



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 9J64 / pdb_00009j64
EMDB ID : EMD-61162
Title : Cryo-EM structure of neddylated Cul2-Rbx1-EloBC-FEM1B homodimer
complexed with FNIP1 degron
Authors : Dai, Z.; Liang, L.; Yin, Y.X.
Deposited on : 2024-08-14
Resolution : 4.28 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

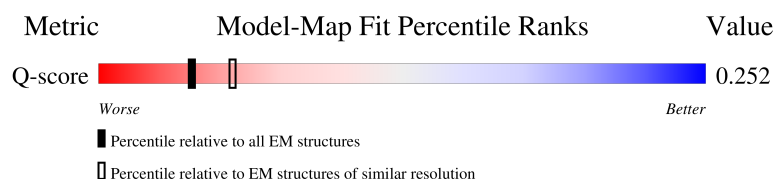
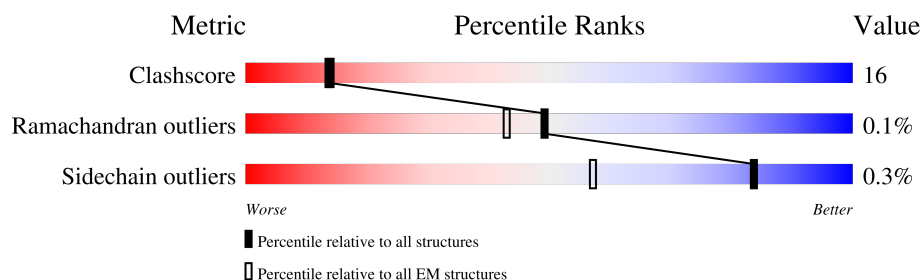
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.28 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	4493 (3.79 - 4.78)

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

Mol	Chain	Length	Quality of chain
1	A	751	
1	D	751	
2	E	108	
2	H	108	

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Mol	Chain	Length	Quality of chain
3	F	98	
4	G	104	
5	I	628	
6	J	467	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16354 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 Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	557	Total	C	N	O	S	0	0
			4558	2897	769	856	36		
1	D	636	Total	C	N	O	S	0	0
			5213	3320	875	979	39		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	746	HIS	-	expression tag	UNP Q13617
A	747	HIS	-	expression tag	UNP Q13617
A	748	HIS	-	expression tag	UNP Q13617
A	749	HIS	-	expression tag	UNP Q13617
A	750	HIS	-	expression tag	UNP Q13617
A	751	HIS	-	expression tag	UNP Q13617
D	746	HIS	-	expression tag	UNP Q13617
D	747	HIS	-	expression tag	UNP Q13617
D	748	HIS	-	expression tag	UNP Q13617
D	749	HIS	-	expression tag	UNP Q13617
D	750	HIS	-	expression tag	UNP Q13617
D	751	HIS	-	expression tag	UNP Q13617

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	72	Total	C	N	O	S	0	0
			601	385	110	97	9		
2	H	70	Total	C	N	O	S	0	0
			589	381	107	93	8		

- Molecule 3 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	90	Total	C	N	O	S	0	0
			714	459	114	135	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	15	MET	-	initiating methionine	UNP Q15369

- Molecule 4 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	86	Total	C	N	O	S	0	0
			685	438	118	125	4		

- Molecule 5 is a protein called Protein fem-1 homolog B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	480	Total	C	N	O	S	1	0
			3822	2391	682	723	26		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	0	GLY	-	expression tag	UNP Q9UK73

- Molecule 6 is a protein called Maltose/maltodextrin-binding periplasmic protein,Folliculin interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	20	Total	C	N	O	S	0	0
			165	101	29	32	3		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	175	MET	-	initiating methionine	UNP P0AEX9
J	176	GLY	-	expression tag	UNP P0AEX9
J	177	HIS	-	expression tag	UNP P0AEX9
J	178	HIS	-	expression tag	UNP P0AEX9
J	179	HIS	-	expression tag	UNP P0AEX9
J	180	HIS	-	expression tag	UNP P0AEX9
J	181	HIS	-	expression tag	UNP P0AEX9

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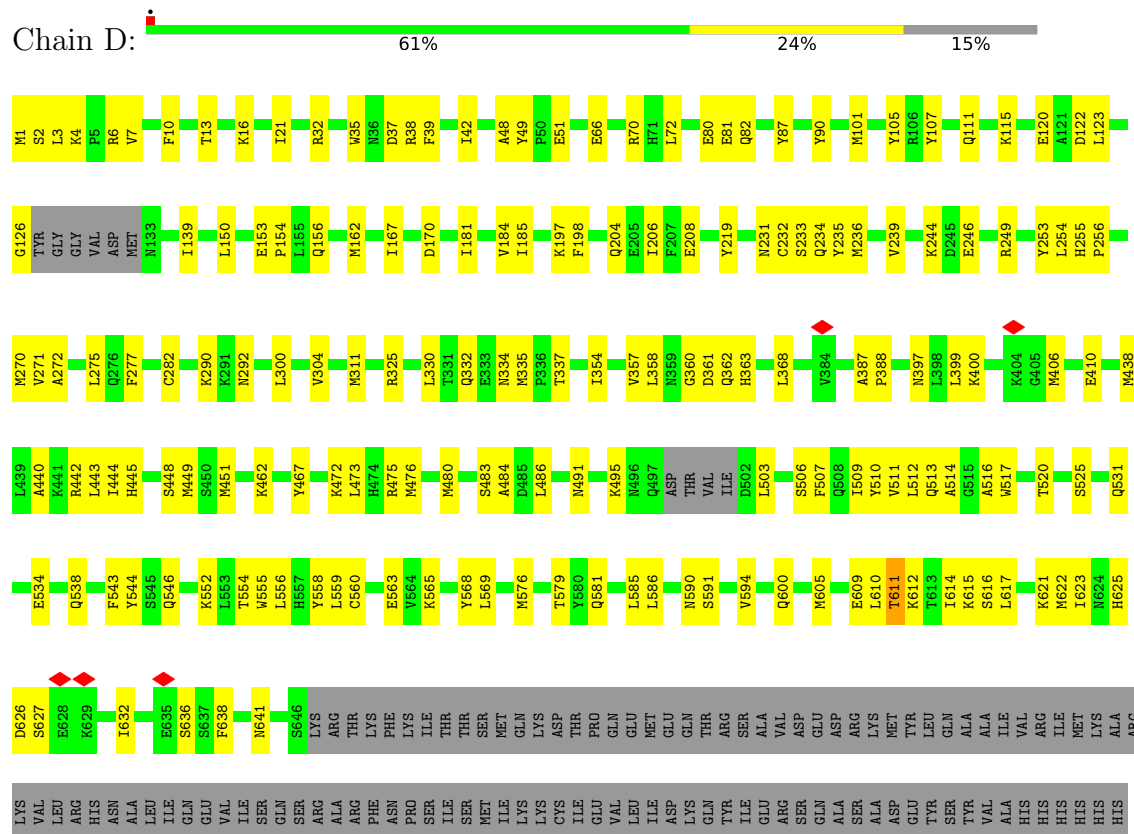
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Chain	Residue	Modelled	Actual	Comment	Reference
J	182	HIS	-	expression tag	UNP P0AEX9
J	549	ASP	-	linker	UNP P0AEX9
J	550	TYR	-	linker	UNP P0AEX9
J	551	ASP	-	linker	UNP P0AEX9
J	552	ILE	-	linker	UNP P0AEX9
J	553	PRO	-	linker	UNP P0AEX9
J	554	THR	-	linker	UNP P0AEX9
J	555	THR	-	linker	UNP P0AEX9
J	556	GLU	-	linker	UNP P0AEX9
J	557	ASN	-	linker	UNP P0AEX9
J	558	LEU	-	linker	UNP P0AEX9
J	559	TYR	-	linker	UNP P0AEX9
J	560	PHE	-	linker	UNP P0AEX9
J	561	GLN	-	linker	UNP P0AEX9
J	562	GLY	-	linker	UNP P0AEX9

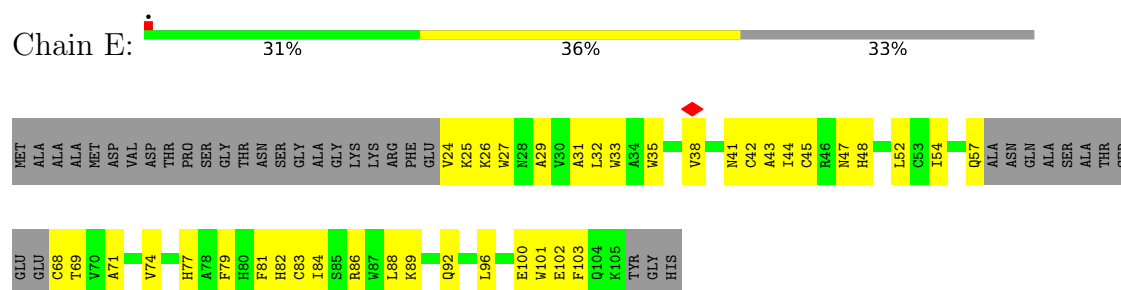
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	E	3	Total 3	Zn 3	0
7	H	3	Total 3	Zn 3	0
7	I	1	Total 1	Zn 1	0

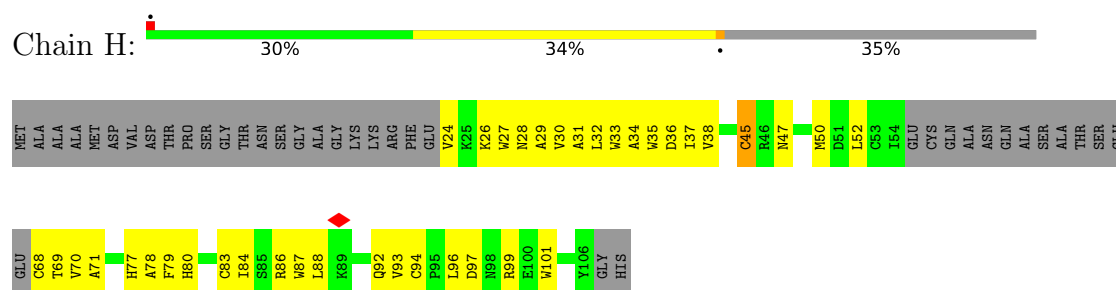
- Molecule 1: Cullin-2



- Molecule 2: E3 ubiquitin-protein ligase RBX1



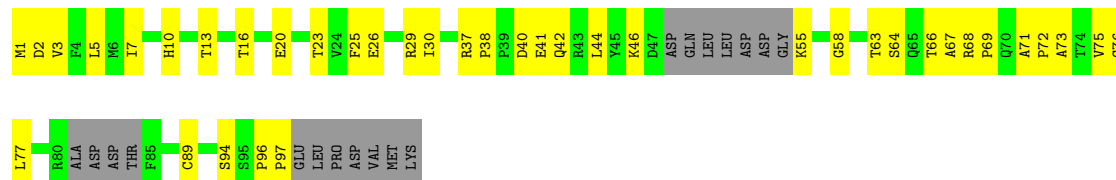
- Molecule 2: E3 ubiquitin-protein ligase RBX1



