



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 09:00 PM UTC

PDB ID : 8RBZ / pdb_00008rbz
EMDB ID : EMD-19040
Title : Structure of Integrator-PP2A-SOSS-CTD post-termination complex
Authors : Fianu, I.; Ochmann, M.; Walshe, J.L.; Cramer, P.
Deposited on : 2023-12-05
Resolution : 3.70 Å(reported)
Based on initial model : ?

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:

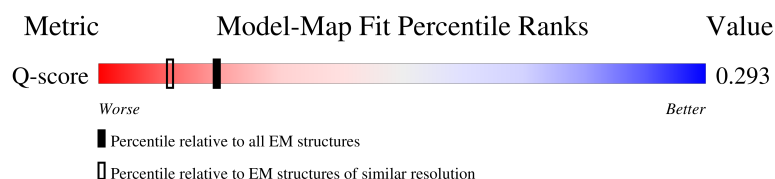
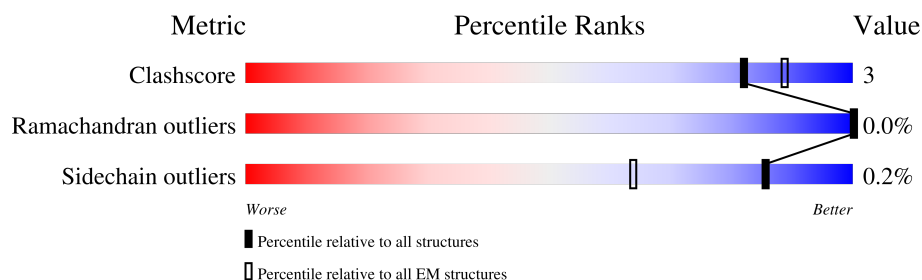
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & 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 3.70 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.



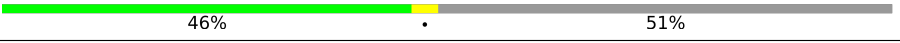
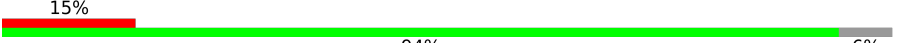
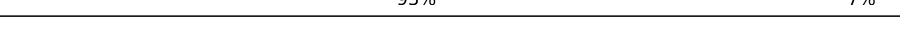
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1	9	100%
2	B	213	48% 50%
3	C	106	37% 63%
4	Y	13	100%

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Mol	Chain	Length	Quality of chain
5	a	2192	
6	b	1204	
7	c	1042	
8	d	963	
9	e	1021	
10	f	889	
11	g	964	
12	h	995	
13	i	658	
14	j	710	
15	k	602	
16	n	518	
17	o	451	
18	p	591	
19	q	311	
20	r	27	
21	m	706	

2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 74102 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 UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	1	9	Total	C	N	O	0	0
			45	27	9	9		

- Molecule 2 is a protein called SOSS complex subunit B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			806	516	135	151	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP Q9BQ15
B	0	ASN	-	expression tag	UNP Q9BQ15

- Molecule 3 is a protein called SOSS complex subunit C.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	39	Total	C	N	O	0	0
			296	190	56	50		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP Q9NRY2
C	0	ASN	-	expression tag	UNP Q9NRY2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	Y	13	Total	C	N	O	0	0
			95	60	13	22		

- Molecule 5 is a protein called Integrator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	a	1085	Total	C	N	O	S	0	0
			8525	5425	1502	1547	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 6 is a protein called Integrator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	1051	Total	C	N	O	S	0	0
			7988	5120	1352	1454	62		

- Molecule 7 is a protein called Integrator complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	463	Total	C	N	O	S	0	0
			3717	2380	646	662	29		

- Molecule 8 is a protein called Integrator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	818	Total	C	N	O	S	0	0
			6395	4081	1091	1189	34		

- Molecule 9 is a protein called Integrator complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	855	Total	C	N	O	S	0	0
			6253	3974	1139	1114	26		

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 10 is a protein called Integrator complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	544	Total	C	N	O	S	0	0
			4137	2653	701	758	25		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	-1	SER	-	expression tag	UNP Q9UL03
f	0	ASN	-	expression tag	UNP Q9UL03

- Molecule 11 is a protein called Integrator complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	886	Total	C	N	O	S	0	0
			6725	4261	1169	1255	40		

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 12 is a protein called Integrator complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	887	Total	C	N	O	S	0	0
			6748	4333	1156	1221	38		

- Molecule 13 is a protein called Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	626	Total	C	N	O	S	0	0
			4867	3134	792	908	33		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	j	668	Total	C	N	O	0	0
			3313	1976	668	669		

- Molecule 15 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	551	Total	C	N	O	S	0	0
			4079	2613	706	734	26		

There are 4 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
k	487	GLU	ASP	conflict	UNP Q5TA45

- Molecule 16 is a protein called Integrator complex subunit 14.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	n	204	Total	C	N	O	0	0
			1007	599	204	204		

- Molecule 17 is a protein called Integrator complex subunit 15.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	o	367	Total	C	N	O	0	0
			1824	1090	367	367		

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 18 is a protein called Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	p	580	Total	C	N	O	S	0	0
			4432	2822	753	831	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	q	290	Total	C	N	O	S	0	0
			2322	1467	403	437	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 20 is a protein called DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	r	27	Total	C	N	O	S	0	0
			237	146	37	53	1		

- Molecule 21 is a protein called Integrator complex subunit 13.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	m	35	Total	C	N	O	0	0
			287	175	61	51		

- Molecule 22 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 23 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

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.

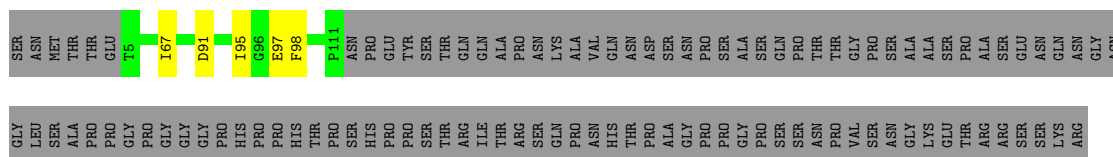
- Molecule 1: UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK-UNK

Chain 1:  100%

There are no outlier residues recorded for this chain.

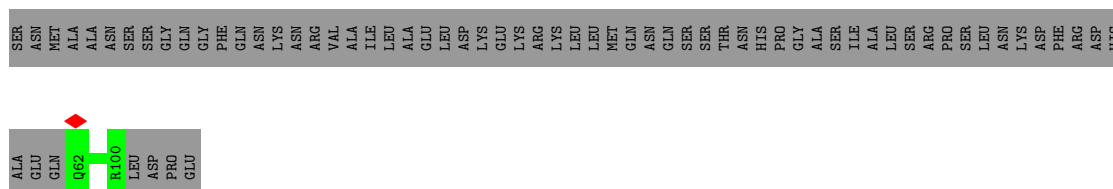
- Molecule 2: SOSS complex subunit B1

Chain B:  48% 50%



- Molecule 3: SOSS complex subunit C

Chain C:  37% 63%



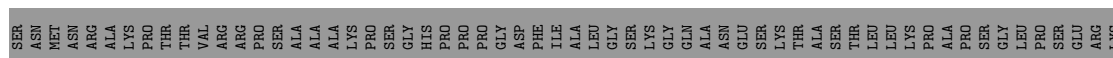
- Molecule 4: DNA-directed RNA polymerase subunit

Chain Y:  100%

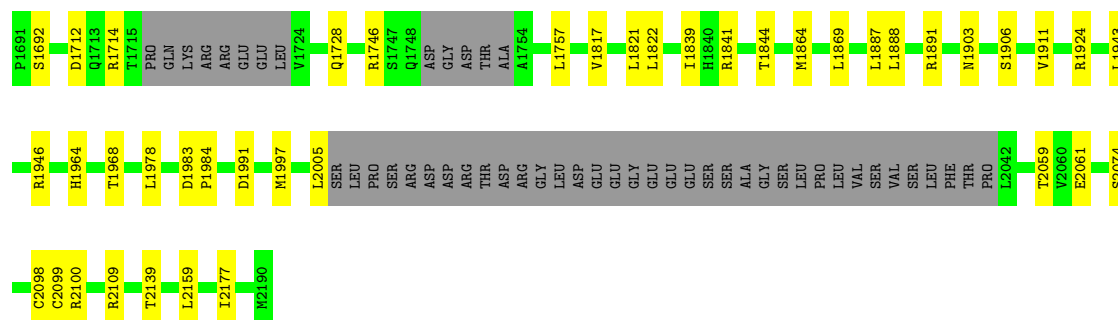
There are no outlier residues recorded for this chain.

- Molecule 5: Integrator complex subunit 1

Chain a:  46% 51%

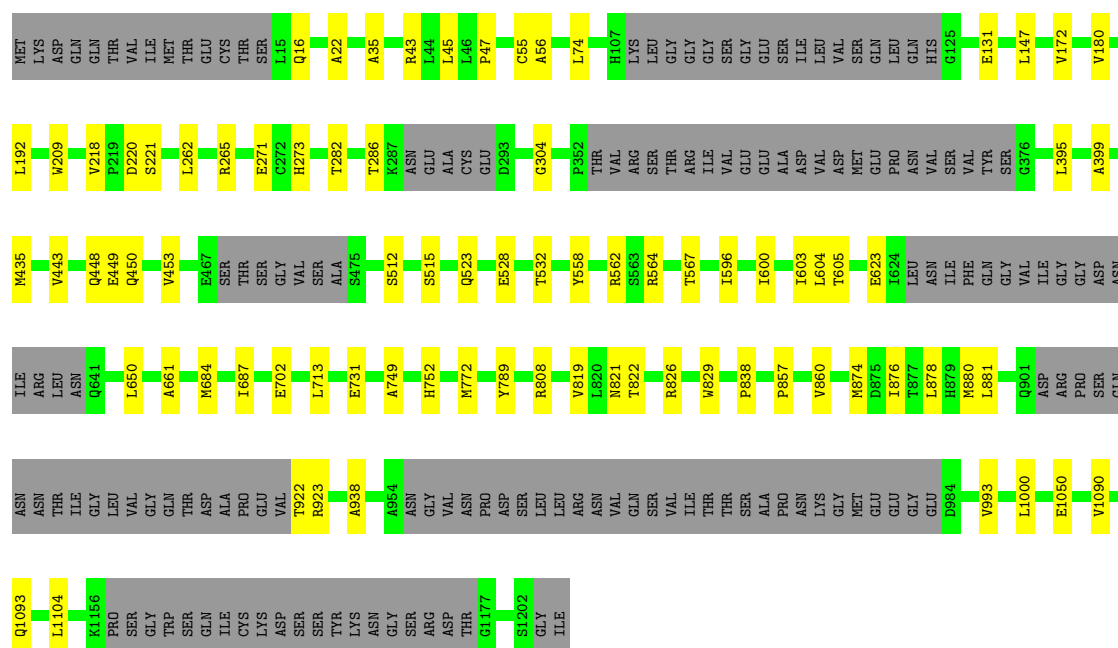






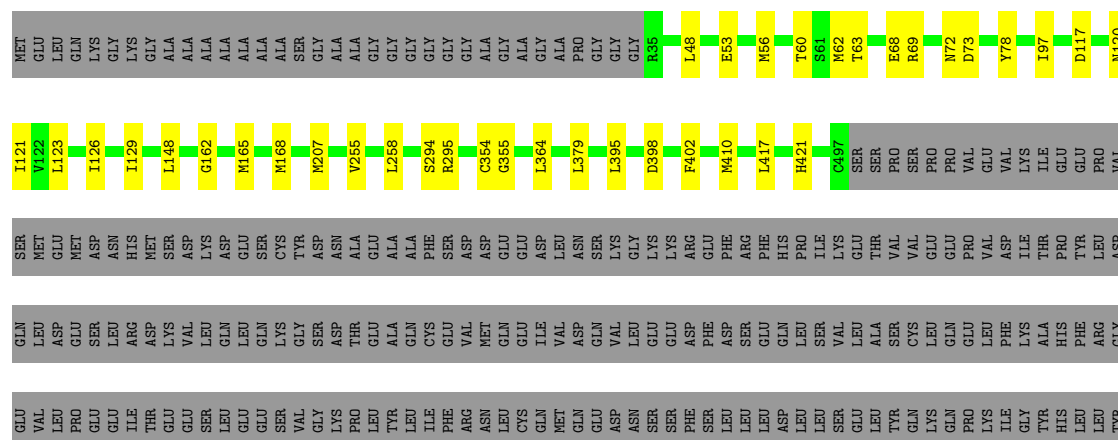
• Molecule 6: Integrator complex subunit 2

