



Full wwPDB EM Validation Report ⓘ

Mar 12, 2026 – 06:20 PM UTC

PDB ID : 8RC4 / pdb_00008rc4
EMDB ID : EMD-19047
Title : Structure of Integrator-PP2A complex
Authors : Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P.
Deposited on : 2023-12-06
Resolution : 3.10 Å(reported)
Based on initial model : 8RBX

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

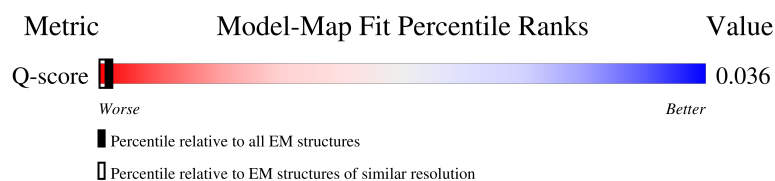
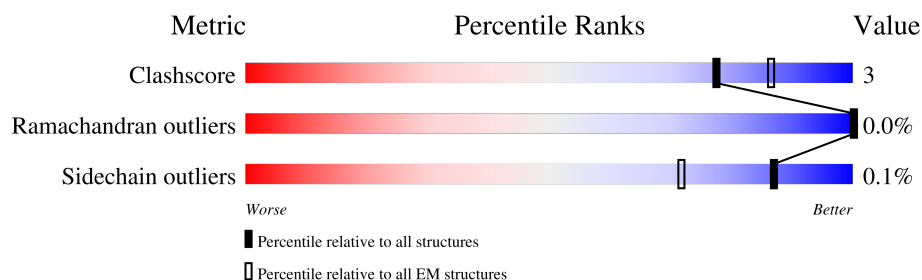
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



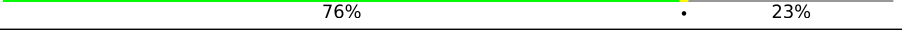
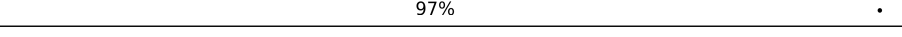
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	p	591	 86% 12% .
2	q	311	 83% 10% 7%
3	r	31	 84% 16%
4	a	2192	 76% 5% 19%

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Mol	Chain	Length	Quality of chain
5	b	1204	
6	d	963	
7	e	1021	
8	f	892	
9	g	964	
10	h	995	
11	i	658	
12	k	602	
13	m	706	
14	j	710	
15	n	518	
16	o	451	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 78273 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	p	580	Total	C	N	O	S	0	0
			4437	2828	753	829	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	-1	SER	-	expression tag	UNP P30153
p	0	ASN	-	expression tag	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	q	290	Total	C	N	O	S	0	0
			2340	1481	405	439	15		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	-1	SER	-	expression tag	UNP P67775
q	0	ASN	-	expression tag	UNP P67775
q	88	ASN	ASP	engineered mutation	UNP P67775

- Molecule 3 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	r	31	Total	C	N	O	S	0	0
			263	161	44	57	1		

- Molecule 4 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	a	1766	Total	C	N	O	S	0	0
			11842	7410	2168	2213	51		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	-1	SER	-	expression tag	UNP Q8N201
a	0	ASN	-	expression tag	UNP Q8N201

- Molecule 5 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	b	1051	Total	C	N	O	S	0	0
			8099	5198	1368	1471	62		

- Molecule 6 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	823	Total	C	N	O	S	0	0
			6443	4112	1099	1196	36		

- Molecule 7 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	873	Total	C	N	O	S	0	0
			6373	4050	1161	1135	27		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
e	-1	SER	-	expression tag	UNP Q6P9B9
e	0	ASN	-	expression tag	UNP Q6P9B9

- Molecule 8 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	561	Total	C	N	O	S	0	0
			4422	2827	754	815	26		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-4	TYR	-	expression tag	UNP Q9UL03
f	-3	PHE	-	expression tag	UNP Q9UL03
f	-2	GLN	-	expression tag	UNP Q9UL03
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

- Molecule 9 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	889	Total	C	N	O	S	0	0
			6764	4283	1173	1267	41		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	-1	SER	-	expression tag	UNP Q9NVH2
g	0	ASN	-	expression tag	UNP Q9NVH2

- Molecule 10 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	h	956	Total	C	N	O	S	0	0
			7623	4877	1297	1403	46		

- Molecule 11 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	i	626	Total	C	N	O	S	0	0
			4871	3137	792	909	33		

- Molecule 12 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	589	Total	C	N	O	S	0	0
			4411	2822	768	790	31		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	-1	SER	-	expression tag	UNP Q5TA45
k	0	ASN	-	expression tag	UNP Q5TA45
k	203	GLN	GLU	engineered mutation	UNP Q5TA45

- Molecule 13 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	m	542	Total	C	N	O	0	0
			2810	1682	568	560		

- Molecule 14 is a protein called Integrator complex subunit 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	653	Total	C	N	O	0	0
			3238	1932	653	653		

- Molecule 15 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	n	503	Total	C	N	O	0	0
			2484	1478	503	503		

- Molecule 16 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	o	372	Total	C	N	O	0	0
			1849	1105	372	372		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
o	-1	SER	-	expression tag	UNP Q96N11
o	0	ASN	-	expression tag	UNP Q96N11

- Molecule 17 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	q	2	Total	Mn	0
			2	2	

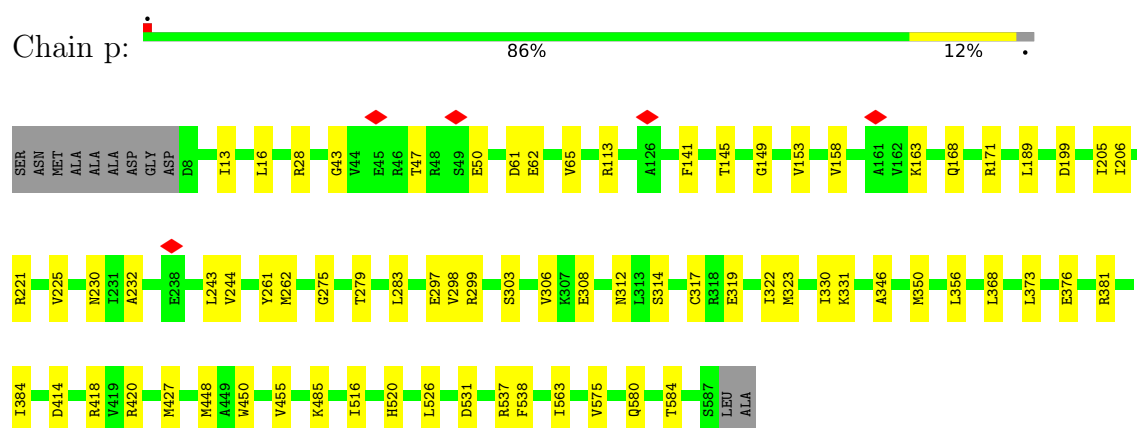
- Molecule 18 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
18	k	2	Total	Zn	0
			2	2	

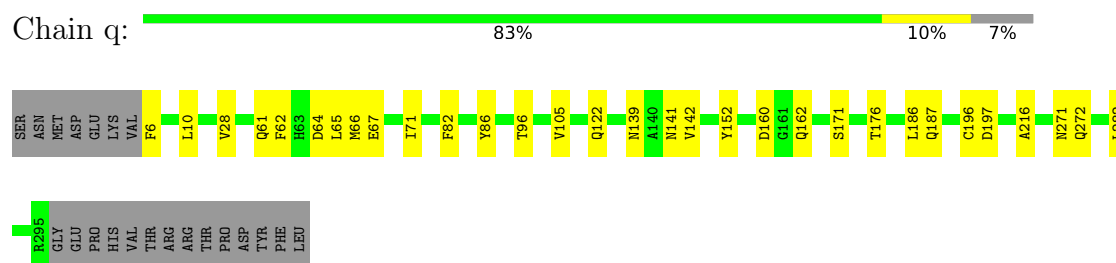
3 Residue-property plots [i](#)

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.

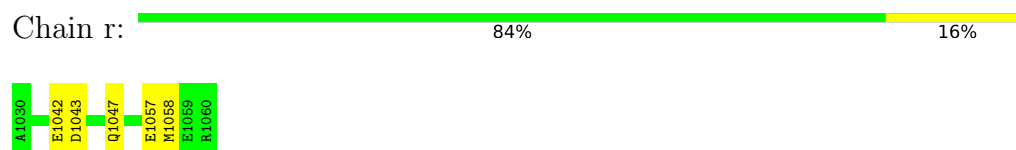
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



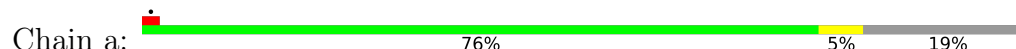
- Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

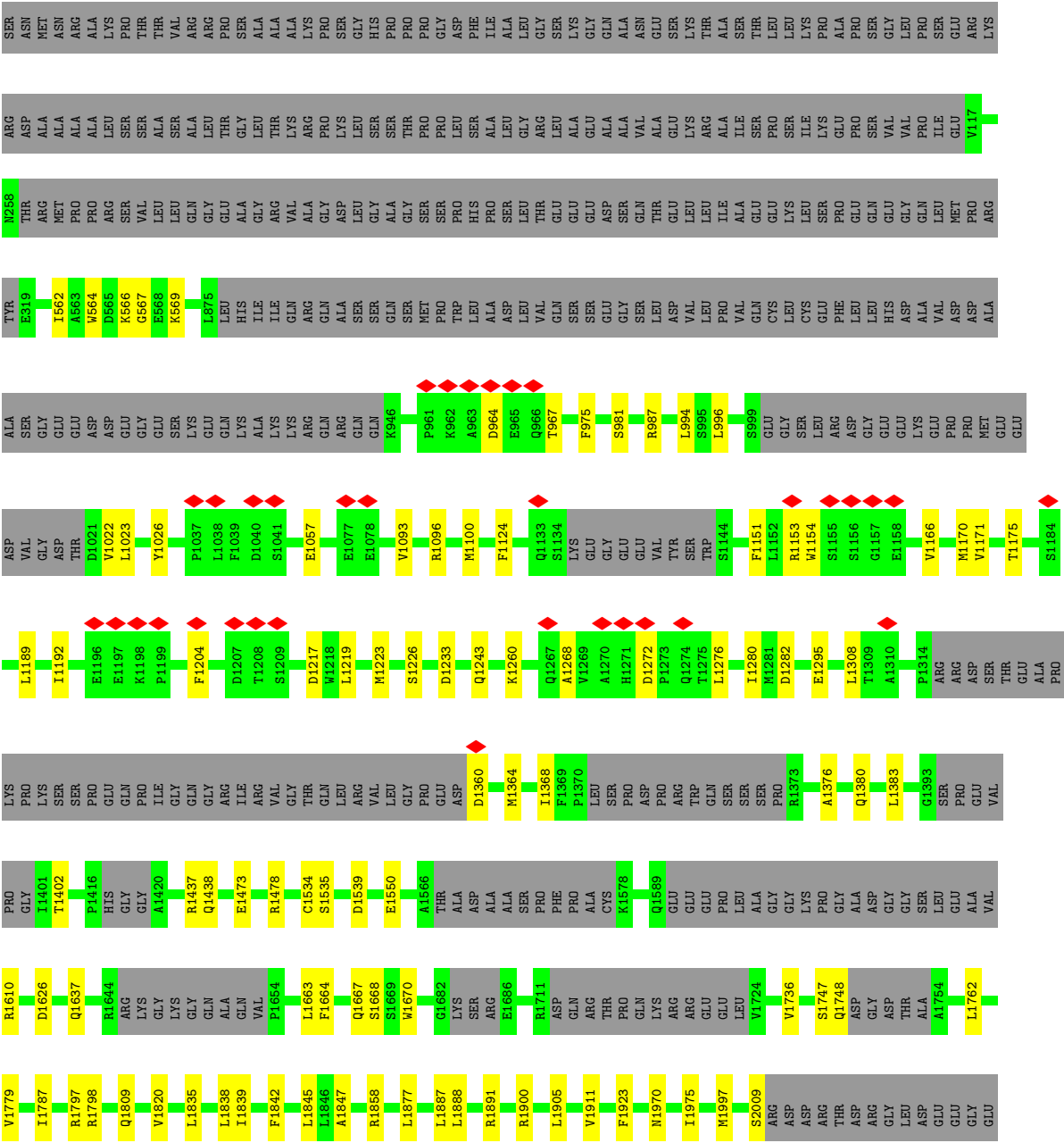


- Molecule 3: DSS1

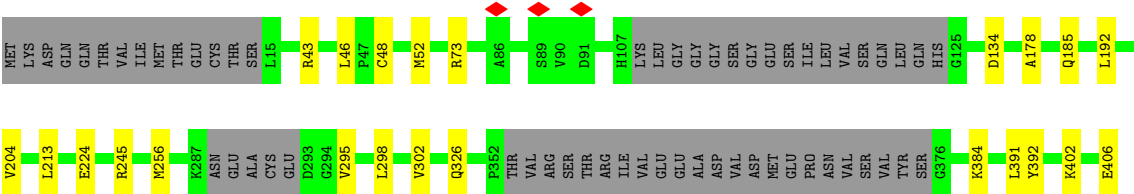
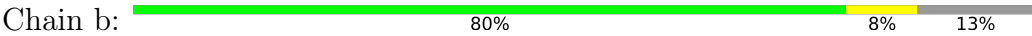


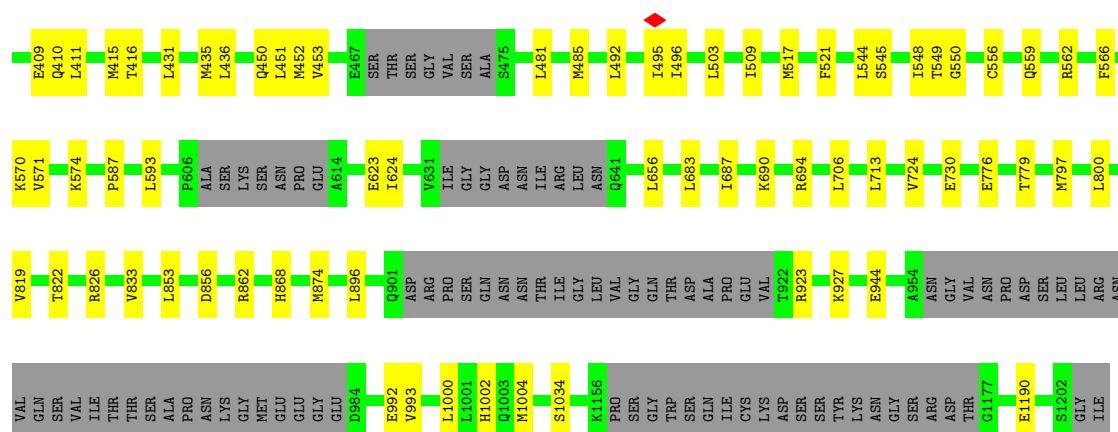
- Molecule 4: Integrator complex subunit 1





