



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:37 AM UTC

PDB ID : 9QO2 / pdb_00009qo2
EMDB ID : EMD-53254
Title : Dissociation-state-1 of 9-subunit CSN and SCF (SKP1-SKP2-CKS1) complex
Authors : Ding, S.; Clapperton, J.A.; Maeots, M.E.; Enchev, R.I.
Deposited on : 2025-03-25
Resolution : 3.80 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:

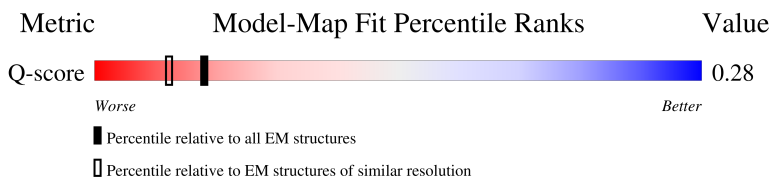
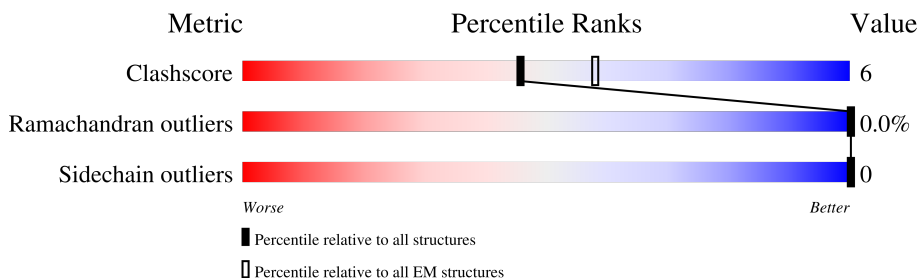
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 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	10198 (3.30 - 4.30)

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	B	443	 82% 9% 9%
2	C	423	 71% 11% 17%
3	D	406	 79% 15% 6%
4	E	334	 26% 73%

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Mol	Chain	Length	Quality of chain
5	F	327	
6	G	264	
7	H	209	
8	I	776	
9	J	108	
10	L	163	
11	M	424	
12	N	79	
13	P	57	
14	A	491	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 26494 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 COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	404	Total	C	N	O	S	0	0
			3305	2101	567	622	15		

- Molecule 2 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	350	Total	C	N	O	S	0	0
			2809	1793	471	522	23		

- Molecule 3 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	381	Total	C	N	O	S	0	0
			3067	1938	531	585	13		

- Molecule 4 is a protein called COP9 signalosome complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	90	Total	C	N	O	S	0	0
			713	448	122	141	2		

- Molecule 5 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	99	Total	C	N	O	S	0	0
			790	506	131	146	7		

- Molecule 6 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	214	Total	C	N	O	S	0	0
			1694	1074	288	326	6		

- Molecule 7 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	171	Total	C	N	O	S	0	0
			1359	868	235	252	4		

- Molecule 8 is a protein called Cullin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	625	Total	C	N	O	S	0	0
			4583	2918	798	847	20		

- Molecule 9 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	79	Total	C	N	O	S	0	0
			661	423	120	109	9		

- Molecule 10 is a protein called S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	127	Total	C	N	O	S	0	0
			1021	651	167	198	5		

- Molecule 11 is a protein called S-phase kinase-associated protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	324	Total	C	N	O	S	0	0
			2561	1627	441	477	16		

- Molecule 12 is a protein called Cyclin-dependent kinases regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	71	Total	C	N	O	S	0	0
			614	398	105	108	3		

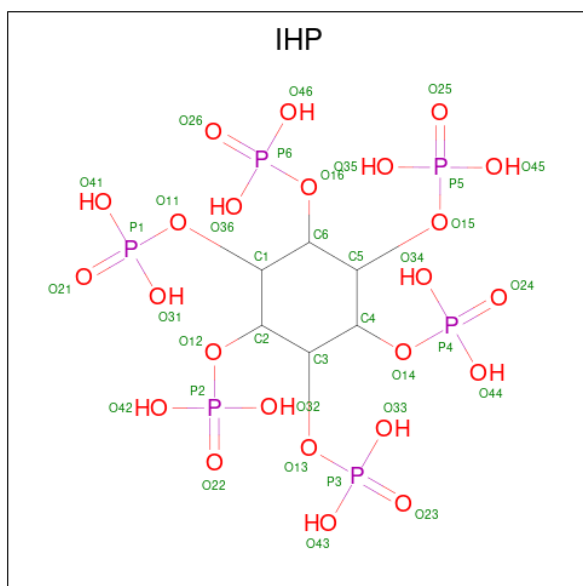
- Molecule 13 is a protein called COP9 signalosome complex subunit 9.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	21	Total	C	N	O	0	0
			179	113	26	40		

- Molecule 14 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	406	Total	C	N	O	S	0	0
			3099	1969	529	579	22		

- Molecule 15 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
15	B	1	Total	C	O	P	0
			36	6	24	6	


- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

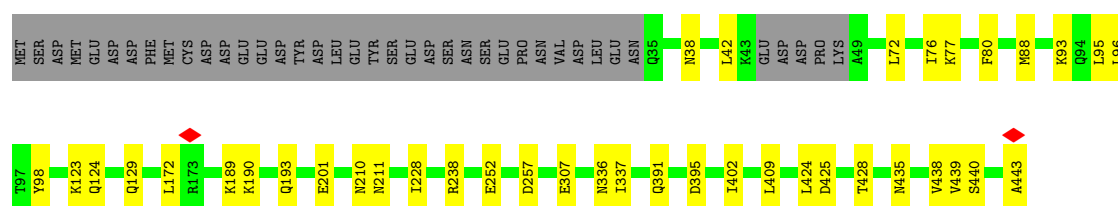
Mol	Chain	Residues	Atoms		AltConf
16	J	3	Total	Zn	0
			3	3	

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.