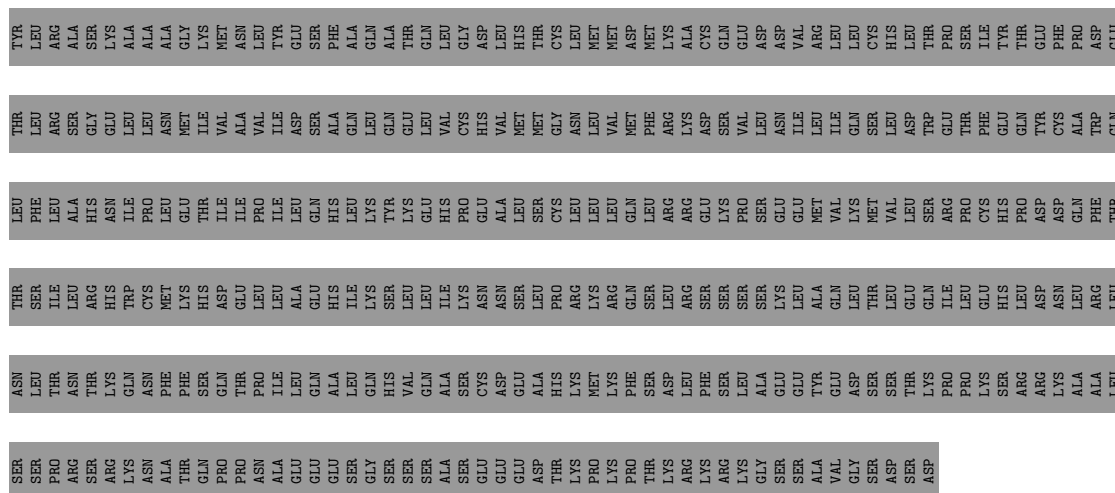
Chain b: 80% 7% 13%



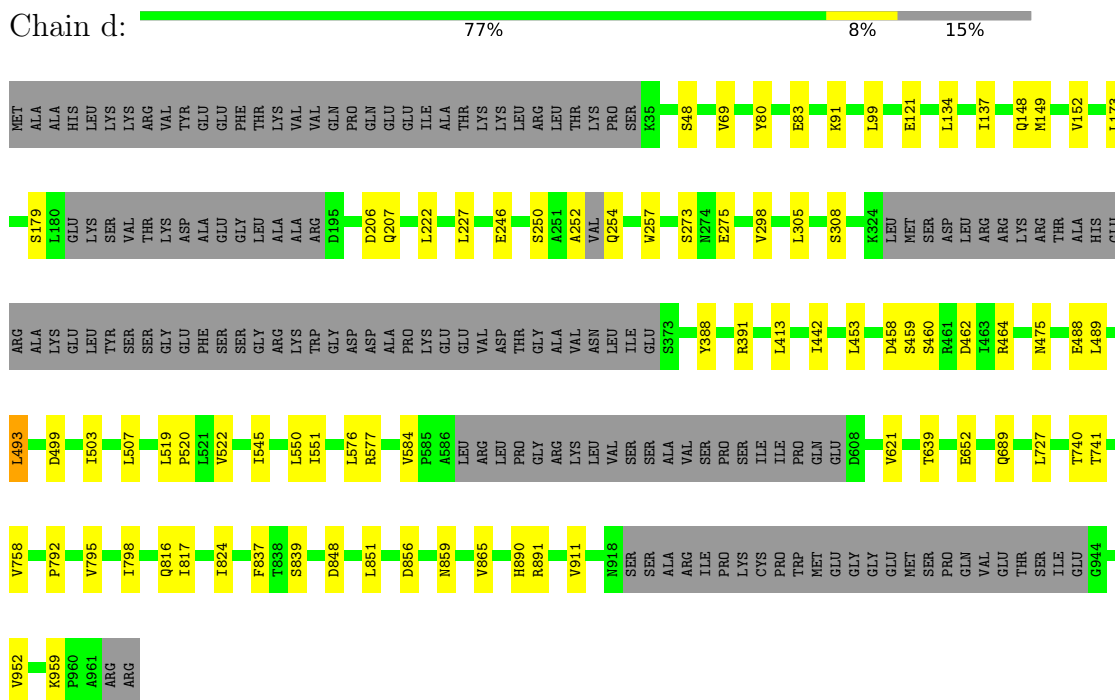
• Molecule 7: Integrator complex subunit 3

Chain c: 41% 1% 56%

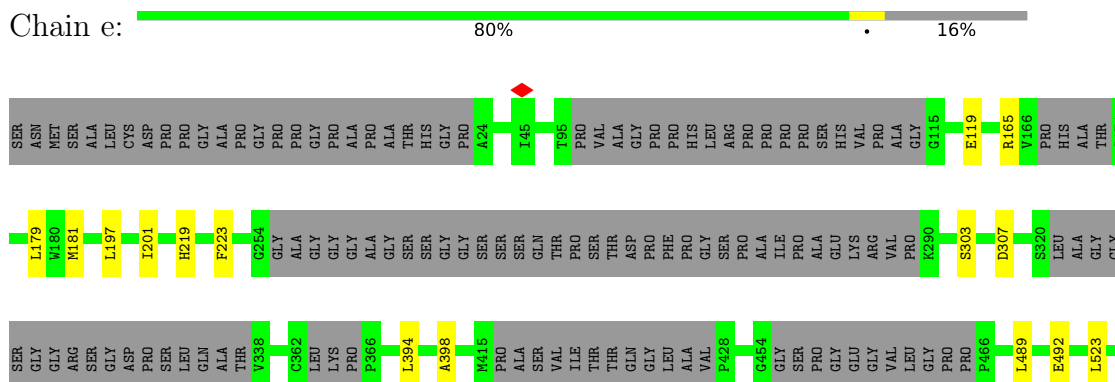


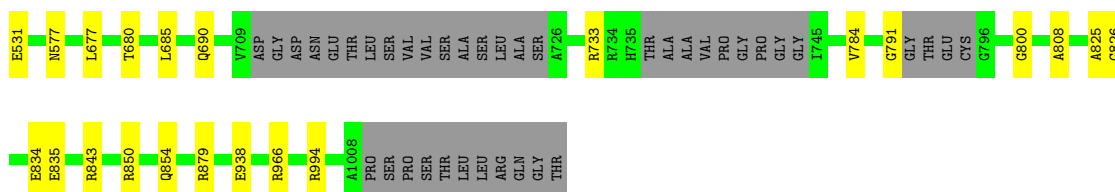


- Molecule 8: Integrator complex subunit 4



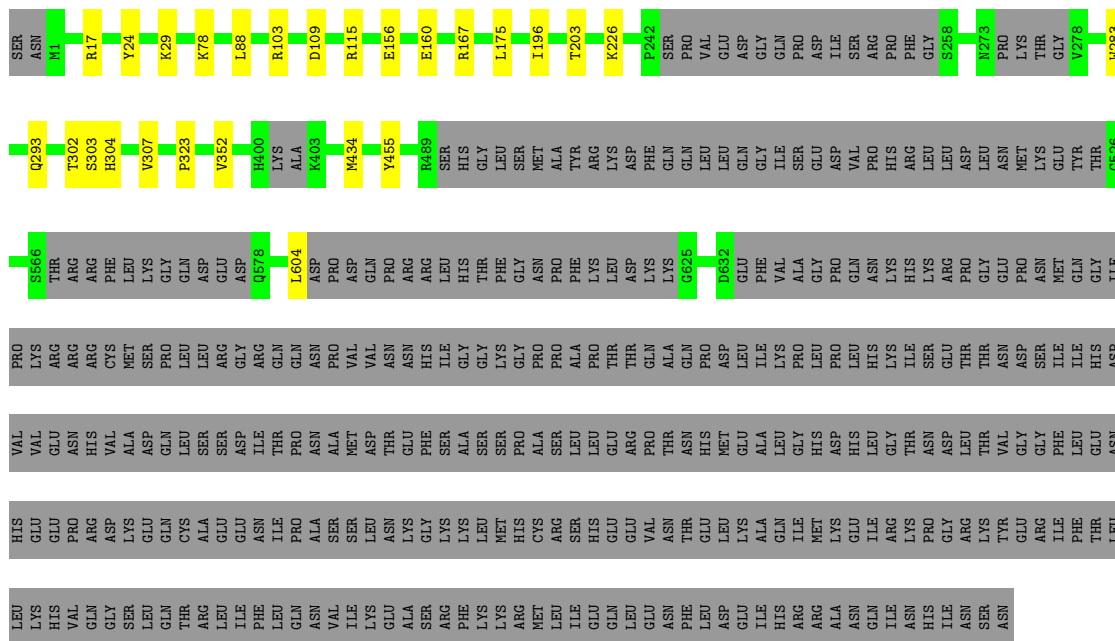
- Molecule 9: Integrator complex subunit 5





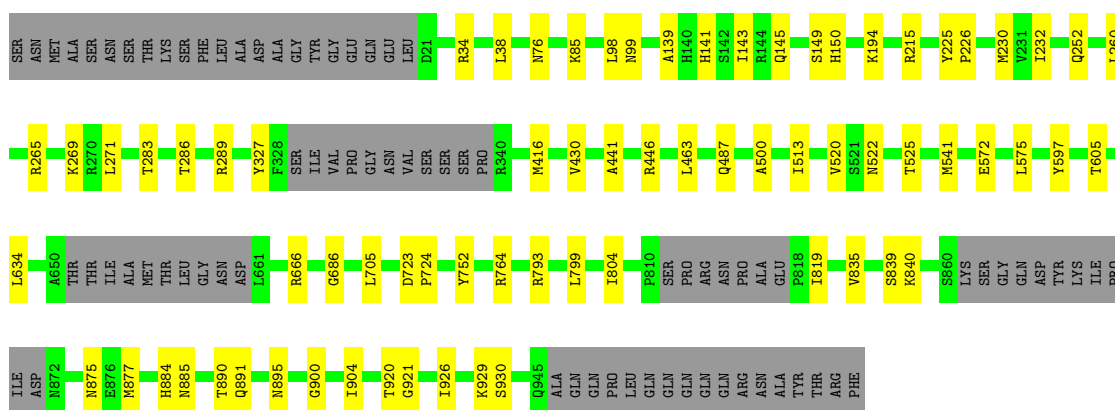
• Molecule 10: Integrator complex subunit 6

Chain f:  58% 39%



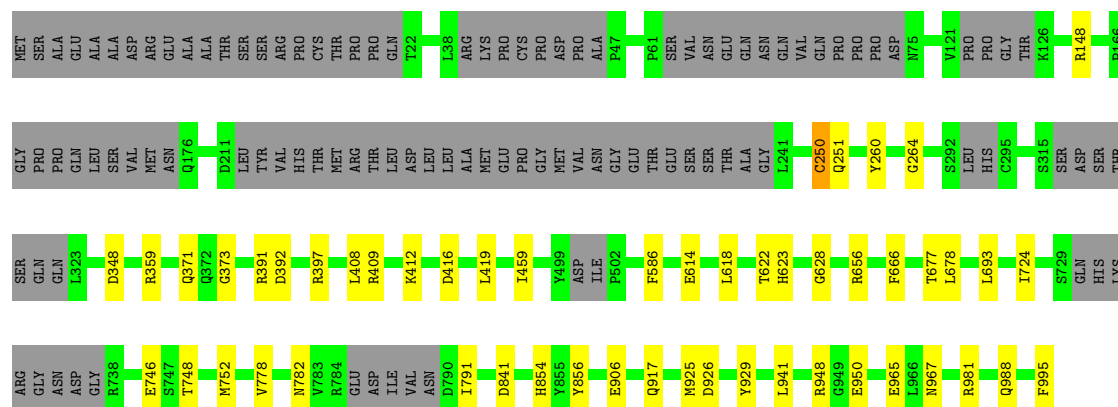
• Molecule 11: Integrator complex subunit 7

Chain g:  84% 7% 8%



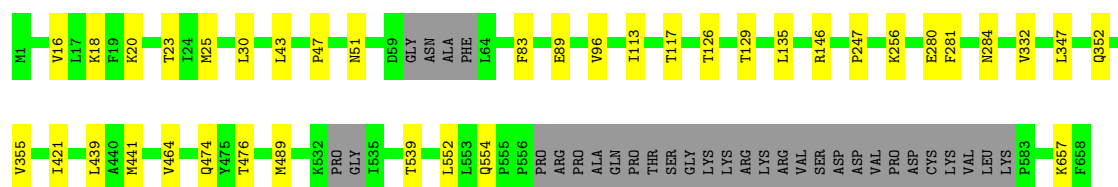
• Molecule 12: Integrator complex subunit 8

Chain h:  84% 5% 11%



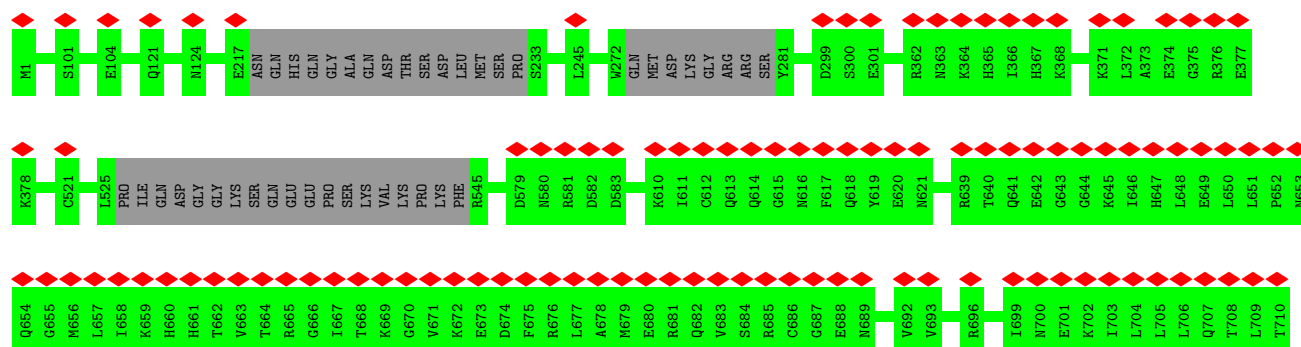
• Molecule 13: Integrator complex subunit 9

Chain i: 89% 6% 5%



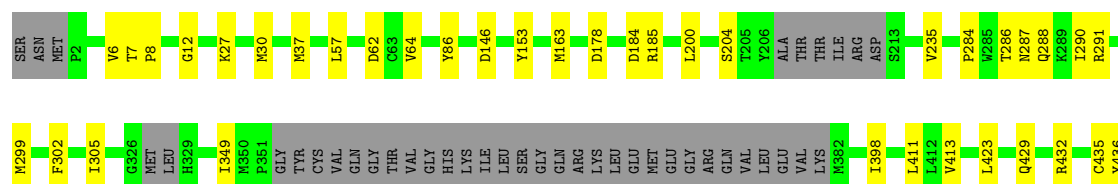
• Molecule 14: Integrator complex subunit 10

