



Full wwPDB EM Validation Report ⓘ

Jul 17, 2023 – 10:15 PM JST

PDB ID : 8GRO
EMDB ID : EMD-34210
Title : AtOSCA3.1 contracted state
Authors : Zhang, M.F.
Deposited on : 2022-09-02
Resolution : 3.50 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.dev50
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.34

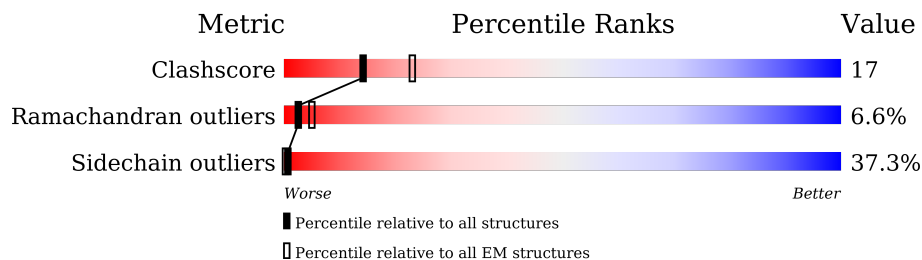
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	724	 8% 43% 35% 11% • 9%
1	B	724	 8% 44% 34% 12% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10624 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.

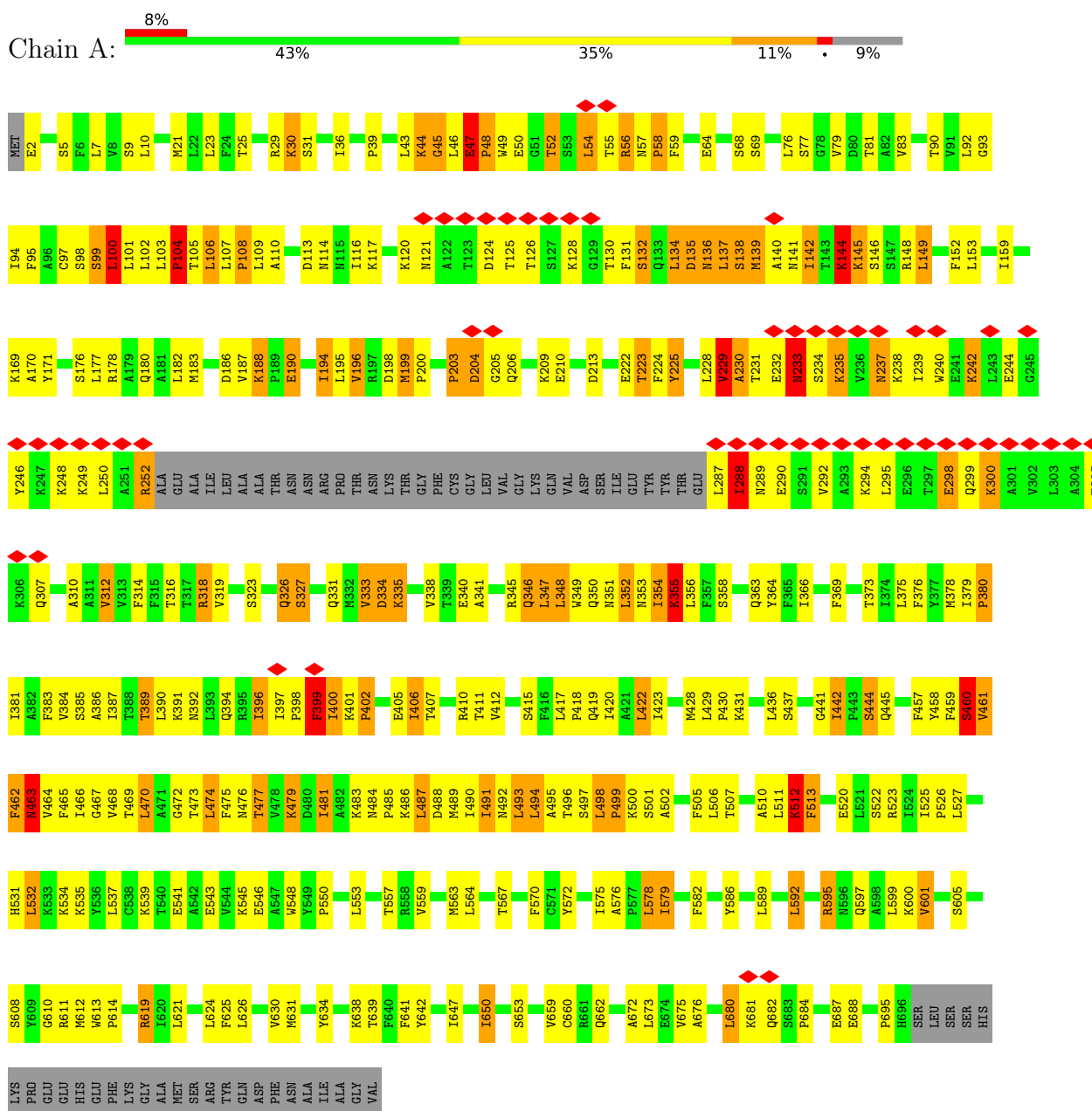
- Molecule 1 is a protein called CSC1-like protein ERD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	661	Total	C	N	O	S	0	0
			5312	3530	850	914	18		
1	B	661	Total	C	N	O	S	0	0
			5312	3530	850	914	18		

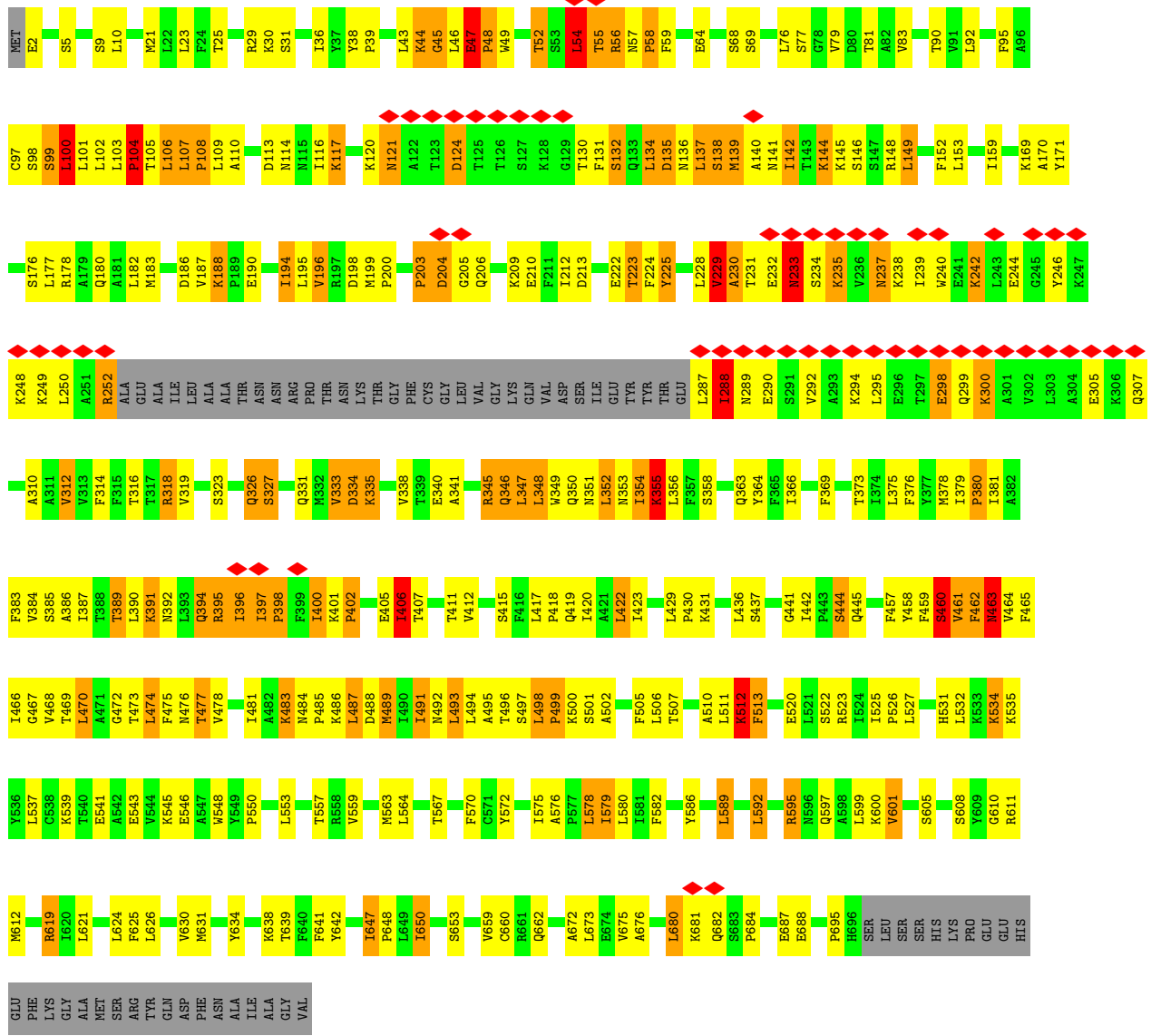
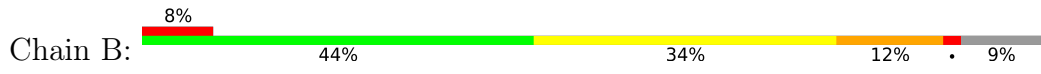
3 Residue-property plots

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: CSC1-like protein ERD4



● Molecule 1: C5C1-like protein ERD4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.695	Depositor
Minimum map value	-0.474	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	266.88, 266.88, 266.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.834, 0.834, 0.834	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	0.62	2/5453 (0.0%)	0.71	3/7412 (0.0%)
1	B	0.61	2/5453 (0.0%)	0.71	3/7412 (0.0%)
All	All	0.61	4/10906 (0.0%)	0.71	6/14824 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	PHE	C-O	-5.09	1.13	1.23
1	B	95	PHE	C-O	-5.09	1.13	1.23
1	A	389	THR	N-CA	5.02	1.56	1.46
1	B	389	THR	N-CA	5.02	1.56	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	PRO	CA-N-CD	-5.89	103.25	111.50
1	B	380	PRO	CA-N-CD	-5.89	103.25	111.50
1	A	145	LYS	N-CA-C	-5.82	95.29	111.00
1	B	145	LYS	N-CA-C	-5.82	95.29	111.00
1	A	104	PRO	CA-N-CD	-5.15	104.29	111.50
1	B	104	PRO	CA-N-CD	-5.15	104.29	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	ASN	Mainchain
1	B	233	ASN	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5312	0	5478	208	0
1	B	5312	0	5478	208	0
All	All	10624	0	10956	376	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 17.