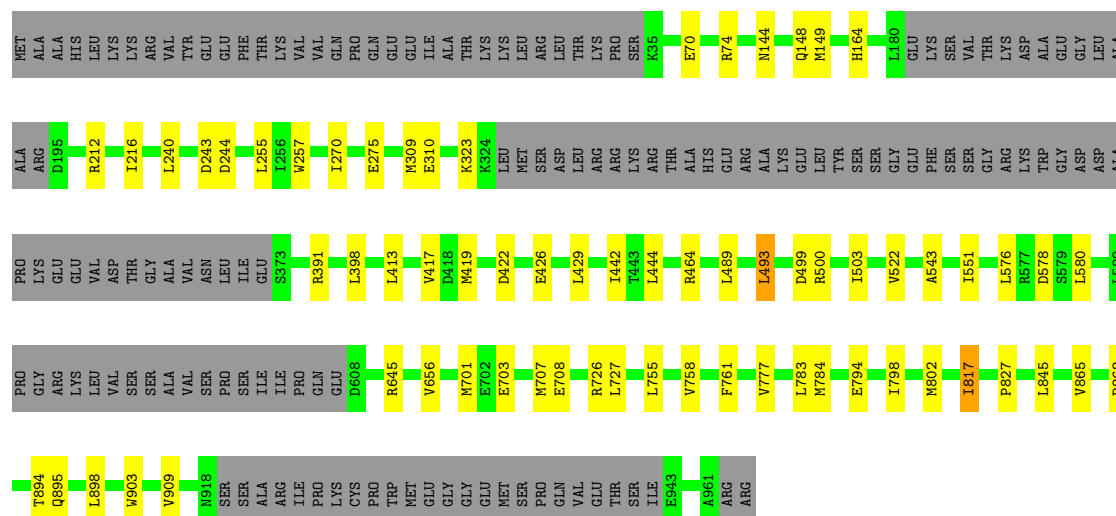
● Molecule 5: Integrator complex subunit 2





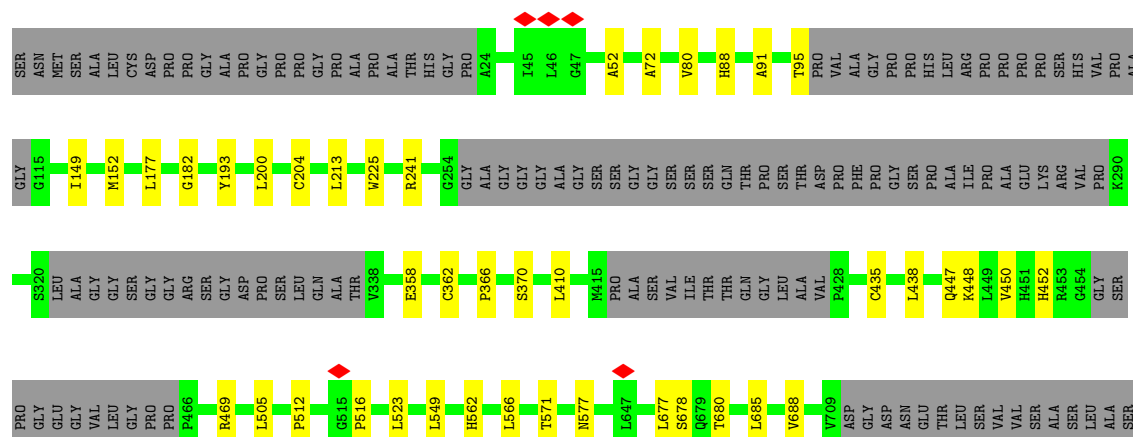
• Molecule 6: Integrator complex subunit 4

Chain d: 79% 7% 15%



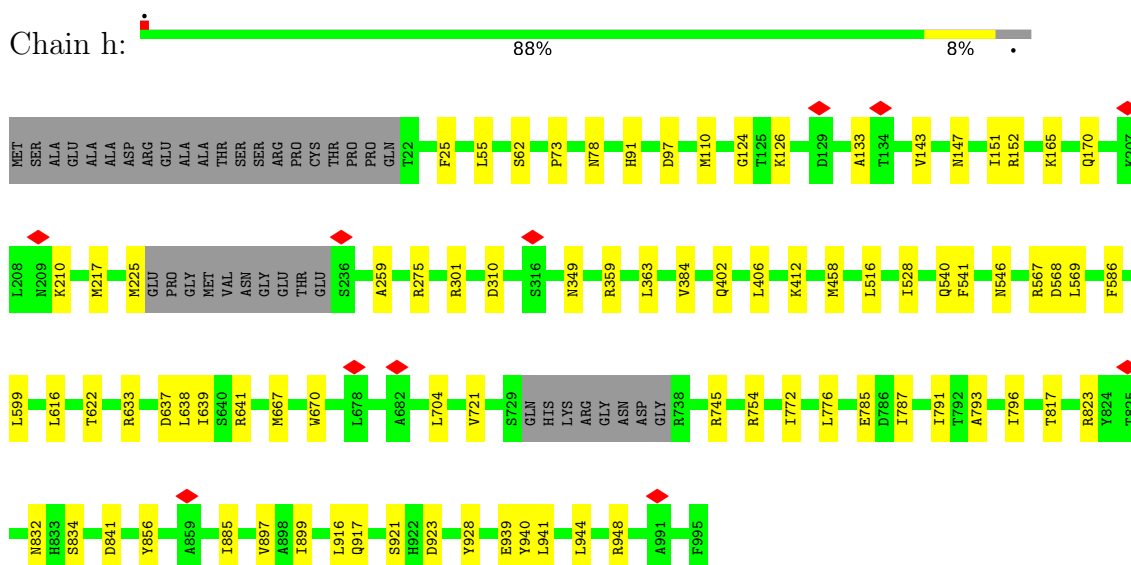
• Molecule 7: Integrator complex subunit 5

Chain e: 78% 8% 14%

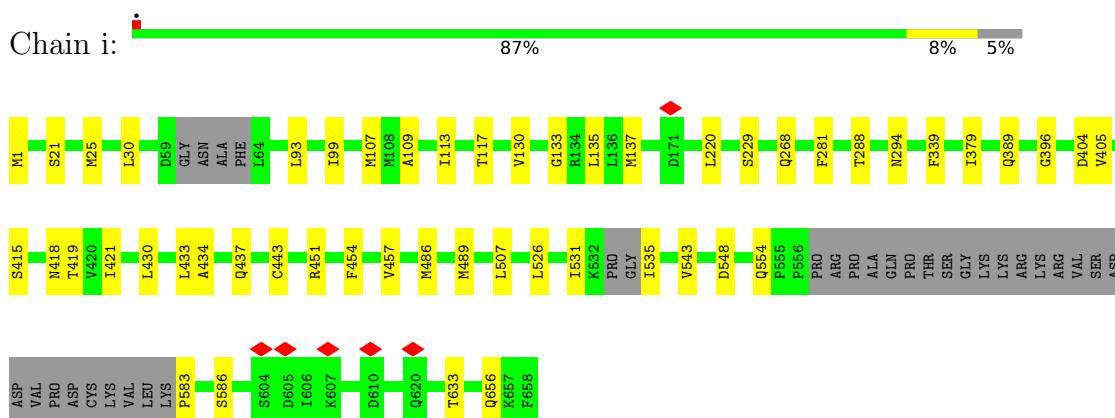




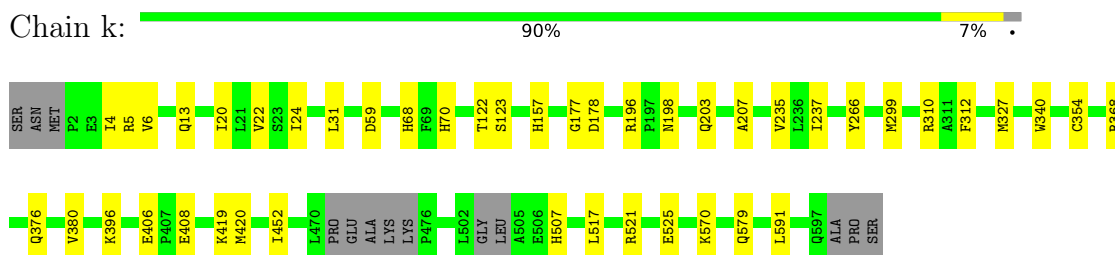
- Molecule 10: Integrator complex subunit 8



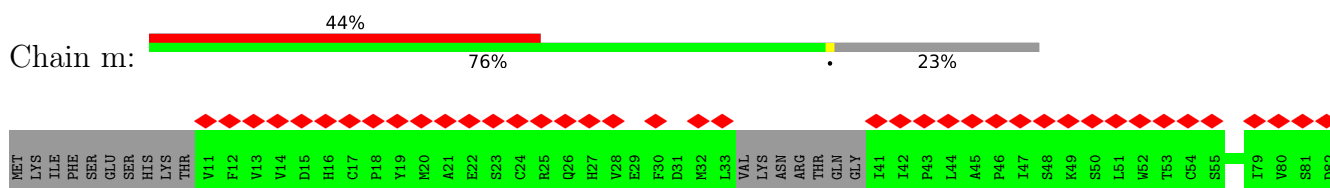
- Molecule 11: Integrator complex subunit 9

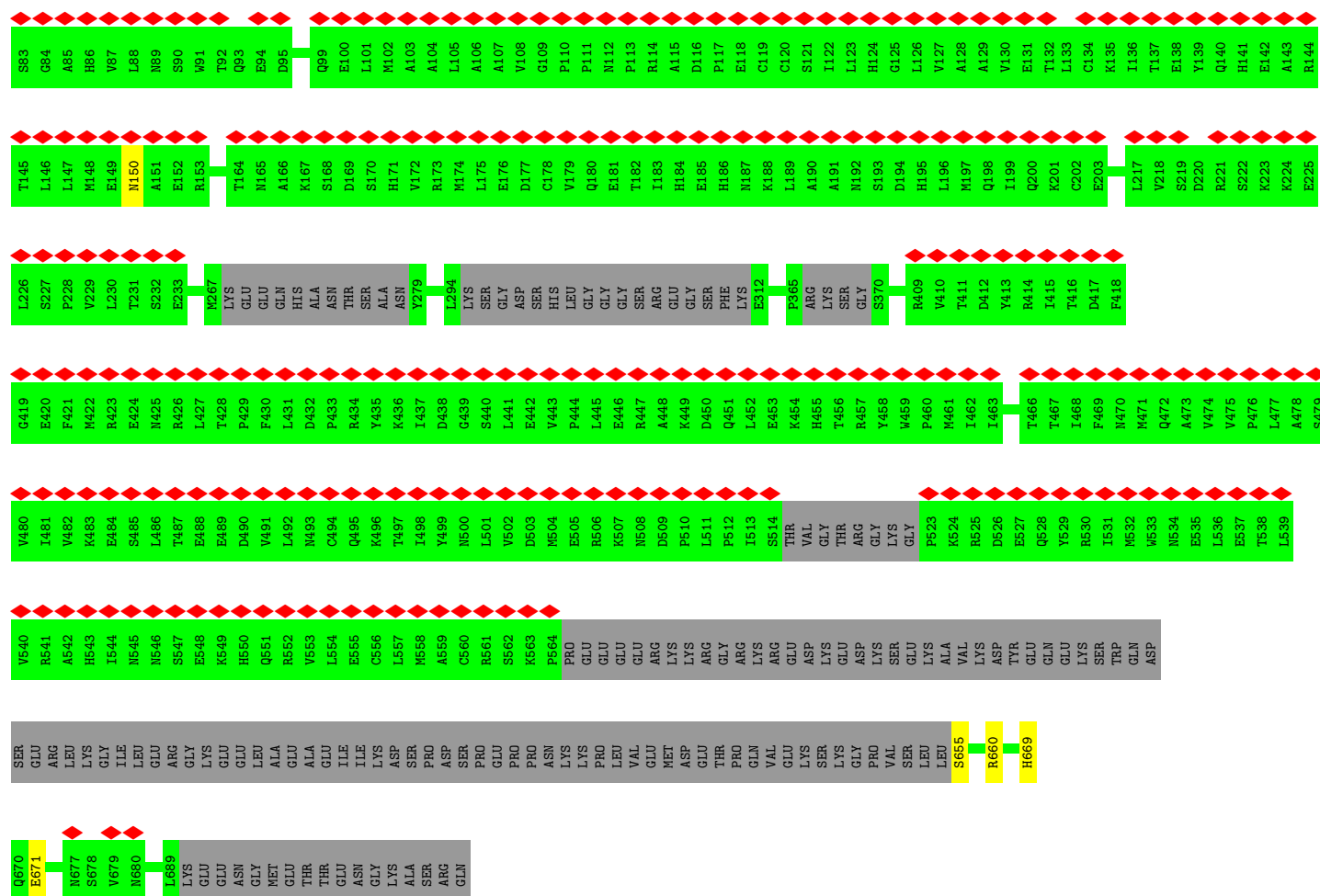


- Molecule 12: Integrator complex subunit 11

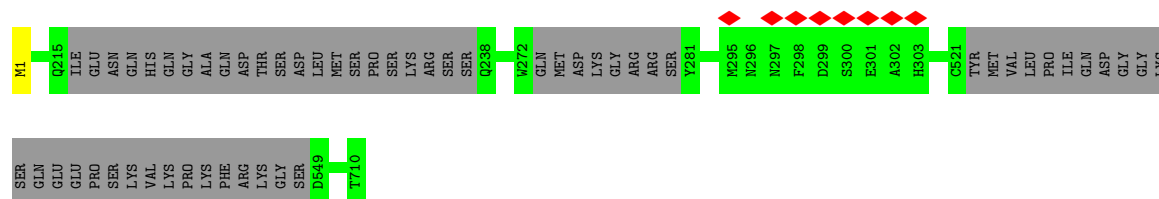
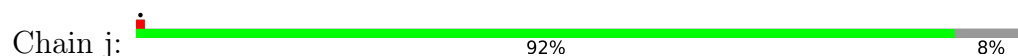


