



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 04:09 PM UTC

PDB ID : 8HME / pdb_00008hme
EMDB ID : EMD-34897
Title : head module state 1 of Tetrahymena IFT-A
Authors : Ma, Y.; Wu, J.; Lei, M.
Deposited on : 2022-12-03
Resolution : 4.20 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.dev132
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

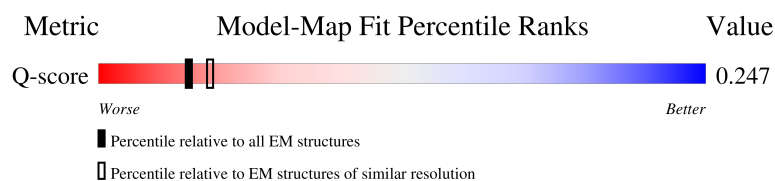
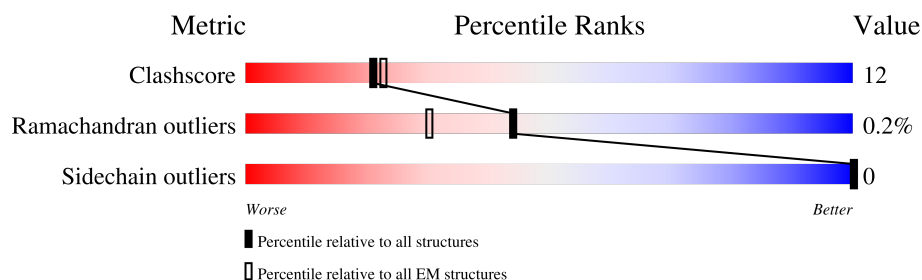
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1251	 31% 11% 57%
2	D	1407	 56% 21% 23%
3	E	1387	 54% 27% 19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22169 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 Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	532	Total	C	N	O	S	0	0
			4380	2797	726	834	23		

- Molecule 2 is a protein called Intraflagellar transporter.

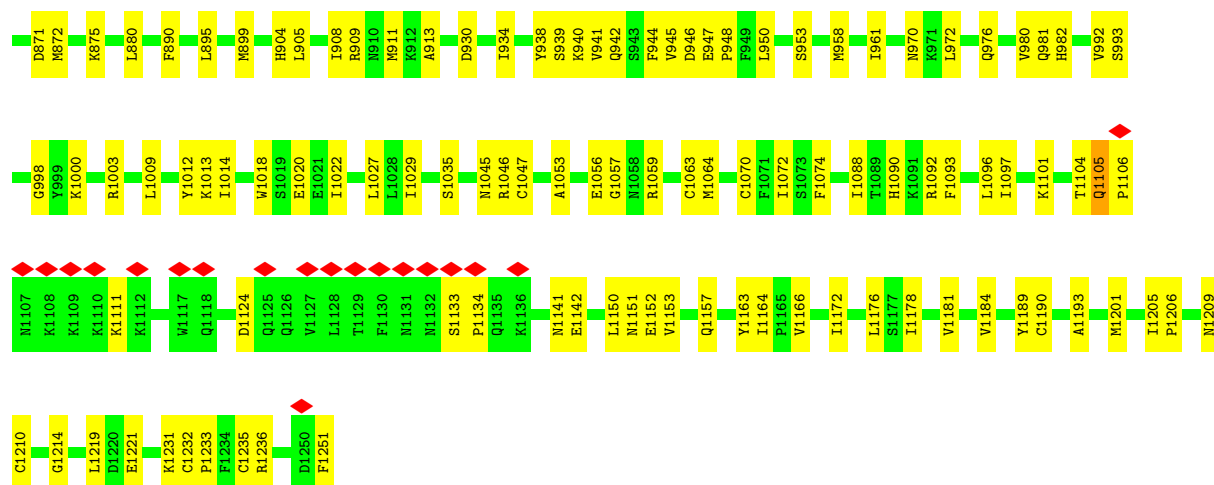
Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	1084	Total	C	N	O	S	0	0
			8740	5502	1505	1689	44		

- Molecule 3 is a protein called WD40 repeat protein.

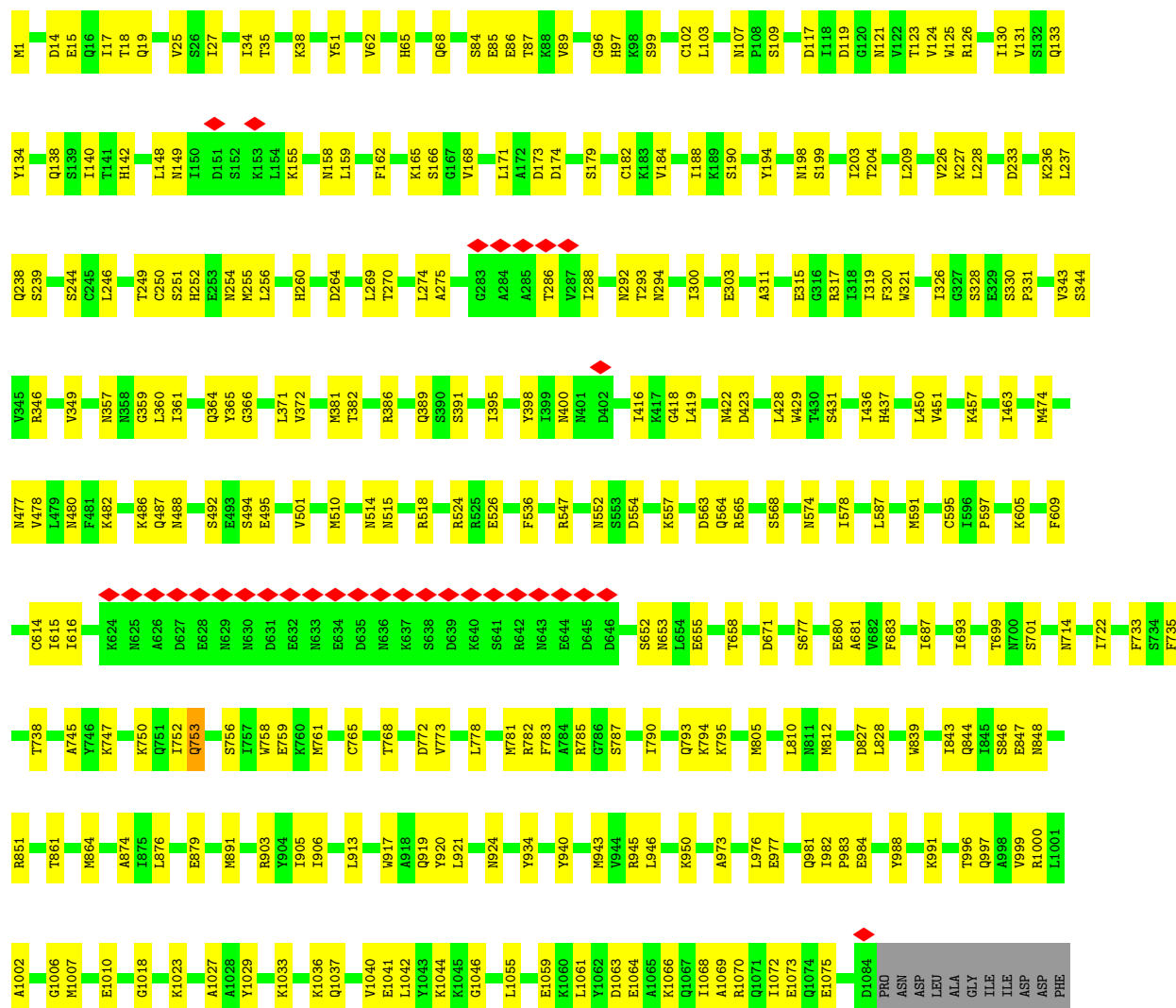
Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1129	Total	C	N	O	S	0	0
			9047	5763	1524	1727	33		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Zn	0
			2	2	



• Molecule 2: Intraflagellar transporter



- Molecule 3: WD40 repeat protein



C984	ASN	HIS	Y1077	C984
D985	GLU	GLU	L1078	D985
V989	ARG	ARG	I1085	V989
C990	LEU	LEU	D1086	C990
V991	PHE	PHE	D1087	V991
V992	PRO	PRO	M1088	V992
V993	THR	THR	I1089	V993
	HIS	HIS	D1090	
	ALA	ALA	L1091	
V996	VAL	VAL	L1091	V996
V1007	ASN	ASN		V1007
E1008	ILE	ILE	R1094	E1008
F1009	LEU	LEU	N1095	F1009
L1010	HIS	HIS		L1010
L1011	ASN	ASN	Q1098	L1011
L1012	VAL	VAL		L1012
A1013	ALA	ALA	L1101	A1013
G1014	ILE	ILE	L1105	G1014
K1015	PRO	PRO	L1106	K1015
K1016	PHE	PHE		K1016
	ASP	ASP		
A1019	LEU	LEU	L1110	A1019
F1020	GLN	GLN	E1111	F1020
Q1021	LYS	LYS	G1112	Q1021
K1022	ASN	ASN	E1113	K1022
Q1024	ARG	ARG	K1114	Q1024
	PRO	PRO	P1115	
V1028	LEU	LEU	K1116	V1028
M1029	ALA	ALA	D1117	M1029
D1030	TYR	TYR	F1118	D1030
A1031	LYS	LYS	I1119	A1031
Y1032	TRP	TRP		Y1032
S1033	SER	SER	K1123	S1033
	VAL	VAL		
M1036	LEU	LEU	G1129	M1036
	ARG	ARG	ASN	
T1040	TYR	TYR	ILE	T1040
R1044	LEU	LEU	GLN	R1044
L1045	ALA	ALA	SER	L1045
R1046	LYS	LYS	LEU	R1046
I1047	ARG	ARG	VAL	I1047
A1048	HIS	HIS	LYS	A1048
	ILE	ILE	ILE	
K1059	ASP	ASP	ALA	K1059
A1060	LYS	LYS	ILE	A1060
A1061	GLU	GLU	THR	A1061
	LYS	LYS	ILE	
F1064	LEU	LEU	ALA	F1064
E1065	ALA	ALA	SER	E1065
	TRP	TRP	ASP	
K1068	ILE	ILE	GLU	K1068
	GLU	GLU	HIS	
	LEU	LEU	ASP	
K1072	ASN	ASN	GLN	K1072
S1073	ILE	ILE	GLY	S1073
L1074	ALA	ALA	ASN	L1074
K1075	ARG	ARG	TYR	K1075
L1076	VAL	VAL	LYS	L1076
	ASN	ASN	ILE	
	PRO	PRO	ALA	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	386801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.036	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size ($\text{\AA}$)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.12	0/4481	0.31	0/6048
2	D	0.11	0/8887	0.32	0/11981
3	E	0.12	0/9217	0.36	0/12450
All	All	0.12	0/22585	0.34	0/30479