All (376) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:VAL:HG21	1:B:364:TYR:CE1	1.41	1.52
1:A:364:TYR:CE1	1:B:659:VAL:HG21	1.41	1.52
1:B:240:TRP:CD1	1:B:298:GLU:OE1	1.83	1.31
1:A:240:TRP:CD1	1:A:298:GLU:OE1	1.83	1.30
1:A:327:SER:HA	1:B:326:GLN:OE1	1.45	1.16
1:A:326:GLN:OE1	1:B:327:SER:HA	1.45	1.14
1:A:364:TYR:CZ	1:B:659:VAL:HG11	1.82	1.14
1:A:659:VAL:HG11	1:B:364:TYR:CZ	1.82	1.14
1:A:195:LEU:HD11	1:A:352:LEU:CD1	1.77	1.13
1:B:195:LEU:HD11	1:B:352:LEU:CD1	1.77	1.13
1:A:364:TYR:CE1	1:B:659:VAL:CG2	2.32	1.11
1:A:659:VAL:CG2	1:B:364:TYR:CE1	2.32	1.11
1:A:195:LEU:HD11	1:A:352:LEU:HD11	1.41	1.02
1:B:195:LEU:HD11	1:B:352:LEU:HD11	1.41	0.98
1:A:364:TYR:HE1	1:B:659:VAL:HG21	1.17	0.97
1:A:240:TRP:HD1	1:A:298:GLU:OE1	1.29	0.92
1:B:240:TRP:HD1	1:B:298:GLU:OE1	1.29	0.91
1:B:195:LEU:HD11	1:B:352:LEU:HD13	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:VAL:HG21	1:B:364:TYR:HE1	1.17	0.89
1:B:252:ARG:NH2	1:B:546:GLU:OE1	2.05	0.89
1:A:195:LEU:HD11	1:A:352:LEU:HD13	1.51	0.89
1:A:364:TYR:CD1	1:B:659:VAL:HG21	2.09	0.88
1:A:252:ARG:NH2	1:A:546:GLU:OE1	2.05	0.88
1:A:659:VAL:HG21	1:B:364:TYR:CD1	2.09	0.88
1:A:477:THR:HG23	1:A:493:LEU:HB3	1.54	0.87
1:A:326:GLN:OE1	1:B:327:SER:CA	2.23	0.86
1:B:473:THR:HA	1:B:497:SER:HB2	1.58	0.86
1:A:473:THR:HA	1:A:497:SER:CB	2.06	0.86
1:A:473:THR:HA	1:A:497:SER:HB2	1.58	0.85
1:B:473:THR:HA	1:B:497:SER:CB	2.06	0.84
1:A:195:LEU:CD1	1:A:352:LEU:HD11	2.07	0.84
1:B:195:LEU:CD1	1:B:352:LEU:HD11	2.07	0.84
1:A:659:VAL:HG11	1:B:364:TYR:OH	1.78	0.83
1:A:327:SER:CA	1:B:326:GLN:OE1	2.23	0.83
1:A:364:TYR:OH	1:B:659:VAL:HG11	1.78	0.81
1:B:139:MET:HG2	1:B:141:ASN:H	1.47	0.79
1:B:204:ASP:OD1	1:B:205:GLY:N	2.16	0.79
1:A:204:ASP:OD1	1:A:205:GLY:N	2.16	0.79
1:B:233:ASN:O	1:B:237:ASN:HB3	1.83	0.78
1:A:204:ASP:OD1	1:A:204:ASP:C	2.22	0.78
1:A:139:MET:HG2	1:A:141:ASN:H	1.47	0.78
1:A:233:ASN:O	1:A:237:ASN:HB3	1.83	0.77
1:A:140:ALA:HB2	1:A:496:THR:HA	1.67	0.77
1:B:204:ASP:OD1	1:B:204:ASP:C	2.22	0.77
1:B:140:ALA:HB2	1:B:496:THR:HA	1.67	0.75
1:A:659:VAL:CG1	1:B:364:TYR:CZ	2.68	0.75
1:B:195:LEU:CD1	1:B:352:LEU:CD1	2.62	0.75
1:A:139:MET:HA	1:A:499:PRO:HG2	1.69	0.73
1:A:327:SER:OG	1:B:673:LEU:HD11	1.88	0.73
1:A:364:TYR:OH	1:B:659:VAL:CG1	2.37	0.73
1:A:364:TYR:CZ	1:B:659:VAL:CG1	2.68	0.73
1:A:673:LEU:HD11	1:B:327:SER:OG	1.88	0.73
1:B:237:ASN:HD22	1:B:295:LEU:HD11	1.54	0.72
1:A:659:VAL:CG1	1:B:364:TYR:OH	2.37	0.72
1:B:391:LYS:NZ	1:B:394:GLN:HG2	2.04	0.72
1:A:398:PRO:HB2	1:A:402:PRO:HD3	1.71	0.72
1:B:139:MET:HA	1:B:499:PRO:HG2	1.69	0.71
1:A:237:ASN:HD22	1:A:295:LEU:HD11	1.54	0.71
1:A:364:TYR:HE1	1:B:659:VAL:CG2	1.86	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:ASN:HD22	1:A:497:SER:HB3	1.57	0.70
1:B:476:ASN:HD22	1:B:497:SER:HB3	1.57	0.70
1:A:659:VAL:CG2	1:B:364:TYR:HE1	1.86	0.69
1:B:99:SER:O	1:B:100:LEU:C	2.30	0.69
1:A:99:SER:O	1:A:100:LEU:C	2.30	0.68
1:B:495:ALA:O	1:B:499:PRO:HD2	1.95	0.67
1:B:235:LYS:O	1:B:239:ILE:HG12	1.95	0.66
1:A:235:LYS:O	1:A:239:ILE:HG12	1.95	0.66
1:A:495:ALA:O	1:A:499:PRO:HD2	1.95	0.66
1:A:327:SER:OG	1:B:673:LEU:CD1	2.45	0.65
1:B:240:TRP:NE1	1:B:298:GLU:OE1	2.30	0.65
1:A:673:LEU:CD1	1:B:327:SER:OG	2.45	0.65
1:A:195:LEU:CD1	1:A:352:LEU:CD1	2.62	0.65
1:A:238:LYS:HE2	1:A:239:ILE:CD1	2.27	0.65
1:A:397:ILE:HB	1:A:398:PRO:HD3	1.78	0.64
1:A:139:MET:HG2	1:A:141:ASN:N	2.12	0.64
1:B:238:LYS:HE2	1:B:239:ILE:CD1	2.27	0.64
1:A:318:ARG:HB2	1:A:676:ALA:HB1	1.78	0.64
1:B:376:PHE:O	1:B:380:PRO:HD2	1.98	0.64
1:A:376:PHE:O	1:A:380:PRO:HD2	1.98	0.63
1:B:139:MET:HG2	1:B:141:ASN:N	2.12	0.63
1:B:318:ARG:HB2	1:B:676:ALA:HB1	1.78	0.63
1:B:237:ASN:HB2	1:B:295:LEU:CD1	2.29	0.63
1:A:373:THR:HB	1:A:459:PHE:HZ	1.64	0.62
1:A:473:THR:HA	1:A:497:SER:HB3	1.80	0.62
1:A:237:ASN:HB2	1:A:295:LEU:CD1	2.29	0.62
1:A:373:THR:HB	1:A:459:PHE:CZ	2.35	0.62
1:B:131:PHE:CZ	1:B:496:THR:HG23	2.35	0.62
1:B:373:THR:HB	1:B:459:PHE:CZ	2.35	0.62
1:A:83:VAL:HG21	1:A:610:GLY:HA2	1.82	0.61
1:A:137:LEU:HB2	1:A:576:ALA:HA	1.83	0.61
1:B:473:THR:HA	1:B:497:SER:HB3	1.80	0.61
1:B:373:THR:HB	1:B:459:PHE:HZ	1.64	0.61
1:A:131:PHE:CZ	1:A:496:THR:HG23	2.35	0.61
1:A:238:LYS:CE	1:A:239:ILE:CD1	2.79	0.61
1:A:240:TRP:NE1	1:A:298:GLU:OE1	2.30	0.61
1:B:238:LYS:CE	1:B:239:ILE:CD1	2.79	0.61
1:A:396:ILE:HG21	1:A:479:LYS:HG2	1.83	0.60
1:A:232:GLU:HG3	1:A:349:TRP:HB3	1.82	0.60
1:A:326:GLN:O	1:B:326:GLN:O	2.18	0.60
1:B:83:VAL:HG21	1:B:610:GLY:HA2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:SER:HB3	1:B:149:LEU:HB2	1.84	0.60
1:B:137:LEU:HB2	1:B:576:ALA:HA	1.83	0.60
1:A:103:LEU:O	1:A:104:PRO:C	2.38	0.60
1:A:493:LEU:O	1:A:496:THR:HB	2.02	0.60
1:B:232:GLU:HG3	1:B:349:TRP:HB3	1.82	0.60
1:A:477:THR:CG2	1:A:493:LEU:HB3	2.27	0.59
1:A:200:PRO:HG3	1:A:335:LYS:HG2	1.84	0.59
1:A:238:LYS:HE2	1:A:239:ILE:HD13	1.83	0.59
1:B:238:LYS:CE	1:B:239:ILE:HD13	2.33	0.59
1:A:238:LYS:CE	1:A:239:ILE:HD13	2.33	0.59
1:B:502:ALA:HB2	1:B:572:TYR:CE1	2.38	0.59
1:B:103:LEU:O	1:B:104:PRO:C	2.38	0.59
1:B:513:PHE:HB2	1:B:586:TYR:HD1	1.68	0.59
1:A:139:MET:H	1:A:139:MET:CE	2.16	0.59
1:B:238:LYS:HE2	1:B:239:ILE:HD13	1.83	0.59
1:A:502:ALA:HB2	1:A:572:TYR:CE1	2.38	0.58
1:B:493:LEU:O	1:B:496:THR:HB	2.02	0.58
1:B:200:PRO:HG3	1:B:335:LYS:HG2	1.84	0.58
1:A:146:SER:HB3	1:A:149:LEU:HB2	1.84	0.58
1:B:139:MET:CE	1:B:139:MET:H	2.16	0.58
1:A:513:PHE:HB2	1:A:586:TYR:HD1	1.68	0.57
1:B:510:ALA:HB2	1:B:582:PHE:CE2	2.40	0.56
1:A:510:ALA:HB2	1:A:582:PHE:CE2	2.40	0.56
1:B:525:ILE:HB	1:B:526:PRO:HD3	1.88	0.55
1:A:525:ILE:HB	1:A:526:PRO:HD3	1.88	0.55
1:B:213:ASP:HA	1:B:224:PHE:CZ	2.41	0.55
1:A:213:ASP:HA	1:A:224:PHE:CZ	2.41	0.55
1:A:331:GLN:HG2	1:B:672:ALA:CB	2.37	0.55
1:A:481:ILE:HG13	1:A:490:ILE:HG23	1.88	0.55
1:A:659:VAL:CB	1:B:364:TYR:CE1	2.90	0.55
1:A:672:ALA:CB	1:B:331:GLN:HG2	2.37	0.54
1:A:460:SER:O	1:A:461:VAL:C	2.45	0.54
1:A:142:ILE:HD13	1:A:149:LEU:HD11	1.88	0.54
1:A:364:TYR:CE1	1:B:659:VAL:CB	2.90	0.54
1:B:142:ILE:HD13	1:B:149:LEU:HD11	1.88	0.54
1:A:109:LEU:O	1:A:148:ARG:NH2	2.41	0.54
1:B:109:LEU:O	1:B:148:ARG:NH2	2.41	0.53
1:B:460:SER:O	1:B:461:VAL:C	2.45	0.52
1:A:672:ALA:HB3	1:B:331:GLN:HG2	1.91	0.52
1:B:100:LEU:O	1:B:104:PRO:HD2	2.10	0.52
1:B:139:MET:CE	1:B:141:ASN:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:CE	1:A:141:ASN:HB3	2.39	0.52
1:B:474:LEU:O	1:B:475:PHE:C	2.48	0.52
1:A:100:LEU:O	1:A:104:PRO:HD2	2.10	0.52
1:B:461:VAL:O	1:B:462:PHE:C	2.48	0.52
1:A:104:PRO:O	1:A:108:PRO:HD2	2.10	0.52
1:A:331:GLN:HG2	1:B:672:ALA:HB3	1.91	0.52
1:B:106:LEU:HG	1:B:152:PHE:CE2	2.45	0.51
1:A:106:LEU:HG	1:A:152:PHE:CE2	2.45	0.51
1:A:461:VAL:O	1:A:462:PHE:C	2.48	0.51
1:B:104:PRO:O	1:B:108:PRO:HD2	2.10	0.51
1:A:326:GLN:O	1:B:326:GLN:HB2	2.10	0.51
1:A:326:GLN:HB2	1:B:326:GLN:O	2.10	0.51
1:B:398:PRO:HB2	1:B:402:PRO:HD3	1.92	0.51
1:A:474:LEU:O	1:A:475:PHE:C	2.48	0.50
1:A:137:LEU:O	1:A:138:SER:C	2.50	0.50
1:B:239:ILE:HA	1:B:242:LYS:HE3	1.94	0.50
1:B:137:LEU:O	1:B:138:SER:C	2.50	0.50
1:B:464:VAL:HG12	1:B:505:PHE:CZ	2.47	0.49
1:B:397:ILE:HB	1:B:398:PRO:HD3	1.93	0.49
1:A:238:LYS:NZ	1:A:239:ILE:HD11	2.27	0.49
1:B:134:LEU:HD22	1:B:137:LEU:HD11	1.94	0.49
1:A:134:LEU:HD22	1:A:137:LEU:HD11	1.94	0.49
1:A:464:VAL:HG12	1:A:505:PHE:CZ	2.47	0.49
1:B:467:GLY:O	1:B:468:VAL:C	2.50	0.48
1:A:131:PHE:HZ	1:A:496:THR:HG23	1.77	0.48
1:B:238:LYS:NZ	1:B:239:ILE:HD11	2.27	0.48
1:A:239:ILE:HA	1:A:242:LYS:HE3	1.94	0.48
1:B:210:GLU:HA	1:B:213:ASP:HB2	1.96	0.48
1:B:139:MET:HE3	1:B:141:ASN:HB3	1.94	0.48
1:A:57:ASN:O	1:A:58:PRO:C	2.52	0.48
1:A:131:PHE:CE1	1:A:496:THR:HG23	2.48	0.48
1:B:512:LYS:O	1:B:513:PHE:C	2.50	0.48
1:A:199:MET:HE3	1:A:199:MET:HB3	1.79	0.48
1:A:467:GLY:O	1:A:468:VAL:C	2.50	0.48
1:A:387:ILE:HG22	1:A:418:PRO:HG3	1.96	0.48
1:B:534:LYS:HE3	1:B:534:LYS:HB3	1.71	0.48
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.74	0.48
1:A:495:ALA:HB3	1:A:638:LYS:NZ	2.29	0.48
1:B:57:ASN:O	1:B:58:PRO:C	2.52	0.48
1:B:131:PHE:CE1	1:B:496:THR:HG23	2.48	0.48
1:A:210:GLU:HA	1:A:213:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LYS:O	1:A:513:PHE:C	2.50	0.47
1:A:355:LYS:HD2	1:A:355:LYS:HA	1.55	0.47
1:A:228:LEU:HB3	1:A:312:VAL:HG23	1.96	0.47
1:A:400:ILE:H	1:A:400:ILE:HG13	1.33	0.47
1:B:477:THR:HG23	1:B:493:LEU:HB3	1.96	0.47
1:B:495:ALA:HB3	1:B:638:LYS:NZ	2.29	0.47
1:A:288:ILE:H	1:A:288:ILE:HG13	1.36	0.47