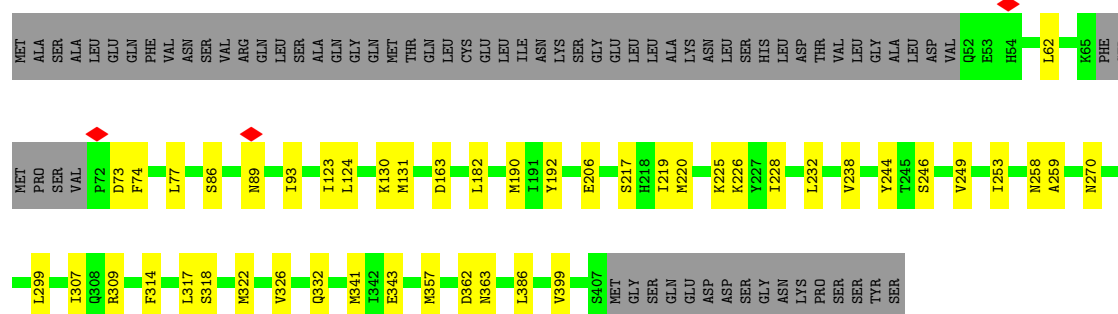
• Molecule 1: COP9 signalosome complex subunit 2

Chain B: 




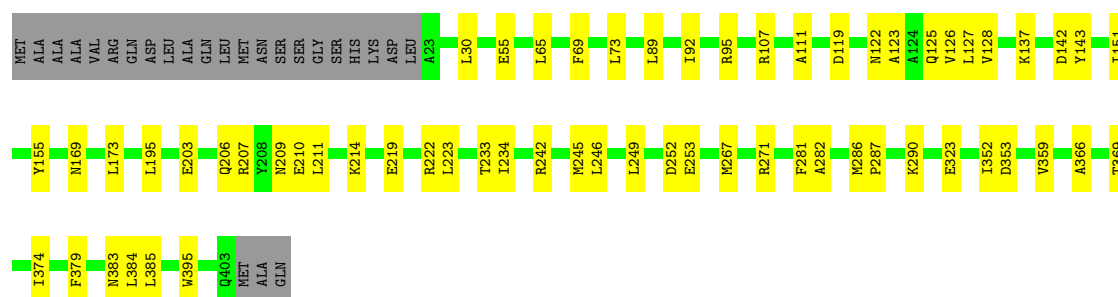
• Molecule 2: COP9 signalosome complex subunit 3

Chain C: 



• Molecule 3: COP9 signalosome complex subunit 4

Chain D: 

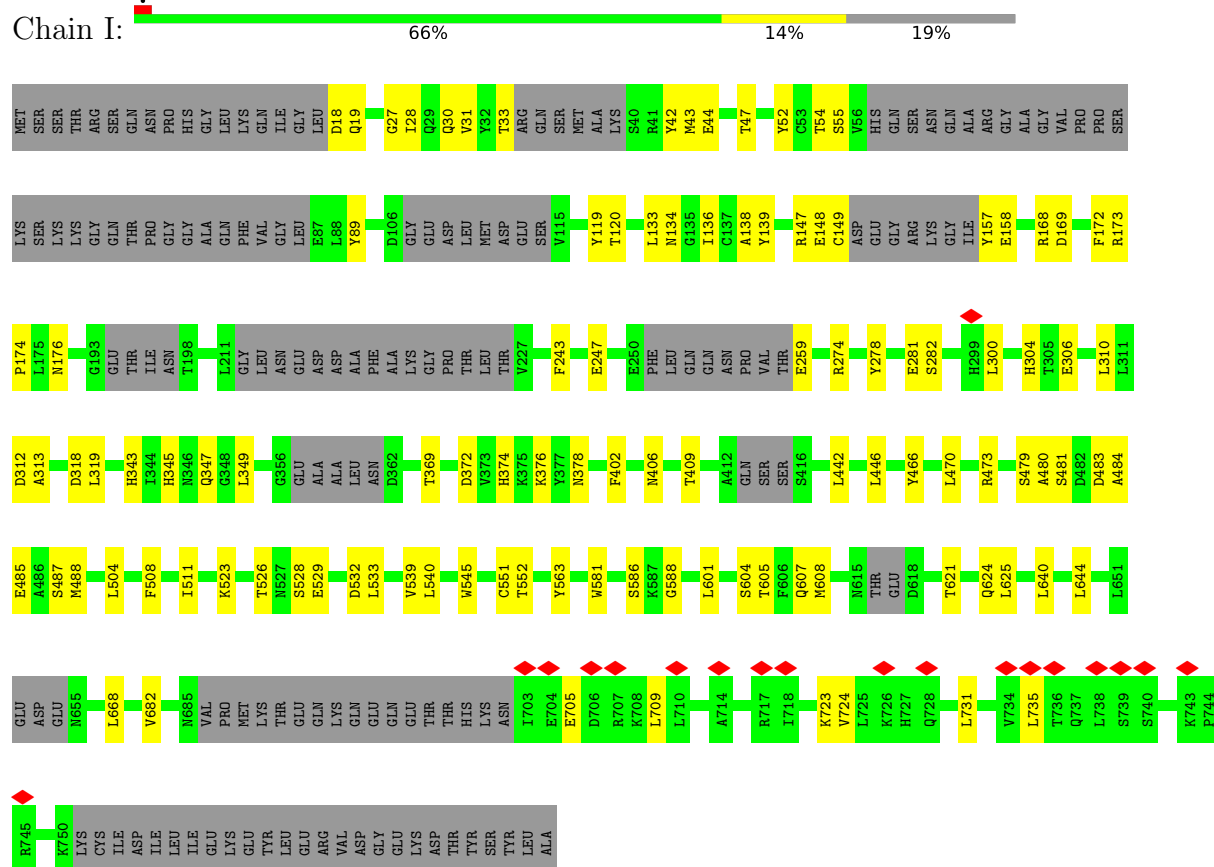






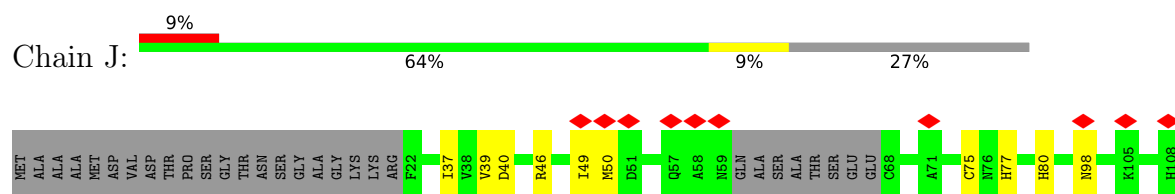
• Molecule 8: Cullin-1

Chain I:



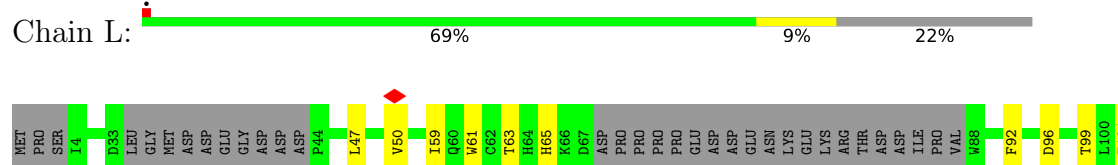
• Molecule 9: E3 ubiquitin-protein ligase RBX1

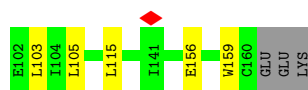
Chain J:



• Molecule 10: S-phase kinase-associated protein 1

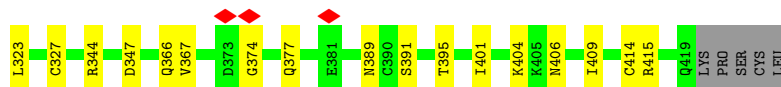
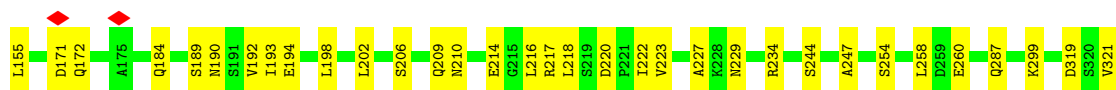
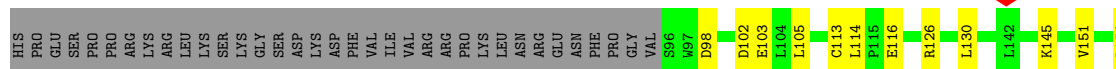
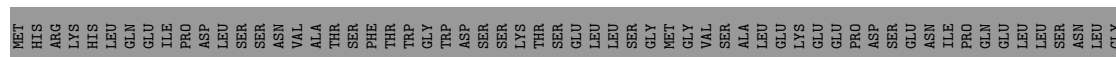
Chain L:





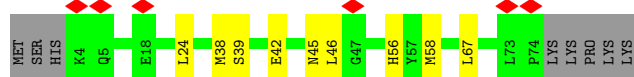
- Molecule 11: S-phase kinase-associated protein 2

Chain M: 62% 15% 24%



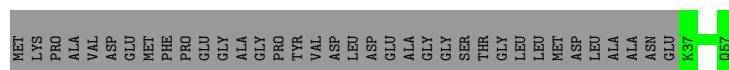
- Molecule 12: Cyclin-dependent kinases regulatory subunit 1

Chain N: 8% 78% 11% 10%



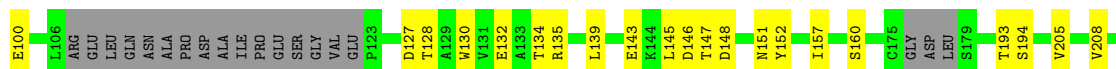
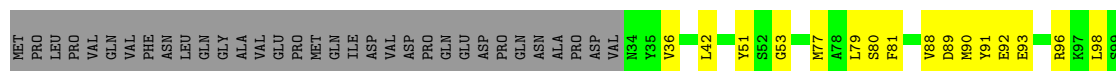
- Molecule 13: COP9 signalosome complex subunit 9

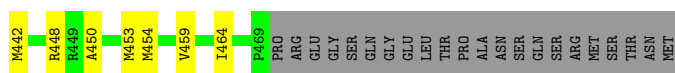
Chain P: 37% 63%



- Molecule 14: COP9 signalosome complex subunit 1

Chain A: 68% 14% 17%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1015152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.032	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.0094	Depositor
Map size (\AA)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	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: IHP, 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	B	0.15	0/3361	0.38	0/4519
2	C	0.15	0/2863	0.33	0/3863
3	D	0.14	0/3118	0.36	0/4214
4	E	0.13	0/720	0.26	0/967
5	F	0.15	0/806	0.33	0/1091
6	G	0.13	0/1714	0.32	0/2319
7	H	0.14	0/1390	0.30	0/1889
8	I	0.16	0/4646	0.35	0/6312
9	J	0.12	0/682	0.31	0/925
10	L	0.12	0/1036	0.33	0/1398
11	M	0.12	0/2611	0.32	0/3544
12	N	0.11	0/635	0.29	0/860
13	P	0.14	0/183	0.27	0/245
14	A	0.17	0/3151	0.42	0/4270
All	All	0.15	0/26916	0.35	0/36416