- Molecule 13: Integrator complex subunit 13

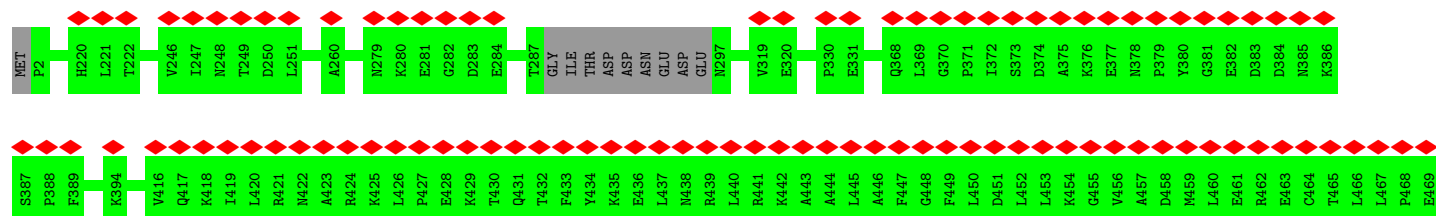


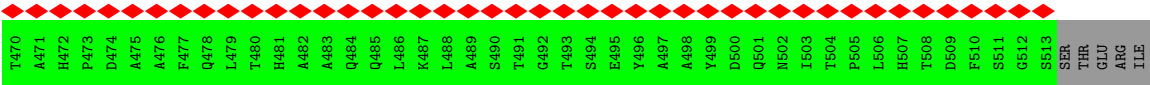


• Molecule 14: Integrator complex subunit 10

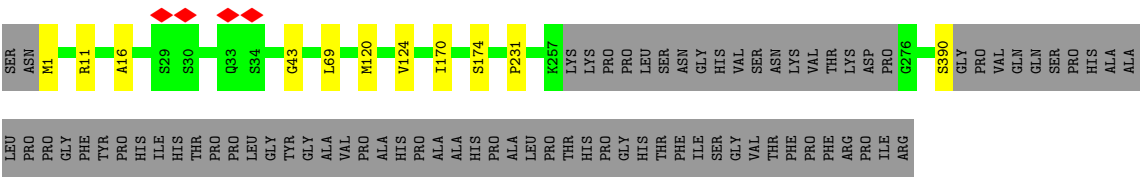
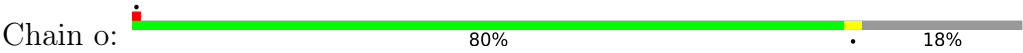


• Molecule 15: Integrator complex subunit 14





• Molecule 16: Integrator complex subunit 15



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2335349	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 ($e^-/\text{\AA}^2$)	40.49	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.185	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.00502	Depositor
Map size ($\text{\AA}$)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	p	0.26	0/4511	0.49	0/6136
2	q	0.35	0/2397	0.50	0/3250
3	r	0.26	0/267	0.55	0/362
4	a	0.19	0/11994	0.45	0/16391
5	b	0.24	0/8242	0.47	0/11212
6	d	0.21	0/6568	0.48	1/8919 (0.0%)
7	e	0.25	0/6520	0.47	0/8895
8	f	0.22	0/4531	0.42	0/6154
9	g	0.22	0/6874	0.42	0/9324
10	h	0.22	0/7768	0.42	0/10530
11	i	0.21	0/4990	0.45	0/6802
12	k	0.19	0/4508	0.47	0/6119
13	m	0.11	0/2809	0.35	0/3897
14	j	0.14	0/3234	0.39	0/4505
15	n	0.12	0/2482	0.37	0/3453
16	o	0.16	0/1847	0.44	0/2576
All	All	0.21	0/79542	0.45	1/108525 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	d	701	MET	CB-CG-SD	5.77	130.02	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	p	4437	0	4508	42	0
2	q	2340	0	2248	20	0
3	r	263	0	229	5	0
4	a	11842	0	10065	67	0
5	b	8099	0	8211	56	0
6	d	6443	0	6483	43	0
7	e	6373	0	6187	48	0
8	f	4422	0	4393	22	0
9	g	6764	0	6747	56	0
10	h	7623	0	7779	48	0
11	i	4871	0	4849	32	0
12	k	4411	0	4248	29	0
13	m	2810	0	1353	4	0
14	j	3238	0	1433	1	0
15	n	2484	0	1104	0	0
16	o	1849	0	811	6	0
17	q	2	0	0	0	0
18	k	2	0	0	0	0
All	All	78273	0	70648	433	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 3.