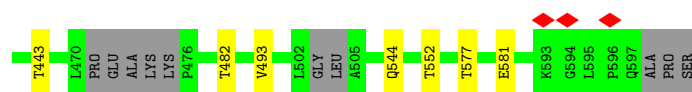
Chain j: 15% 94% 6%



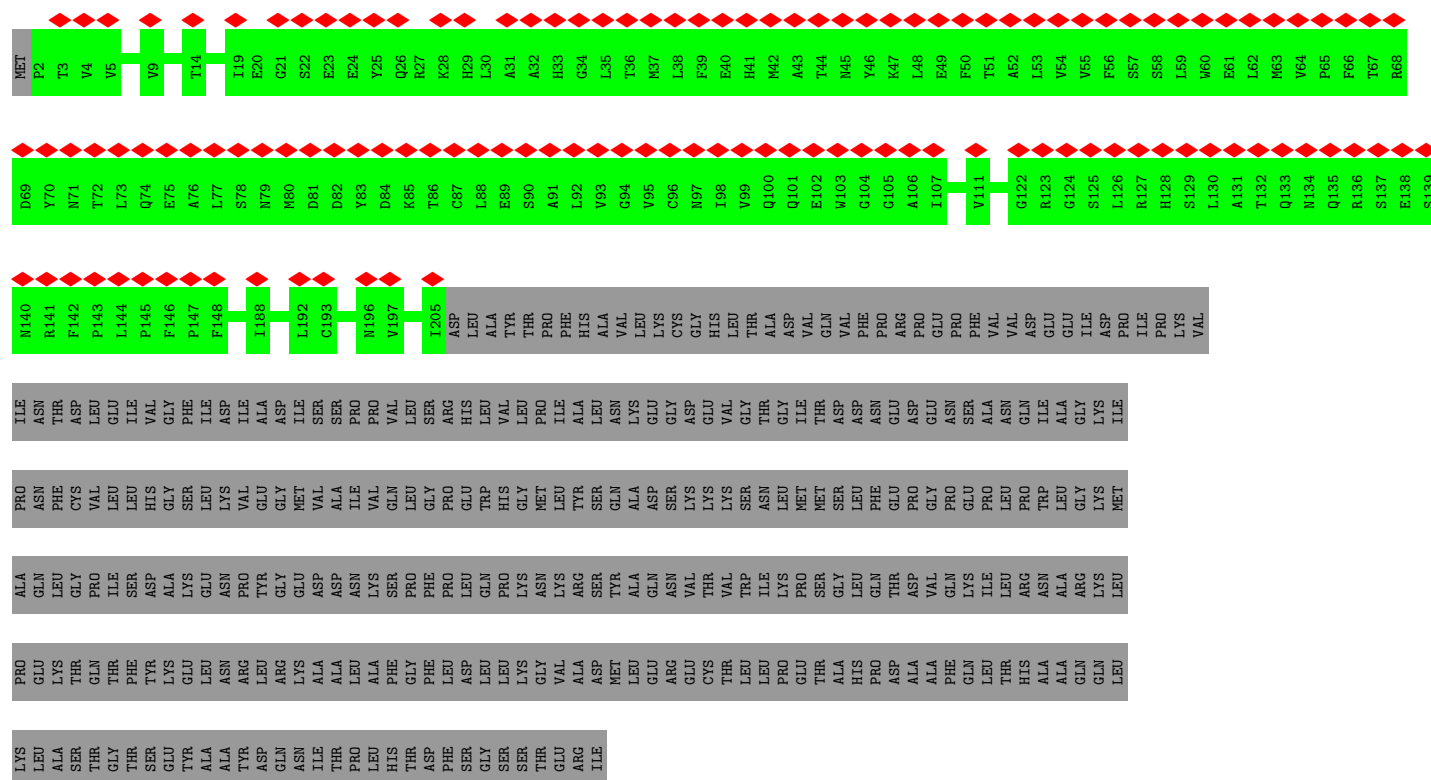
• Molecule 15: Integrator complex subunit 11

Chain k: 84% 7% 8%

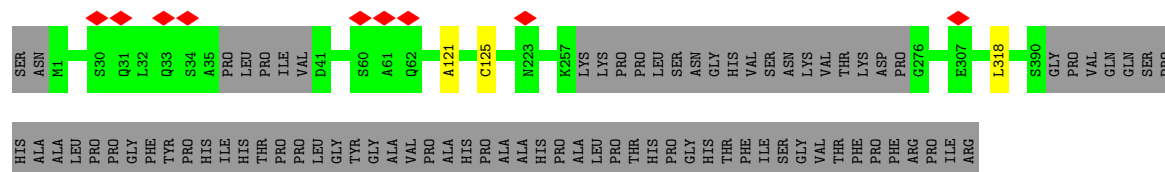
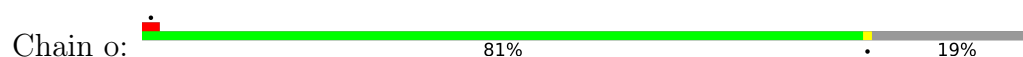




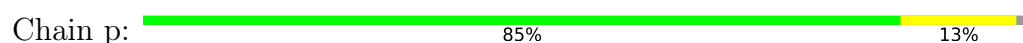
• Molecule 16: Integrator complex subunit 14



• Molecule 17: Integrator complex subunit 15



• Molecule 18: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



L689
LYS
GLU
GLU
ASN
GLY
MET
GLU
THR
THR
GLU
ASN
GLY
LYS
ALA
SER
ARG
GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	236382	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 ($e^-/\text{\AA}^2$)	39.93	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	0.195	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.00308	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: ZN, MN