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	4380	0	4277	96	0
2	D	8740	0	8711	185	0
3	E	9047	0	9073	262	0
4	A	2	0	0	0	0
All	All	22169	0	22061	526	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (526) 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)
3:E:192:ALA:O	3:E:205:THR:HB	1.74	0.88
3:E:382:ARG:HD2	3:E:385:GLN:HB3	1.63	0.81
1:A:958:MET:HG3	1:A:992:VAL:HG23	1.62	0.80
2:D:940:TYR:HA	2:D:943:MET:HE2	1.66	0.76
1:A:1157:GLN:HE22	1:A:1164:ILE:HB	1.50	0.76
2:D:209:LEU:HB2	2:D:226:VAL:HB	1.66	0.76
3:E:227:LEU:HD13	3:E:269:ARG:HH12	1.51	0.74
2:D:1040:VAL:HG22	2:D:1055:LEU:HD13	1.71	0.73
2:D:1044:LYS:NZ	2:D:1064:GLU:OE1	2.23	0.72
1:A:981:GLN:HB3	3:E:743:ASN:HD22	1.55	0.71
2:D:510:MET:SD	2:D:518:ARG:HB2	2.31	0.71
2:D:386:ARG:HB2	2:D:398:TYR:HB2	1.73	0.70
2:D:431:SER:O	2:D:457:LYS:NZ	2.23	0.70
2:D:782:ARG:HH12	3:E:783:GLN:HB2	1.57	0.70
2:D:275:ALA:HB2	2:D:293:THR:HG21	1.75	0.69
1:A:953:SER:HA	2:D:945:ARG:HH21	1.58	0.69
3:E:451:ASN:OD1	3:E:452:GLU:N	2.24	0.68
1:A:754:VAL:HG12	1:A:756:LYS:H	1.59	0.67
3:E:856:SER:HB2	3:E:861:ASP:HB3	1.75	0.67
3:E:966:ASN:HA	3:E:970:LEU:HB2	1.76	0.67
1:A:1153:VAL:HG11	1:A:1166:VAL:HG12	1.76	0.67
3:E:568:ARG:HB3	3:E:586:GLN:HE22	1.60	0.67
3:E:107:ILE:HG22	3:E:118:ILE:HG22	1.76	0.66
2:D:591:MET:HE1	2:D:595:CYS:HB2	1.78	0.66
2:D:905:ILE:HG13	2:D:913:LEU:HB3	1.78	0.66
2:D:361:ILE:HB	2:D:372:VAL:HB	1.78	0.66
3:E:193:ARG:NH1	3:E:203:GLN:OE1	2.30	0.65
2:D:326:ILE:HG13	2:D:615:ILE:HG21	1.79	0.65
3:E:1061:ALA:HB1	3:E:1077:TYR:HE1	1.62	0.65
3:E:831:LYS:NZ	3:E:848:CYS:SG	2.71	0.64
2:D:557:LYS:HB3	2:D:578:ILE:HD11	1.80	0.64
1:A:1184:VAL:HG22	1:A:1209:ASN:HD21	1.64	0.63
1:A:1009:LEU:HD21	1:A:1014:ILE:HD13	1.81	0.62
3:E:24:TRP:HH2	3:E:338:LEU:HB3	1.64	0.62
3:E:166:LEU:HB2	3:E:180:ILE:HB	1.81	0.62
1:A:1210:CYS:O	1:A:1214:GLY:N	2.32	0.62
2:D:733:PHE:HD1	2:D:745:ALA:HB1	1.65	0.62
2:D:328:SER:OG	2:D:565:ARG:NH1	2.32	0.62
3:E:416:VAL:HB	3:E:439:ARG:HB3	1.80	0.61
2:D:17:ILE:HA	2:D:35:THR:HG22	1.82	0.61
3:E:503:SER:O	3:E:527:GLN:NE2	2.34	0.61
3:E:407:HIS:HB2	3:E:450:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:642:LEU:HD23	3:E:656:LEU:HD22	1.80	0.61
3:E:1088:MET:HE3	3:E:1088:MET:O	1.99	0.61
2:D:138:GLN:HE22	2:D:165:LYS:HE2	1.65	0.61
3:E:662:LEU:HD13	3:E:681:GLN:HE22	1.66	0.61
1:A:871:ASP:OD1	1:A:872:MET:N	2.34	0.61
3:E:129:ASN:O	3:E:133:GLN:N	2.34	0.60
3:E:563:GLU:OE1	3:E:564:HIS:ND1	2.34	0.60
1:A:942:GLN:HA	1:A:945:VAL:HG12	1.83	0.60
2:D:134:TYR:OH	2:D:173:ASP:O	2.20	0.60
2:D:844:GLN:O	2:D:848:ASN:ND2	2.34	0.60
3:E:1020:PHE:HE2	3:E:1046:ARG:HH21	1.47	0.60
3:E:467:THR:HG23	3:E:477:GLN:HE21	1.67	0.60
2:D:782:ARG:NH1	3:E:783:GLN:OE1	2.34	0.60
2:D:107:ASN:ND2	2:D:109:SER:OG	2.32	0.60
3:E:86:TRP:HE1	3:E:91:ASN:HA	1.66	0.60
2:D:148:LEU:O	2:D:155:LYS:NZ	2.35	0.60
3:E:242:GLN:HG3	3:E:286:CYS:HA	1.83	0.59
2:D:237:LEU:HD13	2:D:251:SER:HB2	1.83	0.59
3:E:512:LEU:O	3:E:515:GLN:NE2	2.34	0.59
3:E:683:LEU:HD11	3:E:710:LYS:HG2	1.85	0.59
2:D:595:CYS:HB3	2:D:614:CYS:HB3	1.84	0.59
1:A:770:GLY:O	1:A:774:VAL:HG23	2.02	0.59
2:D:735:PHE:O	2:D:738:THR:OG1	2.21	0.59
2:D:51:TYR:OH	2:D:85:GLU:OE2	2.18	0.59
2:D:227:LYS:NZ	2:D:228:LEU:O	2.35	0.59
3:E:398:PRO:HG3	3:E:410:ALA:HB1	1.83	0.58
3:E:803:ILE:HA	3:E:806:ARG:HE	1.68	0.58
1:A:872:MET:HA	1:A:875:LYS:HD3	1.84	0.58
3:E:217:MET:O	3:E:226:PRO:HA	2.03	0.58
1:A:1206:PRO:HB2	1:A:1219:LEU:HD12	1.85	0.58
2:D:609:PHE:HE1	2:D:658:THR:HB	1.68	0.58
2:D:1027:ALA:HB2	2:D:1042:LEU:HD23	1.86	0.58
3:E:87:ASN:O	3:E:91:ASN:N	2.37	0.58
3:E:721:LEU:HB2	3:E:736:ILE:HG21	1.86	0.58
3:E:1085:ILE:HG23	3:E:1105:LEU:HD11	1.86	0.58
2:D:652:SER:HB3	2:D:677:SER:HA	1.84	0.58
2:D:140:ILE:HG21	2:D:162:PHE:HB2	1.85	0.57
2:D:778:LEU:HA	2:D:781:MET:HG2	1.87	0.57
3:E:141:LYS:NZ	3:E:169:SER:OG	2.38	0.57
1:A:730:ILE:HG12	1:A:749:TYR:HE1	1.70	0.57
1:A:938:TYR:HA	1:A:941:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:462:LYS:NZ	3:E:463:CYS:O	2.37	0.57
3:E:85:LEU:HB3	3:E:94:GLU:HG2	1.86	0.57
2:D:158:ASN:ND2	2:D:174:ASP:OD1	2.30	0.57
1:A:1151:ASN:OD1	1:A:1152:GLU:N	2.38	0.56
3:E:1059:LYS:NZ	3:E:1059:LYS:O	2.36	0.56
2:D:747:LYS:HA	2:D:750:LYS:HD3	1.87	0.56
3:E:449:ARG:HB3	3:E:493:LEU:HD12	1.86	0.56
2:D:19:GLN:HB3	2:D:34:ILE:HB	1.88	0.56
3:E:923:LEU:HA	3:E:926:MET:SD	2.45	0.56
2:D:25:VAL:O	2:D:357:ASN:ND2	2.39	0.56
3:E:1008:GLU:HA	3:E:1011:LEU:HD12	1.87	0.56
1:A:1014:ILE:HD12	1:A:1018:TRP:HB2	1.86	0.56
3:E:601:ASN:HD22	3:E:761:LEU:HD21	1.71	0.56
2:D:260:HIS:O	2:D:264:ASP:HA	2.06	0.55
2:D:292:ASN:ND2	2:D:315:GLU:OE2	2.38	0.55
3:E:158:ILE:HG23	3:E:189:LEU:HD13	1.87	0.55
1:A:909:ARG:NH1	1:A:1189:TYR:O	2.40	0.55
1:A:1027:LEU:HD22	3:E:497:PHE:CE1	2.41	0.55
3:E:968:ASP:OD2	3:E:969:LYS:NZ	2.39	0.55
3:E:1116:LYS:HG2	3:E:1117:ASP:H	1.72	0.55
2:D:781:MET:HB2	2:D:783:PHE:HB2	1.88	0.55
3:E:791:LEU:O	3:E:795:ILE:HG12	2.07	0.55
2:D:494:SER:O	2:D:514:ASN:ND2	2.34	0.55
3:E:923:LEU:O	3:E:927:ILE:HG12	2.07	0.55
1:A:852:ALA:O	2:D:851:ARG:NH2	2.39	0.55
2:D:787:SER:OG	3:E:781:ASP:OD2	2.25	0.55
2:D:790:ILE:HD13	2:D:805:MET:HE1	1.89	0.54
3:E:157:LEU:HB3	3:E:169:SER:HB2	1.88	0.54
3:E:572:VAL:HG22	3:E:584:VAL:HG22	1.88	0.54
2:D:246:LEU:HB2	2:D:330:SER:HB3	1.88	0.54
2:D:381:MET:HE2	2:D:683:PHE:CE2	2.42	0.54
3:E:1065:GLU:HG3	3:E:1091:LEU:HD13	1.89	0.54
3:E:809:PHE:O	3:E:812:GLU:HG3	2.07	0.54
1:A:859:GLU:HA	1:A:862:LYS:HG2	1.90	0.54
2:D:920:TYR:O	2:D:924:ASN:ND2	2.41	0.54
2:D:552:ASN:ND2	2:D:554:ASP:OD1	2.41	0.54
3:E:789:LEU:HD21	3:E:807:LEU:HD21	1.88	0.54
3:E:407:HIS:HE1	3:E:420:LEU:HD12	1.73	0.53
3:E:1074:LEU:HD22	3:E:1101:LEU:HB3	1.89	0.53
3:E:458:LEU:HD11	3:E:491:ILE:HG21	1.90	0.53
3:E:302:ILE:HB	3:E:318:ILE:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:LEU:HD22	1:A:1022:ILE:HG21	1.90	0.53
2:D:827:ASP:OD1	2:D:828:LEU:N	2.42	0.53
1:A:1104:THR:HG23	1:A:1111:LYS:HB2	1.90	0.53
2:D:547:ARG:NH1	2:D:563:ASP:OD1	2.41	0.53
2:D:349:VAL:HA	2:D:365:TYR:HB3	1.90	0.53
2:D:123:THR:OG1	2:D:133:GLN:OE1	2.27	0.52
2:D:524:ARG:HG2	2:D:526:GLU:H	1.74	0.52
3:E:330:MET:HG2	3:E:341:VAL:HG22	1.90	0.52
3:E:800:GLU:OE1	3:E:830:ASN:ND2	2.40	0.52
2:D:246:LEU:HD22	2:D:331:PRO:HD2	1.91	0.52
3:E:412:ILE:HG22	3:E:415:ASN:HB2	1.91	0.52
3:E:690:ASN:HA	3:E:693:ILE:HG12	1.91	0.52
3:E:868:ILE:O	3:E:872:LEU:HD23	2.08	0.52
3:E:742:ILE:HB	3:E:748:ILE:HD11	1.91	0.52
3:E:746:ASN:HB3	3:E:769:SER:HB3	1.91	0.52
1:A:772:VAL:HG21	1:A:802:TYR:CD1	2.44	0.52
2:D:274:LEU:HD21	2:D:317:ARG:HH11	1.74	0.52
3:E:501:LEU:HD21	3:E:528:LEU:HB3	1.92	0.52
1:A:1072:ILE:HD11	1:A:1233:PRO:HG2	1.91	0.52
2:D:84:SER:HB3	2:D:89:VAL:HG22	1.91	0.52
3:E:802:PHE:HA	3:E:844:HIS:HE2	1.72	0.52
2:D:360:LEU:HD11	2:D:371:LEU:HD22	1.90	0.52
3:E:543:PHE:HE1	3:E:547:GLY:HA2	1.74	0.52
3:E:895:ALA:HB2	3:E:910:LEU:HD22	1.92	0.52
3:E:242:GLN:NE2	3:E:285:LEU:O	2.43	0.52
3:E:1119:ILE:HG13	3:E:1123:LYS:HE2	1.91	0.52
3:E:993:VAL:O	3:E:996:VAL:HG22	2.09	0.52
3:E:290:ILE:HD12	3:E:335:ASN:HA	1.92	0.52
3:E:129:ASN:O	3:E:133:GLN:CA	2.58	0.52
3:E:117:VAL:HG21	3:E:157:LEU:HD22	1.91	0.51
3:E:206:ILE:HB	3:E:218:TYR:HB3	1.92	0.51
3:E:739:PHE:HE2	3:E:755:ILE:HG13	1.75	0.51
3:E:1072:LYS:HA	3:E:1075:LYS:HG2	1.92	0.51
1:A:857:TYR:HD2	1:A:880:LEU:HD11	1.75	0.51
3:E:1086:ASP:HA	3:E:1089:ILE:HD12	1.93	0.51
2:D:364:GLN:NE2	2:D:366:GLY:O	2.41	0.51
3:E:206:ILE:HD12	3:E:218:TYR:HD2	1.75	0.51
2:D:1018:GLY:O	2:D:1023:LYS:NZ	2.43	0.51
3:E:24:TRP:NE1	3:E:332:TRP:O	2.43	0.51
3:E:60:LYS:O	3:E:78:GLU:N	2.44	0.51
3:E:243:LEU:HD11	3:E:247:GLY:HA2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:412:ILE:HG13	3:E:413:ASN:H	1.74	0.51
3:E:967:LEU:HD11	3:E:996:VAL:HG12	1.92	0.51
3:E:1048:ALA:HB1	3:E:1064:PHE:CE1	2.45	0.51
2:D:99:SER:HB2	2:D:117:ASP:HB2	1.93	0.51
3:E:1048:ALA:HB1	3:E:1064:PHE:HE1	1.75	0.51
3:E:475:LYS:NZ	3:E:476:ASP:O	2.38	0.51
2:D:18:THR:OG1	2:D:34:ILE:O	2.28	0.51
2:D:389:GLN:NE2	2:D:391:SER:O	2.44	0.51
3:E:748:ILE:O	3:E:752:ILE:HG12	2.11	0.51
