Full wwPDB EM Validation Report ⓘ

Sep 2, 2026 – 09:10 PM EDT

PDB ID	:	9ZO5 / pdb_00009zo5
EMDB ID	:	EMD-74466
Title	:	Cryo-EM structure of the complete Pyrococcus furiosus RNA polymerase in open clamp conformation
Authors	:	Fordjour, G.N.R.; Armache, J.-P.; Murakami, K.S.
Deposited on	:	2025-12-15
Resolution	:	4.05 Å(reported)

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:

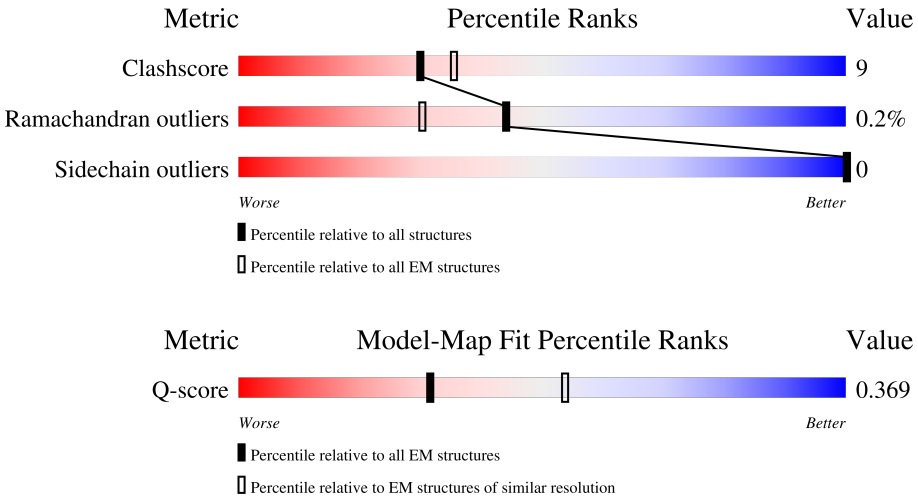
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.05 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	6569 (3.55 - 4.55)

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 <=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	907	77% 22% .
2	B	1117	74% 23% .
3	C	397	74% 24% .
4	D	275	76% 18% 6%

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Mol	Chain	Length	Quality of chain
5	E	189	67% 31%
6	F	120	79% 21%
7	L	95	79% 20%
8	H	82	78% 15% 7%
9	N	65	82% 18%
10	K	57	65% 32%
11	P	49	69% 29%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 26194 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 DNA-directed RNA polymerase subunit Rpo1N.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	901	Total	C	N	O	S	0	0
			7197	4541	1282	1335	39		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1076	Total	C	N	O	S	0	0
			8637	5474	1533	1596	34		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit Rpo1C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	388	Total	C	N	O	S	0	0
			3041	1921	525	585	10		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit Rpo3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	258	Total	C	N	O	S	0	0
			2086	1358	330	396	2		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	262	TRP	-	expression tag	UNP Q8U0E4
D	263	SER	-	expression tag	UNP Q8U0E4
D	264	HIS	-	expression tag	UNP Q8U0E4
D	265	PRO	-	expression tag	UNP Q8U0E4
D	266	GLN	-	expression tag	UNP Q8U0E4
D	267	PHE	-	expression tag	UNP Q8U0E4
D	268	GLU	-	expression tag	UNP Q8U0E4
D	269	LYS	-	expression tag	UNP Q8U0E4
D	270	HIS	-	expression tag	UNP Q8U0E4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	271	HIS	-	expression tag	UNP Q8U0E4
D	272	HIS	-	expression tag	UNP Q8U0E4
D	273	HIS	-	expression tag	UNP Q8U0E4
D	274	HIS	-	expression tag	UNP Q8U0E4
D	275	HIS	-	expression tag	UNP Q8U0E4

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit Rpo7.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	185	Total	C	N	O	S	0	0
			1496	971	247	272	6		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit Rpo4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	120	Total	C	N	O	S	0	0
			986	627	163	189	7		

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit Rpo11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	94	Total	C	N	O	S	0	0
			777	500	129	146	2		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit Rpo5.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	76	Total	C	N	O	0	0
			609	398	100	111		

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit Rpo10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	65	Total	C	N	O	S	0	0
			543	345	94	97	7		

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit Rpo6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	55	Total	C	N	O	S	0	0
			424	281	71	71	1		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit Rpo12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	48	Total	C	N	O	S	0	0
			393	251	75	63	4		

- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	A	2	Total	Zn	0
			2	2	
12	B	1	Total	Zn	0
			1	1	
12	N	1	Total	Zn	0
			1	1	
12	P	1	Total	Zn	0
			1	1	

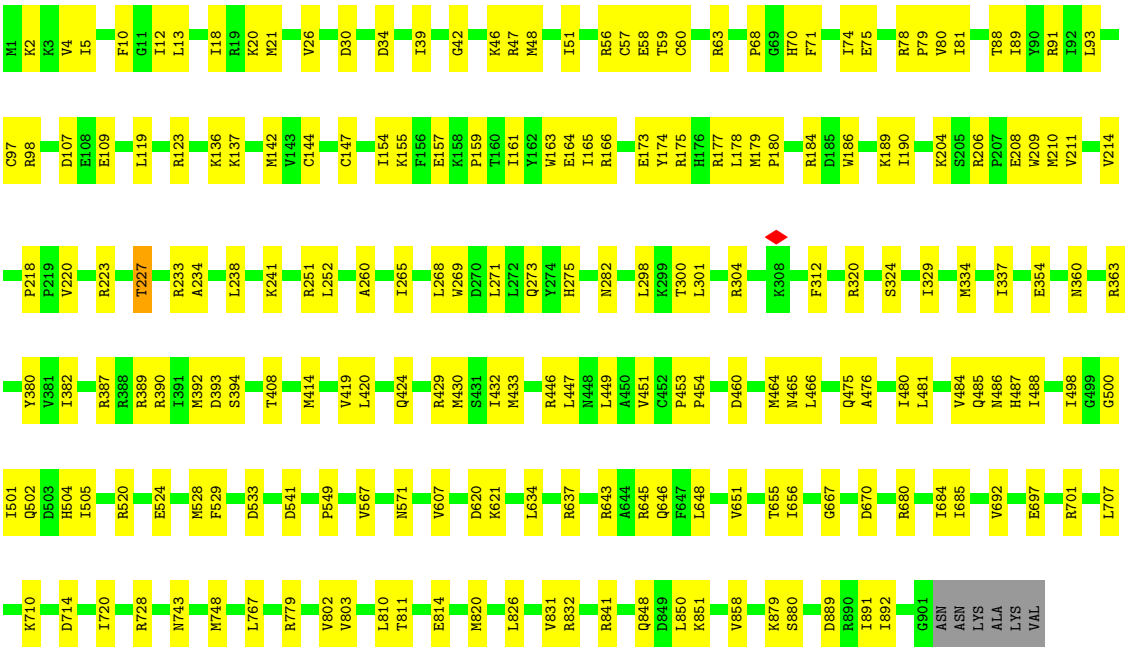
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase subunit Rpo1N

Chain A:

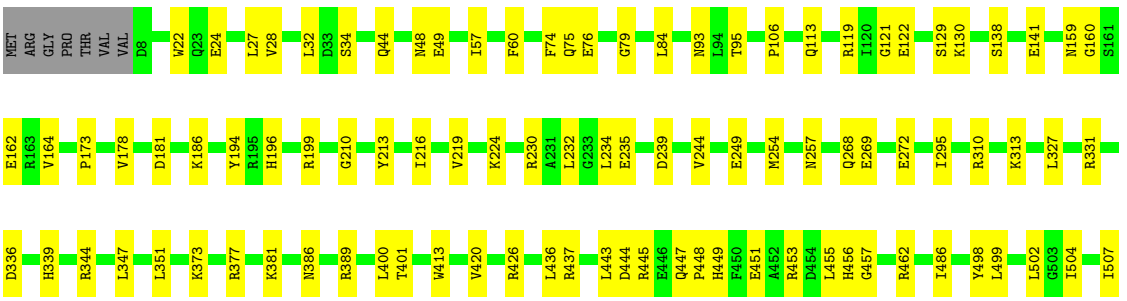


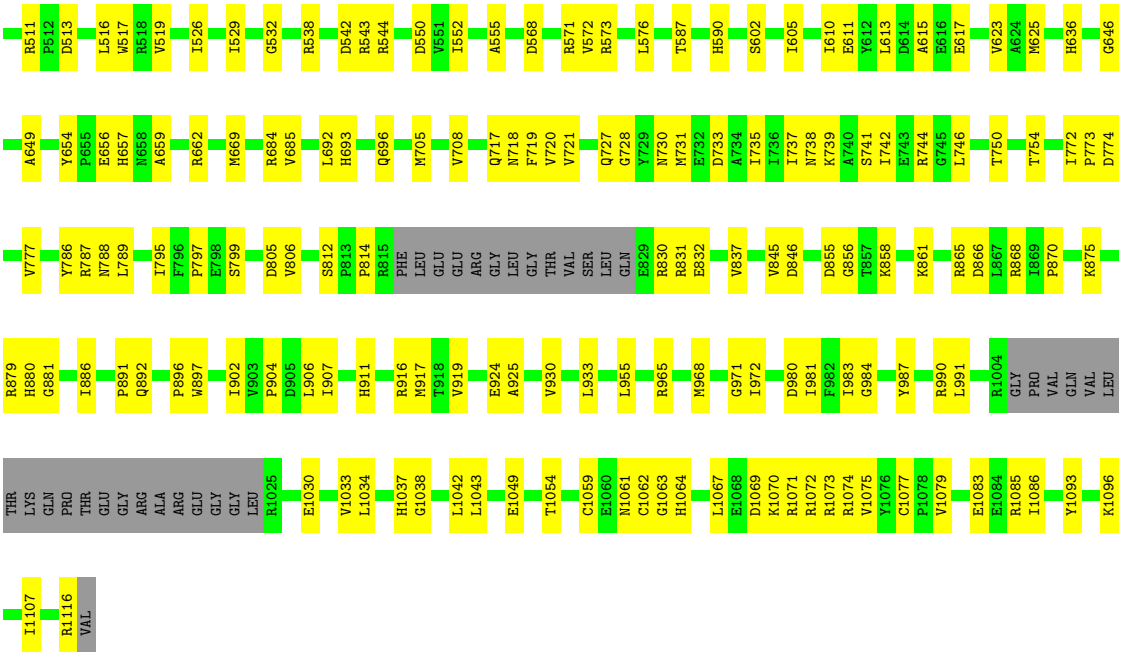


• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain B:



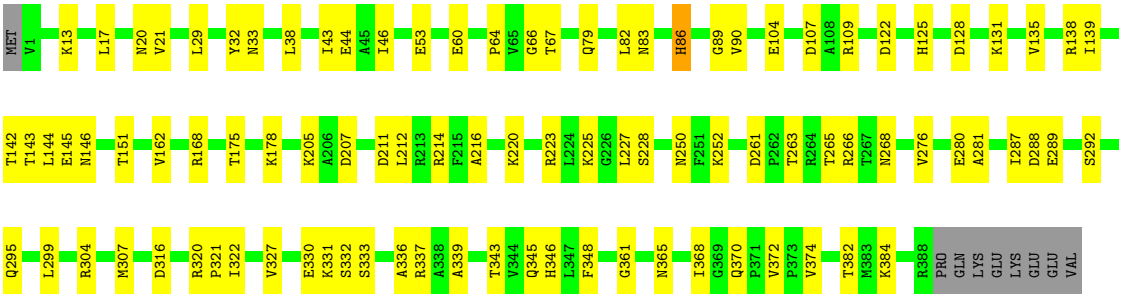




• Molecule 3: DNA-directed RNA polymerase subunit Rpo1C

Chain C:

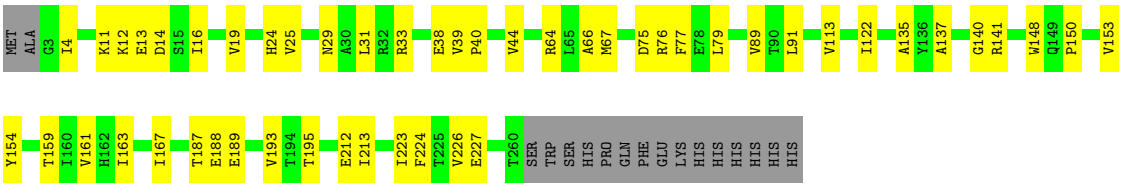




• Molecule 4: DNA-directed RNA polymerase subunit Rpo3

Chain D:

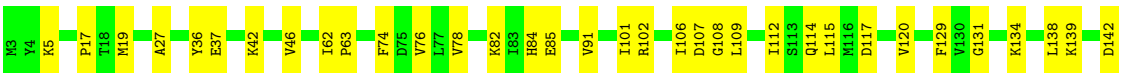


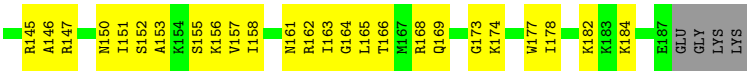


• Molecule 5: DNA-directed RNA polymerase subunit Rpo7

Chain E:



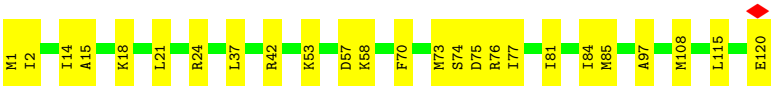




• Molecule 6: DNA-directed RNA polymerase subunit Rpo4

Chain F:

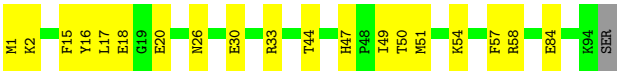




• Molecule 7: DNA-directed RNA polymerase subunit Rpo11

Chain L:

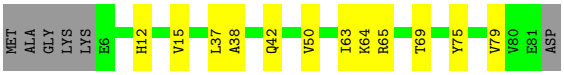




• Molecule 8: DNA-directed RNA polymerase subunit Rpo5

Chain H:

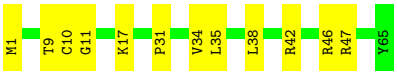




• Molecule 9: DNA-directed RNA polymerase subunit Rpo10

Chain N:

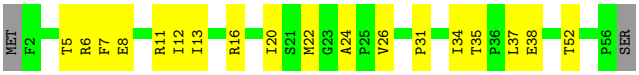




• Molecule 10: DNA-directed RNA polymerase subunit Rpo6

Chain K:





• Molecule 11: DNA-directed RNA polymerase subunit Rpo12

Chain P:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	142876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	-800	Depositor
Maximum defocus (nm)	-2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.961	Depositor
Minimum map value	-1.287	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.041	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	377.6, 377.6, 377.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.944, 0.944, 0.944	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.14	0/7338	0.38	0/9907
2	B	0.14	0/8811	0.37	1/11905 (0.0%)
3	C	0.13	0/3081	0.37	0/4156
4	D	0.13	0/2133	0.31	0/2894
5	E	0.16	0/1524	0.45	0/2052
6	F	0.13	0/1000	0.36	0/1338
7	L	0.16	0/792	0.45	0/1067
8	H	0.13	0/622	0.38	0/841
9	N	0.16	0/553	0.41	0/740
10	K	0.14	0/433	0.37	0/588
11	P	0.17	0/400	0.47	0/534
All	All	0.14	0/26687	0.38	1/36022 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	919	VAL	N-CA-C	-5.59	107.37	112.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	7197	0	7263	154	0
2	B	8637	0	8708	173	0
3	C	3041	0	3151	67	0
4	D	2086	0	2109	34	0
5	E	1496	0	1555	46	0
6	F	986	0	1001	19	0
7	L	777	0	788	18	0
8	H	609	0	634	12	0
9	N	543	0	541	10	0
10	K	424	0	460	15	0
11	P	393	0	423	10	0
12	A	2	0	0	0	0
12	B	1	0	0	0	0
12	N	1	0	0	0	0
12	P	1	0	0	0	0
All	All	26194	0	26633	479	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 9.