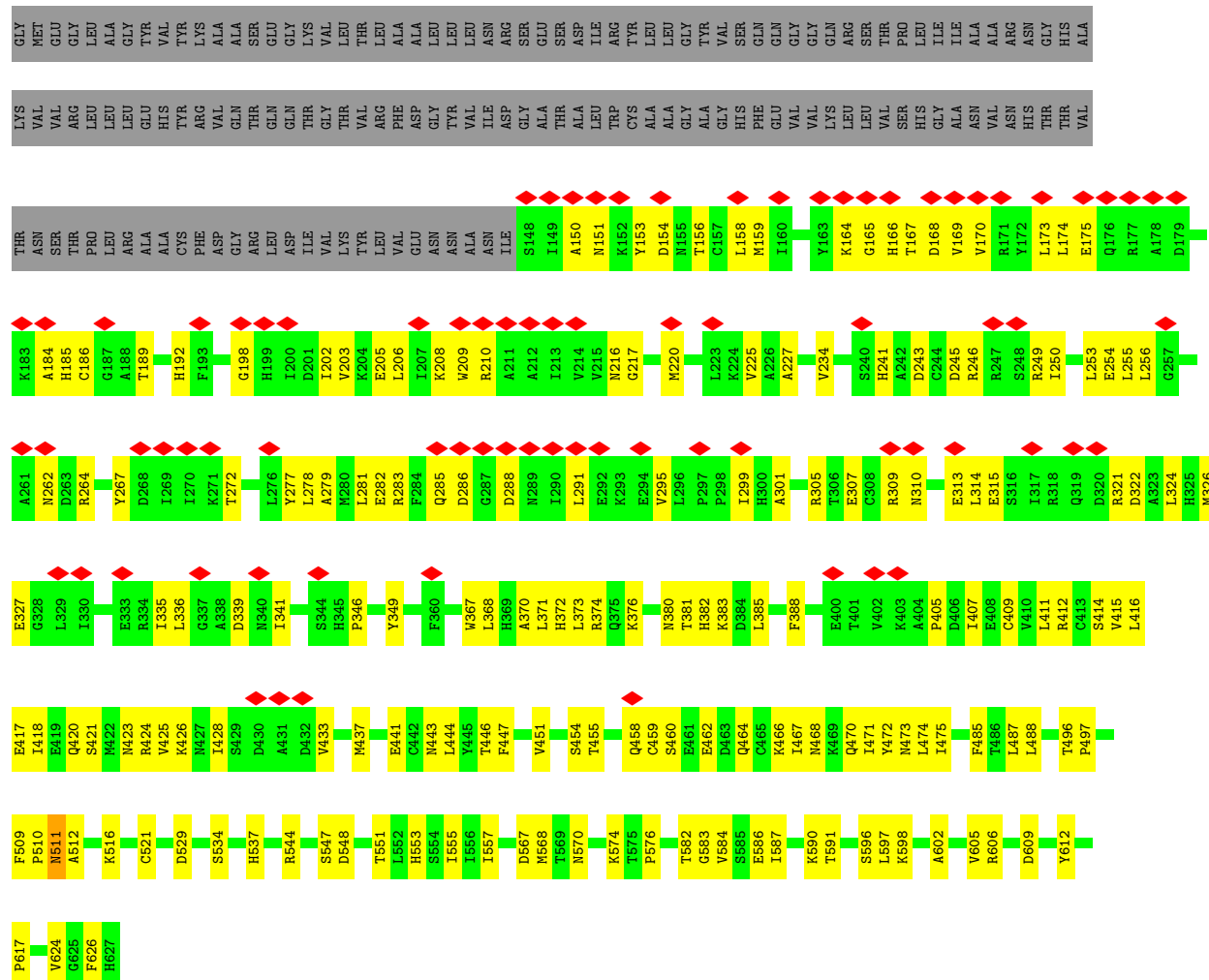
- Molecule 3: Elongin-C



- Molecule 4: Elongin-B



- Molecule 5: Protein fem-1 homolog B



- Chain J: 96%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110858	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48.69	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.514	Depositor
Minimum map value	-0.825	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	A	0.22	0/4649	0.40	0/6257
1	D	0.29	0/5320	0.54	1/7170 (0.0%)
2	E	0.12	0/619	0.30	0/841
2	H	0.21	0/608	0.40	0/827
3	F	0.36	0/729	0.64	0/984
4	G	0.30	0/698	0.50	0/938
5	I	0.17	0/3889	0.36	0/5268
6	J	0.10	0/168	0.26	0/224
All	All	0.24	0/16680	0.45	1/22509 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	520	THR	CB-CA-C	-5.31	110.47	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4558	0	4507	141	0
1	D	5213	0	5160	142	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	601	0	567	41	0
2	H	589	0	560	40	0
3	F	714	0	711	31	0
4	G	685	0	698	26	0
5	I	3822	0	3788	132	0
6	J	165	0	154	6	0
7	E	3	0	0	0	0
7	H	3	0	0	0	0
7	I	1	0	0	0	0
All	All	16354	0	16145	511	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 16.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LYS:HZ2	1:D:292:ASN:H	1.28	0.82
2:E:42:CYS:HB3	2:E:45:CYS:SG	2.19	0.81
4:G:68:ARG:HB2	4:G:71:ALA:H	1.48	0.79
1:A:286:ILE:HD12	1:A:318:HIS:HB2	1.64	0.77
2:E:52:LEU:HB2	2:E:57:GLN:HB2	1.66	0.77
1:D:80:GLU:HG3	1:D:81:GLU:HG3	1.70	0.73
1:D:156:GLN:HG3	1:D:206:ILE:HD11	1.70	0.73
1:D:32:ARG:NH1	3:F:49:PRO:O	2.22	0.72
1:D:486:LEU:HD11	1:D:509:ILE:HG12	1.72	0.72
1:D:170:ASP:O	1:D:249:ARG:NH2	2.22	0.72
2:E:71:ALA:HB2	2:E:81:PHE:HD1	1.55	0.72
1:D:239:VAL:HG22	1:D:270:MET:HE3	1.71	0.71
1:A:240:LEU:HD21	1:A:300:LEU:HD21	1.72	0.71
2:E:88:LEU:HD21	2:E:101:TRP:HB3	1.71	0.71
1:A:70:ARG:HH12	1:A:74:LYS:HG2	1.56	0.71
1:A:606:ASN:HD21	1:A:609:GLU:HG2	1.54	0.71
1:A:302:ARG:HA	1:A:308:LEU:HD21	1.75	0.69
4:G:23:THR:HG1	4:G:55:LYS:N	1.91	0.68
6:J:576:ARG:HH22	6:J:586:SER:HA	1.58	0.68
1:D:272:ALA:HB2	1:D:304:VAL:HG11	1.76	0.67
1:D:473:LEU:HD23	1:D:476:MET:HE3	1.76	0.67
1:A:330:LEU:HD13	1:A:335:MET:HE1	1.76	0.67
3:F:102:GLU:HA	3:F:105:MET:HG3	1.77	0.67
5:I:262:ASN:HB3	5:I:346:PRO:HB3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:TRP:NE1	2:H:93:VAL:O	2.26	0.66
1:A:564:VAL:HA	2:E:25:LYS:HB2	1.77	0.65
5:I:254:GLU:OE2	5:I:283:ARG:NH1	2.26	0.65
1:A:565:LYS:HB2	1:A:574:VAL:HG22	1.78	0.65
1:D:621:LYS:O	1:D:641:ASN:ND2	2.29	0.65
1:D:552:LYS:HB3	2:H:36:ASP:HA	1.78	0.65
1:A:503:LEU:HG	1:A:505:ILE:H	1.62	0.64
2:E:86:ARG:HG2	2:E:89:LYS:HZ1	1.63	0.64
1:A:67:ASN:O	1:A:71:HIS:ND1	2.29	0.64
5:I:174:LEU:HD12	5:I:205:GLU:HG3	1.80	0.64
1:D:10:PHE:HA	1:D:13:THR:HG22	1.78	0.64
1:A:476:MET:HB3	1:A:516:ALA:HB1	1.80	0.63
2:E:83:CYS:SG	2:E:86:ARG:NH2	2.71	0.63
4:G:44:LEU:HD22	4:G:77:LEU:HD23	1.80	0.63
2:H:50:MET:HE1	2:H:69:THR:HG22	1.79	0.63
5:I:264:ARG:HH11	5:I:349:TYR:HD1	1.47	0.63
5:I:374:ARG:NH2	5:I:380:ASN:O	2.32	0.63
5:I:423:ASN:HA	5:I:426:LYS:HD3	1.81	0.63
1:D:234:GLN:N	1:D:234:GLN:OE1	2.33	0.62
1:D:605:MET:SD	1:D:610:LEU:HB2	2.39	0.62
1:D:37:ASP:OD1	3:F:63:ARG:NH2	2.32	0.62
5:I:412:ARG:HH12	5:I:470:GLN:HB2	1.65	0.62
1:D:563:GLU:O	2:H:24:VAL:N	2.32	0.61
1:A:169:ASN:HB3	1:A:174:GLU:HB3	1.82	0.61
1:D:42:ILE:HD13	1:D:105:TYR:HB3	1.82	0.61
1:D:514:ALA:HA	2:H:32:LEU:HD11	1.82	0.61
5:I:174:LEU:HD11	5:I:206:LEU:HD23	1.83	0.61
5:I:587:ILE:HA	5:I:590:LYS:HD2	1.82	0.61
1:D:271:VAL:HG21	1:D:300:LEU:HD11	1.83	0.60
6:J:578:PRO:O	6:J:581:ASN:ND2	2.34	0.60
3:F:83:TYR:HB3	3:F:90:ILE:HD12	1.83	0.60
5:I:370:ALA:HA	5:I:373:LEU:HD12	1.83	0.60
1:D:510:TYR:CD2	2:H:31:ALA:HB3	2.37	0.60
4:G:67:ALA:HA	4:G:73:ALA:H	1.66	0.60
2:H:94:CYS:HB3	2:H:99:ARG:H	1.67	0.60
1:D:625:HIS:CE1	1:D:627:SER:HB2	2.37	0.60
1:D:531:GLN:HE21	1:D:586:LEU:HD22	1.66	0.60
1:D:80:GLU:O	1:D:82:GLN:NE2	2.35	0.59
1:D:406:MET:HB3	1:D:410:GLU:HG3	1.84	0.59
3:F:83:TYR:HE2	4:G:69:PRO:HG2	1.67	0.59
4:G:25:PHE:O	4:G:29:ARG:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:412:ARG:HA	5:I:415:VAL:HG22	1.82	0.59
1:A:336:PRO:HA	1:A:390:LEU:HD13	1.82	0.59
1:D:544:TYR:HH	2:H:33:TRP:CD1	2.20	0.59
3:F:22:ILE:HG22	3:F:61:ASN:HA	1.84	0.59
3:F:96:ALA:HB3	3:F:99:ILE:HD11	1.84	0.59
6:J:573:GLU:HB3	6:J:575:ILE:HG12	1.83	0.59
1:A:74:LYS:HD3	1:A:77:LEU:HD21	1.84	0.59
1:D:334:ASN:HB3	1:D:337:THR:HB	1.85	0.59
1:A:563:GLU:HA	1:A:576:MET:HA	1.84	0.59
1:A:246:GLU:HG3	1:A:249:ARG:NH1	2.17	0.59
1:A:258:SER:HA	1:A:261:LYS:HE2	1.83	0.59
1:A:512:LEU:HD22	1:A:517:TRP:NE1	2.18	0.59
1:A:585:LEU:HA	1:A:588:PHE:HD2	1.68	0.59
1:A:607:GLU:O	1:A:611:THR:N	2.36	0.59
2:E:74:VAL:HG22	2:E:102:GLU:HG3	1.85	0.58
5:I:299:ILE:HG22	5:I:301:ALA:H	1.69	0.58
1:A:254:LEU:HD21	1:A:258:SER:HB2	1.84	0.58
1:D:120:GLU:HA	1:D:123:LEU:HD12	1.86	0.58
1:A:440:ALA:HA	1:A:517:TRP:HZ3	1.69	0.58
5:I:534:SER:H	5:I:537:HIS:HB2	1.68	0.58
1:D:451:MET:HA	1:D:451:MET:HE3	1.86	0.58
1:A:603:THR:HB	1:A:605:MET:HG3	1.86	0.58
1:D:507:PHE:HB3	2:H:29:ALA:HB3	1.86	0.57
1:D:556:LEU:H	2:H:31:ALA:HB2	1.69	0.57
3:F:41:THR:HG22	3:F:45:MET:HE2	1.84	0.57
2:H:88:LEU:HD11	2:H:101:TRP:HD1	1.68	0.57
1:A:428:LYS:HG2	1:D:467:TYR:CD1	2.39	0.57
5:I:606:ARG:HD3	5:I:609:ASP:OD1	2.04	0.57
1:A:75:ARG:NH2	1:A:90:TYR:OH	2.37	0.57
5:I:605:VAL:O	5:I:609:ASP:N	2.24	0.57
1:A:256:PRO:HA	1:A:259:TYR:CE2	2.39	0.57
5:I:512:ALA:HA	5:I:555:ILE:HD11	1.85	0.57
1:D:626:ASP:H	1:D:638:PHE:HA	1.69	0.57
5:I:412:ARG:HD3	5:I:467:ILE:HG12	1.86	0.57
5:I:459:CYS:SG	5:I:460:SER:N	2.70	0.57
5:I:264:ARG:HD2	5:I:349:TYR:HB2	1.86	0.56
1:A:618:LEU:HD11	1:A:638:PHE:HE2	1.70	0.56
1:A:512:LEU:N	2:E:31:ALA:O	2.36	0.56
1:A:543:PHE:O	1:A:547:HIS:ND1	2.31	0.56
1:A:69:VAL:HG13	1:A:151:MET:HE1	1.88	0.56
1:D:4:LYS:HB3	1:D:49:TYR:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:GLU:HA	1:D:612:LYS:HB3	1.87	0.56
1:A:250:CYS:O	1:A:254:LEU:N	2.39	0.55
1:D:66:GLU:OE2	1:D:70:ARG:NH2	2.39	0.55
5:I:412:ARG:NH1	5:I:470:GLN:HB2	2.21	0.55
2:H:79:PHE:HB2	2:H:84:ILE:HD11	1.88	0.55
5:I:405:PRO:HG2	5:I:459:CYS:HB2	1.87	0.55
5:I:186:CYS:O	5:I:217:GLY:N	2.39	0.55
3:F:101:LEU:HG	3:F:105:MET:HG2	1.89	0.55
4:G:5:LEU:HD11	4:G:16:THR:HG22	1.89	0.55
4:G:5:LEU:HD21	4:G:16:THR:HG23	1.89	0.55
1:A:401:LYS:N	1:A:447:LEU:O	2.39	0.55
5:I:336:LEU:HD12	5:I:341:ILE:HB	1.89	0.55
1:A:346:VAL:HA	1:A:349:LYS:HE3	1.89	0.55
1:D:6:ARG:HG3	1:D:7:VAL:HG13	1.88	0.54
5:I:381:THR:HG22	5:I:385:LEU:HG	1.88	0.54
1:D:473:LEU:HA	1:D:476:MET:HG3	1.89	0.54
3:F:79:TYR:OH	3:F:91:PRO:O	2.24	0.54
1:D:512:LEU:HD11	1:D:517:TRP:CD1	2.42	0.54
5:I:255:LEU:HD11	5:I:335:ILE:HG21	1.89	0.54
5:I:310:ASN:OD1	5:I:313:GLU:N	2.36	0.54
1:A:291:LYS:HZ3	1:A:353:LEU:HD12	1.72	0.54
1:A:491:ASN:O	1:A:495:LYS:NZ	2.36	0.54
1:D:153:GLU:HB2	1:D:154:PRO:HD3	1.90	0.54
2:E:68:CYS:SG	2:E:69:THR:N	2.78	0.54
2:H:77:HIS:CG	2:H:96:LEU:HD12	2.43	0.54
5:I:381:THR:O	5:I:385:LEU:N	2.37	0.54
1:A:510:TYR:N	2:E:29:ALA:O	2.39	0.54
5:I:277:TYR:HD1	5:I:314:LEU:HD23	1.73	0.54
1:D:491:ASN:O	1:D:495:LYS:NZ	2.40	0.54
1:A:579:THR:OG1	2:E:27:TRP:NE1	2.33	0.53
1:D:354:ILE:HG22	1:D:360:GLY:HA2	1.90	0.53
1:A:215:THR:HG22	1:A:219:TYR:CE2	2.43	0.53
1:A:611:THR:HG23	1:A:632:ILE:HB	1.88	0.53
3:F:40:GLY:O	3:F:43:LYS:HG2	2.08	0.53
1:D:503:LEU:HD12	2:H:24:VAL:HG13	1.89	0.53
5:I:462:GLU:OE1	5:I:466:LYS:NZ	2.30	0.53
5:I:464:GLN:O	5:I:468:ASN:N	2.33	0.53
5:I:470:GLN:HA	5:I:473:ASN:ND2	2.23	0.53
5:I:281:LEU:O	5:I:285:GLN:N	2.42	0.53
5:I:283:ARG:HA	5:I:291:LEU:HD12	1.91	0.53
1:D:611:THR:HA	1:D:614:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:150:ALA:HB2	5:I:156:THR:HG22	1.91	0.52
1:D:231:ASN:ND2	1:D:234:GLN:OE1	2.43	0.52
2:H:80:HIS:O	2:H:84:ILE:HG12	2.09	0.52
5:I:455:THR:O	5:I:458:GLN:NE2	2.43	0.52
1:D:231:ASN:OD1	1:D:232:CYS:N	2.43	0.52
5:I:153:TYR:HH	6:J:587:HIS:CD2	2.26	0.52
5:I:189:THR:H	5:I:192:HIS:HB3	1.73	0.52