1:A:1153:VAL:O	1:A:1157:GLN:HG2	2.11	0.50
2:D:1:MET:HE1	2:D:681:ALA:HB2	1.94	0.50
2:D:138:GLN:HB3	2:D:166:SER:HB3	1.93	0.50
2:D:203:ILE:HG13	2:D:209:LEU:HD13	1.93	0.50
3:E:152:ASN:HB3	3:E:156:LEU:H	1.76	0.50
3:E:819:GLU:OE1	3:E:819:GLU:N	2.42	0.50
3:E:562:LEU:HB3	3:E:565:PHE:CE2	2.46	0.50
3:E:1024:GLN:HE22	3:E:1046:ARG:HE	1.59	0.50
2:D:99:SER:OG	2:D:119:ASP:OD2	2.29	0.50
3:E:1061:ALA:HA	3:E:1064:PHE:HD2	1.76	0.50
1:A:854:GLN:OE1	1:A:856:ARG:NH2	2.42	0.50
3:E:129:ASN:O	3:E:133:GLN:HA	2.11	0.50
3:E:450:LEU:HD13	3:E:455:ALA:HB2	1.93	0.50
3:E:1010:LEU:HD13	3:E:1019:ALA:HB2	1.92	0.50
1:A:1045:ASN:O	1:A:1046:ARG:HG2	2.12	0.50
2:D:171:LEU:HB3	2:D:179:SER:HB2	1.94	0.50
2:D:843:ILE:HD11	2:D:861:THR:HG21	1.93	0.50
2:D:1:MET:HE3	2:D:680:GLU:HB3	1.94	0.50
2:D:436:ILE:HG23	2:D:451:VAL:HB	1.93	0.50
3:E:357:PHE:HB3	3:E:369:LEU:HB3	1.94	0.50
3:E:76:LEU:HD22	3:E:107:ILE:HG23	1.94	0.50
2:D:250:CYS:HB2	2:D:256:LEU:HD13	1.94	0.49
2:D:344:SER:O	2:D:346:ARG:NH2	2.44	0.49
2:D:752:ILE:O	2:D:753:GLN:HG3	2.12	0.49
3:E:143:SER:OG	3:E:163:GLU:OE1	2.23	0.49
3:E:334:ASN:OD1	3:E:335:ASN:N	2.45	0.49
1:A:1056:GLU:OE1	1:A:1057:GLY:N	2.39	0.49
3:E:240:ASP:OD2	3:E:242:GLN:NE2	2.45	0.49
3:E:182:VAL:HG12	3:E:183:GLN:N	2.27	0.49
3:E:472:ASN:OD1	3:E:473:ASN:N	2.45	0.49
2:D:756:SER:O	2:D:759:GLU:HG3	2.11	0.49
3:E:61:VAL:HA	3:E:77:GLN:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:182:VAL:HG12	3:E:183:GLN:H	1.77	0.49
1:A:1133:SER:OG	1:A:1134:PRO:HD3	2.12	0.49
2:D:480:ASN:HD21	2:D:482:LYS:HB2	1.76	0.49
3:E:946:TYR:HB3	3:E:969:LYS:HD2	1.95	0.49
3:E:34:CYS:HB2	3:E:40:VAL:HG13	1.94	0.49
3:E:976:ALA:O	3:E:980:LEU:HD23	2.13	0.49
2:D:733:PHE:CG	2:D:761:MET:HE1	2.48	0.49
2:D:795:LYS:HD2	2:D:795:LYS:O	2.13	0.49
2:D:976:LEU:HB3	2:D:981:GLN:HB3	1.93	0.49
3:E:420:LEU:HB2	3:E:436:ILE:HD11	1.94	0.49
3:E:159:THR:OG1	3:E:167:THR:OG1	2.31	0.49
3:E:1029:MET:HE3	3:E:1033:SER:HB3	1.95	0.49
2:D:238:GLN:HE21	2:D:300:ILE:HG12	1.77	0.48
2:D:810:LEU:HB3	2:D:812:MET:HE1	1.93	0.48
3:E:402:SER:HB3	3:E:409:ALA:HB3	1.95	0.48
3:E:288:ASN:O	3:E:292:TYR:HA	2.13	0.48
1:A:911:MET:HG3	1:A:913:ALA:H	1.77	0.48
2:D:131:VAL:HG11	2:D:174:ASP:HB2	1.94	0.48
1:A:762:TYR:O	1:A:766:ASN:N	2.46	0.48
3:E:693:ILE:O	3:E:696:GLN:HG3	2.14	0.48
1:A:972:LEU:HD21	1:A:980:VAL:HG21	1.96	0.48
3:E:459:THR:O	3:E:461:GLY:N	2.47	0.48
1:A:1210:CYS:O	1:A:1214:GLY:CA	2.62	0.48
3:E:678:PHE:O	3:E:682:ASN:ND2	2.46	0.48
1:A:904:HIS:O	1:A:908:ILE:HG13	2.13	0.48
1:A:1205:ILE:HD12	1:A:1206:PRO:HD2	1.96	0.48
3:E:79:ASN:HB3	3:E:103:LYS:HE2	1.94	0.48
3:E:717:LEU:HD13	3:E:740:GLN:HG2	1.95	0.48
3:E:992:MET:O	3:E:996:VAL:HG13	2.14	0.48
2:D:102:CYS:SG	2:D:103:LEU:N	2.87	0.48
2:D:793:GLN:HB3	2:D:805:MET:HE2	1.95	0.48
3:E:248:TYR:HB3	3:E:260:HIS:HE2	1.79	0.47
3:E:288:ASN:HB2	3:E:332:TRP:CE3	2.49	0.47
3:E:989:VAL:HA	3:E:992:MET:HE2	1.96	0.47
3:E:828:VAL:HA	3:E:831:LYS:HE2	1.96	0.47
2:D:846:SER:O	2:D:851:ARG:N	2.43	0.47
2:D:1023:LYS:HD3	2:D:1046:GLY:HA2	1.94	0.47
3:E:712:LEU:HD11	3:E:752:ILE:HD12	1.96	0.47
3:E:831:LYS:HE3	3:E:845:ASN:HA	1.96	0.47
3:E:985:ASP:OD1	3:E:985:ASP:N	2.47	0.47
1:A:899:MET:HE2	1:A:899:MET:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:ASP:O	1:A:934:ILE:HG12	2.14	0.47
1:A:1105:GLN:HB2	1:A:1106:PRO:HD3	1.96	0.47
3:E:378:VAL:HG22	3:E:389:VAL:HG12	1.96	0.47
3:E:438:LYS:NZ	3:E:440:ASP:OD1	2.48	0.47
1:A:1093:PHE:O	1:A:1097:ILE:HG12	2.15	0.47
1:A:1090:HIS:HA	1:A:1093:PHE:HB3	1.97	0.47
2:D:65:HIS:CG	2:D:68:GLN:HB2	2.50	0.47
2:D:605:LYS:HB2	2:D:687:ILE:HD11	1.96	0.47
2:D:996:THR:HA	2:D:999:VAL:HG12	1.96	0.47
1:A:746:GLY:O	1:A:750:ILE:HG12	2.14	0.47
1:A:1003:ARG:NH2	1:A:1029:ILE:O	2.47	0.47
2:D:1063:ASP:O	2:D:1066:LYS:HG2	2.15	0.47
3:E:19:LYS:HZ1	3:E:62:ILE:HA	1.80	0.47
3:E:678:PHE:O	3:E:681:GLN:HG3	2.14	0.47
2:D:320:PHE:HE2	2:D:343:VAL:HG23	1.80	0.47
2:D:495:GLU:HG3	3:E:1015:LYS:HZ3	1.80	0.47
2:D:946:LEU:O	2:D:950:LYS:NZ	2.48	0.47
3:E:306:ASN:OD1	3:E:307:LEU:N	2.48	0.47
1:A:1056:GLU:OE2	1:A:1059:ARG:HB2	2.15	0.46
2:D:386:ARG:HH12	2:D:400:ASN:N	2.13	0.46
3:E:110:SER:HB3	3:E:113:HIS:O	2.15	0.46
3:E:795:ILE:HG13	3:E:796:ALA:N	2.30	0.46
1:A:970:ASN:ND2	1:A:1053:ALA:O	2.32	0.46
2:D:772:ASP:OD1	2:D:773:VAL:N	2.48	0.46
3:E:852:ILE:HA	3:E:855:THR:HG22	1.96	0.46
1:A:802:TYR:O	1:A:805:GLU:HG3	2.16	0.46
2:D:35:THR:OG1	2:D:38:LYS:O	2.33	0.46
2:D:303:GLU:HG2	2:D:359:GLY:HA2	1.96	0.46
2:D:1072:ILE:O	2:D:1075:GLU:HG2	2.15	0.46
3:E:808:ALA:O	3:E:811:ILE:HG22	2.16	0.46
2:D:839:TRP:CD1	2:D:864:MET:HE2	2.51	0.46
3:E:142:HIS:CD2	3:E:146:ILE:HD13	2.49	0.46
2:D:422:ASN:ND2	2:D:463:ILE:HG12	2.31	0.46
2:D:14:ASP:OD1	2:D:15:GLU:N	2.49	0.46
3:E:1011:LEU:HD23	3:E:1016:LYS:HE2	1.96	0.46
1:A:729:LEU:HD23	1:A:752:ALA:HB2	1.97	0.46
2:D:782:ARG:NH1	3:E:782:ILE:O	2.49	0.46
2:D:1070:ARG:O	2:D:1073:GLU:HG3	2.15	0.46
3:E:185:GLU:O	3:E:211:SER:N	2.46	0.46
3:E:458:LEU:HD11	3:E:491:ILE:HD13	1.96	0.46
3:E:795:ILE:HG13	3:E:796:ALA:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:959:TRP:CH2	3:E:989:VAL:HG11	2.51	0.46
1:A:1064:MET:HB2	1:A:1163:TYR:HB2	1.98	0.46
3:E:292:TYR:OH	3:E:308:GLY:N	2.48	0.45
2:D:565:ARG:HH21	2:D:568:SER:H	1.63	0.45
3:E:12:ASP:HB3	3:E:346:GLY:HA3	1.97	0.45
2:D:149:ASN:HB2	2:D:198:ASN:HD21	1.82	0.45
3:E:87:ASN:O	3:E:91:ASN:CA	2.64	0.45
3:E:739:PHE:CE2	3:E:755:ILE:HG13	2.51	0.45
3:E:885:CYS:SG	3:E:894:ALA:HB2	2.56	0.45
3:E:990:CYS:HA	3:E:993:VAL:HG12	1.98	0.45
2:D:233:ASP:O	2:D:251:SER:OG	2.34	0.45
2:D:1069:ALA:HA	2:D:1072:ILE:HG22	1.98	0.45
3:E:392:ILE:HG23	3:E:433:GLY:HA3	1.98	0.45
3:E:883:VAL:O	3:E:886:GLU:HG3	2.16	0.45
2:D:782:ARG:NH1	3:E:783:GLN:HB2	2.28	0.45
3:E:148:THR:HG21	3:E:187:SER:HA	1.98	0.45
1:A:1092:ARG:HH11	1:A:1096:LEU:HD12	1.82	0.45
1:A:1231:LYS:HD2	1:A:1236:ARG:HH21	1.80	0.45
2:D:785:ARG:HG3	3:E:735:THR:HG21	1.99	0.45
1:A:1141:ASN:OD1	1:A:1142:GLU:N	2.48	0.45
2:D:501:VAL:HG12	2:D:510:MET:HB3	1.99	0.45
2:D:733:PHE:CD1	2:D:761:MET:HE1	2.51	0.45
2:D:759:GLU:N	2:D:781:MET:HE1	2.31	0.45
1:A:1124:ASP:OD1	1:A:1124:ASP:N	2.49	0.45
2:D:699:THR:HG22	2:D:701:SER:H	1.81	0.45
3:E:210:LEU:HB3	3:E:214:SER:HB3	1.98	0.45
3:E:758:GLN:HE21	3:E:761:LEU:HD13	1.82	0.45
2:D:765:CYS:HA	2:D:768:THR:HG22	1.99	0.45
2:D:117:ASP:OD2	2:D:121:ASN:HB2	2.17	0.45
2:D:123:THR:HG21	2:D:130:ILE:HG12	1.98	0.45
2:D:194:TYR:HB3	2:D:199:SER:HB2	1.99	0.45
1:A:1009:LEU:HA	1:A:1012:TYR:HB2	1.99	0.44
2:D:477:ASN:HB3	2:D:488:ASN:CG	2.42	0.44
2:D:574:ASN:HA	2:D:597:PRO:HD2	1.98	0.44
3:E:854:ARG:HB3	3:E:881:ILE:HD12	1.99	0.44
3:E:1074:LEU:O	3:E:1078:LEU:HG	2.18	0.44
2:D:874:ALA:HB3	2:D:891:MET:HE1	1.99	0.44
3:E:262:SER:H	3:E:272:ILE:HG13	1.82	0.44
3:E:590:LEU:HB2	3:E:626:THR:HB	2.00	0.44
2:D:244:SER:N	2:D:330:SER:OG	2.50	0.44
2:D:844:GLN:O	2:D:847:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:34:CYS:HB3	3:E:64:LEU:HD22	2.00	0.44
1:A:733:ALA:O	1:A:737:VAL:HG23	2.16	0.44
3:E:805:ARG:NH1	3:E:847:LEU:HD13	2.33	0.44
3:E:938:LYS:O	3:E:941:GLU:HG3	2.18	0.44
3:E:977:ILE:HG12	3:E:1009:PHE:HZ	1.83	0.44
1:A:1063:CYS:O	1:A:1064:MET:HE2	2.18	0.44
2:D:395:ILE:HD12	2:D:419:LEU:HD11	2.00	0.44
2:D:480:ASN:HB3	2:D:486:LYS:NZ	2.32	0.44
2:D:1007:MET:HB3	2:D:1010:GLU:OE1	2.17	0.44
3:E:6:LYS:HD3	3:E:9:GLU:HG3	1.99	0.44
3:E:182:VAL:HG11	3:E:216:LEU:HD13	1.99	0.44
3:E:808:ALA:HA	3:E:811:ILE:HG22	1.99	0.44
1:A:1070:CYS:O	1:A:1074:PHE:N	2.41	0.44
2:D:616:ILE:HD11	2:D:655:GLU:HG3	2.00	0.44
3:E:214:SER:OG	3:E:229:LEU:O	2.22	0.44
3:E:265:LEU:HD12	3:E:268:LEU:HD12	2.00	0.44
3:E:362:TYR:H	3:E:403:LEU:HD23	1.83	0.44
1:A:1020:GLU:OE2	1:A:1020:GLU:N	2.37	0.43
1:A:1072:ILE:HG21	1:A:1221:GLU:HB3	1.99	0.43
2:D:416:ILE:HD12	2:D:428:LEU:HD13	2.00	0.43
3:E:337:GLN:HE22	3:E:356:PRO:HD2	1.82	0.43
1:A:993:SER:OG	1:A:998:GLY:O	2.36	0.43
3:E:285:LEU:HG	3:E:294:LEU:HD11	2.00	0.43
1:A:1012:TYR:HA	3:E:745:LYS:HE3	2.00	0.43
3:E:235:TYR:HB3	3:E:253:PHE:CD2	2.53	0.43