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	$\# Z > 5$
2	B	0.21	0/820	0.47	0/1109
3	C	0.17	0/304	0.38	0/413
4	Y	0.18	0/100	0.38	0/139
5	a	0.21	0/8682	0.46	0/11763
6	b	0.25	0/8128	0.51	0/11072
7	c	0.22	0/3791	0.45	0/5134
8	d	0.21	0/6519	0.47	0/8853
9	e	0.21	0/6390	0.45	0/8706
10	f	0.20	0/4240	0.46	0/5784
11	g	0.21	0/6835	0.46	0/9271
12	h	0.20	0/6867	0.44	0/9330
13	i	0.21	0/4986	0.48	0/6798
14	j	0.14	0/3309	0.37	0/4608
15	k	0.21	0/4168	0.47	0/5665
16	n	0.12	0/1006	0.34	0/1399
17	o	0.15	0/1821	0.41	0/2538
18	p	0.26	0/4506	0.53	0/6130
19	q	0.18	0/2378	0.44	0/3228
20	r	0.15	0/241	0.39	0/327
21	m	0.17	0/292	0.57	0/393
All	All	0.21	0/75383	0.46	0/102660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1	45	0	12	0	0
2	B	806	0	806	3	0
3	C	296	0	286	0	0
4	Y	95	0	82	0	0
5	a	8525	0	8673	38	0
6	b	7988	0	8032	48	0
7	c	3717	0	3806	20	0
8	d	6395	0	6420	48	0
9	e	6253	0	6063	24	0
10	f	4137	0	3989	15	0
11	g	6725	0	6694	40	0
12	h	6748	0	6613	35	0
13	i	4867	0	4840	22	0
14	j	3313	0	1464	0	0
15	k	4079	0	3873	24	0
16	n	1007	0	439	0	0
17	o	1824	0	802	1	0
18	p	4432	0	4487	49	0
19	q	2322	0	2215	20	0
20	r	237	0	201	1	0
21	m	287	0	275	3	0
22	k	2	0	0	0	0
23	q	2	0	0	0	0
All	All	74102	0	70072	362	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 (362) 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)
18:p:245:MET:SD	18:p:245:MET:N	2.69	0.66
9:e:966:ARG:NH2	12:h:373:GLY:O	2.29	0.65
6:b:623:GLU:HG3	6:b:687:ILE:HG22	1.80	0.64
18:p:424:ILE:O	18:p:465:ASN:ND2	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:i:30:LEU:HD21	13:i:83:PHE:HB3	1.81	0.63
5:a:1076:VAL:O	5:a:1130:ARG:NH1	2.32	0.63
12:h:917:GLN:O	12:h:948:ARG:NH2	2.31	0.63
19:q:271:ASN:ND2	19:q:272:GLN:O	2.32	0.63
6:b:47:PRO:HG3	6:b:180:VAL:HG13	1.81	0.62
6:b:564:ARG:NH2	6:b:605:THR:OG1	2.33	0.61
11:g:215:ARG:NH1	11:g:252:GLN:OE1	2.34	0.60
13:i:113:ILE:O	13:i:117:THR:OG1	2.18	0.60
7:c:379:LEU:HD21	7:c:395:LEU:HD11	1.83	0.60
6:b:558:TYR:OH	6:b:562:ARG:NH2	2.35	0.60
9:e:677:LEU:O	9:e:680:THR:OG1	2.20	0.59
7:c:295:ARG:NH2	7:c:398:ASP:OD1	2.35	0.59
9:e:825:ALA:O	9:e:843:ARG:NH1	2.35	0.59
8:d:522:VAL:HG22	8:d:551:ILE:HD12	1.85	0.59
8:d:460:SER:OG	8:d:462:ASP:OD1	2.21	0.59
6:b:731:GLU:OE2	11:g:85:LYS:NZ	2.34	0.59
6:b:1090:VAL:HG13	12:h:950:GLU:HB3	1.85	0.59
18:p:392:ASN:ND2	18:p:433:GLN:OE1	2.36	0.58
15:k:429:GLN:O	15:k:432:ARG:NH1	2.36	0.58
6:b:821:ASN:OD1	6:b:829:TRP:NE1	2.35	0.58
11:g:705:LEU:O	11:g:752:TYR:OH	2.21	0.58
9:e:690:GLN:OE1	12:h:988:GLN:NE2	2.36	0.58
19:q:28:VAL:HG11	19:q:142:VAL:HG23	1.84	0.58
10:f:88:LEU:HD21	10:f:196:ILE:HD13	1.85	0.58
11:g:416:MET:HE2	11:g:430:VAL:HG13	1.84	0.58
11:g:724:PRO:O	11:g:764:ARG:NH1	2.36	0.58
6:b:604:LEU:HD11	6:b:661:ALA:HB1	1.86	0.58
15:k:37:MET:SD	15:k:37:MET:N	2.76	0.57
5:a:1712:ASP:O	5:a:1714:ARG:NH1	2.37	0.57
10:f:17:ARG:O	12:h:967:ASN:ND2	2.37	0.57
8:d:464:ARG:NH1	8:d:499:ASP:OD2	2.37	0.57
15:k:6:VAL:HG12	15:k:8:PRO:HD3	1.86	0.57
10:f:167:ARG:NH2	10:f:226:LYS:O	2.37	0.56
12:h:412:LYS:NZ	12:h:416:ASP:OD2	2.38	0.56
5:a:1172:ILE:O	5:a:1175:THR:OG1	2.21	0.56
7:c:62:MET:HE1	7:c:78:TYR:HB2	1.88	0.56
15:k:544:GLN:NE2	15:k:552:THR:O	2.38	0.56
12:h:925:MET:SD	12:h:925:MET:N	2.77	0.55
15:k:435:CYS:SG	15:k:436:TYR:N	2.79	0.55
15:k:12:GLY:HA2	15:k:413:VAL:HG12	1.86	0.55
18:p:451:LEU:HB3	18:p:489:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:68:GLU:O	7:c:72:ASN:ND2	2.39	0.55
9:e:850:ARG:NH2	9:e:854:GLN:OE1	2.38	0.55
11:g:513:ILE:HB	11:g:541:MET:HE1	1.88	0.55
7:c:117:ASP:O	11:g:34:ARG:NH1	2.40	0.55
13:i:439:LEU:HD13	13:i:441:MET:HB3	1.89	0.55
12:h:348:ASP:OD2	12:h:391:ARG:NH1	2.39	0.55
5:a:1888:LEU:HD23	5:a:1891:ARG:HH12	1.72	0.54
6:b:262:LEU:HD22	6:b:265:ARG:HH21	1.72	0.54
7:c:364:LEU:HD12	7:c:410:MET:HE1	1.89	0.54
13:i:539:THR:HG22	13:i:657:LYS:HB3	1.90	0.54
19:q:254:ARG:NH2	19:q:284:TYR:OH	2.40	0.54
10:f:103:ARG:NH2	10:f:109:ASP:OD1	2.39	0.54
12:h:623:HIS:O	12:h:628:GLY:N	2.40	0.54
12:h:724:ILE:O	12:h:748:THR:OG1	2.25	0.54
5:a:1997:MET:SD	5:a:1997:MET:N	2.80	0.54
9:e:800:GLY:O	12:h:409:ARG:NH1	2.40	0.54
6:b:443:VAL:O	6:b:448:GLN:NE2	2.41	0.54
11:g:441:ALA:O	11:g:446:ARG:NH1	2.40	0.54
18:p:421:LEU:HA	18:p:424:ILE:HD12	1.88	0.54
11:g:260:LEU:O	11:g:269:LYS:NZ	2.41	0.54
8:d:519:LEU:HA	8:d:522:VAL:HG23	1.89	0.54
5:a:2074:SER:OG	5:a:2109:ARG:NH1	2.41	0.53
5:a:1887:LEU:HD21	8:d:520:PRO:HG3	1.90	0.53
11:g:875:ASN:ND2	11:g:895:ASN:OD1	2.40	0.53
8:d:252:ALA:O	8:d:254:GLN:N	2.42	0.53
9:e:523:LEU:O	9:e:577:ASN:ND2	2.40	0.53
13:i:16:VAL:HG22	13:i:25:MET:HG2	1.91	0.53
18:p:518:THR:HA	18:p:522:LEU:HD23	1.91	0.53
5:a:1817:VAL:HG11	5:a:1821:LEU:HD12	1.90	0.53
11:g:232:ILE:HG23	11:g:271:LEU:HD22	1.91	0.53
18:p:343:SER:O	18:p:383:ASN:ND2	2.41	0.53
7:c:162:GLY:HA2	7:c:165:MET:HE2	1.89	0.53
10:f:283:TRP:NE1	10:f:323:PRO:O	2.41	0.53
8:d:250:SER:HB3	8:d:298:VAL:HG22	1.91	0.53
9:e:826:GLY:O	9:e:879:ARG:NH1	2.38	0.52
5:a:2098:CYS:SG	5:a:2099:CYS:N	2.83	0.52
6:b:16:GLN:O	6:b:209:TRP:NE1	2.42	0.52
8:d:91:LYS:NZ	13:i:89:GLU:O	2.42	0.52
8:d:493:LEU:HD22	8:d:503:ILE:HD13	1.92	0.52
19:q:228:PHE:O	19:q:232:ASN:ND2	2.42	0.52
8:d:413:LEU:HD21	8:d:442:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:e:791:GLY:O	12:h:409:ARG:NH2	2.42	0.52
18:p:29:LEU:HD22	18:p:65:VAL:HG12	1.90	0.52
18:p:233:GLN:OE1	18:p:233:GLN:N	2.43	0.52
10:f:115:ARG:NH1	10:f:302:THR:O	2.42	0.52
8:d:222:LEU:HD21	8:d:227:LEU:HD23	1.92	0.51
6:b:876:ILE:O	6:b:880:MET:HG3	2.10	0.51
12:h:614:GLU:OE2	12:h:656:ARG:NH1	2.42	0.51
18:p:187:SER:HB3	18:p:223:LEU:HD23	1.92	0.51
6:b:35:ALA:HA	6:b:74:LEU:HD13	1.92	0.51
18:p:414:ASP:O	18:p:420:ARG:NH1	2.42	0.51
15:k:30:MET:HB3	15:k:64:VAL:HA	1.92	0.51
11:g:38:LEU:HD13	11:g:76:ASN:HD21	1.76	0.51
5:a:2159:LEU:HD12	5:a:2177:ILE:HG23	1.92	0.51
8:d:621:VAL:HG21	8:d:639:THR:HG21	1.93	0.51
15:k:184:ASP:OD1	15:k:185:ARG:N	2.43	0.51
5:a:1943:LEU:HD11	5:a:1984:PRO:HB3	1.93	0.51
6:b:528:GLU:O	6:b:532:THR:OG1	2.20	0.50
13:i:280:GLU:O	13:i:284:ASN:ND2	2.45	0.50
15:k:577:THR:O	15:k:581:GLU:N	2.43	0.50
17:o:121:ALA:O	17:o:125:CYS:N	2.44	0.50
18:p:454:HIS:O	18:p:459:ARG:NH1	2.45	0.50
19:q:53:THR:OG1	19:q:277:GLU:OE1	2.27	0.50
12:h:148:ARG:NH1	12:h:251:GLN:OE1	2.44	0.50
15:k:443:THR:H	21:m:681:ASN:HB3	1.76	0.50
18:p:483:ILE:HD12	18:p:521:MET:HE1	1.93	0.50
5:a:1888:LEU:HD21	5:a:1911:VAL:HG11	1.94	0.50
6:b:819:VAL:O	6:b:822:THR:OG1	2.24	0.50
7:c:120:ASN:OD1	7:c:121:ILE:N	2.44	0.50
11:g:572:GLU:OE2	11:g:597:TYR:OH	2.29	0.50
6:b:395:LEU:O	6:b:399:ALA:HB3	2.12	0.50
10:f:604:LEU:O	18:p:258:ARG:NH2	2.41	0.50
6:b:220:ASP:OD1	11:g:666:ARG:NH2	2.44	0.50
12:h:586:PHE:HB3	12:h:622:THR:HG22	1.94	0.50
6:b:922:THR:OG1	6:b:923:ARG:N	2.44	0.50
7:c:73:ASP:OD1	11:g:99:ASN:ND2	2.45	0.50
6:b:874:MET:HG2	6:b:993:VAL:HG13	1.93	0.50
8:d:689:GLN:HE22	11:g:686:GLY:HA2	1.77	0.50
11:g:141:HIS:NE2	11:g:145:GLN:OE1	2.45	0.50
18:p:26:GLN:O	18:p:30:ASN:ND2	2.43	0.50
15:k:299:MET:SD	15:k:299:MET:N	2.79	0.49
11:g:900:GLY:N	11:g:930:SER:OG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:h:693:LEU:HD22	12:h:752:MET:HE1	1.94	0.49
5:a:1978:LEU:HD13	5:a:2005:LEU:HD21	1.93	0.49
5:a:1240:GLU:OE1	5:a:1243:GLN:NE2	2.45	0.49
8:d:865:VAL:HG23	8:d:911:VAL:HG12	1.94	0.49
9:e:834:GLU:N	9:e:834:GLU:OE1	2.45	0.49
15:k:287:ASN:OD1	15:k:288:GLN:N	2.46	0.49
5:a:1839:ILE:HG22	5:a:1869:LEU:HD13	1.95	0.49
6:b:838:PRO:HG3	9:e:733:ARG:HH22	1.76	0.49
11:g:230:MET:SD	11:g:230:MET:N	2.75	0.49
12:h:841:ASP:OD1	12:h:856:TYR:OH	2.20	0.49
9:e:938:GLU:OE2	9:e:994:ARG:NH1	2.46	0.49
15:k:27:LYS:NZ	15:k:146:ASP:OD1	2.41	0.49
5:a:1070:LEU:O	5:a:1074:THR:OG1	2.20	0.49
5:a:1690:ASP:OD2	5:a:1692:SER:OG	2.26	0.49
6:b:564:ARG:HH22	6:b:567:THR:HG21	1.78	0.49
8:d:179:SER:HA	8:d:227:LEU:HD13	1.95	0.48
9:e:966:ARG:NH1	12:h:371:GLN:O	2.46	0.48
13:i:281:PHE:HD1	13:i:421:ILE:HG21	1.79	0.48
18:p:138:GLY:O	18:p:144:ARG:NH1	2.46	0.48
8:d:545:ILE:HG23	8:d:576:LEU:HD11	1.95	0.48
6:b:752:HIS:O	6:b:789:TYR:OH	2.31	0.48
10:f:307:VAL:HG12	10:f:352:VAL:HG12	1.95	0.48
19:q:177:LEU:HD21	19:q:234:LEU:HD11	1.94	0.48
6:b:684:MET:O	6:b:826:ARG:NH2	2.47	0.48
9:e:303:SER:O	9:e:307:ASP:N	2.47	0.48
5:a:1946:ARG:NH1	5:a:1991:ASP:OD2	2.47	0.48
8:d:80:TYR:OH	8:d:121:GLU:OE1	2.29	0.48
9:e:784:VAL:HG12	12:h:408:LEU:HD11	1.96	0.48
10:f:203:THR:HA	10:f:304:HIS:HE1	1.79	0.47
13:i:25:MET:HB2	13:i:96:VAL:HG21	1.95	0.47
7:c:168:MET:HE1	7:c:207:MET:HB3	1.96	0.47
5:a:1746:ARG:HG3	5:a:1757:LEU:HD22	1.96	0.47
10:f:24:TYR:OH	10:f:175:LEU:O	2.31	0.47
15:k:398:ILE:HG21	15:k:423:LEU:HD21	1.95	0.47
18:p:52:LEU:HD22	18:p:92:PRO:HG3	1.96	0.47
11:g:884:HIS:O	11:g:884:HIS:ND1	2.48	0.47
18:p:229:VAL:HG11	18:p:266:LYS:HB2	1.97	0.47
8:d:149:MET:HA	8:d:152:VAL:HG22	1.97	0.47
19:q:120:SER:OG	19:q:188:GLU:OE2	2.26	0.47
8:d:824:ILE:HB	8:d:952:VAL:HG21	1.97	0.47
13:i:43:LEU:HD13	13:i:146:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:k:200:LEU:O	15:k:411:LEU:N	2.45	0.47
13:i:18:LYS:NZ	13:i:20:LYS:O	2.47	0.47
6:b:749:ALA:O	6:b:752:HIS:ND1	2.44	0.46
13:i:554:GLN:N	13:i:554:GLN:OE1	2.48	0.46
18:p:454:HIS:HB3	19:q:287:LEU:HD22	1.97	0.46
13:i:247:PRO:HA	13:i:347:LEU:HA	1.96	0.46
18:p:206:ILE:HG21	18:p:243:LEU:HB3	1.96	0.46
5:a:1196:GLU:N	5:a:1196:GLU:OE1	2.49	0.46
6:b:449:GLU:O	6:b:453:VAL:HG13	2.16	0.46
19:q:137:TYR:O	19:q:139:ASN:ND2	2.48	0.46
5:a:1822:LEU:O	5:a:1924:ARG:NH2	2.47	0.46
6:b:600:ILE:HA	6:b:603:ILE:HD12	1.98	0.46
19:q:204:ASP:OD1	19:q:205:ASP:N	2.48	0.46
10:f:293:GLN:N	10:f:293:GLN:OE1	2.48	0.46
11:g:487:GLN:HB3	11:g:525:THR:HG21	1.97	0.46
8:d:134:LEU:HA	8:d:137:ILE:HG22	1.98	0.46
6:b:271:GLU:O	6:b:273:HIS:ND1	2.48	0.46
8:d:848:ASP:OD1	8:d:891:ARG:NH1	2.49	0.46
18:p:260:ARG:NH2	18:p:295:GLU:OE2	2.49	0.46
18:p:394:VAL:HG23	18:p:395:ILE:HG12	1.98	0.46
18:p:565:GLU:O	18:p:568:THR:OG1	2.34	0.46
8:d:489:LEU:HD22	8:d:503:ILE:HG23	1.97	0.46
10:f:29:LYS:NZ	19:q:207:GLY:O	2.49	0.46
11:g:283:THR:HG1	11:g:286:THR:HG1	1.64	0.46
15:k:286:THR:HB	15:k:290:ILE:HD12	1.97	0.46
8:d:257:TRP:NE1	8:d:308:SER:OG	2.49	0.46
8:d:273:SER:OG	8:d:275:GLU:OE1	2.34	0.46
10:f:156:GLU:OE2	10:f:455:TYR:OH	2.34	0.46
11:g:723:ASP:N	11:g:723:ASP:OD1	2.48	0.46
13:i:256:LYS:HA	13:i:464:VAL:HG13	1.97	0.46
11:g:194:LYS:NZ	11:g:225:TYR:OH	2.48	0.45
19:q:279:ASP:OD1	19:q:283:LYS:N	2.47	0.45
5:a:1964:HIS:O	5:a:1968:THR:OG1	2.30	0.45
8:d:577:ARG:NH1	8:d:584:VAL:O	2.49	0.45
12:h:419:LEU:HD11	12:h:459:ILE:HG13	1.98	0.45
8:d:837:PHE:O	8:d:959:LYS:N	2.49	0.45
18:p:207:PRO:O	18:p:210:SER:OG	2.28	0.45
10:f:78:LYS:NZ	19:q:204:ASP:OD2	2.37	0.45
12:h:677:THR:HG23	12:h:678:LEU:HG	1.98	0.45
18:p:100:GLU:N	18:p:100:GLU:OE1	2.49	0.45
2:B:91:ASP:N	2:B:91:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:b:512:SER:O	6:b:515:SER:OG	2.28	0.45
7:c:417:LEU:O	7:c:421:HIS:ND1	2.49	0.45
15:k:482:THR:OG1	15:k:493:VAL:O	2.30	0.45
8:d:305:LEU:O	8:d:308:SER:OG	2.35	0.45
15:k:153:TYR:N	15:k:163:MET:O	2.44	0.45
19:q:159:VAL:HB	19:q:163:ILE:HB	1.99	0.45
6:b:22:ALA:HB1	6:b:45:LEU:HD11	1.99	0.45
9:e:394:LEU:O	9:e:398:ALA:HB3	2.16	0.45
18:p:295:GLU:HG2	18:p:298:VAL:HG12	1.97	0.45
6:b:43:ARG:HH22	6:b:180:VAL:HG21	1.81	0.45
11:g:877:MET:SD	11:g:877:MET:N	2.90	0.45
12:h:791:ILE:HG23	12:h:841:ASP:HB2	1.99	0.45
18:p:295:GLU:N	18:p:295:GLU:OE1	2.50	0.45
18:p:52:LEU:HD23	18:p:55:LEU:HD12	1.99	0.44
18:p:499:MET:HE1	18:p:536:VAL:HA	1.99	0.44
2:B:67:ILE:HG22	2:B:95:ILE:HD13	1.99	0.44
5:a:984:VAL:HG22	5:a:987:ARG:HH12	1.82	0.44
6:b:1093:GLN:N	12:h:926:ASP:OD2	2.50	0.44
18:p:297:GLU:OE1	18:p:297:GLU:N	2.47	0.44
18:p:299:ARG:O	18:p:303:SER:OG	2.32	0.44
6:b:702:GLU:OE1	6:b:702:GLU:N	2.50	0.44
9:e:119:GLU:OE1	9:e:119:GLU:N	2.50	0.44
12:h:348:ASP:OD2	12:h:359:ARG:NH1	2.45	0.44
6:b:147:LEU:HD21	6:b:192:LEU:HD11	2.00	0.44
7:c:60:THR:O	7:c:63:THR:OG1	2.32	0.44
12:h:965:GLU:OE2	12:h:981:ARG:NH2	2.46	0.44
18:p:180:MET:SD	18:p:180:MET:N	2.90	0.44
5:a:1171:VAL:HG11	5:a:1219:LEU:HD21	2.00	0.44
11:g:890:THR:OG1	11:g:891:GLN:N	2.50	0.44
13:i:23:THR:HG23	13:i:96:VAL:HA	2.00	0.44
5:a:1864:MET:HA	5:a:1864:MET:HE2	2.00	0.44
8:d:48:SER:OG	8:d:83:GLU:OE1	2.34	0.44
9:e:685:LEU:HD21	9:e:808:ALA:HB2	1.99	0.44
12:h:778:VAL:HG13	12:h:791:ILE:HB	2.00	0.44
19:q:65:LEU:HD22	19:q:96:THR:HG23	1.99	0.44
12:h:782:ASN:ND2	12:h:791:ILE:O	2.49	0.44
5:a:1236:LEU:HD21	5:a:1261:LEU:HD22	1.99	0.43
8:d:576:LEU:HB3	8:d:584:VAL:HG21	1.99	0.43
8:d:839:SER:N	8:d:959:LYS:O	2.51	0.43
18:p:453:ASP:OD1	18:p:454:HIS:N	2.51	0.43
7:c:48:LEU:HD21	7:c:129:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:d:727:LEU:HD11	8:d:758:VAL:HG22	2.00	0.43
12:h:260:TYR:O	12:h:264:GLY:N	2.49	0.43
13:i:352:GLN:HA	13:i:355:VAL:HG22	1.99	0.43
5:a:1294:HIS:NE2	5:a:1300:GLY:O	2.47	0.43
18:p:63:ASP:OD1	18:p:63:ASP:N	2.50	0.43
18:p:350:MET:O	18:p:353:SER:OG	2.36	0.43
8:d:134:LEU:HB3	8:d:173:LEU:HD11	2.00	0.43
8:d:507:LEU:HB3	8:d:550:LEU:HB2	2.01	0.43
18:p:72:GLN:O	18:p:75:THR:OG1	2.34	0.43
5:a:1627:PRO:HG3	6:b:772:MET:HG2	2.00	0.43
18:p:109:VAL:HA	18:p:112:LEU:HD12	2.00	0.43
6:b:450:GLN:HA	6:b:453:VAL:HG22	2.00	0.43
5:a:1841:ARG:O	5:a:1844:THR:OG1	2.35	0.43
6:b:1050:GLU:OE1	6:b:1050:GLU:N	2.51	0.43
7:c:69:ARG:HD3	11:g:98:LEU:HD11	2.00	0.43
8:d:246:GLU:OE1	8:d:246:GLU:N	2.52	0.43
8:d:856:ASP:OD2	8:d:859:ASN:ND2	2.52	0.43
7:c:294:SER:OG	7:c:295:ARG:N	2.52	0.43
9:e:165:ARG:HG2	9:e:179:LEU:HD13	2.00	0.43
13:i:476:THR:HA	13:i:489:MET:HE1	2.01	0.43
11:g:839:SER:OG	11:g:840:LYS:N	2.52	0.43
8:d:442:ILE:O	8:d:475:ASN:ND2	2.45	0.42
18:p:84:GLU:O	18:p:87:HIS:NE2	2.51	0.42
18:p:133:LYS:HD3	18:p:169:TYR:CZ	2.54	0.42
18:p:414:ASP:OD1	18:p:415:ALA:N	2.51	0.42
6:b:881:LEU:HD21	6:b:938:ALA:HB1	2.01	0.42
15:k:62:ASP:OD1	15:k:62:ASP:N	2.51	0.42
18:p:82:GLY:O	18:p:86:VAL:HG23	2.19	0.42
19:q:56:GLY:N	19:q:261:SER:OG	2.46	0.42
6:b:304:GLY:HA3	11:g:605:THR:HG23	2.00	0.42
9:e:197:LEU:O	9:e:201:ILE:N	2.52	0.42
11:g:463:LEU:HD11	11:g:500:ALA:HA	2.00	0.42
12:h:623:HIS:HD2	12:h:666:PHE:HE1	1.68	0.42
13:i:126:THR:O	13:i:129:THR:OG1	2.29	0.42
13:i:281:PHE:CD1	13:i:421:ILE:HG21	2.54	0.42
5:a:2059:THR:OG1	5:a:2061:GLU:OE1	2.37	0.42
6:b:772:MET:HE1	6:b:808:ARG:HG2	2.01	0.42
7:c:123:LEU:HA	7:c:126:ILE:HD12	2.02	0.42
7:c:255:VAL:HA	7:c:258:LEU:HD12	2.01	0.42
2:B:97:GLU:OE1	2:B:98:PHE:N	2.52	0.42
11:g:149:SER:OG	11:g:150:HIS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:g:920:THR:OG1	11:g:921:GLY:N	2.52	0.42
18:p:418:ARG:NH2	19:q:67:GLU:OE1	2.52	0.42
5:a:1098:THR:HB	6:b:172:VAL:HG23	2.02	0.42
5:a:1728:GLN:OE1	5:a:1728:GLN:N	2.52	0.42
5:a:2100:ARG:HE	5:a:2139:THR:HG21	1.84	0.42
11:g:804:ILE:HD12	11:g:835:VAL:HG12	2.01	0.42
13:i:135:LEU:HB3	13:i:332:VAL:HG21	2.01	0.42
19:q:239:ARG:NH2	19:q:241:HIS:HB3	2.35	0.42
6:b:596:ILE:HD12	6:b:650:LEU:HD12	2.01	0.42
7:c:97:ILE:HG21	7:c:148:LEU:HD22	2.01	0.42
11:g:520:VAL:HG12	11:g:522:ASN:H	1.85	0.42
5:a:1057:GLU:OE2	5:a:1059:ASP:N	2.53	0.42
8:d:453:LEU:HB3	8:d:488:GLU:HG2	2.01	0.42
8:d:740:THR:HG23	8:d:741:THR:HG23	2.01	0.42
11:g:904:ILE:HB	11:g:926:ILE:HG13	2.02	0.42
6:b:218:VAL:O	6:b:221:SER:OG	2.34	0.42
11:g:793:ARG:HH21	11:g:799:LEU:HD11	1.84	0.42
15:k:7:THR:HB	21:m:675:ARG:HH21	1.85	0.42
8:d:206:ASP:OD1	8:d:207:GLN:N	2.53	0.41
9:e:835:GLU:OE1	9:e:835:GLU:N	2.53	0.41
13:i:47:PRO:O	13:i:51:ASN:ND2	2.53	0.41
6:b:878:LEU:HB3	6:b:1000:LEU:HD22	2.02	0.41
8:d:458:ASP:OD1	8:d:459:SER:N	2.52	0.41
8:d:816:GLN:OE1	8:d:817:ILE:N	2.53	0.41
9:e:219:HIS:HB2	9:e:223:PHE:HE2	1.84	0.41
12:h:929:TYR:CD1	12:h:941:LEU:HD21	2.55	0.41
8:d:792:PRO:HA	8:d:795:VAL:HG12	2.02	0.41
18:p:276:PRO:O	18:p:279:THR:OG1	2.37	0.41
8:d:69:VAL:HG13	8:d:99:LEU:HD22	2.02	0.41
8:d:851:LEU:O	8:d:890:HIS:N	2.50	0.41
11:g:226:PRO:O	11:g:265:ARG:NH1	2.51	0.41
15:k:544:GLN:N	15:k:544:GLN:OE1	2.54	0.41
7:c:53:GLU:HA	7:c:56:MET:HG2	2.01	0.41
19:q:119:GLU:N	19:q:119:GLU:OE1	2.53	0.41
6:b:55:CYS:SG	6:b:56:ALA:N	2.91	0.41
6:b:857:PRO:O	6:b:860:VAL:HG12	2.21	0.41
9:e:489:LEU:HD22	9:e:531:GLU:HB3	2.03	0.41
11:g:819:ILE:O	11:g:929:LYS:N	2.51	0.41
8:d:795:VAL:HA	8:d:798:ILE:HG22	2.02	0.41
11:g:139:ALA:O	11:g:143:ILE:HG12	2.20	0.41
13:i:474:GLN:OE1	13:i:474:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:c:354:CYS:SG	7:c:355:GLY:N	2.93	0.41
12:h:392:ASP:OD1	12:h:397:ARG:NH2	2.53	0.41
12:h:618:LEU:O	12:h:622:THR:HG23	2.21	0.41
15:k:235:VAL:HG11	15:k:349:ILE:HD12	2.03	0.41
18:p:46:ARG:NH1	18:p:50:GLU:OE2	2.54	0.41
18:p:102:THR:HG22	18:p:105:ARG:HH22	1.86	0.41
19:q:52:VAL:HA	19:q:79:ASN:HB2	2.03	0.41
9:e:492:GLU:OE1	9:e:492:GLU:N	2.54	0.41
10:f:160:GLU:OE1	10:f:303:SER:OG	2.26	0.41
11:g:289:ARG:NE	11:g:327:TYR:O	2.53	0.41
15:k:57:LEU:HD12	15:k:86:TYR:HB2	2.03	0.41
20:r:47:GLN:O	20:r:52:GLN:NE2	2.54	0.41
5:a:1903:ASN:O	5:a:1906:SER:OG	2.25	0.40
8:d:388:TYR:HA	8:d:391:ARG:HE	1.86	0.40
5:a:1643:SER:OG	5:a:1644:ARG:N	2.54	0.40
8:d:652:GLU:OE1	8:d:652:GLU:N	2.53	0.40
12:h:854:HIS:CE1	12:h:995:PHE:HA	2.57	0.40
18:p:434:LEU:HD21	18:p:438:PHE:HD2	1.86	0.40
21:m:656:LEU:HD23	21:m:656:LEU:HA	1.87	0.40
8:d:148:GLN:O	8:d:152:VAL:HG13	2.21	0.40
12:h:250:CYS:SG	12:h:251:GLN:N	2.94	0.40
5:a:1098:THR:OG1	6:b:131:GLU:OE2	2.38	0.40
5:a:1178:PRO:HA	5:a:1179:PRO:HD3	2.00	0.40
6:b:713:LEU:HD13	6:b:713:LEU:HA	1.90	0.40
12:h:906:GLU:OE1	12:h:906:GLU:N	2.55	0.40
18:p:319:GLU:OE1	18:p:319:GLU:N	2.54	0.40
18:p:333:LEU:HD23	18:p:345:LEU:HD22	2.03	0.40
18:p:381:ARG:HD2	18:p:411:LEU:HD11	2.03	0.40
6:b:282:THR:O	6:b:286:THR:HG23	2.22	0.40
15:k:284:PRO:HA	15:k:291:ARG:HD3	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	
2	B	105/213 (49%)	100 (95%)	5 (5%)	0	100	100
3	C	37/106 (35%)	37 (100%)	0	0	100	100
4	Y	11/13 (85%)	11 (100%)	0	0	100	100
5	a	1061/2192 (48%)	1031 (97%)	29 (3%)	1 (0%)	48	78
6	b	1033/1204 (86%)	981 (95%)	52 (5%)	0	100	100
7	c	461/1042 (44%)	447 (97%)	14 (3%)	0	100	100
8	d	806/963 (84%)	787 (98%)	19 (2%)	0	100	100
9	e	833/1021 (82%)	800 (96%)	33 (4%)	0	100	100
10	f	530/889 (60%)	512 (97%)	18 (3%)	0	100	100
11	g	876/964 (91%)	848 (97%)	27 (3%)	1 (0%)	48	78
12	h	865/995 (87%)	837 (97%)	28 (3%)	0	100	100
13	i	618/658 (94%)	595 (96%)	23 (4%)	0	100	100
14	j	660/710 (93%)	643 (97%)	17 (3%)	0	100	100
15	k	539/602 (90%)	513 (95%)	25 (5%)	1 (0%)	43	72
16	n	202/518 (39%)	197 (98%)	5 (2%)	0	100	100
17	o	361/451 (80%)	343 (95%)	17 (5%)	1 (0%)	36	65
18	p	578/591 (98%)	561 (97%)	17 (3%)	0	100	100
19	q	288/311 (93%)	275 (96%)	13 (4%)	0	100	100
20	r	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
21	m	33/706 (5%)	30 (91%)	3 (9%)	0	100	100
All	All	9922/14176 (70%)	9572 (96%)	346 (4%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	a	1630	VAL
11	g	885	ASN
15	k	305	ILE
17	o	318	LEU