5:I:208:LYS:O	5:I:210:ARG:NH2	2.42	0.52
1:D:3:LEU:HD13	3:F:101:LEU:HD22	1.91	0.52
5:I:485:PHE:H	5:I:529:ASP:CG	2.17	0.52
1:A:200:LEU:O	1:A:204:GLN:N	2.38	0.52
1:A:285:ILE:HG23	1:A:293:ASP:HB3	1.91	0.52
1:D:525:SER:HB2	1:D:605:MET:HA	1.90	0.52
1:D:611:THR:HA	1:D:614:ILE:HB	1.92	0.52
5:I:198:GLY:HA2	5:I:234:VAL:HG21	1.91	0.52
5:I:295:VAL:HA	5:I:307:GLU:HB3	1.92	0.52
5:I:151:ASN:HD21	5:I:153:TYR:HB2	1.74	0.52
5:I:216:ASN:HD21	5:I:220:MET:HE3	1.75	0.52
1:D:617:LEU:HB3	1:D:622:MET:SD	2.50	0.51
1:D:509:ILE:HG13	1:D:511:VAL:HG13	1.93	0.51
1:A:59:THR:O	1:A:63:ILE:HG12	2.09	0.51
1:A:396:ASP:HA	1:A:399:LEU:HB2	1.91	0.51
1:A:457:MET:N	1:A:457:MET:HE2	2.26	0.51
4:G:40:ASP:OD1	4:G:41:GLU:N	2.44	0.51
1:A:450:SER:OG	1:A:452:ASP:OD1	2.24	0.51
1:A:514:ALA:HB2	2:E:32:LEU:HD13	1.92	0.51
2:E:43:ALA:HB3	2:E:79:PHE:HE1	1.75	0.51
5:I:277:TYR:OH	5:I:315:GLU:OE2	2.25	0.51
5:I:426:LYS:HG2	5:I:437:MET:HE1	1.93	0.51
1:D:219:TYR:OH	1:D:246:GLU:OE2	2.28	0.51
1:D:625:HIS:CE1	1:D:632:ILE:HG12	2.45	0.51
2:H:94:CYS:N	2:H:99:ARG:O	2.44	0.51
1:A:76:VAL:O	1:A:79:SER:OG	2.28	0.51
1:A:548:PHE:HB3	1:A:551:ARG:HD2	1.92	0.51
2:E:77:HIS:CD2	2:E:96:LEU:HD12	2.45	0.51
5:I:437:MET:O	5:I:441:GLU:N	2.32	0.51
4:G:10:HIS:NE2	4:G:89:CYS:HB3	2.26	0.51
1:D:443:LEU:HD13	1:D:480:MET:SD	2.51	0.51
1:A:581:GLN:O	1:A:585:LEU:N	2.32	0.50
5:I:241:HIS:ND1	5:I:243:ASP:O	2.42	0.50
1:A:182:HIS:ND1	1:A:252:LYS:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HG3	1:A:447:LEU:HB3	1.92	0.50
1:A:625:HIS:CD2	1:A:627:SER:H	2.30	0.50
1:D:72:LEU:HD11	1:D:90:TYR:CE1	2.46	0.50
2:E:69:THR:O	2:E:81:PHE:N	2.40	0.50
1:D:554:THR:HG23	1:D:555:TRP:H	1.75	0.50
3:F:39:SER:OG	3:F:40:GLY:N	2.43	0.50
3:F:68:HIS:NE2	4:G:94:SER:O	2.43	0.50
5:I:156:THR:OG1	5:I:159:MET:HG2	2.11	0.50
1:A:170:ASP:CG	1:A:249:ARG:HE	2.20	0.50
1:D:253:TYR:O	1:D:254:LEU:HD23	2.11	0.50
5:I:322:ASP:O	5:I:326:MET:N	2.42	0.50
1:D:3:LEU:HG	1:D:4:LYS:H	1.77	0.50
1:D:332:GLN:HA	1:D:335:MET:HE2	1.94	0.50
3:F:42:ILE:HA	3:F:45:MET:HE3	1.93	0.50
5:I:283:ARG:HB3	5:I:291:LEU:HB2	1.94	0.50
5:I:443:ASN:O	5:I:446:THR:OG1	2.24	0.50
1:D:399:LEU:O	1:D:449:MET:HG2	2.12	0.50
1:A:428:LYS:H	1:D:467:TYR:HD1	1.60	0.50
1:D:357:VAL:HG12	1:D:358:LEU:HD23	1.92	0.50
3:F:76:TYR:CE2	5:I:597:LEU:HD11	2.47	0.50
4:G:76:GLY:C	4:G:77:LEU:HD12	2.37	0.50
5:I:496:THR:OG1	5:I:497:PRO:HD3	2.12	0.50
1:A:373:THR:O	1:A:377:ASN:N	2.40	0.49
5:I:253:LEU:HB3	5:I:279:ALA:HB2	1.94	0.49
1:D:506:SER:O	2:H:26:LYS:NZ	2.37	0.49
3:F:80:LYS:NZ	5:I:597:LEU:HD13	2.26	0.49
5:I:305:ARG:NH2	5:I:327:GLU:HB2	2.28	0.49
1:A:262:VAL:O	1:A:265:GLU:HG3	2.13	0.49
5:I:203:VAL:HA	5:I:206:LEU:HD12	1.95	0.49
1:A:475:ARG:NH2	2:H:97:ASP:O	2.35	0.49
3:F:99:ILE:CG2	3:F:103:LEU:HB2	2.42	0.49
5:I:602:ALA:O	5:I:605:VAL:HG12	2.13	0.49
1:D:87:TYR:CE2	1:D:184:VAL:HG23	2.47	0.49
2:H:35:TRP:HE3	2:H:38:VAL:HG21	1.78	0.49
5:I:367:TRP:O	5:I:371:LEU:N	2.44	0.49
1:D:534:GLU:O	1:D:538:GLN:NE2	2.46	0.48
2:E:88:LEU:O	2:E:92:GLN:NE2	2.46	0.48
4:G:37:ARG:HB2	4:G:42:GLN:NE2	2.28	0.48
1:D:568:TYR:CZ	1:D:569:LEU:HG	2.48	0.48
3:F:32:LYS:HB2	3:F:35:HIS:CE1	2.48	0.48
5:I:510:PRO:O	5:I:511:ASN:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ALA:O	1:D:444:ILE:HG12	2.13	0.48
1:D:483:SER:OG	1:D:484:ALA:N	2.45	0.48
5:I:382:HIS:HE2	5:I:383:LYS:HE2	1.79	0.48
5:I:516:LYS:HE3	5:I:555:ILE:HD13	1.96	0.48
1:A:530:PRO:HB3	1:A:586:LEU:HD11	1.94	0.48
1:A:596:TYR:HE2	1:A:607:GLU:HB3	1.78	0.48
1:D:282:CYS:SG	1:D:311:MET:HG2	2.53	0.48
4:G:63:THR:HG23	4:G:66:THR:H	1.78	0.48
1:D:556:LEU:HB3	2:H:31:ALA:HA	1.95	0.48
5:I:335:ILE:HG22	5:I:336:LEU:HD22	1.96	0.48
5:I:388:PHE:HZ	5:I:411:LEU:HD22	1.78	0.48
1:A:551:ARG:HD3	2:E:33:TRP:NE1	2.28	0.48
1:D:444:ILE:HG13	1:D:445:HIS:N	2.29	0.48
3:F:75:MET:HE1	4:G:72:PRO:HD3	1.95	0.48
5:I:267:TYR:OH	5:I:321:ARG:NH1	2.43	0.48
1:A:404:LYS:O	1:A:404:LYS:HD3	2.13	0.48
1:A:566:MET:SD	1:A:566:MET:N	2.87	0.48
1:D:556:LEU:H	2:H:31:ALA:CB	2.27	0.48
3:F:110:LEU:O	3:F:111:ASP:C	2.57	0.48
5:I:487:LEU:HG	5:I:488:LEU:HD22	1.95	0.48
1:A:330:LEU:HD22	1:A:338:LEU:HB3	1.95	0.48
1:D:21:ILE:HB	1:D:101:MET:HE1	1.96	0.48
1:D:622:MET:SD	1:D:623:ILE:HG23	2.54	0.48
2:E:45:CYS:HB2	2:E:54:ILE:H	1.79	0.48
5:I:417:GLU:HA	5:I:420:GLN:HB3	1.94	0.47
1:D:397:ASN:HA	1:D:400:LYS:HB2	1.96	0.47
5:I:544:ARG:HB3	5:I:547:SER:HB2	1.96	0.47
1:A:162:MET:O	1:A:166:GLU:HG2	2.15	0.47
1:A:354:ILE:HA	1:A:358:LEU:HD13	1.95	0.47
5:I:245:ASP:OD1	5:I:245:ASP:N	2.47	0.47
1:A:76:VAL:HG13	1:A:83:VAL:HG13	1.95	0.47
5:I:164:LYS:HE2	5:I:164:LYS:HA	1.95	0.47
5:I:596:SER:OG	5:I:597:LEU:N	2.47	0.47
1:A:452:ASP:OD1	1:A:453:SER:N	2.48	0.47
5:I:509:PHE:N	5:I:510:PRO:CD	2.78	0.47
1:A:242:ARG:O	1:A:245:ASP:N	2.48	0.47
1:D:400:LYS:HA	1:D:448:SER:HB3	1.95	0.47
1:D:476:MET:HE1	1:D:517:TRP:N	2.29	0.47
1:D:552:LYS:HE3	2:H:34:ALA:HB3	1.97	0.47
1:D:560:CYS:O	1:D:579:THR:OG1	2.32	0.47
2:E:84:ILE:HG21	2:E:103:PHE:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:80:LYS:O	3:F:84:THR:OG1	2.32	0.47
5:I:227:ALA:HB1	5:I:256:LEU:HB2	1.95	0.47
4:G:68:ARG:H	4:G:72:PRO:HA	1.80	0.47
5:I:158:LEU:HD12	5:I:159:MET:HE2	1.95	0.47
5:I:372:HIS:HB3	5:I:376:LYS:NZ	2.29	0.47
1:D:560:CYS:HB3	2:H:28:ASN:O	2.14	0.47
1:A:579:THR:HA	1:A:582:MET:SD	2.55	0.46
2:H:71:ALA:HB1	2:H:101:TRP:HZ2	1.79	0.46
1:A:557:HIS:HB2	1:A:580:TYR:HE1	1.81	0.46
1:D:197:LYS:HE2	1:D:198:PHE:CE2	2.50	0.46
1:D:244:LYS:HB3	1:D:244:LYS:HE2	1.65	0.46
2:E:27:TRP:CZ3	2:E:29:ALA:HB2	2.50	0.46
3:F:39:SER:HB3	3:F:42:ILE:HD12	1.96	0.46
5:I:553:HIS:O	5:I:557:ILE:HG13	2.16	0.46
2:H:70:VAL:HG23	2:H:78:ALA:HB1	1.96	0.46
1:D:438:MET:O	1:D:442:ARG:HD3	2.15	0.46
1:D:510:TYR:HB3	2:H:30:VAL:HA	1.96	0.46
2:E:79:PHE:HB2	2:E:84:ILE:HG13	1.98	0.46
1:A:137:MET:SD	1:A:142:LEU:HB2	2.55	0.46
1:A:415:LEU:HD13	1:A:457:MET:CE	2.45	0.46
1:D:181:ILE:HA	1:D:184:VAL:HG12	1.98	0.46
1:D:581:GLN:NE2	1:D:585:LEU:HD21	2.30	0.46
5:I:548:ASP:HB3	5:I:551:THR:OG1	2.15	0.46
1:A:184:VAL:HG12	1:A:188:PHE:CE2	2.50	0.46
1:A:239:VAL:HG22	1:A:242:ARG:HH22	1.80	0.46
2:E:42:CYS:N	2:E:47:ASN:O	2.24	0.46
1:A:308:LEU:HA	1:A:311:MET:HE3	1.96	0.46
1:D:475:ARG:NH1	1:D:513:GLN:HB2	2.30	0.46
5:I:420:GLN:O	5:I:424:ARG:N	2.35	0.46
1:D:594:VAL:HB	1:D:638:PHE:CZ	2.50	0.46
5:I:433:VAL:O	5:I:437:MET:HG2	2.16	0.46
5:I:471:ILE:HG21	5:I:521:CYS:SG	2.55	0.46
1:A:274:HIS:HA	1:A:277:PHE:CE2	2.51	0.46
5:I:421:SER:O	5:I:425:VAL:N	2.38	0.46
5:I:583:GLY:O	5:I:587:ILE:HG13	2.16	0.46
1:A:565:LYS:HE3	1:A:572:PRO:HB3	1.96	0.46
1:D:150:LEU:HA	1:D:150:LEU:HD23	1.61	0.46
1:D:558:TYR:HD2	1:D:559:LEU:HD13	1.81	0.46
2:H:88:LEU:O	2:H:92:GLN:NE2	2.49	0.46
1:A:605:MET:HE1	1:A:609:GLU:HB2	1.96	0.45
5:I:272:THR:HG22	5:I:324:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:107:ALA:HB3	5:I:598:LYS:HD3	1.98	0.45
1:D:255:HIS:CG	1:D:256:PRO:HD2	2.50	0.45
2:E:92:GLN:HB3	2:E:100:GLU:OE1	2.16	0.45
5:I:339:ASP:HB3	5:I:341:ILE:HG13	1.98	0.45
5:I:582:THR:O	5:I:586:GLU:HG3	2.17	0.45
1:D:576:MET:SD	1:D:576:MET:N	2.90	0.45
1:A:443:LEU:HD12	1:A:517:TRP:CZ2	2.51	0.45
1:A:554:THR:HB	2:E:32:LEU:HB2	1.99	0.45
1:D:462:LYS:O	1:D:467:TYR:HD2	1.99	0.45
1:D:632:ILE:HG23	1:D:636:SER:HB2	1.98	0.45
1:A:270:MET:O	1:A:274:HIS:CD2	2.70	0.45
2:H:83:CYS:N	2:H:86:ARG:HH21	2.14	0.45
1:A:491:ASN:O	1:A:495:LYS:HG2	2.17	0.45
4:G:26:GLU:O	4:G:30:ILE:HG13	2.16	0.45
1:A:72:LEU:HD23	1:A:75:ARG:HD3	1.99	0.45
1:D:495:LYS:HA	1:D:495:LYS:HD3	1.85	0.45
2:E:41:ASN:HA	2:E:48:HIS:HA	1.98	0.44
2:E:77:HIS:CE1	2:E:96:LEU:HB2	2.52	0.44
2:E:102:GLU:N	2:E:102:GLU:OE1	2.50	0.44
5:I:192:HIS:NE2	5:I:225:VAL:HG21	2.32	0.44
5:I:464:GLN:HA	5:I:467:ILE:HB	1.98	0.44
1:D:107:TYR:CE1	1:D:111:GLN:HG3	2.52	0.44
5:I:174:LEU:HD23	5:I:174:LEU:HA	1.84	0.44
5:I:451:VAL:O	5:I:455:THR:N	2.40	0.44
5:I:587:ILE:O	5:I:591:THR:HG23	2.18	0.44
5:I:516:LYS:HE2	5:I:555:ILE:HA	1.99	0.44
1:D:509:ILE:HG23	1:D:511:VAL:HG22	1.99	0.44
4:G:20:GLU:OE2	4:G:58:GLY:N	2.51	0.44
