



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 05:16 PM UTC

PDB ID : 8EAS / pdb\_00008eas  
EMDB ID : EMD-27984  
Title : Yeast VO in complex with Vma12-22p  
Authors : Wang, H.; Bueler, S.A.; Rubinstein, J.L.  
Deposited on : 2022-08-29  
Resolution : 2.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

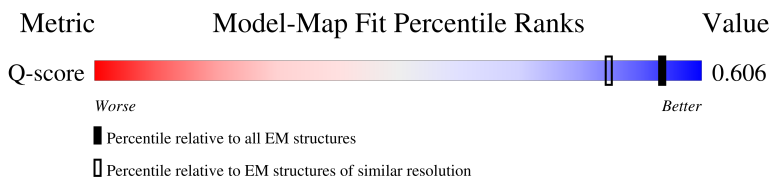
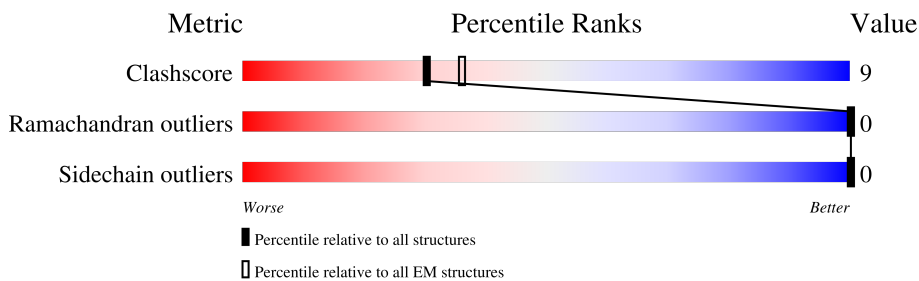
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : 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 2.60 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	8728 ( 2.10 - 3.10 )

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

Mol	Chain	Length	Quality of chain
1	A	181	
2	B	147	
3	F	118	
4	a	840	

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Mol	Chain	Length	Quality of chain
5	b	265	 15% 81%
6	c	213	 73% 20% 7%
7	d	345	 76% 22%
8	e	73	 74% 22%
9	f	85	 74% 8% 18%
10	g	160	 71% 28%
10	h	160	 78% 21%
10	i	160	 74% 25%
10	j	160	 84% 16%
10	k	160	 81% 18%
10	l	160	 78% 21%
10	m	160	 81% 18%
10	n	160	 76% 23%
11	o	164	 67% 29%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 24802 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 Vacuolar ATPase assembly protein VMA22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	130	1044	666	168	207	3	0	0

- Molecule 2 is a protein called V-type proton ATPase assembly factor Vma12p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	139	995	640	175	177	3	0	0

- Molecule 3 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	F	115	919	581	157	181	0	0

- Molecule 4 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	a	742	5948	3881	973	1059	35	0	0

- Molecule 5 is a protein called V0 assembly protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	b	50	385	254	55	74	2	0	0

- Molecule 6 is a protein called V-type proton ATPase subunit c”.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	c	198	1473	980	228	258	7	0	0

- Molecule 7 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	d	338	2740	1742	445	540	13	0	0

- Molecule 8 is a protein called V-type proton ATPase subunit e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	e	70	565	378	92	89	6	0	0

- Molecule 9 is a protein called Yeast V-ATPase subunit f.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	f	70	506	332	81	90	3	0	0

- Molecule 10 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	g	158	1132	746	181	198	7	0	0
10	h	159	1139	749	182	200	8	0	0
10	i	159	1139	749	182	200	8	0	0
10	j	159	1136	746	182	200	8	0	0
10	k	159	1136	748	182	198	8	0	0
10	l	158	1129	745	181	196	7	0	0
10	m	159	1137	748	182	199	8	0	0
10	n	159	1139	749	182	200	8	0	0

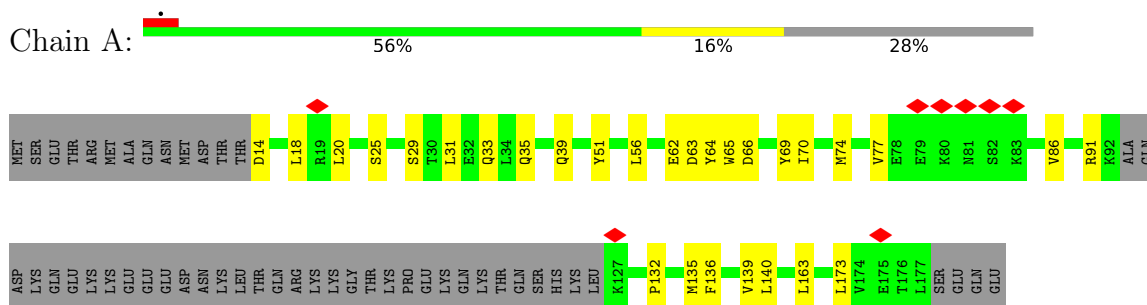
- Molecule 11 is a protein called V-type proton ATPase subunit c'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	o	158	1140	752	177	199	12	0	0

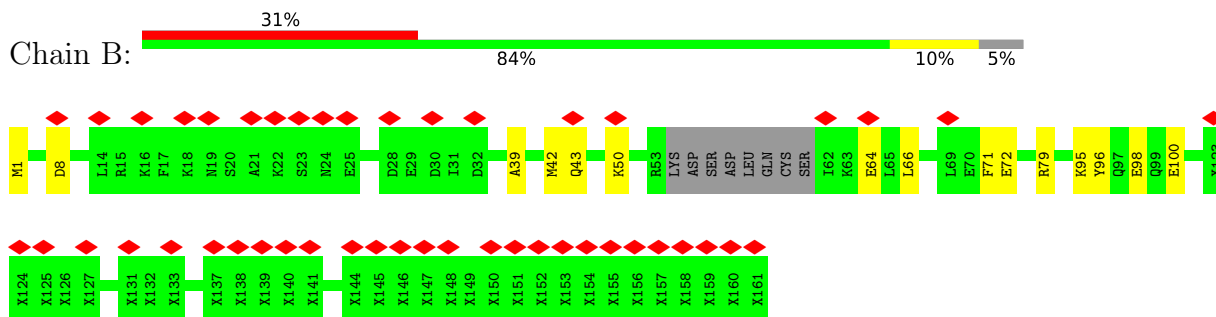
### 3 Residue-property plots [i](#)

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.

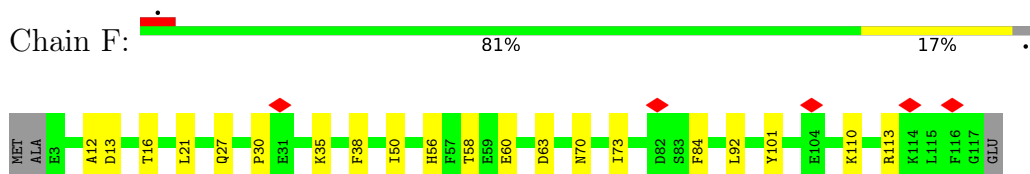
- Molecule 1: Vacuolar ATPase assembly protein VMA22



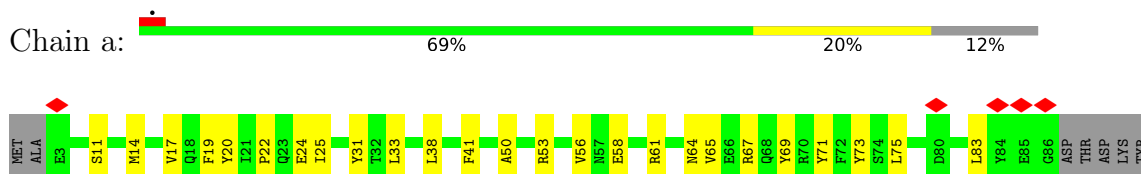
- Molecule 2: V-type proton ATPase assembly factor Vma12p




- Molecule 3: V-type proton ATPase subunit F



- Molecule 4: V-type proton ATPase subunit a, vacuolar isoform





Chain d:  76% 22%



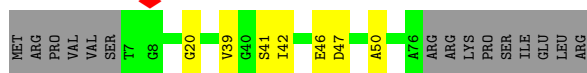
- Molecule 8: V-type proton ATPase subunit e

Chain e:  74% 22%



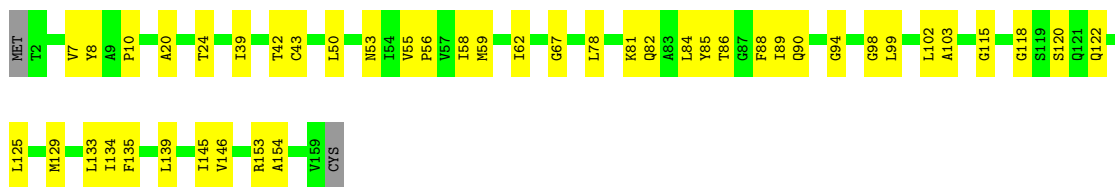
- Molecule 9: Yeast V-ATPase subunit f

Chain f:  74% 8% 18%




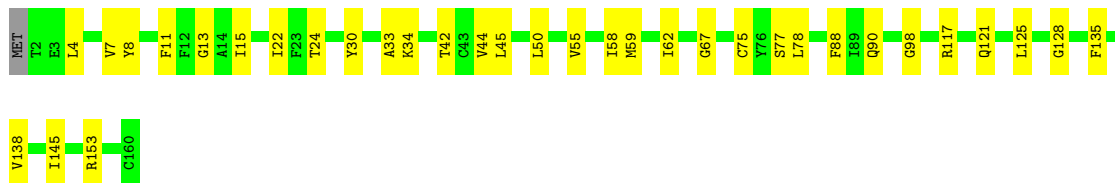
- Molecule 10: V-type proton ATPase subunit c

Chain g:  71% 28%



- Molecule 10: V-type proton ATPase subunit c

Chain h:  78% 21%

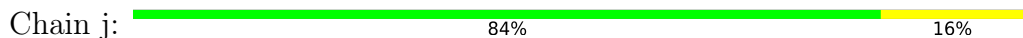


- Molecule 10: V-type proton ATPase subunit c

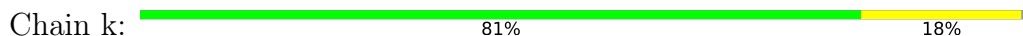
Chain i:  74% 25%



- Molecule 10: V-type proton ATPase subunit c



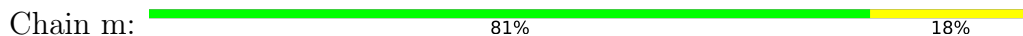
- Molecule 10: V-type proton ATPase subunit c



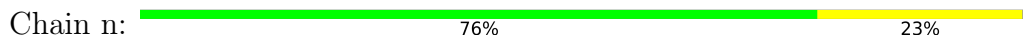
- Molecule 10: V-type proton ATPase subunit c



- Molecule 10: V-type proton ATPase subunit c

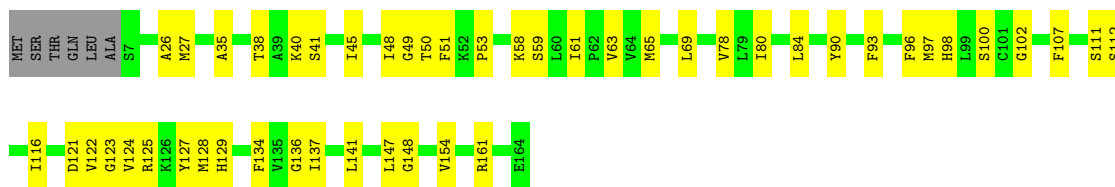


- Molecule 10: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c'

Chain o:  67% 29%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	308537	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	12.719	Depositor
Minimum map value	-6.486	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.311	Depositor
Recommended contour level	1.1	Depositor
Map size (Å)	329.59998, 329.59998, 329.59998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.23	0/1060	0.35	0/1433
2	B	0.14	0/815	0.26	0/1089
3	F	0.17	0/934	0.31	0/1263
4	a	0.20	0/6095	0.33	0/8254
5	b	0.26	0/391	0.35	0/535
6	c	0.30	0/1503	0.41	0/2041
7	d	0.25	0/2797	0.34	0/3793
8	e	0.20	0/582	0.31	0/794
9	f	0.15	0/518	0.26	0/710
10	g	0.31	0/1150	0.42	0/1564
10	h	0.30	0/1157	0.40	0/1572
10	i	0.30	0/1157	0.39	0/1572
10	j	0.26	0/1154	0.35	0/1568
10	k	0.27	0/1154	0.37	0/1568
10	l	0.27	0/1147	0.37	0/1560
10	m	0.28	0/1155	0.39	0/1569
10	n	0.27	0/1157	0.39	0/1572
11	o	0.29	0/1163	0.43	0/1576
All	All	0.25	0/25089	0.36	0/34033