1:A:496:THR:HG22	1:A:497:SER:N	2.30	0.47
1:B:117:LYS:HB2	1:B:117:LYS:HE2	1.60	0.47
1:B:194:ILE:HA	1:B:194:ILE:HD12	1.75	0.47
1:B:228:LEU:HB3	1:B:312:VAL:HG23	1.96	0.47
1:B:229:VAL:HB	1:B:230:ALA:H	1.44	0.47
1:B:121:ASN:HD22	1:B:121:ASN:HA	1.54	0.46
1:B:387:ILE:HG22	1:B:418:PRO:HG3	1.96	0.46
1:A:240:TRP:HB2	1:A:295:LEU:HD13	1.98	0.46
1:B:137:LEU:N	1:B:139:MET:SD	2.77	0.46
1:B:97:CYS:O	1:B:98:SER:C	2.54	0.46
1:B:400:ILE:H	1:B:400:ILE:HG13	1.69	0.46
1:A:229:VAL:HB	1:A:230:ALA:H	1.44	0.46
1:B:56:ARG:O	1:B:57:ASN:C	2.53	0.46
1:B:463:ASN:O	1:B:464:VAL:C	2.52	0.46
1:A:463:ASN:O	1:A:464:VAL:C	2.52	0.46
1:B:496:THR:HG22	1:B:497:SER:N	2.30	0.46
1:A:56:ARG:O	1:A:57:ASN:C	2.53	0.46
1:A:104:PRO:O	1:A:105:THR:C	2.55	0.46
1:A:235:LYS:HA	1:A:235:LYS:HD3	1.52	0.46
1:B:461:VAL:HG13	1:B:626:LEU:HD22	1.98	0.46
1:B:470:LEU:HD13	1:B:470:LEU:HA	1.81	0.46
1:B:90:THR:HG21	1:B:170:ALA:HB2	1.99	0.45
1:A:101:LEU:O	1:A:102:LEU:C	2.55	0.45
1:B:131:PHE:HZ	1:B:496:THR:HG23	1.77	0.45
1:B:619:ARG:HA	1:B:619:ARG:HD3	1.67	0.45
1:B:355:LYS:HD2	1:B:355:LYS:HA	1.55	0.45
1:A:532:LEU:HD22	1:A:532:LEU:HA	1.70	0.45
1:A:137:LEU:N	1:A:139:MET:SD	2.77	0.45
1:A:461:VAL:HG13	1:A:626:LEU:HD22	1.98	0.45
1:B:240:TRP:HB2	1:B:295:LEU:HD13	1.98	0.45
1:B:391:LYS:NZ	1:B:394:GLN:CG	2.77	0.45
1:A:491:ILE:H	1:A:491:ILE:HG12	1.28	0.45
1:B:132:SER:C	1:B:134:LEU:H	2.21	0.45
1:B:499:PRO:O	1:B:502:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ILE:H	1:B:406:ILE:HG12	1.32	0.45
1:A:110:ALA:HB1	1:A:139:MET:CE	2.46	0.44
1:A:132:SER:C	1:A:134:LEU:H	2.21	0.44
1:B:239:ILE:HG12	1:B:239:ILE:H	1.65	0.44
1:A:97:CYS:O	1:A:98:SER:C	2.54	0.44
1:B:457:PHE:O	1:B:458:TYR:C	2.54	0.44
1:B:589:LEU:HD23	1:B:589:LEU:HA	1.81	0.44
1:A:90:THR:HG21	1:A:170:ALA:HB2	1.99	0.44
1:B:110:ALA:HB1	1:B:139:MET:CE	2.46	0.44
1:B:101:LEU:O	1:B:102:LEU:C	2.55	0.44
1:B:489:MET:HE2	1:B:489:MET:HB2	1.90	0.44
1:B:578:LEU:HD23	1:B:578:LEU:HA	1.74	0.44
1:A:134:LEU:HD22	1:A:134:LEU:HA	1.68	0.44
1:A:190:GLU:H	1:A:190:GLU:HG3	1.65	0.44
1:A:196:VAL:O	1:A:310:ALA:HA	2.18	0.44
1:A:470:LEU:HD13	1:A:470:LEU:HA	1.81	0.44
1:A:592:LEU:HD23	1:A:592:LEU:HA	1.73	0.44
1:B:110:ALA:HB1	1:B:139:MET:HE1	2.00	0.44
1:B:223:THR:HG22	1:B:316:THR:HB	1.98	0.44
1:B:391:LYS:HZ3	1:B:394:GLN:HG2	1.80	0.44
1:B:502:ALA:HB2	1:B:572:TYR:CD1	2.53	0.44
1:A:476:ASN:HD22	1:A:497:SER:CB	2.28	0.44
1:B:345:ARG:H	1:B:345:ARG:HG3	1.39	0.44
1:A:49:TRP:HE1	1:A:52:THR:HA	1.83	0.44
1:A:499:PRO:O	1:A:502:ALA:HB3	2.17	0.44
1:B:49:TRP:HE1	1:B:52:THR:HA	1.83	0.44
1:B:476:ASN:HD22	1:B:497:SER:CB	2.28	0.44
1:B:483:LYS:H	1:B:483:LYS:HG3	1.52	0.44
1:B:592:LEU:HD23	1:B:592:LEU:HA	1.73	0.44
1:B:597:GLN:HA	1:B:601:VAL:HG12	1.99	0.44
1:A:399:PHE:HB3	1:A:400:ILE:H	1.70	0.44
1:A:429:LEU:O	1:A:430:PRO:C	2.56	0.44
1:A:625:PHE:HE1	1:A:650:ILE:HG23	1.83	0.44
1:B:196:VAL:O	1:B:310:ALA:HA	2.18	0.44
1:B:347:LEU:O	1:B:348:LEU:C	2.55	0.44
1:A:347:LEU:O	1:A:348:LEU:C	2.55	0.43
1:A:502:ALA:HB2	1:A:572:TYR:CD1	2.53	0.43
1:B:235:LYS:HA	1:B:235:LYS:HD3	1.52	0.43
1:B:369:PHE:HD2	1:B:436:LEU:HD11	1.83	0.43
1:B:491:ILE:H	1:B:491:ILE:HG12	1.28	0.43
1:A:30:LYS:HB3	1:A:30:LYS:HE3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:THR:HG22	1:A:316:THR:HB	1.98	0.43
1:A:465:PHE:HE2	1:A:630:VAL:HG21	1.83	0.43
1:A:493:LEU:HD12	1:A:493:LEU:HA	1.78	0.43
1:B:44:LYS:O	1:B:45:GLY:C	2.57	0.43
1:B:465:PHE:HE2	1:B:630:VAL:HG21	1.83	0.43
1:B:465:PHE:O	1:B:466:ILE:C	2.56	0.43
1:B:625:PHE:HE1	1:B:650:ILE:HG23	1.83	0.43
1:A:300:LYS:HB3	1:A:300:LYS:HE3	1.22	0.43
1:B:203:PRO:HD2	1:B:206:GLN:HB2	1.99	0.43
1:A:203:PRO:HD2	1:A:206:GLN:HB2	1.99	0.43
1:A:462:PHE:O	1:A:463:ASN:C	2.55	0.43
1:B:300:LYS:HE3	1:B:300:LYS:HB3	1.22	0.43
1:A:288:ILE:O	1:A:292:VAL:HG13	2.19	0.43
1:A:477:THR:HG21	1:A:494:LEU:HD12	2.01	0.43
1:B:429:LEU:O	1:B:430:PRO:C	2.56	0.43
1:B:462:PHE:O	1:B:463:ASN:C	2.55	0.43
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.83	0.43
1:A:44:LYS:O	1:A:45:GLY:C	2.57	0.43
1:A:595:ARG:C	1:A:597:GLN:H	2.22	0.43
1:A:136:ASN:HD22	1:A:136:ASN:HA	1.62	0.43
1:B:104:PRO:O	1:B:105:THR:C	2.55	0.43
1:B:680:LEU:HD13	1:B:684:PRO:HG3	2.01	0.43
1:A:113:ASP:HB3	1:A:141:ASN:O	2.19	0.43
1:A:597:GLN:HA	1:A:601:VAL:HG12	1.99	0.43
1:B:288:ILE:O	1:B:292:VAL:HG13	2.19	0.43
1:B:595:ARG:C	1:B:597:GLN:H	2.22	0.43
1:A:428:MET:HE2	1:A:428:MET:HB2	1.90	0.43
1:B:387:ILE:HD13	1:B:387:ILE:HA	1.87	0.43
1:A:369:PHE:HD2	1:A:436:LEU:HD11	1.83	0.42
1:A:379:ILE:HB	1:A:380:PRO:HD2	2.00	0.42
1:B:113:ASP:HB3	1:B:141:ASN:O	2.19	0.42
1:B:134:LEU:HD22	1:B:134:LEU:HA	1.68	0.42
1:B:238:LYS:CE	1:B:239:ILE:HD11	2.49	0.42
1:A:465:PHE:O	1:A:466:ILE:C	2.56	0.42
1:B:212:ILE:H	1:B:212:ILE:HG13	1.66	0.42
1:A:346:GLN:O	1:A:444:SER:HA	2.19	0.42
1:A:458:TYR:O	1:A:459:PHE:C	2.57	0.42
1:A:680:LEU:HD13	1:A:684:PRO:HG3	2.01	0.42
1:B:54:LEU:HB3	1:B:55:THR:H	1.53	0.42
1:A:386:ALA:O	1:A:387:ILE:C	2.58	0.42
1:B:346:GLN:O	1:B:444:SER:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PRO:O	1:B:383:PHE:HB3	2.20	0.42
1:B:580:LEU:HD23	1:B:580:LEU:HA	1.77	0.42
1:B:242:LYS:HB2	1:B:242:LYS:HE2	1.71	0.42
1:A:380:PRO:O	1:A:383:PHE:HB3	2.20	0.42
1:A:459:PHE:O	1:A:460:SER:C	2.58	0.42
1:A:522:SER:O	1:A:523:ARG:C	2.58	0.42
1:A:100:LEU:O	1:A:101:LEU:C	2.58	0.42
1:A:331:GLN:HE21	1:B:672:ALA:H	1.68	0.42
1:A:672:ALA:H	1:B:331:GLN:HE21	1.68	0.42
1:B:39:PRO:HB3	1:B:548:TRP:HZ3	1.85	0.42
1:B:100:LEU:O	1:B:101:LEU:C	2.58	0.42
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.74	0.42
1:A:47:GLU:O	1:A:48:PRO:C	2.57	0.42
1:A:442:ILE:H	1:A:442:ILE:HG12	1.53	0.42
1:A:457:PHE:O	1:A:458:TYR:C	2.54	0.42
1:A:473:THR:HG22	1:A:498:LEU:N	2.35	0.41
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.81	0.41
1:B:458:TYR:O	1:B:459:PHE:C	2.57	0.41
1:A:39:PRO:HB3	1:A:548:TRP:HZ3	1.85	0.41
1:A:145:LYS:H	1:A:145:LYS:HG2	1.58	0.41
1:A:149:LEU:HD12	1:A:149:LEU:HA	1.81	0.41
1:A:194:ILE:HD12	1:A:194:ILE:HA	1.75	0.41
1:B:379:ILE:HB	1:B:380:PRO:HD2	2.00	0.41
1:A:138:SER:HB2	1:A:152:PHE:CE2	2.55	0.41
1:A:469:THR:O	1:A:473:THR:HG23	2.20	0.41
1:A:106:LEU:HG	1:A:152:PHE:CD2	2.55	0.41
1:A:182:LEU:HB3	1:A:675:VAL:HG11	2.02	0.41
1:A:335:LYS:HB2	1:A:335:LYS:HE2	1.39	0.41
1:A:578:LEU:HD23	1:A:578:LEU:HA	1.74	0.41
1:B:47:GLU:O	1:B:48:PRO:C	2.57	0.41
1:B:54:LEU:HD13	1:B:54:LEU:HA	1.91	0.41
1:B:394:GLN:O	1:B:395:ARG:C	2.58	0.41
1:A:242:LYS:HB2	1:A:242:LYS:HE2	1.71	0.41
1:A:364:TYR:CE2	1:B:659:VAL:HG11	2.48	0.41
1:A:613:TRP:O	1:A:614:PRO:C	2.58	0.41
1:A:659:VAL:CB	1:B:364:TYR:CZ	3.03	0.41
1:B:138:SER:HB2	1:B:152:PHE:CE2	2.55	0.41
1:B:386:ALA:O	1:B:387:ILE:C	2.58	0.41
1:A:364:TYR:CZ	1:B:659:VAL:CB	3.03	0.41
1:B:647:ILE:O	1:B:648:PRO:C	2.57	0.41
1:A:144:LYS:HB3	1:A:144:LYS:HE3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD12	1:A:348:LEU:HA	1.82	0.41
1:A:619:ARG:HD3	1:A:619:ARG:HA	1.67	0.41
1:B:107:LEU:HD22	1:B:107:LEU:HA	1.82	0.41
1:A:23:LEU:HD23	1:A:23:LEU:HA	1.81	0.41
1:B:182:LEU:HB3	1:B:675:VAL:HG11	2.02	0.41
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.86	0.41
1:A:238:LYS:CE	1:A:239:ILE:HD11	2.49	0.41
1:A:472:GLY:O	1:A:473:THR:C	2.59	0.41
1:B:106:LEU:HG	1:B:152:PHE:CD2	2.55	0.41
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.86	0.41
1:B:397:ILE:H	1:B:397:ILE:HG12	1.65	0.41
1:B:472:GLY:O	1:B:473:THR:C	2.59	0.41
1:B:495:ALA:HB1	1:B:634:TYR:CE1	2.56	0.41
1:B:522:SER:O	1:B:523:ARG:C	2.58	0.41
1:A:237:ASN:HB2	1:A:295:LEU:HD11	2.00	0.41
1:A:352:LEU:HD22	1:A:352:LEU:HA	1.79	0.41
1:A:495:ALA:HB1	1:A:634:TYR:CE1	2.56	0.41
1:B:459:PHE:O	1:B:460:SER:C	2.58	0.41
1:A:237:ASN:HB2	1:A:295:LEU:HD12	2.03	0.40
1:B:38:TYR:N	1:B:39:PRO:HD3	2.37	0.40
1:B:237:ASN:HB2	1:B:295:LEU:HD11	2.00	0.40
1:A:49:TRP:HB2	1:A:50:GLU:H	1.68	0.40
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.88	0.40
1:B:469:THR:O	1:B:473:THR:HG23	2.20	0.40
1:A:495:ALA:HB1	1:A:638:LYS:HE2	2.03	0.40
1:B:225:TYR:HB3	1:B:314:PHE:O	2.21	0.40
1:B:473:THR:HG22	1:B:498:LEU:N	2.35	0.40
1:A:93:GLY:O	1:A:94:ILE:C	2.60	0.40
1:A:225:TYR:HB3	1:A:314:PHE:O	2.21	0.40
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.81	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	657/724 (91%)	506 (77%)	108 (16%)	43 (6%)	1	14
1	B	657/724 (91%)	507 (77%)	106 (16%)	44 (7%)	1	13
All	All	1314/1448 (91%)	1013 (77%)	214 (16%)	87 (7%)	2	13