All (433) 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)
11:i:633:THR:HG1	12:k:507:HIS:HE2	1.24	0.85
8:f:324:PHE:HB2	8:f:382:MET:HE1	1.74	0.69
6:d:783:LEU:HD21	6:d:802:MET:HE1	1.77	0.66
1:p:62:GLU:HB2	1:p:65:VAL:HG12	1.79	0.65
12:k:70:HIS:CE1	12:k:157:HIS:NE2	2.64	0.65
4:a:1997:MET:SD	4:a:1997:MET:N	2.69	0.64
5:b:436:LEU:HD21	5:b:452:MET:HE2	1.80	0.64
5:b:392:TYR:HB3	5:b:435:MET:HE1	1.79	0.63
7:e:824:ALA:HB1	7:e:827:ALA:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:k:299:MET:SD	12:k:299:MET:N	2.72	0.63
8:f:380:PHE:HB3	8:f:382:MET:HE3	1.80	0.62
11:i:415:SER:OG	11:i:418:ASN:ND2	2.32	0.62
4:a:1057:GLU:O	4:a:1096:ARG:NH2	2.33	0.62
4:a:1626:ASP:OD2	4:a:1637:GLN:NE2	2.33	0.62
4:a:1166:VAL:HG22	4:a:1170:MET:HE2	1.81	0.61
12:k:5:ARG:NH2	13:m:671:GLU:OE2	2.33	0.61
5:b:574:LYS:NZ	5:b:623:GLU:OE1	2.32	0.61
11:i:531:ILE:O	11:i:535:ILE:N	2.33	0.61
12:k:340:TRP:O	12:k:376:GLN:NE2	2.33	0.61
8:f:214:ARG:NH2	8:f:218:GLN:OE1	2.29	0.61
11:i:288:THR:HG21	11:i:419:THR:HG22	1.83	0.61
9:g:474:LEU:HD23	9:g:493:LEU:HD21	1.83	0.60
4:a:1835:LEU:HD22	4:a:1838:LEU:HD21	1.83	0.60
6:d:578:ASP:OD1	9:g:144:ARG:NH1	2.34	0.60
11:i:526:LEU:O	13:m:655:SER:N	2.34	0.60
10:h:124:GLY:O	10:h:126:LYS:NZ	2.32	0.60
10:h:721:VAL:HG11	10:h:776:LEU:HD21	1.83	0.60
6:d:212:ARG:NH1	6:d:243:ASP:OD2	2.35	0.60
4:a:1276:LEU:HA	4:a:1280:ILE:HD12	1.82	0.60
6:d:149:MET:SD	6:d:149:MET:N	2.75	0.59
7:e:896:ASP:OD2	7:e:898:THR:OG1	2.20	0.59
2:q:61:GLN:NE2	2:q:64:ASP:OD2	2.34	0.59
4:a:1473:GLU:O	4:a:1478:ARG:NH2	2.36	0.59
7:e:410:LEU:HD11	7:e:438:LEU:HD11	1.86	0.58
11:i:294:ASN:ND2	11:i:389:GLN:O	2.36	0.58
12:k:196:ARG:NH2	12:k:406:GLU:OE1	2.36	0.58
1:p:189:LEU:HD11	1:p:205:ILE:HG23	1.86	0.58
9:g:390:LEU:HB3	9:g:416:MET:HE2	1.84	0.58
4:a:1762:LEU:HD21	4:a:1809:GLN:HG3	1.85	0.58
1:p:427:MET:HE3	1:p:450:TRP:HH2	1.69	0.58
7:e:523:LEU:O	7:e:577:ASN:ND2	2.35	0.58
7:e:213:LEU:HD11	7:e:241:ARG:HB3	1.85	0.57
9:g:626:ASP:OD2	9:g:684:ARG:NH2	2.38	0.57
12:k:517:LEU:HD22	12:k:591:LEU:HD22	1.85	0.57
10:h:899:ILE:HD11	10:h:928:TYR:HB3	1.86	0.57
5:b:593:LEU:HD11	5:b:706:LEU:HD13	1.85	0.57
4:a:1842:PHE:HA	4:a:1845:LEU:HB2	1.86	0.57
5:b:868:HIS:HA	5:b:874:MET:HE3	1.86	0.57
2:q:171:SER:HB2	2:q:197:ASP:HB2	1.86	0.57
4:a:2065:GLU:OE1	10:h:745:ARG:NH2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:178:ALA:HB1	5:b:213:LEU:HD11	1.87	0.57
4:a:1664:PHE:O	4:a:1668:SER:OG	2.20	0.57
5:b:544:LEU:HA	5:b:548:ILE:HD11	1.86	0.57
6:d:426:GLU:HA	6:d:429:LEU:HD12	1.87	0.57
7:e:52:ALA:HB1	7:e:80:VAL:HG22	1.85	0.57
1:p:322:ILE:HG21	1:p:356:LEU:HD11	1.87	0.57
1:p:418:ARG:NH2	2:q:67:GLU:OE1	2.37	0.57
10:h:97:ASP:OD1	10:h:152:ARG:NH2	2.38	0.57
5:b:624:ILE:HD11	5:b:683:LEU:HD21	1.87	0.56
9:g:399:GLN:NE2	9:g:440:SER:O	2.39	0.56
5:b:492:LEU:HA	5:b:495:ILE:HD12	1.86	0.56
6:d:413:LEU:HD21	6:d:442:ILE:HD12	1.86	0.56
4:a:1550:GLU:OE2	4:a:1610:ARG:N	2.39	0.56
10:h:586:PHE:HB3	10:h:622:THR:HG22	1.87	0.56
5:b:406:GLU:OE2	5:b:410:GLN:NE2	2.37	0.55
3:r:1057:GLU:OE2	9:g:555:SER:N	2.39	0.55
5:b:896:LEU:HD11	5:b:927:LYS:HB2	1.88	0.55
5:b:224:GLU:OE2	9:g:666:ARG:NH2	2.38	0.55
4:a:1217:ASP:OD1	4:a:1243:GLN:NE2	2.40	0.55
7:e:938:GLU:OE2	7:e:994:ARG:NH1	2.39	0.55
4:a:1022:VAL:HG22	4:a:1023:LEU:HD22	1.89	0.55
5:b:687:ILE:O	5:b:826:ARG:NH2	2.39	0.55
7:e:447:GLN:HA	7:e:505:LEU:HD11	1.88	0.55
7:e:730:ASP:OD1	7:e:734:ARG:NH1	2.40	0.55
10:h:540:GLN:OE1	10:h:567:ARG:NH1	2.40	0.54
4:a:1223:MET:O	4:a:1226:SER:OG	2.22	0.54
4:a:1839:ILE:HD11	4:a:1877:LEU:HD13	1.89	0.54
1:p:299:ARG:O	1:p:303:SER:OG	2.24	0.54
7:e:88:HIS:NE2	7:e:182:GLY:O	2.41	0.54
8:f:49:ARG:NH2	8:f:121:GLU:OE2	2.40	0.54
7:e:981:GLY:O	7:e:985:LEU:N	2.41	0.54
12:k:59:ASP:O	13:m:669:HIS:NE2	2.40	0.54
7:e:677:LEU:O	7:e:680:THR:OG1	2.26	0.54
7:e:953:HIS:O	7:e:959:LYS:NZ	2.40	0.54
8:f:574:GLN:N	8:f:578:GLN:OE1	2.41	0.54
10:h:754:ARG:NH1	10:h:817:THR:OG1	2.41	0.53
11:i:454:PHE:HA	11:i:457:VAL:HG12	1.90	0.53
6:d:270:ILE:HD12	6:d:275:GLU:HB2	1.89	0.53
6:d:212:ARG:NH2	11:i:548:ASP:OD1	2.41	0.53
5:b:496:ILE:HD12	5:b:509:ILE:HG13	1.91	0.53
10:h:639:ILE:HG23	10:h:667:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:271:ASN:ND2	2:q:272:GLN:O	2.41	0.53
6:d:391:ARG:NH1	6:d:422:ASP:OD2	2.42	0.53
9:g:94:LEU:HD22	9:g:129:LEU:HD23	1.90	0.53
9:g:839:SER:OG	9:g:840:LYS:N	2.41	0.53
11:i:586:SER:O	11:i:656:GLN:N	2.41	0.53
5:b:409:GLU:OE1	5:b:410:GLN:NE2	2.42	0.52
6:d:464:ARG:NH1	6:d:499:ASP:OD2	2.42	0.52
7:e:450:VAL:O	10:h:546:ASN:ND2	2.41	0.52
11:i:434:ALA:O	11:i:437:GLN:HG3	2.09	0.52
9:g:705:LEU:O	9:g:752:TYR:OH	2.27	0.52
5:b:1002:HIS:ND1	5:b:1034:SER:OG	2.40	0.52
5:b:450:GLN:HA	5:b:453:VAL:HG22	1.91	0.52
5:b:833:VAL:HG11	5:b:853:LEU:HD21	1.92	0.52
6:d:164:HIS:NE2	11:i:21:SER:O	2.38	0.52
7:e:745:ILE:HG23	8:f:565:LYS:HE3	1.89	0.52
6:d:868:PRO:HD3	6:d:909:VAL:HG22	1.91	0.52
3:r:1042:GLU:OE1	9:g:528:ARG:NH1	2.43	0.52
5:b:48:CYS:O	5:b:52:MET:HG3	2.09	0.52
8:f:146:LEU:HD22	8:f:161:PRO:HG2	1.92	0.52
10:h:151:ILE:HG23	10:h:259:ALA:HB2	1.92	0.52
4:a:1295:GLU:OE1	5:b:73:ARG:NH2	2.42	0.52
8:f:259:GLN:OE1	8:f:261:TRP:NE1	2.41	0.52
10:h:921:SER:OG	10:h:923:ASP:OD1	2.26	0.51
7:e:435:CYS:HA	7:e:438:LEU:HG	1.91	0.51
1:p:448:MET:HG3	1:p:485:LYS:HD2	1.91	0.51
4:a:1233:ASP:OD1	4:a:1260:LYS:NZ	2.43	0.51
10:h:841:ASP:OD1	10:h:856:TYR:OH	2.27	0.51
4:a:1747:SER:O	4:a:1798:ARG:NH2	2.43	0.51
5:b:43:ARG:HG2	5:b:46:LEU:HD22	1.93	0.51
11:i:379:ILE:HD11	11:i:404:ASP:HB3	1.93	0.51
4:a:1437:ARG:HH21	9:g:353:TYR:HA	1.76	0.51
10:h:133:ALA:O	10:h:210:LYS:NZ	2.44	0.51
4:a:2149:LEU:HD21	4:a:2183:ILE:HG23	1.92	0.51
6:d:70:GLU:OE2	6:d:74:ARG:NH1	2.44	0.51
7:e:994:ARG:O	10:h:301:ARG:NH2	2.44	0.51
10:h:62:SER:HB3	10:h:73:PRO:HD3	1.91	0.51
6:d:755:LEU:HD12	6:d:784:MET:HE1	1.91	0.50
14:j:1:MET:N	16:o:390:SER:O	2.44	0.50
1:p:61:ASP:OD1	1:p:61:ASP:N	2.43	0.50
11:i:583:PRO:HG3	12:k:579:GLN:HG2	1.93	0.50
4:a:2168:TYR:OH	5:b:1190:GLU:OE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:h:916:LEU:HD22	10:h:941:LEU:HD21	1.93	0.50
1:p:531:ASP:O	1:p:537:ARG:NH1	2.40	0.50
12:k:517:LEU:N	12:k:570:LYS:O	2.41	0.50
11:i:543:VAL:HG13	11:i:554:GLN:HB2	1.92	0.50
1:p:206:ILE:HG21	1:p:243:LEU:HD22	1.94	0.50
1:p:279:THR:HA	1:p:283:LEU:HD13	1.93	0.50
4:a:981:SER:O	4:a:987:ARG:NH2	2.45	0.50
10:h:73:PRO:O	10:h:78:ASN:ND2	2.44	0.50
4:a:1151:PHE:N	4:a:1204:PHE:O	2.42	0.50
12:k:327:MET:HE2	12:k:354:CYS:H	1.76	0.50
5:b:485:MET:HE1	5:b:556:CYS:HB3	1.93	0.50
5:b:694:ARG:NH1	5:b:730:GLU:OE1	2.40	0.50
10:h:704:LEU:HD11	10:h:772:ILE:HD11	1.94	0.50
6:d:489:LEU:HD23	6:d:503:ILE:HG23	1.94	0.50
11:i:1:MET:O	11:i:507:LEU:N	2.44	0.50
9:g:70:ASP:OD1	9:g:73:ARG:NH2	2.43	0.49
9:g:854:VAL:HG11	9:g:894:LEU:HD11	1.94	0.49
11:i:93:LEU:HD13	11:i:113:ILE:HG23	1.94	0.49
1:p:168:GLN:OE1	1:p:171:ARG:NH1	2.46	0.49
4:a:1380:GLN:NE2	4:a:1438:GLN:OE1	2.45	0.49
10:h:633:ARG:NH1	10:h:670:TRP:O	2.46	0.49
6:d:216:ILE:HD11	6:d:240:LEU:HD13	1.93	0.49
7:e:366:PRO:O	7:e:370:SER:N	2.46	0.49
5:b:298:LEU:O	5:b:302:VAL:HG22	2.12	0.49
1:p:526:LEU:HD22	1:p:563:ILE:HG13	1.94	0.49
6:d:413:LEU:HD11	6:d:442:ILE:HB	1.93	0.49
7:e:358:GLU:O	7:e:362:CYS:N	2.46	0.49
7:e:727:SER:O	7:e:731:THR:OG1	2.27	0.49
9:g:594:LEU:O	9:g:598:HIS:ND1	2.44	0.49
4:a:2089:GLN:HG2	4:a:2124:THR:HG21	1.95	0.48
11:i:229:SER:O	11:i:229:SER:OG	2.25	0.48
1:p:580:GLN:O	1:p:584:THR:HG23	2.14	0.48
9:g:119:ARG:NH1	9:g:154:GLU:OE1	2.46	0.48
4:a:1923:PHE:O	4:a:1970:ASN:ND2	2.47	0.48
6:d:708:GLU:OE1	6:d:726:ARG:NH2	2.40	0.48
1:p:306:VAL:HG11	1:p:330:ILE:HD11	1.95	0.48
1:p:314:SER:HG	1:p:317:CYS:HG	1.61	0.48
9:g:192:ASP:OD1	9:g:193:LEU:N	2.46	0.48
9:g:307:LEU:O	9:g:311:MET:HG3	2.14	0.48
9:g:856:SER:OG	9:g:874:THR:OG1	2.29	0.48
4:a:1787:ILE:HG21	4:a:1820:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:1970:ASN:OD1	4:a:1970:ASN:N	2.46	0.48
6:d:794:GLU:O	6:d:798:ILE:HG22	2.14	0.48
1:p:225:VAL:HG23	1:p:262:MET:HG3	1.96	0.48
6:d:500:ARG:HG2	6:d:500:ARG:HH11	1.78	0.48
1:p:314:SER:OG	1:p:317:CYS:SG	2.71	0.48
4:a:1153:ARG:NH2	4:a:1154:TRP:O	2.47	0.47
5:b:944:GLU:OE1	7:e:729:LEU:N	2.41	0.47
9:g:435:LEU:HD22	9:g:470:ASP:HB2	1.95	0.47
2:q:122:GLN:N	2:q:122:GLN:OE1	2.48	0.47
2:q:160:ASP:OD1	2:q:162:GLN:NE2	2.44	0.47
4:a:1839:ILE:HD12	4:a:1842:PHE:CE1	2.50	0.47
9:g:847:ILE:HG23	9:g:910:VAL:HG13	1.96	0.47
10:h:363:LEU:HD13	10:h:384:VAL:HG23	1.95	0.47
2:q:122:GLN:HE22	10:h:170:GLN:HE21	1.62	0.47
7:e:366:PRO:O	7:e:370:SER:OG	2.27	0.47
10:h:832:ASN:OD1	10:h:834:SER:OG	2.32	0.47
12:k:70:HIS:HE1	12:k:157:HIS:NE2	2.08	0.47
4:a:564:TRP:HA	4:a:569:LYS:HA	1.95	0.47
6:d:645:ARG:NH2	9:g:244:SER:O	2.37	0.47
8:f:57:GLU:O	8:f:61:ALA:N	2.47	0.47
12:k:13:GLN:HA	12:k:420:MET:HE1	1.97	0.47
4:a:1189:LEU:HD12	4:a:1192:ILE:HD11	1.96	0.47
4:a:1534:CYS:SG	4:a:1535:SER:N	2.88	0.47
4:a:1887:LEU:O	4:a:1891:ARG:NH1	2.47	0.47
9:g:877:MET:HE2	9:g:892:PHE:HD1	1.80	0.47
5:b:724:VAL:HG11	9:g:121:ILE:HD11	1.97	0.47
7:e:685:LEU:HD21	7:e:808:ALA:HB2	1.95	0.47
11:i:281:PHE:HD1	11:i:421:ILE:HG21	1.80	0.47
5:b:481:LEU:HB3	5:b:485:MET:HE3	1.97	0.47
6:d:576:LEU:HD12	6:d:580:LEU:HD12	1.97	0.47
9:g:104:VAL:HG21	9:g:133:ILE:HG21	1.97	0.47
9:g:445:ALA:O	9:g:449:MET:HG3	2.15	0.47
5:b:411:LEU:O	5:b:415:MET:HG3	2.14	0.46
8:f:292:ASP:N	8:f:292:ASP:OD1	2.48	0.46
4:a:1171:VAL:O	4:a:1175:THR:HG23	2.15	0.46
5:b:549:THR:OG1	5:b:550:GLY:N	2.48	0.46
5:b:856:ASP:OD2	5:b:862:ARG:NH2	2.45	0.46
1:p:13:ILE:HG21	1:p:50:GLU:HB3	1.96	0.46
12:k:68:HIS:CE1	12:k:178:ASP:HB2	2.50	0.46
10:h:516:LEU:HB2	10:h:528:ILE:HG21	1.97	0.46
7:e:916:GLU:OE2	10:h:402:GLN:NE2	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:k:521:ARG:HE	12:k:525:GLU:HG2	1.79	0.46
1:p:376:GLU:O	1:p:381:ARG:NH2	2.49	0.46
6:d:144:ASN:O	6:d:148:GLN:NE2	2.45	0.46
7:e:91:ALA:O	7:e:95:THR:OG1	2.32	0.46
10:h:917:GLN:O	10:h:948:ARG:NH2	2.44	0.46
5:b:431:LEU:HD23	5:b:503:LEU:HD23	1.97	0.46
1:p:346:ALA:HB1	1:p:384:ILE:HG12	1.97	0.46
6:d:493:LEU:HD23	6:d:543:ALA:HA	1.97	0.46
12:k:452:ILE:HD12	13:m:660:ARG:HD3	1.98	0.46
9:g:357:ARG:NH2	9:g:400:ASP:OD2	2.49	0.46
6:d:522:VAL:HG22	6:d:551:ILE:HG12	1.98	0.45
11:i:135:LEU:HD11	11:i:339:PHE:HD2	1.80	0.45
1:p:538:PHE:HB3	1:p:575:VAL:HA	1.97	0.45
2:q:62:PHE:CE1	2:q:66:MET:HE3	2.51	0.45
8:f:575:ASP:OD1	8:f:576:GLU:N	2.49	0.45
9:g:285:HIS:HB3	9:g:322:ILE:HD11	1.96	0.45
9:g:383:GLU:OE2	9:g:425:HIS:NE2	2.44	0.45
1:p:261:TYR:HB2	1:p:298:VAL:HG12	1.98	0.45
4:a:1124:PHE:HE1	4:a:1166:VAL:HG23	1.82	0.45
11:i:396:GLY:HA3	11:i:405:VAL:HB	1.98	0.45