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	1044	0	1019	24	0
2	B	995	0	803	13	0
3	F	919	0	912	14	0
4	a	5948	0	5877	122	0
5	b	385	0	399	8	0
6	c	1473	0	1540	36	0
7	d	2740	0	2631	53	0
8	e	565	0	584	14	0
9	f	506	0	487	6	0
10	g	1132	0	1202	43	0
10	h	1139	0	1207	28	0
10	i	1139	0	1207	33	0
10	j	1136	0	1198	20	0
10	k	1136	0	1205	25	0
10	l	1129	0	1200	29	0
10	m	1137	0	1202	24	0
10	n	1139	0	1207	32	0
11	o	1140	0	1180	43	0
All	All	24802	0	25060	451	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 (451) 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)
10:g:115:GLY:HA3	10:g:129:MET:HG3	1.49	0.95
10:i:59:MET:HE2	10:i:137:GLU:HG3	1.49	0.91
11:o:65:MET:HE1	11:o:141:LEU:HB3	1.59	0.83
10:g:78:LEU:O	10:h:153:ARG:NH2	2.14	0.80
4:a:788:MET:HE2	10:h:138:VAL:HG11	1.63	0.79
6:c:169:THR:HG22	7:d:303:GLN:HG2	1.64	0.78
11:o:61:ILE:HG22	11:o:65:MET:HE2	1.64	0.78
7:d:18:ARG:NH2	7:d:300:PHE:O	2.17	0.78
10:h:55:VAL:HG12	10:h:59:MET:HE2	1.64	0.78
6:c:77:TRP:CD1	6:c:161:ILE:HG12	2.20	0.76
5:b:254:LEU:O	10:h:121:GLN:NE2	2.18	0.76
7:d:105:ASP:OD1	7:d:185:TYR:OH	2.04	0.74
1:A:25:SER:OG	2:B:43:GLN:OE1	2.05	0.73
10:g:42:THR:HG23	10:g:120:SER:HB2	1.70	0.73
4:a:795:LEU:HD11	10:g:55:VAL:HG13	1.69	0.72
3:F:13:ASP:OD1	3:F:70:ASN:ND2	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:n:24:THR:HG23	10:n:98:GLY:HA2	1.72	0.72
8:e:40:THR:HG22	8:e:44:MET:HE2	1.72	0.72
4:a:150:GLU:O	4:a:214:LYS:NZ	2.24	0.71
4:a:422:MET:HG2	4:a:736:LEU:HA	1.72	0.70
6:c:132:ASN:O	6:c:138:ASN:ND2	2.25	0.69
6:c:87:ILE:HG21	10:g:115:GLY:HA2	1.75	0.69
10:i:78:LEU:O	10:j:153:ARG:NH2	2.23	0.69
4:a:391:GLN:OE1	4:a:406:ASN:ND2	2.26	0.68
10:m:24:THR:HG23	10:m:98:GLY:HA2	1.74	0.68
6:c:72:VAL:HG13	10:g:139:LEU:HB3	1.75	0.68
10:g:7:VAL:HG12	10:h:4:LEU:HD23	1.75	0.68
10:k:75:CYS:O	10:l:153:ARG:NH1	2.27	0.67
4:a:419:PHE:CE1	4:a:432:MET:HE1	2.29	0.66
10:l:34:LYS:HG2	10:l:113:ASP:HB2	1.76	0.66
10:h:77:SER:OG	10:h:90:GLN:NE2	2.25	0.65
4:a:501:LYS:HG3	4:a:504:GLU:HB2	1.80	0.64
8:e:68:ARG:NH1	9:f:46:GLU:OE1	2.30	0.64
11:o:45:ILE:HD12	11:o:59:SER:HB2	1.78	0.64
1:A:56:LEU:HD13	7:d:109:LEU:HA	1.79	0.64
11:o:90:TYR:OH	11:o:98:HIS:ND1	2.27	0.63
6:c:74:GLY:HA3	6:c:157:LEU:HA	1.80	0.63
10:j:22:ILE:HG12	10:k:99:LEU:HB2	1.80	0.63
10:g:50:LEU:HD11	10:h:128:GLY:HA3	1.80	0.63
10:m:75:CYS:O	10:n:153:ARG:NH1	2.31	0.63
7:d:32:ASN:HB3	7:d:45:GLN:HE21	1.63	0.63
4:a:73:TYR:HB2	4:a:827:MET:HE3	1.81	0.62
4:a:17:VAL:HG12	4:a:370:VAL:HG22	1.81	0.62
6:c:177:ASP:HB3	6:c:180:LEU:HD12	1.82	0.62
7:d:248:LEU:HD23	7:d:256:LEU:HD11	1.82	0.62
10:i:22:ILE:HG12	10:j:99:LEU:HB2	1.82	0.62
4:a:67:ARG:NH2	4:a:118:GLU:OE2	2.32	0.62
4:a:525:THR:HG21	8:e:62:PRO:HB3	1.82	0.62
10:h:22:ILE:HG12	10:i:99:LEU:HB2	1.82	0.61
10:k:156:GLN:NE2	10:k:157:ASP:OD1	2.33	0.61
4:a:754:THR:OG1	4:a:755:ILE:N	2.34	0.61
10:j:24:THR:HG23	10:j:98:GLY:HA2	1.82	0.61
1:A:74:MET:HE2	1:A:91:ARG:HB2	1.81	0.61
4:a:64:ASN:OD1	4:a:67:ARG:NH1	2.33	0.61
10:k:59:MET:HE2	10:k:137:GLU:HG3	1.83	0.61
4:a:451:ARG:NH1	4:a:456:ASP:OD1	2.31	0.60
11:o:40:LYS:HE2	11:o:121:ASP:OD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:193:ARG:NH2	4:a:218:ILE:O	2.33	0.60
10:n:78:LEU:O	11:o:161:ARG:NH2	2.32	0.60
1:A:35:GLN:O	1:A:39:GLN:HG3	2.02	0.60
4:a:556:LEU:HD12	4:a:572:PHE:CE2	2.37	0.60
10:i:56:PRO:HG3	10:i:133:LEU:HD11	1.83	0.60
1:A:66:ASP:H	1:A:135:MET:HE3	1.67	0.59
6:c:108:GLU:HG3	10:g:135:PHE:CD1	2.37	0.59
10:n:21:ILE:HD11	11:o:154:VAL:HG21	1.83	0.59
11:o:41:SER:O	11:o:45:ILE:HG12	2.02	0.59
7:d:336:GLU:HG2	7:d:337:ARG:HG3	1.85	0.59
10:l:24:THR:HG23	10:l:98:GLY:HA2	1.84	0.58
4:a:24:GLU:HG2	4:a:25:ILE:HG23	1.85	0.58
6:c:172:ILE:HG13	7:d:303:GLN:HE22	1.67	0.58
10:i:24:THR:HG23	10:i:98:GLY:HA2	1.86	0.58
10:m:59:MET:SD	10:m:133:LEU:HB3	2.44	0.58
10:l:22:ILE:HG12	10:m:99:LEU:HB2	1.86	0.58
3:F:38:PHE:HE2	3:F:50:ILE:HG22	1.69	0.58
4:a:73:TYR:OH	4:a:828:GLU:OE2	2.16	0.58
4:a:109:ASP:OD1	4:a:112:ARG:NH2	2.37	0.58
4:a:731:ALA:HB1	10:g:145:ILE:HD11	1.86	0.58
7:d:36:CYS:O	7:d:335:ARG:NH1	2.37	0.57
7:d:149:TYR:HA	7:d:153:LEU:HB2	1.86	0.57
10:n:156:GLN:NE2	10:n:157:ASP:OD1	2.37	0.57
1:A:77:VAL:HG22	1:A:86:VAL:HG22	1.86	0.57
4:a:33:LEU:HD13	4:a:41:PHE:HZ	1.68	0.57
1:A:18:LEU:HD21	2:B:50:LYS:HD3	1.86	0.57
10:i:7:VAL:HG12	10:j:4:LEU:HD23	1.86	0.56
10:k:24:THR:HG23	10:k:98:GLY:HA2	1.86	0.56
6:c:108:GLU:HG3	10:g:135:PHE:HD1	1.71	0.56
4:a:421:ILE:HG21	4:a:736:LEU:HD23	1.88	0.56
7:d:103:MET:HG3	7:d:131:GLY:HA2	1.88	0.55
10:m:78:LEU:O	10:n:153:ARG:NH1	2.39	0.55
4:a:14:MET:HB2	4:a:377:PRO:HB3	1.87	0.55
10:n:49:LEU:O	10:n:53:ASN:ND2	2.40	0.55
11:o:58:LYS:HB2	11:o:128:MET:HE1	1.89	0.55
4:a:24:GLU:OE1	4:a:333:LYS:NZ	2.36	0.55
10:k:55:VAL:O	10:k:59:MET:HG3	2.06	0.55
6:c:201:VAL:HG21	11:o:27:MET:SD	2.47	0.55
10:j:126:PHE:O	10:j:130:ILE:HG12	2.06	0.54
7:d:186:LYS:HG3	7:d:243:PRO:HA	1.89	0.54
10:m:34:LYS:HG2	10:m:113:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:556:LEU:HD12	4:a:572:PHE:CZ	2.42	0.54
6:c:82:THR:HG21	6:c:103:SER:HB2	1.88	0.54
7:d:14:GLU:OE2	7:d:18:ARG:NH1	2.33	0.54
10:l:77:SER:OG	10:l:90:GLN:NE2	2.36	0.54
10:m:126:PHE:CE2	10:m:130:ILE:HD11	2.43	0.54
10:m:22:ILE:HG12	10:n:99:LEU:HB2	1.89	0.54
4:a:19:PHE:HB2	4:a:337:ALA:HB3	1.88	0.54
4:a:419:PHE:HE1	4:a:432:MET:HE1	1.72	0.54
4:a:464:ILE:HG22	4:a:468:MET:HE2	1.89	0.54
10:k:118:GLY:O	10:k:122:GLN:N	2.41	0.54
10:m:43:CYS:HB2	10:n:125:LEU:HD13	1.89	0.54
7:d:67:LEU:HD22	7:d:71:TYR:HE1	1.73	0.53
7:d:194:ASN:O	7:d:198:GLU:HG2	2.08	0.53
10:k:22:ILE:HG12	10:l:99:LEU:HB2	1.89	0.53
7:d:17:VAL:HG21	7:d:309:VAL:HG22	1.90	0.53
10:h:50:LEU:HD11	10:i:128:GLY:HA3	1.89	0.53
3:F:12:ALA:HB1	3:F:16:THR:HB	1.91	0.53
3:F:27:GLN:OE1	3:F:35:LYS:NZ	2.42	0.53
4:a:436:ALA:HB2	4:a:465:ILE:HG22	1.91	0.53
11:o:26:ALA:HB2	11:o:102:GLY:HA2	1.90	0.53
10:h:24:THR:OG1	10:h:67:GLY:HA3	2.08	0.53
10:i:55:VAL:O	10:i:59:MET:HG3	2.09	0.53
10:n:50:LEU:HD21	11:o:136:GLY:HA3	1.91	0.53
4:a:71:TYR:CZ	4:a:75:LEU:HD11	2.44	0.53
4:a:758:ALA:HB2	4:a:773:LEU:HD12	1.90	0.53
4:a:11:SER:O	4:a:403:ARG:NH1	2.36	0.53
4:a:206:VAL:HG23	4:a:207:LEU:HD12	1.91	0.53
7:d:272:VAL:HG21	7:d:275:TYR:HD2	1.74	0.53
10:m:104:ALA:O	10:m:108:ILE:HG12	2.08	0.53
10:k:50:LEU:HD11	10:l:128:GLY:HA3	1.91	0.52
11:o:112:SER:OG	11:o:148:GLY:N	2.42	0.52
4:a:118:GLU:O	4:a:122:ILE:HG13	2.08	0.52
10:g:115:GLY:HA3	10:g:129:MET:CG	2.32	0.52
10:k:59:MET:SD	10:k:133:LEU:HB3	2.50	0.52
1:A:62:GLU:HA	1:A:65:TRP:CD2	2.45	0.52
4:a:131:ILE:HG22	4:a:288:LEU:HD12	1.91	0.52
10:l:55:VAL:O	10:l:59:MET:HG2	2.08	0.52
10:g:118:GLY:O	10:g:122:GLN:N	2.37	0.52
11:o:80:ILE:HG23	11:o:98:HIS:CG	2.44	0.52
4:a:135:LYS:HD2	4:a:285:TYR:HE2	1.73	0.52
10:n:37:VAL:HG22	11:o:122:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:21:LEU:HD21	3:F:27:GLN:HG2	1.92	0.51
6:c:73:VAL:HG22	10:g:103:ALA:HB2	1.91	0.51
10:g:86:THR:HG22	10:g:90:GLN:NE2	2.25	0.51
10:m:24:THR:OG1	10:m:67:GLY:HA3	2.10	0.51
7:d:1:MET:HB3	7:d:4:VAL:HG23	1.91	0.51
10:h:24:THR:HG23	10:h:98:GLY:HA2	1.91	0.51
10:k:66:TYR:CD2	10:k:144:LEU:HD22	2.44	0.51
2:B:64:GLU:HG2	2:B:66:LEU:H	1.75	0.51
1:A:25:SER:HB2	2:B:42:MET:HB3	1.93	0.51
4:a:65:VAL:HG21	4:a:111:VAL:HG22	1.92	0.51
10:n:21:ILE:HG12	10:n:71:SER:OG	2.09	0.51
7:d:91:THR:O	7:d:95:MET:HG3	2.11	0.51
4:a:799:ARG:HH21	10:g:134:ILE:HG23	1.75	0.51
11:o:45:ILE:HD13	11:o:124:VAL:HG11	1.92	0.51
1:A:163:LEU:HD23	3:F:92:LEU:HD11	1.93	0.51
4:a:407:ALA:O	4:a:411:THR:OG1	2.29	0.51
6:c:69:GLY:HA3	10:g:99:LEU:HD23	1.93	0.51
6:c:90:GLY:HA3	10:g:125:LEU:HD21	1.92	0.50
2:B:71:PHE:H	3:F:113:ARG:NH2	2.09	0.50
4:a:583:PHE:CD1	4:a:730:THR:HG21	2.46	0.50
6:c:92:ARG:NH2	7:d:50:ASP:OD2	2.38	0.50
2:B:100:GLU:OE1	4:a:53:ARG:NH2	2.40	0.50
6:c:56:PRO:HD2	6:c:133:MET:HE2	1.91	0.50
7:d:153:LEU:HD13	7:d:162:PHE:CZ	2.46	0.50
7:d:225:LEU:HD11	7:d:279:LEU:HD21	1.92	0.50
7:d:216:ALA:HB1	7:d:243:PRO:HB2	1.94	0.50
7:d:251:LEU:HD22	10:m:121:GLN:NE2	2.26	0.50
10:h:7:VAL:HG12	10:i:4:LEU:HD23	1.93	0.50
10:i:53:ASN:O	10:i:56:PRO:HD2	2.12	0.50
10:n:75:CYS:HA	10:n:78:LEU:HD12	1.94	0.50
5:b:222:GLY:HA2	5:b:225:MET:HE2	1.94	0.50
10:k:75:CYS:HA	10:k:78:LEU:HD12	1.92	0.50
1:A:66:ASP:HA	7:d:116:HIS:HB3	1.94	0.50
11:o:38:THR:HG23	11:o:63:VAL:HG13	1.94	0.50
1:A:66:ASP:H	1:A:135:MET:CE	2.25	0.50
7:d:128:HIS:CE1	7:d:130:LEU:HB2	2.46	0.50
10:j:7:VAL:HG12	10:k:4:LEU:HD23	1.92	0.49
5:b:215:LEU:HD11	6:c:50:PHE:HA	1.94	0.49
11:o:127:TYR:HB3	11:o:137:ILE:HD12	1.93	0.49
4:a:465:ILE:HA	4:a:468:MET:HE3	1.94	0.49
11:o:124:VAL:HA	11:o:127:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:556:LEU:HB2	4:a:572:PHE:CE1	2.48	0.49
10:g:58:ILE:HG12	10:h:135:PHE:CZ	2.47	0.49
10:i:59:MET:HE2	10:i:137:GLU:CG	2.32	0.49
10:k:43:CYS:HB2	10:l:125:LEU:HD13	1.94	0.49
11:o:49:GLY:O	11:o:50:THR:HG22	2.13	0.49
1:A:51:TYR:HA	7:d:289:TYR:OH	2.12	0.49
3:F:56:HIS:HA	3:F:60:GLU:OE1	2.13	0.49
10:g:56:PRO:HG3	10:g:133:LEU:HD11	1.95	0.49
11:o:121:ASP:OD1	11:o:125:ARG:NH2	2.46	0.49
2:B:79:ARG:NH2	7:d:330:ILE:O	2.45	0.49
10:i:39:ILE:HG12	10:i:53:ASN:HB3	1.95	0.49
10:i:59:MET:HB3	10:i:137:GLU:OE2	2.12	0.49
10:l:42:THR:HG21	10:l:117:ARG:HA	1.94	0.49
10:l:8:TYR:HA	10:m:88:PHE:HE2	1.77	0.49
4:a:53:ARG:HB2	4:a:56:VAL:HG22	1.95	0.49
10:j:156:GLN:NE2	10:j:157:ASP:OD1	2.46	0.49
4:a:31:TYR:CE2	4:a:319:ILE:HD13	2.48	0.48
4:a:424:GLY:HA3	4:a:479:TYR:CE2	2.47	0.48
10:n:66:TYR:CD1	10:n:144:LEU:HD22	2.48	0.48
4:a:486:THR:HG21	4:a:523:HIS:HB2	1.95	0.48
4:a:333:LYS:HD2	4:a:333:LYS:O	2.13	0.48
10:k:80:GLN:NE2	10:l:4:LEU:HD13	2.28	0.48
1:A:139:VAL:HG12	1:A:140:LEU:HG	1.95	0.48
4:a:754:THR:HA	4:a:773:LEU:HD22	1.95	0.48
10:i:115:GLY:HA3	10:i:129:MET:HG3	1.94	0.48
10:g:53:ASN:O	10:g:56:PRO:HD2	2.13	0.48
4:a:83:LEU:HD21	4:a:306:LEU:HD23	1.96	0.48
4:a:273:GLN:O	4:a:277:VAL:HG23	2.13	0.48
4:a:799:ARG:NH2	10:g:134:ILE:HG23	2.29	0.48
4:a:480:ASN:O	4:a:486:THR:HG22	2.14	0.47
4:a:428:HIS:CE1	4:a:785:LEU:HD13	2.48	0.47
4:a:795:LEU:HD13	10:g:58:ILE:HB	1.96	0.47
7:d:151:THR:HG22	7:d:152:VAL:HG23	1.96	0.47
10:l:11:PHE:HB2	10:m:88:PHE:CZ	2.49	0.47
11:o:69:LEU:HD11	11:o:116:ILE:HD12	1.96	0.47
4:a:353:LEU:HD12	4:a:368:ILE:HD11	1.95	0.47
7:d:289:TYR:HB3	7:d:342:ILE:HG13	1.96	0.47
4:a:429:GLY:O	4:a:433:THR:OG1	2.31	0.47
10:h:42:THR:HG21	10:h:117:ARG:HA	1.96	0.47
1:A:31:LEU:HD23	1:A:163:LEU:HD21	1.96	0.47
11:o:112:SER:OG	11:o:147:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:144:ILE:HD12	4:a:261:TYR:HD2	1.79	0.47
7:d:34:THR:O	7:d:335:ARG:NH2	2.39	0.47
10:g:10:PRO:HA	10:g:82:GLN:NE2	2.29	0.47
10:k:24:THR:OG1	10:k:67:GLY:HA3	2.14	0.47
10:l:24:THR:OG1	10:l:67:GLY:HA3	2.13	0.47
10:n:22:ILE:HG12	11:o:107:PHE:HB2	1.96	0.47
6:c:117:ILE:HG13	6:c:152:VAL:HG11	1.96	0.47
10:j:24:THR:OG1	10:j:67:GLY:HA3	2.15	0.47
4:a:205:ARG:NH1	7:d:155:ASP:OD2	2.47	0.47
6:c:68:VAL:HG21	10:g:146:VAL:HG21	1.97	0.47
10:h:125:LEU:O	10:h:125:LEU:HD23	2.14	0.47
4:a:540:SER:HB3	4:a:733:TYR:O	2.15	0.47
10:i:24:THR:OG1	10:i:67:GLY:HA3	2.15	0.47
10:i:113:ASP:OD1	10:i:117:ARG:NH1	2.48	0.47
6:c:162:ALA:HB2	11:o:35:ALA:HB1	1.96	0.46
10:g:59:MET:O	10:g:62:ILE:HG22	2.15	0.46
10:h:11:PHE:HB2	10:i:88:PHE:CE2	2.50	0.46
10:l:39:ILE:HG12	10:l:53:ASN:HB3	1.96	0.46
4:a:341:ILE:HD13	4:a:349:LEU:HD22	1.98	0.46
4:a:437:LEU:HA	4:a:440:VAL:HG22	1.98	0.46