All (479) 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:656:ILE:HD11	2:B:728:GLY:HA3	1.67	0.77
1:A:505:ILE:HD11	1:A:621:LYS:HA	1.66	0.76
1:A:528:MET:HE1	7:L:58:ARG:HE	1.51	0.76
1:A:430:MET:HE1	1:A:487:HIS:HB3	1.69	0.75
1:A:10:PHE:HB3	2:B:1107:ILE:HD11	1.69	0.74
1:A:123:ARG:NH1	8:H:38:ALA:O	2.20	0.73
7:L:15:PHE:HB3	7:L:57:PHE:HB2	1.70	0.72
1:A:60:CYS:SG	1:A:70:HIS:CE1	2.82	0.72
3:C:333:SER:HB3	3:C:336:ALA:HB3	1.71	0.71
11:P:27:CYS:HB3	11:P:30:CYS:SG	2.31	0.71
6:F:37:LEU:H	6:F:42:ARG:HH12	1.39	0.70
2:B:568:ASP:H	2:B:571:ARG:HH21	1.38	0.70
4:D:91:LEU:HB2	4:D:135:ALA:HB3	1.75	0.69
1:A:892:ILE:HD13	3:C:46:ILE:HG12	1.76	0.68
2:B:576:LEU:HD12	2:B:613:LEU:HD12	1.76	0.68
1:A:475:GLN:HB3	10:K:37:LEU:HD22	1.77	0.67
10:K:20:ILE:HD11	10:K:26:VAL:HG22	1.75	0.67
1:A:851:LYS:HD3	3:C:374:VAL:HG22	1.77	0.66
2:B:1075:VAL:HG23	2:B:1086:ILE:HD13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:372:VAL:HG12	3:C:374:VAL:H	1.62	0.65
4:D:38:GLU:OE2	4:D:141:ARG:NH1	2.30	0.64
1:A:60:CYS:HA	2:B:1069:ASP:HA	1.80	0.64
2:B:744:ARG:HA	4:D:67:MET:HE1	1.80	0.64
1:A:832:ARG:HH21	3:C:82:LEU:H	1.46	0.63
2:B:106:PRO:HG2	2:B:113:GLN:HB2	1.80	0.63
2:B:230:ARG:NH1	2:B:235:GLU:O	2.32	0.63
4:D:44:VAL:HB	4:D:66:ALA:HA	1.79	0.63
4:D:153:VAL:HG12	4:D:226:VAL:HA	1.81	0.63
2:B:971:GLY:O	4:D:33:ARG:NH2	2.32	0.62
5:E:114:GLN:O	5:E:168:ARG:NH1	2.32	0.62
1:A:155:LYS:H	1:A:164:GLU:HA	1.65	0.62
5:E:37:GLU:OE1	6:F:24:ARG:NH2	2.32	0.62
1:A:382:ILE:HB	1:A:408:THR:HB	1.81	0.62
2:B:739:LYS:HB3	2:B:891:PRO:HA	1.82	0.62
9:N:10:CYS:SG	9:N:11:GLY:N	2.72	0.62
2:B:718:ASN:O	9:N:47:ARG:NH1	2.33	0.62
1:A:392:MET:SD	1:A:393:ASP:N	2.72	0.62
6:F:70:PHE:HB3	6:F:73:MET:HB3	1.82	0.61
1:A:811:THR:OG1	1:A:814:GLU:OE1	2.18	0.61
1:A:354:GLU:OE2	1:A:360:ASN:ND2	2.33	0.61
2:B:705:MET:HA	2:B:708:VAL:HG12	1.82	0.61
2:B:1064:HIS:CG	2:B:1077:CYS:SG	2.93	0.61
5:E:157:VAL:O	5:E:161:ASN:ND2	2.33	0.61
1:A:21:MET:HB3	2:B:1079:VAL:HB	1.82	0.61
1:A:4:VAL:HA	3:C:370:GLN:HE22	1.65	0.61
2:B:504:ILE:HA	2:B:529:ILE:HD11	1.82	0.61
1:A:271:LEU:O	1:A:275:HIS:ND1	2.33	0.60
1:A:419:VAL:HG11	1:A:466:LEU:HD12	1.83	0.60
1:A:488:ILE:HA	1:A:498:ILE:HD12	1.83	0.60
2:B:730:ASN:ND2	2:B:907:ILE:O	2.35	0.60
6:F:76:ARG:HG3	6:F:77:ILE:HD12	1.84	0.60
2:B:925:ALA:HB1	2:B:984:GLY:HA3	1.83	0.60
9:N:17:LYS:HB3	9:N:38:LEU:HD21	1.83	0.60
3:C:304:ARG:HE	8:H:69:THR:HG21	1.67	0.59
1:A:57:CYS:SG	1:A:59:THR:OG1	2.60	0.59
1:A:500:GLY:HA3	1:A:504:HIS:HB2	1.84	0.59
5:E:82:LYS:HE3	5:E:85:GLU:HB2	1.84	0.59
1:A:528:MET:HG3	7:L:44:THR:HG23	1.85	0.59
1:A:177:ARG:NH1	1:A:178:LEU:O	2.36	0.59
1:A:707:LEU:HD13	3:C:90:VAL:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:LEU:HD21	3:C:43:ILE:HD12	1.84	0.59
5:E:19:MET:HE2	5:E:27:ALA:HA	1.84	0.59
5:E:174:LYS:H	5:E:177:TRP:HD1	1.51	0.58
1:A:154:ILE:HG23	1:A:164:GLU:HB3	1.85	0.58
4:D:24:HIS:ND1	7:L:30:GLU:OE2	2.32	0.58
2:B:972:ILE:O	7:L:26:ASN:ND2	2.36	0.58
1:A:571:ASN:HD22	1:A:607:VAL:HG23	1.68	0.58
5:E:106:ILE:HD13	5:E:158:ILE:HG12	1.85	0.58
6:F:85:MET:HE1	6:F:115:LEU:HD22	1.85	0.58
1:A:20:LYS:NZ	2:B:1079:VAL:O	2.35	0.57
5:E:109:LEU:HB3	5:E:162:ARG:HH22	1.70	0.57
3:C:60:GLU:OE2	10:K:6:ARG:NH1	2.38	0.56
3:C:128:ASP:HB3	3:C:131:LYS:HB2	1.86	0.56
1:A:5:ILE:HD12	3:C:370:GLN:HE21	1.70	0.56
2:B:738:ASN:OD1	2:B:741:SER:N	2.38	0.56
1:A:60:CYS:SG	1:A:70:HIS:HE1	2.23	0.56
4:D:227:GLU:OE2	9:N:42:ARG:NH2	2.38	0.56
1:A:2:LYS:HB2	5:E:62:ILE:HD13	1.86	0.56
1:A:334:MET:HG2	7:L:47:HIS:H	1.71	0.56
1:A:637:ARG:NH2	1:A:880:SER:O	2.39	0.56
1:A:850:LEU:HB2	3:C:66:GLY:HA3	1.86	0.56
2:B:1038:GLY:HA3	10:K:7:PHE:HE1	1.71	0.56
4:D:19:VAL:HG22	4:D:223:ILE:HG12	1.87	0.56
5:E:145:ARG:NH1	5:E:173:GLY:O	2.38	0.55
1:A:520:ARG:HB2	1:A:549:PRO:HG2	1.89	0.55
3:C:337:ARG:HH12	3:C:346:HIS:HB2	1.69	0.55
1:A:831:VAL:HG21	2:B:448:PRO:HB3	1.88	0.55
2:B:870:PRO:HG3	2:B:990:ARG:HH12	1.71	0.55
1:A:184:ARG:NH2	1:A:211:VAL:O	2.40	0.55
3:C:316:ASP:OD1	3:C:320:ARG:NH2	2.39	0.55
1:A:119:LEU:O	1:A:123:ARG:NH2	2.39	0.55
1:A:460:ASP:O	2:B:875:LYS:NZ	2.39	0.55
1:A:820:MET:HG2	2:B:455:LEU:HB3	1.88	0.55
3:C:139:ILE:HA	3:C:227:LEU:HD23	1.87	0.55
5:E:101:ILE:O	5:E:108:GLY:N	2.38	0.55
1:A:89:ILE:HG13	1:A:210:MET:HE2	1.89	0.55
1:A:480:ILE:O	1:A:486:ASN:ND2	2.40	0.55
3:C:343:THR:OG1	3:C:345:GLN:OE1	2.25	0.55
1:A:449:LEU:HD22	2:B:731:MET:HE3	1.89	0.55
2:B:162:GLU:OE2	2:B:684:ARG:NH2	2.39	0.55
1:A:56:ARG:HH21	1:A:63:ARG:HE	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:ILE:O	2:B:511:ARG:NH2	2.40	0.54
4:D:12:LYS:HG3	4:D:13:GLU:H	1.72	0.54
2:B:122:GLU:H	2:B:401:THR:HG22	1.73	0.54
1:A:227:THR:HA	1:A:234:ALA:H	1.72	0.54
1:A:643:ARG:NH1	1:A:646:GLN:OE1	2.41	0.54
2:B:897:TRP:CD1	4:D:154:TYR:HB2	2.43	0.54
2:B:95:THR:HG22	2:B:159:ASN:H	1.72	0.54
2:B:138:SER:OG	2:B:141:GLU:OE1	2.21	0.54
4:D:39:VAL:HB	4:D:150:PRO:HG3	1.88	0.54
1:A:891:ILE:HD12	3:C:53:GLU:HG3	1.90	0.54
3:C:143:THR:HB	3:C:223:ARG:HH12	1.72	0.54
1:A:420:LEU:HD13	1:A:432:ILE:HD11	1.90	0.53
2:B:447:GLN:HG3	2:B:449:HIS:NE2	2.23	0.53
5:E:42:LYS:NZ	5:E:153:ALA:O	2.41	0.53
5:E:84:HIS:O	5:E:147:ARG:NH1	2.41	0.53
4:D:187:THR:OG1	4:D:188:GLU:N	2.42	0.53
3:C:345:GLN:HA	3:C:348:PHE:HD2	1.74	0.53
6:F:14:ILE:HG12	6:F:18:LYS:HE2	1.90	0.53
1:A:697:GLU:HB3	1:A:701:ARG:HH21	1.74	0.53
2:B:513:ASP:HB2	2:B:516:LEU:HD23	1.90	0.53
2:B:555:ALA:HB2	2:B:617:GLU:HA	1.91	0.53
2:B:1062:CYS:SG	2:B:1063:GLY:N	2.82	0.53
4:D:29:ASN:OD1	4:D:33:ARG:NH2	2.42	0.53
1:A:567:VAL:HG11	1:A:634:LEU:HG	1.90	0.52
1:A:97:CYS:O	1:A:186:TRP:NE1	2.38	0.52
1:A:337:ILE:HD13	1:A:648:LEU:HD23	1.90	0.52
1:A:524:GLU:OE1	7:L:33:ARG:NH1	2.42	0.52
2:B:933:LEU:O	9:N:46:ARG:NH1	2.43	0.52
1:A:13:LEU:HD13	1:A:18:ILE:HD13	1.92	0.52
1:A:165:ILE:HG22	1:A:173:GLU:HG3	1.91	0.52
5:E:63:PRO:HG3	10:K:11:ARG:HH12	1.73	0.52
2:B:721:VAL:HG22	2:B:906:LEU:HB3	1.91	0.52
5:E:155:SER:OG	5:E:161:ASN:ND2	2.43	0.52
5:E:174:LYS:H	5:E:177:TRP:CD1	2.28	0.52
10:K:35:THR:HB	10:K:38:GLU:HG3	1.92	0.52
2:B:654:TYR:HB3	2:B:657:HIS:HD2	1.75	0.52
3:C:86:HIS:NE2	3:C:89:GLY:O	2.43	0.52
1:A:779:ARG:NH2	2:B:336:ASP:OD1	2.43	0.52
1:A:251:ARG:HG2	1:A:268:LEU:HD21	1.91	0.51
1:A:392:MET:SD	1:A:394:SER:N	2.79	0.51
2:B:772:ILE:HD12	2:B:789:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:115:LEU:HG	5:E:129:PHE:HE2	1.75	0.51
2:B:568:ASP:O	2:B:571:ARG:NH2	2.43	0.51
2:B:587:THR:OG1	2:B:590:HIS:ND1	2.38	0.51
2:B:656:GLU:OE1	2:B:656:GLU:N	2.43	0.51
2:B:786:TYR:OH	2:B:832:GLU:OE1	2.27	0.51
3:C:79:GLN:HG2	3:C:299:LEU:HD21	1.92	0.51
3:C:292:SER:HA	3:C:295:GLN:HE21	1.75	0.51
1:A:710:LYS:HB3	1:A:714:ASP:HB2	1.92	0.51
2:B:846:ASP:OD1	2:B:865:ARG:NH1	2.43	0.51
5:E:117:ASP:OD1	5:E:117:ASP:N	2.43	0.51
2:B:1059:CYS:HA	2:B:1086:ILE:HA	1.93	0.51
1:A:420:LEU:HD11	2:B:1042:LEU:HD11	1.93	0.51
3:C:144:LEU:HB3	3:C:220:LYS:HA	1.92	0.51
9:N:9:THR:OG1	9:N:47:ARG:NH2	2.44	0.51
1:A:80:VAL:HA	1:A:273:GLN:HE22	1.76	0.51
2:B:543:ARG:NH1	2:B:552:ILE:O	2.43	0.51
3:C:228:SER:O	3:C:250:ASN:ND2	2.44	0.51
4:D:14:ASP:N	4:D:14:ASP:OD1	2.44	0.51
1:A:282:ASN:ND2	1:A:298:LEU:O	2.41	0.51
1:A:387:ARG:HH12	1:A:389:ARG:HH11	1.59	0.51
2:B:75:GLN:NE2	2:B:76:GLU:O	2.44	0.51
2:B:445:ARG:O	2:B:453:ARG:NH2	2.44	0.51
2:B:880:HIS:NE2	2:B:924:GLU:OE1	2.30	0.51
10:K:20:ILE:HA	10:K:24:ALA:HB3	1.93	0.51
1:A:312:PHE:HB3	3:C:339:ALA:HA	1.93	0.50
2:B:772:ILE:HD12	2:B:773:PRO:HD2	1.93	0.50
1:A:485:GLN:OE1	1:A:645:ARG:NE	2.44	0.50
2:B:75:GLN:NE2	2:B:79:GLY:O	2.41	0.50
11:P:11:CYS:SG	11:P:13:ARG:NH1	2.85	0.50
5:E:5:LYS:HB3	5:E:78:VAL:HG23	1.93	0.50
5:E:17:PRO:HB3	10:K:24:ALA:HB2	1.93	0.50
2:B:27:LEU:O	2:B:437:ARG:NH1	2.44	0.50
3:C:143:THR:HG23	3:C:145:GLU:H	1.77	0.50
6:F:108:MET:HE3	6:F:108:MET:O	2.11	0.50
2:B:268:GLN:HG3	2:B:269:GLU:H	1.77	0.50
5:E:106:ILE:HB	5:E:158:ILE:HD11	1.93	0.50
1:A:166:ARG:N	1:A:174:TYR:O	2.45	0.50
1:A:481:LEU:O	1:A:487:HIS:NE2	2.44	0.50
2:B:685:VAL:HG23	2:B:754:THR:HG21	1.94	0.50
4:D:89:VAL:HB	4:D:137:ALA:HB3	1.92	0.50
2:B:866:ASP:OD2	2:B:868:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:64:ARG:HD2	4:D:122:ILE:HA	1.94	0.49
4:D:66:ALA:HB2	11:P:48:ALA:HB1	1.93	0.49
1:A:810:LEU:HD12	1:A:814:GLU:HB3	1.94	0.49
2:B:210:GLY:O	2:B:257:ASN:ND2	2.41	0.49
2:B:812:SER:O	2:B:831:ARG:N	2.45	0.49
5:E:17:PRO:HG2	10:K:22:MET:HB3	1.93	0.49
7:L:15:PHE:HE2	7:L:17:LEU:HD12	1.77	0.49
1:A:81:ILE:HG12	1:A:180:PRO:HG3	1.95	0.49
1:A:238:LEU:HD21	1:A:300:THR:HA	1.94	0.49
2:B:550:ASP:O	2:B:573:ARG:NH1	2.37	0.49
2:B:968:MET:HE3	2:B:981:ILE:HD11	1.94	0.49
4:D:167:ILE:HD11	4:D:212:GLU:HB3	1.95	0.49
5:E:82:LYS:HE2	6:F:76:ARG:NH2	2.27	0.49
1:A:190:ILE:O	1:A:206:ARG:NH2	2.46	0.49
4:D:163:ILE:HD13	4:D:213:ILE:HD12	1.94	0.49
1:A:68:PRO:O	2:B:1096:LYS:NZ	2.40	0.49
2:B:44:GLN:NE2	2:B:48:ASN:OD1	2.37	0.49
2:B:696:GLN:HB3	2:B:717:GLN:HA	1.93	0.49
2:B:1034:LEU:HD22	2:B:1043:LEU:HB2	1.93	0.49
2:B:544:ARG:NH1	2:B:611:GLU:OE2	2.46	0.49
3:C:143:THR:OG1	3:C:220:LYS:O	2.26	0.49
4:D:189:GLU:OE2	4:D:189:GLU:N	2.42	0.49
1:A:186:TRP:HA	1:A:189:LYS:HE3	1.95	0.48
2:B:444:ASP:OD2	2:B:447:GLN:NE2	2.46	0.48
2:B:788:ASN:ND2	2:B:799:SER:OG	2.45	0.48
2:B:858:LYS:HG3	11:P:25:LEU:HD11	1.95	0.48
2:B:902:ILE:HD11	9:N:42:ARG:HB2	1.94	0.48
2:B:1083:GLU:HG2	6:F:1:MET:HG3	1.95	0.48
2:B:1072:ARG:HB3	2:B:1074:ARG:HH11	1.78	0.48
5:E:46:VAL:HG11	5:E:158:ILE:HD12	1.95	0.48
5:E:112:ILE:HA	5:E:115:LEU:HD23	1.94	0.48
2:B:1054:THR:HB	2:B:1093:TYR:HE1	1.79	0.48
5:E:178:ILE:O	5:E:182:LYS:N	2.40	0.48
2:B:980:ASP:OD1	2:B:980:ASP:N	2.45	0.48
2:B:1116:ARG:HH12	5:E:62:ILE:HG23	1.79	0.48
2:B:244:VAL:HG21	2:B:254:MET:HG2	1.96	0.48
1:A:60:CYS:HB3	2:B:1067:LEU:HG	1.96	0.48
2:B:805:ASP:OD1	2:B:806:VAL:N	2.46	0.48
1:A:728:ARG:NH1	1:A:767:LEU:O	2.47	0.48
1:A:453:PRO:HG3	1:A:501:ILE:HD11	1.94	0.48
3:C:281:ALA:HB2	8:H:15:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ARG:HH12	7:L:49:ILE:HG13	1.79	0.47
2:B:310:ARG:HA	2:B:313:LYS:HE2	1.96	0.47
2:B:1074:ARG:HE	5:E:156:LYS:HE2	1.78	0.47
2:B:351:LEU:HD13	2:B:413:TRP:HE1	1.79	0.47
2:B:733:ASP:OD1	2:B:916:ARG:NH2	2.47	0.47
1:A:78:ARG:HB3	1:A:269:TRP:CE2	2.49	0.47
2:B:443:LEU:HB3	2:B:449:HIS:CE1	2.50	0.47
2:B:693:HIS:HE2	2:B:750:THR:HG1	1.57	0.47
3:C:316:ASP:HB2	8:H:42:GLN:HE21	1.79	0.47
1:A:56:ARG:HH11	2:B:1070:LYS:HD3	1.79	0.47
1:A:380:TYR:OH	1:A:390:ARG:NH2	2.41	0.47
1:A:433:MET:HE3	1:A:484:VAL:HA	1.95	0.47
3:C:280:GLU:OE2	8:H:65:ARG:NE	2.46	0.47
9:N:31:PRO:HA	9:N:34:VAL:HG12	1.96	0.47
1:A:47:ARG:HG3	1:A:58:GLU:HG3	1.97	0.47
1:A:637:ARG:HH12	1:A:879:LYS:C	2.22	0.47
2:B:462:ARG:HH12	2:B:615:ALA:N	2.12	0.47
2:B:662:ARG:NH2	2:B:881:GLY:O	2.41	0.47
3:C:268:ASN:ND2	3:C:289:GLU:OE1	2.48	0.47
5:E:36:TYR:HE2	6:F:2:ILE:HD11	1.79	0.47
5:E:91:VAL:HA	5:E:101:ILE:HA	1.97	0.47
9:N:35:LEU:HD13	9:N:46:ARG:HG2	1.96	0.47
1:A:165:ILE:HA	1:A:175:ARG:HA	1.97	0.47