5:I:570:ASN:O	5:I:574:LYS:HE2	2.17	0.44
1:A:211:PHE:O	1:A:215:THR:OG1	2.27	0.44
1:A:472:LYS:H	1:A:472:LYS:HG2	1.61	0.44
1:A:641:ASN:HB3	1:A:644:PHE:HB2	2.00	0.44
1:D:48:ALA:HB3	1:D:51:GLU:O	2.18	0.44
1:D:204:GLN:HG2	1:D:208:GLU:OE2	2.16	0.44
1:D:232:CYS:SG	1:D:233:SER:N	2.91	0.44
1:D:330:LEU:HB3	1:D:335:MET:SD	2.58	0.44
5:I:151:ASN:ND2	6:J:579:ASN:OD1	2.50	0.44
5:I:584:VAL:HA	5:I:587:ILE:HD12	1.99	0.44
1:A:400:LYS:HG3	1:A:447:LEU:HD22	2.00	0.44
5:I:368:LEU:HD23	5:I:372:HIS:CE1	2.53	0.44
1:D:605:MET:HE1	1:D:609:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:167:THR:HG23	5:I:202:ILE:HA	1.99	0.44
5:I:485:PHE:N	5:I:529:ASP:OD1	2.45	0.44
2:E:44:ILE:HB	2:E:83:CYS:HB3	1.98	0.44
5:I:175:GLU:HA	5:I:209:TRP:CZ3	2.53	0.44
5:I:568:MET:HE1	5:I:626:PHE:HD1	1.83	0.44
1:A:243:LEU:HD21	1:A:270:MET:HE1	2.00	0.43
3:F:17:MET:HE2	3:F:17:MET:HB3	1.89	0.43
5:I:426:LYS:HA	5:I:433:VAL:HG11	2.00	0.43
1:A:156:GLN:HA	1:A:159:LEU:HG	1.99	0.43
1:A:582:MET:HA	1:A:585:LEU:HB2	2.00	0.43
4:G:3:VAL:HG22	4:G:67:ALA:HB3	2.00	0.43
5:I:407:ILE:O	5:I:411:LEU:HG	2.17	0.43
1:A:281:GLU:O	1:A:285:ILE:HG13	2.18	0.43
1:D:4:LYS:HE3	5:I:617:PRO:HA	2.01	0.43
1:D:614:ILE:O	1:D:617:LEU:HB2	2.18	0.43
2:H:47:ASN:HB3	2:H:52:LEU:HG	2.01	0.43
1:A:513:GLN:HG3	2:E:33:TRP:O	2.19	0.43
2:H:47:ASN:HB2	2:H:80:HIS:CE1	2.53	0.43
2:H:88:LEU:HD11	2:H:101:TRP:CD1	2.50	0.43
5:I:367:TRP:O	5:I:371:LEU:HG	2.18	0.43
1:A:165:ARG:HH21	1:A:168:LYS:HB3	1.83	0.43
1:D:625:HIS:NE2	1:D:636:SER:HB3	2.33	0.43
5:I:444:LEU:O	5:I:447:PHE:HB2	2.18	0.43
1:A:596:TYR:CD2	1:A:634:ALA:HA	2.54	0.43
4:G:46:LYS:HD3	4:G:76:GLY:O	2.19	0.43
6:J:576:ARG:HH21	6:J:577:THR:HB	1.84	0.43
1:A:148:ARG:HD2	1:A:202:PHE:CE2	2.54	0.43
1:A:149:LYS:O	1:A:154:PRO:HD3	2.18	0.43
1:A:151:MET:C	1:A:154:PRO:HD2	2.44	0.43
1:A:264:HIS:O	1:A:268:GLN:HG2	2.18	0.43
1:A:271:VAL:HG22	1:A:275:LEU:HB3	2.01	0.43
1:A:271:VAL:O	1:A:273:ASP:N	2.52	0.43
1:D:72:LEU:HD12	1:D:72:LEU:HA	1.80	0.43
1:D:235:TYR:O	1:D:239:VAL:HG23	2.19	0.43
1:D:290:LYS:NZ	1:D:292:ASN:H	2.08	0.43
5:I:468:ASN:HA	5:I:471:ILE:HD12	2.00	0.43
1:A:88:HIS:NE2	1:A:183:GLY:HA3	2.33	0.43
1:A:584:VAL:HG12	1:A:588:PHE:HE2	1.83	0.43
2:E:68:CYS:HA	2:E:82:HIS:HE1	1.83	0.43
5:I:164:LYS:HB3	5:I:166:HIS:CD2	2.54	0.43
5:I:278:LEU:O	5:I:282:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:612:TYR:CG	5:I:624:VAL:HG11	2.53	0.43
1:A:324:LEU:O	1:A:327:THR:OG1	2.28	0.42
1:D:1:MET:HB3	1:D:2:SER:H	1.72	0.42
5:I:246:ARG:CZ	5:I:250:ILE:HD11	2.49	0.42
5:I:414:SER:O	5:I:418:ILE:HG12	2.19	0.42
1:A:354:ILE:HG22	1:A:360:GLY:HA2	2.00	0.42
1:A:426:ASP:OD1	1:A:426:ASP:N	2.51	0.42
1:D:4:LYS:HA	1:D:4:LYS:HD3	1.67	0.42
1:D:600:GLN:NE2	1:D:605:MET:O	2.47	0.42
5:I:425:VAL:HA	5:I:428:ILE:HD12	2.00	0.42
1:A:215:THR:HG22	1:A:219:TYR:HE2	1.82	0.42
1:A:449:MET:SD	1:A:449:MET:N	2.90	0.42
1:D:590:ASN:OD1	1:D:591:SER:N	2.52	0.42
2:E:38:VAL:HG13	2:H:96:LEU:HD22	2.01	0.42
5:I:309:ARG:CD	5:I:310:ASN:HD22	2.32	0.42
1:A:153:GLU:HB2	1:A:154:PRO:HD3	2.01	0.42
1:A:236:MET:HE2	1:A:300:LEU:HB2	2.01	0.42
1:A:506:SER:HB3	2:E:26:LYS:NZ	2.35	0.42
3:F:23:SER:OG	3:F:70:LEU:HD22	2.20	0.42
4:G:38:PRO:O	4:G:42:GLN:HG2	2.19	0.42
1:A:242:ARG:O	1:A:243:LEU:C	2.62	0.42
1:A:596:TYR:HD2	1:A:634:ALA:HA	1.83	0.42
1:D:325:ARG:HD2	1:D:325:ARG:O	2.20	0.42
1:D:472:LYS:HZ2	1:D:516:ALA:HB2	1.84	0.42
1:D:581:GLN:O	1:D:585:LEU:HG	2.19	0.42
1:A:70:ARG:O	1:A:70:ARG:NH1	2.53	0.42
1:D:438:MET:C	1:D:442:ARG:HD3	2.44	0.42
1:D:611:THR:HG22	1:D:615:LYS:HZ2	1.85	0.42
5:I:367:TRP:HA	5:I:370:ALA:HB3	2.00	0.42
5:I:609:ASP:OD1	5:I:612:TYR:OH	2.37	0.42
1:A:58:TYR:HE1	1:A:139:ILE:HA	1.85	0.42
1:A:221:GLN:OE1	1:A:225:ASN:ND2	2.46	0.42
1:A:584:VAL:HG13	1:A:599:LEU:HD13	2.01	0.42
1:D:543:PHE:O	1:D:546:GLN:NE2	2.53	0.42
1:A:354:ILE:HD12	1:A:358:LEU:HD22	2.02	0.42
1:A:505:ILE:HD13	2:E:24:VAL:O	2.19	0.42
1:A:550:GLY:O	2:E:35:TRP:NE1	2.52	0.42
1:A:554:THR:N	2:E:32:LEU:O	2.52	0.42
1:A:625:HIS:NE2	1:A:636:SER:HB3	2.35	0.42
1:D:162:MET:HE2	1:D:162:MET:HB2	1.78	0.42
1:D:185:ILE:HD13	1:D:185:ILE:HA	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:LEU:HD11	2:E:101:TRP:HD1	1.85	0.42
5:I:154:ASP:HB2	5:I:185:HIS:N	2.34	0.42
5:I:168:ASP:OD1	5:I:169:VAL:N	2.51	0.42
1:D:472:LYS:NZ	1:D:516:ALA:HB2	2.35	0.41
2:H:26:LYS:HE3	2:H:27:TRP:O	2.20	0.41
2:H:45:CYS:SG	2:H:83:CYS:SG	3.18	0.41
1:A:512:LEU:O	2:E:33:TRP:N	2.51	0.41
1:A:512:LEU:HB2	2:E:32:LEU:HD23	2.01	0.41
1:D:510:TYR:HB2	2:H:31:ALA:H	1.86	0.41
2:E:77:HIS:HB2	2:E:101:TRP:CZ3	2.55	0.41
4:G:1:MET:SD	4:G:2:ASP:HB2	2.59	0.41
5:I:165:GLY:HA2	5:I:202:ILE:HD11	2.02	0.41
1:D:16:LYS:HB3	1:D:38:ARG:NH2	2.35	0.41
1:D:361:ASP:OD2	1:D:363:HIS:HB2	2.20	0.41
1:D:368:LEU:HD23	1:D:368:LEU:HA	1.81	0.41
4:G:7:ILE:O	4:G:13:THR:HA	2.19	0.41
5:I:154:ASP:HB2	5:I:184:ALA:C	2.46	0.41
5:I:286:ASP:OD2	5:I:288:ASP:HB2	2.20	0.41
1:A:80:GLU:C	1:A:82:GLN:H	2.29	0.41
1:A:301:LEU:HB3	1:A:311:MET:HE1	2.02	0.41
1:D:167:ILE:HD13	1:D:167:ILE:HA	1.96	0.41
5:I:451:VAL:HA	5:I:454:SER:HB2	2.03	0.41
1:D:483:SER:HA	1:D:509:ILE:HG21	2.03	0.41
1:D:611:THR:O	1:D:615:LYS:N	2.48	0.41
5:I:472:TYR:HA	5:I:475:ILE:HD12	2.01	0.41
1:A:271:VAL:HG23	1:A:274:HIS:CE1	2.56	0.41
1:A:316:GLN:HG3	1:A:367:ALA:HB1	2.01	0.41
4:G:2:ASP:H	4:G:64:SER:HB3	1.86	0.41
5:I:209:TRP:C	5:I:210:ARG:HG2	2.46	0.41
5:I:470:GLN:O	5:I:474:LEU:HG	2.20	0.41
5:I:597:LEU:HD12	5:I:597:LEU:HA	1.65	0.41
1:A:282:CYS:O	1:A:286:ILE:HG12	2.20	0.41
1:A:433:LYS:HE2	1:A:433:LYS:HB3	1.73	0.41
3:F:76:TYR:HB3	3:F:80:LYS:NZ	2.36	0.41
2:H:80:HIS:O	2:H:84:ILE:N	2.44	0.41
5:I:264:ARG:HA	5:I:349:TYR:CD1	2.55	0.41
1:A:198:PHE:HA	1:A:201:LYS:HD3	2.02	0.41
1:A:380:GLU:HB3	1:A:381:PRO:HD3	2.03	0.41
4:G:96:PRO:HA	4:G:97:PRO:HD3	1.93	0.41
1:A:268:GLN:O	1:A:272:ALA:HB3	2.20	0.41
1:A:357:VAL:HB	1:A:358:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:MET:HE2	1:D:236:MET:HA	2.03	0.41
1:D:387:ALA:HB3	1:D:388:PRO:HD3	2.03	0.41
4:G:46:LYS:NZ	4:G:75:VAL:HB	2.36	0.41
2:H:96:LEU:HD23	2:H:96:LEU:HA	1.87	0.41
1:A:298:TYR:OH	1:A:302:ARG:NH1	2.54	0.41
1:D:38:ARG:HD3	1:D:38:ARG:HA	1.64	0.41
1:D:361:ASP:OD1	1:D:362:GLN:N	2.54	0.41
3:F:69:VAL:HG23	3:F:70:LEU:HD12	2.03	0.41
5:I:416:LEU:HD13	5:I:470:GLN:HB3	2.02	0.41
1:A:330:LEU:HD21	1:A:342:SER:HB3	2.03	0.40
1:A:600:GLN:HG3	1:A:607:GLU:HG2	2.02	0.40
1:D:512:LEU:HD11	1:D:517:TRP:CG	2.56	0.40
2:H:36:ASP:OD1	2:H:37:ILE:HG12	2.21	0.40
5:I:246:ARG:HG3	5:I:249:ARG:HE	1.87	0.40
1:A:257:SER:O	1:A:261:LYS:NZ	2.42	0.40
1:A:335:MET:HE3	1:A:335:MET:O	2.20	0.40
1:D:139:ILE:HD13	1:D:139:ILE:HA	1.92	0.40
3:F:97:PRO:HG2	3:F:98:GLU:CD	2.47	0.40
3:F:99:ILE:HA	3:F:102:GLU:OE2	2.22	0.40
1:A:70:ARG:HH22	1:A:74:LYS:HE3	1.86	0.40
1:A:361:ASP:HB3	1:A:364:PHE:CD2	2.57	0.40
1:D:32:ARG:O	1:D:35:TRP:HB3	2.21	0.40
1:D:39:PHE:CE2	3:F:45:MET:HG3	2.57	0.40
1:D:115:LYS:HA	1:D:115:LYS:HD3	1.74	0.40
1:D:122:ASP:O	1:D:126:GLY:N	2.46	0.40
1:D:290:LYS:HA	1:D:290:LYS:HD2	1.94	0.40
1:D:556:LEU:HG	1:D:558:TYR:CZ	2.56	0.40
5:I:368:LEU:O	5:I:371:LEU:HB2	2.21	0.40
5:I:409:CYS:SG	5:I:467:ILE:HG13	2.61	0.40
1:A:477:TYR:O	1:A:480:MET:HG3	2.22	0.40
1:D:476:MET:HE1	1:D:517:TRP:HB2	2.02	0.40
1:D:552:LYS:HZ2	2:H:34:ALA:H	1.70	0.40
1:D:565:LYS:H	2:H:24:VAL:HG23	1.86	0.40
2:E:82:HIS:O	2:E:86:ARG:HG3	2.22	0.40
5:I:170:VAL:HA	5:I:173:LEU:HD12	2.03	0.40
5:I:567:ASP:HA	5:I:576:PRO:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/751 (73%)	541 (98%)	9 (2%)	1 (0%)	43	77
1	D	630/751 (84%)	597 (95%)	33 (5%)	0	100	100
2	E	68/108 (63%)	68 (100%)	0	0	100	100
2	H	66/108 (61%)	62 (94%)	4 (6%)	0	100	100
3	F	86/98 (88%)	74 (86%)	12 (14%)	0	100	100
4	G	80/104 (77%)	77 (96%)	3 (4%)	0	100	100
5	I	479/628 (76%)	458 (96%)	20 (4%)	1 (0%)	43	77
6	J	18/467 (4%)	18 (100%)	0	0	100	100
All	All	1978/3015 (66%)	1895 (96%)	81 (4%)	2 (0%)	49	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	511	ASN
1	A	272	ALA

