



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 11:00 PM UTC

PDB ID : 9ARJ / pdb_00009arj
EMDB ID : EMD-43784
Title : CryoEM structure of BoNT-NTNH-OrfX2 complex from Clostridium botulinum E1, major class
Authors : Gao, L.
Deposited on : 2024-02-23
Resolution : 3.40 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

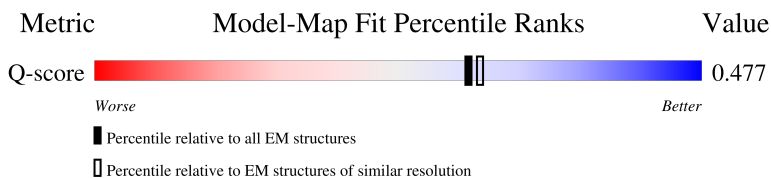
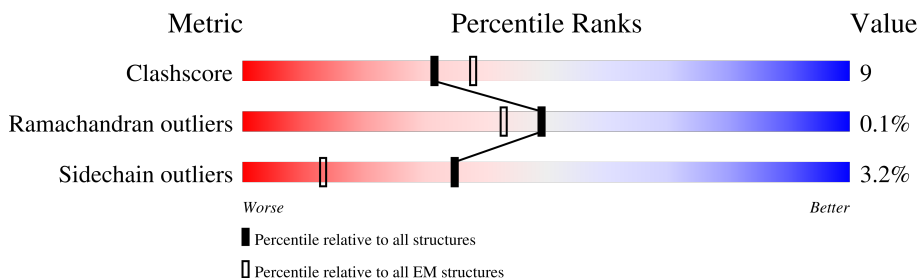
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	C	748	
2	A	1252	
3	B	1163	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24188 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 Toxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	578	Total	C	N	O	S	0	0
			4550	2917	749	877	7		

- Molecule 2 is a protein called Botulinum neurotoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1241	Total	C	N	O	S	0	0
			9965	6344	1658	1941	22		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	212	ALA	HIS	engineered mutation	UNP A8Y875
A	213	ALA	GLU	engineered mutation	UNP A8Y875
A	216	ALA	HIS	engineered mutation	UNP A8Y875

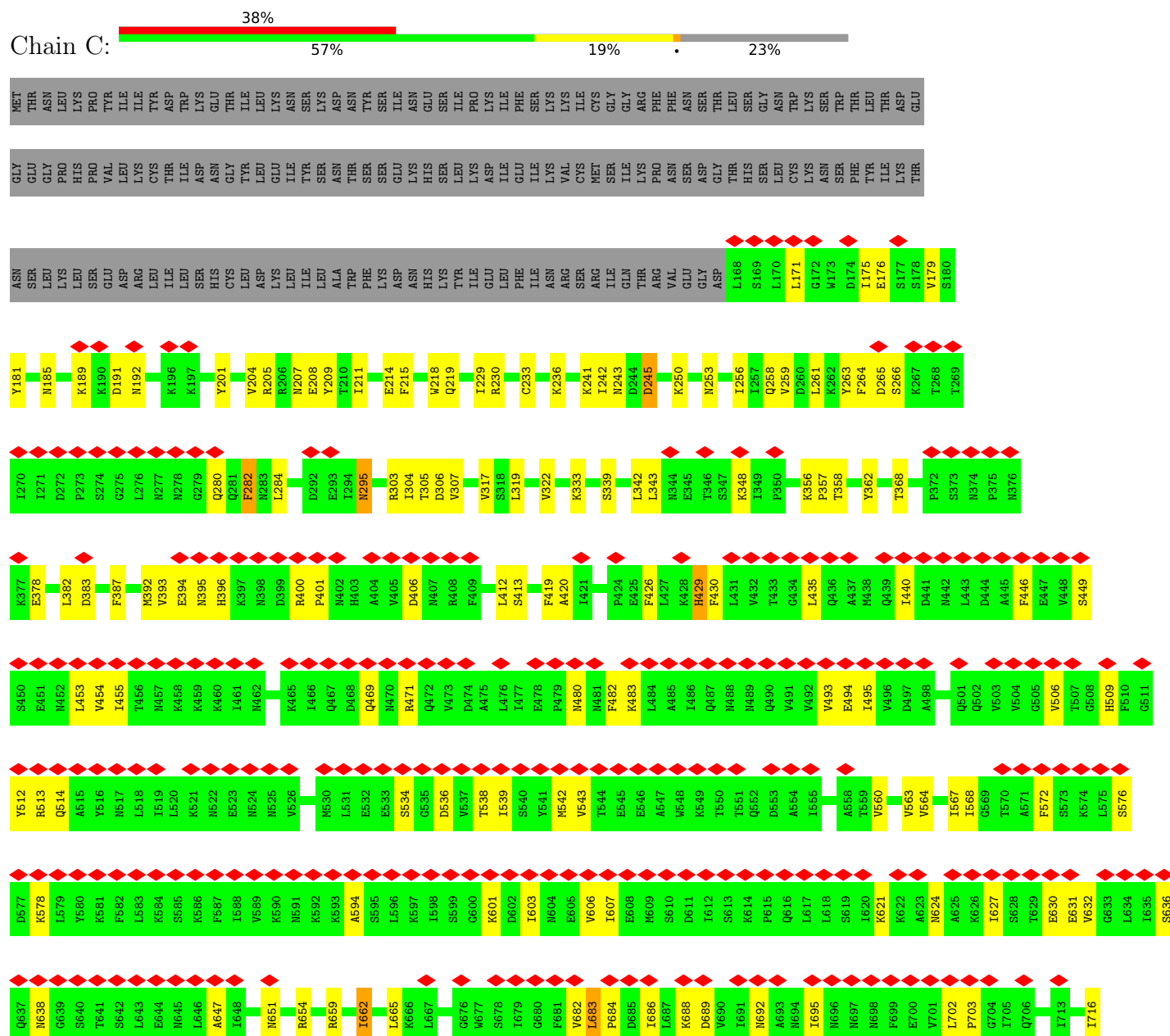
- Molecule 3 is a protein called Peptidase M27.

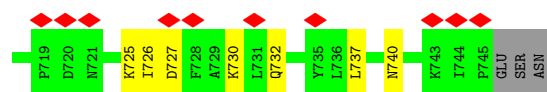
Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	1163	Total	C	N	O	S	0	0
			9673	6242	1553	1853	25		

3 Residue-property plots

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.