1:A:282:ASN:HD21	1:A:298:LEU:HB2	1.80	0.47
1:A:429:ARG:O	2:B:1037:HIS:NE2	2.44	0.47
2:B:1054:THR:HB	2:B:1093:TYR:CE1	2.50	0.47
1:A:123:ARG:NH2	8:H:42:GLN:OE1	2.42	0.47
2:B:129:SER:OG	2:B:130:LYS:N	2.46	0.47
2:B:719:PHE:HD2	2:B:906:LEU:HD22	1.79	0.47
3:C:175:THR:H	3:C:178:LYS:HE2	1.79	0.47
4:D:11:LYS:HB2	4:D:16:ILE:HG13	1.97	0.47
11:P:31:GLY:O	11:P:33:LYS:NZ	2.47	0.47
2:B:669:MET:HB3	2:B:991:LEU:HD11	1.97	0.46
4:D:4:ILE:HD11	7:L:84:GLU:HB3	1.97	0.46
5:E:19:MET:HE3	5:E:19:MET:O	2.15	0.46
1:A:430:MET:HG3	1:A:454:PRO:HB3	1.95	0.46
2:B:735:ILE:HD12	2:B:906:LEU:HD11	1.96	0.46
4:D:161:VAL:HB	4:D:193:VAL:HB	1.97	0.46
6:F:15:ALA:HA	6:F:18:LYS:HE3	1.97	0.46
7:L:1:MET:HE2	7:L:20:GLU:OE2	2.16	0.46
1:A:476:ALA:HB1	10:K:13:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:805:ASP:H	2:B:837:VAL:HG12	1.79	0.46
3:C:146:ASN:O	3:C:168:ARG:NH1	2.48	0.46
2:B:774:ASP:HB3	2:B:777:VAL:HG13	1.97	0.46
3:C:287:ILE:HD11	3:C:307:MET:HA	1.97	0.46
7:L:2:LYS:HG3	7:L:18:GLU:HB3	1.97	0.46
2:B:386:ASN:HB3	2:B:389:ARG:HG2	1.97	0.46
4:D:40:PRO:HG2	4:D:79:LEU:HD22	1.98	0.46
1:A:109:GLU:OE2	1:A:137:LYS:NZ	2.45	0.46
2:B:232:LEU:HD22	2:B:295:ILE:HD11	1.98	0.46
2:B:623:VAL:HG22	2:B:636:HIS:HB2	1.98	0.46
7:L:51:MET:HG3	7:L:54:LYS:HB3	1.98	0.46
1:A:748:MET:SD	2:B:911:HIS:HD2	2.39	0.46
2:B:413:TRP:CD1	2:B:420:VAL:HG21	2.51	0.46
2:B:499:LEU:HB3	2:B:504:ILE:HD12	1.98	0.46
4:D:24:HIS:CD2	4:D:25:VAL:H	2.34	0.46
5:E:134:LYS:HZ3	5:E:184:LYS:HD3	1.81	0.46
2:B:121:GLY:HA3	2:B:400:LEU:HD23	1.97	0.46
2:B:426:ARG:HG3	2:B:684:ARG:HH21	1.81	0.46
3:C:361:GLY:O	3:C:365:ASN:ND2	2.48	0.46
7:L:20:GLU:N	7:L:20:GLU:OE1	2.50	0.45
1:A:848:GLN:HA	3:C:67:THR:HB	1.98	0.45
1:A:685:ILE:HD13	1:A:803:VAL:HG13	1.98	0.45
2:B:347:LEU:HD21	2:B:486:ILE:HG21	1.98	0.45
4:D:140:GLY:HA3	4:D:148:TRP:CE2	2.51	0.45
1:A:252:LEU:HD21	1:A:269:TRP:HA	1.98	0.45
2:B:879:ARG:NH2	2:B:924:GLU:OE2	2.49	0.45
2:B:904:PRO:HG3	2:B:983:ILE:HD12	1.99	0.45
5:E:166:THR:OG1	5:E:168:ARG:NH1	2.44	0.45
1:A:48:MET:HA	1:A:70:HIS:HB2	1.99	0.45
1:A:841:ARG:O	1:A:841:ARG:NH1	2.50	0.45
2:B:119:ARG:NH1	2:B:122:GLU:OE2	2.49	0.45
2:B:972:ILE:O	4:D:29:ASN:ND2	2.50	0.45
7:L:16:TYR:CE1	7:L:54:LYS:HD2	2.52	0.45
9:N:1:MET:SD	9:N:1:MET:N	2.86	0.45
10:K:5:THR:OG1	10:K:8:GLU:OE1	2.33	0.45
1:A:260:ALA:HB3	1:A:265:ILE:HD11	1.98	0.45
2:B:814:PRO:HD3	2:B:830:ARG:HA	1.98	0.45
3:C:104:GLU:HG3	3:C:109:ARG:HG3	1.98	0.45
1:A:12:ILE:N	1:A:204:LYS:O	2.49	0.45
1:A:107:ASP:OD1	1:A:107:ASP:N	2.50	0.45
5:E:147:ARG:N	5:E:166:THR:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:20:SER:C	11:P:23:ARG:HH22	2.24	0.45
1:A:30:ASP:HB2	1:A:42:GLY:HA3	1.98	0.45
3:C:205:LYS:HD2	3:C:205:LYS:HA	1.79	0.45
1:A:446:ARG:HH22	7:L:49:ILE:HG13	1.82	0.45
5:E:169:GLN:HE21	6:F:97:ALA:HB3	1.81	0.45
2:B:855:ASP:OD1	2:B:856:GLY:N	2.50	0.44
1:A:892:ILE:HG21	3:C:32:TYR:HD2	1.81	0.44
2:B:24:GLU:OE1	2:B:602:SER:N	2.43	0.44
2:B:451:GLU:OE1	2:B:451:GLU:N	2.42	0.44
2:B:896:PRO:HB2	2:B:968:MET:SD	2.57	0.44
1:A:301:LEU:HA	1:A:304:ARG:HE	1.82	0.44
2:B:737:ILE:HD11	2:B:886:ILE:HG21	1.98	0.44
3:C:64:PRO:HB2	3:C:67:THR:HG22	1.99	0.44
3:C:332:SER:O	3:C:337:ARG:NE	2.43	0.44
2:B:336:ASP:OD2	2:B:339:HIS:N	2.50	0.44
2:B:858:LYS:HZ3	11:P:23:ARG:HE	1.64	0.44
3:C:265:THR:O	8:H:12:HIS:NE2	2.41	0.44
6:F:74:SER:OG	6:F:75:ASP:N	2.51	0.44
11:P:14:GLU:OE1	11:P:14:GLU:N	2.50	0.44
3:C:266:ARG:NH1	3:C:288:ASP:OD2	2.50	0.44
1:A:26:VAL:HB	1:A:74:ILE:HG13	2.00	0.44
1:A:98:ARG:O	1:A:189:LYS:NZ	2.39	0.44
1:A:218:PRO:HG2	1:A:223:ARG:HE	1.83	0.44
8:H:64:LYS:HE3	8:H:64:LYS:HB2	1.84	0.44
1:A:30:ASP:HB3	1:A:39:ILE:HD12	1.99	0.44
5:E:139:LYS:N	5:E:142:ASP:OD2	2.44	0.44
8:H:50:VAL:HG21	8:H:79:VAL:HG11	2.00	0.44
2:B:1070:LYS:HG3	2:B:1071:ARG:HD3	1.98	0.44
1:A:692:VAL:HG22	1:A:720:ILE:HD12	2.00	0.44
2:B:32:LEU:HD11	2:B:129:SER:HA	2.00	0.44
3:C:151:THR:HA	3:C:162:VAL:HA	1.98	0.44
4:D:75:ASP:O	4:D:77:PHE:N	2.50	0.44
1:A:46:LYS:HB2	1:A:58:GLU:HG2	1.99	0.43
1:A:184:ARG:HE	1:A:211:VAL:HB	1.84	0.43
1:A:502:GLN:HB3	2:B:911:HIS:ND1	2.33	0.43
3:C:316:ASP:OD1	3:C:316:ASP:N	2.47	0.43
5:E:129:PHE:HB3	5:E:138:LEU:HB2	2.00	0.43
1:A:541:ASP:OD1	1:A:541:ASP:N	2.49	0.43
4:D:89:VAL:HG11	4:D:113:VAL:HG11	2.00	0.43
1:A:157:GLU:HB3	1:A:161:ILE:HB	2.00	0.43
2:B:22:TRP:HZ3	2:B:708:VAL:HB	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:164:VAL:HG21	2:B:436:LEU:HD23	2.01	0.43
3:C:327:VAL:HA	3:C:330:GLU:HG2	1.99	0.43
4:D:140:GLY:HA3	4:D:148:TRP:CD2	2.53	0.43
5:E:166:THR:HG1	5:E:168:ARG:HH11	1.65	0.43
2:B:34:SER:HB2	2:B:347:LEU:HD13	1.99	0.43
3:C:212:LEU:O	3:C:216:ALA:N	2.52	0.43
1:A:157:GLU:HB2	1:A:163:TRP:HD1	1.84	0.43
2:B:646:GLY:H	2:B:649:ALA:HB3	1.83	0.43
2:B:1030:GLU:HA	2:B:1033:VAL:HG12	2.01	0.43
11:P:22:THR:HG22	11:P:24:ASP:H	1.84	0.43
1:A:21:MET:HE1	1:A:71:PHE:HD2	1.83	0.43
2:B:57:ILE:HG13	2:B:60:PHE:HD2	1.84	0.43
2:B:685:VAL:HG21	2:B:861:LYS:HD3	2.01	0.43
3:C:122:ASP:OD1	3:C:122:ASP:N	2.52	0.43
1:A:51:ILE:HG23	1:A:220:VAL:HG13	1.99	0.43
2:B:181:ASP:OD1	2:B:186:LYS:N	2.52	0.43
2:B:462:ARG:HB3	2:B:572:VAL:HG11	2.00	0.43
4:D:159:THR:O	4:D:195:THR:OG1	2.29	0.43
5:E:120:VAL:HG13	5:E:131:GLY:HA2	2.00	0.43
1:A:88:THR:OG1	1:A:91:ARG:NH2	2.52	0.43
1:A:206:ARG:HB3	1:A:209:TRP:CD2	2.54	0.43
1:A:767:LEU:HD13	1:A:802:VAL:HG21	2.01	0.43
1:A:164:GLU:HG2	1:A:178:LEU:HG	2.01	0.43
1:A:779:ARG:O	2:B:457:GLY:N	2.52	0.43
2:B:269:GLU:HA	2:B:272:GLU:HB2	2.01	0.43
2:B:502:LEU:HD11	2:B:538:ARG:HG2	2.00	0.43
3:C:125:HIS:CD2	3:C:131:LYS:HB3	2.54	0.43
1:A:533:ASP:OD1	1:A:533:ASP:N	2.50	0.43
1:A:667:GLY:H	2:B:965:ARG:HH21	1.67	0.43
2:B:692:LEU:HD21	2:B:717:GLN:NE2	2.33	0.43
5:E:152:SER:N	5:E:162:ARG:O	2.51	0.43
1:A:447:LEU:HD11	1:A:451:VAL:HB	2.01	0.42
1:A:670:ASP:OD1	1:A:743:ASN:ND2	2.51	0.42
2:B:216:ILE:HB	2:B:219:VAL:HG12	2.01	0.42
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.76	0.42
2:B:178:VAL:HG21	2:B:327:LEU:HD21	2.01	0.42
2:B:720:VAL:HG13	2:B:904:PRO:HA	2.00	0.42
2:B:930:VAL:HG23	2:B:955:LEU:HD12	2.02	0.42
5:E:147:ARG:NE	5:E:169:GLN:OE1	2.52	0.42
1:A:850:LEU:HD12	1:A:858:VAL:HG12	2.01	0.42
2:B:498:TYR:OH	2:B:542:ASP:OD2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:605:ILE:HD13	2:B:610:ILE:HB	2.01	0.42
5:E:74:PHE:HE2	5:E:76:VAL:HB	1.84	0.42
2:B:517:TRP:NE1	2:B:532:GLY:H	2.18	0.42
2:B:797:PRO:HD2	11:P:40:PRO:HD3	2.00	0.42
3:C:207:ASP:OD1	3:C:207:ASP:N	2.52	0.42
5:E:150:ASN:O	5:E:164:GLY:N	2.50	0.42
6:F:21:LEU:HA	6:F:24:ARG:HB3	2.01	0.42
1:A:424:GLN:OE1	1:A:465:ASN:ND2	2.38	0.42
1:A:889:ASP:OD1	1:A:889:ASP:N	2.51	0.42
6:F:18:LYS:HZ3	6:F:53:LYS:H	1.66	0.42
7:L:47:HIS:CE1	7:L:50:THR:HG22	2.54	0.42
1:A:320:ARG:NH2	1:A:324:SER:OG	2.52	0.42
3:C:135:VAL:HG12	3:C:138:ARG:HH21	1.84	0.42
3:C:211:ASP:OD1	3:C:214:ARG:NH1	2.52	0.42
3:C:368:ILE:HG23	3:C:370:GLN:H	1.84	0.42
2:B:249:GLU:OE2	2:B:331:ARG:NH2	2.44	0.42
2:B:738:ASN:HD21	2:B:892:GLN:HG3	1.83	0.42
2:B:879:ARG:HE	2:B:987:TYR:HB3	1.85	0.42
3:C:82:LEU:HD23	3:C:83:ASN:HB2	2.01	0.42
6:F:81:ILE:HA	6:F:84:ILE:HG22	2.02	0.42
1:A:227:THR:HG23	1:A:233:ARG:HA	2.02	0.42
3:C:261:ASP:OD2	3:C:263:THR:OG1	2.34	0.42
3:C:384:LYS:HD2	3:C:384:LYS:HA	1.81	0.42
2:B:74:PHE:HB2	2:B:84:LEU:HD22	2.02	0.42
3:C:13:LYS:NZ	3:C:44:GLU:OE2	2.53	0.42
1:A:184:ARG:HD3	1:A:208:GLU:HB2	2.02	0.42
1:A:334:MET:HG2	7:L:47:HIS:N	2.35	0.42
2:B:93:ASN:HA	2:B:160:GLY:HA3	2.01	0.42
3:C:33:ASN:HA	3:C:38:LEU:HG	2.02	0.42
4:D:11:LYS:HE2	4:D:11:LYS:HB3	1.86	0.42
10:K:31:PRO:HD2	10:K:34:ILE:HD13	2.01	0.42
1:A:75:GLU:HA	1:A:214:VAL:HG22	2.01	0.41
1:A:571:ASN:HB2	1:A:620:ASP:OD2	2.19	0.41
2:B:787:ARG:HH11	2:B:788:ASN:HB2	1.85	0.41
4:D:31:LEU:HD23	4:D:224:PHE:HE2	1.85	0.41
1:A:179:MET:HE3	1:A:180:PRO:HD2	2.02	0.41
1:A:329:ILE:HD11	1:A:464:MET:HG2	2.02	0.41
2:B:194:TYR:OH	2:B:199:ARG:NH2	2.53	0.41
3:C:382:THR:OG1	10:K:52:THR:O	2.37	0.41
6:F:57:ASP:N	6:F:57:ASP:OD1	2.53	0.41
1:A:529:PHE:HZ	2:B:727:GLN:HE21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:ARG:HH21	1:A:684:ILE:HD11	1.85	0.41
8:H:37:LEU:HD23	8:H:37:LEU:HA	1.93	0.41
1:A:430:MET:CG	1:A:454:PRO:HB3	2.51	0.41
1:A:779:ARG:HB3	2:B:456:HIS:CD2	2.55	0.41
2:B:576:LEU:HD23	2:B:576:LEU:HA	1.91	0.41
2:B:659:ALA:HB2	2:B:917:MET:HB3	2.02	0.41
2:B:742:ILE:HD12	2:B:870:PRO:HG2	2.02	0.41
10:K:16:ARG:HA	10:K:16:ARG:HD2	1.87	0.41
1:A:79:PRO:HD2	1:A:269:TRP:HZ2	1.85	0.41
1:A:165:ILE:HG12	1:A:175:ARG:HG2	2.02	0.41
1:A:241:LYS:HD2	1:A:241:LYS:HA	1.85	0.41
2:B:213:TYR:CZ	2:B:224:LYS:HG2	2.55	0.41
2:B:381:LYS:H	2:B:381:LYS:HG2	1.69	0.41
2:B:529:ILE:HD13	2:B:529:ILE:HA	1.91	0.41
5:E:102:ARG:HA	5:E:107:ASP:HA	2.02	0.41
8:H:63:ILE:HD11	8:H:75:TYR:HD2	1.84	0.41
1:A:504:HIS:NE2	2:B:731:MET:HE1	2.35	0.41
2:B:1059:CYS:HB2	2:B:1064:HIS:HE2	1.85	0.41
3:C:17:LEU:HD23	3:C:21:VAL:HG11	2.02	0.41
2:B:447:GLN:H	2:B:447:GLN:HG2	1.68	0.41
3:C:322:ILE:HD12	3:C:327:VAL:HG21	2.01	0.41
2:B:519:VAL:HG13	2:B:526:ILE:HB	2.02	0.41
2:B:625:MET:HA	2:B:625:MET:HE3	2.03	0.41
3:C:20:ASN:ND2	8:H:69:THR:O	2.54	0.41
3:C:107:ASP:O	3:C:321:PRO:HB3	2.21	0.41
2:B:719:PHE:CZ	2:B:746:LEU:HD21	2.55	0.41
2:B:1085:ARG:HD2	2:B:1085:ARG:HA	1.83	0.41
6:F:75:ASP:N	6:F:75:ASP:OD1	2.53	0.41
10:K:8:GLU:O	10:K:12:ILE:HG12	2.21	0.41
3:C:252:LYS:HB3	3:C:276:VAL:HG11	2.02	0.41
1:A:144:CYS:HB3	1:A:147:CYS:HB2	2.03	0.40
1:A:826:LEU:HD23	1:A:826:LEU:HA	1.92	0.40
2:B:28:VAL:HG11	2:B:436:LEU:HD13	2.02	0.40
5:E:146:ALA:HB3	5:E:165:LEU:HD12	2.03	0.40
1:A:136:LYS:HD3	1:A:136:LYS:HA	1.90	0.40
2:B:234:LEU:HD21	2:B:239:ASP:HB2	2.02	0.40
6:F:58:LYS:HE2	6:F:120:GLU:HG3	2.02	0.40
1:A:34:ASP:N	1:A:34:ASP:OD1	2.51	0.40
1:A:93:LEU:HD11	1:A:154:ILE:HG21	2.03	0.40
1:A:363:ARG:NH1	1:A:414:MET:HE1	2.37	0.40
1:A:651:VAL:O	1:A:655:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:GLU:HG3	2:B:196:HIS:NE2	2.36	0.40
2:B:373:LYS:O	2:B:377:ARG:HG3	2.21	0.40
2:B:1070:LYS:HA	2:B:1073:ARG:NH2	2.37	0.40
5:E:151:ILE:HG23	5:E:163:ILE:HG13	2.03	0.40
1:A:142:MET:HE3	1:A:142:MET:O	2.21	0.40
2:B:173:PRO:HD2	2:B:344:ARG:HG3	2.03	0.40
2:B:795:ILE:HD12	2:B:845:VAL:HG21	2.03	0.40
3:C:142:THR:OG1	3:C:225:LYS:HG3	2.22	0.40
3:C:331:LYS:HG3	3:C:333:SER:HB2	2.04	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	899/907 (99%)	851 (95%)	46 (5%)	2 (0%)	43	75
2	B	1070/1117 (96%)	1018 (95%)	50 (5%)	2 (0%)	43	75
3	C	386/397 (97%)	370 (96%)	15 (4%)	1 (0%)	36	70
4	D	256/275 (93%)	244 (95%)	11 (4%)	1 (0%)	30	65
5	E	183/189 (97%)	168 (92%)	15 (8%)	0	100	100
6	F	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
7	L	92/95 (97%)	81 (88%)	11 (12%)	0	100	100
8	H	74/82 (90%)	70 (95%)	4 (5%)	0	100	100
9	N	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
10	K	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
11	P	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
All	All	3240/3353 (97%)	3070 (95%)	164 (5%)	6 (0%)	44	75