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	A	509/687 (74%)	509 (100%)	0	100	100
1	D	581/687 (85%)	577 (99%)	4 (1%)	76	78
2	E	65/90 (72%)	65 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	63/90 (70%)	61 (97%)	2 (3%)	34	55
3	F	81/86 (94%)	81 (100%)	0	100	100
4	G	76/92 (83%)	76 (100%)	0	100	100
5	I	421/536 (78%)	421 (100%)	0	100	100
6	J	20/389 (5%)	20 (100%)	0	100	100
All	All	1816/2657 (68%)	1810 (100%)	6 (0%)	84	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	275	LEU
1	D	277	PHE
1	D	611	THR
1	D	616	SER
2	H	45	CYS
2	H	68	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	279	HIS
1	A	355	ASN
1	A	377	ASN
1	A	491	ASN
1	D	88	HIS
1	D	268	GLN
1	D	332	GLN
1	D	491	ASN
1	D	513	GLN
1	D	531	GLN
4	G	42	GLN
2	H	76	ASN
5	I	185	HIS
5	I	216	ASN
5	I	218	HIS
5	I	262	ASN
5	I	397	HIS
5	I	423	ASN

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Mol	Chain	Res	Type
5	I	473	ASN
5	I	611	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

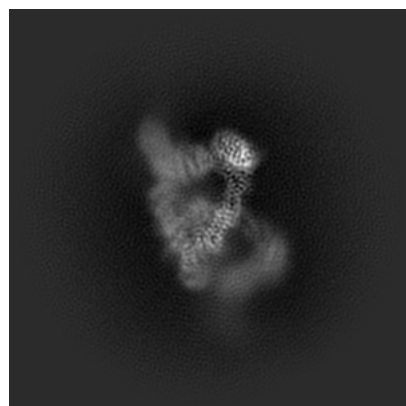
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61162. These allow visual inspection of the internal detail of the map and identification of artifacts.