10:n:11:PHE:HB2	11:o:96:PHE:CE2	2.51	0.46
8:e:15:SER:O	8:e:19:VAL:HG23	2.16	0.46
4:a:594:TRP:CH2	8:e:50:ILE:HG23	2.51	0.46
2:B:79:ARG:NH1	7:d:37:ASP:OD1	2.48	0.46
4:a:203:LEU:HA	4:a:206:VAL:HG22	1.98	0.46
10:g:24:THR:HG23	10:g:98:GLY:HA2	1.97	0.46
10:m:125:LEU:O	10:m:125:LEU:HD23	2.16	0.46
10:n:49:LEU:HG	10:n:53:ASN:HD21	1.81	0.46
4:a:242:GLY:O	4:a:246:ILE:HG12	2.15	0.46
4:a:379:THR:HG21	4:a:400:ALA:HB3	1.97	0.46
7:d:95:MET:HE2	7:d:95:MET:HB3	1.86	0.46
4:a:776:MET:O	4:a:780:LEU:HG	2.16	0.46
10:i:40:CYS:O	10:i:44:VAL:HG23	2.15	0.46
10:j:39:ILE:HG12	10:j:53:ASN:HB3	1.98	0.46
4:a:141:TYR:CD1	4:a:261:TYR:HB3	2.51	0.46
4:a:264:ASP:HB2	4:a:273:GLN:NE2	2.31	0.46
4:a:783:ALA:O	4:a:787:LEU:HB3	2.16	0.46
10:k:59:MET:HB3	10:k:137:GLU:OE2	2.16	0.46
10:k:10:PRO:HA	10:k:82:GLN:NE2	2.30	0.46
10:g:10:PRO:HA	10:g:82:GLN:HE21	1.80	0.45
11:o:124:VAL:HA	11:o:127:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:367:ILE:HG23	4:a:368:ILE:HG12	1.97	0.45
10:m:33:ALA:HA	10:n:111:VAL:HG23	1.99	0.45
10:n:46:ARG:HG2	10:n:48:ASP:OD1	2.17	0.45
4:a:58:GLU:OE1	4:a:61:ARG:NH1	2.50	0.45
10:g:8:TYR:HA	10:h:88:PHE:HE2	1.81	0.45
4:a:126:ASP:O	4:a:130:GLN:HG3	2.16	0.45
4:a:446:ILE:O	4:a:449:MET:HB3	2.16	0.45
6:c:146:PHE:CZ	6:c:150:ILE:HD11	2.51	0.45
10:n:22:ILE:HG12	11:o:107:PHE:CB	2.46	0.45
10:n:29:ALA:HB2	11:o:111:SER:HB3	1.98	0.45
11:o:48:ILE:HD11	11:o:124:VAL:HG13	1.99	0.45
4:a:53:ARG:HB2	4:a:56:VAL:CG2	2.45	0.45
10:g:20:ALA:HB2	10:g:94:GLY:HA2	1.97	0.45
10:n:10:PRO:HA	10:n:82:GLN:HE21	1.81	0.45
4:a:415:PHE:HA	4:a:801:HIS:CE1	2.52	0.45
10:i:11:PHE:HB2	10:j:88:PHE:CE2	2.52	0.45
10:m:6:PRO:HD2	10:m:84:LEU:HB2	1.99	0.45
10:j:66:TYR:CD1	10:j:144:LEU:HD22	2.51	0.45
1:A:29:SER:O	1:A:33:GLN:HG3	2.17	0.45
4:a:144:ILE:HD12	4:a:261:TYR:CD2	2.52	0.45
6:c:125:LEU:O	10:g:153:ARG:HD3	2.16	0.45
10:m:39:ILE:HG12	10:m:53:ASN:HB3	1.99	0.45
8:e:68:ARG:NH2	9:f:39:VAL:O	2.50	0.45
10:i:155:THR:HG22	10:i:155:THR:O	2.17	0.45
3:F:110:LYS:O	3:F:113:ARG:HB2	2.17	0.44
4:a:75:LEU:HD12	4:a:121:LEU:HD23	1.98	0.44
4:a:754:THR:O	4:a:773:LEU:HD13	2.16	0.44
1:A:20:LEU:HB2	1:A:173:LEU:HD22	1.98	0.44
10:i:126:PHE:O	10:i:130:ILE:HG12	2.17	0.44
10:k:8:TYR:HA	10:l:88:PHE:HE2	1.81	0.44
10:n:14:ALA:HB1	11:o:100:SER:HB2	1.99	0.44
5:b:225:MET:HE1	10:g:84:LEU:HD21	1.98	0.44
7:d:220:SER:OG	7:d:243:PRO:HD2	2.17	0.44
10:h:13:GLY:C	10:h:78:LEU:HD21	2.43	0.44
10:n:126:PHE:CZ	10:n:130:ILE:HD11	2.52	0.44
1:A:139:VAL:O	7:d:229:GLN:NE2	2.50	0.44
10:k:118:GLY:HA3	10:k:125:LEU:HD23	2.00	0.44
11:o:40:LYS:HG3	11:o:121:ASP:HB2	1.99	0.44
11:o:125:ARG:O	11:o:129:HIS:ND1	2.51	0.44
4:a:405:ILE:HD11	4:a:557:ALA:HB3	1.98	0.44
4:a:739:LEU:HD11	10:g:62:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:322:ASN:ND2	7:d:342:ILE:O	2.50	0.44
10:g:39:ILE:HG12	10:g:53:ASN:HB3	2.00	0.44
2:B:96:TYR:CZ	4:a:50:ALA:HB2	2.53	0.44
4:a:574:PRO:HB3	4:a:647:TRP:CG	2.53	0.44
4:a:746:LEU:HD23	10:h:145:ILE:HD11	1.99	0.44
10:l:113:ASP:O	10:l:117:ARG:HG3	2.18	0.44
10:m:50:LEU:HD11	10:n:128:GLY:HA3	1.99	0.44
1:A:64:TYR:CD1	1:A:136:PHE:HA	2.53	0.44
3:F:70:ASN:HB2	3:F:73:ILE:HD12	2.00	0.44
9:f:47:ASP:CB	9:f:50:ALA:HB3	2.48	0.44
10:n:10:PRO:HA	10:n:82:GLN:NE2	2.32	0.44
1:A:139:VAL:HB	7:d:178:GLU:OE1	2.16	0.43
4:a:140:GLN:HB3	4:a:190:VAL:HG21	1.98	0.43
4:a:487:MET:HB3	4:a:489:ILE:HG12	1.99	0.43
7:d:220:SER:HA	7:d:242:LEU:HD22	1.99	0.43
7:d:324:THR:O	7:d:328:GLU:HG2	2.18	0.43
10:g:89:ILE:HG21	10:g:154:ALA:HB2	2.00	0.43
10:n:33:ALA:O	10:n:37:VAL:HG23	2.18	0.43
11:o:48:ILE:HD13	11:o:128:MET:HG3	2.00	0.43
5:b:241:LEU:HA	5:b:244:ILE:HG22	2.00	0.43
10:j:31:GLY:HA2	10:j:109:GLY:CA	2.48	0.43
10:l:13:GLY:HA3	10:l:78:LEU:HD21	1.99	0.43
6:c:19:HIS:HA	6:c:22:TYR:HD2	1.82	0.43
7:d:2:GLU:OE1	11:o:40:LYS:HE3	2.18	0.43
8:e:11:PHE:HB2	8:e:45:PHE:CZ	2.53	0.43
10:i:6:PRO:HD2	10:i:84:LEU:HB2	1.99	0.43
4:a:132:GLU:OE2	4:a:288:LEU:HD11	2.18	0.43
11:o:93:PHE:O	11:o:97:MET:HG2	2.18	0.43
4:a:516:ILE:HG13	8:e:48:TRP:HD1	1.83	0.43
6:c:180:LEU:HD11	11:o:50:THR:H	1.83	0.43
10:g:24:THR:OG1	10:g:67:GLY:HA3	2.19	0.43
10:l:89:ILE:HG23	10:l:150:LEU:HG	2.00	0.43
10:l:22:ILE:HD13	10:m:99:LEU:HD12	2.00	0.43
10:m:31:GLY:HA2	10:m:109:GLY:CA	2.48	0.43
10:k:10:PRO:HA	10:k:82:GLN:HE21	1.83	0.43
10:n:34:LYS:HE3	10:n:34:LYS:HB3	1.92	0.43
4:a:424:GLY:HA3	4:a:479:TYR:CD2	2.54	0.43
4:a:804:GLU:N	4:a:804:GLU:OE1	2.52	0.43
6:c:79:ILE:HD12	10:g:139:LEU:HD11	2.00	0.43
10:i:35:SER:HB3	10:i:56:PRO:HB2	2.01	0.43
4:a:332:ARG:O	4:a:333:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:59:MET:SD	10:j:133:LEU:HB3	2.58	0.42
4:a:135:LYS:HD3	4:a:288:LEU:HD13	2.01	0.42
7:d:144:ASP:OD1	7:d:171:GLU:HG2	2.19	0.42
10:h:75:CYS:HA	10:h:78:LEU:HD12	2.01	0.42
10:l:6:PRO:HD2	10:l:84:LEU:HB2	2.01	0.42
10:l:126:PHE:O	10:l:130:ILE:HG12	2.19	0.42
3:F:58:THR:HB	3:F:84:PHE:CE1	2.54	0.42
5:b:221:GLU:O	5:b:225:MET:HG3	2.19	0.42
6:c:58:MET:HB2	10:g:88:PHE:CZ	2.54	0.42
10:i:37:VAL:HG12	10:j:114:ALA:HB2	2.01	0.42
4:a:22:PRO:HD2	4:a:25:ILE:HD11	2.02	0.42
4:a:207:LEU:HD11	4:a:249:ILE:HD11	2.01	0.42
6:c:180:LEU:HD21	11:o:53:PRO:HB3	2.02	0.42
7:d:124:LEU:HD21	7:d:137:PRO:HA	2.00	0.42
8:e:66:ASP:OD1	9:f:41:SER:OG	2.26	0.42
2:B:8:ASP:OD1	2:B:8:ASP:N	2.53	0.42
2:B:95:LYS:O	2:B:98:GLU:HG2	2.19	0.42
7:d:238:LYS:O	7:d:242:LEU:HG	2.20	0.42
7:d:332:GLN:O	7:d:334:GLN:HG2	2.19	0.42
1:A:63:ASP:OD1	7:d:126:ARG:NH2	2.38	0.42
4:a:416:PRO:HA	4:a:468:MET:HG2	2.02	0.42
10:l:7:VAL:HG21	10:m:3:GLU:HG3	2.00	0.42
1:A:69:TYR:OH	1:A:132:PRO:HG3	2.19	0.42
4:a:128:THR:O	4:a:132:GLU:HG2	2.19	0.42
4:a:635:VAL:O	4:a:639:LEU:HD23	2.20	0.42
5:b:243:TRP:HZ2	6:c:77:TRP:CZ3	2.37	0.42
7:d:96:ASP:O	7:d:99:THR:OG1	2.35	0.42
10:n:16:GLY:O	10:n:94:GLY:HA3	2.20	0.42
3:F:63:ASP:OD1	3:F:63:ASP:N	2.50	0.42
10:i:8:TYR:HA	10:j:88:PHE:HE2	1.85	0.42
10:n:30:TYR:CD1	10:n:106:PHE:HA	2.55	0.42
4:a:315:ARG:O	4:a:319:ILE:HG23	2.20	0.42
4:a:542:LEU:O	4:a:546:ILE:HG12	2.20	0.42
4:a:653:PRO:HD3	4:a:715:GLN:HG2	2.00	0.42
4:a:774:PHE:CZ	9:f:20:GLY:HA2	2.55	0.42
10:n:49:LEU:HG	10:n:53:ASN:ND2	2.35	0.42
1:A:14:ASP:OD1	1:A:14:ASP:N	2.53	0.41
6:c:109:VAL:HG12	6:c:113:TYR:CZ	2.55	0.41
10:j:53:ASN:O	10:j:56:PRO:HD2	2.20	0.41
10:l:78:LEU:O	10:m:153:ARG:NH1	2.45	0.41
4:a:20:TYR:CD1	4:a:334:ILE:HD12	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:353:LEU:HD23	4:a:353:LEU:HA	1.85	0.41
4:a:801:HIS:HA	4:a:805:SER:HB3	2.03	0.41
7:d:208:MET:HG2	7:d:307:SER:HB3	2.02	0.41
7:d:336:GLU:H	7:d:336:GLU:CD	2.29	0.41
4:a:542:LEU:HD23	4:a:587:SER:HB3	2.01	0.41
4:a:784:VAL:O	4:a:788:MET:HB3	2.21	0.41
10:h:8:TYR:HA	10:i:88:PHE:HE2	1.84	0.41
10:i:30:TYR:CD1	10:i:106:PHE:HA	2.56	0.41
4:a:478:LEU:HA	4:a:478:LEU:HD23	1.82	0.41
6:c:208:LYS:HE3	11:o:84:LEU:O	2.20	0.41
7:d:142:ALA:O	7:d:148:LEU:HD21	2.19	0.41
10:g:84:LEU:HG	10:g:88:PHE:CE2	2.56	0.41
4:a:529:LEU:HD23	4:a:529:LEU:HA	1.88	0.41
4:a:475:THR:HG22	8:e:47:MET:SD	2.61	0.41
7:d:20:TYR:HB3	7:d:312:TRP:NE1	2.36	0.41
10:h:42:THR:CG2	10:h:117:ARG:HA	2.51	0.41
10:j:43:CYS:HB2	10:k:125:LEU:HD13	2.02	0.41
10:l:7:VAL:HG12	10:m:84:LEU:HD23	2.01	0.41
6:c:59:TRP:HB3	6:c:146:PHE:HB2	2.02	0.41
6:c:77:TRP:HA	6:c:80:PHE:CE1	2.56	0.41
8:e:68:ARG:HH21	8:e:71:PHE:HE2	1.69	0.41
8:e:68:ARG:HD2	9:f:42:ILE:HA	2.02	0.41
10:g:43:CYS:SG	10:g:50:LEU:HA	2.61	0.41
10:i:5:CYS:SG	10:i:160:CYS:HA	2.61	0.41
10:i:45:LEU:HA	10:i:45:LEU:HD23	1.80	0.41
10:k:126:PHE:O	10:k:130:ILE:HG12	2.21	0.41
4:a:107:ILE:O	4:a:111:VAL:HG23	2.21	0.41
4:a:409:LEU:HB3	4:a:410:PRO:HD3	2.02	0.41
4:a:419:PHE:CD1	4:a:468:MET:HB3	2.55	0.41
4:a:459:PHE:O	4:a:462:ARG:NH1	2.43	0.41
5:b:240:ALA:HB2	10:g:102:LEU:HD21	2.02	0.41
6:c:57:TYR:CE2	10:g:85:TYR:HB2	2.56	0.41
7:d:247:LYS:HE3	7:d:274:GLU:HG3	2.01	0.41
8:e:2:SER:HB2	8:e:6:THR:OG1	2.20	0.41
10:g:81:LYS:HE2	10:h:4:LEU:HD11	2.03	0.41
10:h:30:TYR:CE1	10:h:34:LYS:HG3	2.56	0.41
10:i:11:PHE:HB2	10:j:88:PHE:CZ	2.56	0.41
10:j:15:ILE:HD13	10:j:15:ILE:HA	1.95	0.41
11:o:123:GLY:O	11:o:137:ILE:HD13	2.21	0.41
4:a:319:ILE:HG13	4:a:320:PHE:N	2.36	0.41
6:c:204:LEU:HD13	11:o:78:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:d:134:ASP:OD1	7:d:134:ASP:N	2.52	0.41
2:B:39:ALA:HB2	2:B:72:GLU:OE1	2.21	0.40
4:a:418:MET:SD	4:a:736:LEU:HD21	2.61	0.40
10:i:32:THR:HG23	10:i:57:VAL:HG13	2.02	0.40
10:l:66:TYR:CD1	10:l:144:LEU:HD22	2.55	0.40
11:o:49:GLY:C	11:o:51:PHE:H	2.30	0.40
11:o:127:TYR:CD1	11:o:134:PHE:HD1	2.39	0.40
2:B:1:MET:HE1	3:F:101:TYR:HB3	2.02	0.40
4:a:289:LYS:HA	4:a:289:LYS:HD3	1.78	0.40
10:h:33:ALA:HA	10:i:111:VAL:HG23	2.02	0.40
10:l:59:MET:HE3	10:l:137:GLU:HB2	2.03	0.40
4:a:38:LEU:HD13	4:a:345:GLU:HB3	2.02	0.40
4:a:141:TYR:HD1	4:a:261:TYR:HB3	1.86	0.40
4:a:419:PHE:CE1	4:a:468:MET:HB3	2.57	0.40
4:a:530:LEU:HD23	8:e:60:VAL:HG11	2.03	0.40
4:a:583:PHE:CE2	4:a:727:VAL:HG12	2.57	0.40
6:c:193:ILE:O	6:c:197:LEU:HG	2.22	0.40
10:h:15:ILE:HD13	10:h:15:ILE:HA	1.95	0.40
10:h:58:ILE:O	10:h:62:ILE:HG13	2.22	0.40
10:k:40:CYS:HA	10:l:125:LEU:HD11	2.04	0.40
4:a:69:TYR:CZ	4:a:309:TRP:HB3	2.56	0.40
10:n:13:GLY:HA2	10:n:90:GLN:HB2	2.03	0.40
1:A:70:ILE:HG21	3:F:30:PRO:HA	2.04	0.40
10:h:44:VAL:HG12	10:h:45:LEU:HD22	2.03	0.40
10:k:11:PHE:HB2	10:l:88:PHE:CZ	2.57	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	126/181 (70%)	123 (98%)	3 (2%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	96/147 (65%)	94 (98%)	2 (2%)	0	100	100
3	F	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
4	a	734/840 (87%)	715 (97%)	19 (3%)	0	100	100
5	b	48/265 (18%)	47 (98%)	1 (2%)	0	100	100
6	c	196/213 (92%)	196 (100%)	0	0	100	100
7	d	334/345 (97%)	326 (98%)	8 (2%)	0	100	100
8	e	68/73 (93%)	68 (100%)	0	0	100	100
9	f	68/85 (80%)	68 (100%)	0	0	100	100
10	g	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
10	h	157/160 (98%)	157 (100%)	0	0	100	100
10	i	157/160 (98%)	157 (100%)	0	0	100	100
10	j	157/160 (98%)	157 (100%)	0	0	100	100
10	k	157/160 (98%)	156 (99%)	1 (1%)	0	100	100
10	l	156/160 (98%)	154 (99%)	2 (1%)	0	100	100
10	m	157/160 (98%)	155 (99%)	2 (1%)	0	100	100
10	n	157/160 (98%)	157 (100%)	0	0	100	100
11	o	156/164 (95%)	154 (99%)	2 (1%)	0	100	100
All	All	3193/3711 (86%)	3148 (99%)	45 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	115/168 (68%)	115 (100%)	0	100	100
2	B	75/103 (73%)	75 (100%)	0	100	100
3	F	100/104 (96%)	100 (100%)	0	100	100
4	a	631/728 (87%)	631 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	b	45/244 (18%)	45 (100%)	0	100	100
6	c	154/168 (92%)	154 (100%)	0	100	100
7	d	301/309 (97%)	301 (100%)	0	100	100
8	e	63/65 (97%)	63 (100%)	0	100	100
9	f	52/72 (72%)	52 (100%)	0	100	100
10	g	117/119 (98%)	117 (100%)	0	100	100
10	h	118/119 (99%)	118 (100%)	0	100	100
10	i	118/119 (99%)	118 (100%)	0	100	100
10	j	117/119 (98%)	117 (100%)	0	100	100
10	k	117/119 (98%)	117 (100%)	0	100	100
10	l	116/119 (98%)	116 (100%)	0	100	100
10	m	117/119 (98%)	117 (100%)	0	100	100
10	n	118/119 (99%)	118 (100%)	0	100	100
11	o	118/125 (94%)	118 (100%)	0	100	100
All	All	2592/3038 (85%)	2592 (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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
2	B	38	HIS
4	a	273	GLN
4	a	614	ASN
4	a	629	HIS
4	a	715	GLN
4	a	756	GLN
6	c	132	ASN
7	d	27	ASN
7	d	35	GLN
7	d	229	GLN
7	d	303	GLN
7	d	333	ASN
8	e	57	HIS
10	g	121	GLN
10	k	82	GLN