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	THR
2	B	1061	ASN
4	D	76	ARG
3	C	86	HIS
2	B	1049	GLU
1	A	159	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	777/782 (99%)	777 (100%)	0	100	100
2	B	929/962 (97%)	929 (100%)	0	100	100
3	C	336/345 (97%)	336 (100%)	0	100	100
4	D	230/246 (94%)	230 (100%)	0	100	100
5	E	164/167 (98%)	164 (100%)	0	100	100
6	F	103/103 (100%)	103 (100%)	0	100	100
7	L	83/84 (99%)	83 (100%)	0	100	100
8	H	66/70 (94%)	66 (100%)	0	100	100
9	N	60/60 (100%)	60 (100%)	0	100	100
10	K	45/47 (96%)	45 (100%)	0	100	100
11	P	44/45 (98%)	44 (100%)	0	100	100
All	All	2837/2911 (98%)	2837 (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 (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	282	ASN
1	A	525	GLN
1	A	804	ASN
2	B	159	ASN
2	B	174	ASN
2	B	218	ASN
2	B	268	GLN
2	B	393	ASN
2	B	553	ASN
2	B	566	ASN
2	B	658	ASN
2	B	663	ASN
2	B	690	HIS
3	C	33	ASN
3	C	269	ASN
3	C	325	HIS
6	F	68	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