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO
1	A	100	LEU
1	A	144	LYS
1	A	203	PRO
1	A	288	ILE
1	A	333	VAL
1	A	355	LYS
1	A	461	VAL
1	A	485	PRO
1	B	58	PRO
1	B	100	LEU
1	B	144	LYS
1	B	203	PRO
1	B	288	ILE
1	B	333	VAL
1	B	355	LYS
1	B	461	VAL
1	B	485	PRO
1	A	45	GLY
1	A	99	SER
1	A	354	ILE
1	A	406	ILE
1	A	460	SER
1	A	550	PRO
1	A	639	THR
1	B	45	GLY
1	B	99	SER
1	B	354	ILE
1	B	406	ILE
1	B	460	SER
1	B	550	PRO
1	B	639	THR
1	A	188	LYS

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Mol	Chain	Res	Type
1	A	399	PHE
1	A	402	PRO
1	A	487	LEU
1	A	695	PRO
1	B	124	ASP
1	B	188	LYS
1	B	487	LEU
1	B	695	PRO
1	A	47	GLU
1	A	56	ARG
1	A	124	ASP
1	A	132	SER
1	A	135	ASP
1	A	138	SER
1	A	225	TYR
1	A	334	ASP
1	A	353	ASN
1	A	462	PHE
1	A	512	LYS
1	B	47	GLU
1	B	56	ARG
1	B	132	SER
1	B	135	ASP
1	B	138	SER
1	B	225	TYR
1	B	334	ASP
1	B	353	ASN
1	B	462	PHE
1	B	512	LYS
1	A	229	VAL
1	A	341	ALA
1	B	229	VAL
1	B	341	ALA
1	A	48	PRO
1	A	54	LEU
1	A	230	ALA
1	A	444	SER
1	A	463	ASN
1	A	579	ILE
1	B	48	PRO
1	B	54	LEU
1	B	230	ALA

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Mol	Chain	Res	Type
1	B	444	SER
1	B	463	ASN
1	B	579	ILE
1	A	601	VAL
1	B	396	ILE
1	B	398	PRO
1	B	402	PRO
1	B	601	VAL
1	A	441	GLY
1	B	441	GLY
1	A	187	VAL
1	B	187	VAL

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	576/627 (92%)	360 (62%)	216 (38%)	0 1
1	B	576/627 (92%)	362 (63%)	214 (37%)	0 1
All	All	1152/1254 (92%)	722 (63%)	430 (37%)	1 1

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	5	SER
1	A	9	SER
1	A	10	LEU
1	A	21	MET
1	A	25	THR
1	A	29	ARG
1	A	30	LYS
1	A	31	SER
1	A	36	ILE
1	A	43	LEU

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Mol	Chain	Res	Type
1	A	44	LYS
1	A	46	LEU
1	A	47	GLU
1	A	52	THR
1	A	54	LEU
1	A	55	THR
1	A	59	PHE
1	A	64	GLU
1	A	68	SER
1	A	69	SER
1	A	76	LEU
1	A	77	SER
1	A	79	VAL
1	A	81	THR
1	A	92	LEU
1	A	100	LEU
1	A	104	PRO
1	A	106	LEU
1	A	107	LEU
1	A	108	PRO
1	A	114	ASN
1	A	116	ILE
1	A	117	LYS
1	A	120	LYS
1	A	121	ASN
1	A	125	THR
1	A	126	THR
1	A	128	LYS
1	A	130	THR
1	A	134	LEU
1	A	135	ASP
1	A	136	ASN
1	A	137	LEU
1	A	139	MET
1	A	142	ILE
1	A	144	LYS
1	A	149	LEU
1	A	153	LEU
1	A	159	ILE
1	A	169	LYS
1	A	171	TYR
1	A	176	SER

Continued on next page...

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Mol	Chain	Res	Type
1	A	178	ARG
1	A	180	GLN
1	A	183	MET
1	A	186	ASP
1	A	188	LYS
1	A	190	GLU
1	A	194	ILE
1	A	196	VAL
1	A	198	ASP
1	A	199	MET
1	A	204	ASP
1	A	209	LYS
1	A	222	GLU
1	A	223	THR
1	A	229	VAL
1	A	231	THR
1	A	233	ASN
1	A	234	SER
1	A	235	LYS
1	A	237	ASN
1	A	242	LYS
1	A	244	GLU
1	A	246	TYR
1	A	248	LYS
1	A	249	LYS
1	A	250	LEU
1	A	252	ARG
1	A	287	LEU
1	A	288	ILE
1	A	289	ASN
1	A	290	GLU
1	A	294	LYS
1	A	298	GLU
1	A	299	GLN
1	A	300	LYS
1	A	305	GLU
1	A	307	GLN
1	A	312	VAL
1	A	318	ARG
1	A	319	VAL
1	A	323	SER
1	A	326	GLN

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Mol	Chain	Res	Type
1	A	327	SER
1	A	333	VAL
1	A	334	ASP
1	A	335	LYS
1	A	338	VAL
1	A	340	GLU
1	A	345	ARG
1	A	346	GLN
1	A	347	LEU
1	A	348	LEU
1	A	350	GLN
1	A	351	ASN
1	A	352	LEU
1	A	354	ILE
1	A	355	LYS
1	A	356	LEU
1	A	358	SER
1	A	363	GLN
1	A	366	ILE
1	A	375	LEU
1	A	378	MET
1	A	381	ILE
1	A	384	VAL
1	A	385	SER
1	A	389	THR
1	A	390	LEU
1	A	391	LYS
1	A	392	ASN
1	A	394	GLN
1	A	396	ILE
1	A	399	PHE
1	A	400	ILE
1	A	401	LYS
1	A	405	GLU
1	A	406	ILE
1	A	407	THR
1	A	410	ARG
1	A	411	THR
1	A	412	VAL
1	A	415	SER
1	A	417	LEU
1	A	419	GLN

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Mol	Chain	Res	Type
1	A	420	ILE
1	A	422	LEU
1	A	423	ILE
1	A	431	LYS
1	A	437	SER
1	A	442	ILE
1	A	445	GLN
1	A	460	SER
1	A	463	ASN
1	A	470	LEU
1	A	474	LEU
1	A	477	THR
1	A	479	LYS
1	A	481	ILE
1	A	483	LYS
1	A	484	ASN
1	A	486	LYS
1	A	487	LEU
1	A	488	ASP
1	A	489	MET
1	A	491	ILE
1	A	492	ASN
1	A	493	LEU
1	A	494	LEU
1	A	498	LEU
1	A	499	PRO
1	A	500	LYS
1	A	501	SER
1	A	506	LEU
1	A	507	THR
1	A	511	LEU
1	A	512	LYS
1	A	513	PHE
1	A	520	GLU
1	A	527	LEU
1	A	531	HIS
1	A	532	LEU
1	A	534	LYS
1	A	535	LYS
1	A	537	LEU
1	A	539	LYS
1	A	541	GLU