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Mol	Chain	Res	Type
10	k	122	GLN
10	m	151	ASN
10	n	53	ASN
10	n	82	GLN
11	o	159	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	108:LYS	C	123:UNK	N	25.94

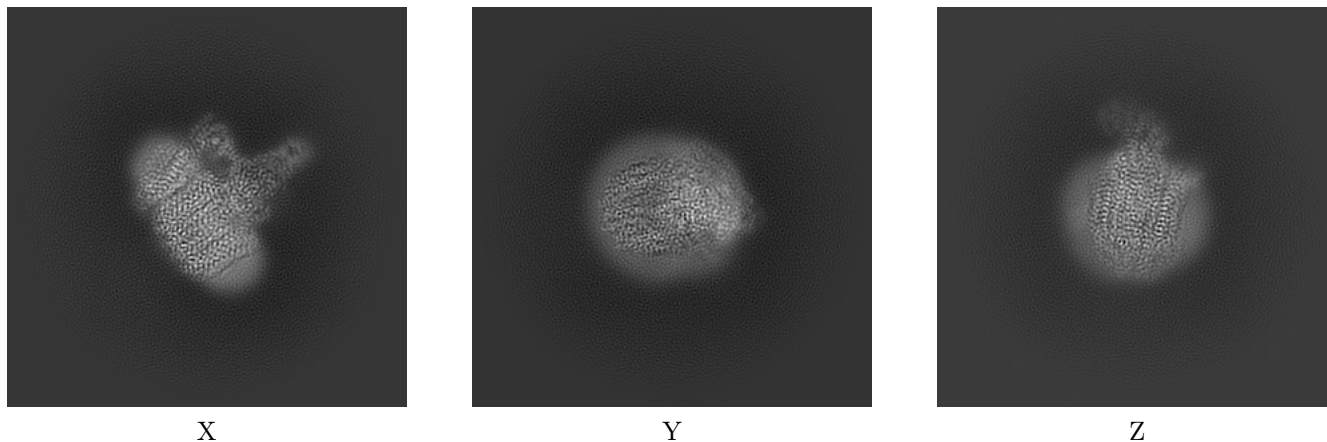
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27984. These allow visual inspection of the internal detail of the map and identification of artifacts.