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 [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	B	3305	0	3353	30	0
2	C	2809	0	2821	36	0
3	D	3067	0	3067	47	0
4	E	713	0	727	4	0
5	F	790	0	784	17	0
6	G	1694	0	1737	20	0
7	H	1359	0	1339	17	0
8	I	4583	0	4221	69	0
9	J	661	0	613	9	0
10	L	1021	0	1023	9	0
11	M	2561	0	2585	39	0
12	N	614	0	594	5	0
13	P	179	0	144	0	0
14	A	3099	0	3018	50	0
15	B	36	0	6	4	0
16	J	3	0	0	0	0
All	All	26494	0	26032	327	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 6.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:206:SER:O	11:M:229:ASN:ND2	2.08	0.86
2:C:307:ILE:HG21	2:C:341:MET:HE1	1.56	0.85
8:I:343:HIS:O	8:I:347:GLN:NE2	2.09	0.85
3:D:379:PHE:O	3:D:383:ASN:ND2	2.11	0.83
2:C:163:ASP:OD1	2:C:192:TYR:OH	1.96	0.83
1:B:391:GLN:NE2	1:B:395:ASP:OD2	2.13	0.81
14:A:53:GLY:O	14:A:211:TYR:OH	1.97	0.81
2:C:93:ILE:HG21	2:C:131:MET:HE1	1.65	0.78
1:B:252:GLU:OE2	9:J:98:ASN:ND2	2.18	0.76
1:B:336:ASN:OD1	1:B:337:ILE:HD12	1.86	0.76
5:F:285:ASP:OD1	14:A:432:ARG:NH1	2.19	0.75
15:B:501:IHP:O25	15:B:501:IHP:O44	2.04	0.75
11:M:299:LYS:NZ	11:M:327:CYS:SG	2.60	0.75
3:D:214:LYS:O	3:D:222:ARG:NH1	2.20	0.75
15:B:501:IHP:O21	15:B:501:IHP:O32	2.05	0.75
2:C:307:ILE:CG2	2:C:341:MET:HE1	2.16	0.74
11:M:98:ASP:O	11:M:126:ARG:NH2	2.20	0.74
8:I:586:SER:OG	8:I:605:THR:OG1	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:129:GLU:OE2	6:G:147:GLN:NE2	2.21	0.73
1:B:190:LYS:NZ	1:B:193:GLN:OE1	2.21	0.73
2:C:362:ASP:OD1	2:C:363:ASN:N	2.21	0.73
8:I:89:TYR:HH	8:I:157:TYR:N	1.86	0.72
11:M:217:ARG:NH1	11:M:218:LEU:O	2.22	0.72
14:A:130:TRP:O	14:A:134:THR:HG23	1.90	0.72
11:M:210:ASN:OD1	11:M:234:ARG:N	2.24	0.71
5:F:297:LYS:NZ	7:H:207:LEU:O	2.23	0.71
6:G:97:LYS:O	6:G:101:ILE:HD12	1.91	0.71
8:I:28:ILE:HG22	8:I:133:LEU:HD22	1.72	0.70
8:I:406:ASN:O	8:I:409:THR:OG1	2.08	0.70
14:A:284:LEU:N	14:A:288:ASN:OD1	2.25	0.70
11:M:202:LEU:HD21	11:M:222:ILE:HG23	1.72	0.70
2:C:130:LYS:C	2:C:131:MET:HE2	2.16	0.69
11:M:323:LEU:N	11:M:347:ASP:OD2	2.26	0.69
5:F:216:THR:N	7:H:208:GLU:OE2	2.27	0.68
11:M:113:CYS:N	11:M:116:GLU:OE2	2.27	0.68
15:B:501:IHP:O46	15:B:501:IHP:O11	2.11	0.67
8:I:473:ARG:NH1	8:I:485:GLU:OE2	2.27	0.67
3:D:395:TRP:CH2	5:F:244:ALA:HB1	2.29	0.67
8:I:43:MET:SD	8:I:44:GLU:N	2.69	0.65
14:A:276:ASP:OD1	14:A:277:HIS:N	2.29	0.65
8:I:481:SER:OG	8:I:483:ASP:OD1	2.16	0.63
8:I:134:ASN:O	8:I:138:ALA:N	2.32	0.63
12:N:39:SER:OG	12:N:42:GLU:OE1	2.06	0.63
11:M:113:CYS:SG	11:M:114:LEU:N	2.72	0.63
14:A:151:ASN:OD1	14:A:152:TYR:N	2.32	0.62
3:D:119:ASP:OD2	3:D:122:ASN:ND2	2.31	0.62
8:I:312:ASP:OD1	8:I:313:ALA:N	2.33	0.62
10:L:96:ASP:O	10:L:99:THR:OG1	2.17	0.62
3:D:55:GLU:OE1	3:D:95:ARG:NH1	2.33	0.61
1:B:76:ILE:HG23	1:B:88:MET:HE3	1.82	0.61
8:I:43:MET:O	8:I:47:THR:HG23	2.01	0.61
3:D:142:ASP:OD1	3:D:143:TYR:N	2.33	0.61
8:I:470:LEU:HD23	8:I:504:LEU:HD11	1.83	0.60
2:C:93:ILE:CG2	2:C:131:MET:HE1	2.32	0.59
5:F:249:GLU:N	5:F:249:GLU:OE1	2.36	0.59
3:D:242:ARG:O	3:D:246:LEU:HD23	2.03	0.59
3:D:233:THR:O	3:D:242:ARG:NH1	2.36	0.58
8:I:18:ASP:OD1	8:I:19:GLN:N	2.36	0.58
11:M:209:GLN:OE1	11:M:209:GLN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:173:LEU:HD11	9:J:39:VAL:HB	1.84	0.58
8:I:54:THR:OG1	8:I:139:TYR:OH	2.16	0.58
10:L:156:GLU:OE2	11:M:154:ARG:NH1	2.36	0.58
8:I:274:ARG:NE	8:I:278:TYR:OH	2.36	0.58
8:I:466:TYR:OH	8:I:488:MET:SD	2.56	0.58
2:C:270:ASN:OD1	2:C:309:ARG:NH2	2.38	0.57
4:E:234:ASP:OD1	4:E:235:ARG:N	2.38	0.57
8:I:532:ASP:OD1	8:I:533:LEU:N	2.37	0.57
8:I:604:SER:O	8:I:608:MET:N	2.37	0.57
8:I:607:GLN:N	8:I:607:GLN:OE1	2.37	0.57
14:A:359:ALA:O	14:A:362:VAL:HG12	2.05	0.57
11:M:220:ASP:OD2	11:M:244:SER:OG	2.23	0.57
3:D:219:GLU:OE2	3:D:222:ARG:NE	2.38	0.57
8:I:30:GLN:O	8:I:33:THR:OG1	2.23	0.57
8:I:621:THR:HG22	8:I:668:LEU:HD22	1.86	0.57
11:M:194:GLU:OE1	11:M:194:GLU:N	2.38	0.57
8:I:621:THR:O	8:I:625:LEU:HD23	2.04	0.57
1:B:129:GLN:N	1:B:129:GLN:OE1	2.38	0.57