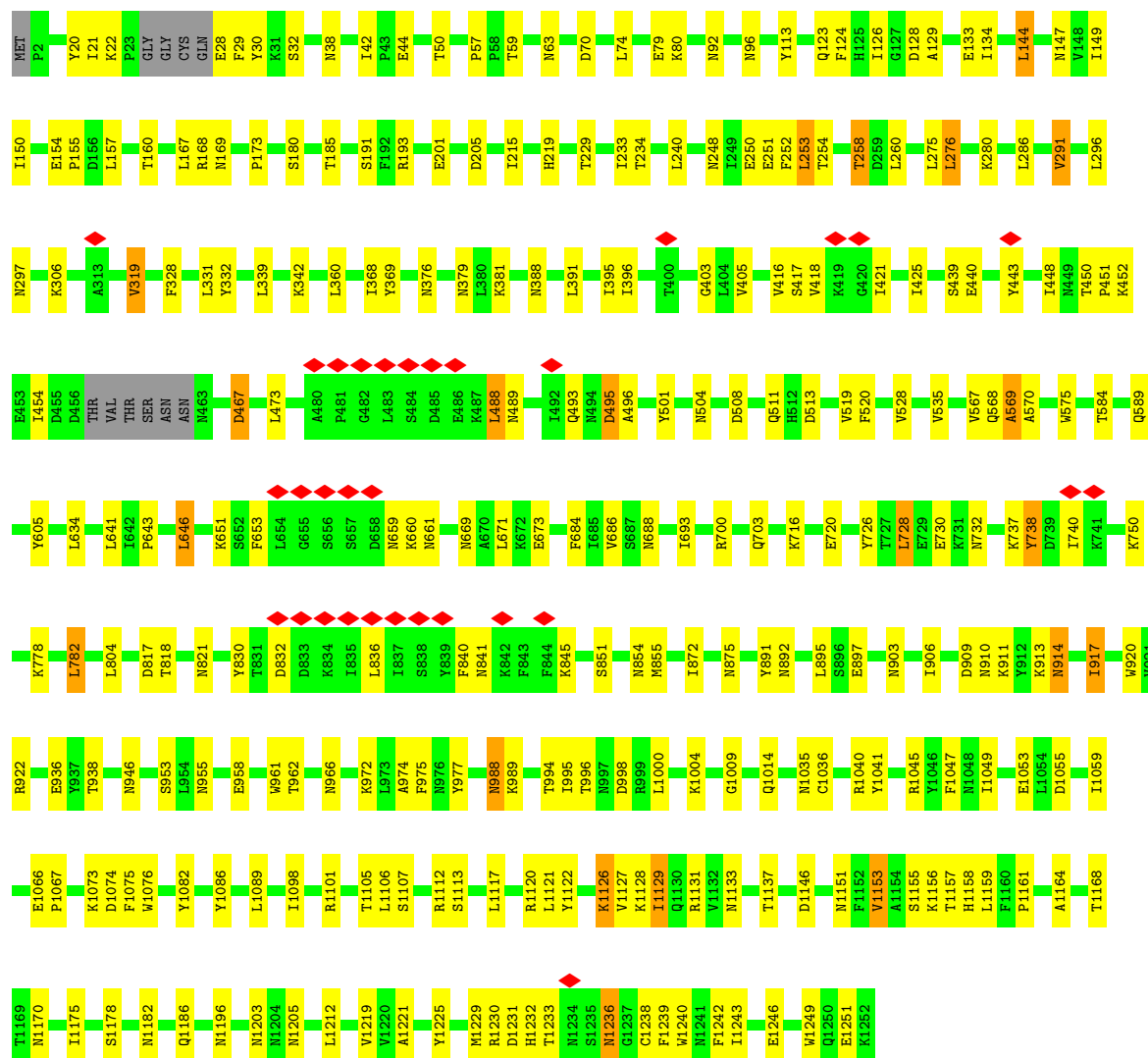
• Molecule 1: Toxin





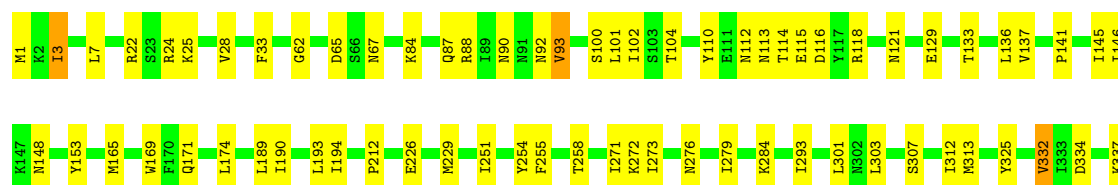
• Molecule 2: Botulinum neurotoxin

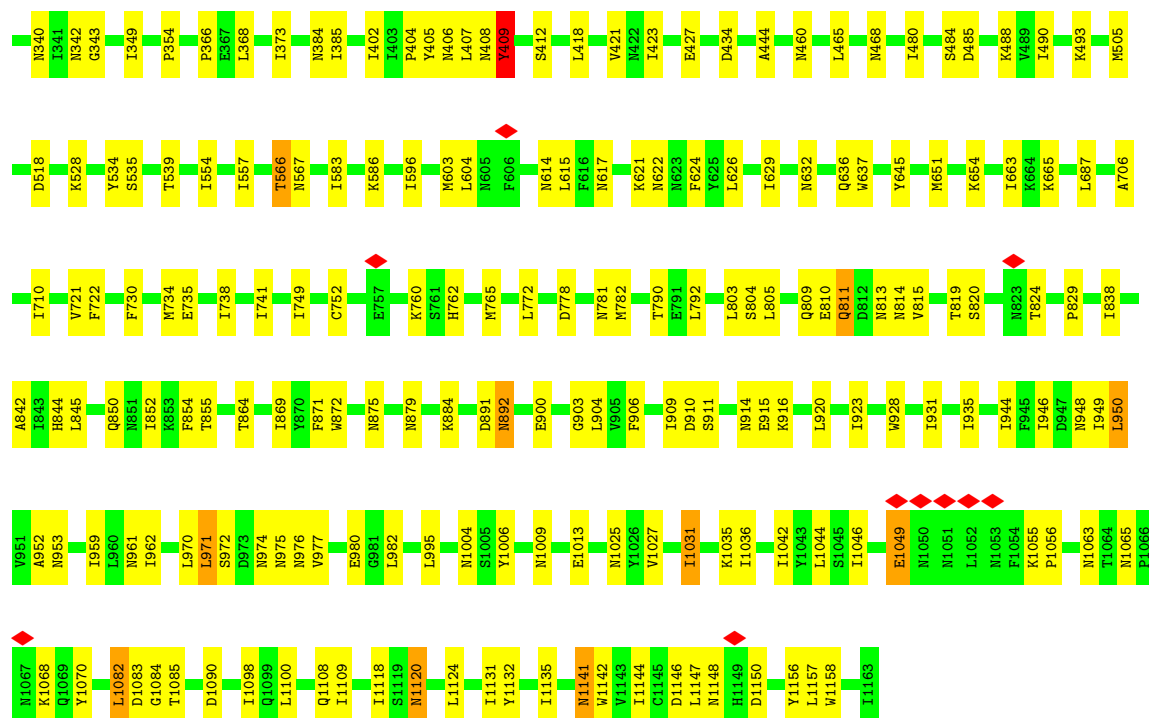
Chain A: 77% 21%



• Molecule 3: Peptidase M27

Chain B: 77% 21%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	384801	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.503	Depositor
Minimum map value	-0.251	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	403.456, 403.456, 403.456	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.788, 0.788, 0.788	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	C	0.09	0/4638	0.25	0/6294
2	A	0.16	0/10163	0.30	0/13790
3	B	0.15	0/9888	0.29	2/13407 (0.0%)
All	All	0.14	0/24689	0.29	2/33491 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	406	ASN	N-CA-C	8.94	121.10	111.36
3	B	409	TYR	N-CA-C	5.71	122.97	110.80