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	
2	B	87/181 (48%)	87 (100%)	0	100	100
3	C	28/87 (32%)	28 (100%)	0	100	100
4	Y	13/13 (100%)	13 (100%)	0	100	100
5	a	946/1909 (50%)	944 (100%)	2 (0%)	87	86
6	b	869/1072 (81%)	866 (100%)	3 (0%)	86	83
7	c	414/927 (45%)	413 (100%)	1 (0%)	87	86
8	d	702/845 (83%)	701 (100%)	1 (0%)	88	88
9	e	616/814 (76%)	615 (100%)	1 (0%)	87	86
10	f	438/798 (55%)	437 (100%)	1 (0%)	87	86
11	g	723/842 (86%)	721 (100%)	2 (0%)	86	83
12	h	700/896 (78%)	698 (100%)	2 (0%)	86	83
13	i	554/600 (92%)	553 (100%)	1 (0%)	87	86
15	k	403/522 (77%)	400 (99%)	3 (1%)	76	77
18	p	485/514 (94%)	484 (100%)	1 (0%)	87	86
19	q	251/276 (91%)	251 (100%)	0	100	100
20	r	27/27 (100%)	27 (100%)	0	100	100
21	m	30/639 (5%)	30 (100%)	0	100	100
All	All	7286/10962 (66%)	7268 (100%)	18 (0%)	85	86

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	a	1630	VAL
5	a	1983	ASP
6	b	435	MET
6	b	523	GLN
6	b	1104	LEU
7	c	402	PHE
8	d	493	LEU

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Mol	Chain	Res	Type
9	e	181	MET
10	f	434	MET
11	g	575	LEU
11	g	634	LEU
12	h	250	CYS
12	h	746	GLU
13	i	552	LEU
15	k	178	ASP
15	k	204	SER
15	k	302	PHE
18	p	245	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	ASN
3	C	78	HIS
5	a	1052	GLN
5	a	1187	GLN
5	a	1426	HIS
5	a	1441	GLN
5	a	1512	GLN
5	a	1857	ASN
5	a	1880	HIS
5	a	2112	GLN
6	b	66	GLN
6	b	491	GLN
6	b	837	GLN
6	b	1093	GLN
6	b	1151	GLN
6	b	1152	GLN
7	c	124	ASN
7	c	194	GLN
7	c	451	HIS
8	d	148	GLN
8	d	403	GLN
9	e	76	HIS
9	e	88	HIS
9	e	136	ASN
9	e	154	GLN
9	e	452	HIS
9	e	653	HIS

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Mol	Chain	Res	Type
9	e	690	GLN
9	e	836	HIS
9	e	899	HIS
10	f	551	ASN
11	g	76	ASN
11	g	93	HIS
11	g	145	GLN
11	g	168	GLN
11	g	205	HIS
11	g	673	GLN
11	g	708	GLN
11	g	797	GLN
11	g	837	HIS
11	g	853	ASN
12	h	623	HIS
12	h	695	GLN
12	h	723	GLN
12	h	831	ASN
12	h	868	ASN
12	h	988	GLN
13	i	37	ASN
13	i	142	ASN
13	i	268	GLN
13	i	385	ASN
18	p	230	ASN
18	p	539	ASN
18	p	580	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.