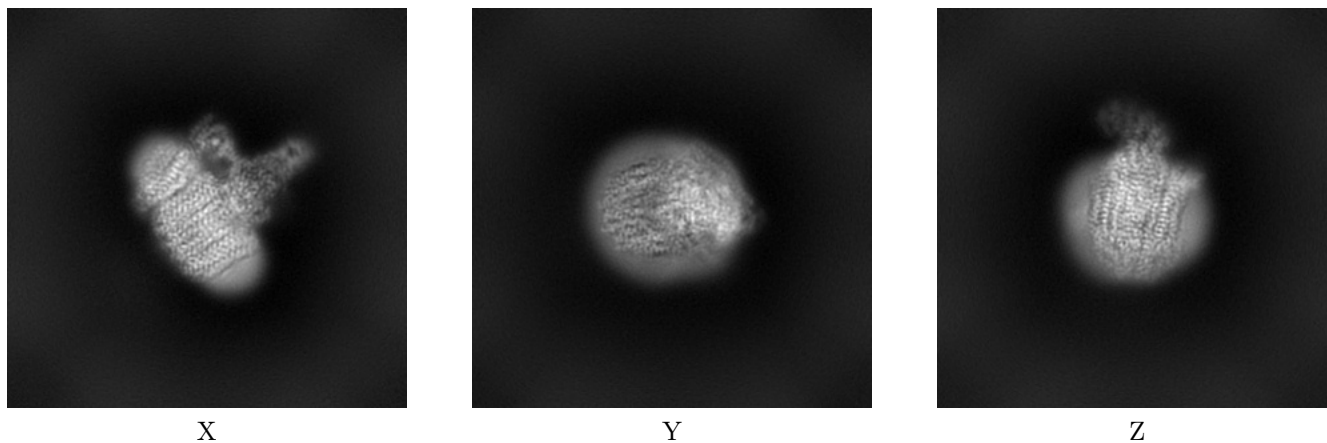
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



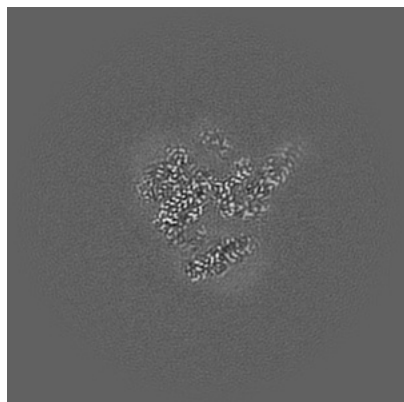
#### 6.1.2 Raw map



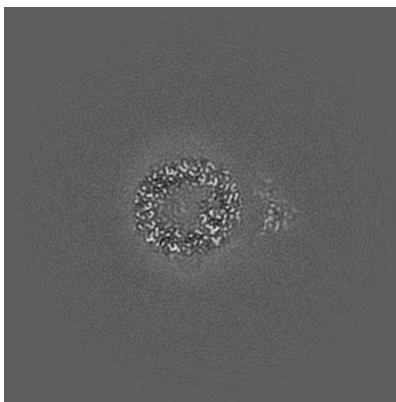
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