2:C:258:ASN:OD1	2:C:259:ALA:N	2.38	0.56
7:H:93:ILE:HD13	7:H:110:ARG:HG3	1.87	0.56
8:I:168:ARG:O	8:I:172:PHE:HB3	2.05	0.56
8:I:300:LEU:O	8:I:304:HIS:ND1	2.39	0.56
12:N:56:HIS:NE2	12:N:58:MET:O	2.36	0.56
7:H:13:PHE:HE1	7:H:105:ILE:HG22	1.69	0.56
8:I:345:HIS:O	8:I:349:LEU:HD23	2.05	0.56
1:B:95:LEU:O	1:B:95:LEU:HD23	2.05	0.56
3:D:89:LEU:HD21	3:D:107:ARG:HH21	1.70	0.56
6:G:20:LYS:HD2	6:G:20:LYS:O	2.06	0.56
6:G:126:ARG:NH2	6:G:129:GLU:OE1	2.39	0.56
7:H:151:GLN:N	7:H:151:GLN:OE1	2.39	0.56
11:M:414:CYS:SG	11:M:415:ARG:N	2.79	0.56
6:G:83:GLU:N	6:G:83:GLU:OE1	2.38	0.56
8:I:551:CYS:SG	8:I:552:THR:N	2.78	0.56
7:H:50:MET:HE2	7:H:50:MET:N	2.19	0.56
11:M:319:ASP:OD1	11:M:344:ARG:NE	2.37	0.55
1:B:172:LEU:HD21	1:B:201:GLU:HB3	1.88	0.55
14:A:454:MET:N	14:A:454:MET:HE2	2.22	0.55
3:D:245:MET:O	3:D:249:LEU:HD23	2.06	0.55
8:I:259:GLU:N	8:I:259:GLU:OE1	2.40	0.55
7:H:97:GLN:N	7:H:97:GLN:OE1	2.39	0.54
8:I:168:ARG:O	8:I:172:PHE:CB	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:484:ALA:O	8:I:487:SER:OG	2.22	0.54
1:B:443:ALA:HB1	2:C:244:TYR:HB3	1.88	0.54
2:C:73:ASP:OD1	2:C:74:PHE:N	2.40	0.54
6:G:22:THR:HG22	6:G:22:THR:O	2.08	0.54
2:C:228:ILE:O	2:C:232:LEU:HD23	2.08	0.54
6:G:98:HIS:CE1	6:G:135:ALA:HB2	2.42	0.54
2:C:131:MET:HE2	2:C:131:MET:N	2.21	0.54
14:A:193:THR:O	14:A:194:SER:OG	2.24	0.54
7:H:13:PHE:CE1	7:H:105:ILE:HG22	2.43	0.54
14:A:79:LEU:HD11	14:A:98:LEU:HG	1.90	0.54
11:M:190:ASN:N	11:M:214:GLU:O	2.40	0.53
14:A:362:VAL:HG13	14:A:363:ARG:N	2.24	0.53
3:D:352:ILE:HD12	3:D:359:VAL:HG22	1.91	0.53
2:C:225:LYS:O	2:C:228:ILE:HG22	2.07	0.53
14:A:222:VAL:HG11	14:A:253:ALA:HB2	1.91	0.53
7:H:49:ASP:C	7:H:50:MET:HE2	2.33	0.53
14:A:36:VAL:HG23	14:A:36:VAL:O	2.09	0.52
1:B:210:ASN:OD1	1:B:211:ASN:N	2.43	0.52
3:D:137:LYS:O	3:D:137:LYS:NZ	2.25	0.52
6:G:101:ILE:HD11	6:G:120:LEU:HD11	1.91	0.52
3:D:206:GLN:O	3:D:210:GLU:OE1	2.27	0.52
14:A:96:ARG:O	14:A:100:GLU:OE1	2.28	0.52
11:M:344:ARG:NH2	12:N:45:ASN:OD1	2.43	0.52
2:C:206:GLU:OE1	14:A:448:ARG:NH2	2.43	0.51
11:M:223:VAL:HB	11:M:247:ALA:HB1	1.92	0.51
9:J:39:VAL:HG13	9:J:40:ASP:N	2.25	0.51
3:D:242:ARG:HH21	3:D:267:MET:HE2	1.76	0.51
14:A:139:LEU:O	14:A:143:GLU:OE1	2.29	0.51
5:F:302:MET:HE3	14:A:453:MET:HE3	1.92	0.51
9:J:75:CYS:SG	9:J:77:HIS:CG	2.87	0.51
11:M:102:ASP:OD1	11:M:103:GLU:N	2.43	0.51
1:B:428:THR:HG22	14:A:442:MET:HE1	1.91	0.51
3:D:195:LEU:HD21	3:D:203:GLU:HB2	1.93	0.50
6:G:147:GLN:O	6:G:147:GLN:HG3	2.10	0.50
5:F:265:HIS:ND1	6:G:106:SER:O	2.45	0.50
14:A:89:ASP:O	14:A:93:GLU:OE1	2.29	0.50
1:B:93:LYS:HA	1:B:96:LEU:HD23	1.94	0.50
10:L:61:TRP:O	10:L:65:HIS:ND1	2.42	0.50
3:D:169:ASN:OD1	9:J:39:VAL:HG21	2.11	0.50
3:D:286:MET:SD	3:D:287:PRO:HD2	2.52	0.50
11:M:409:ILE:HG23	11:M:409:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:218:VAL:O	14:A:222:VAL:HG23	2.12	0.50
1:B:77:LYS:NZ	15:B:501:IHP:O42	2.38	0.49
2:C:86:SER:O	2:C:89:ASN:ND2	2.43	0.49
2:C:343:GLU:OE1	7:H:120:LEU:HD13	2.12	0.49
1:B:228:ILE:HG13	1:B:228:ILE:O	2.11	0.49
6:G:217:LYS:HA	6:G:217:LYS:HE2	1.94	0.49
10:L:59:ILE:O	10:L:63:THR:HG23	2.13	0.49
11:M:404:LYS:O	11:M:406:ASN:ND2	2.43	0.49
8:I:640:LEU:O	8:I:644:LEU:HD23	2.12	0.49
2:C:246:SER:O	2:C:249:VAL:HG22	2.13	0.49
8:I:586:SER:CB	8:I:605:THR:HG1	2.24	0.49
9:J:37:ILE:HD11	9:J:39:VAL:HG12	1.95	0.49
14:A:132:GLU:HA	14:A:135:ARG:CD	2.43	0.49
8:I:147:ARG:HD2	8:I:147:ARG:O	2.11	0.48
8:I:540:LEU:HD23	8:I:545:TRP:CD2	2.48	0.48
11:M:395:THR:HG23	11:M:401:ILE:HD13	1.94	0.48
2:C:314:PHE:CD2	2:C:317:LEU:HD21	2.48	0.48
2:C:275:LEU:C	2:C:275:LEU:HD23	2.38	0.48
14:A:335:GLU:O	14:A:336:SER:OG	2.27	0.48
2:C:182:LEU:HB3	2:C:219:ILE:HG21	1.95	0.48
8:I:621:THR:OG1	8:I:624:GLN:OE1	2.32	0.48
10:L:103:LEU:HD21	10:L:115:LEU:HD21	1.95	0.48
1:B:189:LYS:NZ	1:B:190:LYS:O	2.47	0.48
3:D:219:GLU:O	3:D:223:LEU:HD12	2.14	0.48
5:F:302:MET:HE3	14:A:453:MET:CE	2.43	0.48
2:C:314:PHE:CE2	2:C:317:LEU:HD21	2.48	0.48