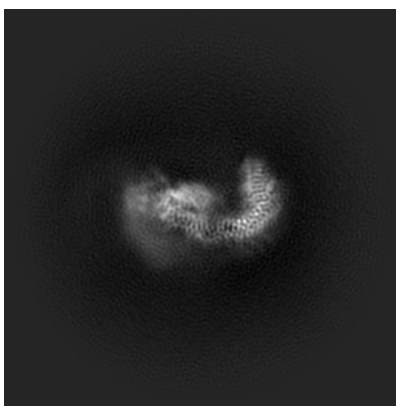
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

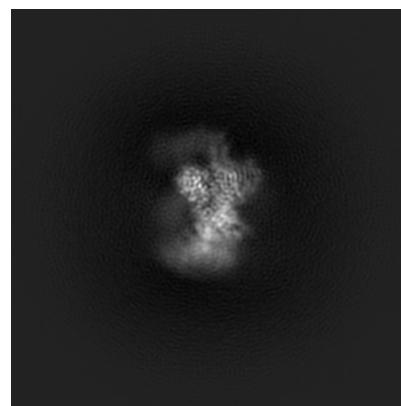
6.1.1 Primary map



X

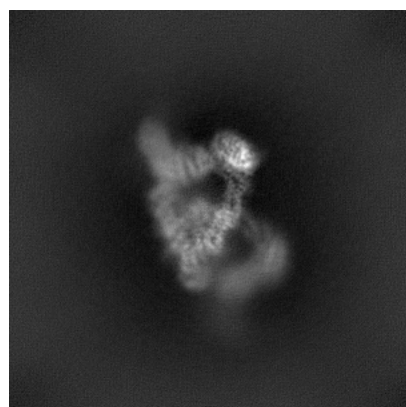


Y

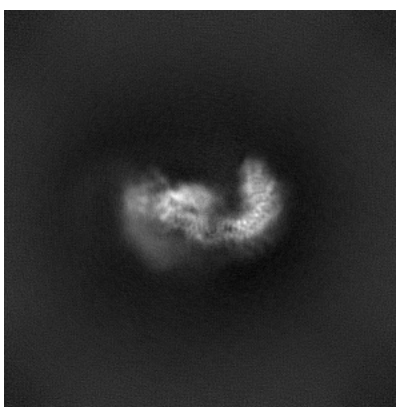


Z

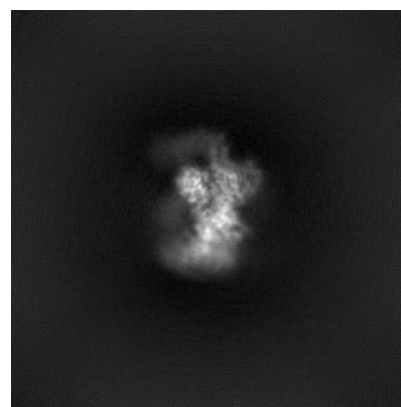
6.1.2 Raw map



X



Y

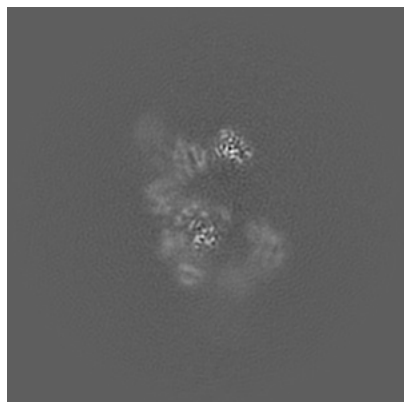


Z

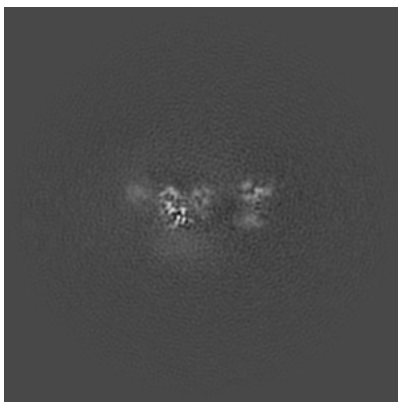
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

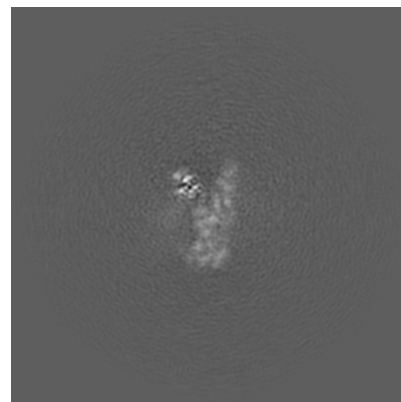
6.2.1 Primary map



X Index: 240

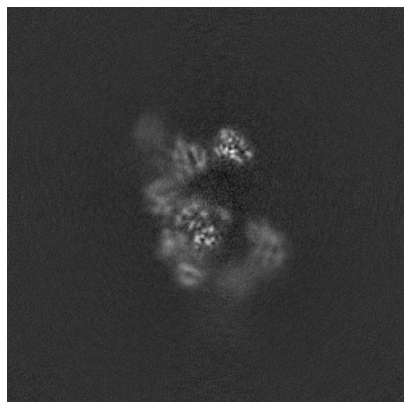


Y Index: 240

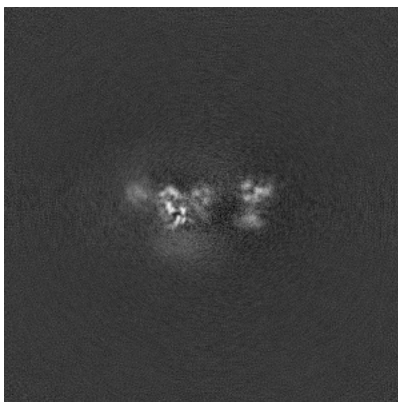


Z Index: 240

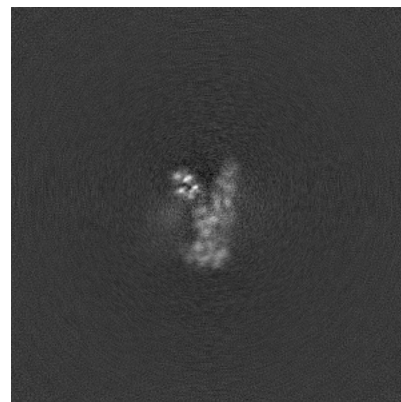
6.2.2 Raw map



X Index: 240



Y Index: 240

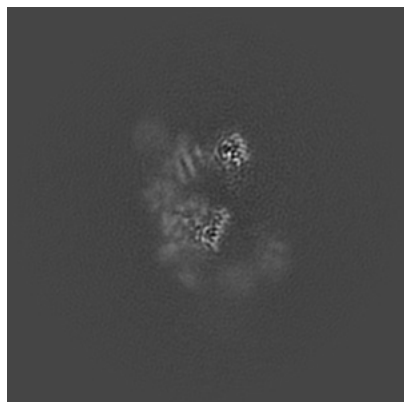


Z Index: 240

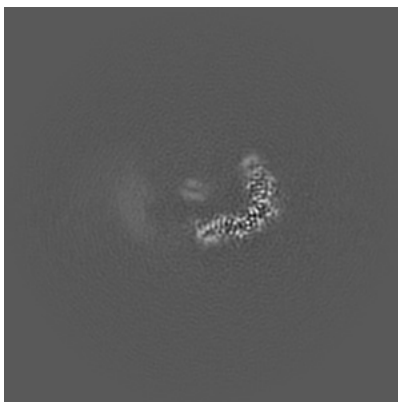
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

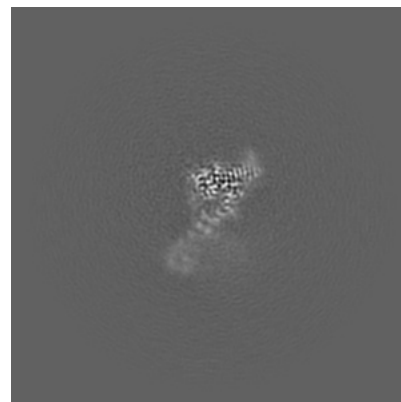
6.3.1 Primary map



X Index: 233

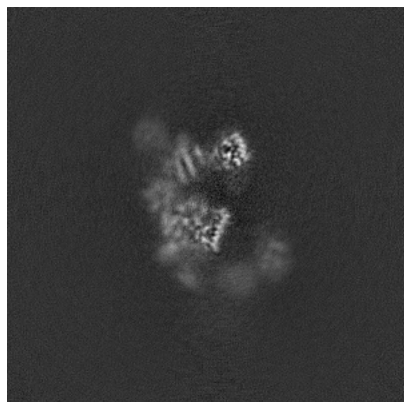


Y Index: 274



Z Index: 308

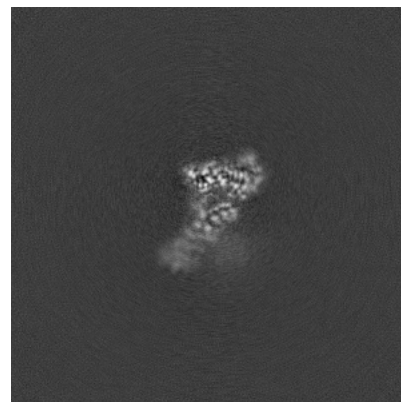
6.3.2 Raw map



X Index: 233



Y Index: 264

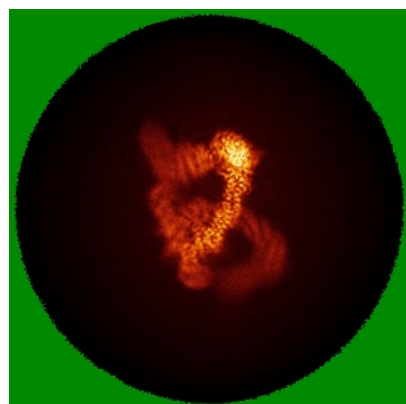


Z Index: 301

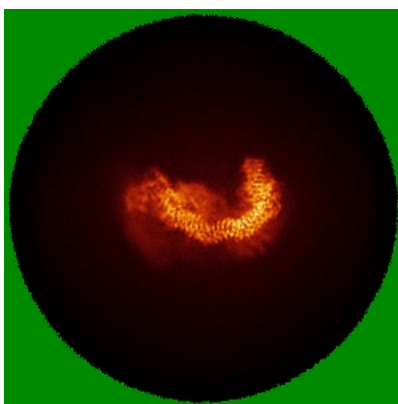
The images above show the largest variance slices of the map in three orthogonal directions.

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

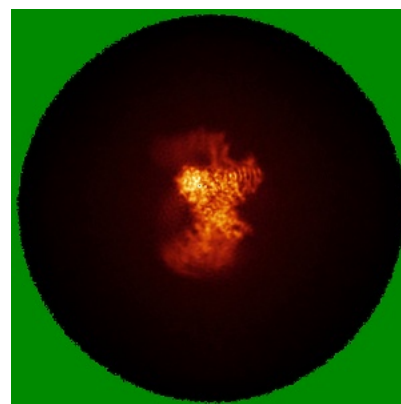
6.4.1 Primary map



X

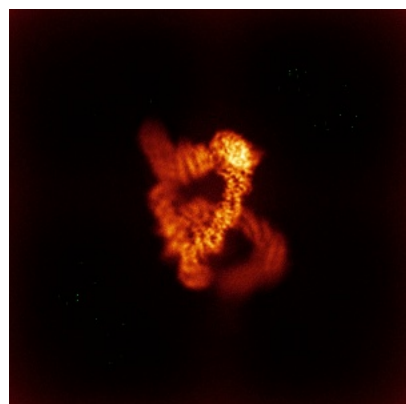


Y



Z

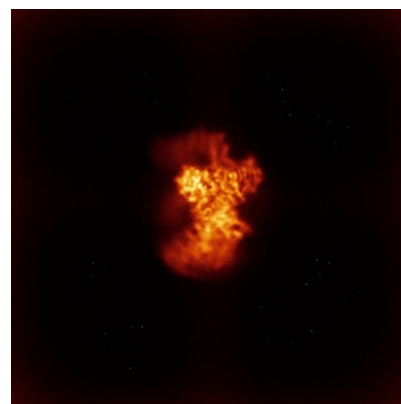
6.4.2 Raw map



X



Y

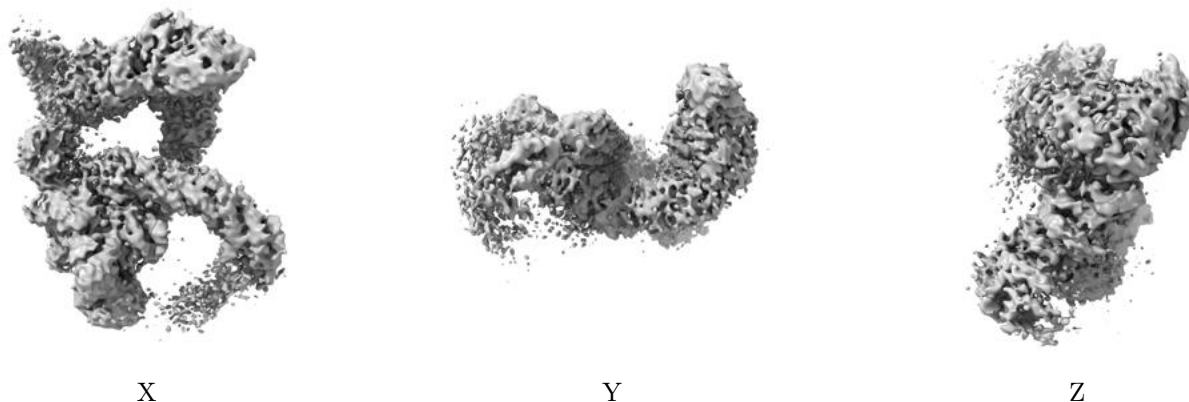


Z

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 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