5:b:185:GLN:NE2	5:b:192:LEU:O	2.45	0.45
6:d:865:VAL:HG11	6:d:898:LEU:HD22	1.98	0.45
7:e:72:ALA:HB2	16:o:69:LEU:HA	1.98	0.45
7:e:914:MET:HE1	7:e:950:LEU:HD11	1.99	0.45
7:e:923:ALA:HB1	7:e:985:LEU:HD21	1.99	0.45
9:g:269:LYS:HD2	9:g:307:LEU:HD13	1.99	0.45
4:a:1845:LEU:HD22	4:a:1858:ARG:HG2	1.98	0.45
6:d:802:MET:HE3	6:d:802:MET:HB2	1.74	0.45
7:e:801:ALA:HB2	10:h:406:LEU:HD23	1.99	0.45
7:e:811:ALA:O	7:e:815:THR:HG22	2.17	0.45
8:f:430:ALA:O	8:f:434:MET:HG2	2.17	0.45
9:g:598:HIS:HA	9:g:601:ILE:HG22	1.99	0.45
12:k:6:VAL:HG22	12:k:22:VAL:HG22	1.99	0.45
5:b:517:MET:O	5:b:521:PHE:HB2	2.17	0.45
5:b:566:PHE:O	5:b:570:LYS:N	2.48	0.45
7:e:828:GLU:O	7:e:879:ARG:NH2	2.42	0.45
1:p:297:GLU:OE2	8:f:602:ARG:NE	2.40	0.45
4:a:1170:MET:HG2	4:a:1189:LEU:HD21	1.99	0.45
4:a:1888:LEU:HD11	4:a:1911:VAL:HG11	1.98	0.45
9:g:232:ILE:HA	9:g:271:LEU:HD22	1.99	0.44
9:g:920:THR:OG1	9:g:921:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:894:THR:OG1	6:d:895:GLN:N	2.50	0.44
10:h:917:GLN:OE1	10:h:940:TYR:OH	2.31	0.44
4:a:1308:LEU:HD23	4:a:1308:LEU:HA	1.85	0.44
5:b:874:MET:HG2	5:b:993:VAL:HG13	2.00	0.44
1:p:319:GLU:O	1:p:323:MET:HG2	2.18	0.44
9:g:422:GLY:O	9:g:423:ARG:NH1	2.50	0.44
1:p:141:PHE:O	1:p:145:THR:HG23	2.18	0.44
11:i:113:ILE:O	11:i:117:THR:OG1	2.31	0.44
16:o:11:ARG:O	16:o:16:ALA:N	2.50	0.44
4:a:1748:GLN:HE22	4:a:1797:ARG:HH12	1.64	0.44
7:e:152:MET:HE1	7:e:193:TYR:CE2	2.53	0.44
7:e:516:PRO:HD3	7:e:549:LEU:HD12	1.99	0.44
12:k:327:MET:HG3	12:k:354:CYS:HA	2.00	0.44
2:q:176:THR:OG1	7:e:842:GLU:OE2	2.36	0.44
6:d:310:GLU:OE1	6:d:310:GLU:N	2.51	0.44
1:p:414:ASP:O	1:p:420:ARG:NH1	2.43	0.43
2:q:187:GLN:HB3	10:h:165:LYS:HG2	1.99	0.43
10:h:412:LYS:HD2	10:h:458:MET:HE1	2.00	0.43
16:o:120:MET:O	16:o:124:VAL:N	2.51	0.43
5:b:416:THR:HG21	5:b:451:LEU:HG	2.00	0.43
7:e:833:PRO:HA	7:e:951:ARG:HD2	2.00	0.43
9:g:473:GLU:HA	9:g:476:LYS:HE3	1.99	0.43
2:q:28:VAL:HG11	2:q:142:VAL:HG13	1.99	0.43
5:b:204:VAL:O	5:b:245:ARG:NH2	2.51	0.43
6:d:827:PRO:HG3	6:d:845:LEU:HD11	1.99	0.43
10:h:91:HIS:HB2	10:h:217:MET:HE1	1.99	0.43
11:i:486:MET:HA	11:i:489:MET:HE2	1.99	0.43
1:p:43:GLY:O	1:p:47:THR:N	2.44	0.43
7:e:452:HIS:HB3	7:e:469:ARG:HH12	1.84	0.43
7:e:882:LEU:HD11	7:e:943:LEU:HB3	1.99	0.43
12:k:198:ASN:HA	12:k:408:GLU:HB3	2.01	0.43
2:q:196:CYS:SG	2:q:216:ALA:HB1	2.58	0.43
4:a:2161:ARG:NH2	7:e:562:HIS:O	2.45	0.43
7:e:200:LEU:O	7:e:204:CYS:N	2.51	0.43
7:e:910:LEU:O	7:e:914:MET:HG3	2.18	0.43
8:f:124:ILE:HG22	8:f:167:ARG:HB2	2.01	0.43
11:i:433:LEU:HD21	11:i:443:CYS:SG	2.58	0.43
4:a:1975:ILE:HD13	4:a:2009:SER:HA	2.00	0.43
5:b:797:MET:HB2	5:b:800:LEU:HD12	2.00	0.43
9:g:349:GLN:NE2	9:g:385:ASP:OD2	2.50	0.43
9:g:393:LEU:HD23	9:g:412:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:h:791:ILE:HG12	10:h:841:ASP:HB3	2.01	0.43
1:p:331:LYS:HG2	1:p:368:LEU:HD21	2.00	0.43
2:q:10:LEU:HD11	2:q:105:VAL:HG12	2.01	0.43
2:q:139:ASN:N	2:q:139:ASN:OD1	2.51	0.43
4:a:975:PHE:HE2	4:a:994:LEU:HB2	1.83	0.43
9:g:808:LEU:HB2	9:g:831:VAL:HG12	2.01	0.43
10:h:541:PHE:N	10:h:568:ASP:OD2	2.52	0.43
1:p:28:ARG:NH1	1:p:62:GLU:OE2	2.52	0.43
4:a:1670:TRP:NE1	5:b:992:GLU:OE2	2.40	0.43
5:b:566:PHE:HD2	5:b:571:VAL:HG13	1.84	0.43
5:b:819:VAL:O	5:b:822:THR:OG1	2.37	0.43
9:g:631:PHE:O	9:g:635:ILE:HG12	2.19	0.43
1:p:221:ARG:O	1:p:225:VAL:HG13	2.19	0.43
10:h:275:ARG:NH2	10:h:310:ASP:OD1	2.52	0.43
11:i:25:MET:HG2	11:i:99:ILE:HG23	2.00	0.43
5:b:896:LEU:HD22	5:b:923:ARG:HD3	2.00	0.43
11:i:220:LEU:HD23	11:i:220:LEU:HA	1.86	0.43
12:k:4:ILE:HG12	12:k:24:ILE:HG13	2.00	0.43
1:p:516:ILE:HG23	1:p:520:HIS:HD2	1.84	0.42
4:a:1383:LEU:HD23	4:a:1402:THR:HG22	1.99	0.42
5:b:559:GLN:OE1	5:b:562:ARG:NH2	2.52	0.42
6:d:417:VAL:HG11	6:d:444:LEU:HD21	2.01	0.42
10:h:885:ILE:HG23	10:h:897:VAL:HG13	2.01	0.42
12:k:235:VAL:HG12	12:k:237:ILE:HG23	2.01	0.42
1:p:232:ALA:HB2	1:p:244:VAL:HG11	2.00	0.42
6:d:727:LEU:HD21	6:d:758:VAL:HG22	2.01	0.42
7:e:448:LYS:HE2	7:e:448:LYS:HA	2.02	0.42
7:e:566:LEU:O	7:e:571:THR:OG1	2.37	0.42
2:q:65:LEU:HD22	2:q:96:THR:HG23	2.01	0.42
4:a:1219:LEU:O	4:a:1223:MET:HG2	2.19	0.42
9:g:390:LEU:HD13	9:g:416:MET:HG3	2.01	0.42
9:g:468:LEU:HD23	9:g:468:LEU:HA	1.89	0.42
10:h:55:LEU:HB3	10:h:110:MET:HE2	2.00	0.42
1:p:275:GLY:O	1:p:279:THR:HG23	2.20	0.42
4:a:964:ASP:OD1	4:a:967:THR:OG1	2.28	0.42
10:h:793:ALA:HB3	10:h:796:ILE:HD13	2.01	0.42
11:i:107:MET:HE1	11:i:130:VAL:HA	2.00	0.42
12:k:368:ARG:HH21	12:k:380:VAL:HA	1.84	0.42
16:o:170:ILE:O	16:o:174:SER:N	2.51	0.42
4:a:562:ILE:O	5:b:326:GLN:NE2	2.53	0.42
4:a:567:GLY:HA3	5:b:402:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:d:243:ASP:OD1	6:d:244:ASP:N	2.53	0.42
7:e:988:LEU:HD21	7:e:1006:PHE:CD1	2.55	0.42
12:k:207:ALA:HB3	12:k:419:LYS:HB3	2.02	0.42
1:p:373:LEU:HD12	1:p:373:LEU:HA	1.90	0.42
6:d:903:TRP:CE2	9:g:893:LEU:HD11	2.55	0.42
5:b:776:GLU:O	5:b:779:THR:OG1	2.34	0.42
9:g:705:LEU:HD11	9:g:745:GLU:HG2	2.01	0.42
10:h:569:LEU:HD23	10:h:599:LEU:HD22	2.01	0.42
12:k:20:ILE:HB	12:k:31:LEU:HB2	2.01	0.42
2:q:82:PHE:HB3	2:q:86:TYR:HE1	1.84	0.42
2:q:141:ASN:OD1	2:q:142:VAL:N	2.53	0.42
8:f:165:ASP:OD1	8:f:165:ASP:N	2.47	0.42
8:f:283:TRP:CZ2	8:f:383:PRO:HG3	2.55	0.42
10:h:637:ASP:OD1	10:h:638:LEU:N	2.53	0.42
11:i:430:LEU:HD23	11:i:430:LEU:HA	1.93	0.42
4:a:1736:VAL:HG11	4:a:1779:VAL:HG21	2.02	0.41
4:a:2088:LEU:HD13	4:a:2107:ALA:HB2	2.02	0.41
6:d:656:VAL:HG22	6:d:817:ILE:HG23	2.00	0.41
6:d:755:LEU:HD13	6:d:755:LEU:HA	1.90	0.41
11:i:586:SER:HA	12:k:507:HIS:H	1.85	0.41
2:q:152:TYR:CE1	2:q:186:LEU:HD21	2.55	0.41
6:d:398:LEU:HD23	6:d:398:LEU:HA	1.88	0.41
8:f:438:ASN:OD1	8:f:438:ASN:N	2.52	0.41
1:p:158:VAL:HG23	1:p:163:LYS:HG3	2.02	0.41
1:p:455:VAL:HG13	2:q:71:ILE:HD13	2.02	0.41
4:a:1268:ALA:O	4:a:1272:ASP:N	2.53	0.41
7:e:149:ILE:HB	7:e:193:TYR:OH	2.20	0.41
8:f:29:LYS:HE2	8:f:80:LEU:HB2	2.02	0.41
7:e:177:LEU:HD23	7:e:225:TRP:HE3	1.86	0.41
4:a:2051:MET:HE1	7:e:512:PRO:N	2.35	0.41
5:b:295:VAL:HG22	5:b:384:LYS:HG2	2.02	0.41
5:b:690:LYS:NZ	5:b:822:THR:O	2.53	0.41
9:g:526:VAL:HG13	9:g:545:LEU:HD22	2.02	0.41
10:h:225:MET:SD	10:h:225:MET:N	2.92	0.41
10:h:349:ASN:OD1	10:h:359:ARG:NH1	2.51	0.41
2:q:282:LEU:HD23	2:q:282:LEU:HA	1.86	0.41
7:e:972:ASP:H	7:e:975:ARG:NH2	2.18	0.41
8:f:25:LEU:HD22	8:f:82:ALA:HB2	2.03	0.41
9:g:107:ILE:HD13	9:g:107:ILE:HA	1.89	0.41
9:g:215:ARG:NH1	9:g:252:GLN:OE1	2.47	0.41
5:b:545:SER:HB2	5:b:587:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:1000:LEU:O	5:b:1004:MET:HG3	2.21	0.41
12:k:177:GLY:O	12:k:203:GLN:HB3	2.21	0.41
4:a:1093:VAL:HA	4:a:1100:MET:SD	2.61	0.41
5:b:656:LEU:HB2	5:b:713:LEU:HD13	2.01	0.41
5:b:724:VAL:HG21	9:g:77:ASN:HB3	2.02	0.41
9:g:80:ARG:HB3	9:g:121:ILE:HG21	2.02	0.41
9:g:634:LEU:HD23	9:g:781:ILE:HD11	2.02	0.41
11:i:133:GLY:O	11:i:137:MET:HG3	2.21	0.41
1:p:113:ARG:NH2	1:p:149:GLY:O	2.54	0.41
4:a:1360:ASP:O	4:a:1364:MET:N	2.52	0.41
4:a:1900:ARG:HH21	4:a:1905:LEU:HD22	1.86	0.41
5:b:256:MET:HE2	5:b:256:MET:HB3	1.85	0.41
6:d:419:MET:HE2	6:d:419:MET:HB2	1.91	0.41
8:f:12:ALA:HB3	10:h:939:GLU:HG3	2.02	0.41
8:f:13:SER:O	8:f:16:GLN:NE2	2.41	0.41
9:g:594:LEU:HD23	9:g:594:LEU:HA	1.96	0.41
9:g:675:MET:SD	9:g:679:ARG:NH2	2.94	0.41
10:h:143:VAL:O	10:h:147:ASN:ND2	2.50	0.41
11:i:25:MET:HB3	11:i:99:ILE:HG12	2.03	0.41
1:p:308:GLU:O	1:p:312:ASN:ND2	2.54	0.41
3:r:1047:GLN:OE1	3:r:1047:GLN:N	2.53	0.41
3:r:1058:MET:HE2	9:g:549:LEU:HD22	2.03	0.41
4:a:1023:LEU:HB3	4:a:1026:TYR:HB2	2.04	0.41
4:a:1368:ILE:HG12	4:a:1376:ALA:HB2	2.02	0.41
4:a:2095:ALA:O	10:h:823:ARG:NH2	2.54	0.41
4:a:2164:LEU:HD23	4:a:2164:LEU:HA	1.93	0.41
6:d:761:PHE:CD1	6:d:777:VAL:HG21	2.56	0.41
1:p:16:LEU:HD11	10:h:25:PHE:HB3	2.03	0.40
5:b:134:ASP:OD1	5:b:134:ASP:N	2.54	0.40
5:b:302:VAL:HG23	5:b:391:LEU:HD11	2.03	0.40
6:d:257:TRP:HD1	6:d:309:MET:HE3	1.87	0.40
7:e:678:SER:HB3	7:e:688:VAL:HG11	2.02	0.40
9:g:491:VAL:HG12	9:g:529:ILE:HG13	2.03	0.40
11:i:30:LEU:HD13	11:i:109:ALA:HB2	2.03	0.40
12:k:122:THR:OG1	12:k:123:SER:N	2.54	0.40
12:k:266:TYR:OH	12:k:312:PHE:N	2.53	0.40
3:r:1043:ASP:OD1	9:g:793:ARG:NH2	2.51	0.40
4:a:1847:ALA:O	4:a:1891:ARG:NH2	2.53	0.40
4:a:2171:MET:H	4:a:2171:MET:HG2	1.74	0.40
6:d:216:ILE:HG23	6:d:255:LEU:HD22	2.04	0.40
10:h:917:GLN:HA	10:h:944:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:a:1663:LEU:O	4:a:1667:GLN:CB	2.70	0.40
9:g:183:MET:HE2	9:g:197:LEU:HD11	2.04	0.40
11:i:268:GLN:OE1	11:i:451:ARG:NH2	2.55	0.40
16:o:1:MET:N	16:o:43:GLY:O	2.54	0.40
1:p:113:ARG:HB2	1:p:153:VAL:HG11	2.03	0.40
6:d:703:GLU:O	6:d:707:MET:HG3	2.21	0.40
8:f:99:LEU:HD23	8:f:99:LEU:HA	1.94	0.40
1:p:199:ASP:OD1	1:p:199:ASP:N	2.54	0.40
4:a:1539:ASP:OD1	4:a:1539:ASP:N	2.55	0.40
4:a:2069:ASP:O	4:a:2073:MET:HG2	2.21	0.40
6:d:323:LYS:O	12:k:396:LYS:NZ	2.52	0.40
9:g:540:ASP:OD1	9:g:540:ASP:N	2.55	0.40
10:h:616:LEU:HD13	10:h:641:ARG:HB3	2.04	0.40
10:h:785:GLU:HB2	10:h:787:ILE:HG23	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	p	578/591 (98%)	567 (98%)	11 (2%)	0	100	100
2	q	288/311 (93%)	273 (95%)	15 (5%)	0	100	100
3	r	29/31 (94%)	29 (100%)	0	0	100	100
4	a	1734/2192 (79%)	1682 (97%)	51 (3%)	1 (0%)	48	78
5	b	1031/1204 (86%)	983 (95%)	48 (5%)	0	100	100
6	d	813/963 (84%)	791 (97%)	22 (3%)	0	100	100
7	e	857/1021 (84%)	824 (96%)	33 (4%)	0	100	100
8	f	551/892 (62%)	535 (97%)	16 (3%)	0	100	100
9	g	879/964 (91%)	847 (96%)	32 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	h	950/995 (96%)	927 (98%)	23 (2%)	0	100	100
11	i	618/658 (94%)	588 (95%)	30 (5%)	0	100	100
12	k	583/602 (97%)	540 (93%)	42 (7%)	1 (0%)	43	73
13	m	528/706 (75%)	491 (93%)	36 (7%)	1 (0%)	43	73
14	j	645/710 (91%)	626 (97%)	19 (3%)	0	100	100
15	n	499/518 (96%)	466 (93%)	33 (7%)	0	100	100
16	o	368/451 (82%)	347 (94%)	20 (5%)	1 (0%)	36	67
All	All	10951/12809 (86%)	10516 (96%)	431 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	k	310	ARG
16	o	231	PRO
4	a	566	LYS
13	m	150	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	p	487/514 (95%)	485 (100%)	2 (0%)	84	86
2	q	255/276 (92%)	254 (100%)	1 (0%)	84	86
3	r	28/28 (100%)	28 (100%)	0	100	100
4	a	931/1909 (49%)	929 (100%)	2 (0%)	87	89
5	b	894/1072 (83%)	894 (100%)	0	100	100
6	d	709/845 (84%)	707 (100%)	2 (0%)	86	87
7	e	630/814 (77%)	630 (100%)	0	100	100
8	f	491/801 (61%)	491 (100%)	0	100	100
9	g	733/842 (87%)	733 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	h	859/896 (96%)	859 (100%)	0	100	100
11	i	555/600 (92%)	555 (100%)	0	100	100
12	k	443/522 (85%)	443 (100%)	0	100	100
13	m	31/639 (5%)	31 (100%)	0	100	100
All	All	7046/9758 (72%)	7039 (100%)	7 (0%)	87	90