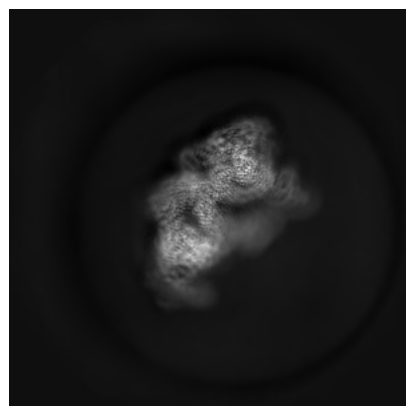
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19040. These allow visual inspection of the internal detail of the map and identification of artifacts.

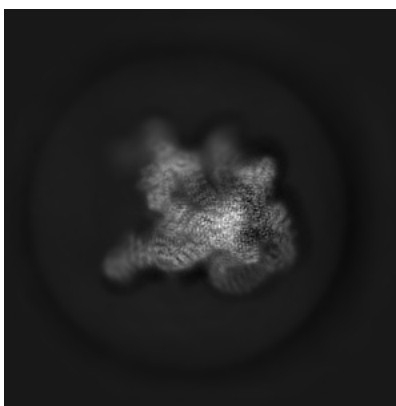
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

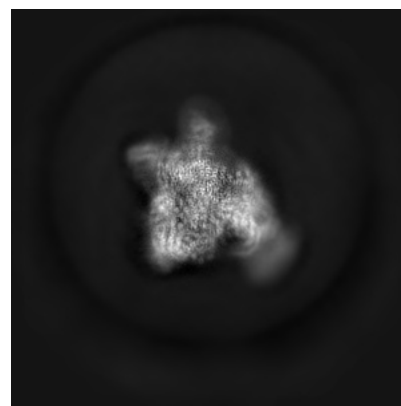
6.1.1 Primary map



X

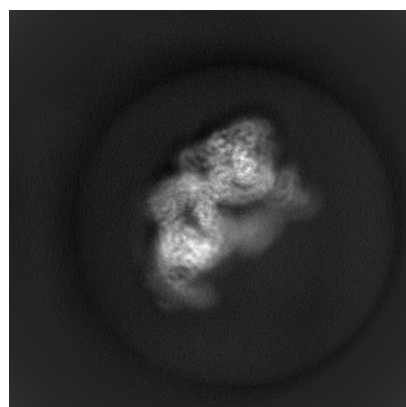


Y

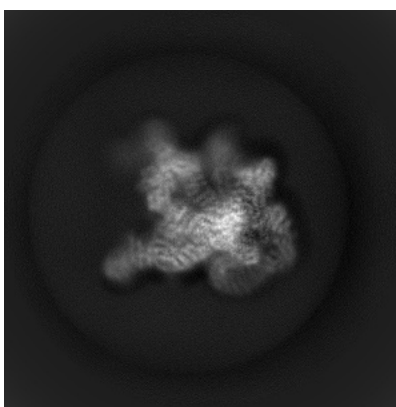


Z

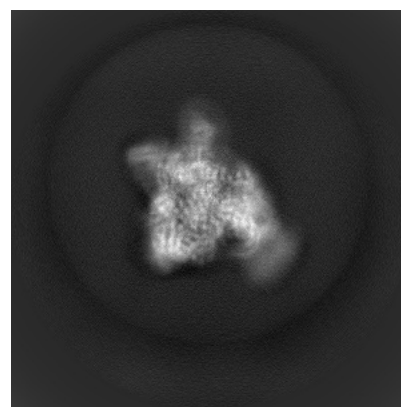
6.1.2 Raw map



X



Y

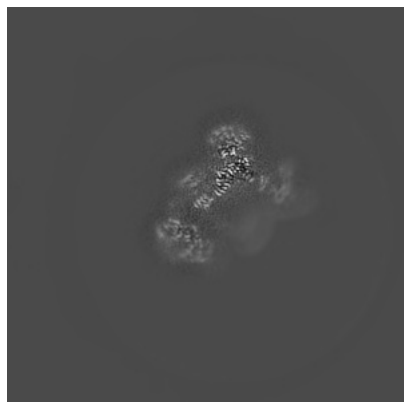


Z

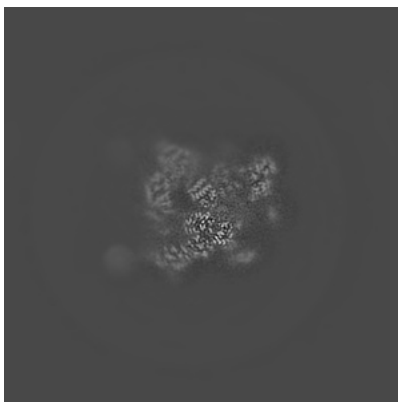
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

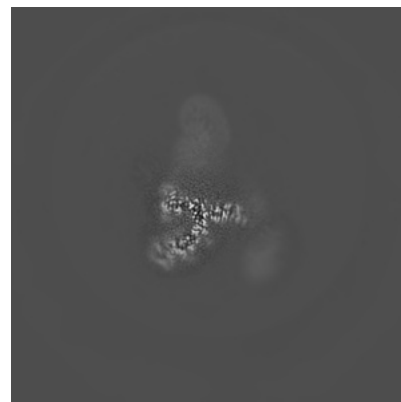
6.2.1 Primary map



X Index: 240

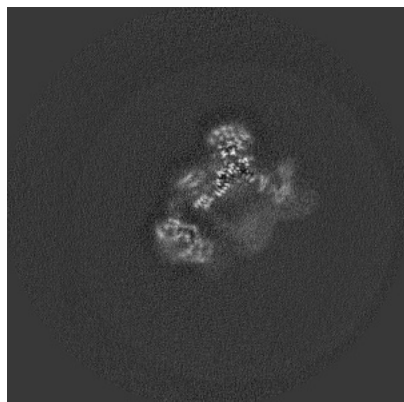


Y Index: 240

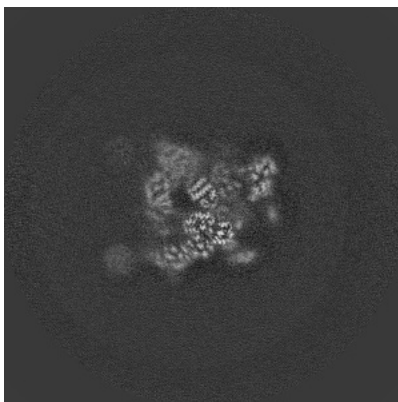


Z Index: 240

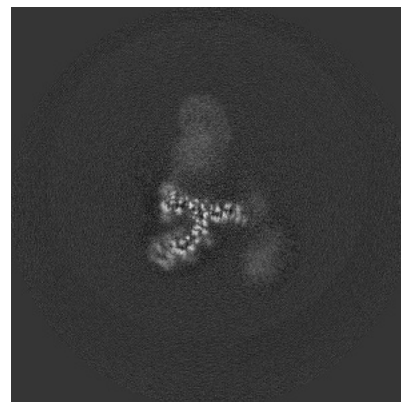
6.2.2 Raw map



X Index: 240



Y Index: 240

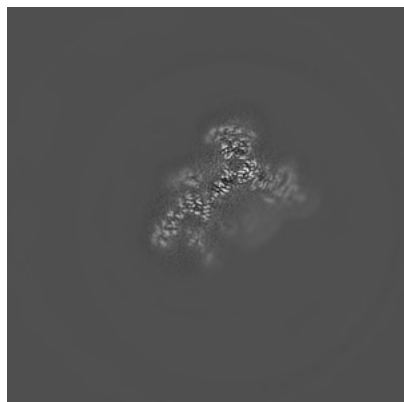


Z Index: 240

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

6.3 Largest variance slices [i](#)

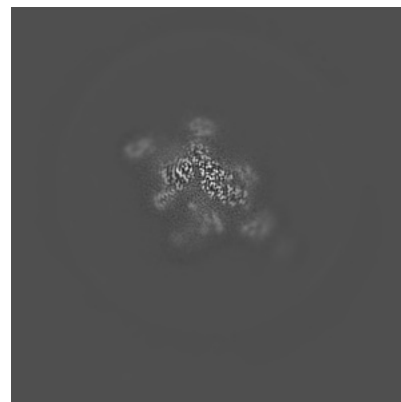
6.3.1 Primary map



X Index: 230

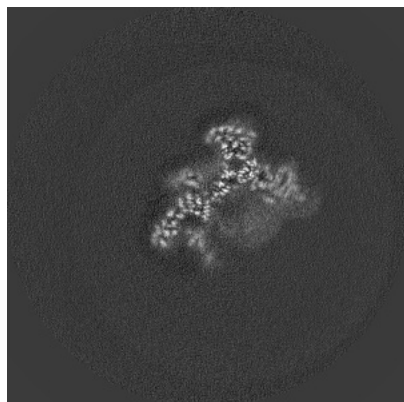


Y Index: 280

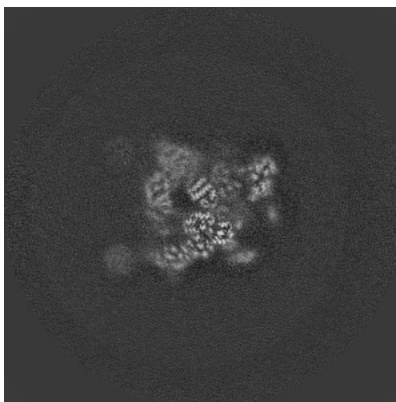


Z Index: 282

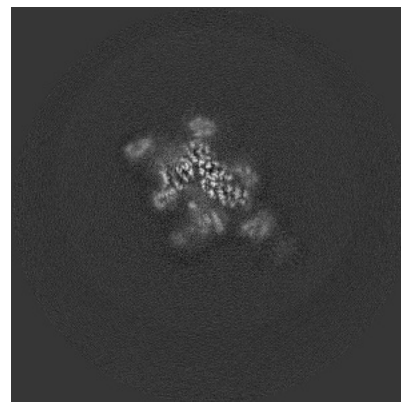
6.3.2 Raw map



X Index: 230



Y Index: 240

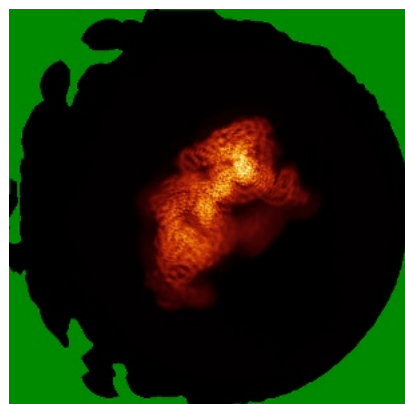


Z Index: 281

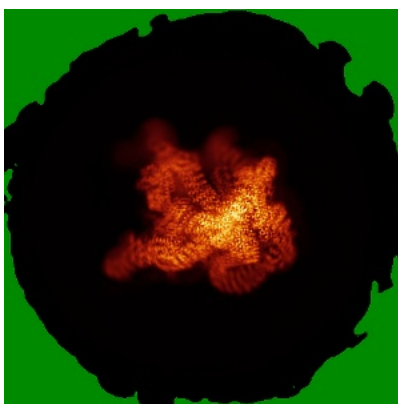
The images above show the largest variance slices of the map in three orthogonal directions.