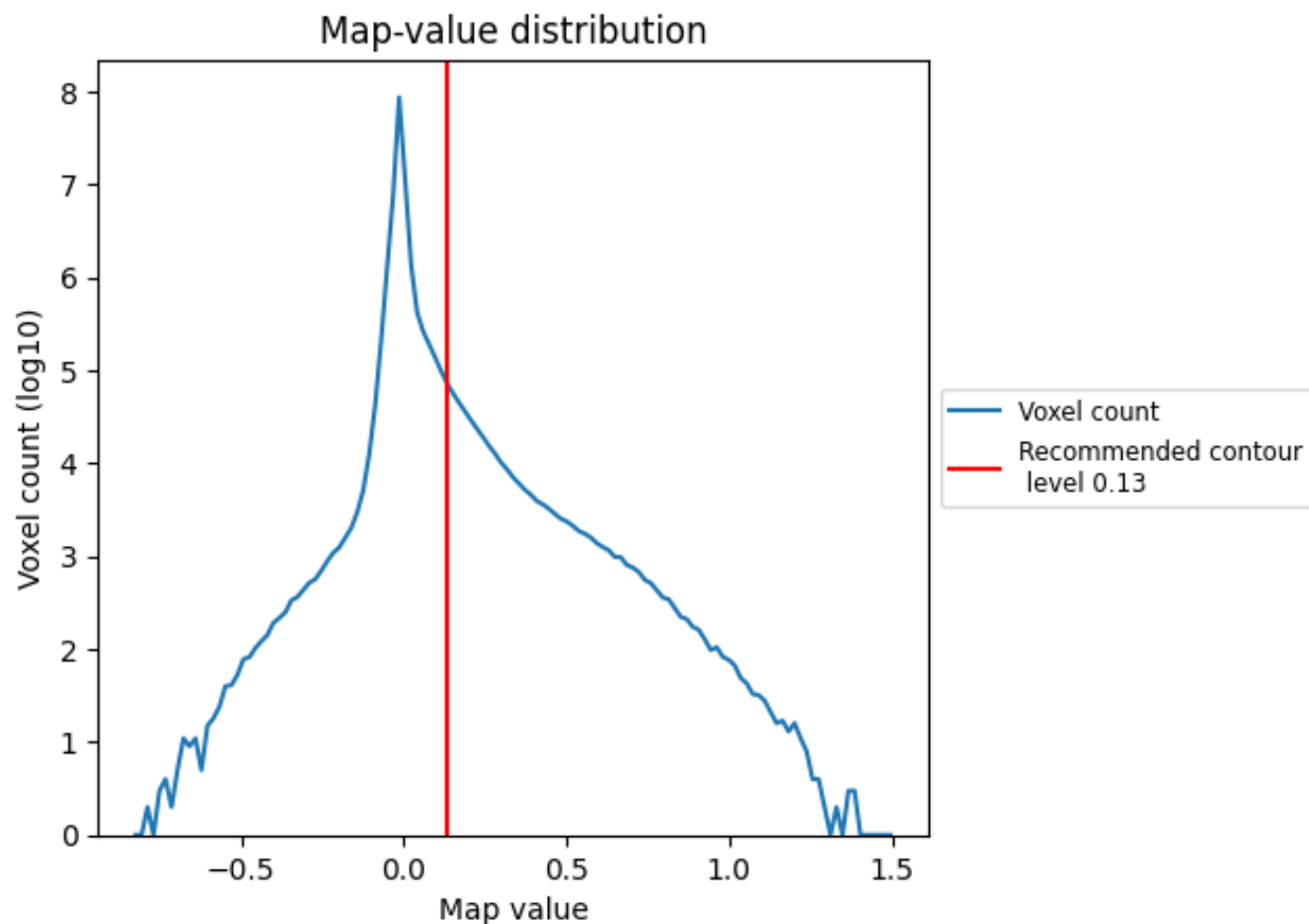
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

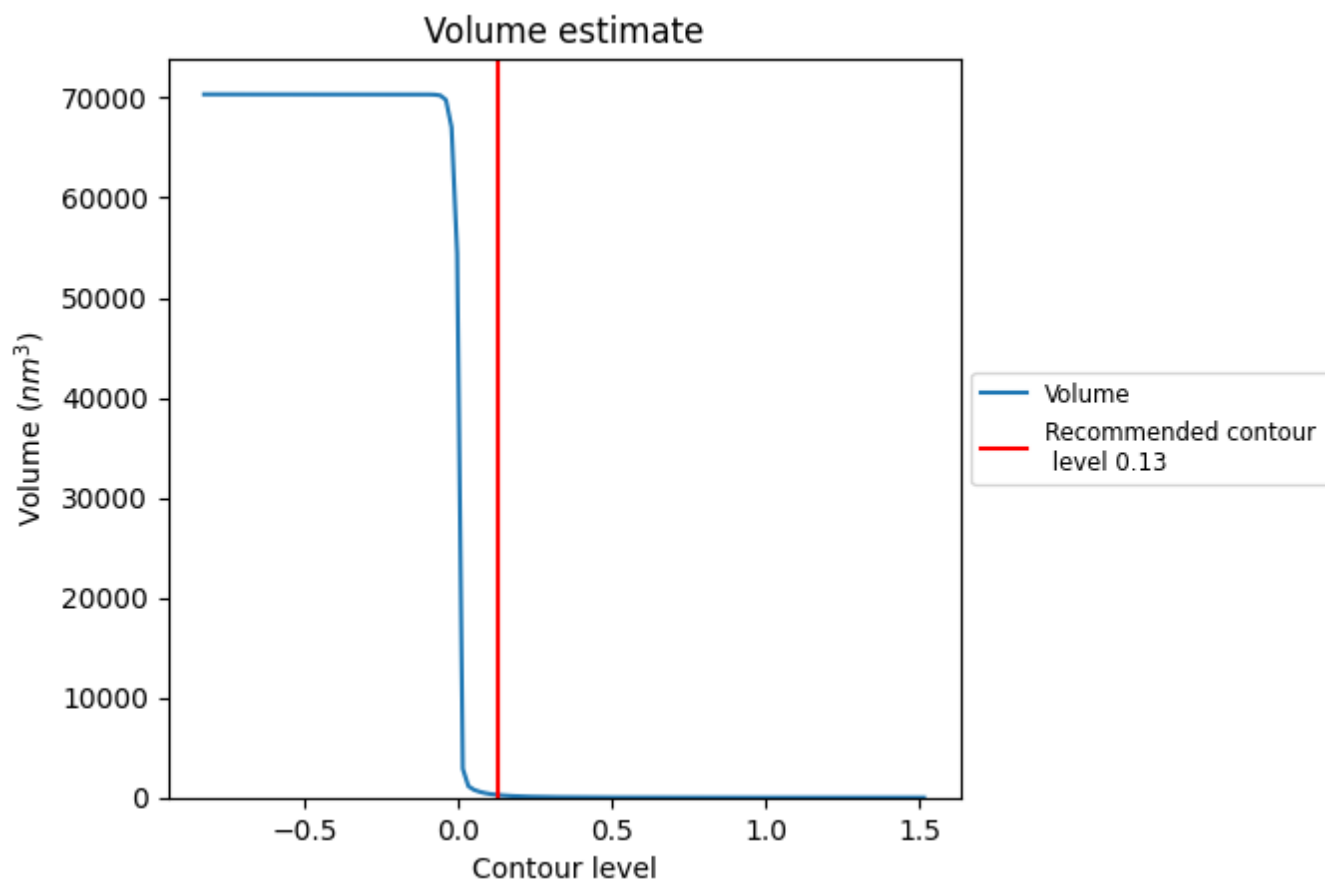
This section contains the results of statistical analysis of the map.

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.

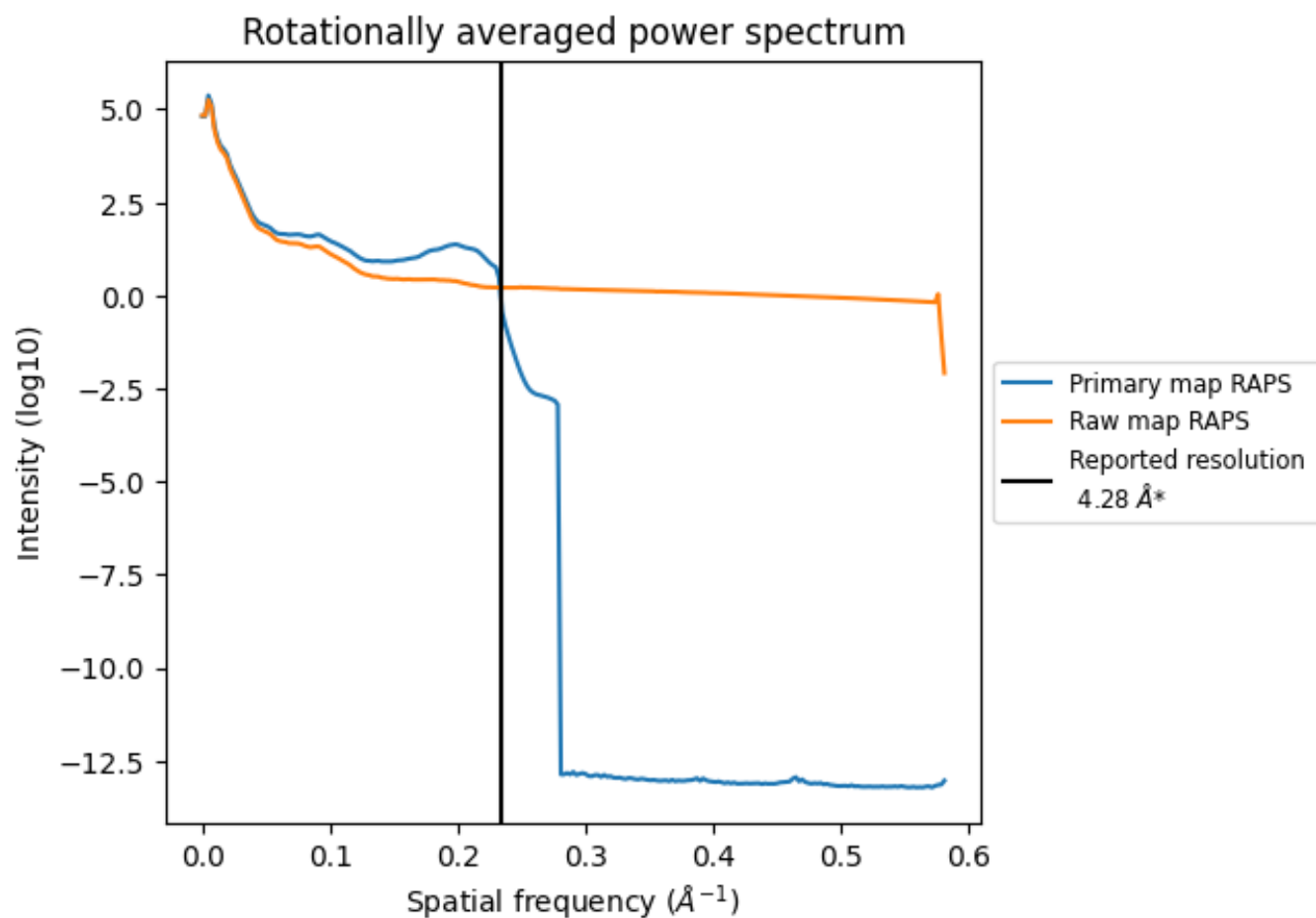
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 258 nm³; this corresponds to an approximate mass of 233 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 ⓘ