3:E:891:TYR:HB3	3:E:910:LEU:HD21	2.00	0.43
3:E:959:TRP:CG	3:E:983:LYS:HD3	2.53	0.43
1:A:726:LYS:HD3	1:A:753:GLU:OE2	2.18	0.43
1:A:948:PRO:O	2:D:919:GLN:NE2	2.51	0.43
1:A:1105:GLN:O	1:A:1111:LYS:NZ	2.52	0.43
2:D:286:THR:HG22	2:D:288:ILE:HG13	1.99	0.43
3:E:379:ASP:HB3	3:E:387:GLN:HB2	1.99	0.43
3:E:89:PHE:CE2	3:E:90:GLN:HG3	2.53	0.43
3:E:420:LEU:HD23	3:E:421:TRP:N	2.34	0.43
3:E:675:HIS:HD2	3:E:698:LEU:HD23	1.83	0.43
3:E:718:ASP:OD1	3:E:718:ASP:N	2.51	0.43
3:E:931:ASN:HA	3:E:934:LYS:HE2	2.01	0.43
2:D:126:ARG:HB3	3:E:1068:LYS:NZ	2.33	0.43
2:D:382:THR:HB	2:D:423:ASP:OD1	2.18	0.43
3:E:66:TRP:CD1	3:E:73:LEU:HD21	2.54	0.43
3:E:889:LYS:HD2	3:E:889:LYS:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:332:TRP:HB3	3:E:336:GLY:HA2	2.00	0.43
3:E:732:MET:O	3:E:736:ILE:HG12	2.19	0.43
1:A:1088:ILE:HA	1:A:1092:ARG:NH2	2.33	0.43
1:A:895:LEU:HD13	1:A:1236:ARG:HG3	2.00	0.43
2:D:25:VAL:HG12	2:D:27:ILE:H	1.84	0.43
2:D:260:HIS:O	2:D:264:ASP:CA	2.67	0.43
3:E:37:SER:C	3:E:38:LYS:HG3	2.44	0.43
1:A:946:ASP:OD1	1:A:947:GLU:N	2.52	0.43
1:A:1045:ASN:C	1:A:1047:CYS:H	2.27	0.43
2:D:437:HIS:NE2	2:D:450:LEU:HD12	2.34	0.43
3:E:990:CYS:HB3	3:E:1013:ALA:HB2	2.00	0.43
3:E:545:ASN:O	3:E:546:LYS:HG2	2.18	0.42
1:A:845:LEU:HB3	1:A:846:PRO:HD3	1.99	0.42
2:D:1006:GLY:O	2:D:1007:MET:HE2	2.19	0.42
3:E:34:CYS:SG	3:E:40:VAL:HG22	2.59	0.42
3:E:528:LEU:HD13	3:E:544:ASP:OD1	2.19	0.42
3:E:751:ASN:HA	3:E:754:MET:HG3	2.00	0.42
3:E:1114:LYS:HB3	3:E:1115:PRO:HD2	2.01	0.42
1:A:1172:ILE:O	1:A:1176:LEU:HG	2.20	0.42
2:D:34:ILE:HD11	2:D:62:VAL:HG21	2.00	0.42
2:D:1059:GLU:HG3	2:D:1061:LEU:HD23	2.01	0.42
3:E:1032:TYR:CE1	3:E:1036:MET:HG3	2.54	0.42
1:A:976:GLN:HA	1:A:982:HIS:NE2	2.35	0.42
2:D:159:LEU:HD22	2:D:171:LEU:HD11	2.00	0.42
2:D:269:LEU:HD13	2:D:321:TRP:CE2	2.54	0.42
2:D:474:MET:HE2	2:D:474:MET:HA	2.00	0.42
3:E:407:HIS:HA	3:E:419:TYR:O	2.18	0.42
1:A:827:ASP:N	1:A:827:ASP:OD1	2.53	0.42
1:A:1056:GLU:CD	1:A:1057:GLY:H	2.23	0.42
2:D:97:HIS:ND1	2:D:117:ASP:OD2	2.52	0.42
3:E:712:LEU:CD1	3:E:752:ILE:HD12	2.50	0.42
3:E:834:ARG:NH1	3:E:837:ASP:HB2	2.34	0.42
1:A:842:ILE:HD12	1:A:842:ILE:H	1.83	0.42
1:A:1190:CYS:SG	1:A:1193:ALA:HB2	2.60	0.42
3:E:362:TYR:HB2	3:E:403:LEU:HG	2.00	0.42
3:E:540:VAL:CG1	3:E:552:PHE:HB3	2.49	0.42
3:E:1029:MET:HE2	3:E:1047:ILE:HG12	2.02	0.42
3:E:1088:MET:CE	3:E:1101:LEU:HD12	2.50	0.42
2:D:124:VAL:HG11	2:D:174:ASP:HA	2.00	0.42
2:D:515:ASN:HB3	2:D:536:PHE:HB3	2.01	0.42
3:E:85:LEU:HB3	3:E:94:GLU:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:TYR:OH	2:D:851:ARG:NH1	2.53	0.42
1:A:890:PHE:HB2	1:A:939:SER:HB3	2.01	0.42
1:A:944:PHE:CD1	1:A:961:ILE:HG13	2.55	0.42
2:D:671:ASP:OD2	2:D:714:ASN:ND2	2.45	0.42
3:E:87:ASN:O	3:E:91:ASN:HA	2.19	0.42
3:E:129:ASN:OD1	3:E:131:LYS:NZ	2.39	0.42
3:E:369:LEU:HD21	3:E:372:PHE:HA	2.02	0.42
3:E:950:GLU:OE2	3:E:966:ASN:ND2	2.53	0.42
1:A:940:LYS:HE3	1:A:940:LYS:HB2	1.83	0.42
2:D:14:ASP:OD1	2:D:15:GLU:HG3	2.20	0.42
2:D:255:MET:SD	2:D:270:THR:HG22	2.60	0.42
2:D:851:ARG:HD2	2:D:851:ARG:O	2.20	0.42
3:E:402:SER:HB2	3:E:448:ILE:HG23	2.02	0.42
3:E:675:HIS:HE2	3:E:697:PHE:HB2	1.84	0.42
3:E:811:ILE:HG21	3:E:823:LEU:HD12	2.02	0.42
3:E:1028:VAL:O	3:E:1028:VAL:HG12	2.20	0.42
1:A:1201:MET:HE3	1:A:1201:MET:HA	2.02	0.41
3:E:187:SER:N	3:E:209:ILE:O	2.53	0.41
3:E:849:PHE:HA	3:E:852:ILE:HG12	2.01	0.41
3:E:1064:PHE:CG	3:E:1076:LEU:HD21	2.55	0.41
3:E:267:GLU:HB3	3:E:272:ILE:HD11	2.01	0.41
3:E:1040:THR:O	3:E:1044:ARG:NH1	2.52	0.41
1:A:1046:ARG:HB2	1:A:1150:LEU:HD11	2.02	0.41
2:D:578:ILE:HG23	2:D:587:LEU:HB2	2.02	0.41
3:E:2:ALA:O	3:E:316:GLN:NE2	2.49	0.41
3:E:150:ASP:HB3	3:E:191:TRP:CZ3	2.55	0.41
3:E:377:ILE:HG22	3:E:390:SER:HB3	2.01	0.41
1:A:905:LEU:HA	1:A:908:ILE:HG13	2.01	0.41
2:D:86:GLU:HG3	2:D:87:THR:HG23	2.03	0.41
2:D:683:PHE:HD1	2:D:693:ILE:HD11	1.84	0.41
3:E:506:LYS:HD2	3:E:508:ARG:HE	1.85	0.41
3:E:834:ARG:HH12	3:E:837:ASP:HB2	1.84	0.41
3:E:1007:VAL:HG13	3:E:1032:TYR:HB2	2.02	0.41
3:E:1117:ASP:N	3:E:1117:ASP:OD1	2.53	0.41
2:D:903:ARG:NH2	2:D:906:ILE:HD12	2.35	0.41
3:E:219:ASP:OD1	3:E:219:ASP:N	2.53	0.41
1:A:981:GLN:HB3	3:E:743:ASN:ND2	2.29	0.41
1:A:1219:LEU:HD23	1:A:1219:LEU:HA	1.86	0.41
2:D:495:GLU:CD	2:D:518:ARG:HH21	2.28	0.41
2:D:790:ILE:HG22	2:D:794:LYS:HE2	2.01	0.41
3:E:254:THR:HG23	3:E:255:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:827:ALA:O	3:E:831:LYS:HG2	2.20	0.41
2:D:168:VAL:HG13	2:D:182:CYS:HA	2.02	0.41
2:D:418:GLY:HA3	2:D:429:TRP:CE2	2.56	0.41
2:D:758:TRP:O	2:D:761:MET:HB2	2.21	0.41
2:D:917:TRP:NE1	2:D:921:LEU:HD11	2.36	0.41
3:E:102:SER:OG	3:E:120:THR:HG21	2.21	0.41
3:E:125:LEU:HB3	3:E:138:THR:OG1	2.20	0.41
3:E:191:TRP:HB3	3:E:203:GLN:HE21	1.85	0.41
3:E:632:VAL:HG11	3:E:646:THR:HG22	2.03	0.41
1:A:733:ALA:HB1	1:A:757:LYS:NZ	2.35	0.41
3:E:288:ASN:HD21	3:E:336:GLY:HA3	1.85	0.41
3:E:401:LEU:HD11	3:E:408:LEU:HD11	2.02	0.41
3:E:457:VAL:HB	3:E:464:ILE:HG22	2.02	0.41
3:E:612:LEU:HD11	3:E:677:ARG:HE	1.85	0.41
3:E:959:TRP:CZ3	3:E:989:VAL:HG11	2.56	0.41
3:E:1022:LYS:HE2	3:E:1022:LYS:HB3	1.74	0.41
3:E:1061:ALA:HB1	3:E:1077:TYR:CE1	2.49	0.41
1:A:1101:LYS:HD2	1:A:1178:ILE:HG12	2.03	0.41
1:A:1157:GLN:OE1	1:A:1164:ILE:N	2.52	0.41
1:A:1232:CYS:HB3	1:A:1235:CYS:HB3	2.03	0.41
2:D:65:HIS:HB3	2:D:68:GLN:O	2.20	0.41
2:D:142:HIS:CE1	2:D:190:SER:HA	2.56	0.41
2:D:188:ILE:HA	2:D:204:THR:HG22	2.03	0.41
2:D:236:LYS:HD3	2:D:252:HIS:HB2	2.03	0.41
2:D:418:GLY:HA3	2:D:429:TRP:CZ2	2.56	0.41
2:D:615:ILE:HD12	2:D:653:ASN:O	2.21	0.41
2:D:934:TYR:HB3	2:D:943:MET:SD	2.61	0.41
2:D:981:GLN:HG3	2:D:984:GLU:HB2	2.02	0.41
3:E:30:TYR:HB3	3:E:42:VAL:HG21	2.02	0.41
3:E:422:LEU:HD12	3:E:431:LYS:HE3	2.03	0.41
3:E:480:PRO:O	3:E:481:GLN:HB2	2.21	0.41
3:E:877:ILE:O	3:E:881:ILE:HG12	2.21	0.41
3:E:936:TYR:O	3:E:940:LYS:HG2	2.21	0.41
3:E:1020:PHE:HE2	3:E:1046:ARG:NH2	2.15	0.41
2:D:96:GLY:HA2	2:D:125:TRP:HH2	1.86	0.41
2:D:173:ASP:OD1	2:D:173:ASP:N	2.54	0.41
2:D:311:ALA:HB3	2:D:319:ILE:HG23	2.02	0.41
2:D:973:ALA:O	2:D:977:GLU:HG2	2.20	0.41
2:D:997:GLN:HE22	2:D:1000:ARG:HH21	1.68	0.41
2:D:1036:LYS:O	2:D:1040:VAL:HG23	2.21	0.41
2:D:1037:GLN:O	2:D:1041:GLU:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:208:ALA:HB3	3:E:216:LEU:HB3	2.03	0.41
3:E:332:TRP:CD1	3:E:339:LEU:HD13	2.56	0.41
3:E:911:TYR:HB3	3:E:920:ALA:HB2	2.03	0.41
1:A:828:GLU:HA	1:A:831:THR:HG22	2.03	0.40
1:A:1000:LYS:HE2	1:A:1035:SER:HA	2.02	0.40
1:A:1178:ILE:O	1:A:1181:VAL:HG22	2.22	0.40
2:D:254:ASN:ND2	2:D:294:ASN:HA	2.36	0.40
2:D:564:GLN:H	2:D:564:GLN:HG3	1.75	0.40
2:D:876:LEU:HA	2:D:879:GLU:CD	2.47	0.40
2:D:988:TYR:HA	2:D:991:LYS:HE2	2.02	0.40
3:E:42:VAL:HG13	3:E:50:LEU:HB2	2.02	0.40
3:E:1030:ASP:OD1	3:E:1030:ASP:N	2.53	0.40
1:A:801:GLN:HG2	1:A:802:TYR:N	2.37	0.40
1:A:950:LEU:HD22	2:D:945:ARG:NH2	2.36	0.40
2:D:239:SER:HB2	2:D:249:THR:HG22	2.03	0.40
2:D:1044:LYS:HD2	2:D:1068:ILE:HD11	2.03	0.40
3:E:1021:GLN:HA	3:E:1024:GLN:OE1	2.22	0.40
3:E:1106:LEU:O	3:E:1110:LEU:HG	2.21	0.40
1:A:866:LYS:HG3	1:A:1251:PHE:CE1	2.56	0.40
2:D:1002:ALA:O	2:D:1006:GLY:N	2.53	0.40
2:D:1029:TYR:O	2:D:1033:LYS:HG2	2.21	0.40
3:E:158:ILE:HG22	3:E:191:TRP:CH2	2.57	0.40
3:E:540:VAL:HG13	3:E:552:PHE:HB3	2.03	0.40
3:E:746:ASN:HD21	3:E:768:LYS:HB3	1.85	0.40
1:A:1013:LYS:HD3	1:A:1013:LYS:HA	1.89	0.40
2:D:492:SER:OG	2:D:495:GLU:OE1	2.28	0.40
3:E:150:ASP:O	3:E:157:LEU:HD12	2.22	0.40
3:E:422:LEU:HD22	3:E:427:ASN:O	2.21	0.40
2:D:478:VAL:HG12	2:D:487:GLN:HG3	2.04	0.40
2:D:982:ILE:HG13	2:D:983:PRO:HD3	2.03	0.40
3:E:451:ASN:CG	3:E:452:GLU:H	2.22	0.40
3:E:675:HIS:NE2	3:E:694:ALA:HA	2.37	0.40
3:E:824:TYR:CZ	3:E:851:GLY:HA3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	530/1251 (42%)	500 (94%)	28 (5%)	2 (0%)	30	66
2	D	1082/1407 (77%)	1045 (97%)	34 (3%)	3 (0%)	36	71
3	E	1127/1387 (81%)	1063 (94%)	64 (6%)	0	100	100
All	All	2739/4045 (68%)	2608 (95%)	126 (5%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	753	GLN
2	D	184	VAL
1	A	1105	GLN
1	A	753	GLU
2	D	722	ILE