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	C	4550	0	4548	88	0
2	A	9965	0	9712	184	0
3	B	9673	0	9516	159	0
All	All	24188	0	23776	418	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 (418) 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:B:408:ASN:ND2	3:B:621:LYS:HD2	1.68	1.07
3:B:408:ASN:HD22	3:B:621:LYS:HD2	1.25	1.00
2:A:840:PHE:HB2	3:B:995:LEU:HD13	1.64	0.78
1:C:543:VAL:O	1:C:594:ALA:HB3	1.82	0.77
2:A:42:ILE:HG13	2:A:149:ILE:HD11	1.67	0.74
1:C:682:VAL:HG12	1:C:684:PRO:HD2	1.69	0.73
3:B:271:ILE:HG22	3:B:272:LYS:HG3	1.70	0.73
3:B:1120:ASN:N	3:B:1120:ASN:OD1	2.22	0.73
2:A:686:VAL:HG11	2:A:830:TYR:HB3	1.71	0.72
2:A:914:ASN:HB3	2:A:998:ASP:HA	1.70	0.72
2:A:1067:PRO:O	2:A:1073:LYS:NZ	2.24	0.71
2:A:922:ARG:NH2	2:A:1246:GLU:OE1	2.24	0.70
3:B:465:LEU:H	3:B:468:ASN:HD22	1.39	0.70
3:B:229:MET:HE2	3:B:255:PHE:HZ	1.55	0.70
1:C:358:THR:HG21	1:C:395:ASN:H	1.57	0.70
3:B:891:ASP:O	3:B:892:ASN:ND2	2.25	0.69
1:C:567:ILE:HG13	1:C:568:ILE:HG12	1.73	0.69
2:A:660:LYS:O	2:A:661:ASN:ND2	2.25	0.69
2:A:1156:LYS:HG2	2:A:1157:THR:HG23	1.75	0.68
1:C:218:TRP:HZ2	1:C:333:LYS:HZ2	1.41	0.67
2:A:1236:ASN:N	2:A:1236:ASN:OD1	2.27	0.67
3:B:1068:LYS:NZ	3:B:1070:TYR:O	2.27	0.67
1:C:176:GLU:HB3	1:C:420:ALA:HB3	1.75	0.67
3:B:484:SER:HB3	3:B:505:MET:HE1	1.76	0.67
3:B:583:ILE:O	3:B:586:LYS:NZ	2.28	0.67
2:A:1133:ASN:HA	3:B:1065:ASN:HD22	1.60	0.67
1:C:725:LYS:HE3	1:C:740:ASN:HB2	1.78	0.66
2:A:21:ILE:HG12	2:A:134:ILE:HG22	1.76	0.66
3:B:113:ASN:HB3	3:B:116:ASP:HB3	1.77	0.66
2:A:167:LEU:HD22	2:A:495:ASP:HB2	1.78	0.66
3:B:141:PRO:HB2	3:B:145:ILE:HA	1.77	0.66
1:C:449:SER:O	1:C:453:LEU:HA	1.96	0.66
2:A:379:ASN:OD1	2:A:903:ASN:ND2	2.29	0.66
2:A:22:LYS:HB3	2:A:133:GLU:HG3	1.78	0.65
2:A:234:THR:HG1	2:A:439:SER:HG	1.44	0.65
2:A:875:ASN:HB2	2:A:897:GLU:HG3	1.79	0.65
3:B:251:ILE:HB	3:B:404:PRO:HG3	1.77	0.65
3:B:554:ILE:HG13	3:B:710:ILE:HD13	1.78	0.64
2:A:92:ASN:O	2:A:96:ASN:ND2	2.31	0.64
2:A:1128:LYS:HD2	2:A:1159:LEU:HD21	1.79	0.64
3:B:1141:ASN:OD1	3:B:1141:ASN:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:879:ASN:ND2	3:B:975:ASN:OD1	2.31	0.63
1:C:662:ILE:HD12	1:C:665:LEU:HD21	1.79	0.63
3:B:803:LEU:HD13	3:B:824:THR:HG21	1.79	0.63
3:B:920:LEU:HD13	3:B:946:ILE:HD11	1.80	0.63
2:A:331:LEU:HD23	2:A:332:TYR:HE1	1.64	0.62
2:A:22:LYS:NZ	2:A:28:GLU:OE1	2.32	0.62
2:A:1175:ILE:HD12	2:A:1212:LEU:HD13	1.81	0.62
2:A:215:ILE:HD11	2:A:339:LEU:HD12	1.82	0.62
2:A:910:ASN:HD21	2:A:913:LYS:HG2	1.65	0.61
3:B:875:ASN:HA	3:B:977:VAL:HG12	1.81	0.61
3:B:596:ILE:HG21	3:B:741:ILE:HD11	1.82	0.61
2:A:1164:ALA:O	2:A:1186:GLN:NE2	2.26	0.61
3:B:557:ILE:HD11	3:B:710:ILE:HD12	1.83	0.61
2:A:778:LYS:HA	2:A:782:LEU:HB2	1.83	0.61
2:A:994:THR:HG21	2:A:1059:ILE:HD12	1.82	0.61
3:B:950:LEU:HD11	3:B:953:ASN:HB2	1.83	0.61
3:B:944:ILE:HB	3:B:952:ALA:HB3	1.81	0.61
2:A:63:ASN:O	2:A:504:ASN:ND2	2.32	0.60
2:A:1074:ASP:OD1	2:A:1075:PHE:N	2.33	0.60
2:A:1155:SER:OG	2:A:1158:HIS:ND1	2.32	0.60
1:C:454:VAL:HG22	1:C:483:LYS:HD2	1.82	0.60
3:B:366:PRO:HB3	3:B:384:ASN:HB3	1.84	0.60
3:B:408:ASN:HD22	3:B:621:LYS:CD	2.08	0.59
3:B:909:ILE:HG12	3:B:915:GLU:HG3	1.84	0.59
2:A:961:TRP:CE2	2:A:995:ILE:HG21	2.36	0.59
2:A:1196:ASN:HB3	2:A:1239:PHE:HB3	1.83	0.59
1:C:513:ARG:HB2	1:C:538:THR:HB	1.84	0.59
2:A:1004:LYS:NZ	2:A:1014:GLN:OE1	2.35	0.59
1:C:654:ARG:HH21	1:C:659:ARG:HH11	1.50	0.59
2:A:395:ILE:HG13	2:A:396:ILE:HG23	1.84	0.59
3:B:368:LEU:HD23	3:B:385:ILE:HD12	1.85	0.59
3:B:1025:ASN:ND2	3:B:1157:LEU:O	2.36	0.59
2:A:128:ASP:OD2	2:A:496:ALA:N	2.36	0.59
2:A:467:ASP:N	2:A:467:ASP:OD1	2.35	0.58
2:A:988:ASN:ND2	2:A:988:ASN:O	2.35	0.58
3:B:121:ASN:HA	3:B:165:MET:HE2	1.85	0.58
2:A:1117:LEU:HD11	3:B:412:SER:HB2	1.85	0.58
2:A:1168:THR:HG22	2:A:1170:ASN:H	1.67	0.58
3:B:276:ASN:O	3:B:284:LYS:NZ	2.33	0.58
2:A:160:THR:HA	2:A:185:THR:O	2.04	0.58
3:B:325:TYR:O	3:B:654:LYS:NZ	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1230:ARG:NH2	3:B:804:SER:OG	2.36	0.58
1:C:692:ASN:HA	1:C:695:ILE:HG12	1.85	0.57
2:A:126:ILE:O	2:A:493:GLN:NE2	2.36	0.57
1:C:317:VAL:HG21	3:B:22:ARG:HH22	1.68	0.57
1:C:636:SER:OG	1:C:638:ASN:OD1	2.21	0.57
2:A:909:ASP:O	2:A:910:ASN:ND2	2.36	0.57
3:B:824:THR:HA	3:B:855:THR:O	2.04	0.57
1:C:413:SER:HA	1:C:730:LYS:HE2	1.86	0.57
1:C:362:TYR:HB2	1:C:387:PHE:HE1	1.70	0.57
2:A:448:ILE:HD11	2:A:643:PRO:HG2	1.85	0.57
1:C:400:ARG:NH1	1:C:401:PRO:O	2.38	0.57
2:A:450:THR:HA	2:A:646:LEU:HD11	1.87	0.57
2:A:584:THR:OG1	2:A:750:LYS:NZ	2.30	0.57
3:B:1:MET:O	3:B:90:ASN:ND2	2.32	0.56
1:C:250:LYS:O	1:C:253:ASN:ND2	2.25	0.56
3:B:842:ALA:HB2	3:B:980:GLU:HB2	1.86	0.56
2:A:989:LYS:HG3	2:A:1076:TRP:HD1	1.69	0.56
3:B:1031:ILE:HD12	3:B:1046:ILE:HD12	1.87	0.56
3:B:1044:LEU:HD13	3:B:1098:ILE:HG22	1.87	0.56
2:A:1101:ARG:NH1	2:A:1105:THR:OG1	2.39	0.56
1:C:284:LEU:HD13	1:C:339:SER:HB3	1.87	0.56
1:C:348:LYS:H	1:C:348:LYS:HD3	1.71	0.56
2:A:1175:ILE:HD11	2:A:1221:ALA:HB2	1.86	0.56
1:C:449:SER:O	1:C:453:LEU:CA	2.54	0.56
1:C:230:ARG:NE	1:C:258:GLN:OE1	2.36	0.55
2:A:855:MET:HE2	2:A:1047:PHE:HB3	1.88	0.55
2:A:1098:ILE:HA	2:A:1107:SER:O	2.06	0.55
3:B:332:VAL:HG22	3:B:354:PRO:HG2	1.88	0.55
3:B:810:GLU:N	3:B:813:ASN:O	2.39	0.55
3:B:1083:ASP:C	3:B:1085:THR:H	2.14	0.55
2:A:855:MET:HG3	2:A:872:ILE:HD13	1.89	0.55
3:B:112:ASN:ND2	3:B:116:ASP:OD2	2.37	0.55
1:C:181:TYR:HD1	1:C:185:ASN:HD21	1.54	0.55
2:A:1230:ARG:HH21	3:B:820:SER:HA	1.72	0.55
1:C:601:LYS:H	1:C:601:LYS:HD3	1.71	0.55
3:B:910:ASP:OD1	3:B:914:ASN:N	2.40	0.55
1:C:392:MET:HB3	1:C:396:HIS:HB2	1.89	0.55
1:C:688:LYS:O	1:C:692:ASN:ND2	2.40	0.55
3:B:113:ASN:OD1	3:B:114:THR:N	2.40	0.55
1:C:683:LEU:HD22	1:C:686:ILE:HD11	1.89	0.54
2:A:730:GLU:OE1	2:A:730:GLU:N	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:102:ILE:HD11	3:B:193:LEU:HB3	1.90	0.54
3:B:1132:TYR:HB3	3:B:1156:TYR:HD1	1.71	0.54
2:A:836:LEU:HD23	2:A:836:LEU:H	1.72	0.54
2:A:895:LEU:HD23	2:A:895:LEU:H	1.72	0.54
1:C:215:PHE:CE1	1:C:233:CYS:HB3	2.42	0.54
1:C:426:PHE:HA	1:C:429:HIS:HD2	1.72	0.54
2:A:488:LEU:HD13	2:A:488:LEU:H	1.71	0.54
1:C:306:ASP:OD1	1:C:307:VAL:N	2.41	0.54
1:C:702:LEU:HD12	1:C:703:PRO:HD2	1.89	0.54
2:A:914:ASN:OD1	2:A:914:ASN:N	2.40	0.54
1:C:689:ASP:HA	1:C:692:ASN:HD21	1.73	0.53
2:A:726:TYR:HB3	2:A:730:GLU:HB2	1.90	0.53
2:A:817:ASP:O	2:A:821:ASN:ND2	2.41	0.53
2:A:1106:LEU:HB2	2:A:1219:VAL:HB	1.90	0.53
3:B:313:MET:HE1	3:B:349:ILE:HG13	1.90	0.53
2:A:193:ARG:HD2	2:A:201:GLU:HB3	1.90	0.53
2:A:331:LEU:HD23	2:A:332:TYR:CE1	2.43	0.53
3:B:615:LEU:HD11	3:B:749:ILE:HD11	1.90	0.53
3:B:408:ASN:ND2	3:B:621:LYS:CD	2.59	0.53
2:A:368:ILE:HG23	2:A:395:ILE:HG22	1.90	0.53
2:A:1112:ARG:NH1	2:A:1120:ARG:O	2.42	0.53
2:A:634:LEU:HD21	2:A:693:ILE:HG23	1.91	0.53
3:B:1035:LYS:HB2	3:B:1042:ILE:HD11	1.91	0.53
2:A:219:HIS:ND1	2:A:250:GLU:OE2	2.41	0.52
2:A:962:THR:OG1	2:A:972:LYS:NZ	2.38	0.52
3:B:603:MET:HE2	3:B:614:ASN:HD22	1.75	0.52
2:A:129:ALA:HB2	2:A:167:LEU:HD21	1.92	0.52
2:A:568:GLN:O	2:A:570:ALA:N	2.42	0.52
3:B:871:PHE:HB3	3:B:982:LEU:HA	1.92	0.52
2:A:417:SER:HB2	2:A:421:ILE:HG23	1.90	0.52
2:A:920:TRP:HB2	2:A:1045:ARG:HG2	1.90	0.52
3:B:1148:ASN:ND2	3:B:1150:ASP:OD1	2.43	0.52
3:B:1146:ASP:OD1	3:B:1147:LEU:N	2.42	0.52
2:A:1203:ASN:OD1	2:A:1205:ASN:ND2	2.43	0.52
1:C:393:VAL:HG12	1:C:394:GLU:H	1.75	0.51
3:B:307:SER:OG	3:B:312:ILE:O	2.25	0.51
1:C:483:LYS:HB2	1:C:494:GLU:HG2	1.92	0.51
3:B:948:ASN:ND2	3:B:995:LEU:HD23	2.26	0.51
1:C:469:GLN:OE1	1:C:471:ARG:NE	2.42	0.51
2:A:30:TYR:HB3	2:A:44:GLU:HG3	1.93	0.51
3:B:809:GLN:HA	3:B:814:ASN:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:TYR:HB3	1:C:282:PHE:CE1	2.46	0.51
3:B:1132:TYR:HB3	3:B:1156:TYR:CD1	2.46	0.50
1:C:241:LYS:NZ	1:C:243:ASN:O	2.44	0.50
2:A:376:ASN:HB3	2:A:381:LYS:HA	1.92	0.50
2:A:961:TRP:CD2	2:A:995:ILE:HG21	2.46	0.50
2:A:1249:TRP:CD1	2:A:1251:GLU:HG3	2.47	0.50
3:B:110:TYR:HB3	3:B:118:ARG:HB2	1.94	0.50
2:A:168:ARG:H	2:A:168:ARG:HD2	1.76	0.50
1:C:534:SER:OG	1:C:536:ASP:OD2	2.23	0.50
2:A:134:ILE:HD13	2:A:144:LEU:HB2	1.93	0.50
2:A:1035:ASN:O	2:A:1035:ASN:ND2	2.45	0.50
3:B:402:ILE:HD12	3:B:402:ILE:N	2.27	0.50
3:B:1042:ILE:HG13	3:B:1100:LEU:HD13	1.94	0.50
3:B:1082:LEU:HD13	3:B:1084:GLY:H	1.77	0.50
3:B:1090:ASP:HA	3:B:1108:GLN:HG2	1.94	0.50
1:C:265:ASP:OD1	1:C:280:GLN:NE2	2.44	0.49
2:A:671:LEU:HD13	2:A:818:THR:HG21	1.94	0.49
3:B:189:LEU:O	3:B:193:LEU:HG	2.12	0.49
2:A:728:LEU:O	2:A:732:ASN:ND2	2.45	0.49
2:A:154:GLU:HB2	2:A:155:PRO:HD2	1.93	0.49
3:B:480:ILE:HD11	3:B:665:LYS:HE2	1.94	0.49
2:A:205:ASP:OD1	2:A:369:TYR:OH	2.25	0.49
3:B:148:ASN:HA	3:B:169:TRP:O	2.12	0.49
3:B:971:LEU:HD12	3:B:972:SER:H	1.78	0.49
3:B:1006:TYR:HE1	3:B:1070:TYR:HB3	1.77	0.49
2:A:1121:LEU:HB3	2:A:1243:ILE:HD13	1.95	0.49
3:B:493:LYS:H	3:B:493:LYS:HD2	1.77	0.49
2:A:508:ASP:OD1	2:A:508:ASP:N	2.46	0.49
1:C:189:LYS:NZ	1:C:218:TRP:O	2.46	0.48
2:A:740:ILE:HD12	2:A:740:ILE:H	1.78	0.48
2:A:1086:TYR:CG	2:A:1242:PHE:HB3	2.48	0.48
2:A:1086:TYR:HE2	2:A:1129:ILE:HD11	1.78	0.48
3:B:88:ARG:HE	3:B:343:GLY:HA2	1.78	0.48
1:C:509:HIS:HB2	1:C:542:MET:O	2.13	0.48
1:C:727:ASP:OD1	1:C:727:ASP:N	2.46	0.48
3:B:340:ASN:HD22	3:B:342:ASN:H	1.62	0.48
3:B:409:TYR:CD1	3:B:409:TYR:N	2.75	0.48
3:B:911:SER:HB2	3:B:961:ASN:HD22	1.78	0.48
2:A:124:PHE:HD2	2:A:296:LEU:HD21	1.79	0.48
3:B:273:ILE:HG23	3:B:279:ILE:HD13	1.95	0.48
2:A:418:VAL:O	2:A:421:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:829:PRO:HG3	3:B:850:GLN:HB3	1.95	0.48
3:B:852:ILE:HB	3:B:970:LEU:HB3	1.94	0.48
3:B:884:LYS:HB2	3:B:971:LEU:HD11	1.94	0.48
2:A:569:ALA:HB2	2:A:730:GLU:HG2	1.95	0.48