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Mol	Chain	Res	Type
1	A	543	GLU
1	A	545	LYS
1	A	553	LEU
1	A	557	THR
1	A	559	VAL
1	A	563	MET
1	A	564	LEU
1	A	567	THR
1	A	570	PHE
1	A	575	ILE
1	A	578	LEU
1	A	579	ILE
1	A	589	LEU
1	A	592	LEU
1	A	595	ARG
1	A	599	LEU
1	A	600	LYS
1	A	605	SER
1	A	608	SER
1	A	611	ARG
1	A	612	MET
1	A	619	ARG
1	A	621	LEU
1	A	624	LEU
1	A	631	MET
1	A	641	PHE
1	A	642	TYR
1	A	647	ILE
1	A	650	ILE
1	A	653	SER
1	A	660	CYS
1	A	662	GLN
1	A	680	LEU
1	A	681	LYS
1	A	682	GLN
1	A	687	GLU
1	A	688	GLU
1	B	2	GLU
1	B	5	SER
1	B	9	SER
1	B	10	LEU
1	B	21	MET

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Mol	Chain	Res	Type
1	B	25	THR
1	B	29	ARG
1	B	30	LYS
1	B	31	SER
1	B	36	ILE
1	B	43	LEU
1	B	44	LYS
1	B	46	LEU
1	B	47	GLU
1	B	52	THR
1	B	54	LEU
1	B	55	THR
1	B	59	PHE
1	B	64	GLU
1	B	68	SER
1	B	69	SER
1	B	76	LEU
1	B	77	SER
1	B	79	VAL
1	B	81	THR
1	B	92	LEU
1	B	100	LEU
1	B	104	PRO
1	B	106	LEU
1	B	107	LEU
1	B	108	PRO
1	B	114	ASN
1	B	116	ILE
1	B	117	LYS
1	B	120	LYS
1	B	121	ASN
1	B	124	ASP
1	B	130	THR
1	B	134	LEU
1	B	135	ASP
1	B	136	ASN
1	B	137	LEU
1	B	139	MET
1	B	142	ILE
1	B	144	LYS
1	B	149	LEU
1	B	153	LEU

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Mol	Chain	Res	Type
1	B	159	ILE
1	B	169	LYS
1	B	171	TYR
1	B	176	SER
1	B	178	ARG
1	B	180	GLN
1	B	183	MET
1	B	186	ASP
1	B	188	LYS
1	B	190	GLU
1	B	194	ILE
1	B	196	VAL
1	B	198	ASP
1	B	199	MET
1	B	204	ASP
1	B	209	LYS
1	B	222	GLU
1	B	223	THR
1	B	229	VAL
1	B	231	THR
1	B	233	ASN
1	B	234	SER
1	B	235	LYS
1	B	237	ASN
1	B	242	LYS
1	B	244	GLU
1	B	246	TYR
1	B	248	LYS
1	B	249	LYS
1	B	250	LEU
1	B	252	ARG
1	B	287	LEU
1	B	288	ILE
1	B	289	ASN
1	B	290	GLU
1	B	294	LYS
1	B	298	GLU
1	B	299	GLN
1	B	300	LYS
1	B	305	GLU
1	B	307	GLN
1	B	312	VAL

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Mol	Chain	Res	Type
1	B	318	ARG
1	B	319	VAL
1	B	323	SER
1	B	326	GLN
1	B	327	SER
1	B	333	VAL
1	B	334	ASP
1	B	335	LYS
1	B	338	VAL
1	B	340	GLU
1	B	345	ARG
1	B	346	GLN
1	B	347	LEU
1	B	348	LEU
1	B	350	GLN
1	B	351	ASN
1	B	352	LEU
1	B	354	ILE
1	B	355	LYS
1	B	356	LEU
1	B	358	SER
1	B	363	GLN
1	B	366	ILE
1	B	375	LEU
1	B	378	MET
1	B	381	ILE
1	B	384	VAL
1	B	385	SER
1	B	389	THR
1	B	390	LEU
1	B	391	LYS
1	B	392	ASN
1	B	394	GLN
1	B	395	ARG
1	B	396	ILE
1	B	397	ILE
1	B	400	ILE
1	B	401	LYS
1	B	405	GLU
1	B	406	ILE
1	B	407	THR
1	B	411	THR

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Mol	Chain	Res	Type
1	B	412	VAL
1	B	415	SER
1	B	417	LEU
1	B	419	GLN
1	B	420	ILE
1	B	422	LEU
1	B	423	ILE
1	B	431	LYS
1	B	437	SER
1	B	442	ILE
1	B	445	GLN
1	B	460	SER
1	B	463	ASN
1	B	470	LEU
1	B	474	LEU
1	B	477	THR
1	B	478	VAL
1	B	481	ILE
1	B	483	LYS
1	B	484	ASN
1	B	486	LYS
1	B	487	LEU
1	B	488	ASP
1	B	489	MET
1	B	491	ILE
1	B	492	ASN
1	B	493	LEU
1	B	494	LEU
1	B	498	LEU
1	B	499	PRO
1	B	500	LYS
1	B	501	SER
1	B	506	LEU
1	B	507	THR
1	B	511	LEU
1	B	512	LYS
1	B	513	PHE
1	B	520	GLU
1	B	527	LEU
1	B	531	HIS
1	B	532	LEU
1	B	534	LYS

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Mol	Chain	Res	Type
1	B	535	LYS
1	B	537	LEU
1	B	539	LYS
1	B	541	GLU
1	B	543	GLU
1	B	545	LYS
1	B	553	LEU
1	B	557	THR
1	B	559	VAL
1	B	563	MET
1	B	564	LEU
1	B	567	THR
1	B	570	PHE
1	B	575	ILE
1	B	578	LEU
1	B	579	ILE
1	B	589	LEU
1	B	592	LEU
1	B	595	ARG
1	B	599	LEU
1	B	600	LYS
1	B	605	SER
1	B	608	SER
1	B	611	ARG
1	B	612	MET
1	B	619	ARG
1	B	621	LEU
1	B	624	LEU
1	B	631	MET
1	B	641	PHE
1	B	642	TYR
1	B	647	ILE
1	B	650	ILE
1	B	653	SER
1	B	660	CYS
1	B	662	GLN
1	B	680	LEU
1	B	681	LYS
1	B	682	GLN
1	B	687	GLU
1	B	688	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	121	ASN
1	A	136	ASN
1	A	237	ASN
1	A	392	ASN
1	A	476	ASN
1	A	617	HIS
1	A	618	GLN
1	B	40	ASN
1	B	121	ASN
1	B	136	ASN
1	B	237	ASN
1	B	476	ASN
1	B	617	HIS
1	B	618	GLN

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 monosaccharides 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

There are no chain breaks in this entry.

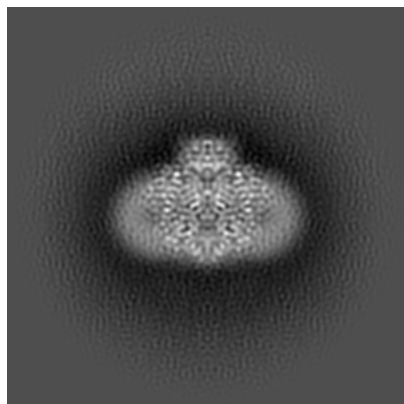
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34210. These allow visual inspection of the internal detail of the map and identification of artifacts.

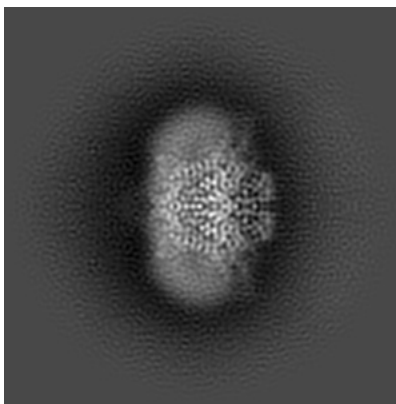
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

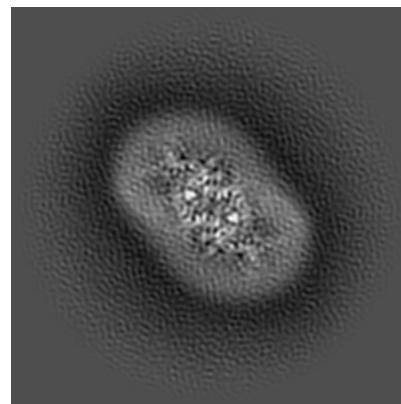
6.1.1 Primary map



X

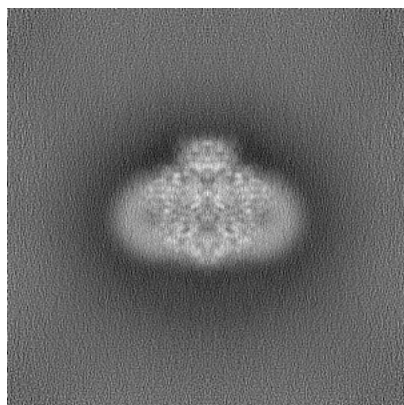


Y

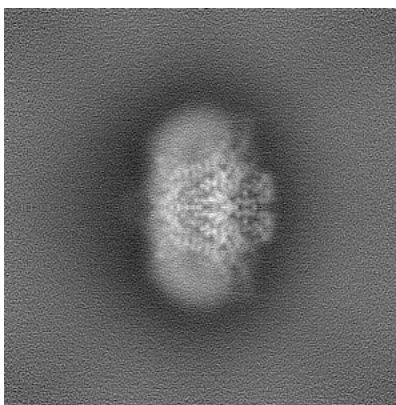


Z

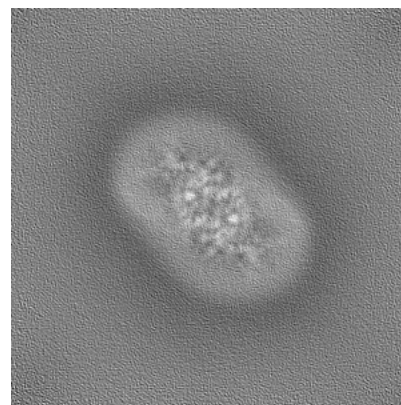
6.1.2 Raw map



X



Y

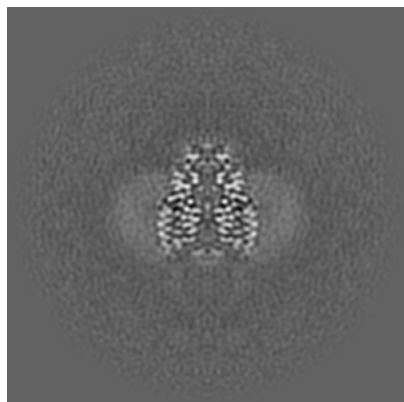


Z

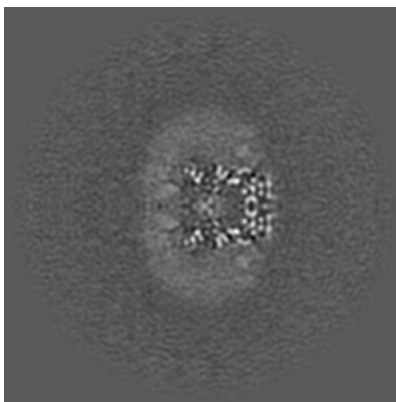
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