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	479/1117 (43%)	479 (100%)	0	100	100
2	D	975/1259 (77%)	975 (100%)	0	100	100
3	E	999/1232 (81%)	999 (100%)	0	100	100
All	All	2453/3608 (68%)	2453 (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 (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	927	GLN
1	A	1049	ASN
1	A	1069	ASN
1	A	1126	GLN
1	A	1209	ASN
2	D	63	GLN
2	D	121	ASN
2	D	238	GLN
2	D	281	GLN
2	D	424	GLN
2	D	515	ASN
2	D	545	GLN
2	D	665	ASN
2	D	754	ASN
2	D	780	ASN
2	D	849	HIS
2	D	873	GLN
2	D	897	GLN
2	D	964	ASN
2	D	981	GLN
2	D	1021	GLN
2	D	1071	GLN
3	E	15	ASN
3	E	113	HIS
3	E	273	GLN
3	E	337	GLN
3	E	556	GLN
3	E	586	GLN
3	E	673	GLN
3	E	681	GLN
3	E	686	HIS
3	E	743	ASN
3	E	863	GLN
3	E	887	ASN
3	E	899	GLN
3	E	1000	GLN
3	E	1027	ASN

5.3.3 RNA ⓘ

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 2 ligands modelled in this entry, 2 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.

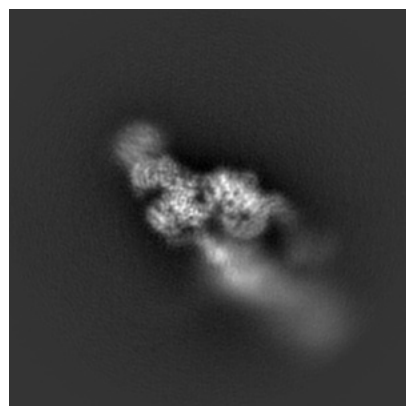
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34897. These allow visual inspection of the internal detail of the map and identification of artifacts.

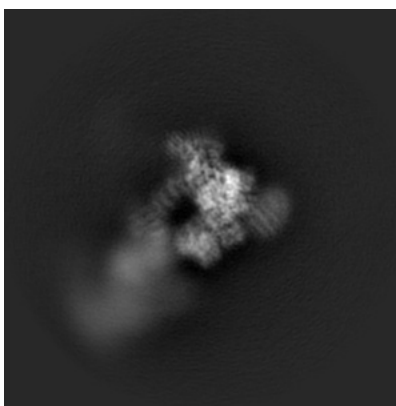
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

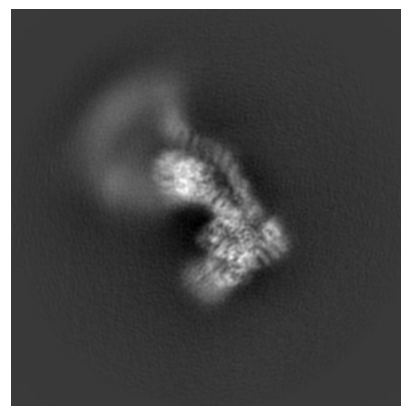
6.1.1 Primary map



X

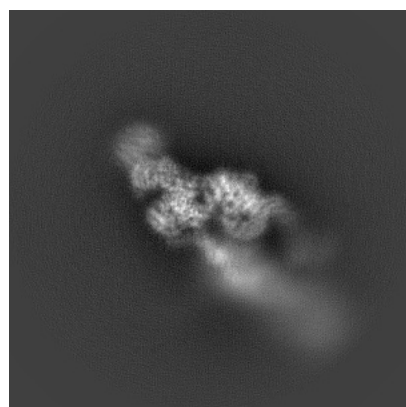


Y

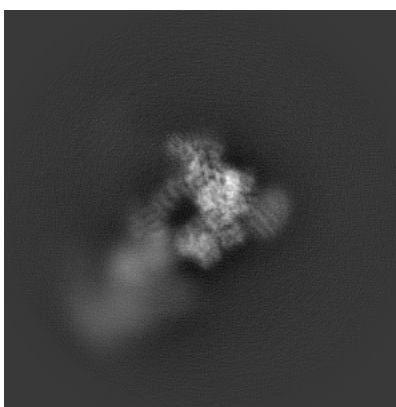


Z

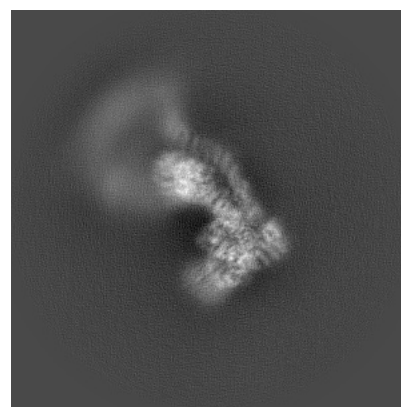
6.1.2 Raw map



X



Y

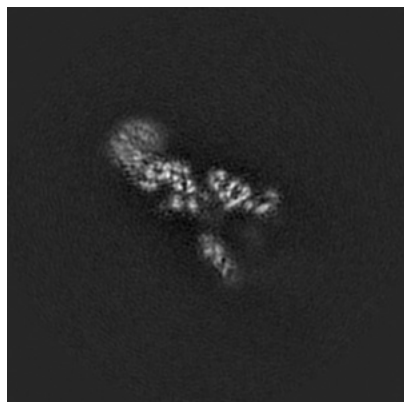


Z

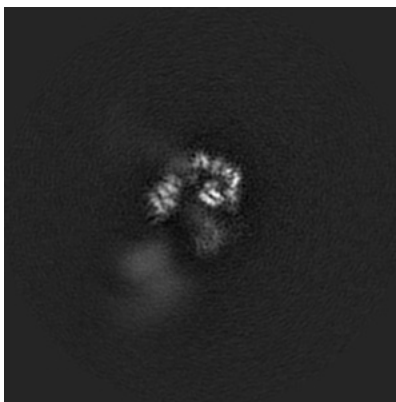
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