2:A:1055:ASP:O	2:A:1059:ILE:HG12	2.14	0.48
1:C:207:ASN:OD1	3:B:118:ARG:NH1	2.47	0.48
2:A:716:LYS:HG3	2:A:738:TYR:CE1	2.48	0.48
1:C:383:ASP:OD1	1:C:383:ASP:N	2.44	0.47
2:A:892:ASN:HD22	2:A:1036:CYS:HB3	1.79	0.47
3:B:730:PHE:O	3:B:734:MET:HG2	2.13	0.47
1:C:624:ASN:O	1:C:627:ILE:HG13	2.14	0.47
2:A:851:SER:OG	2:A:854:ASN:OD1	2.28	0.47
3:B:845:LEU:HD22	3:B:972:SER:HB2	1.95	0.47
2:A:653:PHE:O	2:A:659:ASN:ND2	2.47	0.47
2:A:996:THR:HG22	2:A:1053:GLU:HG3	1.96	0.47
3:B:1042:ILE:HG23	3:B:1100:LEU:HB2	1.96	0.47
2:A:1089:LEU:HD23	2:A:1112:ARG:HH21	1.79	0.47
1:C:560:VAL:HA	1:C:563:VAL:HG22	1.96	0.47
2:A:495:ASP:OD1	2:A:495:ASP:N	2.47	0.47
3:B:1:MET:HE1	3:B:100:SER:HA	1.95	0.47
3:B:916:LYS:HB2	3:B:959:ILE:HD11	1.97	0.47
2:A:126:ILE:HD13	2:A:489:ASN:HD21	1.80	0.47
2:A:443:TYR:HD2	2:A:684:PHE:HZ	1.62	0.47
2:A:1231:ASP:OD1	2:A:1232:HIS:N	2.42	0.47
3:B:752:CYS:O	3:B:760:LYS:NZ	2.40	0.47
3:B:974:ASN:ND2	3:B:974:ASN:O	2.48	0.47
1:C:482:PHE:HA	1:C:495:ILE:HG13	1.97	0.47
2:A:173:PRO:HG2	2:A:180:SER:OG	2.15	0.47
3:B:334:ASP:HB3	3:B:337:LYS:HB3	1.97	0.47
1:C:215:PHE:HE1	1:C:233:CYS:HB3	1.80	0.46
2:A:240:LEU:HD22	2:A:520:PHE:HE2	1.79	0.46
2:A:917:ILE:HG13	2:A:1049:ILE:HG12	1.97	0.46
2:A:946:ASN:ND2	2:A:966:ASN:OD1	2.48	0.46
1:C:449:SER:O	1:C:453:LEU:N	2.48	0.46
3:B:171:GLN:HE21	3:B:174:LEU:HG	1.80	0.46
3:B:485:ASP:HB3	3:B:488:LYS:HB2	1.96	0.46
3:B:1063:ASN:HD22	3:B:1068:LYS:HD3	1.80	0.46
1:C:264:PHE:CE2	1:C:266:SER:HB3	2.51	0.46
3:B:65:ASP:OD1	3:B:67:ASN:N	2.49	0.46
2:A:1126:LYS:HB3	2:A:1153:VAL:HG23	1.98	0.46
3:B:904:LEU:HD11	3:B:931:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:684:PRO:O	1:C:688:LYS:HG2	2.16	0.46
3:B:62:GLY:HA2	3:B:146:ILE:HD11	1.98	0.46
1:C:567:ILE:HB	1:C:607:ILE:HD11	1.96	0.46
3:B:313:MET:HB3	3:B:790:THR:HG23	1.98	0.46
1:C:201:TYR:HE1	1:C:208:GLU:HB3	1.81	0.45
1:C:230:ARG:HG2	1:C:256:ILE:HD11	1.98	0.45
1:C:175:ILE:HG23	1:C:419:PHE:HE1	1.82	0.45
2:A:20:TYR:O	2:A:134:ILE:HA	2.15	0.45
2:A:938:THR:HA	2:A:953:SER:HA	1.99	0.45
2:A:1098:ILE:HD11	2:A:1240:TRP:HZ3	1.81	0.45
2:A:1161:PRO:HG2	2:A:1178:SER:HB3	1.98	0.45
2:A:1229:MET:O	2:A:1233:THR:OG1	2.26	0.45
2:A:891:TYR:CD1	2:A:1041:TYR:HB3	2.52	0.45
3:B:971:LEU:HD12	3:B:972:SER:N	2.32	0.45
1:C:214:GLU:HG3	1:C:236:LYS:HB2	1.97	0.45
2:A:669:ASN:O	2:A:673:GLU:HG2	2.17	0.45
2:A:567:VAL:HG11	2:A:575:TRP:CG	2.52	0.45
3:B:535:SER:O	3:B:539:THR:OG1	2.27	0.45
2:A:280:LYS:HG2	2:A:319:VAL:HG11	1.99	0.45
3:B:1118:ILE:HG12	3:B:1157:LEU:HD13	1.99	0.45
2:A:913:LYS:O	2:A:913:LYS:HG3	2.16	0.44
2:A:1082:TYR:OH	2:A:1146:ASP:OD2	2.34	0.44
3:B:735:GLU:O	3:B:738:ILE:HG13	2.17	0.44
1:C:603:ILE:HA	1:C:606:VAL:HG12	1.99	0.44
1:C:647:ALA:O	1:C:651:ASN:ND2	2.43	0.44
2:A:70:ASP:HB3	2:A:157:LEU:HD11	1.99	0.44
2:A:233:ILE:HD12	2:A:252:PHE:HE2	1.82	0.44
2:A:684:PHE:O	2:A:688:ASN:ND2	2.33	0.44
3:B:7:LEU:HD13	3:B:33:PHE:HB3	2.00	0.44
3:B:407:LEU:CD2	3:B:409:TYR:CE2	3.01	0.44
1:C:730:LYS:NZ	1:C:732:GLN:HE21	2.16	0.44
2:A:128:ASP:OD2	2:A:495:ASP:N	2.50	0.44
3:B:254:TYR:O	3:B:258:THR:OG1	2.27	0.44
3:B:423:ILE:O	3:B:427:GLU:HG2	2.18	0.44
3:B:903:GLY:HA2	3:B:923:ILE:HB	1.99	0.44
1:C:185:ASN:ND2	1:C:219:GLN:HE22	2.15	0.44
2:A:74:LEU:N	2:A:79:GLU:OE1	2.50	0.44
2:A:448:ILE:HA	2:A:646:LEU:HD22	2.00	0.44
3:B:928:TRP:HE1	3:B:1013:GLU:CD	2.25	0.44
1:C:191:ASP:OD1	1:C:192:ASN:N	2.51	0.44
2:A:452:LYS:HD2	2:A:452:LYS:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:342:LYS:HE2	2:A:342:LYS:HB2	1.83	0.44
2:A:388:ASN:HB3	2:A:391:LEU:HB2	2.00	0.44
2:A:448:ILE:HG23	2:A:646:LEU:HB3	1.99	0.44
3:B:88:ARG:HE	3:B:343:GLY:CA	2.30	0.44
3:B:617:ASN:O	3:B:621:LYS:HG2	2.18	0.44
1:C:631:GLU:HG3	1:C:632:VAL:HG23	1.99	0.44
2:A:113:TYR:HE1	2:A:286:LEU:HD13	1.83	0.44
2:A:1131:ARG:NH1	2:A:1137:THR:OG1	2.49	0.44
1:C:229:ILE:HG13	1:C:259:VAL:O	2.18	0.44
2:A:124:PHE:CD2	2:A:296:LEU:HD21	2.53	0.44
2:A:275:LEU:HD23	2:A:328:PHE:CD2	2.52	0.44
2:A:1182:ASN:HD22	2:A:1182:ASN:H	1.65	0.44
3:B:92:ASN:OD1	3:B:93:VAL:N	2.51	0.44
3:B:528:LYS:HG3	3:B:864:THR:HG22	2.00	0.44
2:A:1098:ILE:HD11	2:A:1240:TRP:CZ3	2.52	0.43
2:A:454:ILE:H	2:A:651:LYS:HE3	1.83	0.43
2:A:1009:GLY:HA2	2:A:1059:ILE:HG22	1.99	0.43
3:B:762:HIS:HA	3:B:765:MET:HE2	1.99	0.43
3:B:1131:ILE:O	3:B:1158:TRP:NE1	2.48	0.43
3:B:1049:GLU:H	3:B:1049:GLU:HG3	1.55	0.43
1:C:211:ILE:HD13	1:C:322:VAL:HG13	2.00	0.43
1:C:576:SER:HB2	1:C:578:LYS:HE3	2.00	0.43
2:A:38:ASN:HD22	2:A:147:ASN:ND2	2.15	0.43
3:B:645:TYR:OH	3:B:721:VAL:HG21	2.18	0.43
1:C:204:VAL:HB	1:C:209:TYR:HE1	1.83	0.43
3:B:373:ILE:HD13	3:B:460:ASN:HB3	2.00	0.43
3:B:604:LEU:HD13	3:B:604:LEU:HA	1.91	0.43
1:C:480:ASN:HA	1:C:483:LYS:NZ	2.34	0.43
2:A:511:GLN:NE2	2:A:513:ASP:OD1	2.40	0.43
2:A:922:ARG:HH21	2:A:988:ASN:HD21	1.66	0.43
3:B:121:ASN:OD1	3:B:121:ASN:N	2.51	0.43
1:C:295:ASN:OD1	1:C:295:ASN:N	2.51	0.43
2:A:473:LEU:HD12	3:B:1027:VAL:HG21	2.00	0.43
1:C:563:VAL:O	1:C:567:ILE:HG12	2.19	0.43
2:A:972:LYS:HE3	3:B:772:LEU:HD22	1.99	0.43
2:A:1113:SER:OG	2:A:1120:ARG:NH1	2.52	0.43
2:A:20:TYR:HB3	2:A:29:PHE:HB3	1.99	0.43
2:A:276:LEU:HD22	2:A:280:LYS:HE3	2.00	0.43
3:B:651:MET:HA	3:B:654:LYS:HE3	2.00	0.43
3:B:838:ILE:O	3:B:1004:ASN:ND2	2.49	0.43
3:B:101:LEU:HA	3:B:104:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:810:GLU:HG3	3:B:811:GLN:H	1.84	0.42
2:A:155:PRO:HG2	2:A:501:TYR:CZ	2.54	0.42
3:B:408:ASN:HB3	3:B:624:PHE:HB2	2.02	0.42
2:A:229:THR:HA	2:A:248:ASN:HD21	1.85	0.42
3:B:3:ILE:CD1	3:B:87:GLN:HG3	2.49	0.42
3:B:534:TYR:CD1	3:B:663:ILE:HG13	2.55	0.42
2:A:258:THR:HG21	2:A:832:ASP:HB3	2.01	0.42
2:A:331:LEU:HB3	2:A:332:TYR:HD1	1.84	0.42
3:B:84:LYS:HE2	3:B:84:LYS:HB2	1.85	0.42
2:A:920:TRP:HB2	2:A:1045:ARG:CG	2.50	0.42
3:B:778:ASP:HB3	3:B:781:ASN:HB2	2.01	0.42
3:B:1142:TRP:HB2	3:B:1144:ILE:HG13	2.02	0.42
1:C:564:VAL:HG11	1:C:572:PHE:HB2	2.02	0.42
1:C:683:LEU:HB3	1:C:684:PRO:HD3	2.00	0.42
3:B:153:TYR:CD2	3:B:444:ALA:HB2	2.54	0.42
1:C:261:LEU:HD13	1:C:284:LEU:HB3	2.02	0.42
2:A:589:GLN:HE21	2:A:605:TYR:HD2	1.67	0.42
3:B:749:ILE:HD13	3:B:749:ILE:HA	1.94	0.42
1:C:621:LYS:HD3	1:C:621:LYS:HA	1.90	0.42
2:A:388:ASN:ND2	2:A:391:LEU:HD23	2.34	0.42
2:A:450:THR:OG1	2:A:451:PRO:HD3	2.19	0.42
3:B:301:LEU:HD11	3:B:418:LEU:HD21	2.00	0.42
3:B:1055:LYS:HZ3	3:B:1056:PRO:HD2	1.84	0.42
1:C:512:TYR:HE1	1:C:539:ILE:HG23	1.85	0.42
2:A:922:ARG:NH2	2:A:988:ASN:HD21	2.18	0.42
3:B:25:LYS:HG3	3:B:28:VAL:HG22	2.00	0.42
2:A:191:SER:HB2	2:A:360:LEU:HD11	2.02	0.42
2:A:251:GLU:HA	2:A:254:THR:HG22	2.01	0.42
2:A:841:ASN:O	2:A:845:LYS:N	2.47	0.42
2:A:1151:ASN:HA	2:A:1161:PRO:HA	2.01	0.41
3:B:872:TRP:HB2	3:B:980:GLU:HB3	2.01	0.41
2:A:44:GLU:OE1	2:A:80:LYS:NZ	2.53	0.41
2:A:440:GLU:H	2:A:440:GLU:CD	2.28	0.41
2:A:1117:LEU:HD12	2:A:1117:LEU:HA	1.89	0.41
1:C:454:VAL:HG13	1:C:483:LYS:NZ	2.35	0.41
2:A:700:ARG:NH1	2:A:703:GLN:OE1	2.54	0.41
2:A:920:TRP:NE1	2:A:1066:GLU:OE1	2.33	0.41
3:B:706:ALA:O	3:B:710:ILE:HG12	2.20	0.41
1:C:627:ILE:O	1:C:630:GLU:HG3	2.19	0.41
2:A:253:LEU:HD12	2:A:253:LEU:HA	1.89	0.41
2:A:720:GLU:HG2	2:A:738:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:629:ILE:HD12	3:B:734:MET:HE1	2.02	0.41
2:A:836:LEU:HD21	3:B:949:ILE:HA	2.02	0.41
2:A:1225:TYR:CD2	2:A:1238:CYS:HB3	2.55	0.41
2:A:989:LYS:HG3	2:A:1076:TRP:CD1	2.52	0.41
3:B:303:LEU:HD12	3:B:303:LEU:HA	1.91	0.41
3:B:845:LEU:HD13	3:B:972:SER:OG	2.21	0.41
2:A:660:LYS:NZ	2:A:804:LEU:O	2.48	0.41
2:A:750:LYS:HZ2	2:A:1000:LEU:HD12	1.86	0.41
2:A:975:PHE:CZ	2:A:977:TYR:HB3	2.56	0.41
1:C:446:PHE:HB3	1:C:455:ILE:HD11	2.01	0.41
1:C:654:ARG:HH21	1:C:659:ARG:NH1	2.17	0.41
2:A:123:GLN:HA	2:A:291:VAL:HG12	2.02	0.41
2:A:955:ASN:HB3	2:A:958:GLU:HB3	2.02	0.41
3:B:805:LEU:HD21	3:B:854:PHE:HE1	1.86	0.41
1:C:192:ASN:ND2	1:C:192:ASN:O	2.54	0.41
1:C:357:PRO:HA	1:C:393:VAL:HG22	2.02	0.41
1:C:406:ASP:OD1	1:C:406:ASP:N	2.53	0.41
1:C:726:ILE:HG12	1:C:737:LEU:HD21	2.03	0.41
2:A:974:ALA:HB2	3:B:772:LEU:HD21	2.03	0.41
3:B:190:ILE:O	3:B:194:ILE:HG13	2.21	0.41
3:B:906:PHE:HZ	3:B:935:ILE:HD11	1.86	0.41
1:C:493:VAL:HB	1:C:514:GLN:HG3	2.03	0.41
2:A:57:PRO:HG3	2:A:403:GLY:HA2	2.02	0.41
3:B:405:TYR:O	3:B:405:TYR:CD2	2.74	0.41
3:B:844:HIS:NE2	3:B:976:ASN:OD1	2.45	0.41
3:B:910:ASP:HA	3:B:962:ILE:HG22	2.03	0.41
2:A:169:ASN:ND2	2:A:169:ASN:O	2.53	0.40
3:B:1124:LEU:O	3:B:1131:ILE:HG12	2.21	0.40
3:B:1135:ILE:H	3:B:1135:ILE:HG13	1.69	0.40
1:C:245:ASP:N	1:C:245:ASP:OD1	2.54	0.40
2:A:50:THR:HG22	2:A:501:TYR:CG	2.55	0.40
2:A:306:LYS:HE3	2:A:306:LYS:HB2	1.97	0.40
2:A:737:LYS:HB3	2:A:737:LYS:HE3	1.87	0.40
2:A:821:ASN:ND2	3:B:900:GLU:OE2	2.54	0.40
3:B:622:ASN:O	3:B:626:LEU:HG	2.21	0.40
3:B:637:TRP:CD1	3:B:722:PHE:HB2	2.57	0.40
1:C:205:ARG:NH1	3:B:434:ASP:O	2.53	0.40
1:C:435:LEU:HG	1:C:440:ILE:HD11	2.03	0.40
2:A:493:GLN:OE1	2:A:493:GLN:N	2.39	0.40
2:A:1055:ASP:OD1	2:A:1055:ASP:N	2.46	0.40
2:A:1122:TYR:OH	2:A:1249:TRP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:212:PRO:HA	3:B:226:GLU:HG2	2.03	0.40
3:B:632:ASN:O	3:B:636:GLN:HG3	2.22	0.40
3:B:1031:ILE:H	3:B:1031:ILE:HG13	1.71	0.40
1:C:342:LEU:O	1:C:356:LYS:NZ	2.55	0.40
2:A:32:SER:OG	2:A:42:ILE:HG12	2.21	0.40
2:A:936:GLU:OE2	2:A:953:SER:OG	2.34	0.40
3:B:566:THR:HG22	3:B:567:ASN:H	1.87	0.40
3:B:626:LEU:HD22	3:B:734:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	576/748 (77%)	560 (97%)	16 (3%)	0	100	100
2	A	1235/1252 (99%)	1150 (93%)	84 (7%)	1 (0%)	48	78
3	B	1161/1163 (100%)	1108 (95%)	51 (4%)	2 (0%)	43	71
All	All	2972/3163 (94%)	2818 (95%)	151 (5%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	569	ALA
3	B	409	TYR
3	B	24	ARG