8:I:406:ASN:N	8:I:409:THR:OG1	2.41	0.48
1:B:80:PHE:HB2	1:B:88:MET:HE1	1.95	0.47
2:C:228:ILE:HD11	2:C:238:VAL:HG22	1.96	0.47
3:D:30:LEU:CD2	3:D:65:LEU:HD11	2.43	0.47
6:G:168:ASN:OD1	6:G:169:ASN:N	2.47	0.47
14:A:51:TYR:HE1	14:A:81:PHE:HB3	1.78	0.47
2:C:357:MET:HE2	14:A:420:HIS:HB2	1.95	0.47
3:D:123:ALA:O	3:D:127:LEU:HD23	2.13	0.47
8:I:723:LYS:O	8:I:724:VAL:HG23	2.14	0.47
11:M:184:GLN:OE1	11:M:184:GLN:N	2.47	0.47
1:B:123:LYS:HG3	1:B:124:GLN:H	1.80	0.47
11:M:374:GLY:O	11:M:377:GLN:NE2	2.46	0.47
14:A:298:LEU:HG	14:A:369:ILE:HD12	1.95	0.47
8:I:173:ARG:CB	8:I:174:PRO:HD3	2.45	0.47
8:I:281:GLU:O	8:I:282:SER:OG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:731:LEU:O	8:I:735:LEU:HD13	2.15	0.47
2:C:318:SER:OG	2:C:357:MET:SD	2.65	0.47
5:F:224:GLN:HA	5:F:224:GLN:OE1	2.15	0.47
8:I:318:ASP:OD1	8:I:319:LEU:N	2.48	0.47
8:I:374:HIS:ND1	8:I:378:ASN:OD1	2.47	0.47
1:B:72:LEU:HD11	1:B:98:TYR:CE2	2.50	0.46
8:I:442:LEU:O	8:I:446:LEU:HD23	2.15	0.46
8:I:42:TYR:CD1	8:I:136:ILE:HD11	2.49	0.46
1:B:38:ASN:O	1:B:42:LEU:HD13	2.15	0.46
3:D:352:ILE:CD1	3:D:359:VAL:HG22	2.45	0.46
2:C:123:ILE:HG13	2:C:124:LEU:HD12	1.97	0.46
3:D:352:ILE:HD13	3:D:359:VAL:HG13	1.98	0.46
6:G:66:LEU:HD11	6:G:88:LEU:HD11	1.97	0.46
7:H:34:PRO:N	7:H:35:PRO:HD2	2.31	0.46
2:C:275:LEU:HD22	2:C:299:LEU:HD23	1.98	0.46
2:C:322:MET:O	2:C:326:VAL:HG22	2.16	0.46
3:D:384:LEU:O	3:D:384:LEU:HD23	2.16	0.45
9:J:46:ARG:HG3	9:J:46:ARG:HH11	1.81	0.45
3:D:282:ALA:O	3:D:290:LYS:NZ	2.47	0.45
11:M:198:LEU:HG	11:M:202:LEU:HD23	1.97	0.45
14:A:280:PHE:N	14:A:281:PRO:HD2	2.31	0.45
8:I:601:LEU:HD21	8:I:682:VAL:HG21	1.97	0.45
10:L:47:LEU:HB3	10:L:50:VAL:HG12	1.98	0.45
10:L:101:PHE:O	10:L:105:LEU:HD13	2.17	0.45
3:D:111:ALA:HB1	3:D:127:LEU:HD21	1.98	0.45
8:I:483:ASP:OD1	8:I:483:ASP:N	2.48	0.45
14:A:146:ASP:OD1	14:A:147:THR:N	2.49	0.45
1:B:172:LEU:HD21	1:B:201:GLU:CB	2.46	0.45
3:D:385:LEU:HD22	5:F:234:ARG:HG3	1.99	0.45
9:J:49:ILE:HG23	9:J:50:MET:HG3	1.98	0.45
14:A:143:GLU:O	14:A:146:ASP:OD1	2.35	0.45
8:I:479:SER:OG	8:I:480:ALA:N	2.50	0.45
3:D:234:ILE:HG21	3:D:281:PHE:CE2	2.52	0.45
8:I:168:ARG:O	8:I:169:ASP:C	2.56	0.45
2:C:386:LEU:HD21	14:A:450:ALA:HB1	1.99	0.44
14:A:299:ALA:HB2	14:A:369:ILE:HD11	2.00	0.44
14:A:345:LEU:HD12	14:A:366:TYR:CZ	2.51	0.44
1:B:72:LEU:HD13	1:B:95:LEU:CD2	2.47	0.44
3:D:123:ALA:O	3:D:126:VAL:HG22	2.17	0.44
12:N:38:MET:HE1	12:N:46:LEU:CD1	2.48	0.44
7:H:35:PRO:O	7:H:39:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:376:LYS:C	8:I:376:LYS:HD2	2.43	0.44
14:A:311:ILE:HD11	14:A:331:PHE:CE1	2.53	0.44
8:I:172:PHE:O	8:I:173:ARG:C	2.60	0.44
8:I:605:THR:HA	8:I:608:MET:HB2	1.98	0.44
3:D:384:LEU:HD22	5:F:238:ILE:HD12	1.99	0.44
5:F:300:ASN:C	5:F:300:ASN:HD22	2.26	0.44
7:H:33:THR:O	7:H:36:VAL:HG12	2.17	0.44
8:I:369:THR:O	8:I:372:ASP:OD1	2.35	0.44
12:N:24:LEU:HD11	12:N:67:LEU:HD11	1.98	0.44
1:B:425:ASP:O	1:B:428:THR:OG1	2.29	0.44
3:D:323:GLU:OE1	6:G:147:GLN:NE2	2.47	0.44
7:H:50:MET:HE2	7:H:50:MET:CA	2.48	0.44
14:A:459:VAL:HG23	14:A:464:ILE:HD12	1.99	0.44
3:D:252:ASP:OD1	3:D:253:GLU:N	2.51	0.44
2:C:249:VAL:HG12	2:C:253:ILE:HD13	2.00	0.44
3:D:92:ILE:HG22	3:D:92:ILE:O	2.17	0.43
11:M:366:GLN:NE2	11:M:391:SER:O	2.51	0.43
11:M:367:VAL:N	11:M:389:ASN:OD1	2.47	0.43
6:G:167:ILE:HD12	6:G:167:ILE:H	1.84	0.43
3:D:366:ALA:O	3:D:369:THR:OG1	2.25	0.43
7:H:73:GLY:O	7:H:76:SER:OG	2.27	0.43
8:I:148:GLU:O	8:I:149:CYS:C	2.61	0.43
8:I:172:PHE:O	8:I:176:ASN:CB	2.66	0.43
14:A:88:VAL:O	14:A:92:GLU:OE1	2.37	0.43
8:I:27:GLY:O	8:I:31:VAL:HG23	2.18	0.43
11:M:227:ALA:HB1	11:M:254:SER:OG	2.18	0.43
14:A:454:MET:HE2	14:A:454:MET:CA	2.49	0.43
1:B:238:ARG:NH2	1:B:257:ASP:OD1	2.52	0.43
1:B:435:ASN:HA	1:B:438:VAL:HG12	2.00	0.43
2:C:332:GLN:OE1	2:C:332:GLN:HA	2.19	0.43
8:I:563:TYR:HH	8:I:581:TRP:CD1	2.37	0.43
3:D:374:ILE:HG23	4:E:328:PHE:HE1	1.84	0.43
5:F:221:LEU:HD12	6:G:188:ILE:HG23	2.01	0.43