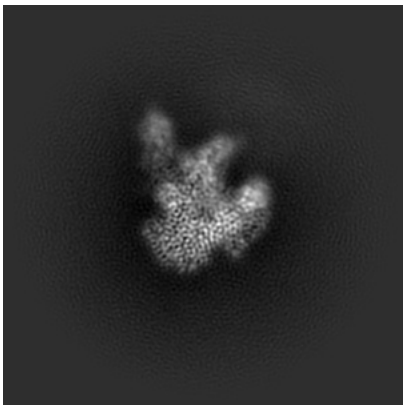
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-74466. These allow visual inspection of the internal detail of the map and identification of artifacts.

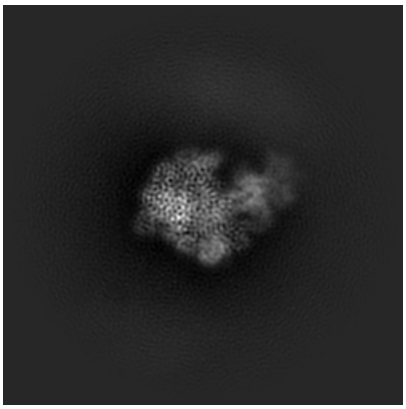
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

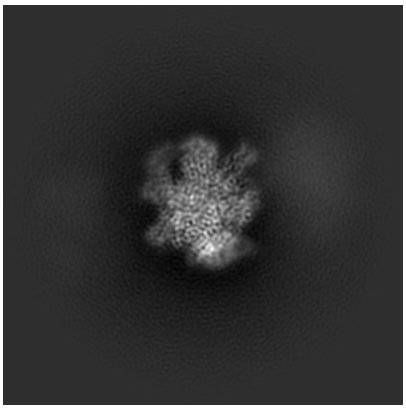
6.1.1 Primary map



X

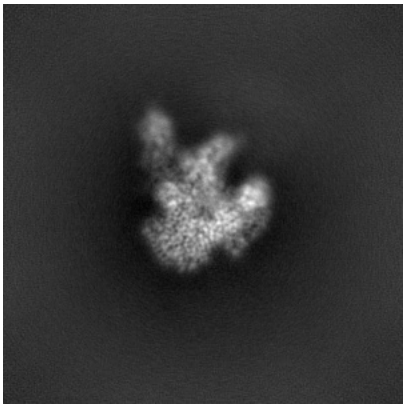


Y

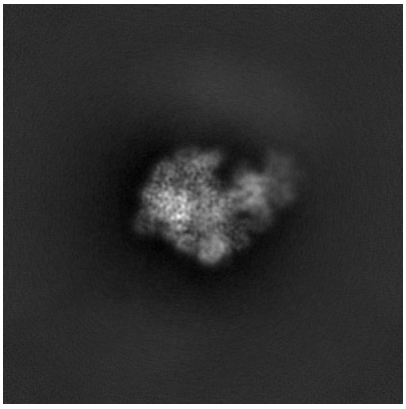


Z

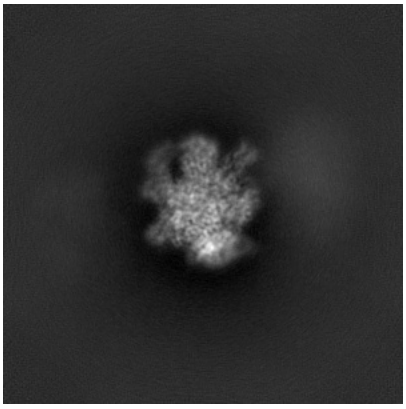
6.1.2 Raw map



X



Y

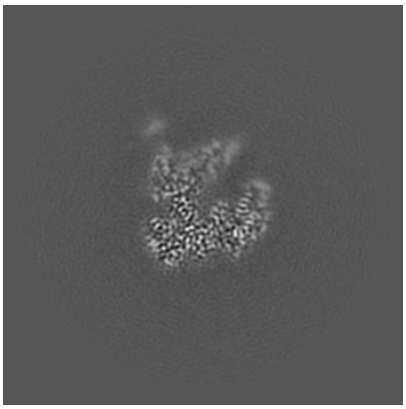


Z

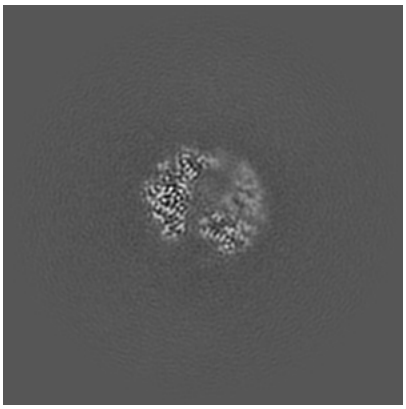
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

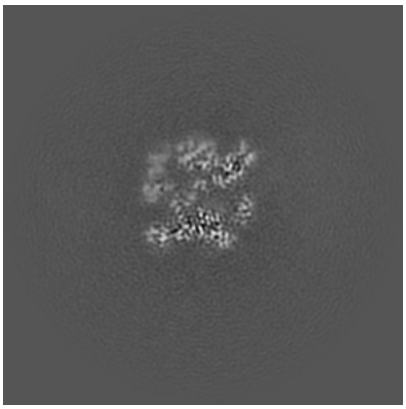
6.2.1 Primary map



X Index: 200

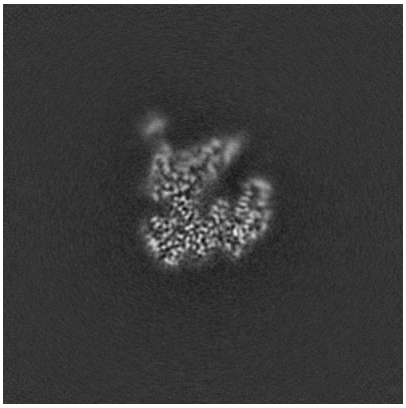


Y Index: 200

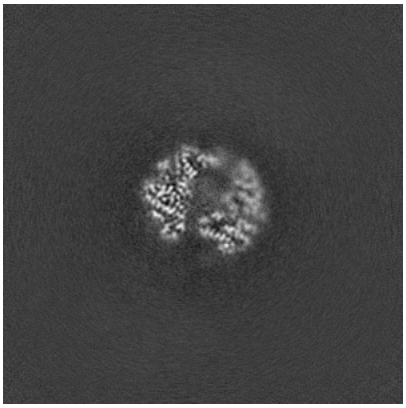


Z Index: 200

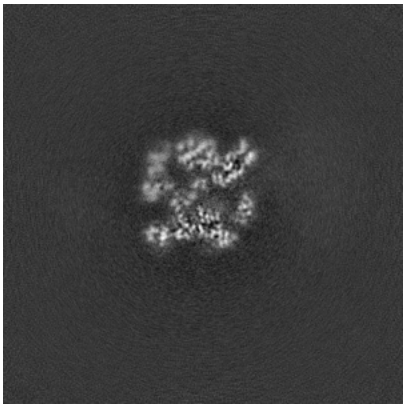
6.2.2 Raw map



X Index: 200



Y Index: 200

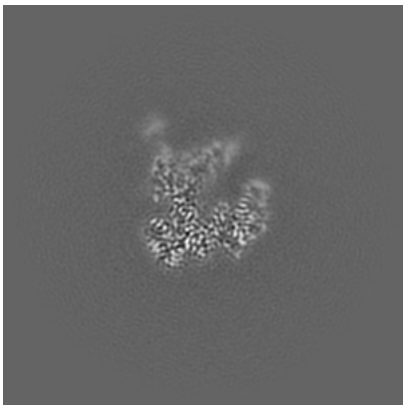


Z Index: 200

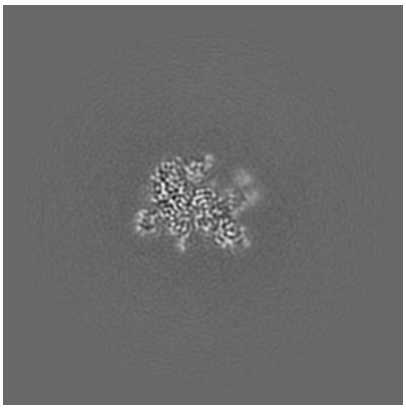
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

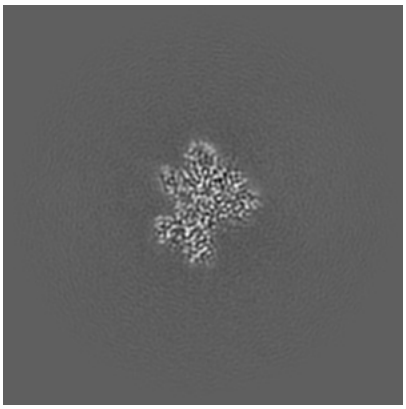
6.3.1 Primary map



X Index: 201

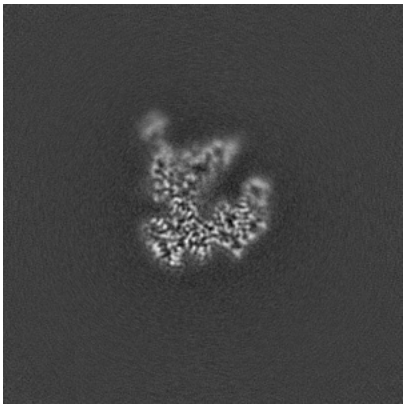


Y Index: 187

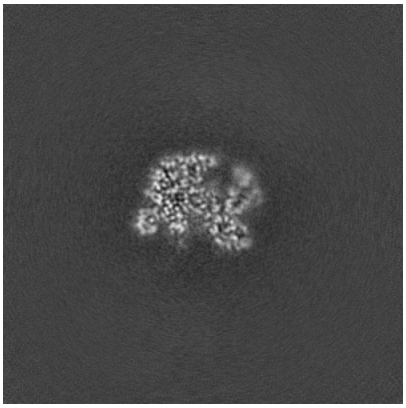


Z Index: 180

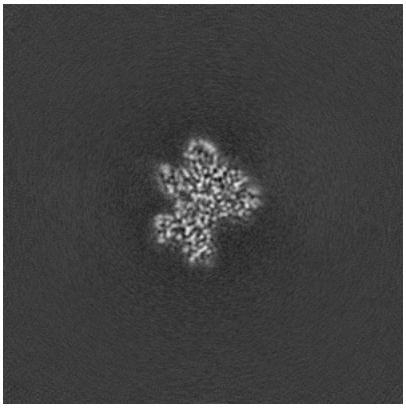
6.3.2 Raw map



X Index: 202



Y Index: 190

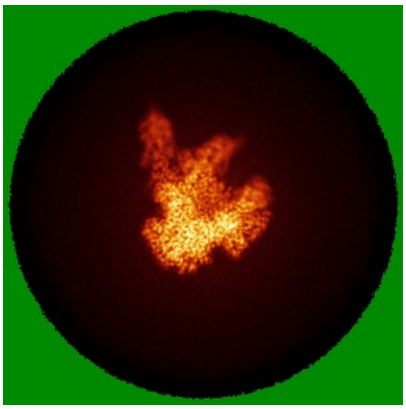


Z Index: 180

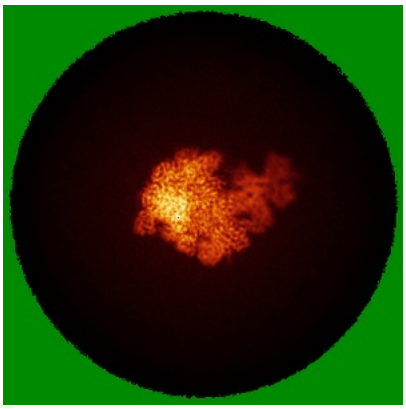
The images above show the largest variance slices of the map in three orthogonal directions.

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

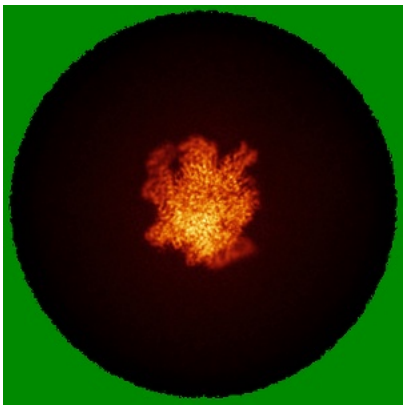
6.4.1 Primary map



X

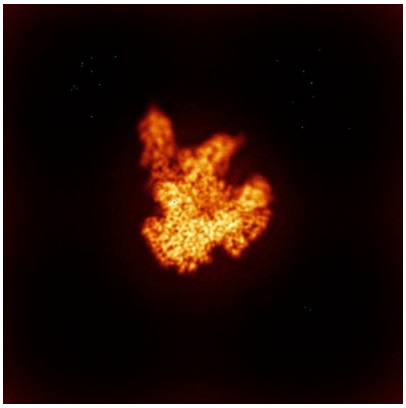


Y

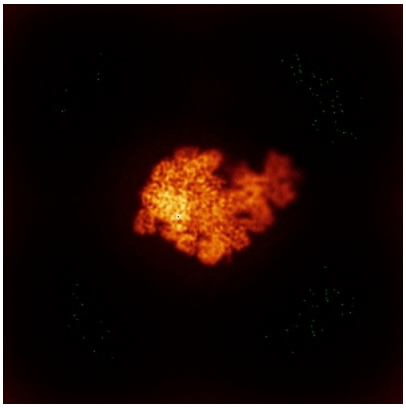


Z

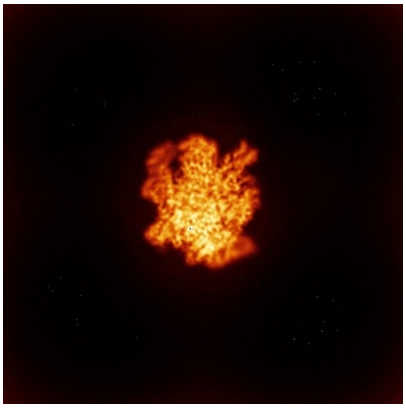
6.4.2 Raw map



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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.16. 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



X Y Z

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.