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	C	507/677 (75%)	486 (96%)	21 (4%)	27	52
2	A	1118/1150 (97%)	1083 (97%)	35 (3%)	35	59
3	B	1102/1103 (100%)	1071 (97%)	31 (3%)	38	60
All	All	2727/2930 (93%)	2640 (97%)	87 (3%)	35	58

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	171	LEU
1	C	179	VAL
1	C	242	ILE
1	C	245	ASP
1	C	282	PHE
1	C	295	ASN
1	C	303	ARG
1	C	304	ILE
1	C	305	THR
1	C	319	LEU
1	C	343	LEU
1	C	368	THR
1	C	378	GLU
1	C	382	LEU
1	C	412	LEU
1	C	429	HIS
1	C	430	PHE
1	C	506	VAL
1	C	662	ILE
1	C	683	LEU
1	C	716	ILE
2	A	59	THR
2	A	144	LEU
2	A	150	ILE
2	A	253	LEU
2	A	258	THR
2	A	260	LEU
2	A	276	LEU
2	A	291	VAL
2	A	297	ASN

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Mol	Chain	Res	Type
2	A	319	VAL
2	A	405	VAL
2	A	416	VAL
2	A	425	ILE
2	A	467	ASP
2	A	488	LEU
2	A	495	ASP
2	A	519	VAL
2	A	528	VAL
2	A	535	VAL
2	A	641	LEU
2	A	646	LEU
2	A	728	LEU
2	A	738	TYR
2	A	782	LEU
2	A	906	ILE
2	A	911	LYS
2	A	914	ASN
2	A	917	ILE
2	A	988	ASN
2	A	1040	ARG
2	A	1126	LYS
2	A	1127	VAL
2	A	1129	ILE
2	A	1153	VAL
2	A	1236	ASN
3	B	3	ILE
3	B	93	VAL
3	B	115	GLU
3	B	129	GLU
3	B	133	THR
3	B	136	LEU
3	B	137	VAL
3	B	293	ILE
3	B	332	VAL
3	B	421	VAL
3	B	490	ILE
3	B	518	ASP
3	B	566	THR
3	B	687	LEU
3	B	782	MET
3	B	792	LEU

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Mol	Chain	Res	Type
3	B	811	GLN
3	B	815	VAL
3	B	819	THR
3	B	869	ILE
3	B	892	ASN
3	B	950	LEU
3	B	971	LEU
3	B	1009	ASN
3	B	1031	ILE
3	B	1036	ILE
3	B	1049	GLU
3	B	1082	LEU
3	B	1109	ILE
3	B	1120	ASN
3	B	1141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	185	ASN
1	C	192	ASN
1	C	344	ASN
1	C	381	ASN
1	C	470	ASN
1	C	637	GLN
1	C	692	ASN
1	C	732	GLN
2	A	147	ASN
2	A	164	ASN
2	A	290	GLN
2	A	390	ASN
2	A	561	ASN
2	A	589	GLN
2	A	736	ASN
2	A	780	ASN
2	A	808	GLN
2	A	821	ASN
2	A	956	HIS
2	A	1022	ASN
2	A	1095	ASN
2	A	1151	ASN
2	A	1182	ASN

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Mol	Chain	Res	Type
3	B	54	ASN
3	B	135	ASN
3	B	311	GLN
3	B	400	ASN
3	B	408	ASN
3	B	452	ASN
3	B	460	ASN
3	B	481	ASN
3	B	568	ASN
3	B	614	ASN
3	B	623	ASN
3	B	736	GLN
3	B	762	HIS
3	B	823	ASN
3	B	878	GLN
3	B	879	ASN
3	B	901	ASN
3	B	948	ASN
3	B	1047	ASN
3	B	1048	ASN
3	B	1065	ASN
3	B	1127	ASN
3	B	1148	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](#)

There are no chain breaks in this entry.

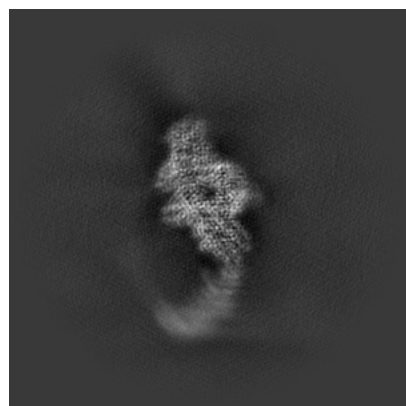
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43784. These allow visual inspection of the internal detail of the map and identification of artifacts.

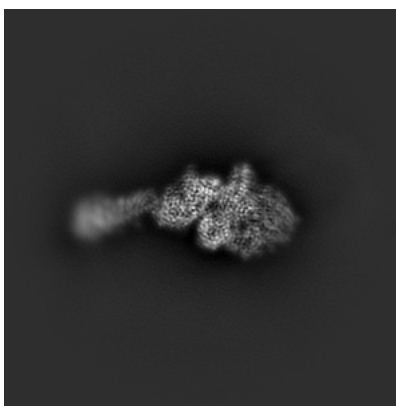
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

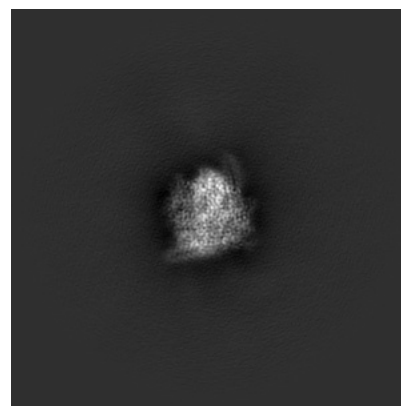
6.1.1 Primary map



X

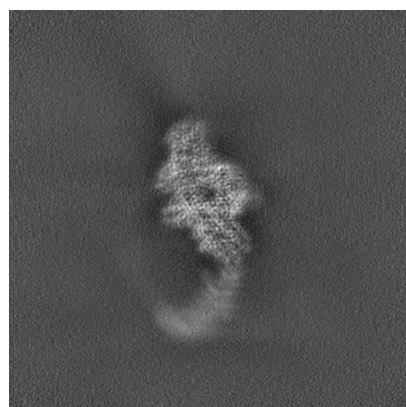


Y

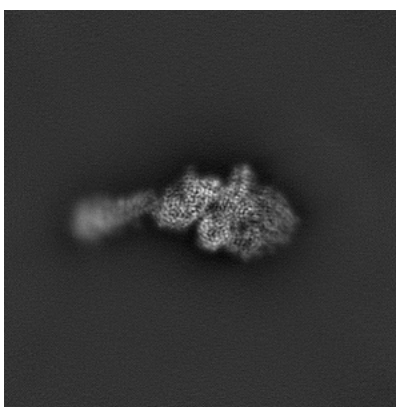


Z

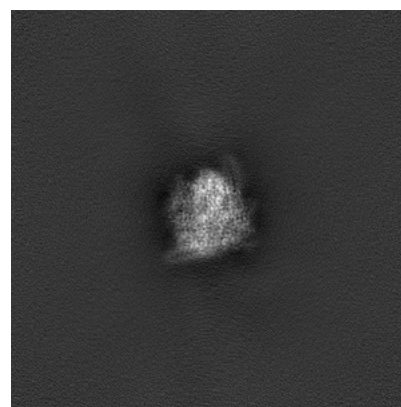
6.1.2 Raw map



X



Y

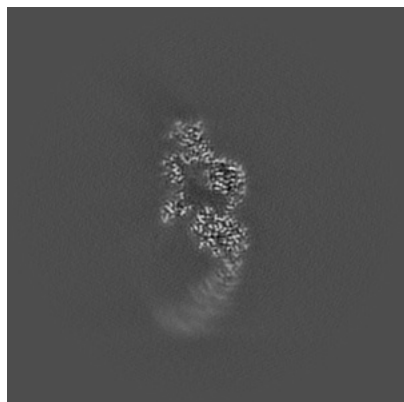


Z

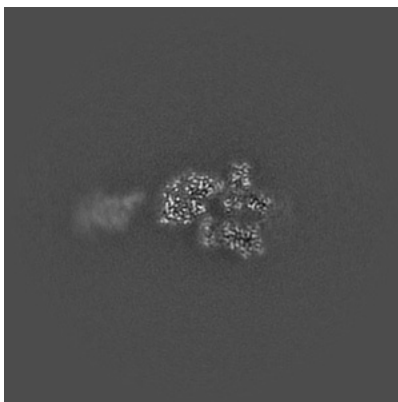
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