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

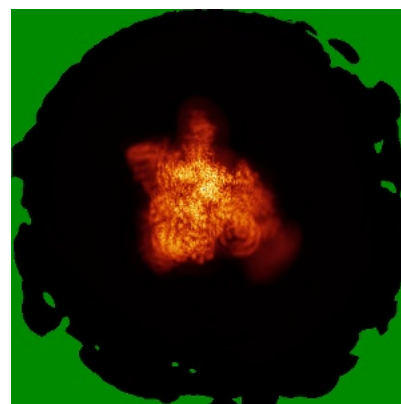
6.4.1 Primary map



X

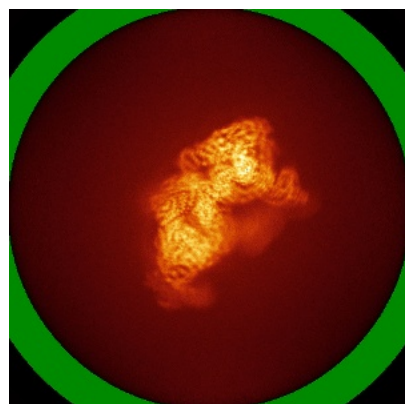


Y

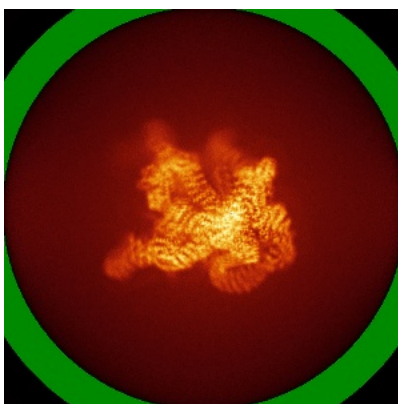


Z

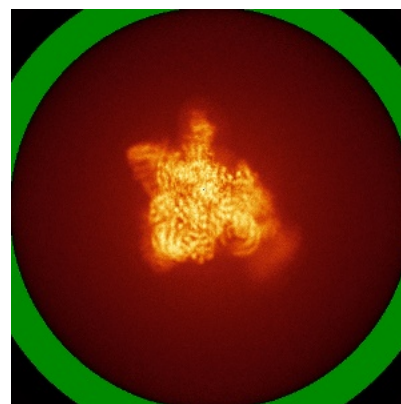
6.4.2 Raw map



X



Y

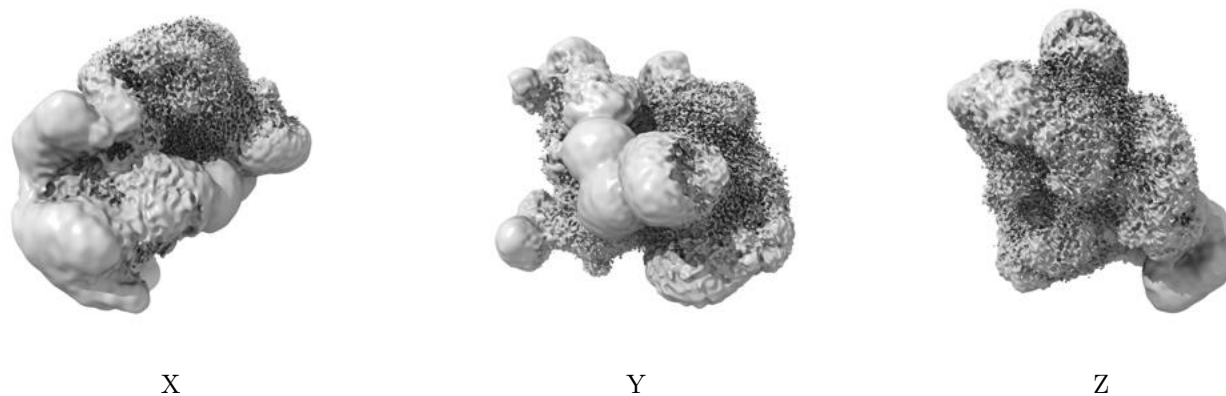


Z

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.

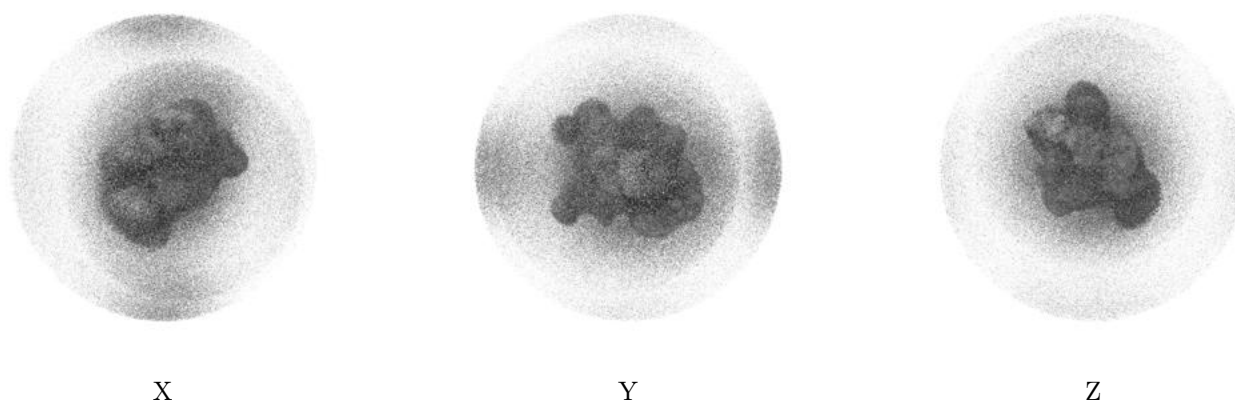
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00308. 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.

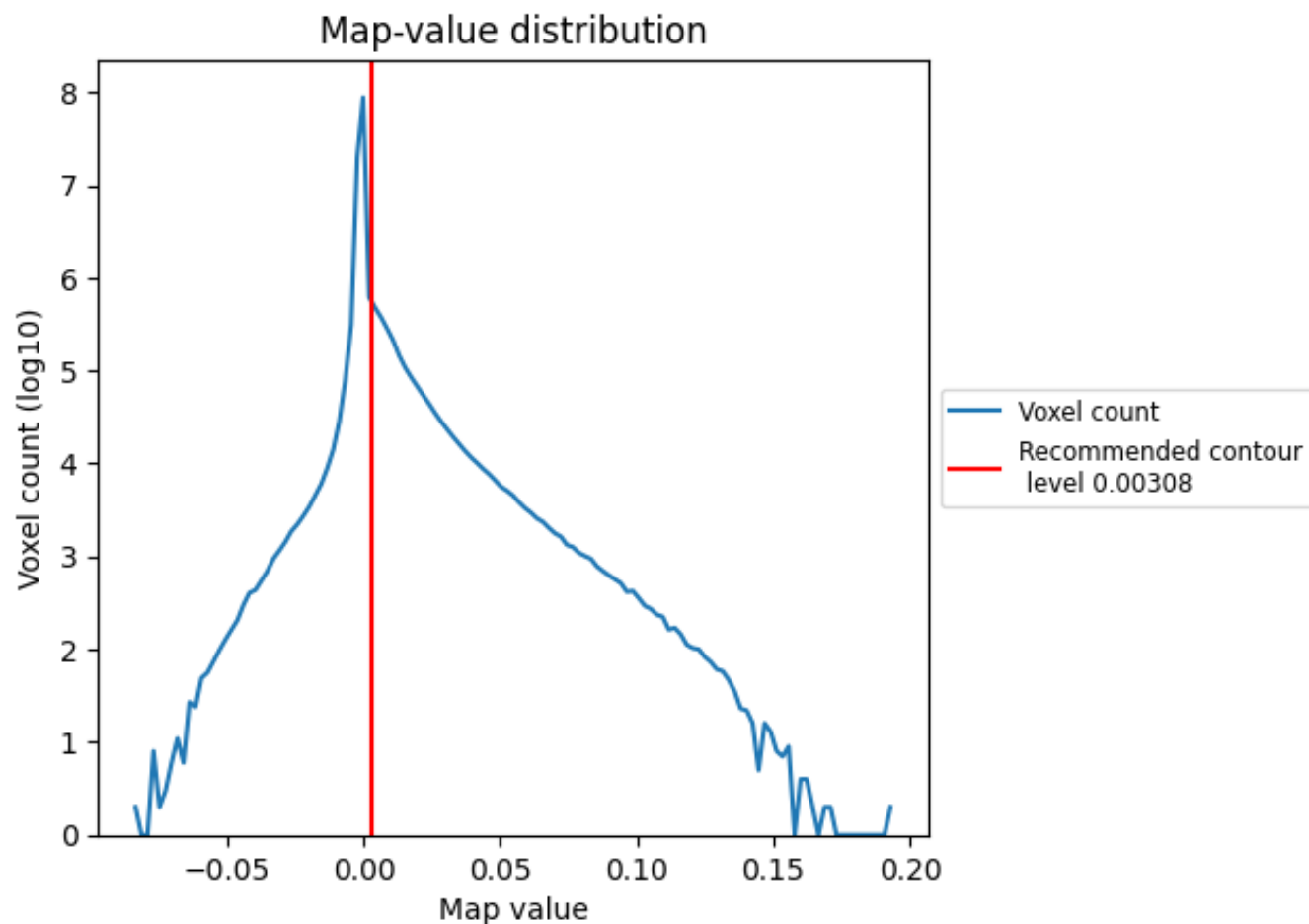
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

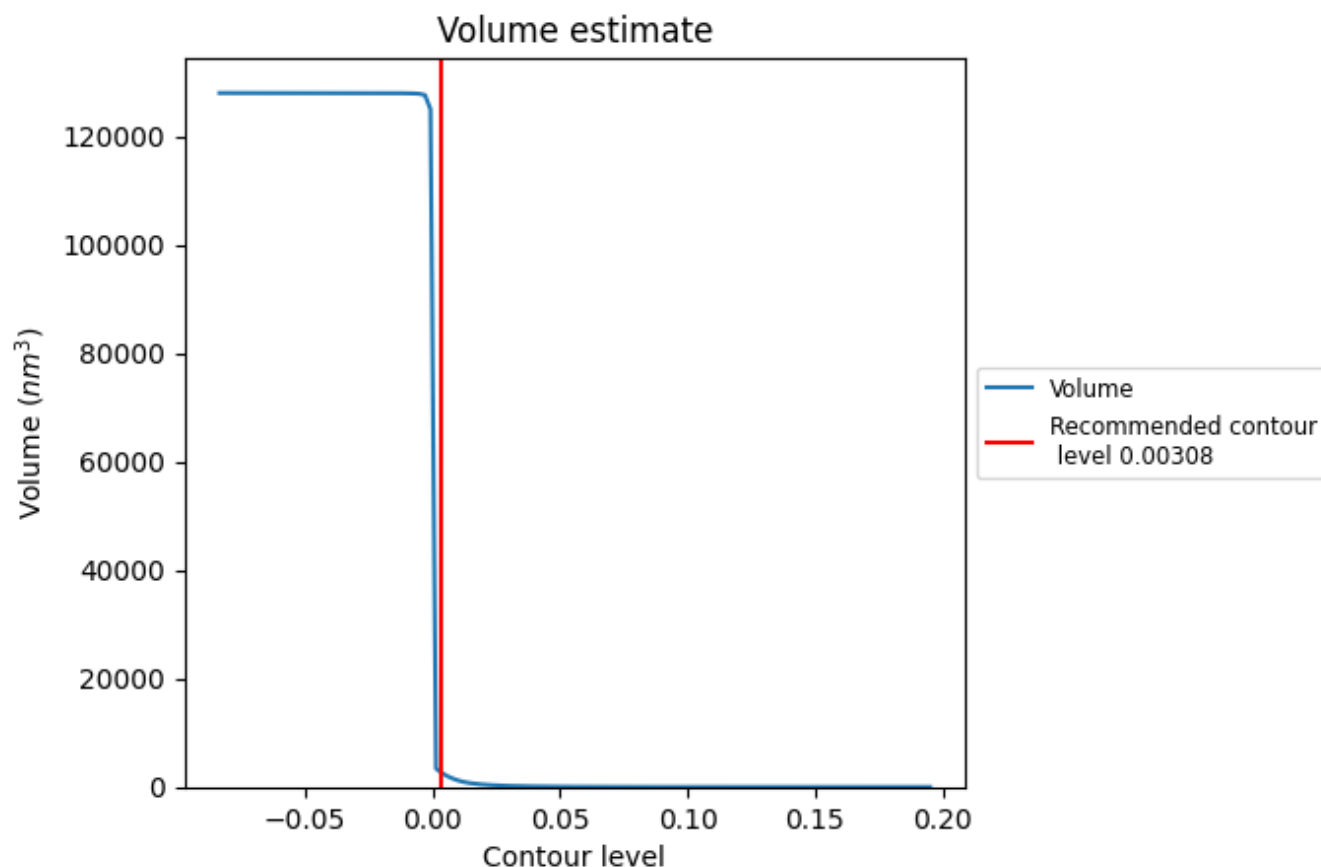
This section contains the results of statistical analysis of the map.

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.

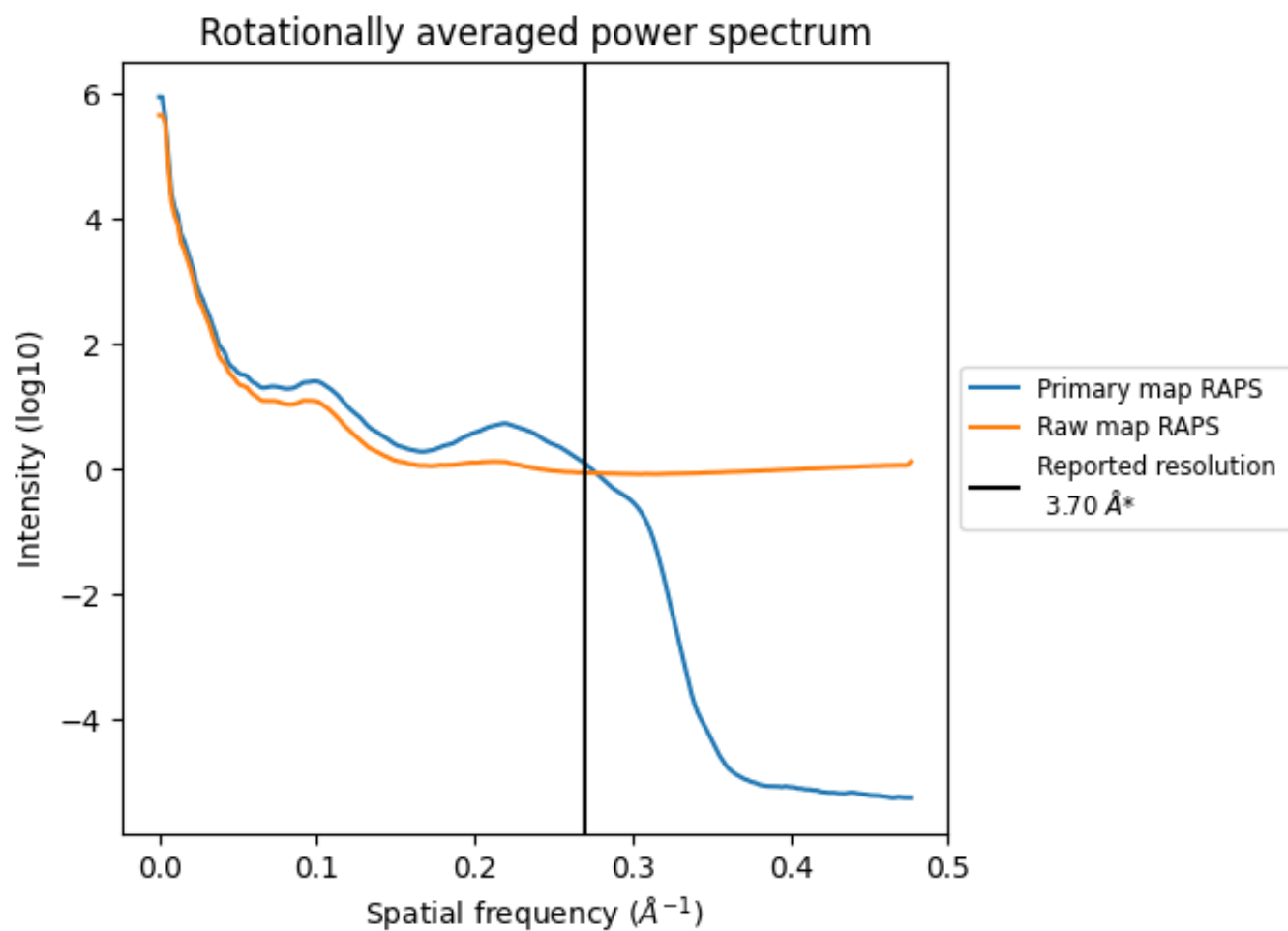
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2799 nm^3 ; this corresponds to an approximate mass of 2528 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 ⓘ