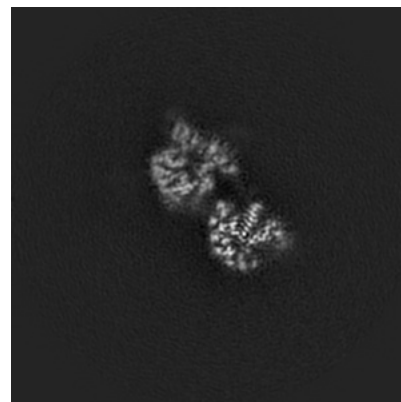
6.2.1 Primary map



X Index: 192

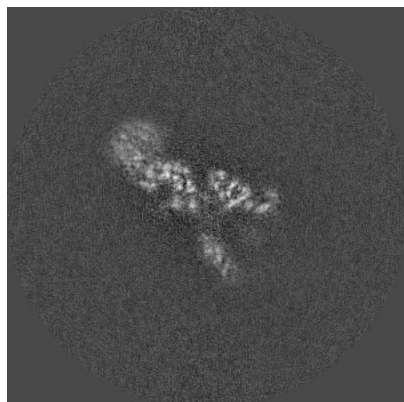


Y Index: 192

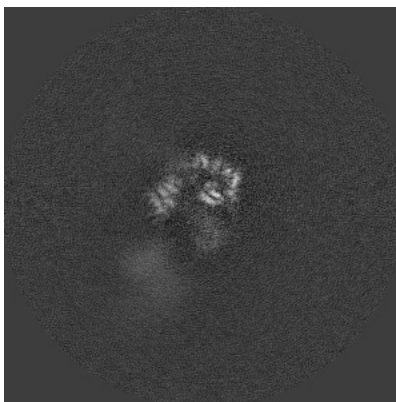


Z Index: 192

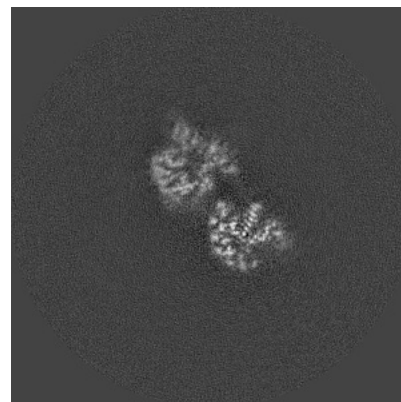
6.2.2 Raw map



X Index: 192



Y Index: 192

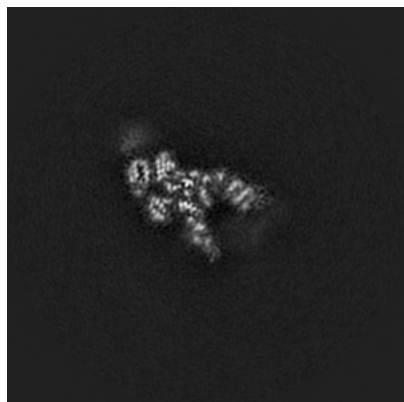


Z Index: 192

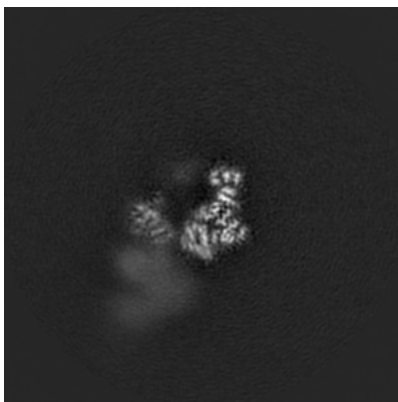
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

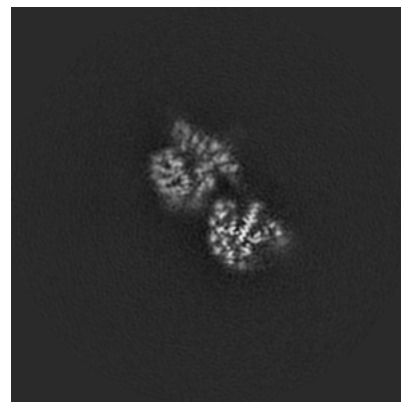
6.3.1 Primary map



X Index: 212

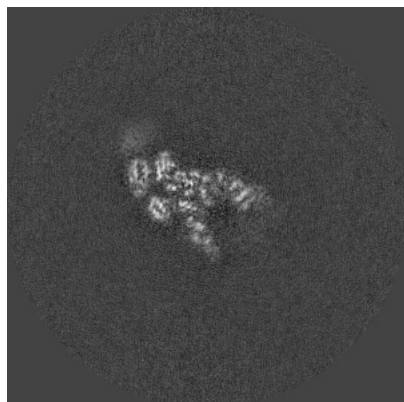


Y Index: 209

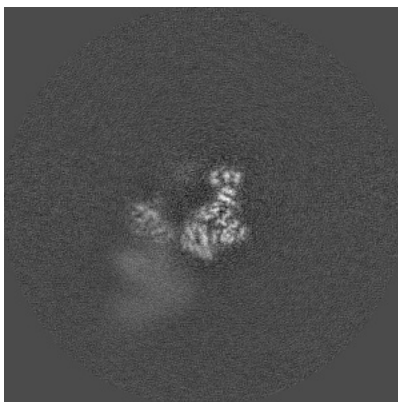


Z Index: 194

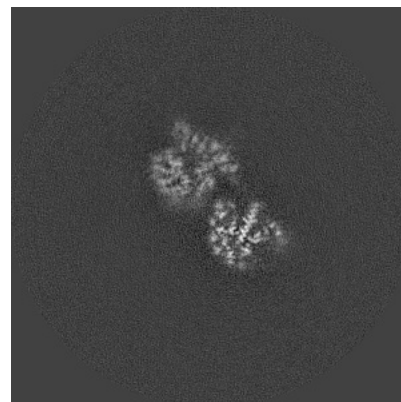
6.3.2 Raw map



X Index: 211



Y Index: 209

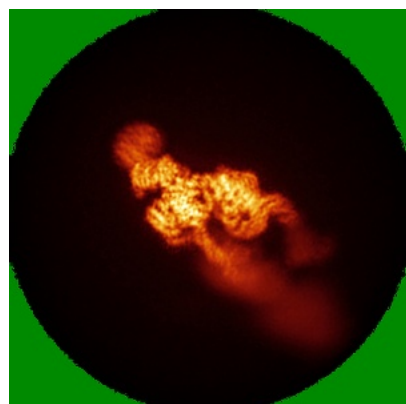


Z Index: 194

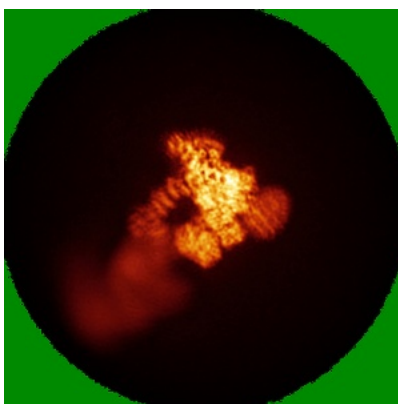
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

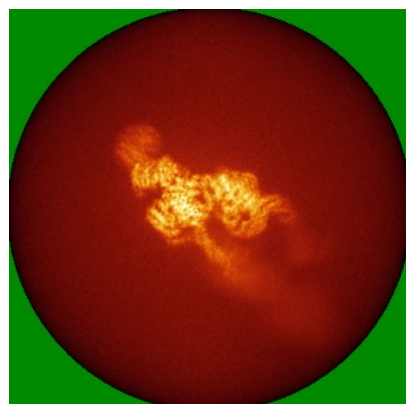


Y

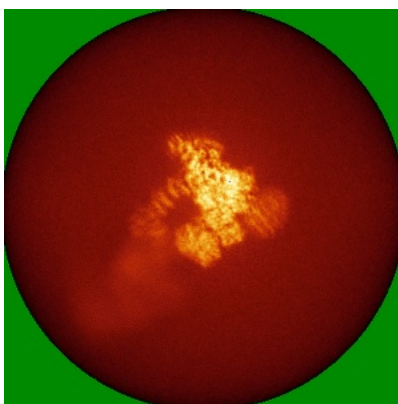


Z

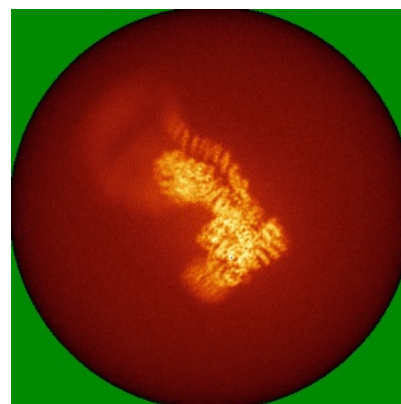
6.4.2 Raw map



X



Y

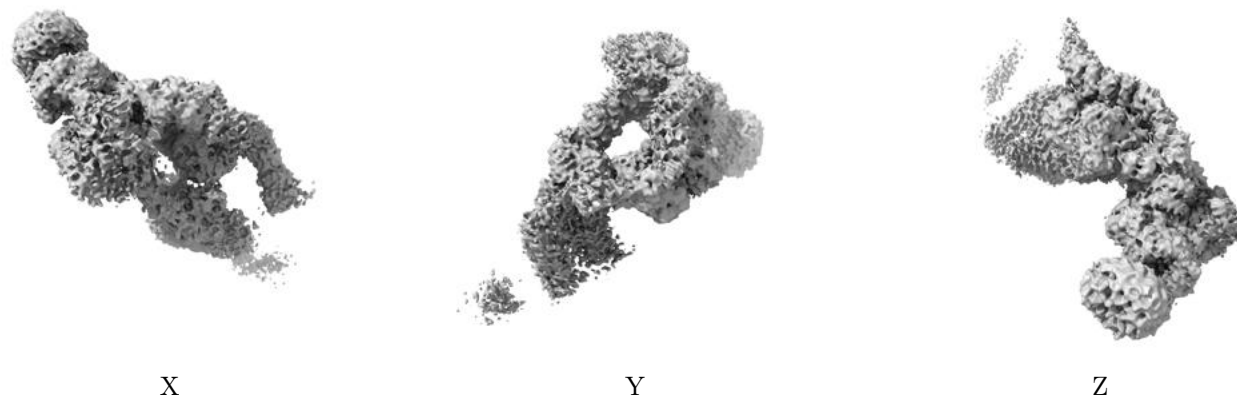


Z

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.

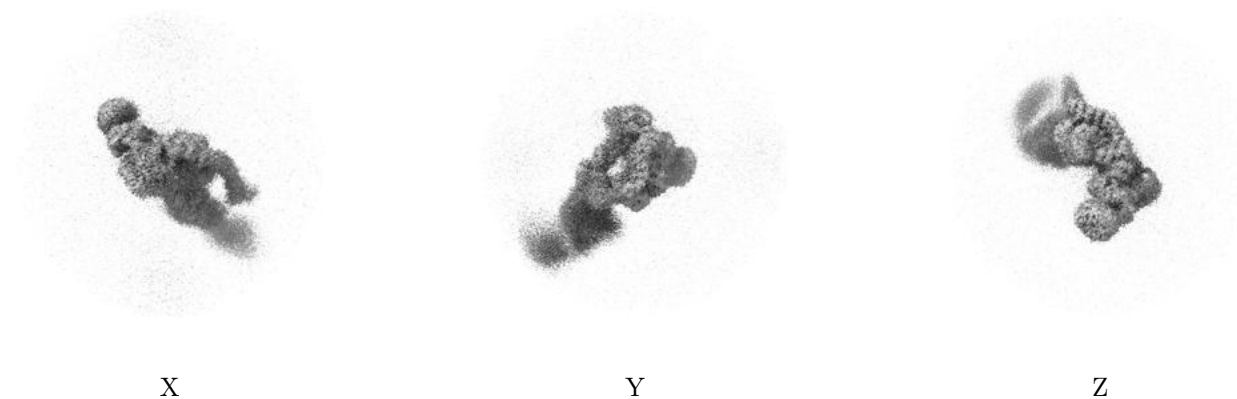
6.5 Orthogonal surface views [i](#)

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.