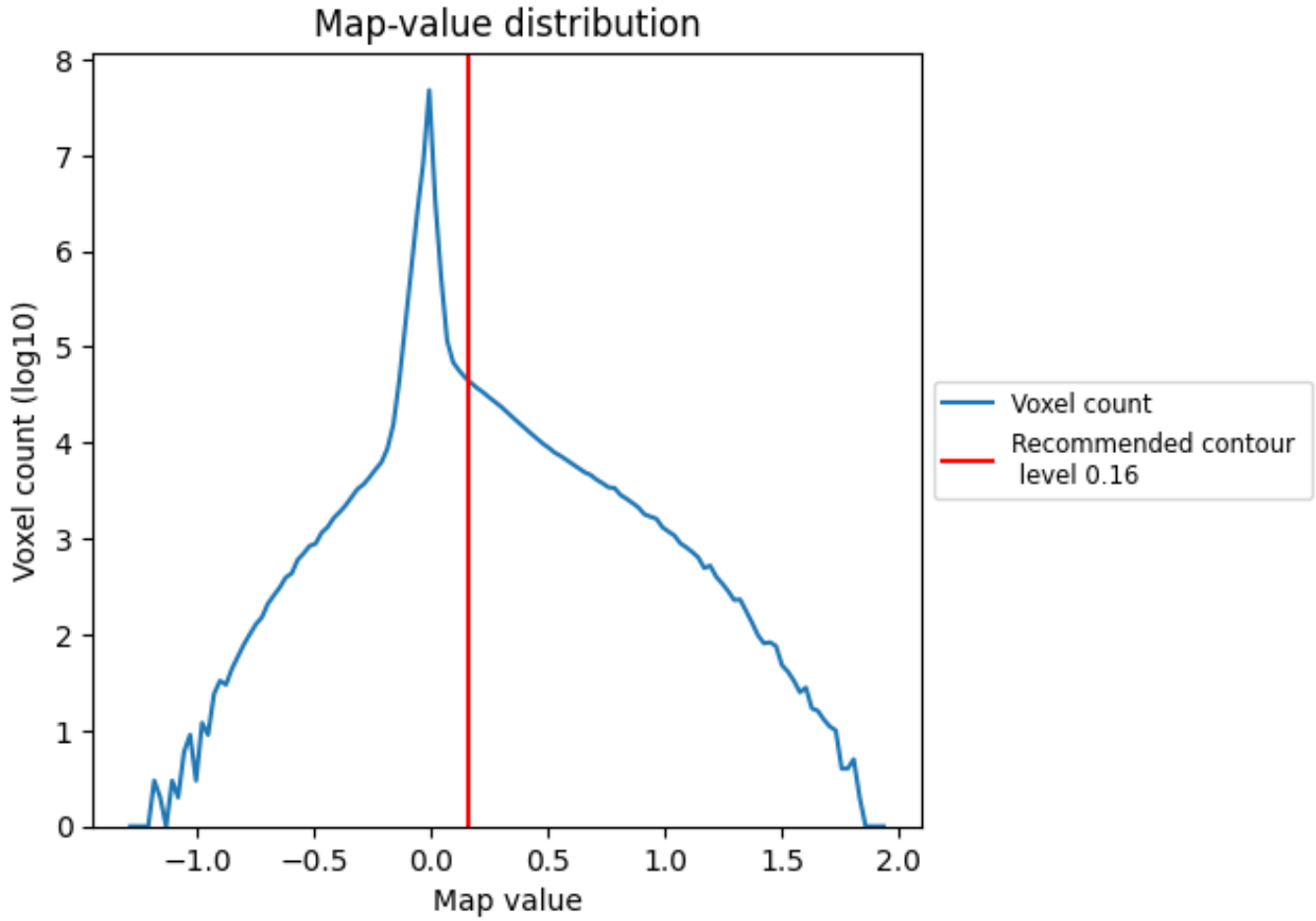
6.6 Mask visualisation (i)

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

7 Map analysis

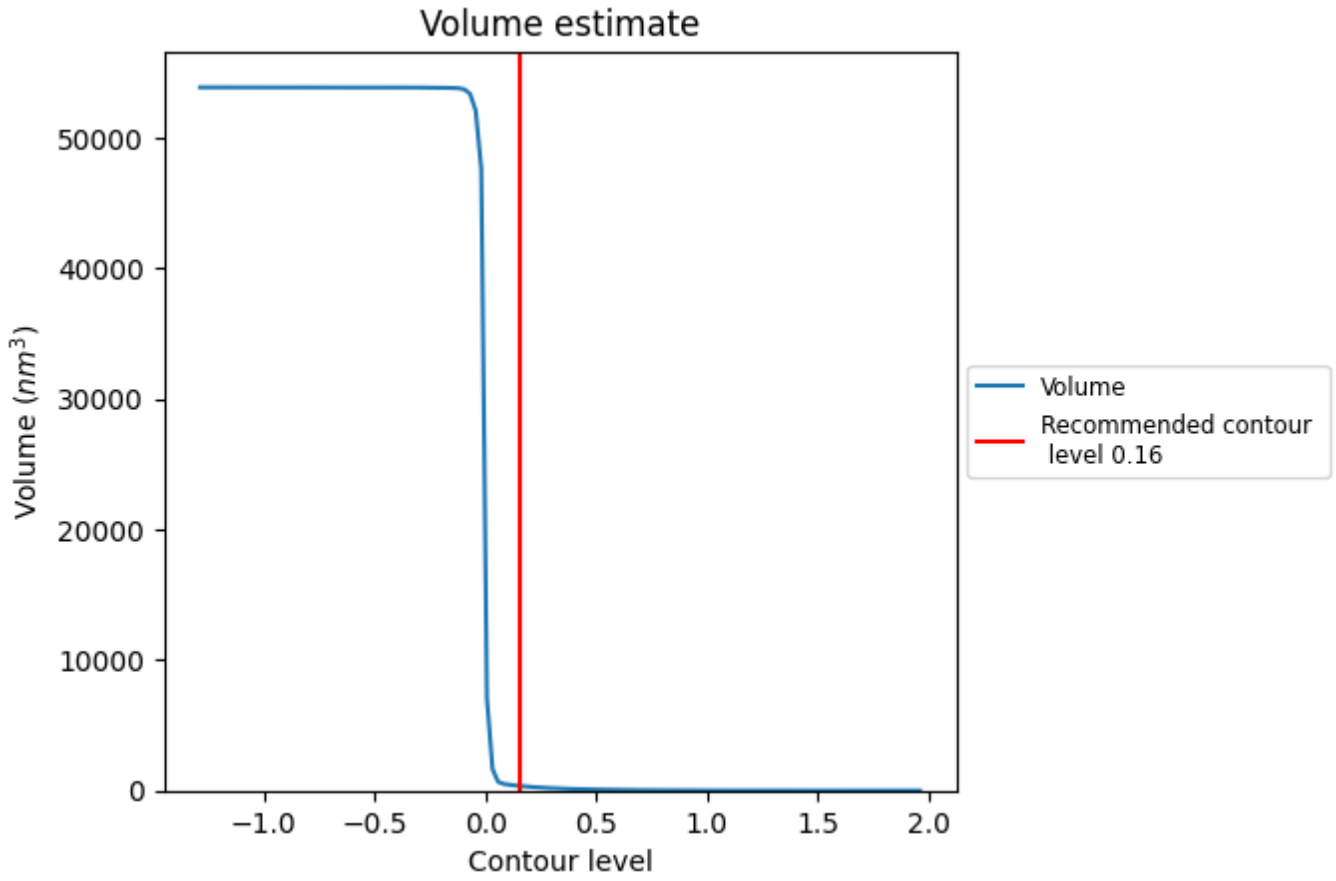
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

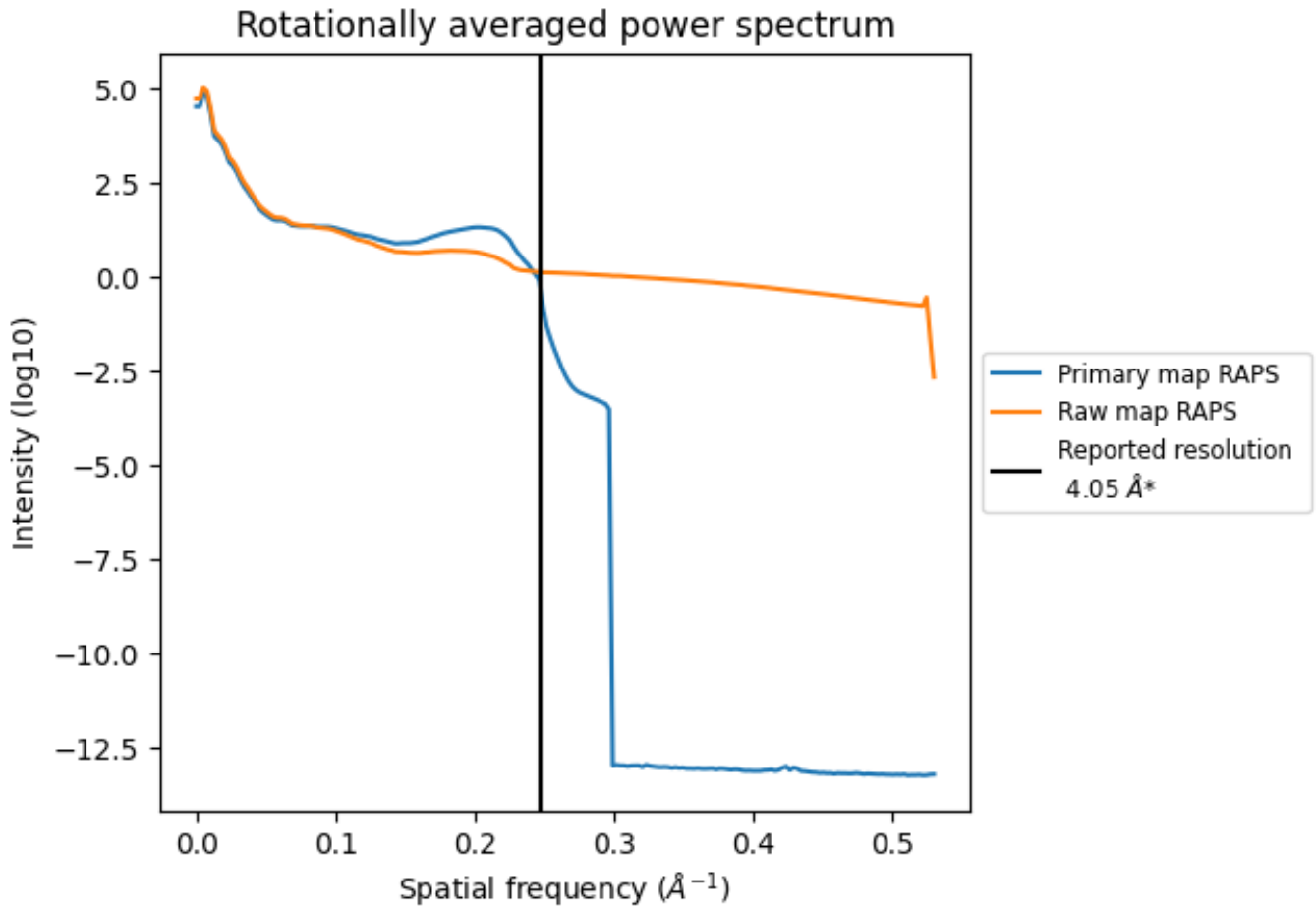
7.2 Volume estimate (i)



The volume at the recommended contour level is 343 nm^3; this corresponds to an approximate mass of 310 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