2:C:217:SER:O	2:C:220:MET:N	2.50	0.43
2:C:228:ILE:CD1	2:C:238:VAL:HG22	2.49	0.43
8:I:243:PHE:O	8:I:247:GLU:OE1	2.37	0.43
8:I:349:LEU:HD22	8:I:402:PHE:CD1	2.53	0.42
11:M:192:VAL:HG13	11:M:192:VAL:O	2.18	0.42
1:B:336:ASN:OD1	1:B:337:ILE:N	2.52	0.42
3:D:151:ILE:HG12	3:D:155:TYR:CE2	2.54	0.42
8:I:446:LEU:HD11	8:I:488:MET:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:159:TRP:O	11:M:145:LYS:NZ	2.50	0.42
11:M:105:LEU:HB2	11:M:130:LEU:HD21	2.00	0.42
1:B:424:LEU:O	1:B:428:THR:HG23	2.19	0.42
10:L:92:PHE:CD1	10:L:92:PHE:C	2.97	0.42
14:A:89:ASP:OD1	14:A:90:MET:N	2.46	0.42
14:A:205:VAL:HA	14:A:208:VAL:HG12	2.01	0.42
11:M:321:VAL:HG22	11:M:321:VAL:O	2.19	0.42
14:A:91:TYR:OH	14:A:127:ASP:OD1	2.33	0.42
1:B:307:GLU:N	1:B:307:GLU:OE1	2.52	0.42
11:M:171:ASP:OD1	11:M:172:GLN:NE2	2.52	0.42
2:C:399:VAL:O	2:C:399:VAL:HG12	2.18	0.42
9:J:49:ILE:O	9:J:80:HIS:NE2	2.53	0.42
14:A:364:THR:HG23	14:A:365:LEU:N	2.35	0.42
8:I:508:PHE:O	8:I:511:ILE:HG22	2.19	0.42
8:I:523:LYS:O	8:I:526:THR:OG1	2.33	0.42
8:I:306:GLU:O	8:I:310:LEU:HD13	2.19	0.42
8:I:528:SER:OG	8:I:529:GLU:N	2.52	0.42
14:A:77:MET:O	14:A:80:SER:OG	2.25	0.42
3:D:374:ILE:HG23	4:E:328:PHE:CE1	2.55	0.42
3:D:385:LEU:HD22	5:F:234:ARG:CG	2.49	0.42
8:I:621:THR:CG2	8:I:668:LEU:HD22	2.48	0.42
11:M:258:LEU:HD12	11:M:258:LEU:O	2.19	0.42
14:A:151:ASN:OD1	14:A:151:ASN:C	2.62	0.42
14:A:89:ASP:O	14:A:90:MET:C	2.63	0.41
14:A:128:THR:O	14:A:132:GLU:OE1	2.38	0.41
3:D:69:PHE:CZ	3:D:73:LEU:HD21	2.55	0.41
3:D:209:ASN:C	3:D:209:ASN:OD1	2.63	0.41
3:D:352:ILE:HG22	3:D:353:ASP:N	2.35	0.41
4:E:315:ILE:HG23	7:H:200:LEU:HD12	2.01	0.41
5:F:217:VAL:O	5:F:217:VAL:HG22	2.20	0.41
8:I:539:VAL:C	8:I:540:LEU:HD12	2.45	0.41
1:B:439:VAL:O	1:B:440:SER:OG	2.29	0.41
6:G:76:PRO:HA	6:G:79:ILE:HG12	2.01	0.41
14:A:145:LEU:O	14:A:148:ASP:OD1	2.38	0.41
14:A:222:VAL:HG13	14:A:249:LEU:HD11	2.02	0.41
2:C:62:LEU:CD2	2:C:77:LEU:HD11	2.50	0.41
3:D:271:ARG:NH2	6:G:137:TYR:O	2.54	0.41
14:A:157:ILE:O	14:A:160:SER:OG	2.38	0.41
11:M:151:VAL:O	11:M:155:LEU:HD13	2.20	0.41
1:B:123:LYS:HG3	1:B:124:GLN:N	2.36	0.41
1:B:402:ILE:HG22	1:B:409:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:52:TYR:O	8:I:55:SER:OG	2.30	0.41
8:I:172:PHE:O	8:I:176:ASN:N	2.35	0.41
11:M:189:SER:O	11:M:190:ASN:C	2.64	0.41
11:M:193:ILE:HD11	11:M:216:LEU:CD1	2.51	0.41
5:F:270:LEU:HD23	5:F:275:PHE:CD1	2.56	0.41
6:G:46:LEU:HD23	6:G:46:LEU:H	1.85	0.41
11:M:260:GLU:OE1	11:M:287:GLN:HB2	2.20	0.41
3:D:207:ARG:O	3:D:211:LEU:HD13	2.21	0.41
8:I:588:GLY:CA	8:I:608:MET:HE1	2.51	0.41
8:I:705:GLU:O	8:I:709:LEU:HD23	2.21	0.41
14:A:88:VAL:O	14:A:91:TYR:HB3	2.21	0.41
3:D:89:LEU:HD21	3:D:107:ARG:NH2	2.36	0.40
8:I:119:TYR:O	8:I:120:THR:C	2.64	0.40
11:M:190:ASN:OD1	11:M:190:ASN:O	2.39	0.40
3:D:125:GLN:O	3:D:128:VAL:HG12	2.21	0.40
3:D:195:LEU:HD21	3:D:203:GLU:CB	2.49	0.40
6:G:69:LEU:O	6:G:73:GLY:N	2.48	0.40
7:H:50:MET:HE2	7:H:50:MET:HA	2.02	0.40
2:C:190:MET:HE2	2:C:226:LYS:HE3	2.02	0.40
5:F:288:LEU:O	5:F:292:LEU:HD23	2.21	0.40
14:A:42:LEU:H	14:A:42:LEU:HD23	1.86	0.40
14:A:93:GLU:O	14:A:96:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	400/443 (90%)	374 (94%)	26 (6%)	0	100	100
2	C	346/423 (82%)	334 (96%)	12 (4%)	0	100	100
3	D	379/406 (93%)	363 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	86/334 (26%)	84 (98%)	2 (2%)	0	100	100
5	F	97/327 (30%)	94 (97%)	3 (3%)	0	100	100
6	G	212/264 (80%)	206 (97%)	6 (3%)	0	100	100
7	H	167/209 (80%)	162 (97%)	5 (3%)	0	100	100
8	I	599/776 (77%)	573 (96%)	25 (4%)	1 (0%)	43	73
9	J	75/108 (69%)	64 (85%)	11 (15%)	0	100	100
10	L	121/163 (74%)	109 (90%)	12 (10%)	0	100	100
11	M	322/424 (76%)	303 (94%)	19 (6%)	0	100	100
12	N	69/79 (87%)	68 (99%)	1 (1%)	0	100	100
13	P	19/57 (33%)	18 (95%)	1 (5%)	0	100	100
14	A	398/491 (81%)	378 (95%)	20 (5%)	0	100	100
All	All	3290/4504 (73%)	3130 (95%)	159 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	158	GLU