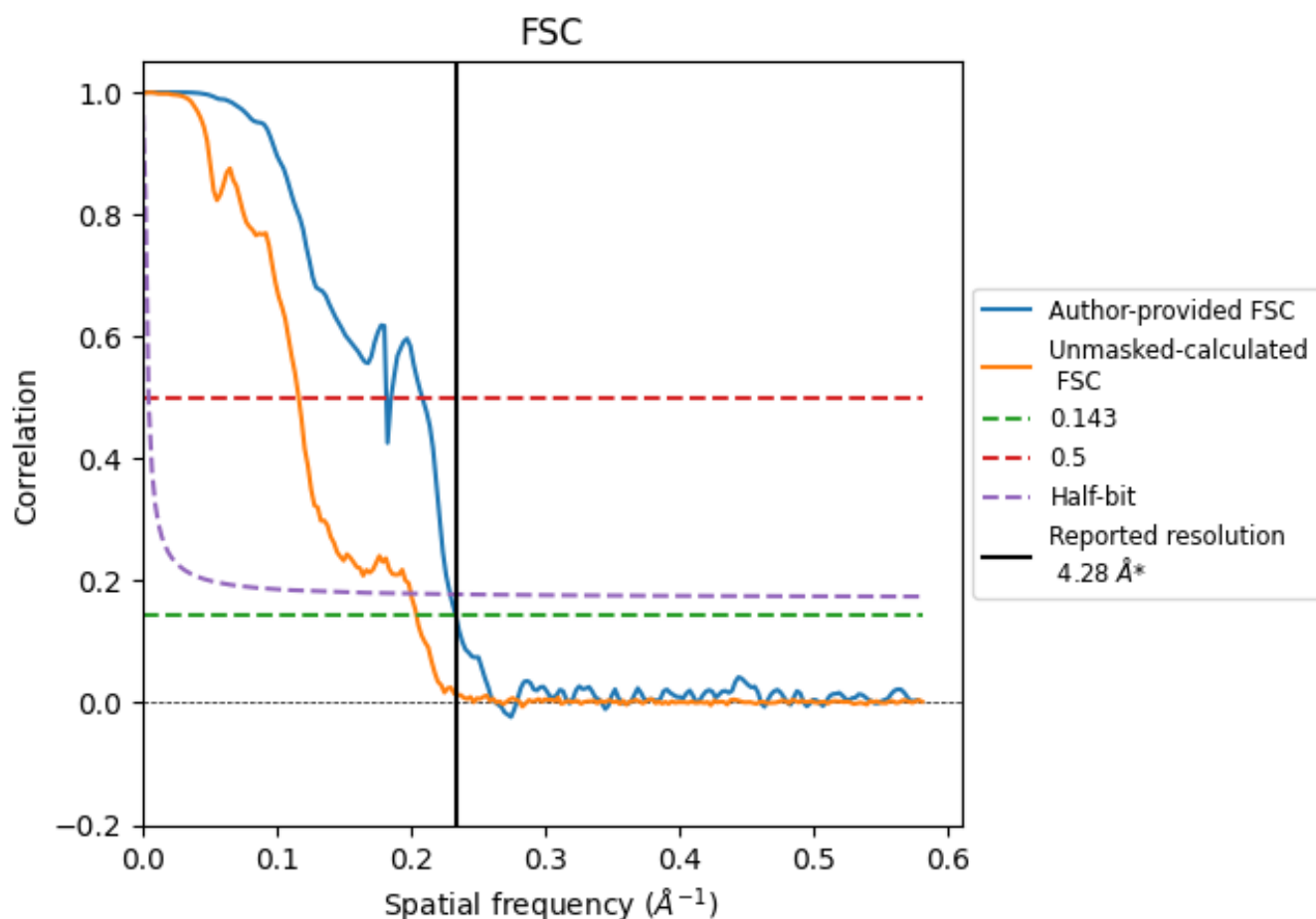


*Reported resolution corresponds to spatial frequency of 0.234 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.234 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

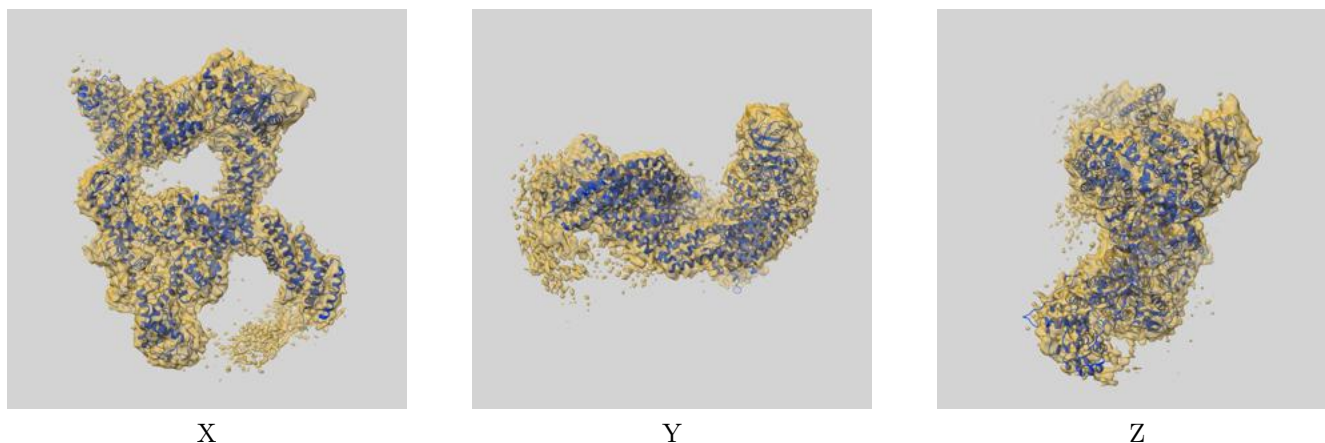
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.28	-	-
Author-provided FSC curve	4.28	5.49	4.35
Unmasked-calculated*	4.89	8.58	4.99

*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 4.89 differs from the reported value 4.28 by more than 10 %

9 Map-model fit [i](#)

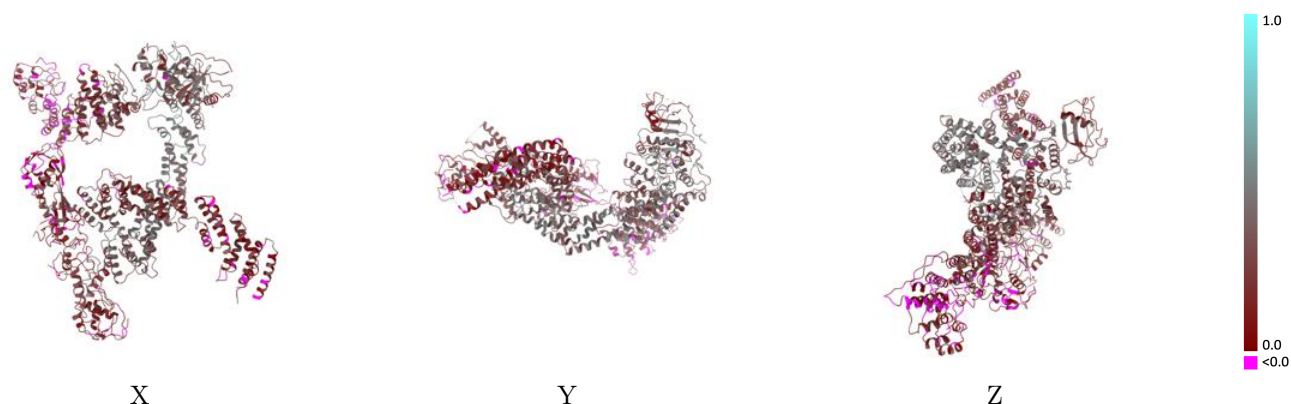
This section contains information regarding the fit between EMDB map EMD-61162 and PDB model 9J64. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



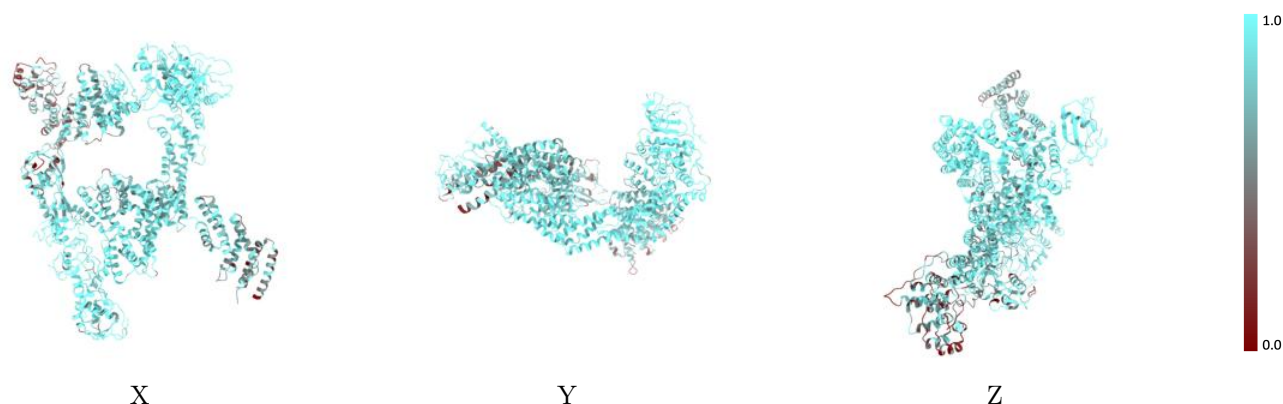
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



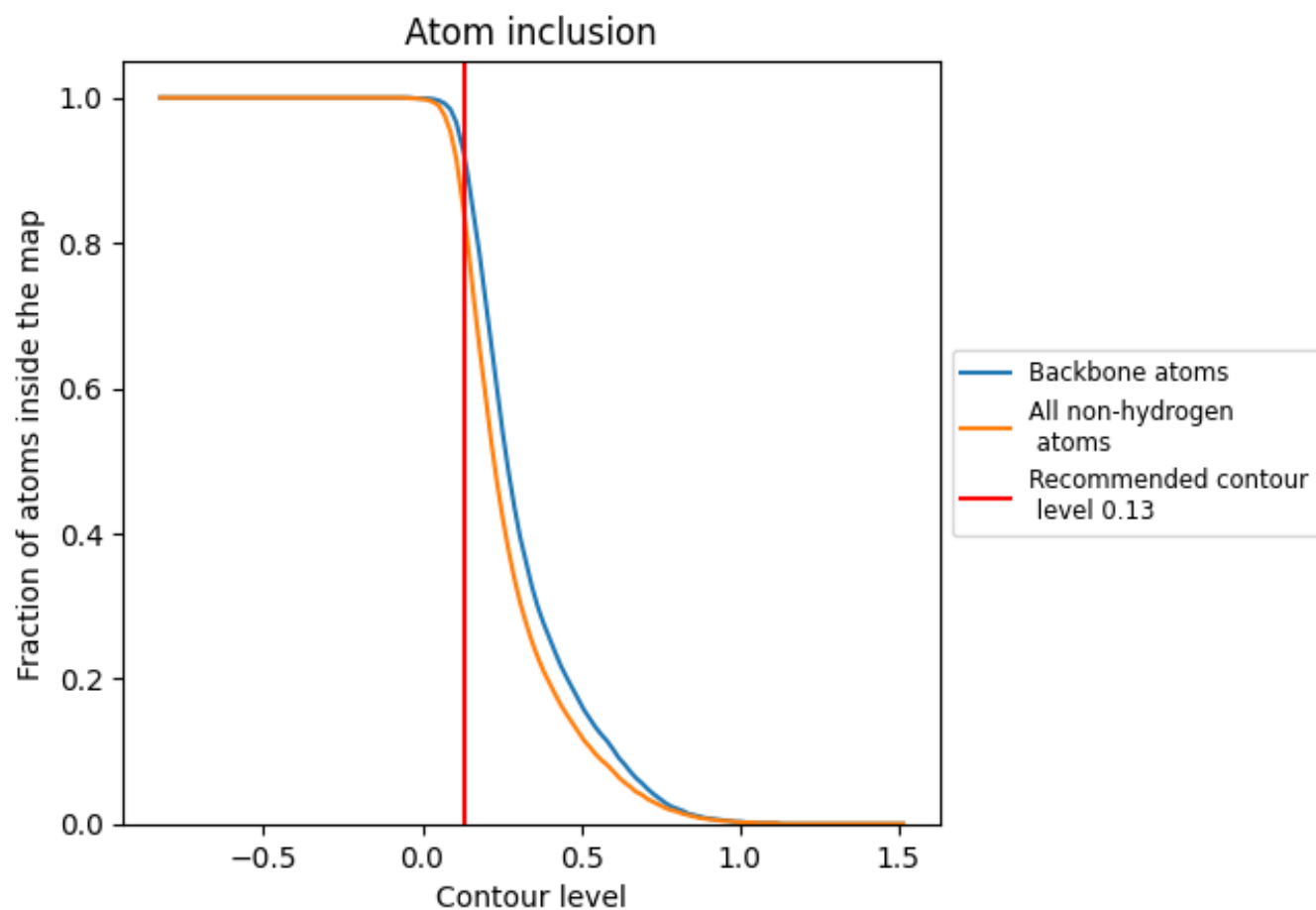
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8450	0.2520
A	0.7730	0.1890
D	0.9510	0.3590
E	0.9240	0.1620
F	0.9490	0.3790
G	0.9490	0.2790
H	0.9450	0.1870
I	0.7350	0.1840
J	0.4570	0.1250

1.0

0.0

<0.0