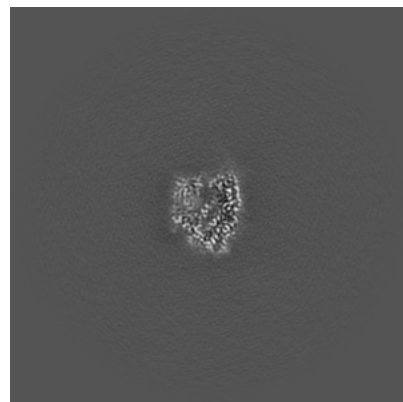
6.2.1 Primary map



X Index: 256

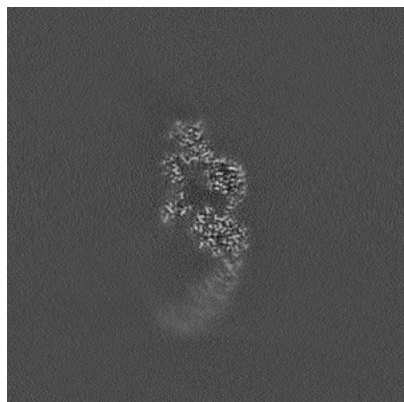


Y Index: 256

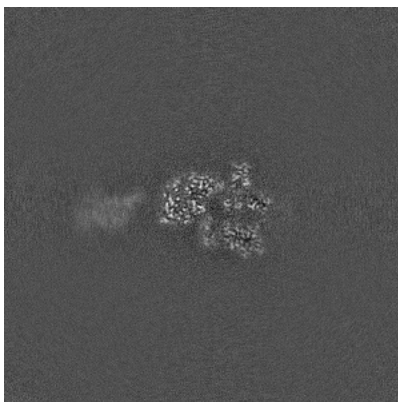


Z Index: 256

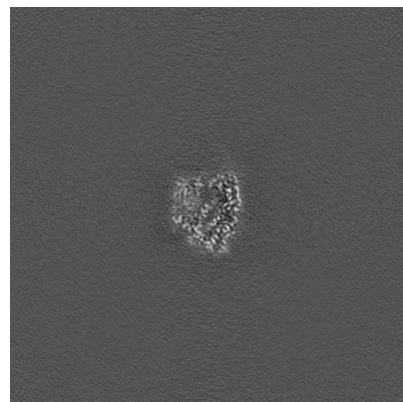
6.2.2 Raw map



X Index: 256



Y Index: 256

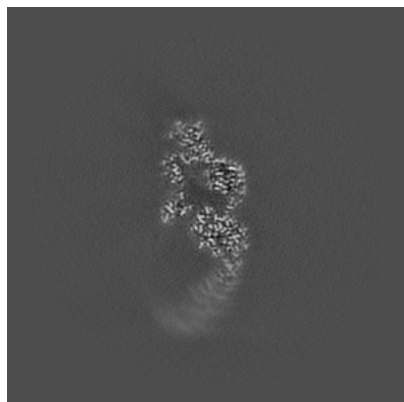


Z Index: 256

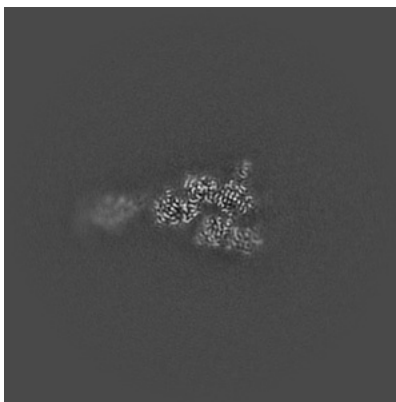
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

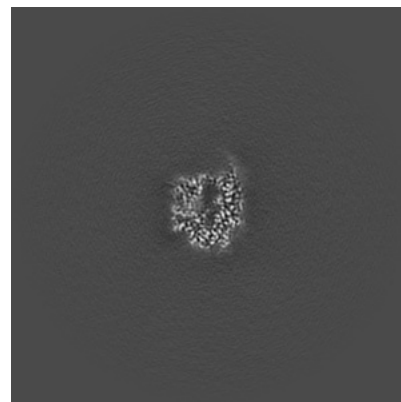
6.3.1 Primary map



X Index: 256

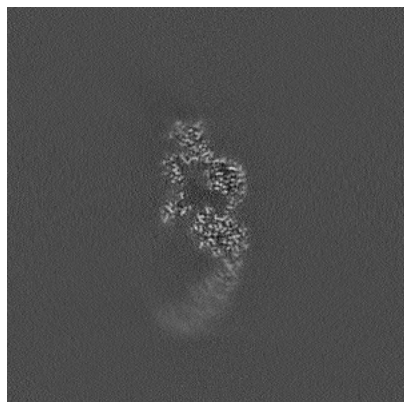


Y Index: 266

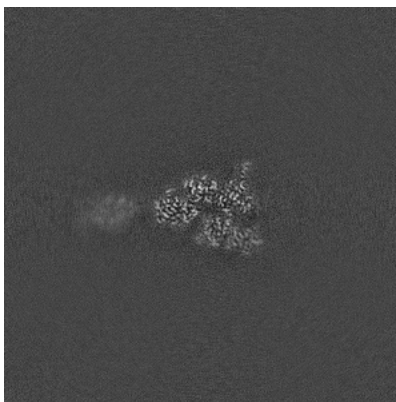


Z Index: 259

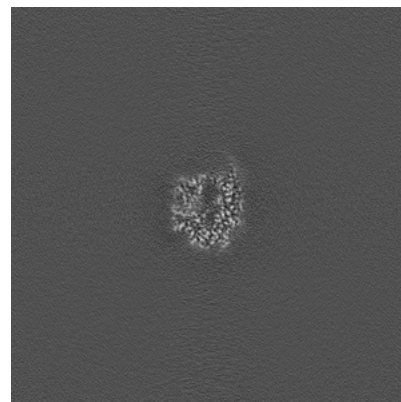
6.3.2 Raw map



X Index: 256



Y Index: 265



Z Index: 259

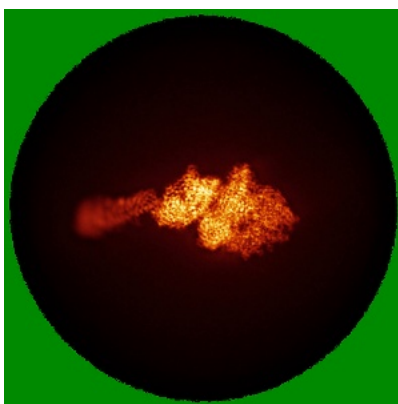
The images above show the largest variance slices of the map in three orthogonal directions.

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

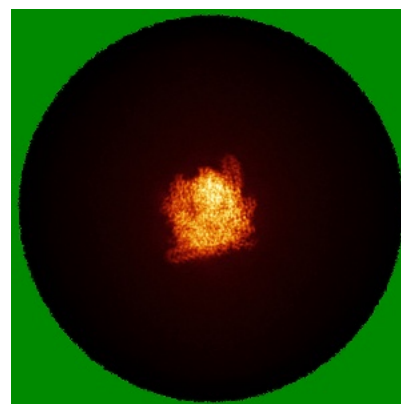
6.4.1 Primary map



X

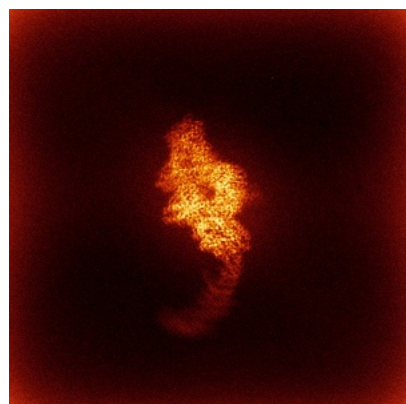


Y

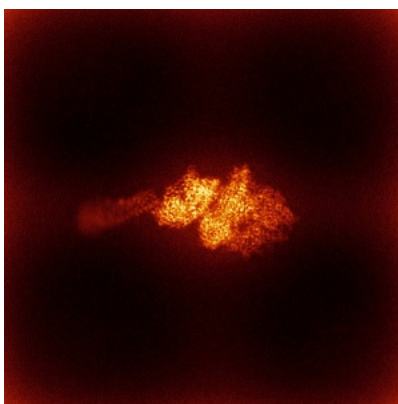


Z

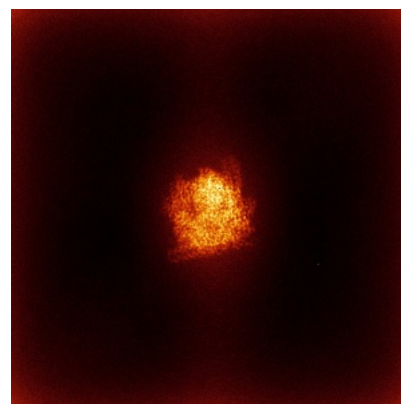
6.4.2 Raw map



X



Y

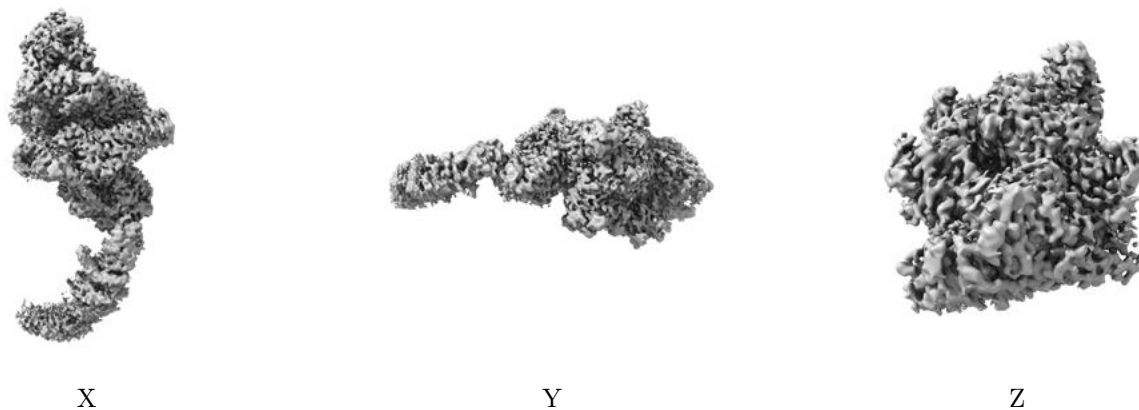


Z

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.

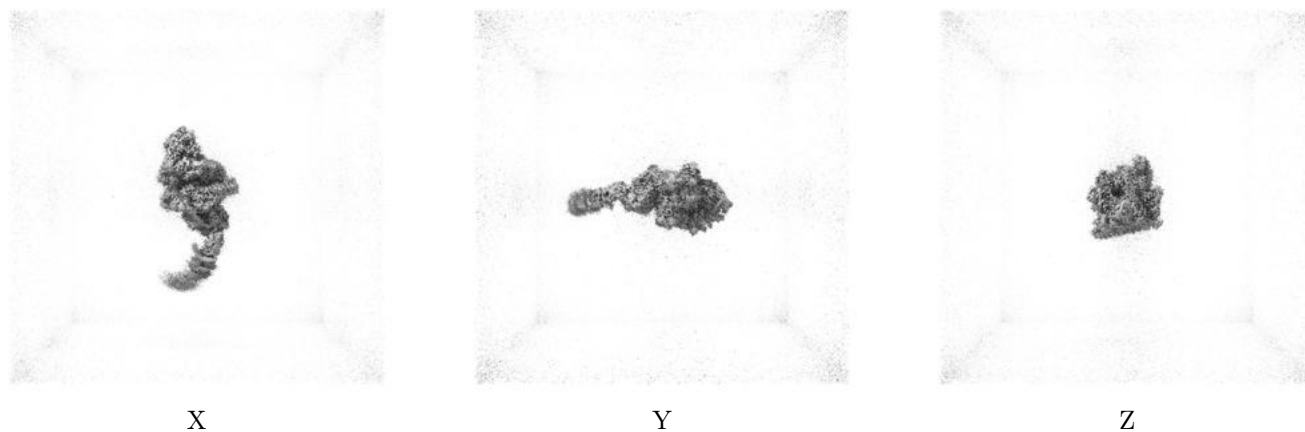
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