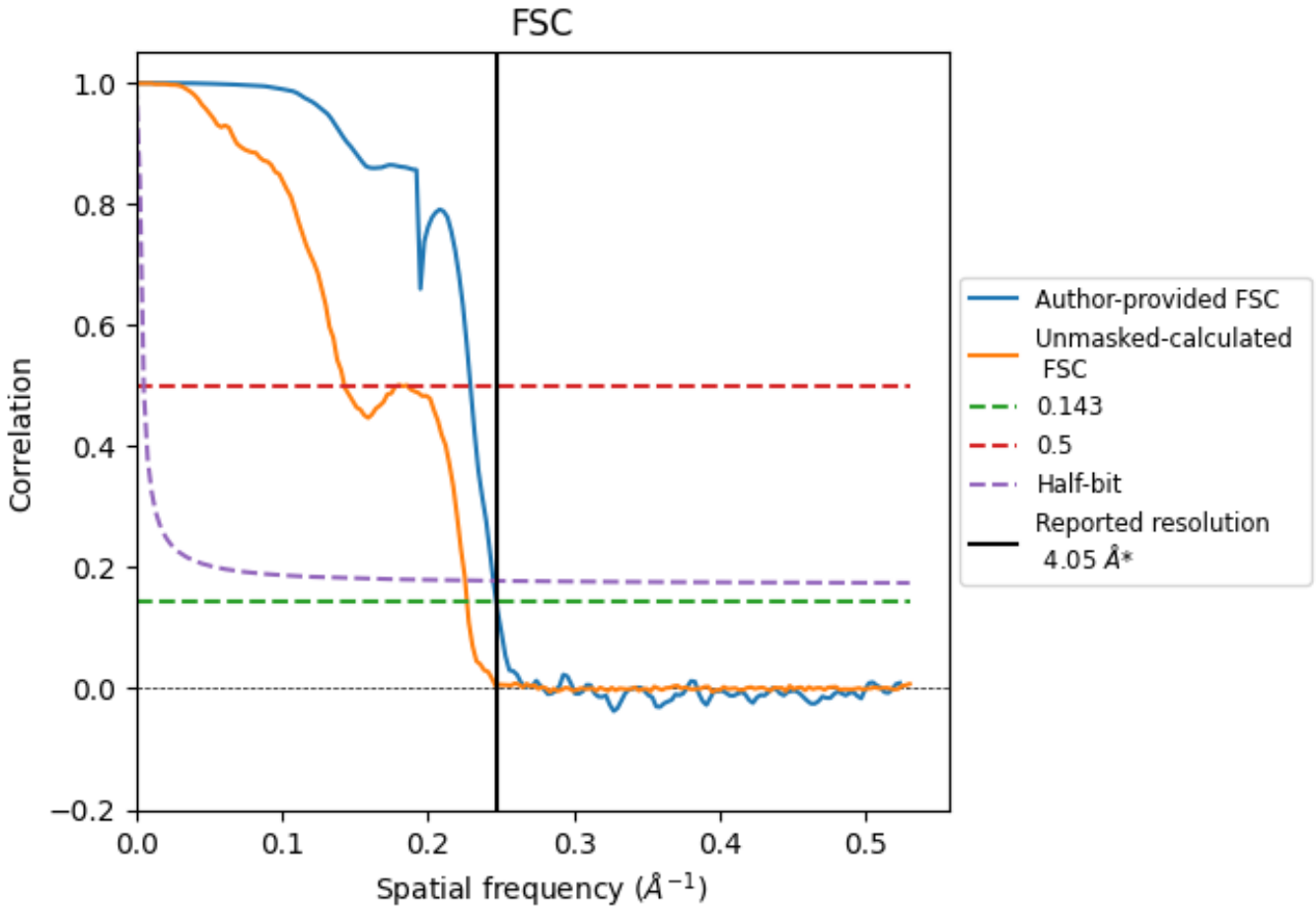


*Reported resolution corresponds to spatial frequency of 0.247 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.247 Å^{-1}

8.2 Resolution estimates (i)

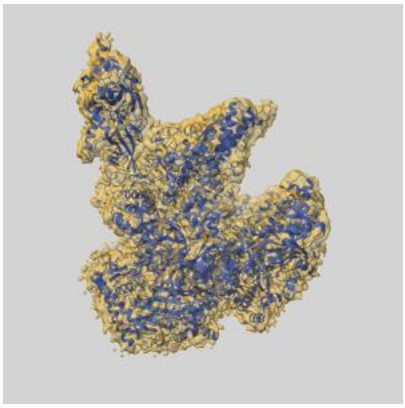
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.05	-	-
Author-provided FSC curve	4.05	4.37	4.09
Unmasked-calculated*	4.41	7.01	4.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

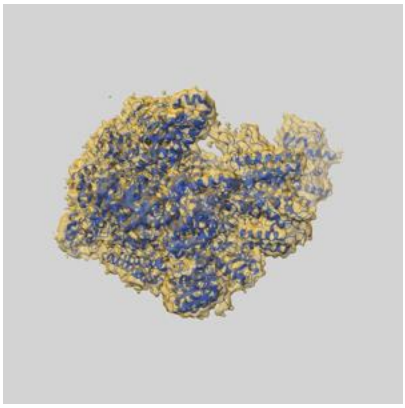
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-74466 and PDB model 9ZO5. Per-residue inclusion information can be found in section 3 on page 7.

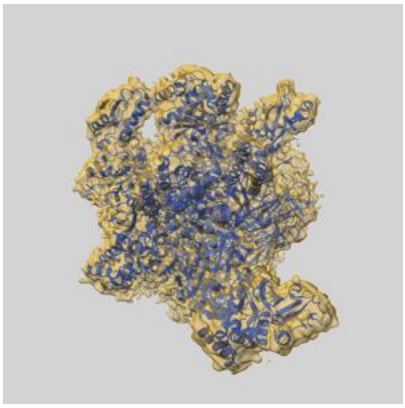
9.1 Map-model overlay



X



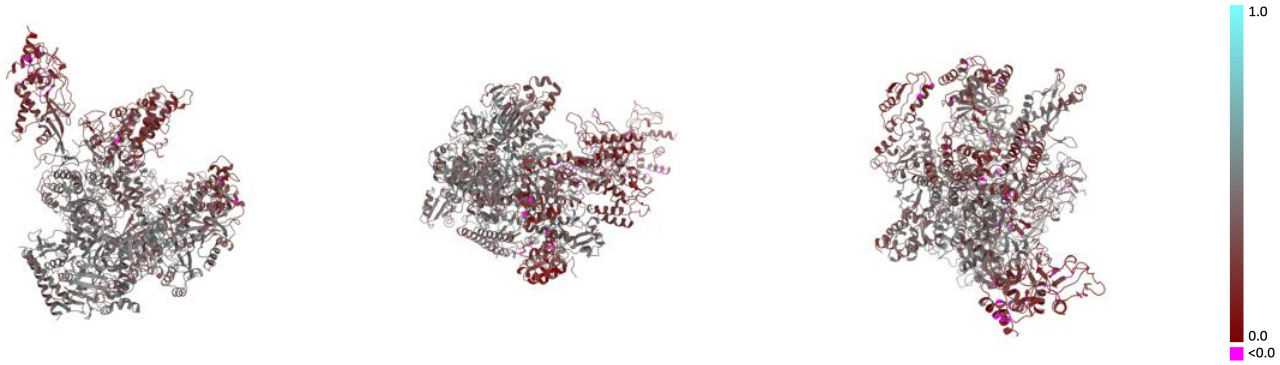
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.16 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.

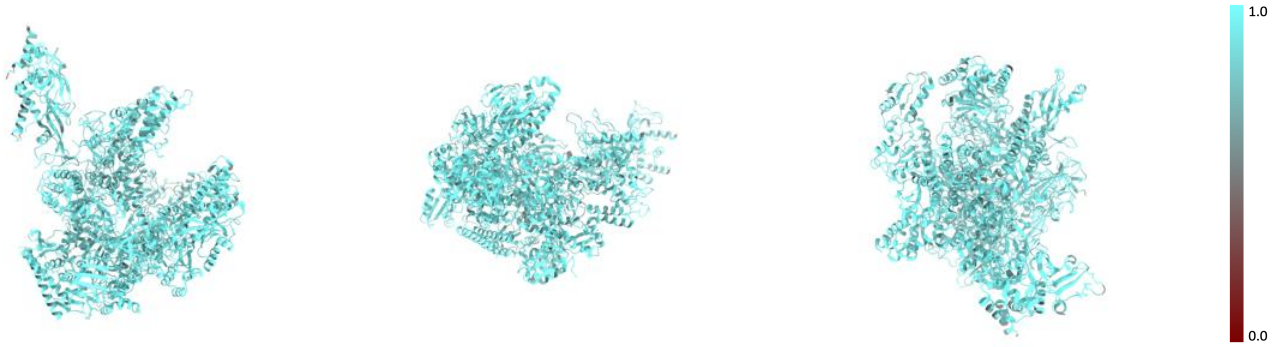
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

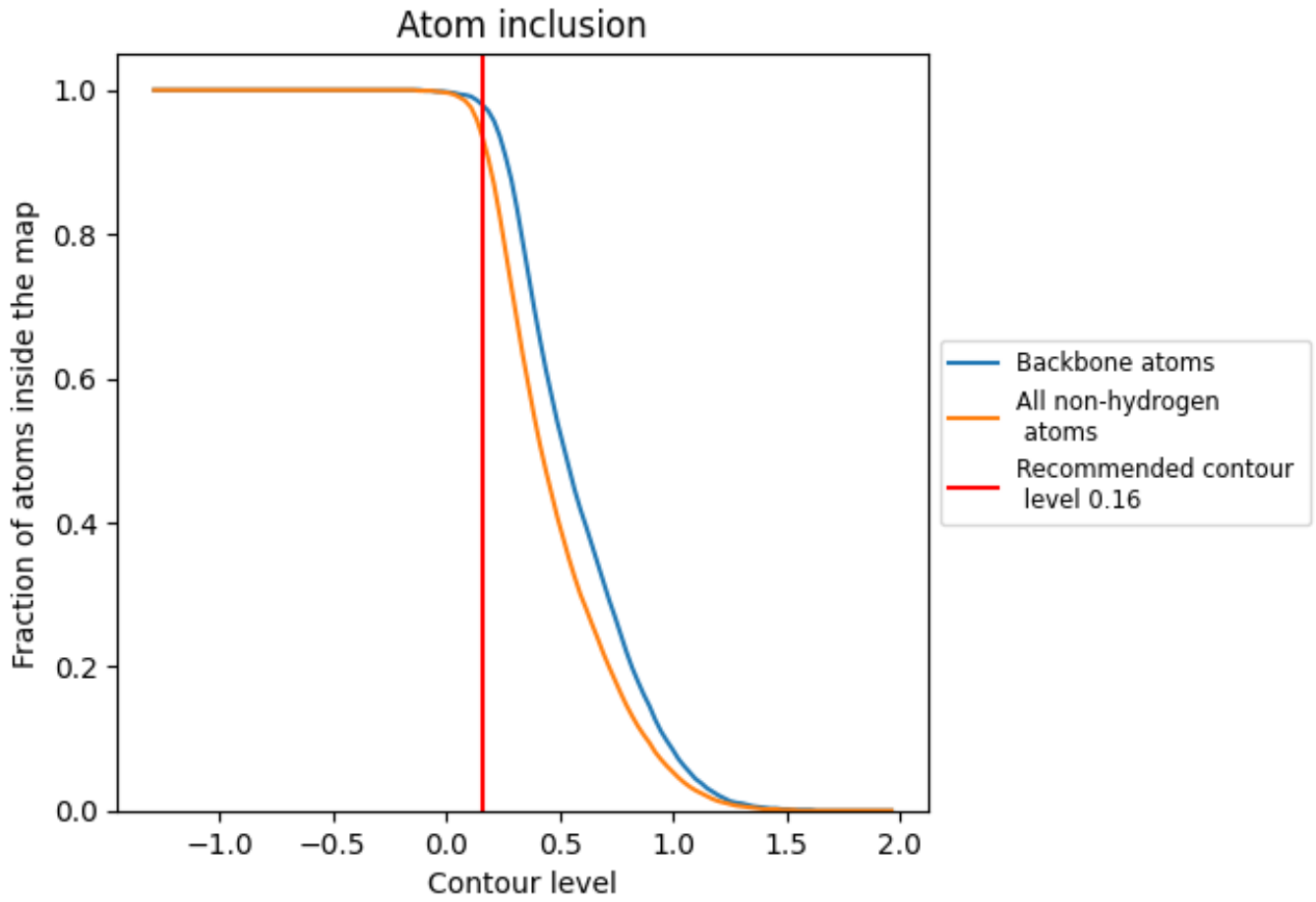
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.16).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9340	0.3690
A	0.9330	0.3650
B	0.9380	0.3960
C	0.9150	0.3240
D	0.9610	0.4380
E	0.9030	0.2390
F	0.8930	0.2100
H	0.9730	0.4160
K	0.9640	0.4110
L	0.9370	0.4290
N	0.9700	0.4500
P	0.9310	0.3830