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	p	230	ASN
1	p	350	MET
2	q	6	PHE
4	a	996	LEU
4	a	1282	ASP
6	d	493	LEU
6	d	817	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	p	26	GLN
1	p	127	HIS
1	p	312	ASN
1	p	479	HIS
2	q	191	HIS
2	q	272	GLN
4	a	1072	GLN
4	a	1242	GLN
4	a	1243	GLN
4	a	1380	GLN
4	a	1381	GLN
4	a	1443	GLN
4	a	1487	GLN
4	a	1555	HIS
4	a	1805	GLN
4	a	1903	ASN
4	a	1921	HIS
4	a	2152	GLN
5	b	103	GLN
5	b	151	ASN

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Mol	Chain	Res	Type
5	b	206	ASN
5	b	232	ASN
5	b	686	GLN
5	b	700	GLN
5	b	747	ASN
5	b	846	GLN
5	b	851	ASN
5	b	1054	GLN
6	d	144	ASN
6	d	223	HIS
6	d	301	GLN
6	d	475	ASN
6	d	611	GLN
6	d	615	GLN
6	d	728	GLN
6	d	853	HIS
7	e	48	HIS
7	e	389	ASN
7	e	537	GLN
7	e	643	GLN
7	e	894	HIS
7	e	899	HIS
7	e	953	HIS
7	e	984	HIS
7	e	1007	GLN
8	f	-2	GLN
8	f	0	ASN
8	f	113	GLN
8	f	141	GLN
8	f	378	ASN
9	g	62	ASN
9	g	89	GLN
9	g	152	ASN
9	g	185	GLN
9	g	236	HIS
9	g	258	GLN
9	g	355	ASN
9	g	406	GLN
9	g	487	GLN
9	g	538	ASN
9	g	573	GLN
9	g	579	GLN

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Mol	Chain	Res	Type
9	g	779	ASN
9	g	792	GLN
10	h	68	GLN
10	h	127	HIS
10	h	170	GLN
10	h	267	ASN
10	h	294	HIS
10	h	330	HIS
10	h	339	GLN
10	h	480	GLN
10	h	781	HIS
11	i	15	ASN
11	i	37	ASN
11	i	230	HIS
11	i	371	ASN
11	i	418	ASN
11	i	468	HIS
12	k	143	GLN
12	k	226	HIS
12	k	288	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

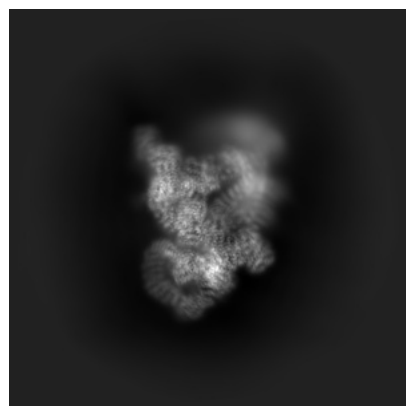
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19047. These allow visual inspection of the internal detail of the map and identification of artifacts.

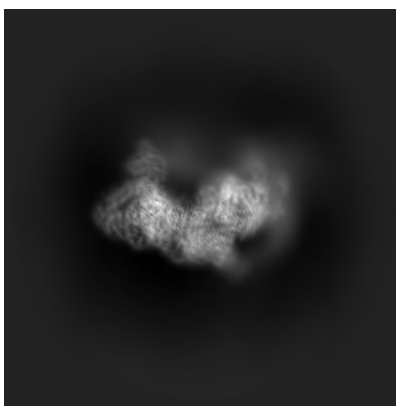
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

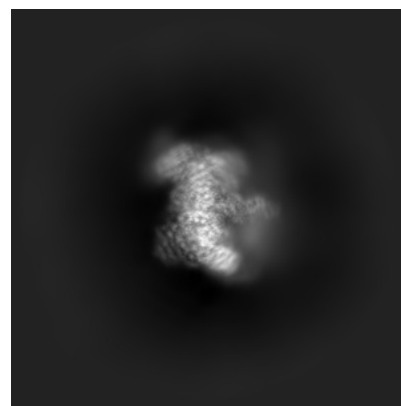
6.1.1 Primary map



X

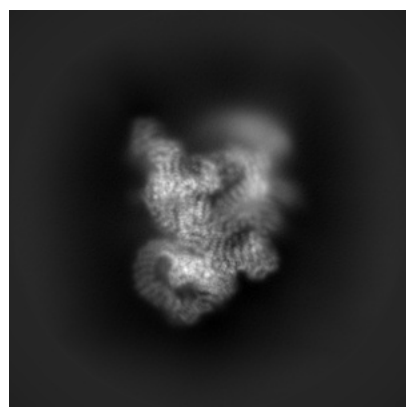


Y

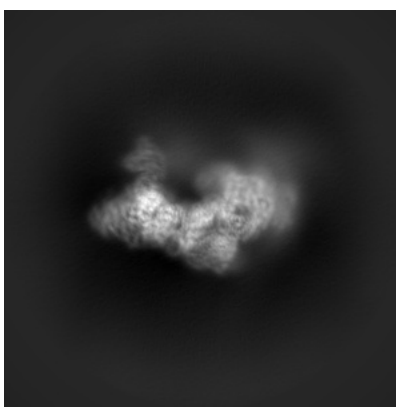


Z

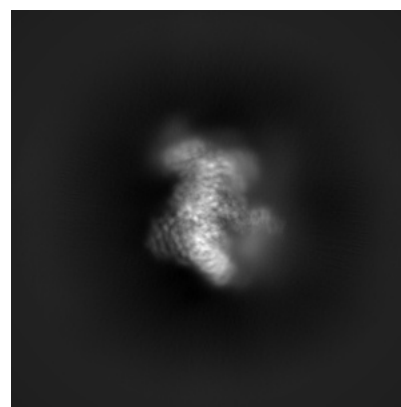
6.1.2 Raw map



X



Y

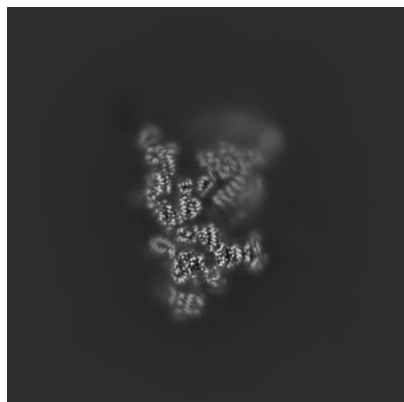


Z

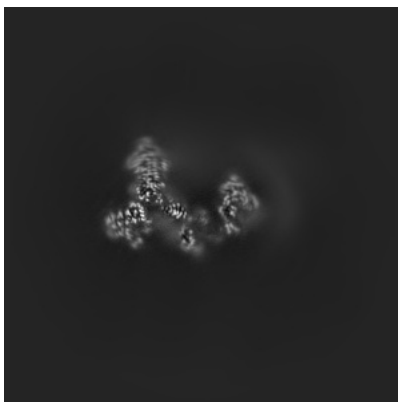
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

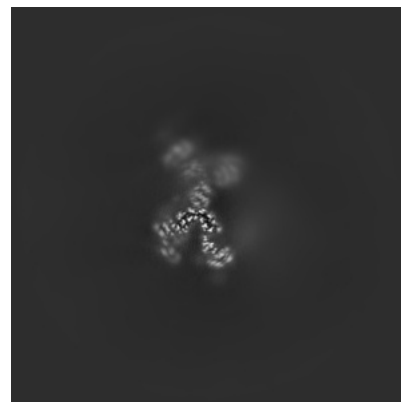
6.2.1 Primary map



X Index: 240

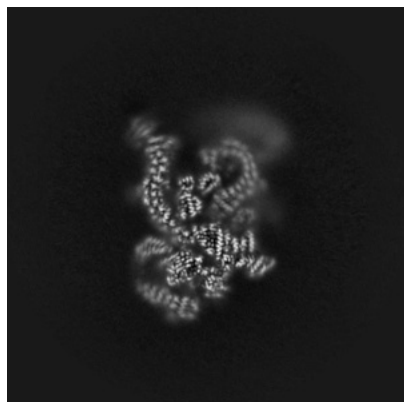


Y Index: 240

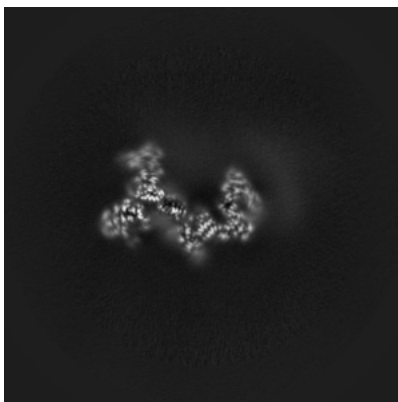


Z Index: 240

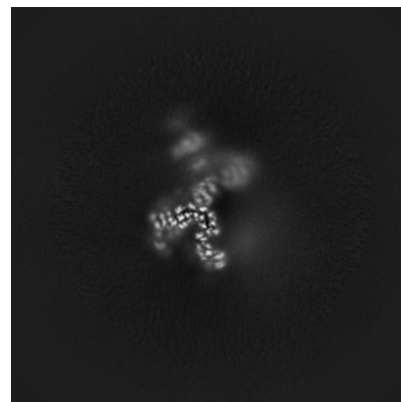
6.2.2 Raw map



X Index: 240



Y Index: 240

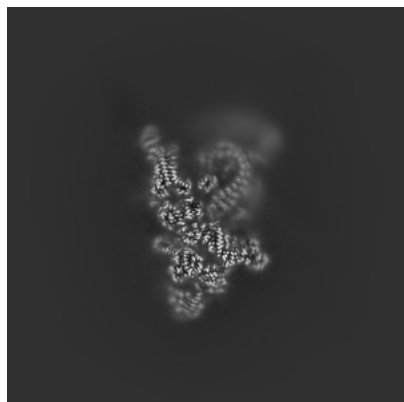


Z Index: 240

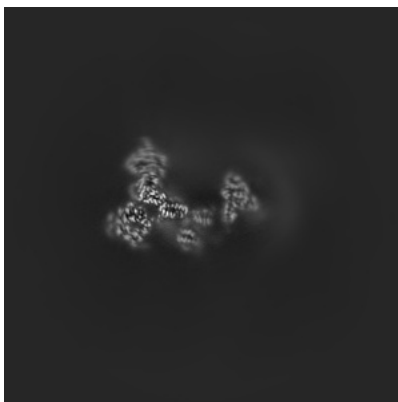
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

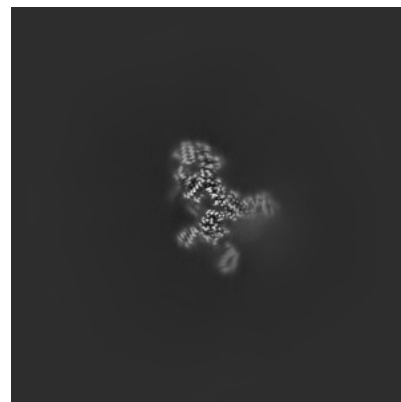
6.3.1 Primary map



X Index: 235

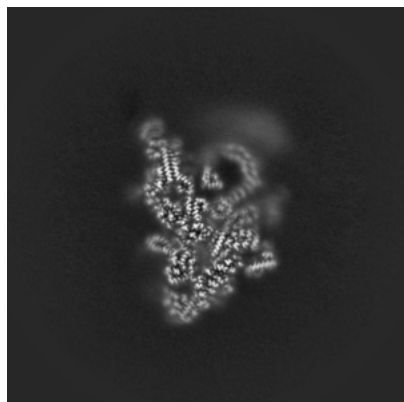


Y Index: 245

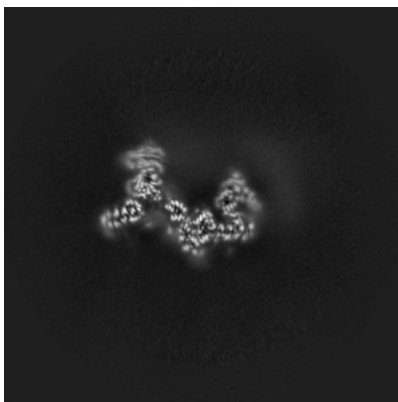


Z Index: 177

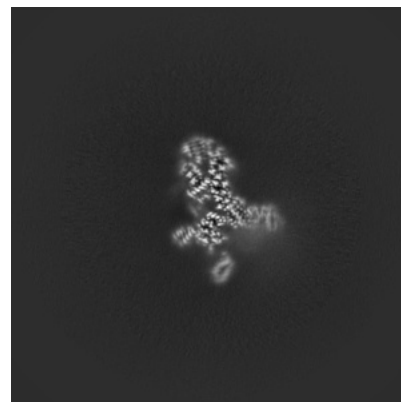
6.3.2 Raw map



X Index: 230



Y Index: 236

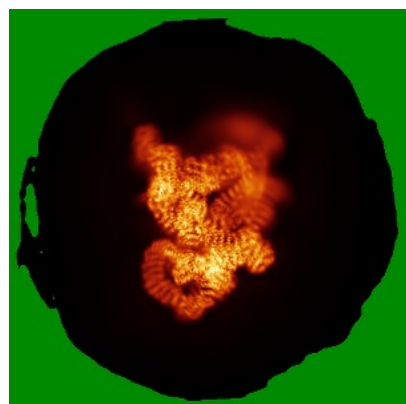


Z Index: 175

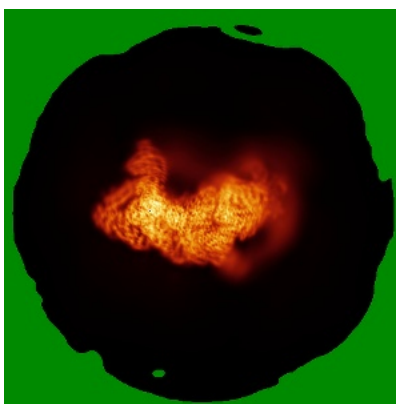
The images above show the largest variance slices of the map in three orthogonal directions.