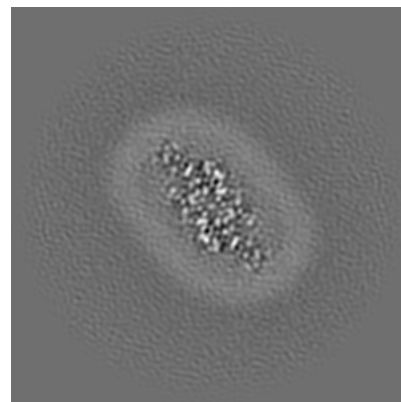
6.2.1 Primary map



X Index: 160

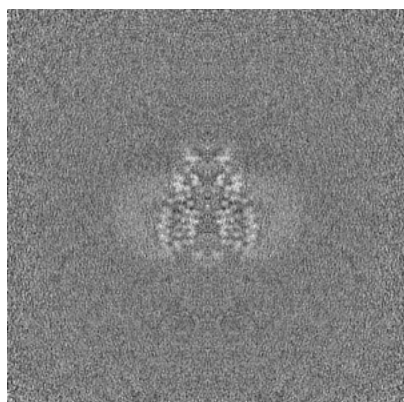


Y Index: 160

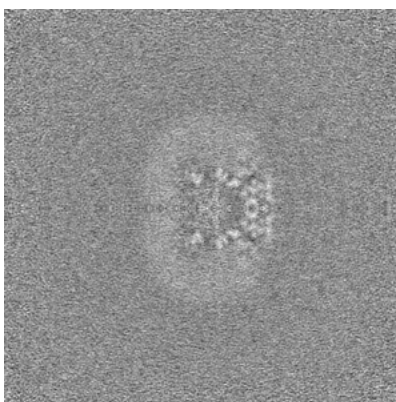


Z Index: 160

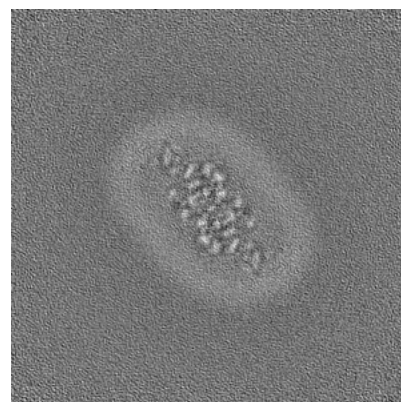
6.2.2 Raw map



X Index: 160



Y Index: 160

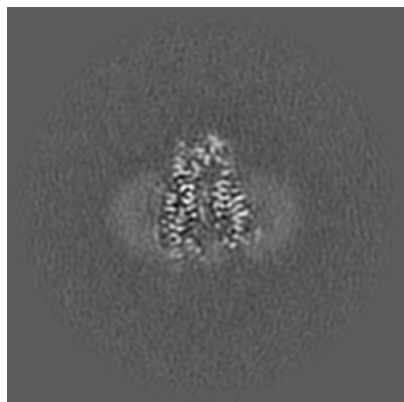


Z Index: 160

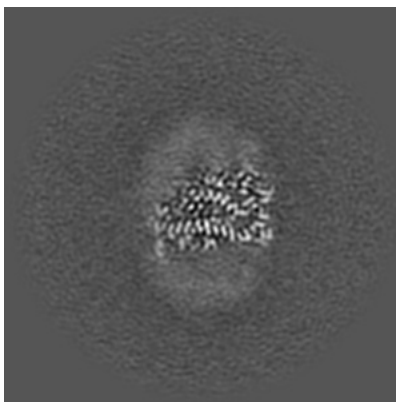
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

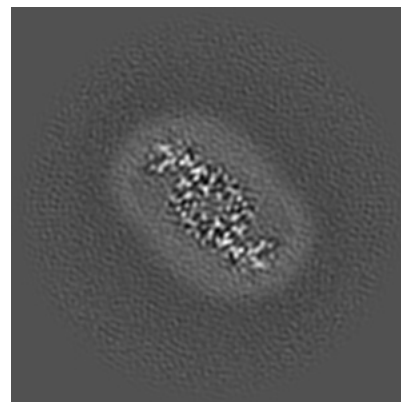
6.3.1 Primary map



X Index: 166

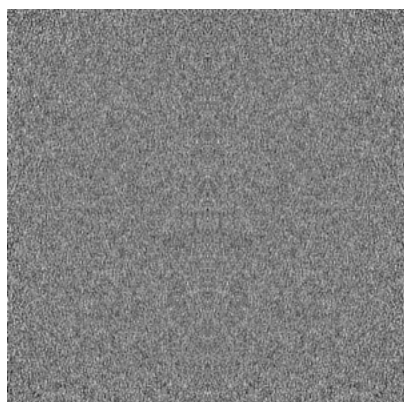


Y Index: 169

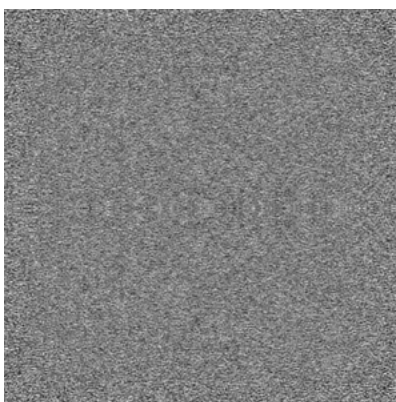


Z Index: 169

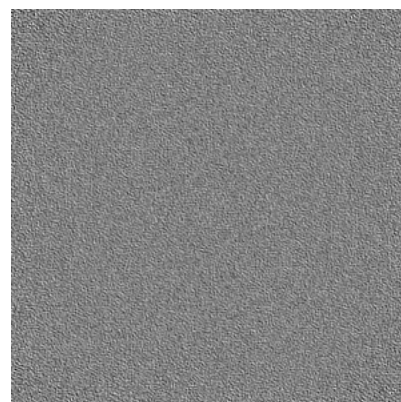
6.3.2 Raw map



X Index: 0



Y Index: 0

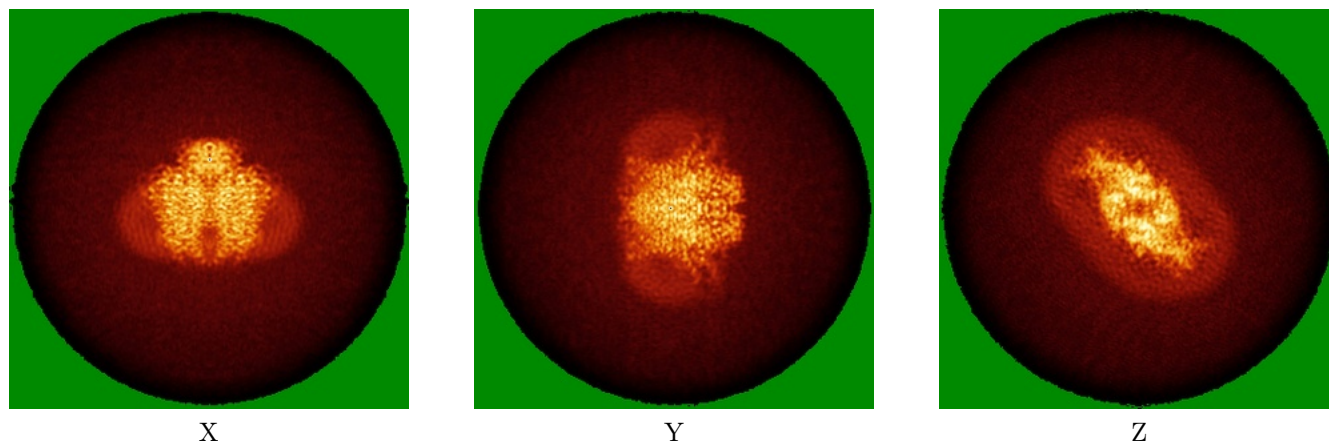


Z Index: 0

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

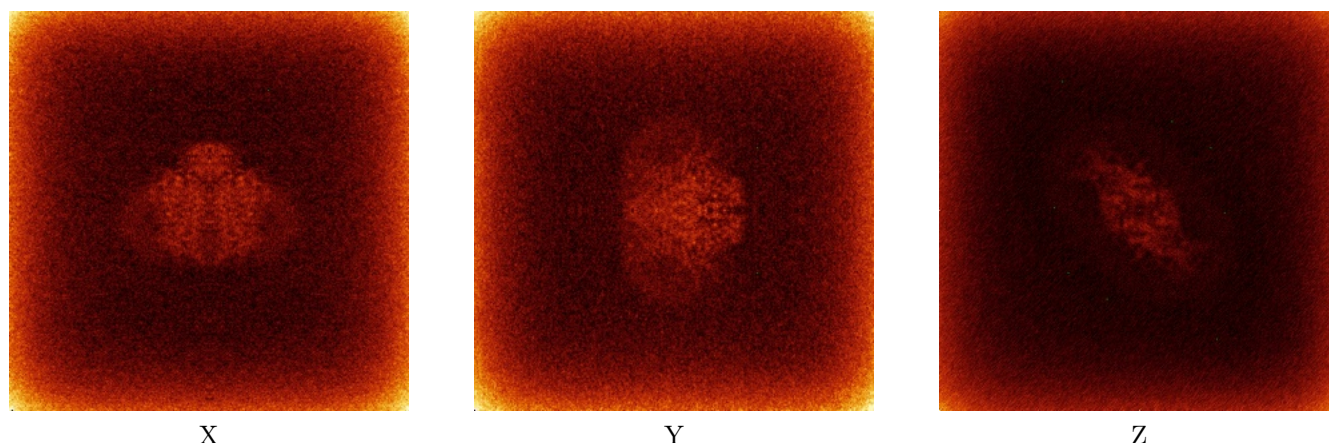


X

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.

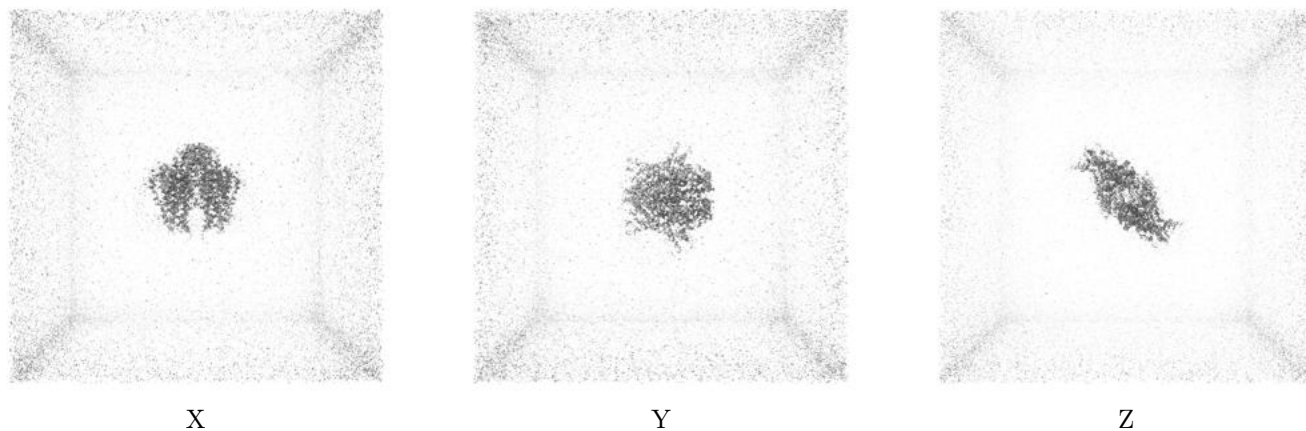
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