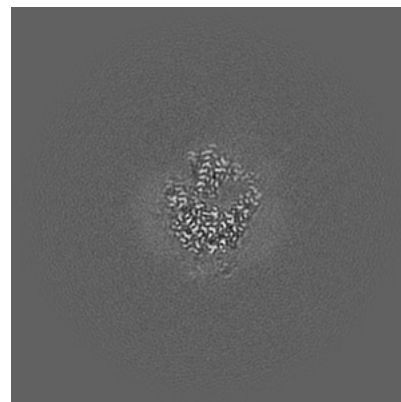
### 6.2.1 Primary map



X Index: 160

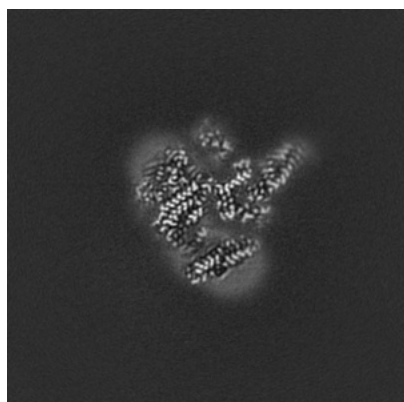


Y Index: 160

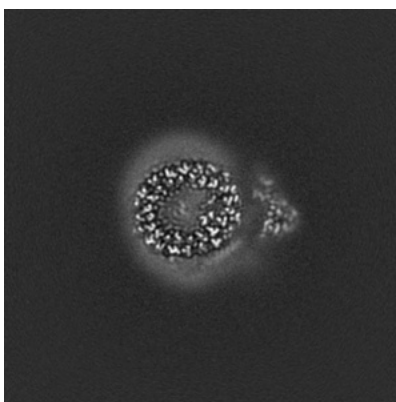


Z Index: 160

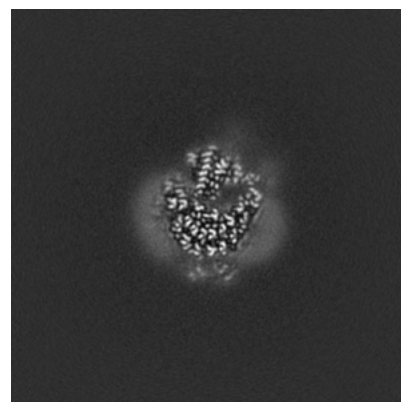
### 6.2.2 Raw map



X Index: 160



Y Index: 160

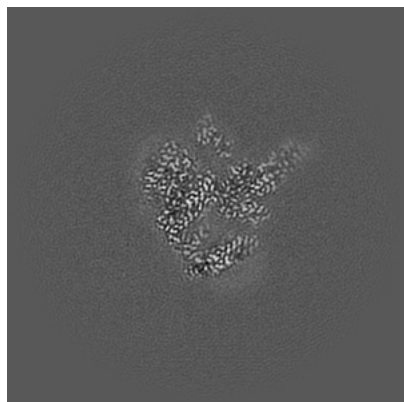


Z Index: 160

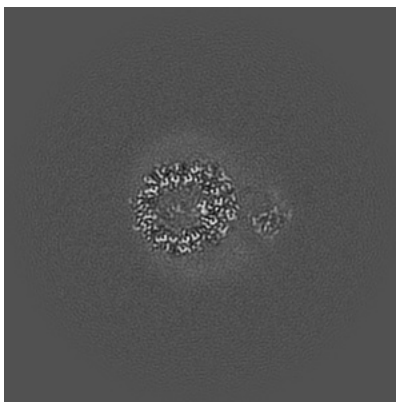
The images above show central slices of the map in three orthogonal directions.

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

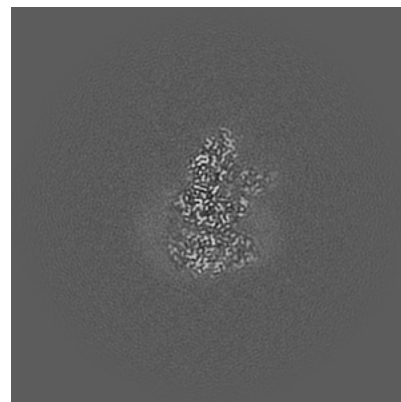
### 6.3.1 Primary map



X Index: 156

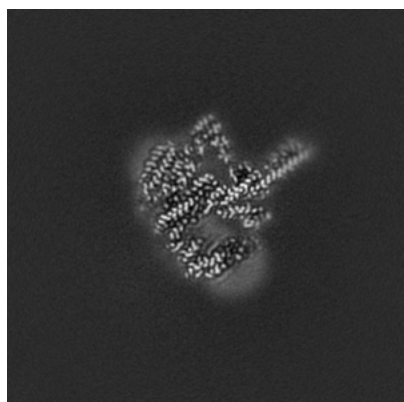


Y Index: 154

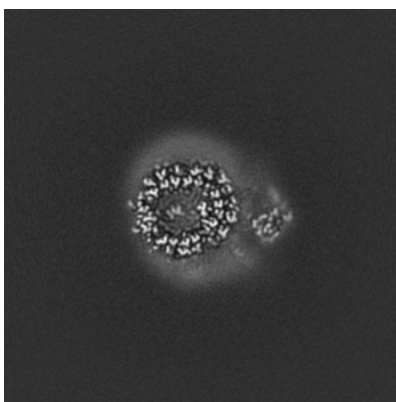


Z Index: 176

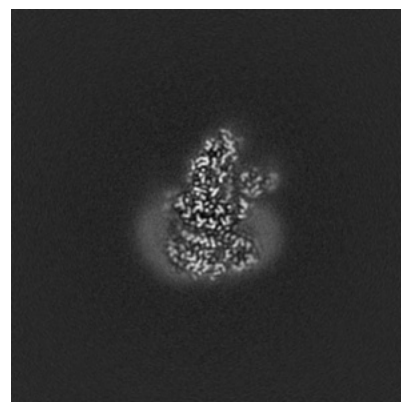
### 6.3.2 Raw map



X Index: 153



Y Index: 154

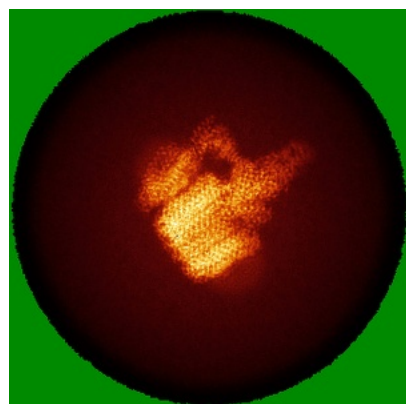


Z Index: 176

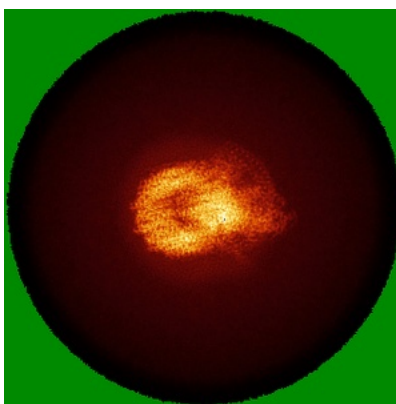
The images above show the largest variance slices of the map in three orthogonal directions.

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

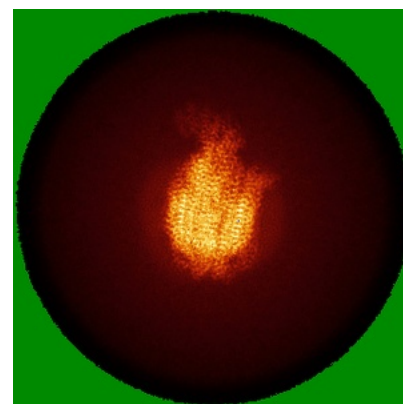
### 6.4.1 Primary map



X

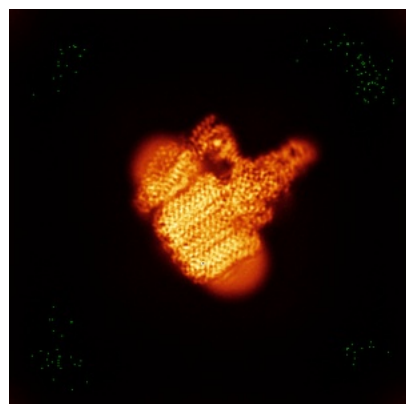


Y

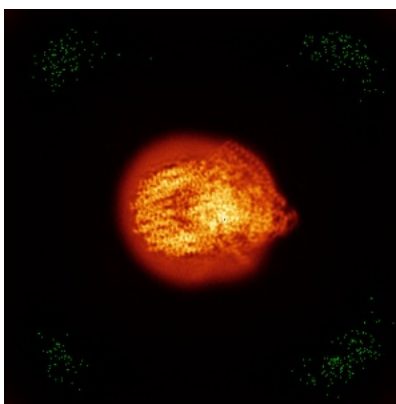


Z

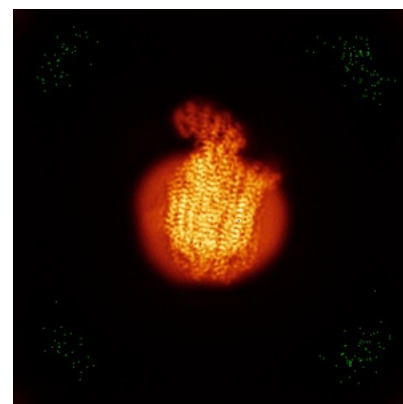
### 6.4.2 Raw map



X



Y

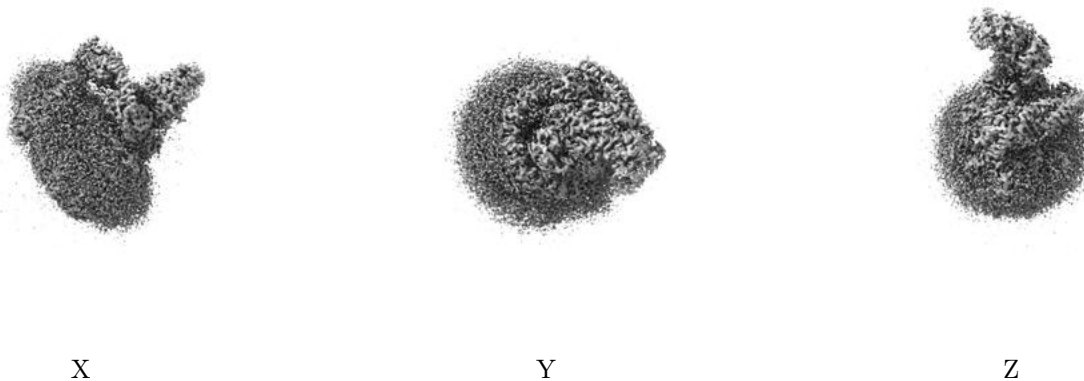


Z

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.

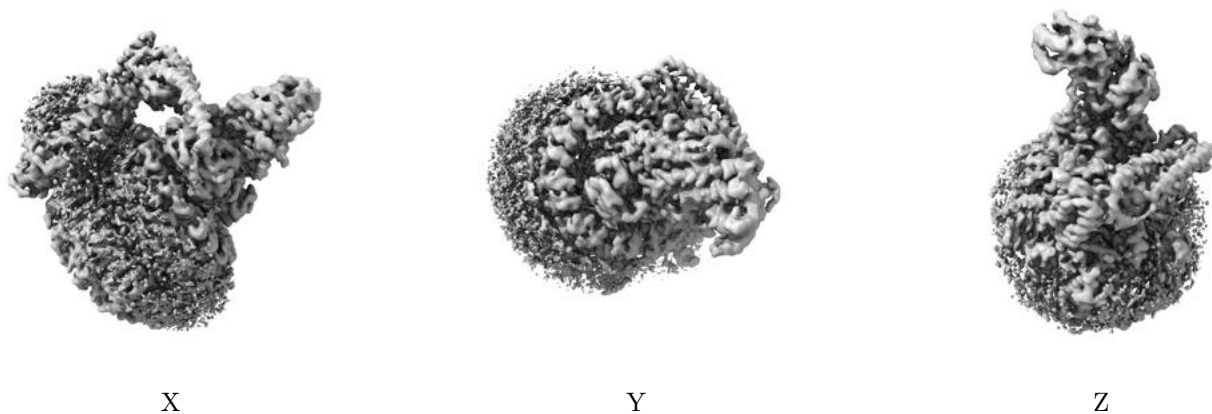
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.1. 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.