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

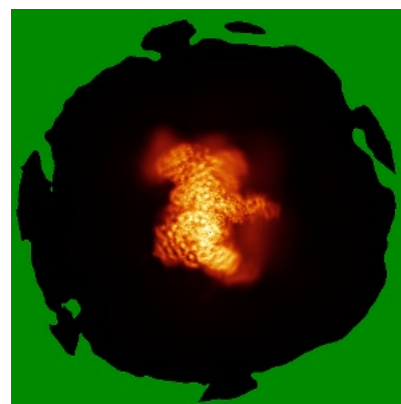
6.4.1 Primary map



X

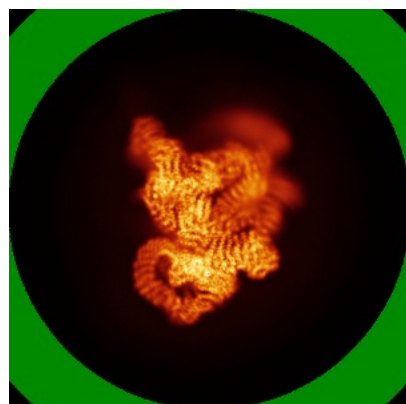


Y



Z

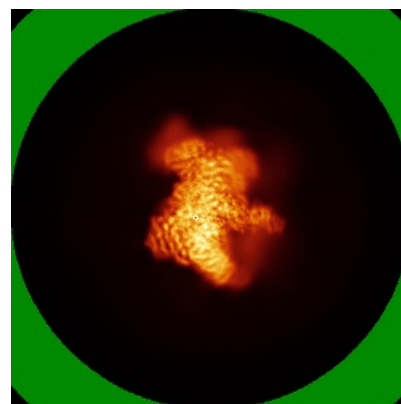
6.4.2 Raw map



X



Y

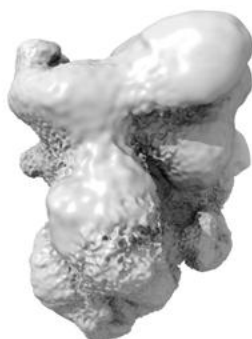


Z

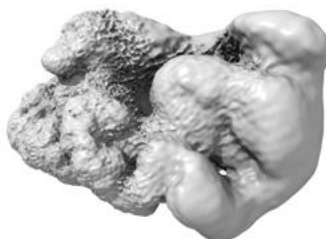
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



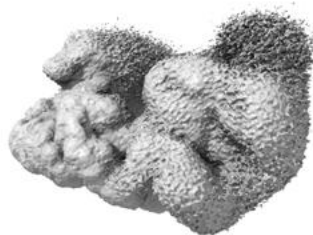
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00502. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

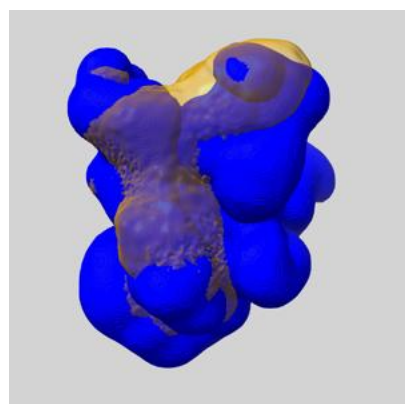
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

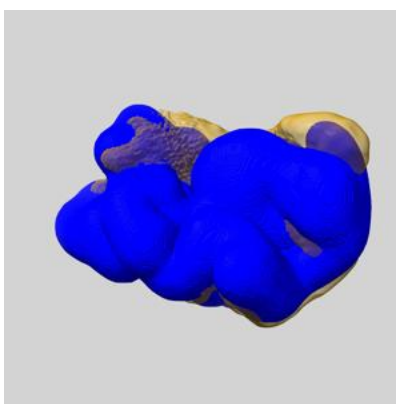
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

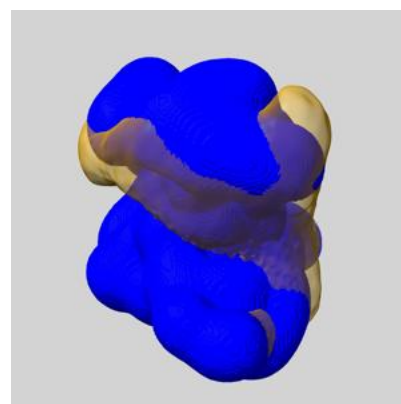
6.6.1 emd_19047_msk_1.map [i](#)



X



Y

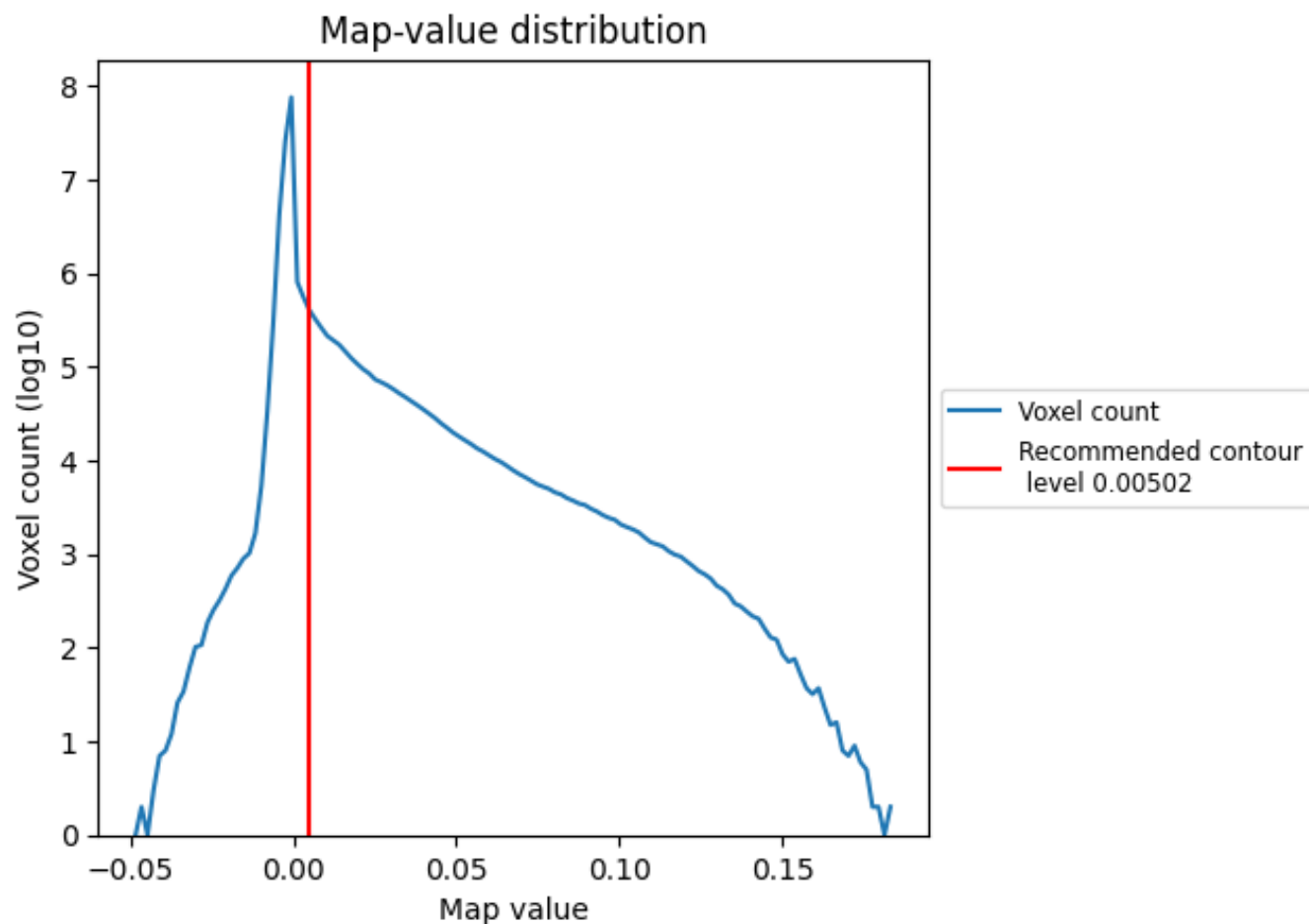


Z

7 Map analysis [i](#)

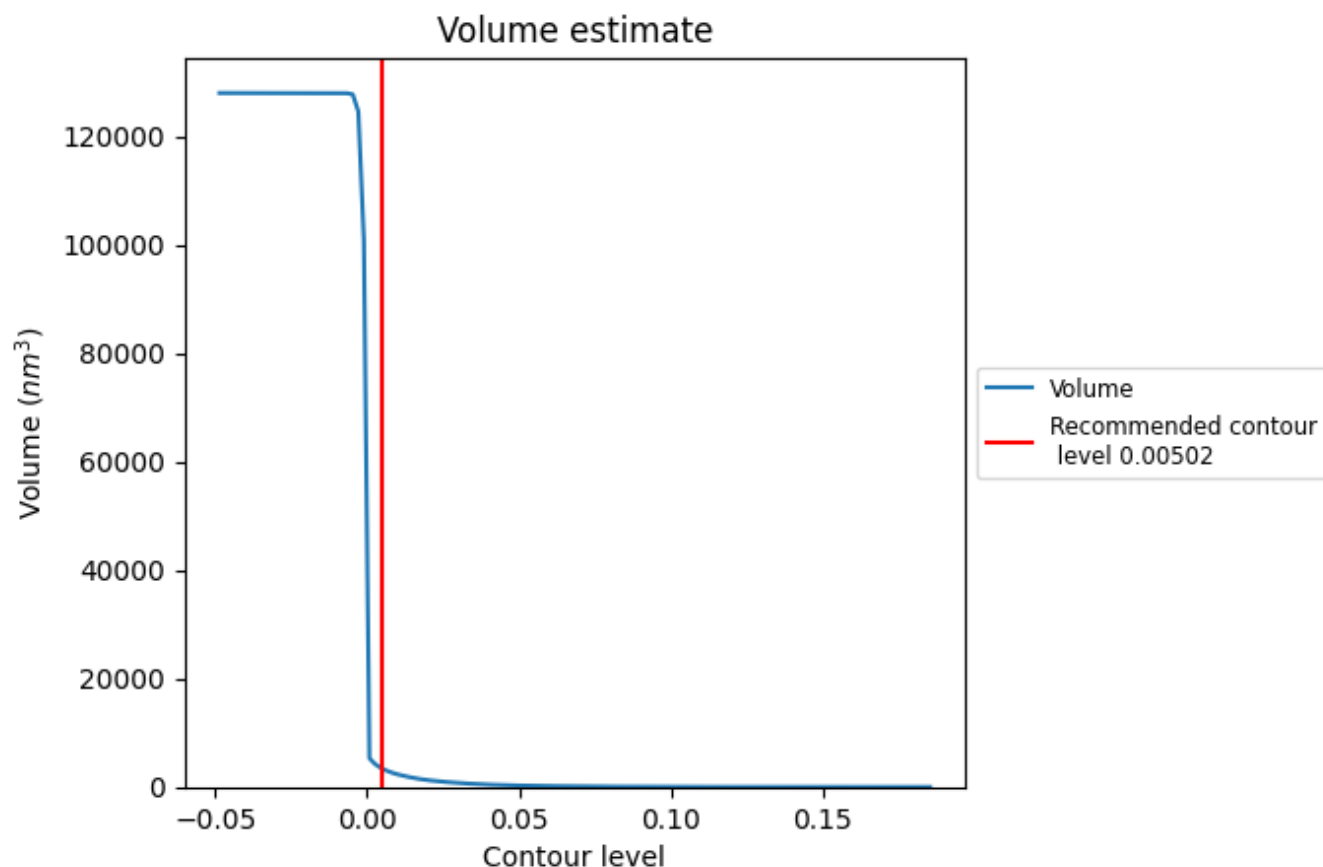
This section contains the results of statistical analysis of the map.

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.

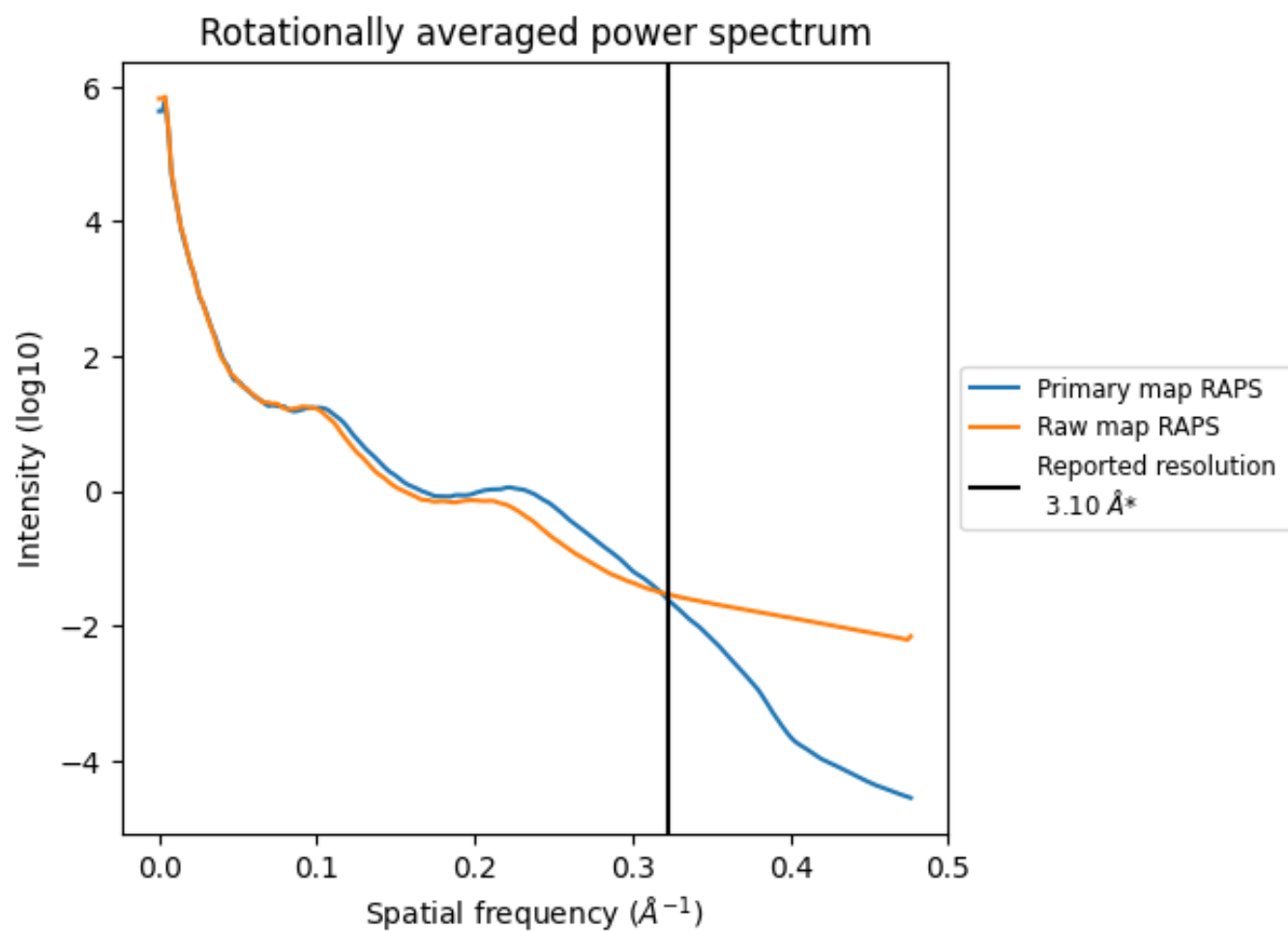
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3389 nm³; this corresponds to an approximate mass of 3061 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 ⓘ