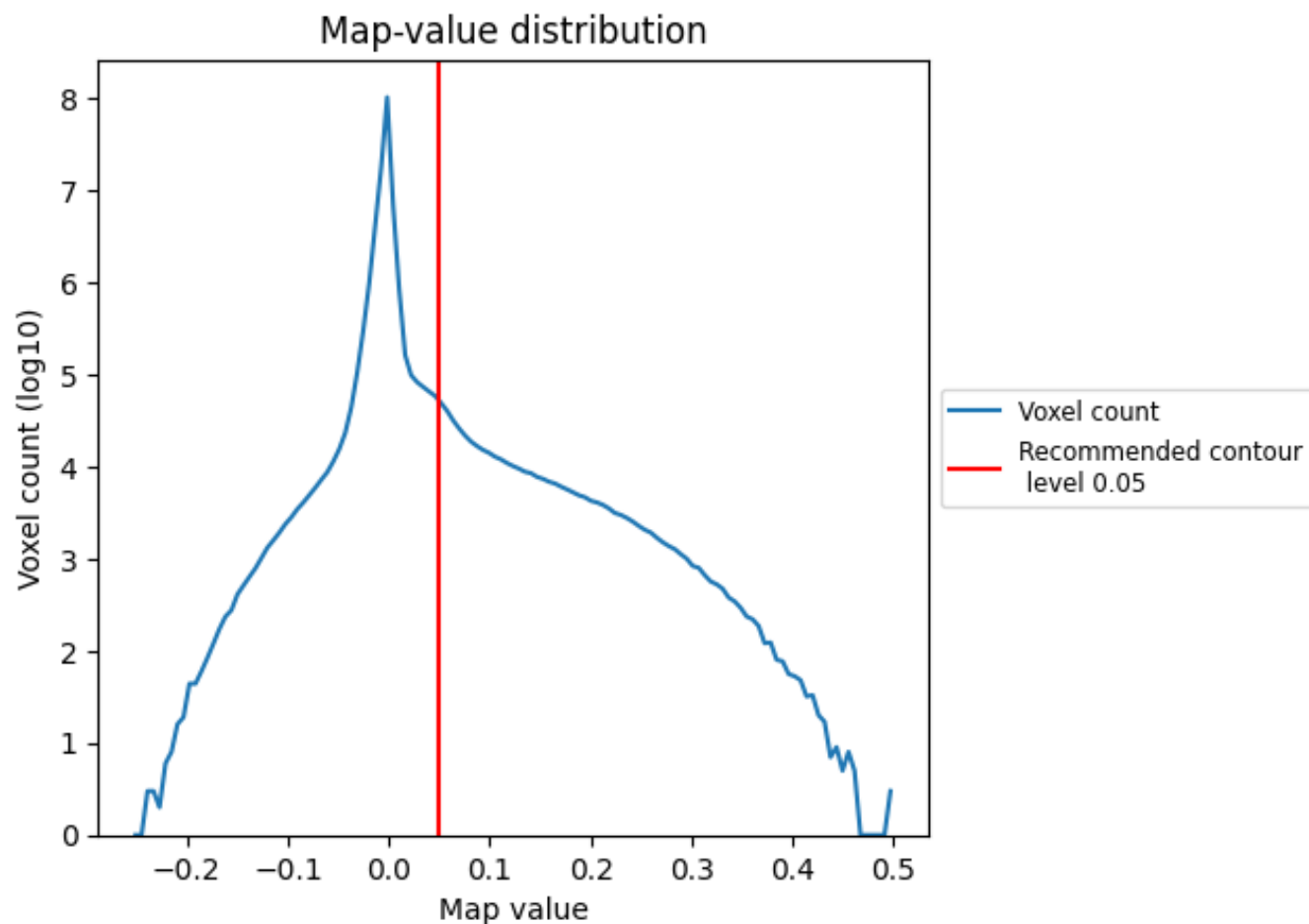
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

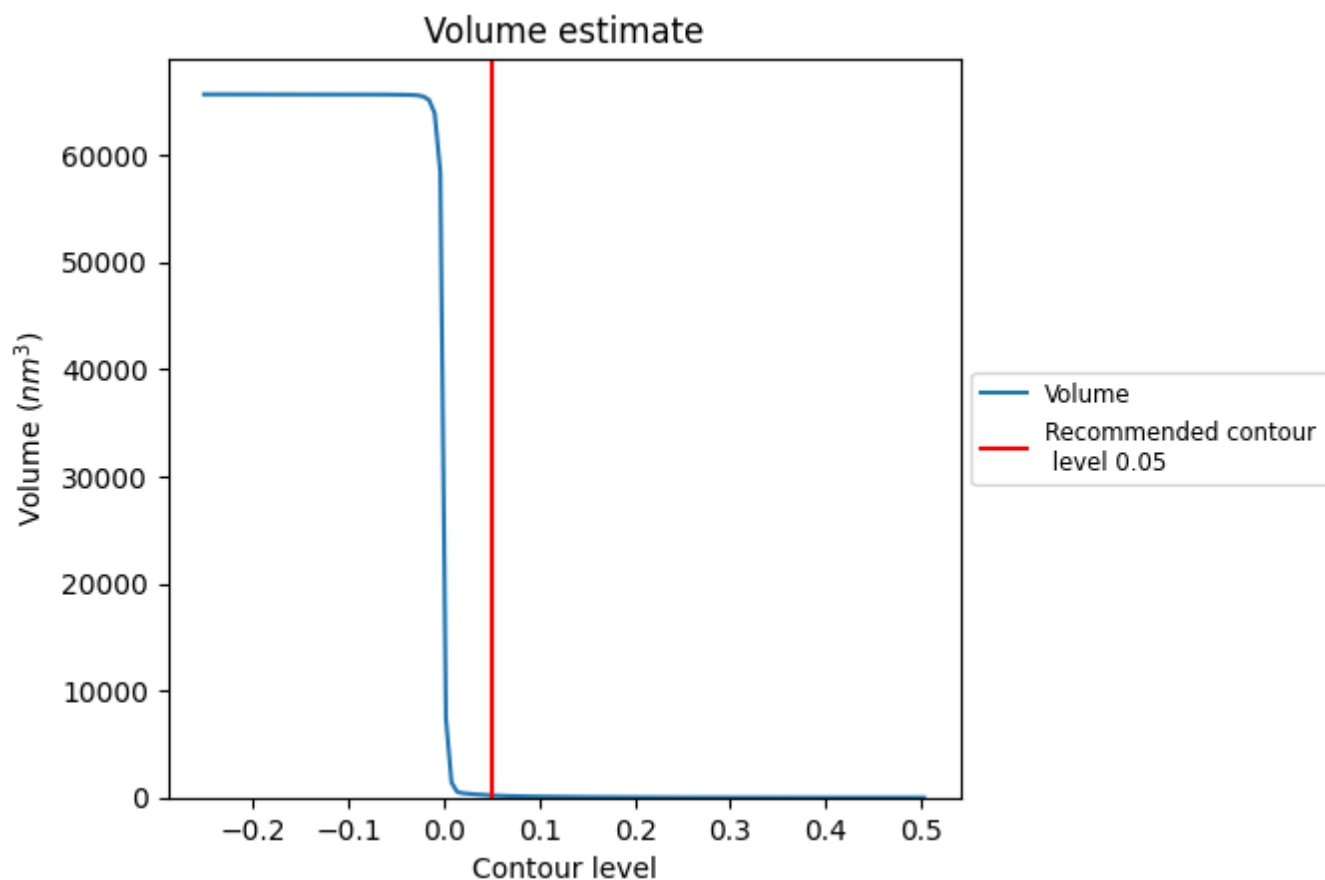
This section contains the results of statistical analysis of the map.

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.

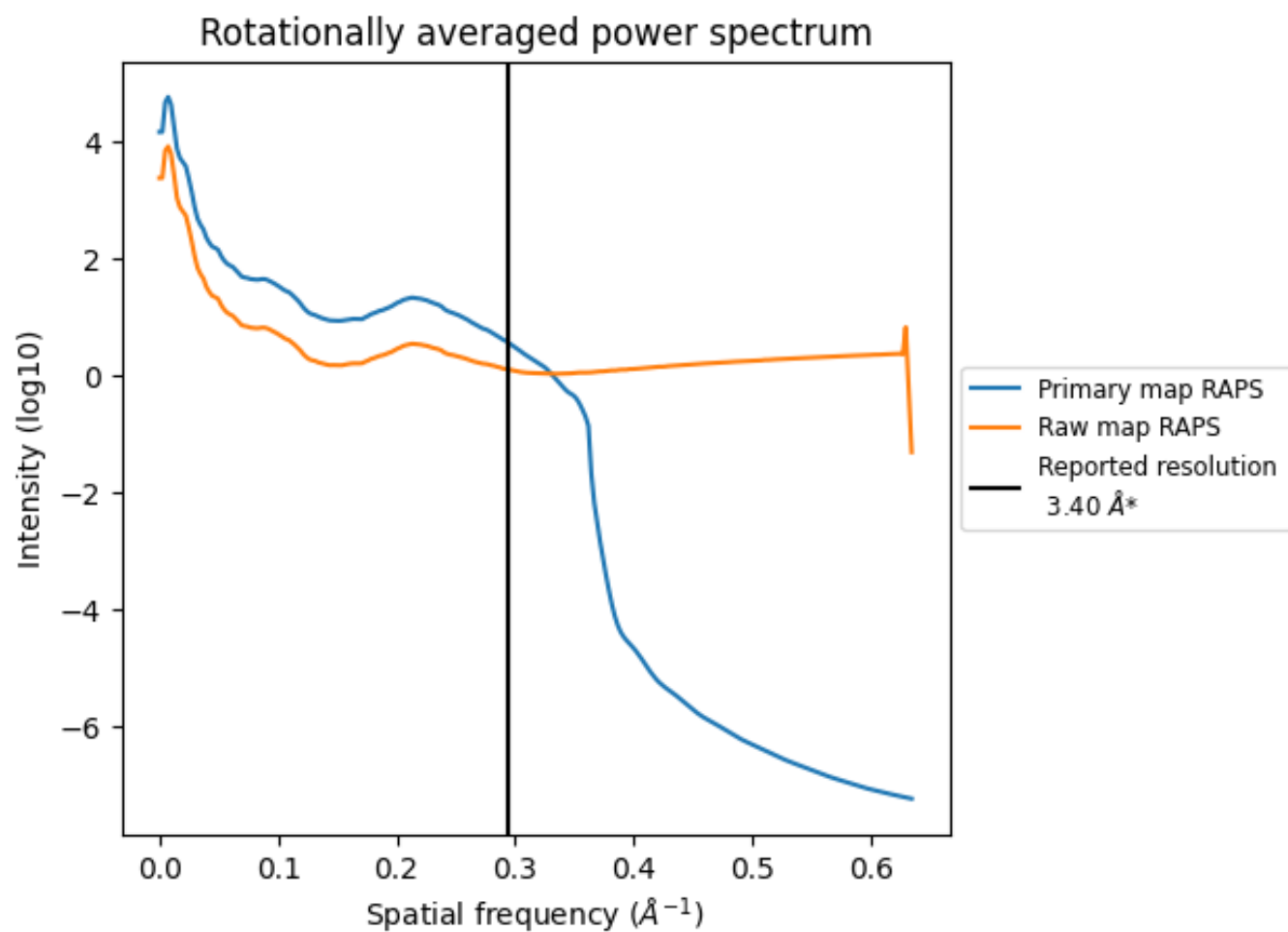
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 208 nm^3 ; this corresponds to an approximate mass of 188 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 ⓘ