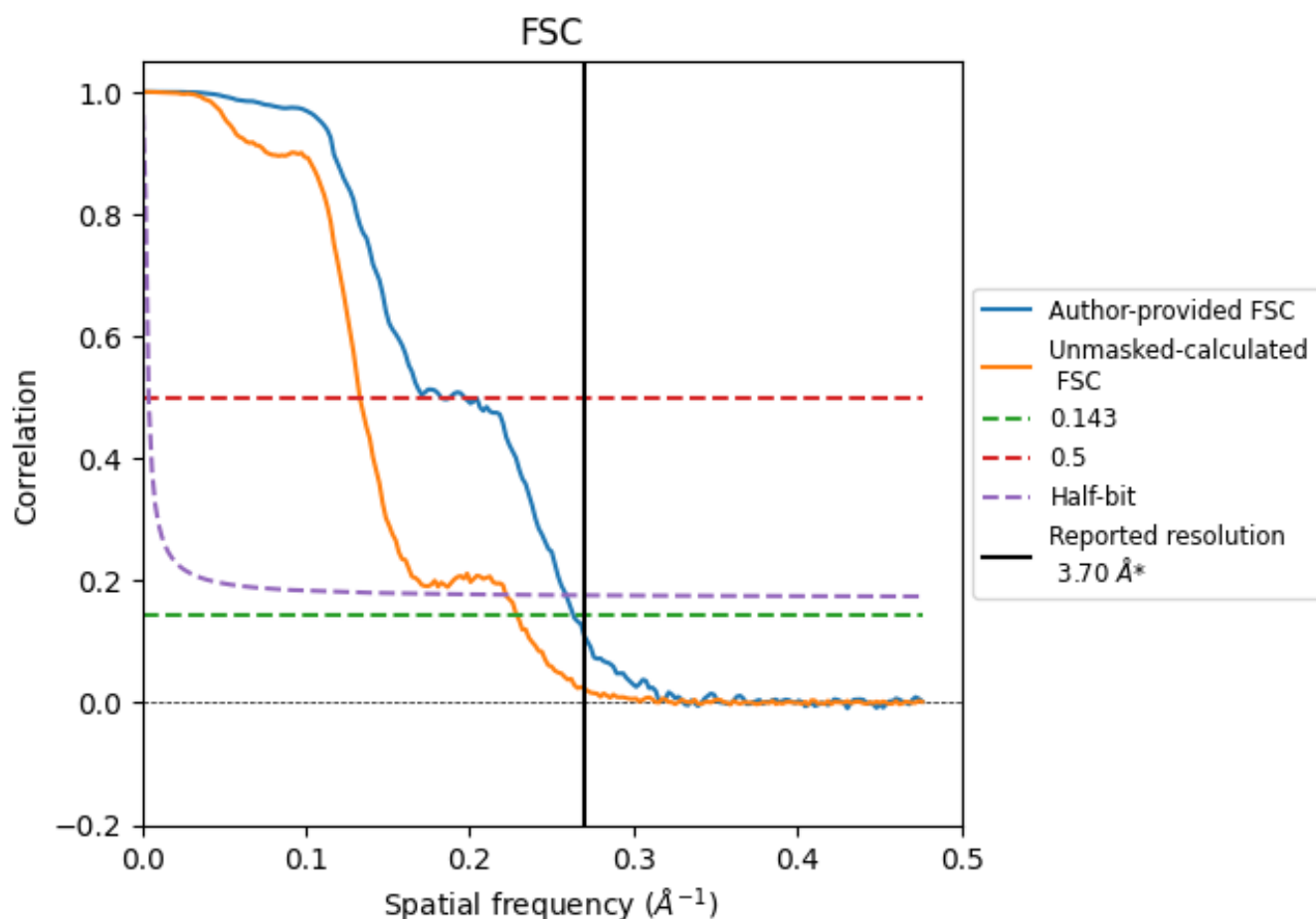


*Reported resolution corresponds to spatial frequency of 0.270 $\text{\AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.80	5.48	3.86
Unmasked-calculated*	4.37	7.53	4.50

*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 4.37 differs from the reported value 3.7 by more than 10 %

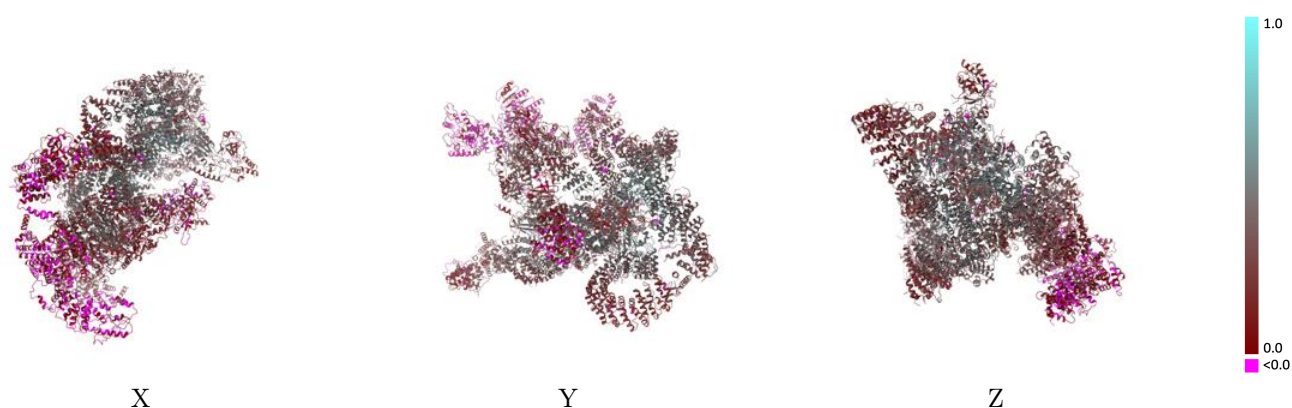
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19040 and PDB model 8RBZ. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)

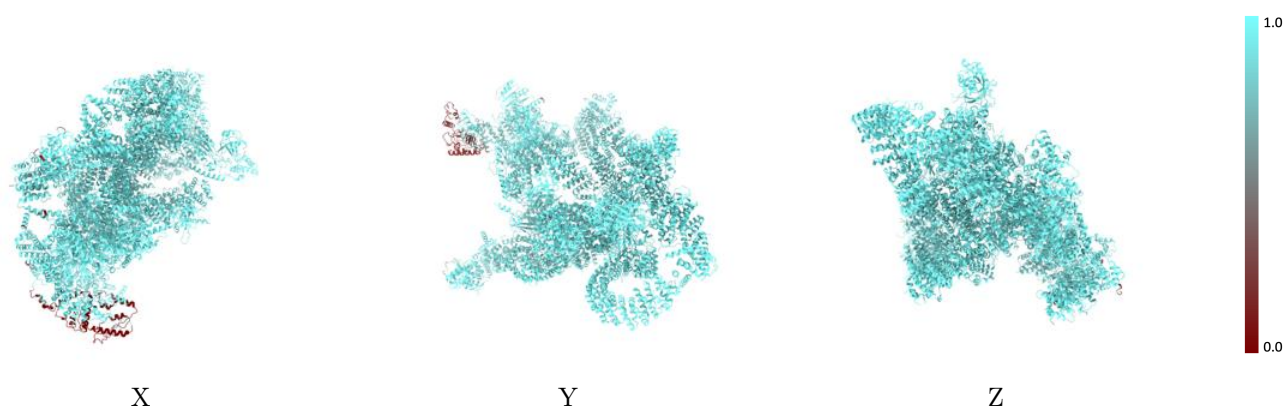
This section was not generated.

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



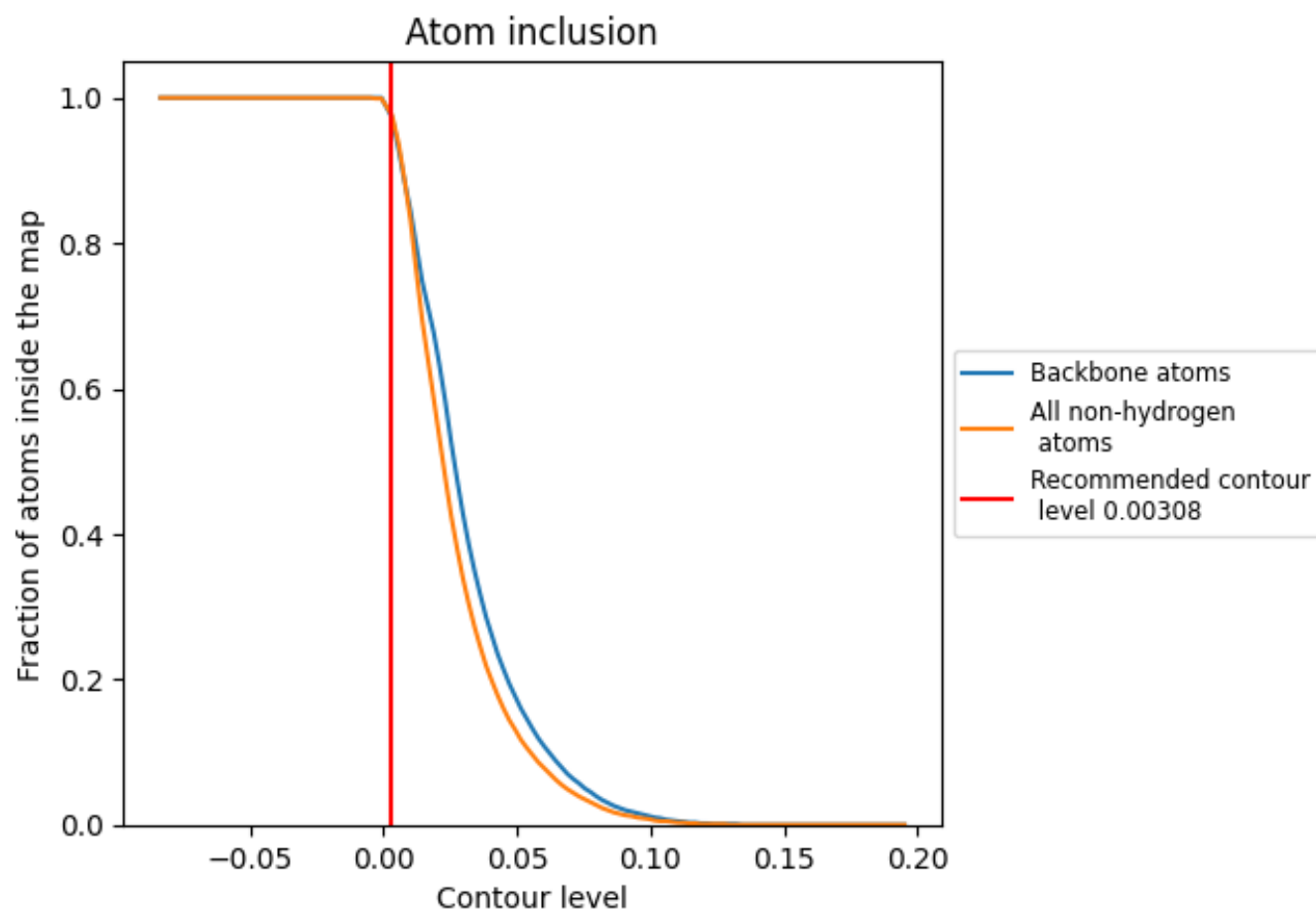
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00308).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.00308) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.2930
1	 1.0000	 0.3650
B	 1.0000	 0.0960
C	 0.9630	 0.0550
Y	 0.9890	 0.5060
a	 0.9830	 0.2600
b	 0.9930	 0.3820
c	 0.9850	 0.1360
d	 0.9970	 0.3340
e	 0.9940	 0.3530
f	 0.9950	 0.3430
g	 0.9930	 0.4080
h	 0.9950	 0.3840
i	 0.9960	 0.2720
j	 0.8400	 0.0330
k	 0.9950	 0.1930
m	 0.9890	 0.0910
n	 0.3880	 0.0150
o	 0.9750	 0.0730
p	 0.9980	 0.2470
q	 0.9940	 0.4750
r	 0.9910	 0.3220