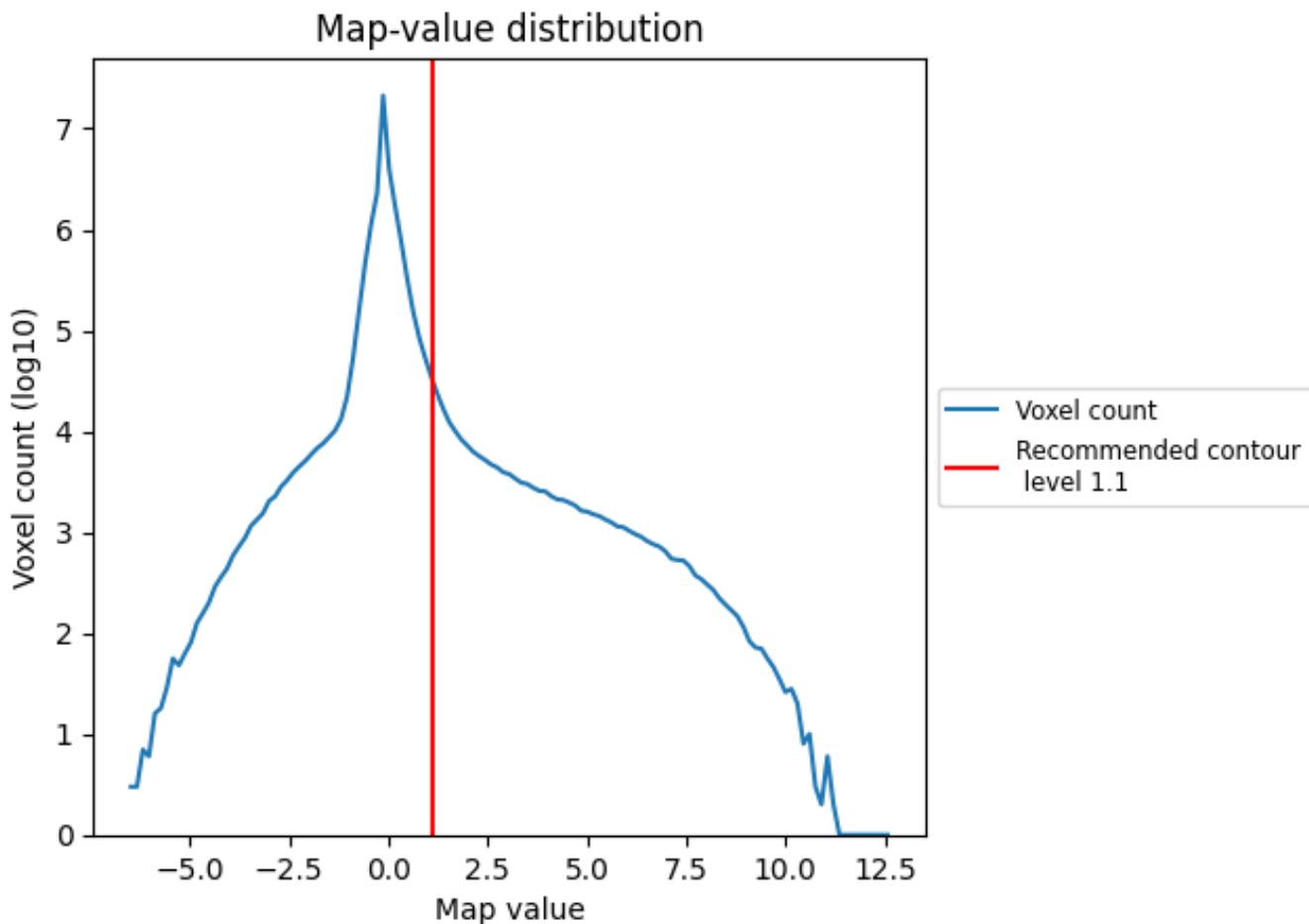
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

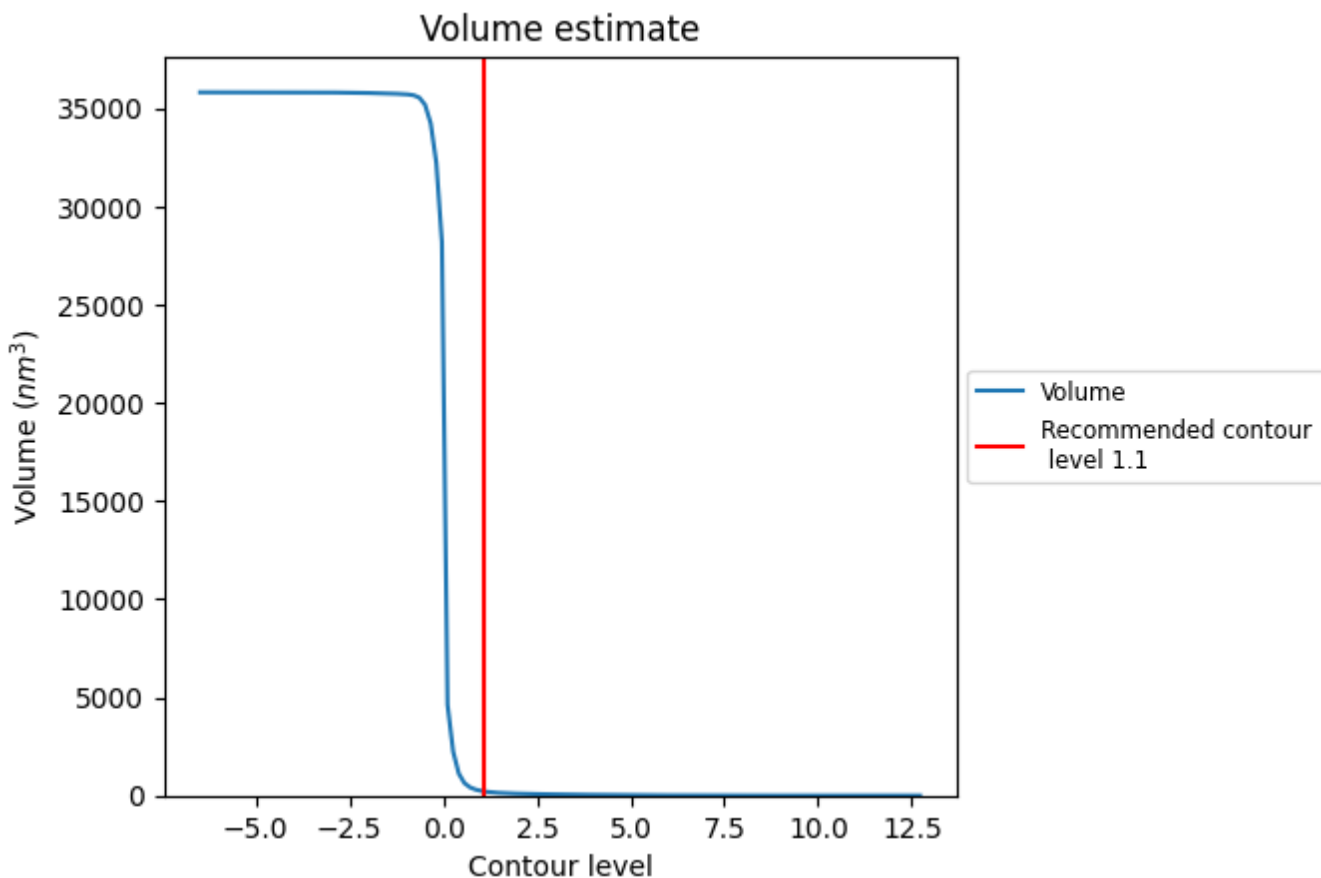
This section contains the results of statistical analysis of the map.

### 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.

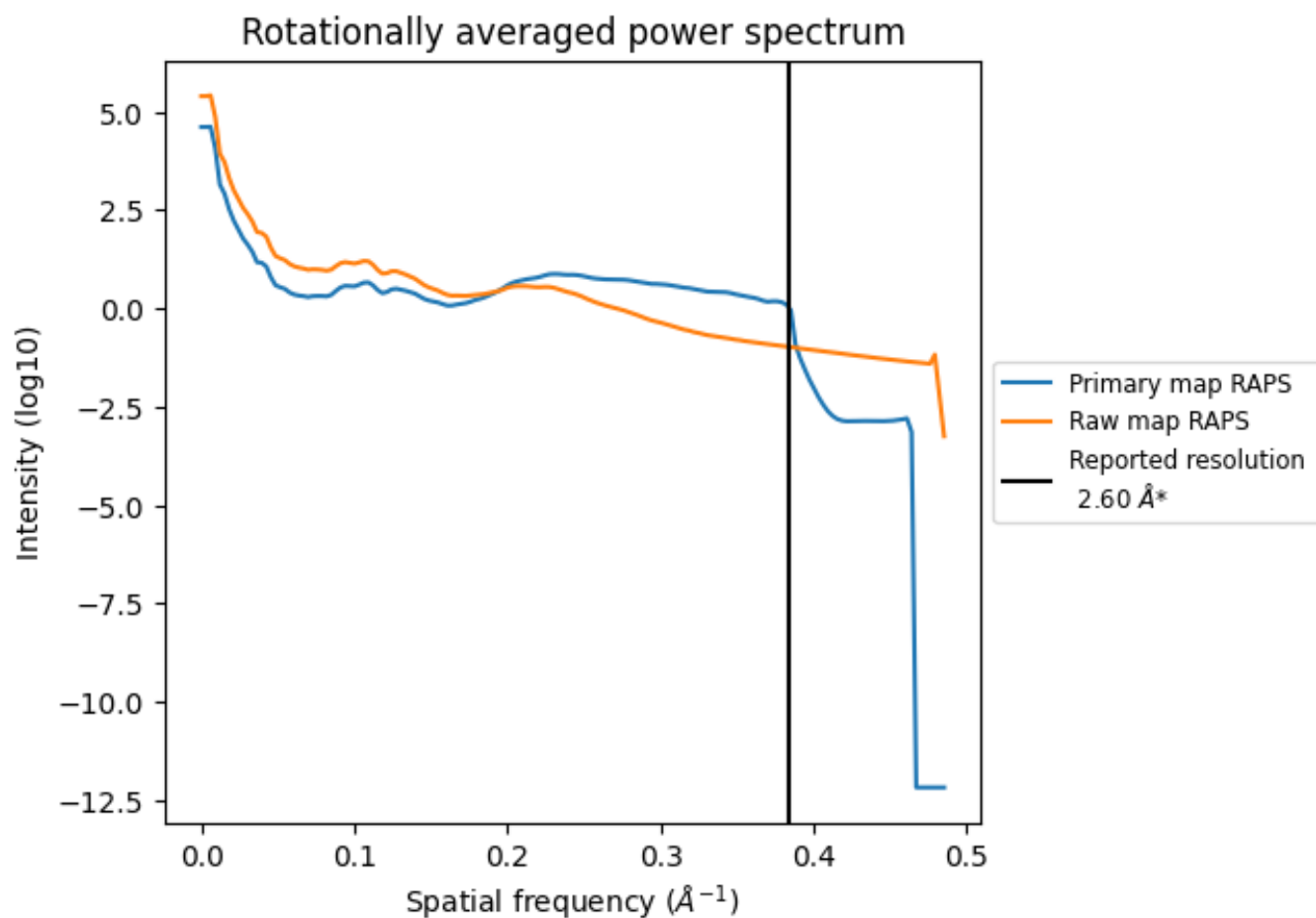
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 210 nm<sup>3</sup>; this corresponds to an approximate mass of 189 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](#)