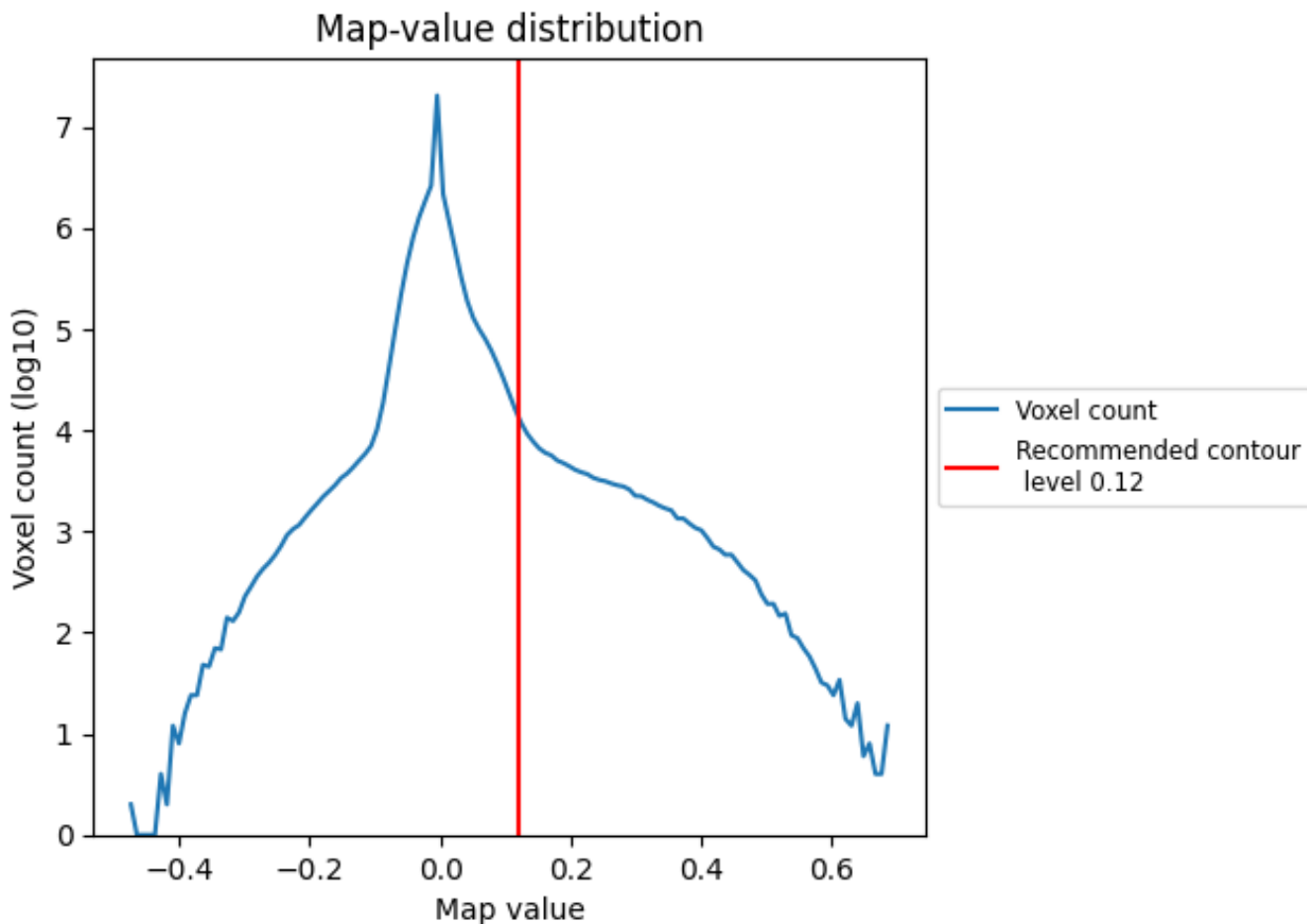
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

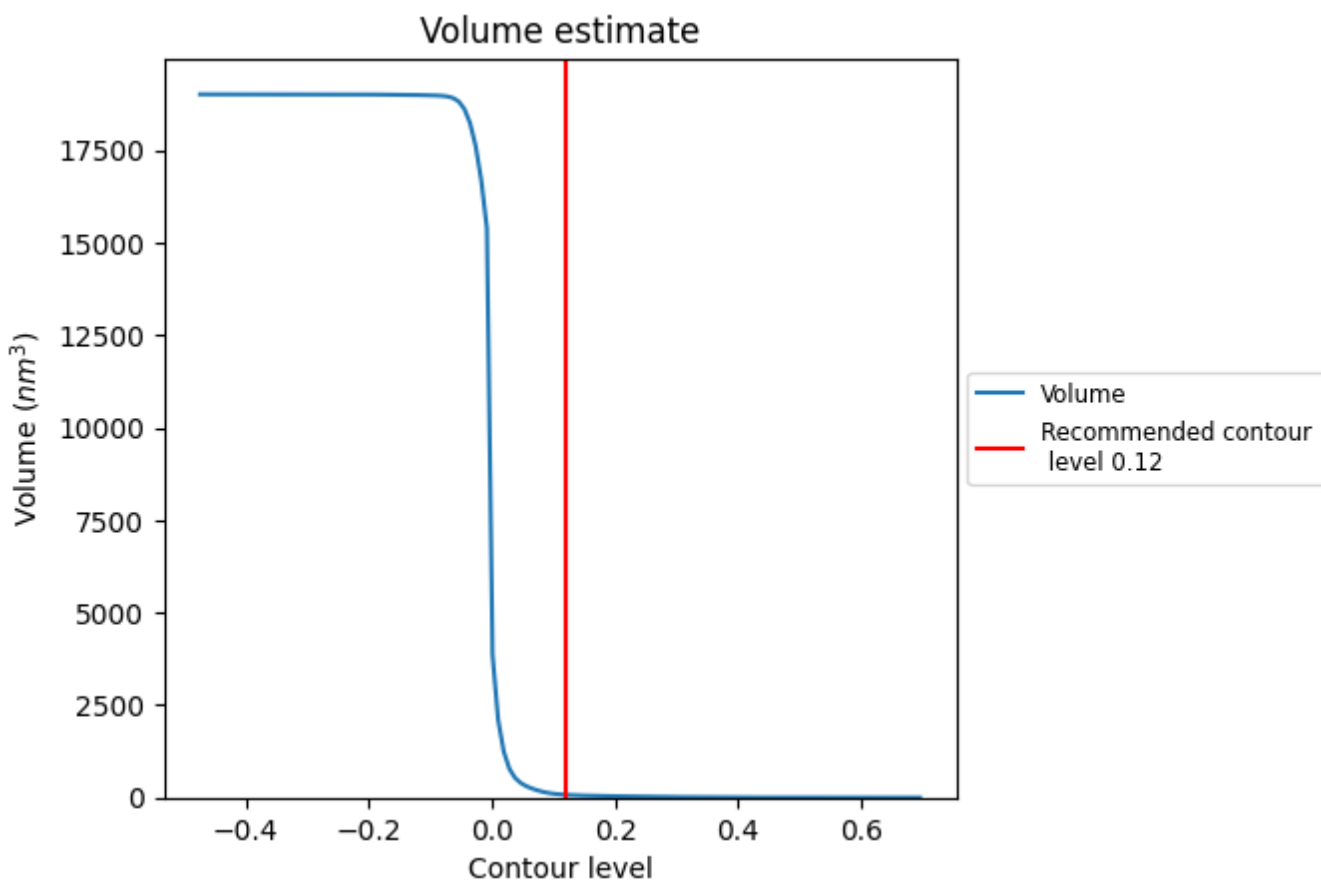
This section contains the results of statistical analysis of the map.

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.

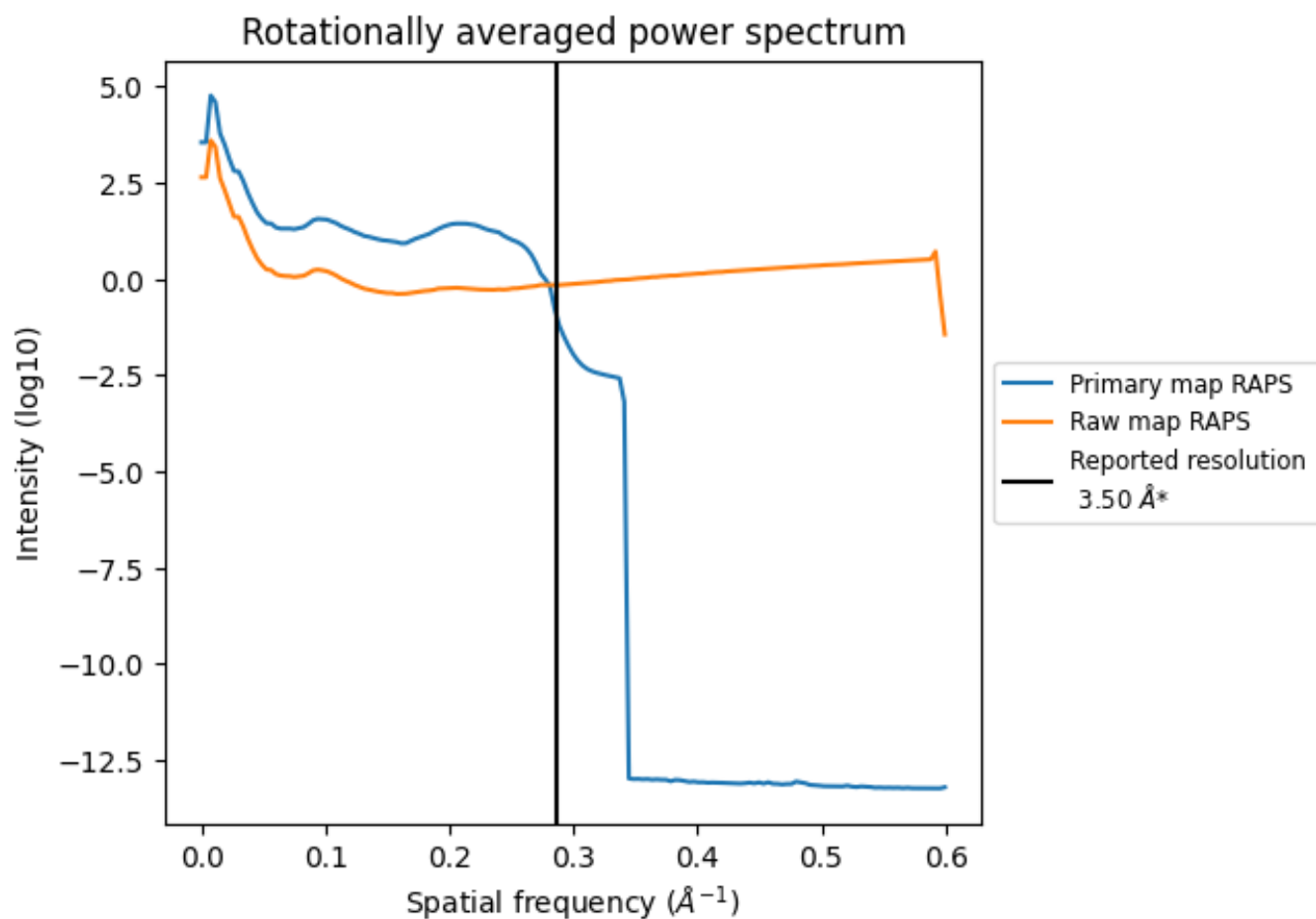
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 73 nm³; this corresponds to an approximate mass of 66 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](#)