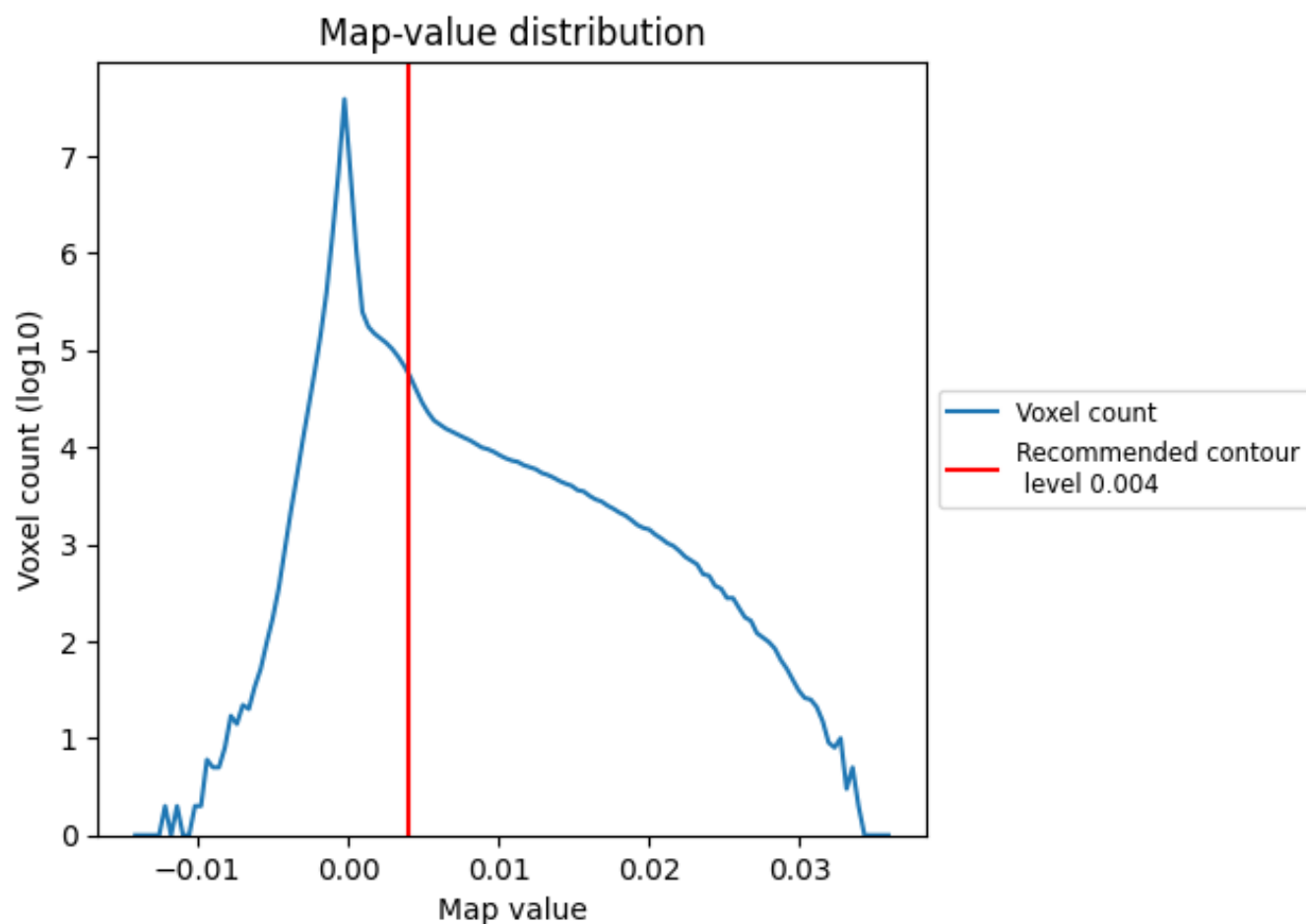
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

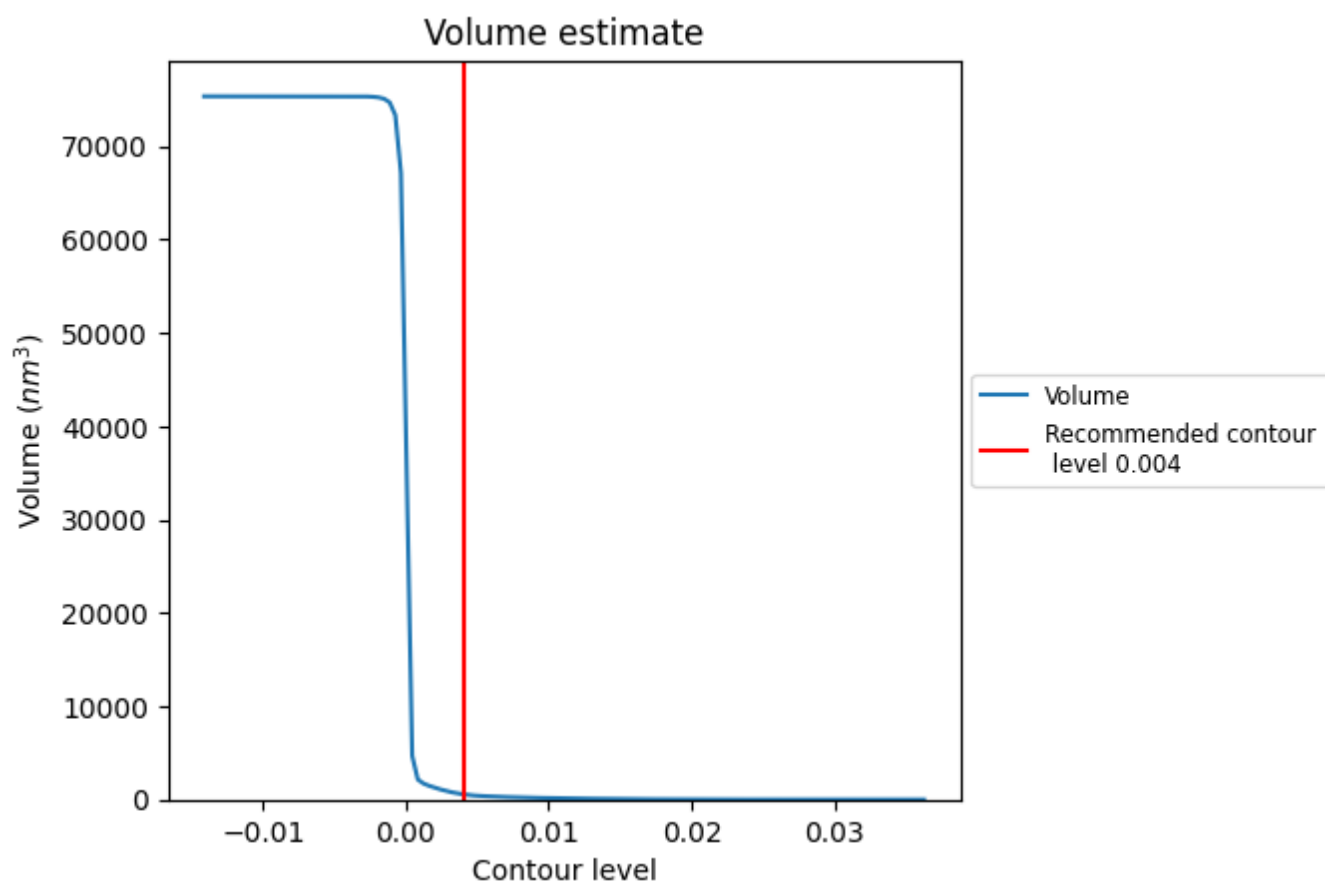
This section contains the results of statistical analysis of the map.

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.

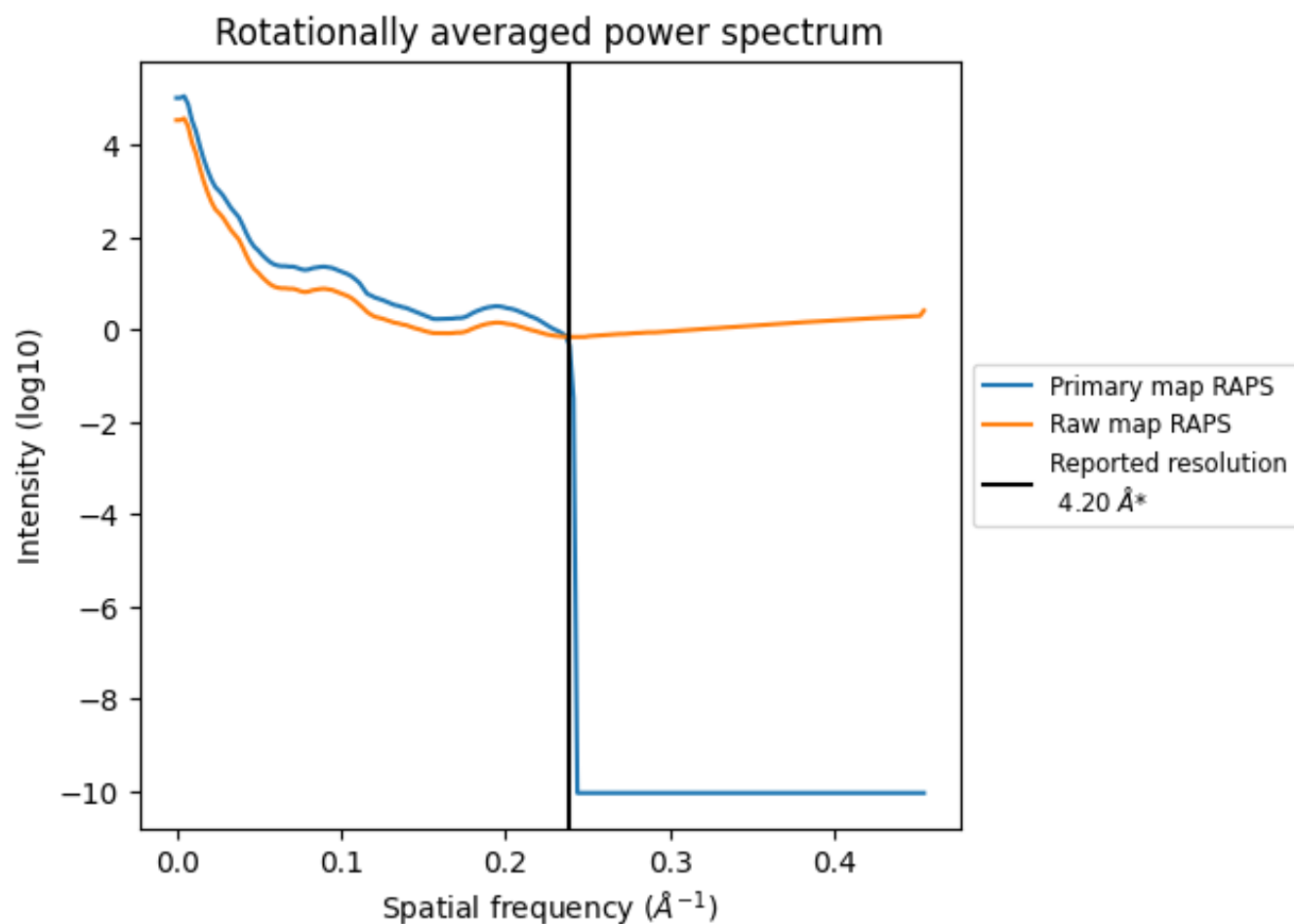
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 566 nm^3 ; this corresponds to an approximate mass of 511 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 ⓘ