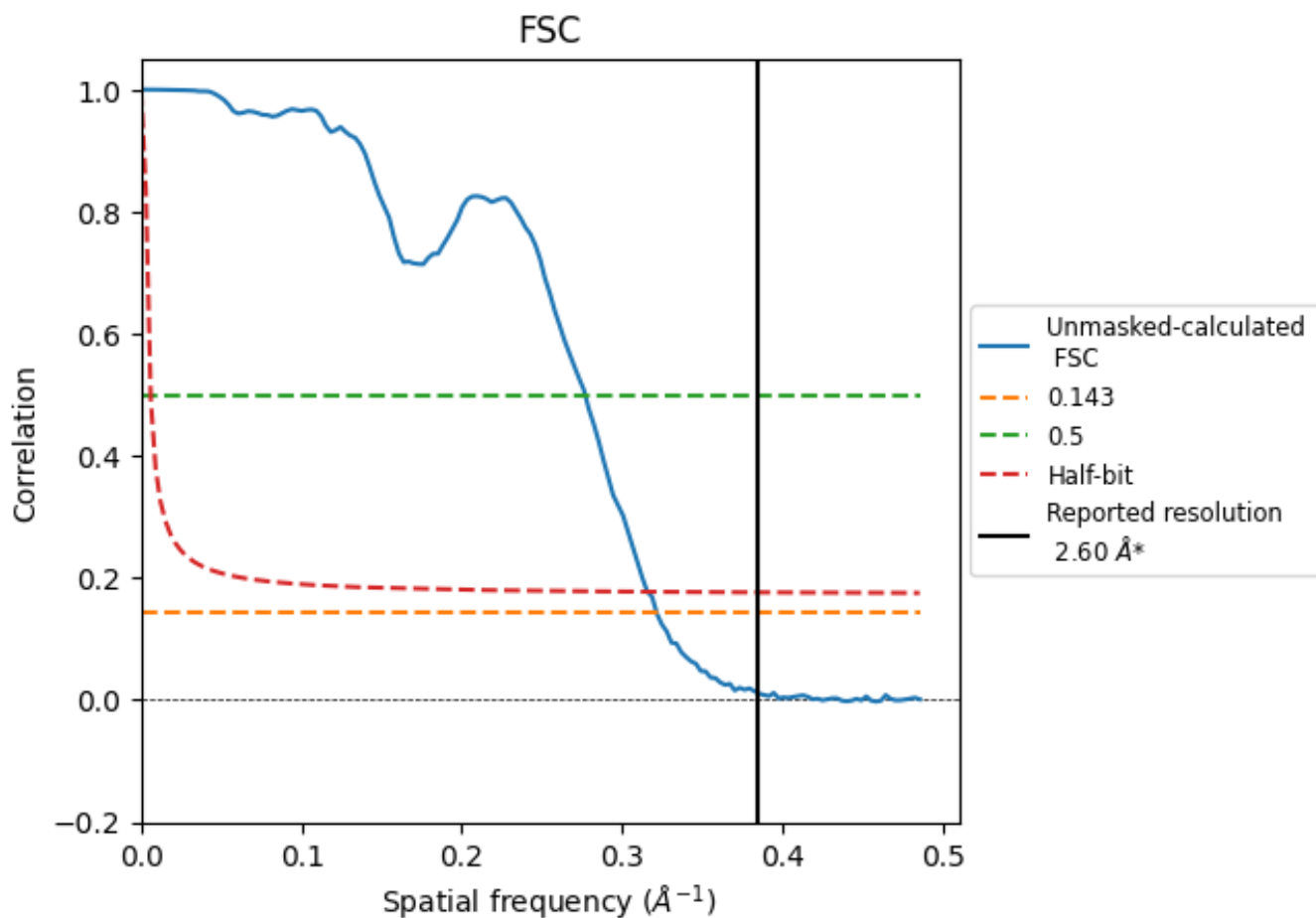


\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.385 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

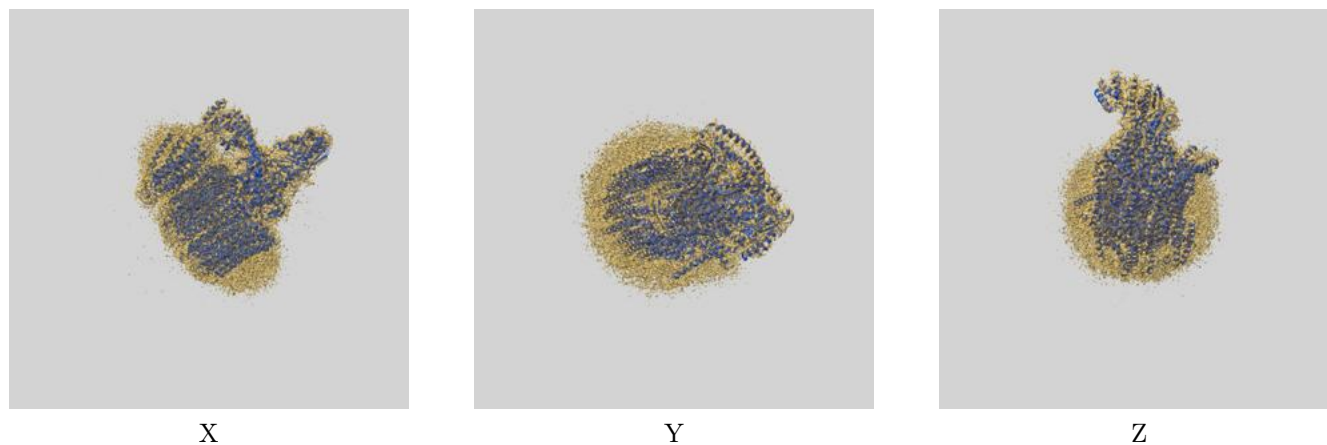
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.61	3.17

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.11 differs from the reported value 2.6 by more than 10 %

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

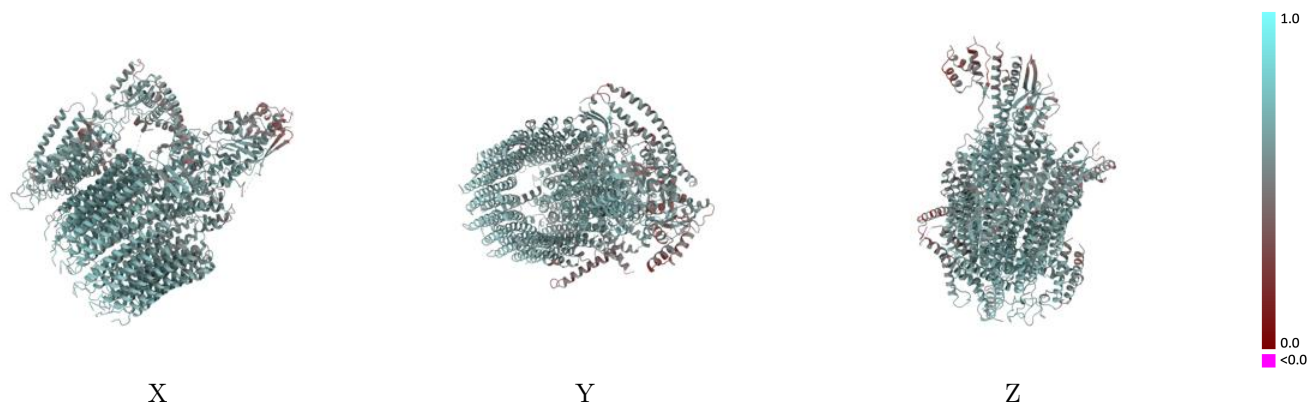
This section contains information regarding the fit between EMDB map EMD-27984 and PDB model 8EAS. Per-residue inclusion information can be found in section 3 on page 6.

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



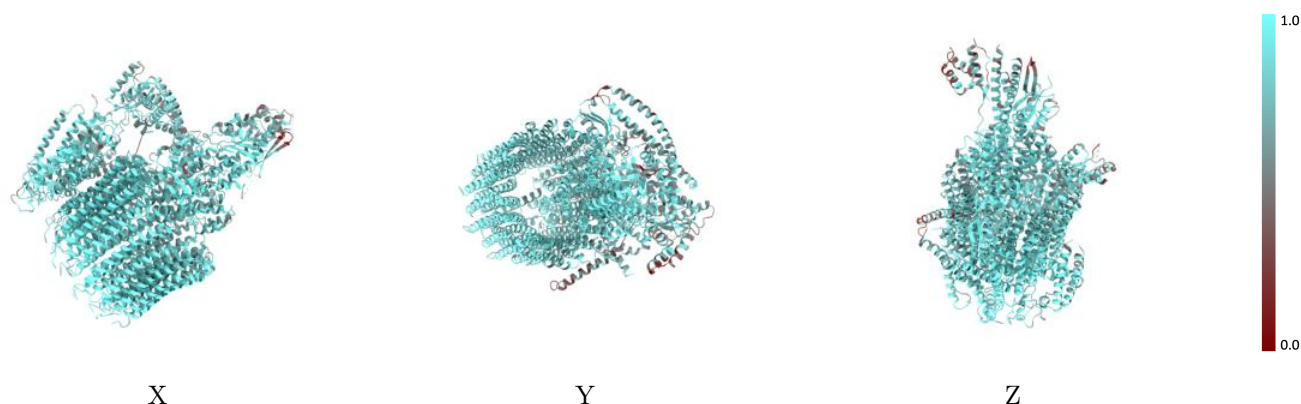
The images above show the 3D surface view of the map at the recommended contour level 1.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



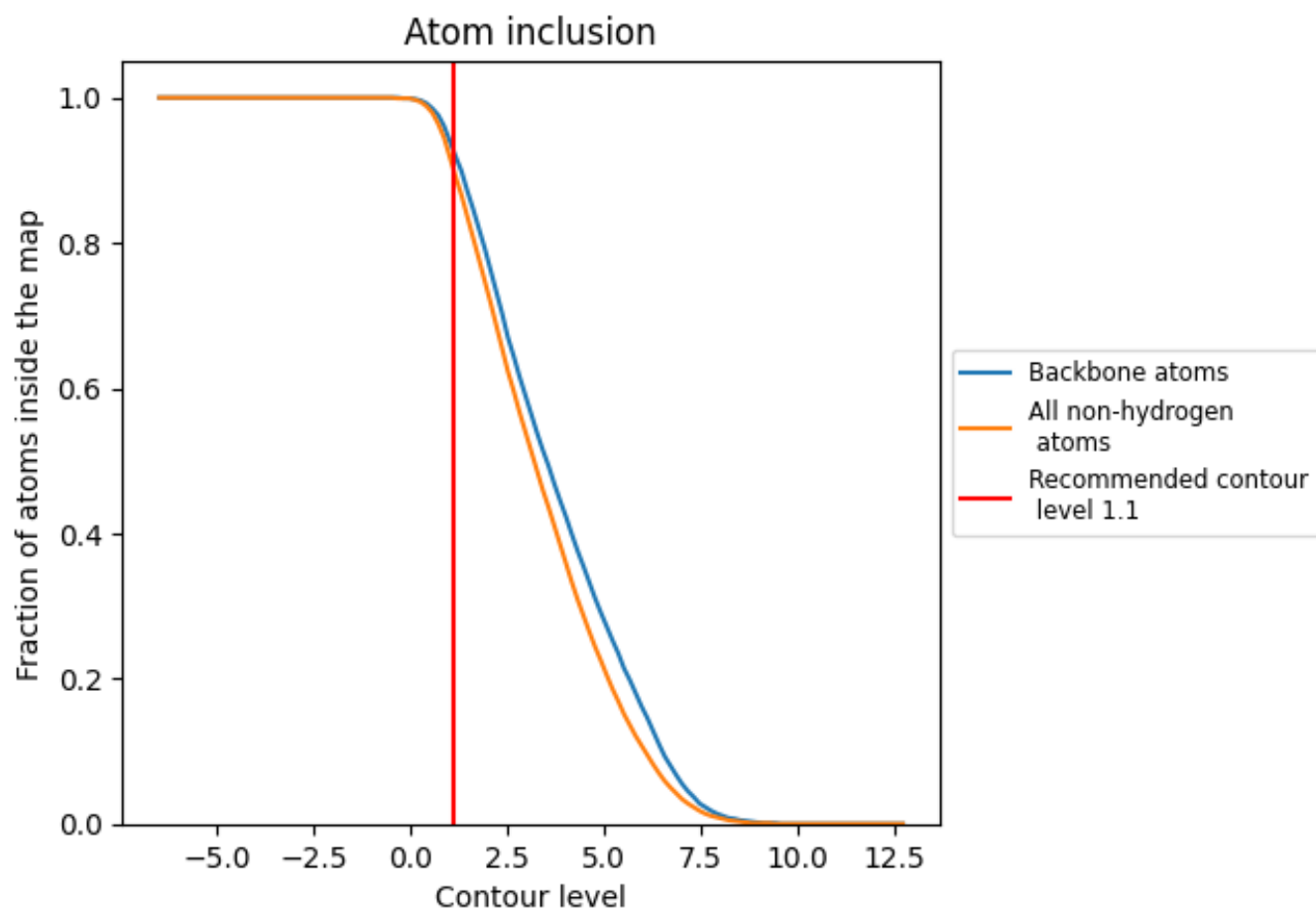
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.1).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (1.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9030	 0.6060
A	 0.8240	 0.5570
B	 0.6070	 0.4430
F	 0.8230	 0.5560
a	 0.8520	 0.5790
b	 0.9320	 0.6330
c	 0.9770	 0.6520
d	 0.9300	 0.6220
e	 0.8990	 0.6120
f	 0.8510	 0.5480
g	 0.9780	 0.6490
h	 0.9840	 0.6560
i	 0.9700	 0.6480
j	 0.9560	 0.6310
k	 0.9470	 0.6260
l	 0.9560	 0.6320
m	 0.9680	 0.6400
n	 0.9310	 0.6250
o	 0.9480	 0.6290