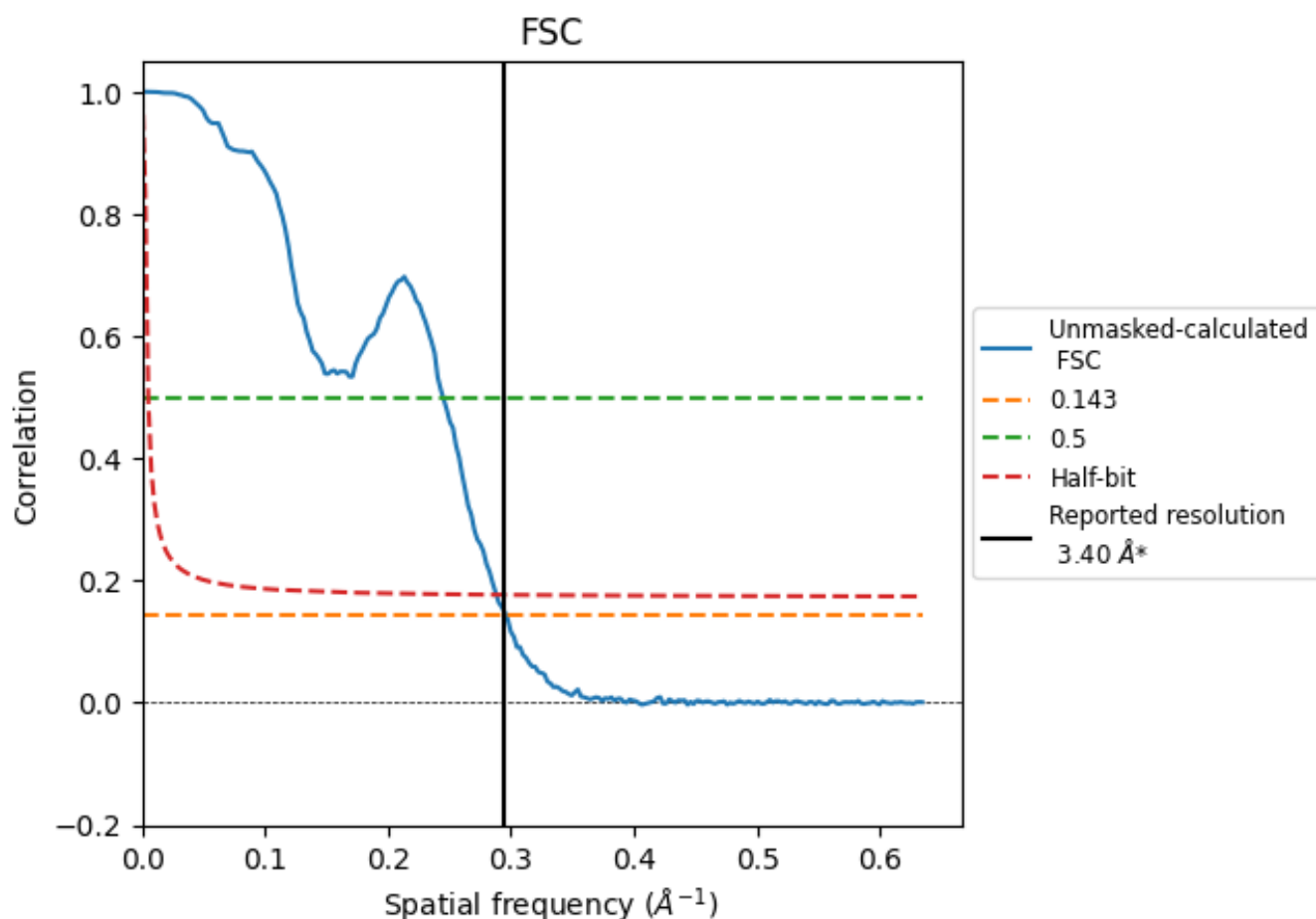


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

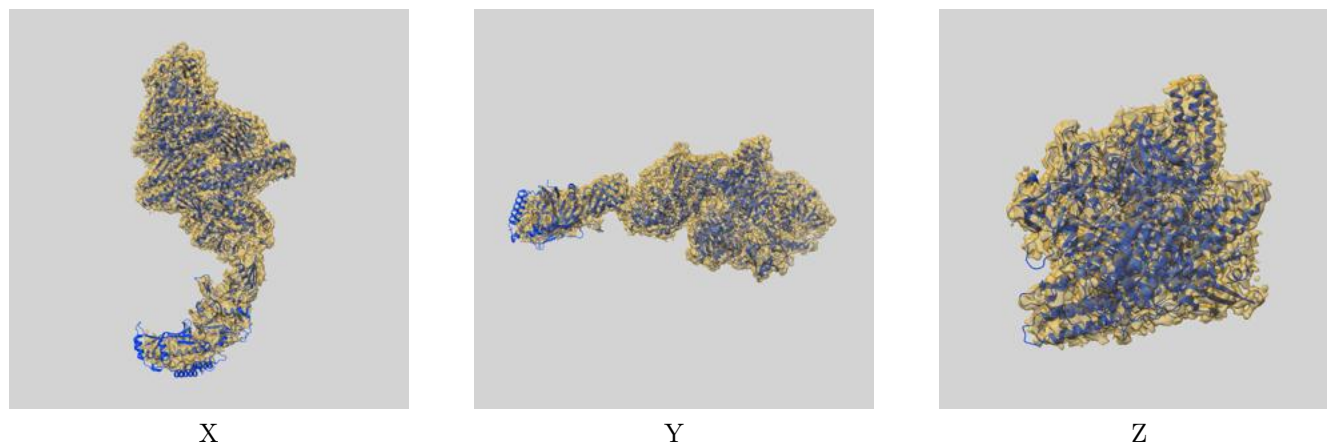
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.38	4.09	3.47

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

9 Map-model fit [i](#)

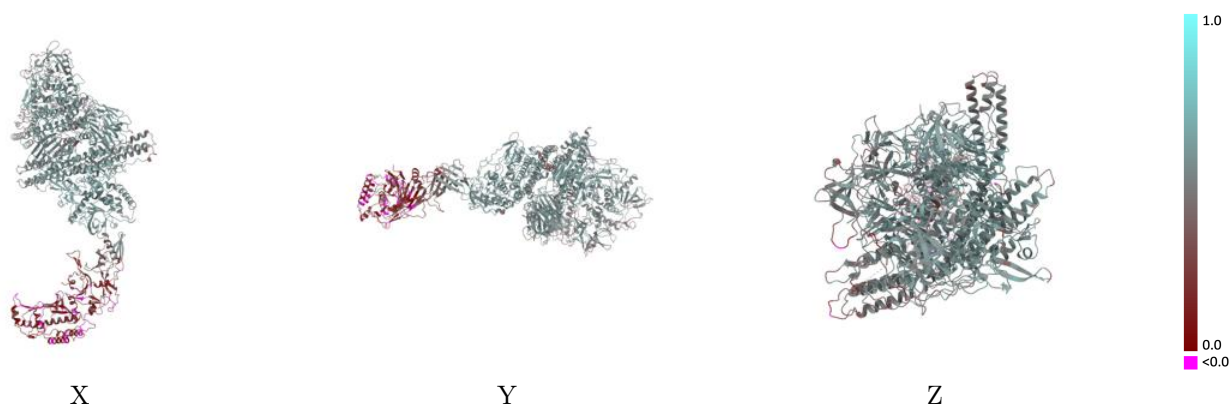
This section contains information regarding the fit between EMDB map EMD-43784 and PDB model 9ARJ. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



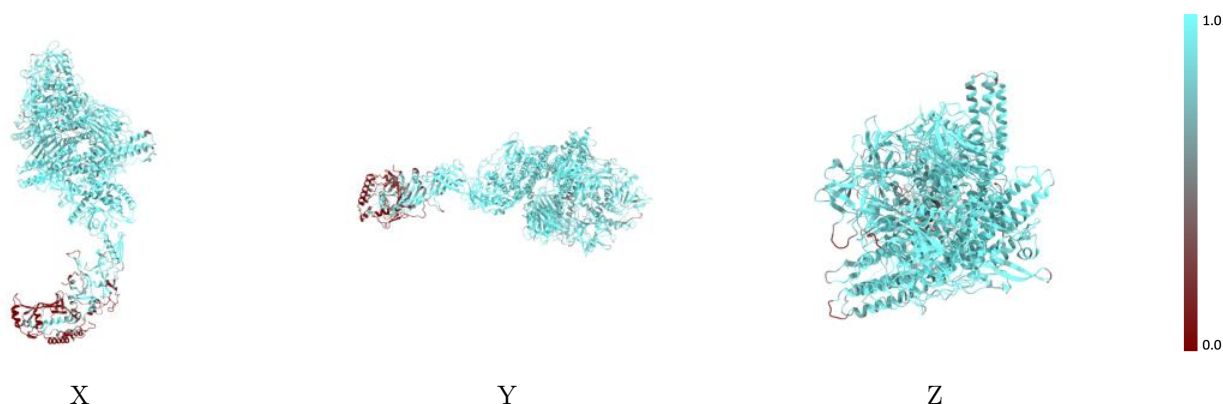
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



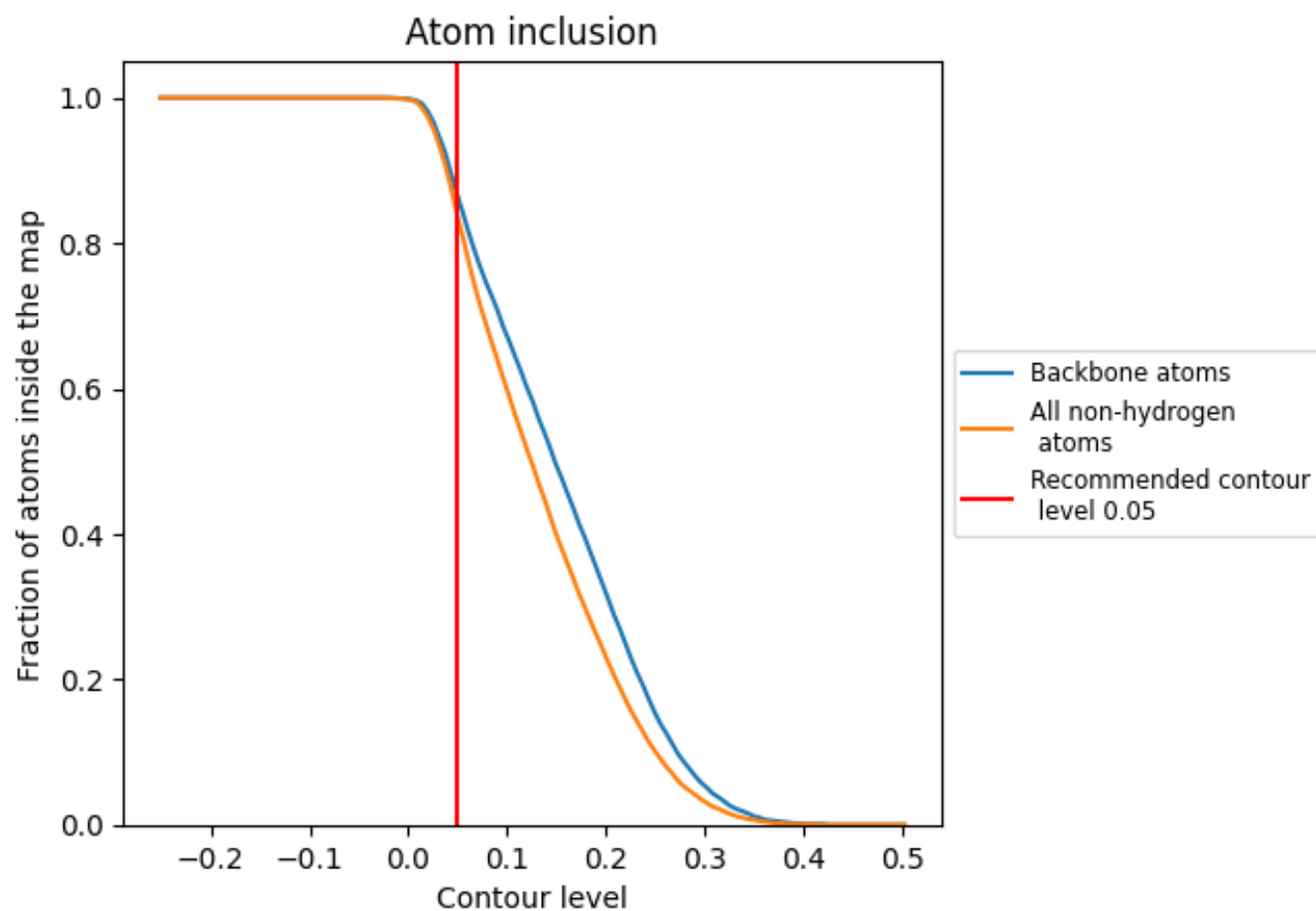
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8370	0.4770
A	0.9080	0.5300
B	0.9390	0.5500
C	0.4690	0.2080

