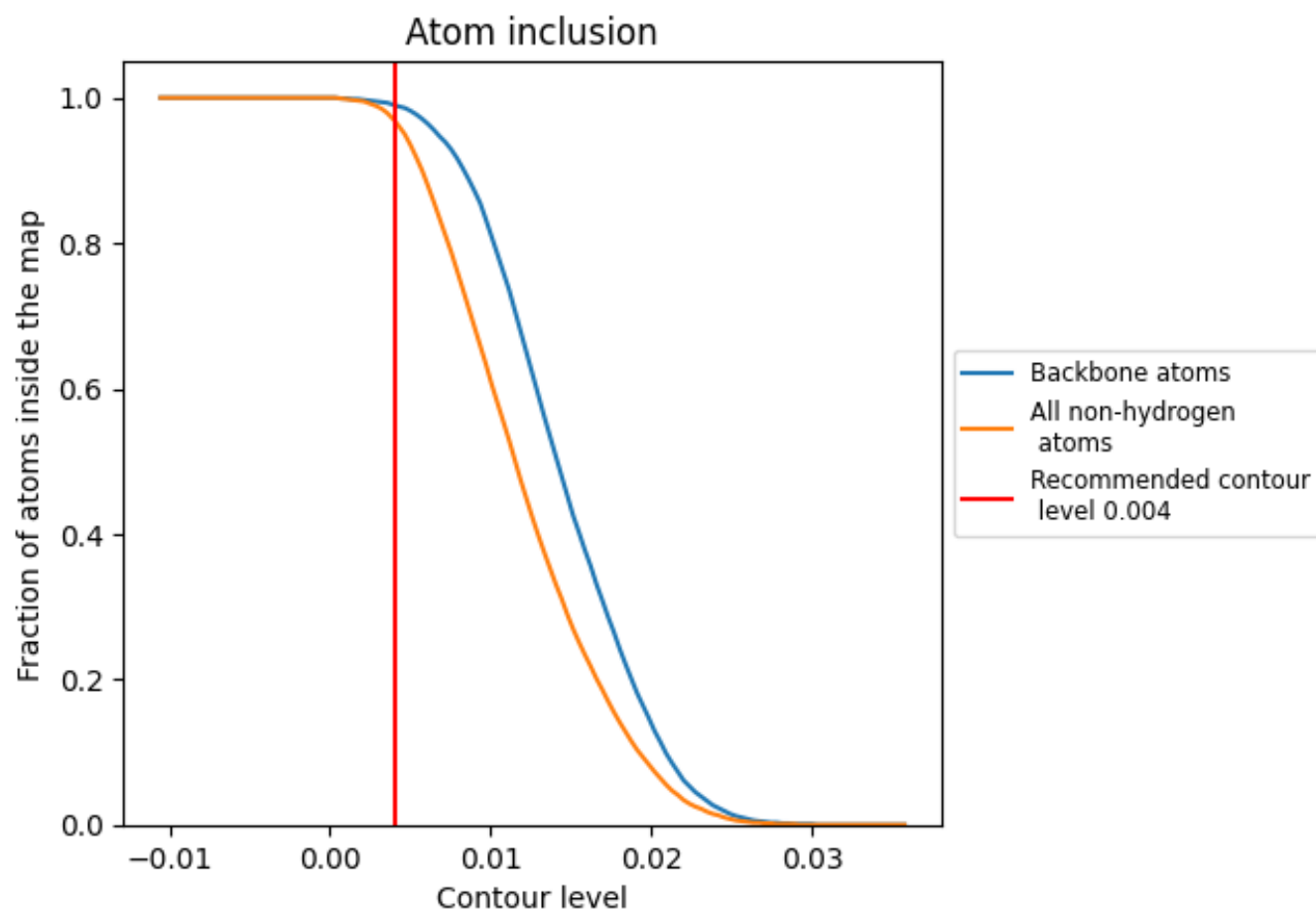
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

## 9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9690	<div><div></div></div> 0.3430
A	<div><div></div></div> 0.9810	<div><div></div></div> 0.3950
B	<div><div></div></div> 0.9610	<div><div></div></div> 0.3080
C	<div><div></div></div> 0.9130	<div><div></div></div> 0.2190
D	<div><div></div></div> 0.9740	<div><div></div></div> 0.3590
E	<div><div></div></div> 0.9780	<div><div></div></div> 0.3780
F	<div><div></div></div> 0.9840	<div><div></div></div> 0.3880
G	<div><div></div></div> 0.9850	<div><div></div></div> 0.3720
H	<div><div></div></div> 0.9330	<div><div></div></div> 0.3450
K	<div><div></div></div> 0.9370	<div><div></div></div> 0.2380
L	<div><div></div></div> 0.9980	<div><div></div></div> 0.3200
M	<div><div></div></div> 0.9870	<div><div></div></div> 0.3110

1.0

0.0

<0.0