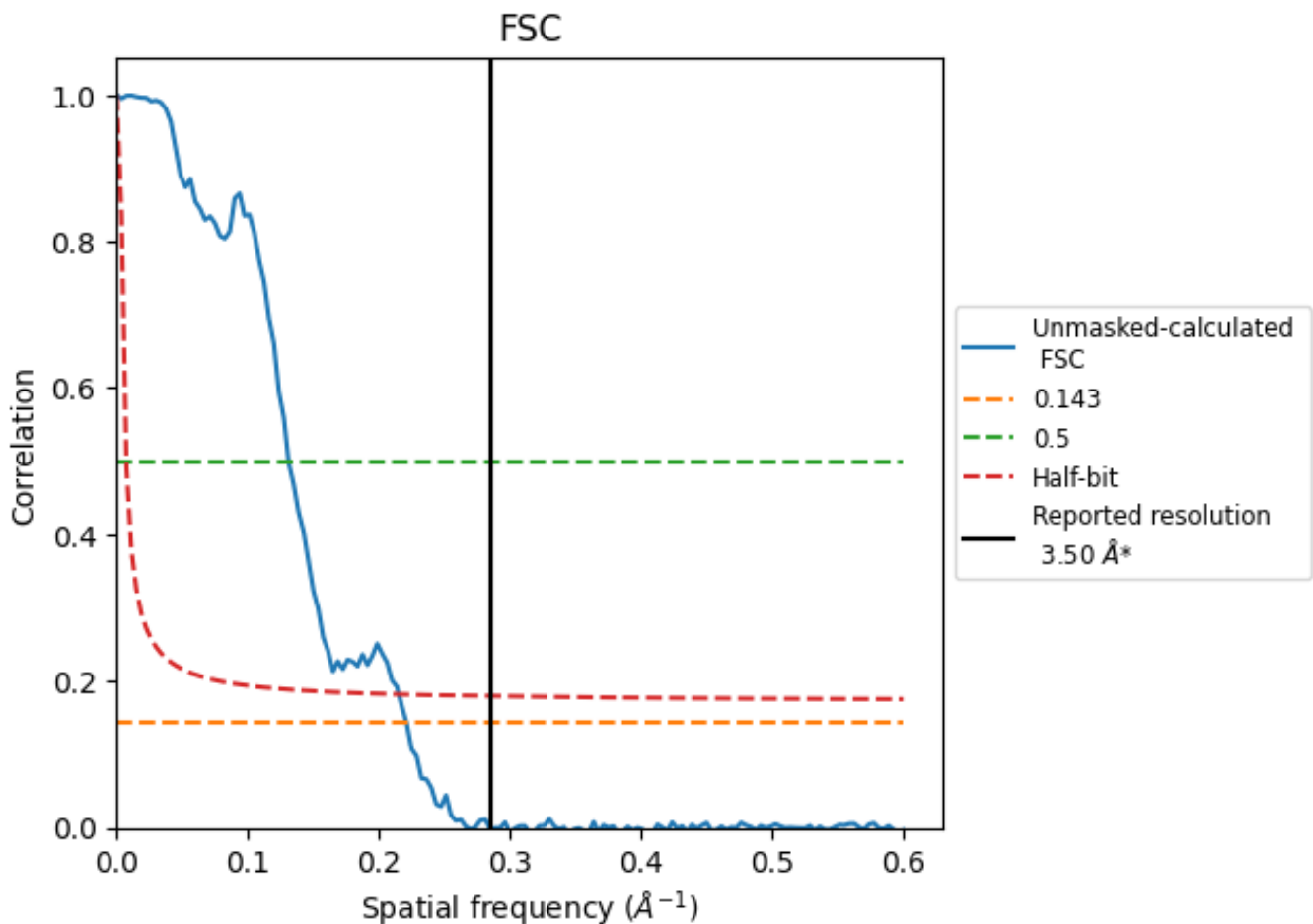


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

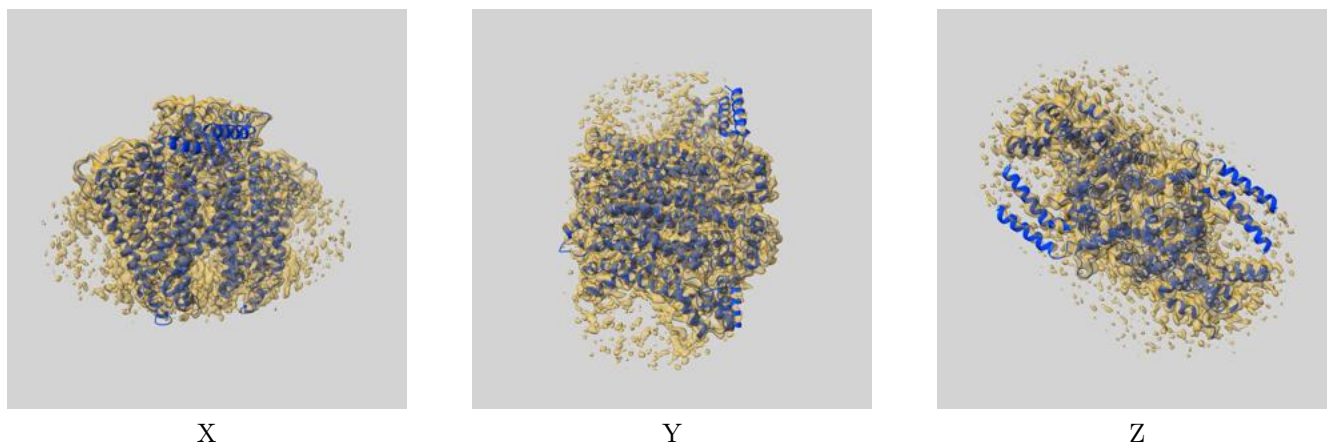
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.53	7.63	4.65

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.53 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

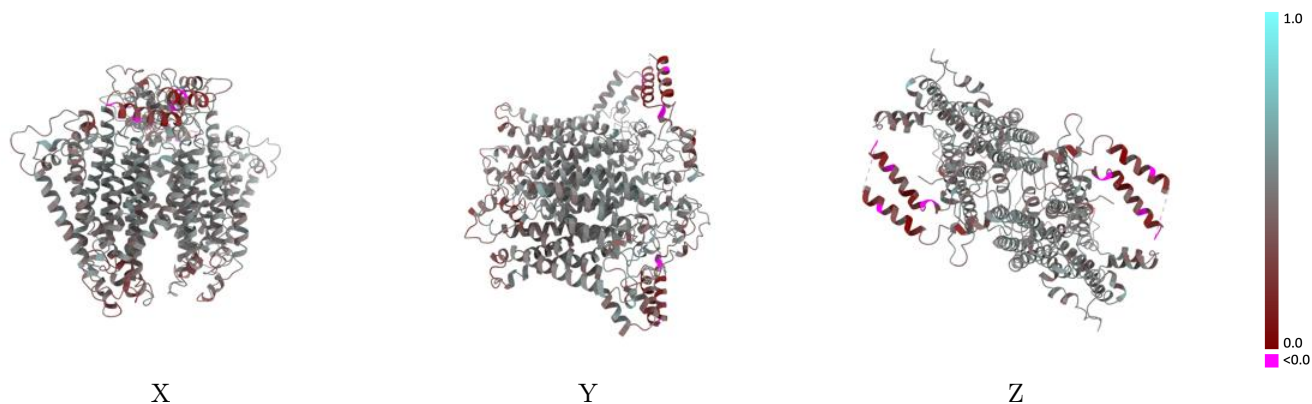
This section contains information regarding the fit between EMDB map EMD-34210 and PDB model 8GRO. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



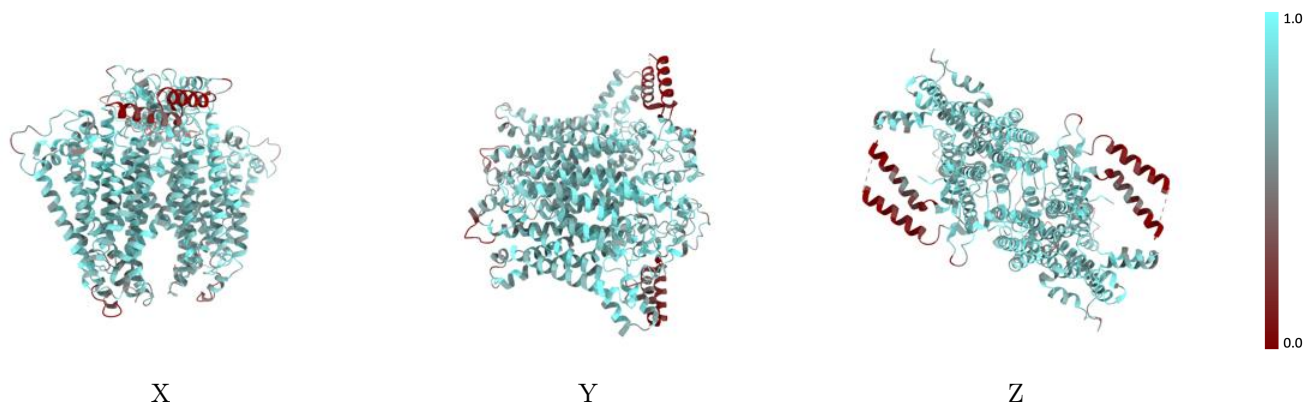
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



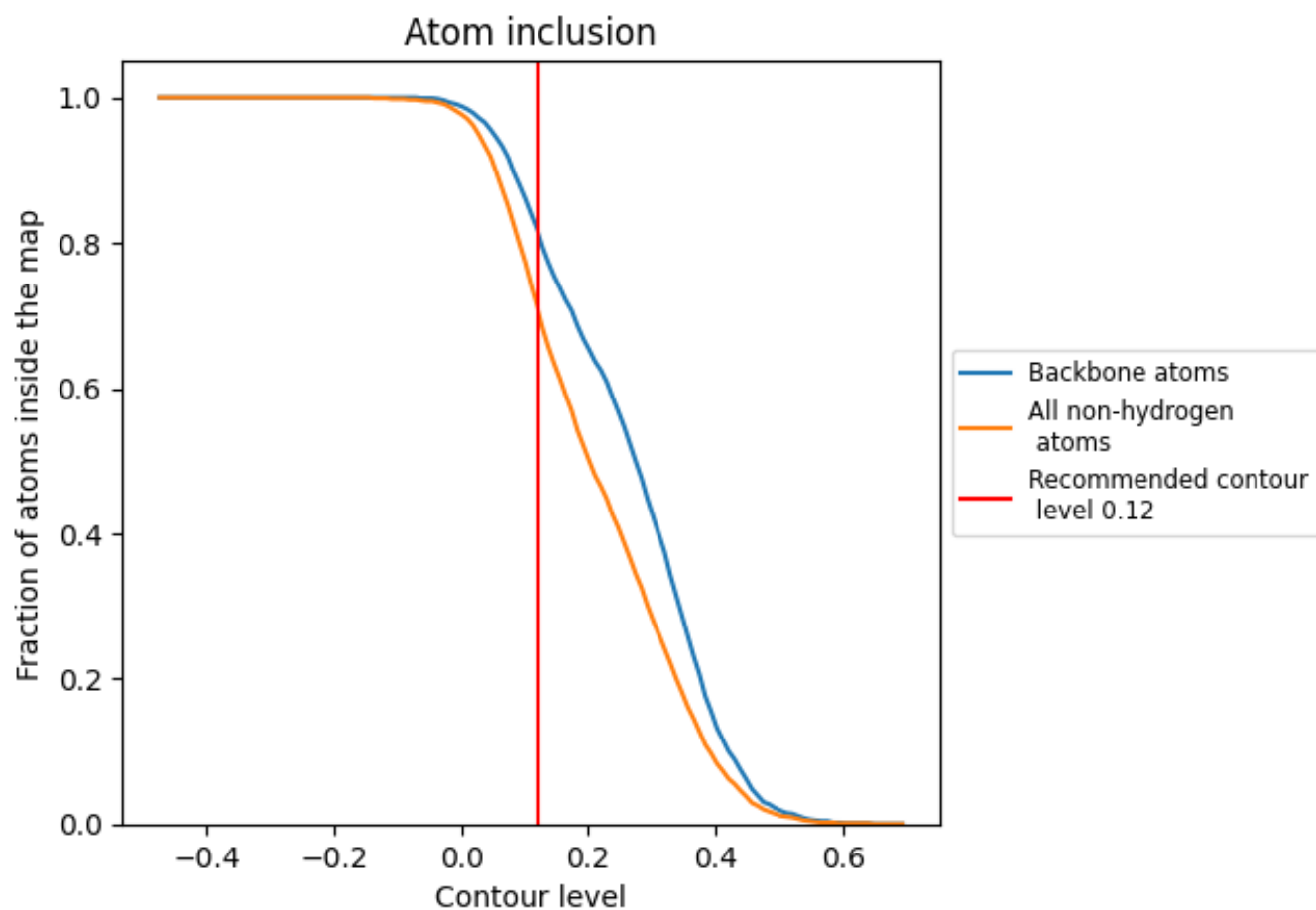
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).







9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7120	 0.4440
A	 0.7120	 0.4440
B	 0.7120	 0.4440