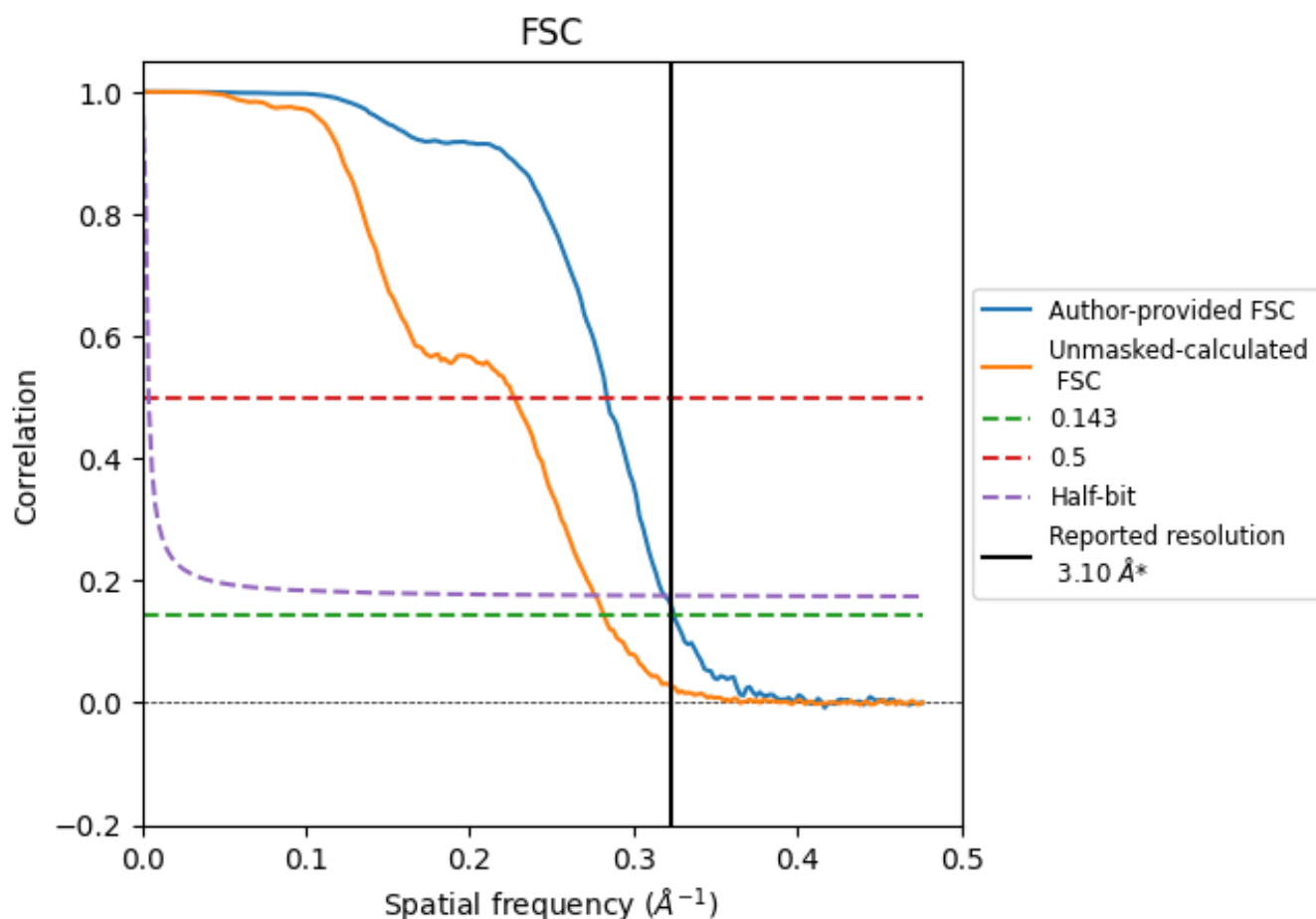


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

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 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

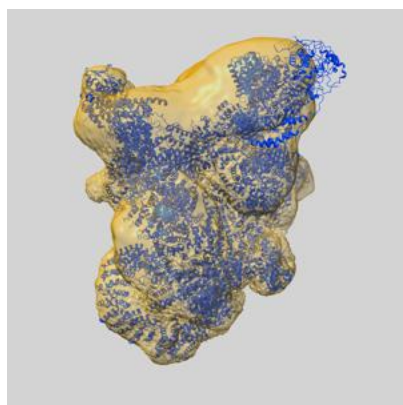
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.52	3.13
Unmasked-calculated*	3.55	4.41	3.62

*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 3.55 differs from the reported value 3.1 by more than 10 %

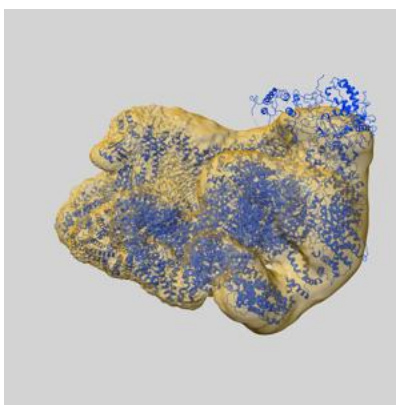
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19047 and PDB model 8RC4. Per-residue inclusion information can be found in section [3](#) on page [8](#).

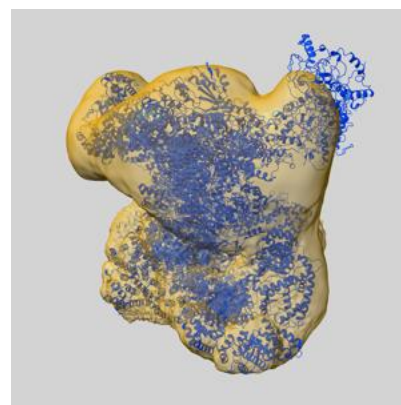
9.1 Map-model overlay [i](#)



X



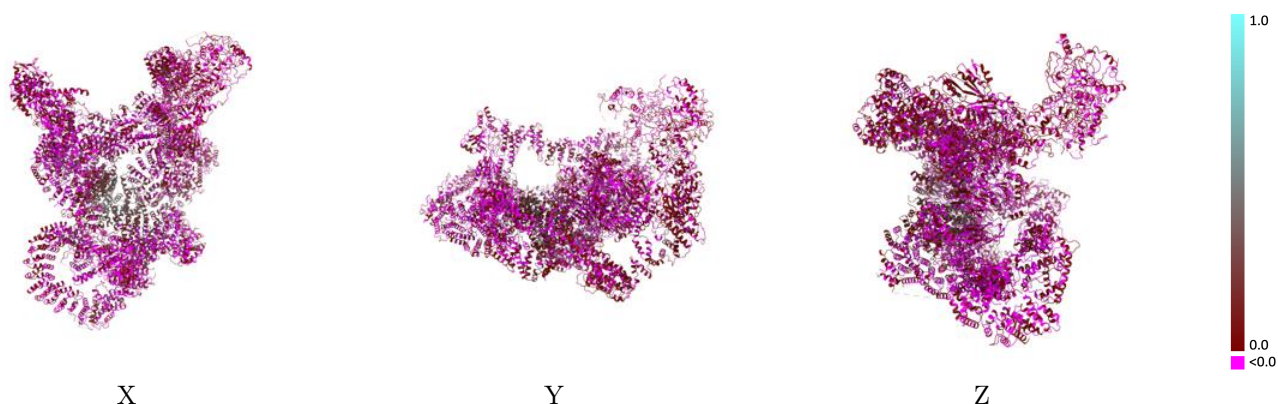
Y



Z

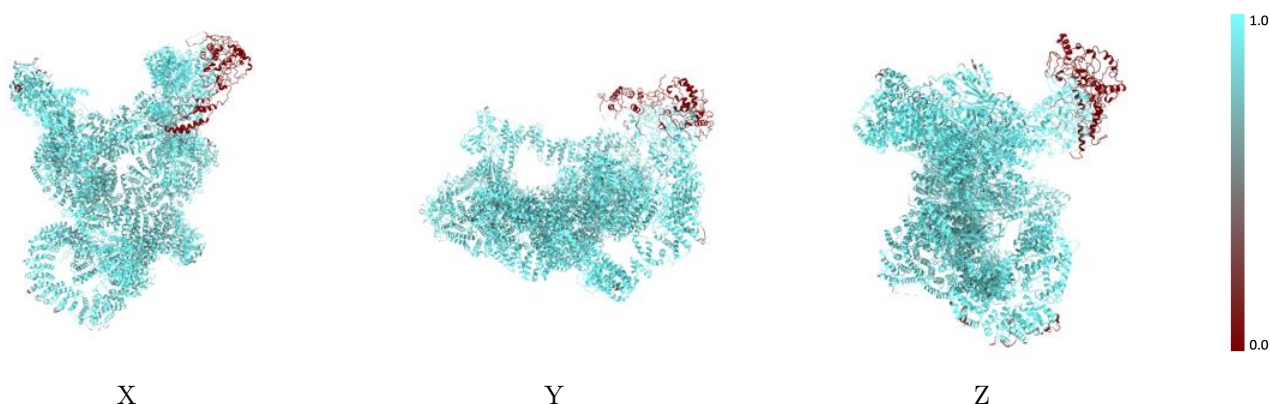
The images above show the 3D surface view of the map at the recommended contour level 0.00502 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



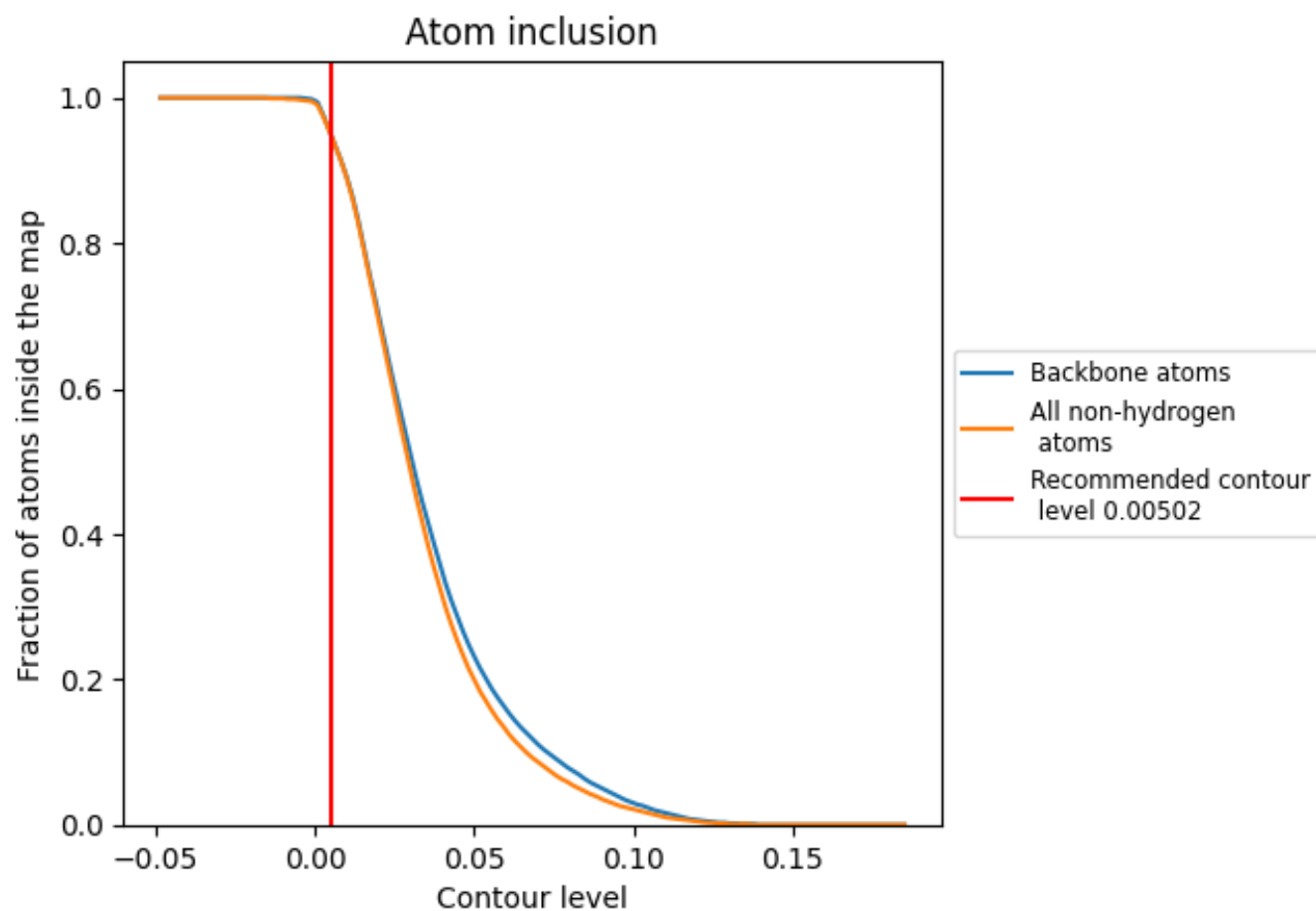
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00502).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.00502) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.0360
a	 0.9690	 0.0540
b	 0.9790	 0.0870
d	 0.9900	 0.0350
e	 0.9700	 0.0110
f	 0.9870	 0.0240
g	 0.9670	 0.0460
h	 0.9630	 0.0100
i	 0.9840	 0.0020
j	 0.9860	 0.0510
k	 0.9990	 0.0440
m	 0.4430	 0.0190
n	 0.7180	 0.0230
o	 0.9890	 0.0540
p	 0.9760	 0.0390
q	 0.9660	 -0.0370
r	 0.9530	 -0.0080