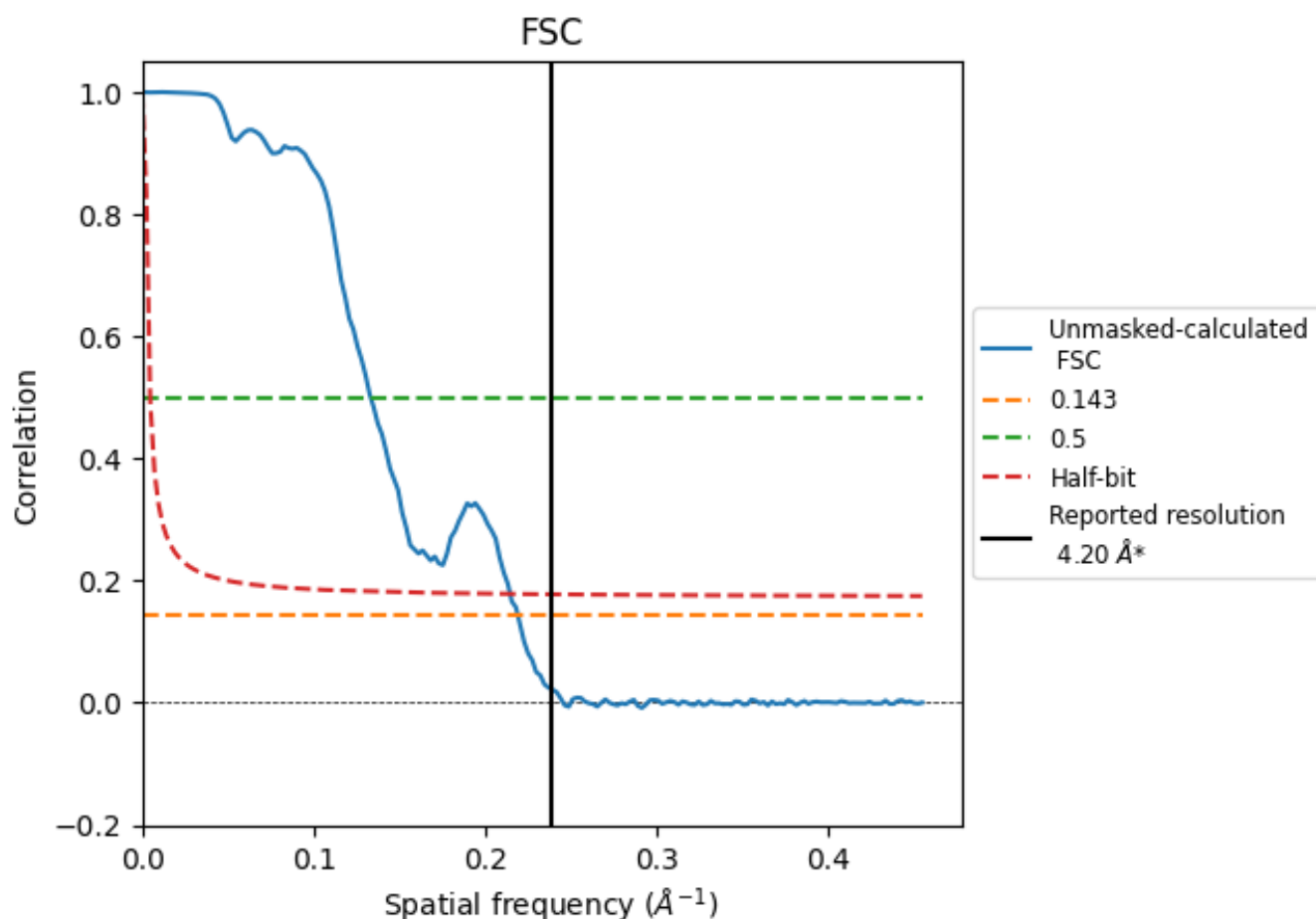


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.238 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

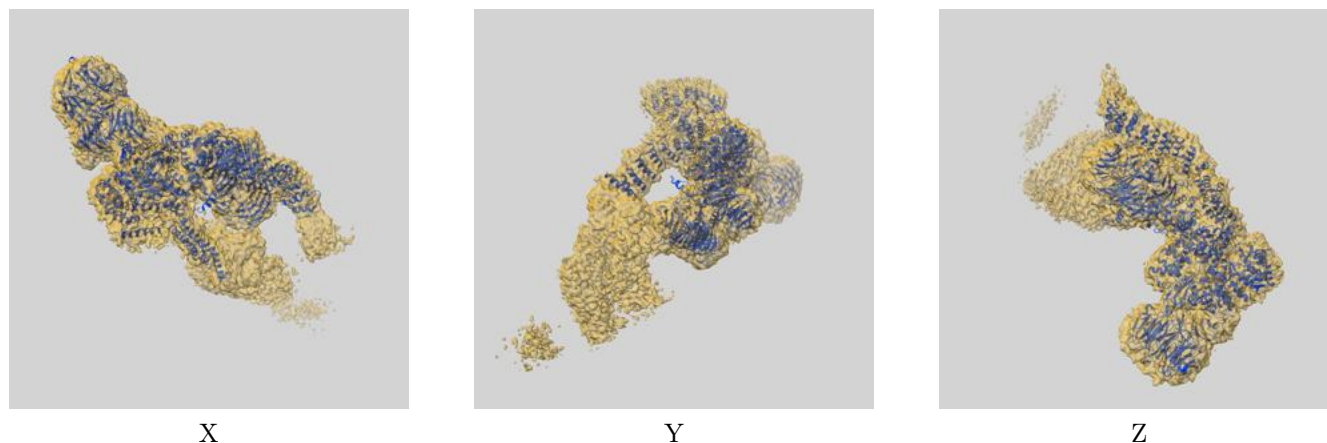
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.57	7.51	4.66

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

9 Map-model fit [i](#)

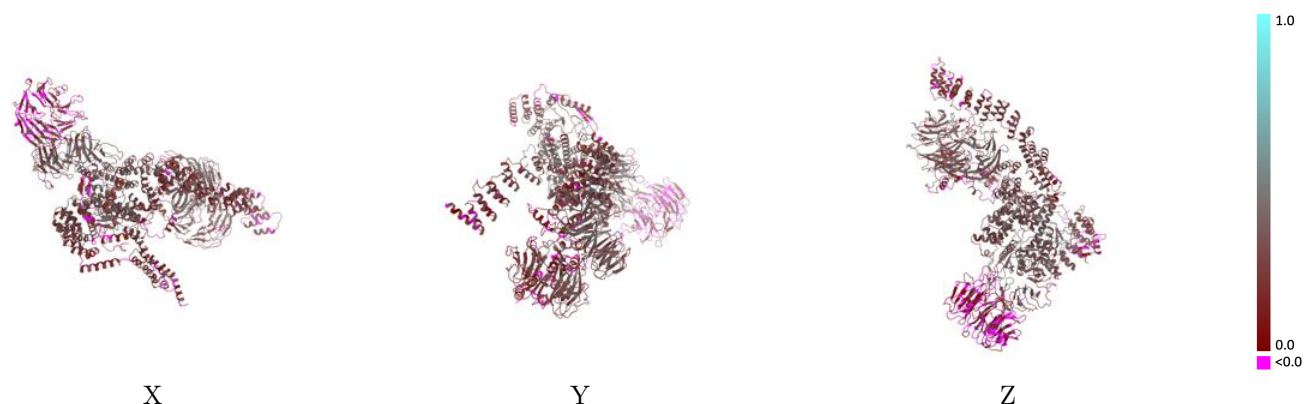
This section contains information regarding the fit between EMDB map EMD-34897 and PDB model 8HME. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



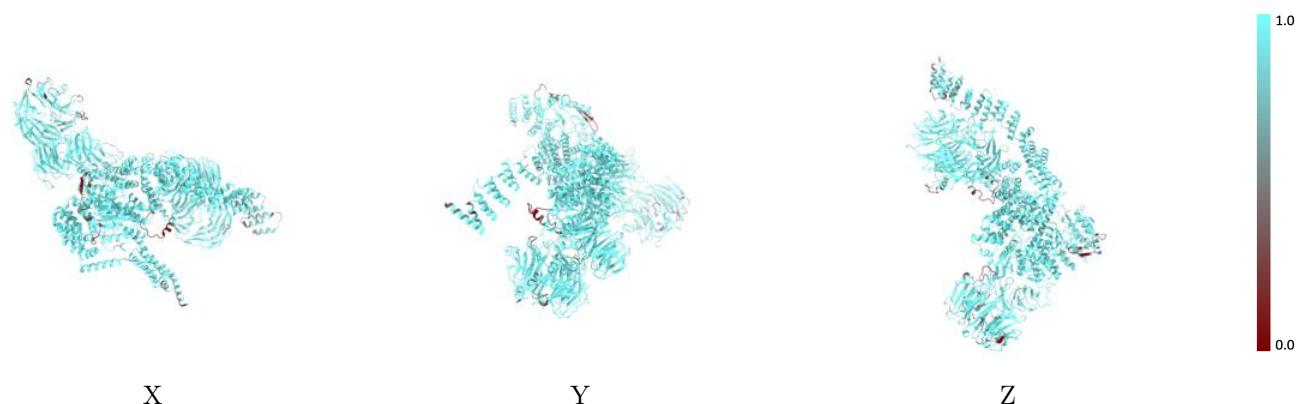
The images above show the 3D surface view of the map at the recommended contour level 0.004 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



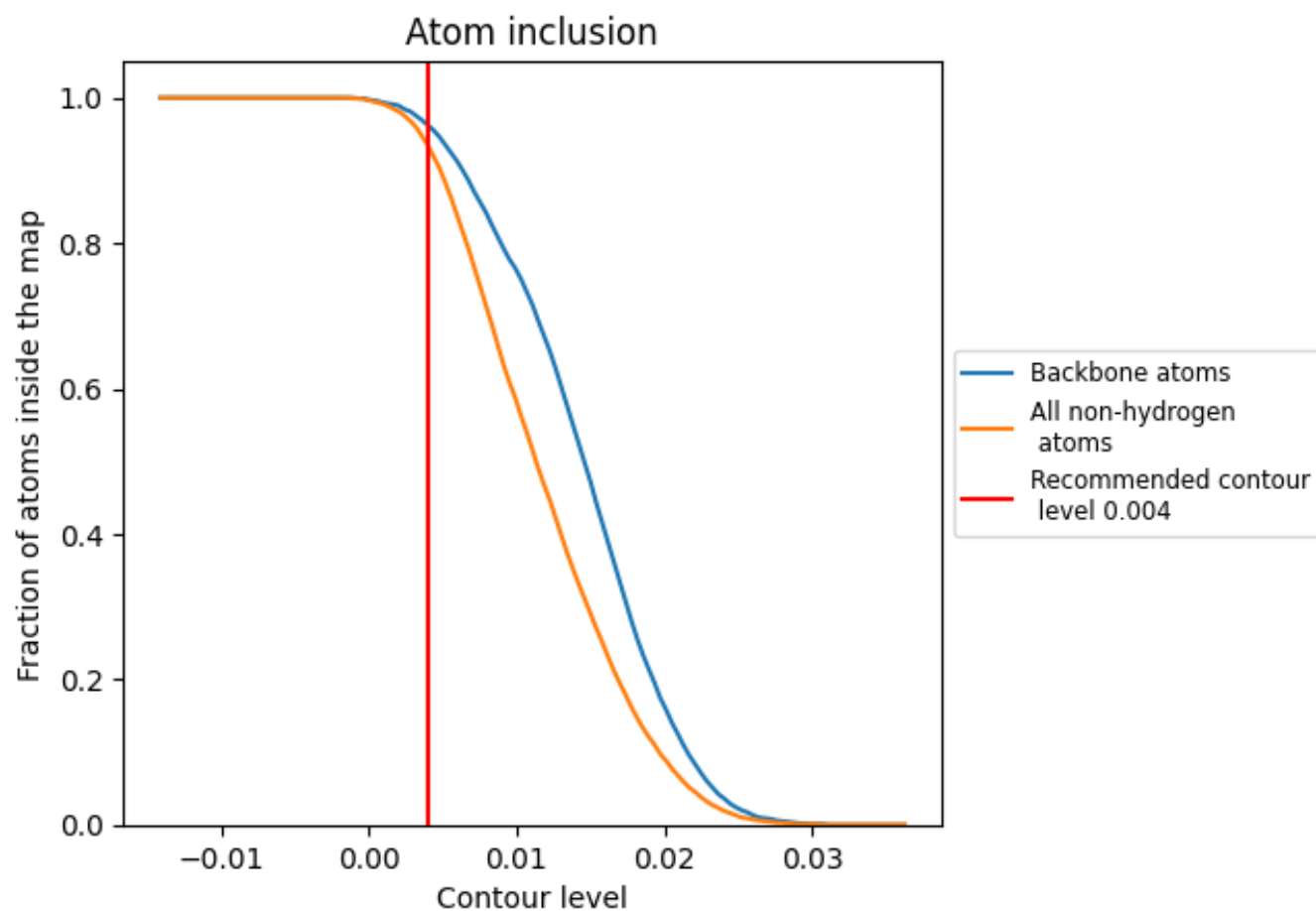
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 96% of all backbone atoms, 93% 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	0.9340	0.2470
A	0.9290	0.2780
D	0.9510	0.2810
E	0.9210	0.2000