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	B	366/405 (90%)	366 (100%)	0	100	100
2	C	314/377 (83%)	314 (100%)	0	100	100
3	D	328/347 (94%)	328 (100%)	0	100	100
4	E	81/283 (29%)	81 (100%)	0	100	100
5	F	88/276 (32%)	88 (100%)	0	100	100
6	G	186/229 (81%)	186 (100%)	0	100	100
7	H	141/173 (82%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	I	432/698 (62%)	432 (100%)	0	100	100
9	J	70/90 (78%)	70 (100%)	0	100	100
10	L	115/150 (77%)	115 (100%)	0	100	100
11	M	299/392 (76%)	299 (100%)	0	100	100
12	N	68/76 (90%)	68 (100%)	0	100	100
13	P	19/45 (42%)	19 (100%)	0	100	100
14	A	320/429 (75%)	320 (100%)	0	100	100
All	All	2827/3970 (71%)	2827 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	370	HIS
1	B	404	GLN
2	C	105	HIS
2	C	180	HIS
2	C	239	GLN
2	C	320	GLN
2	C	353	GLN
3	D	72	HIS
3	D	218	HIS
6	G	98	HIS
6	G	169	ASN
6	G	202	HIS
7	H	68	ASN
8	I	176	ASN
8	I	347	GLN
11	M	172	GLN
11	M	190	ASN
11	M	289	ASN
14	A	447	GLN

5.3.3 RNA ⓘ

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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	IHP	B	501	-	36,36,36	0.69	1 (2%)	60,60,60	0.73	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	IHP	B	501	-	-	11/30/54/54	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	B	501	IHP	P3-O13	3.02	1.64	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	B	501	IHP	P6-O16-C6	2.63	130.47	123.43
15	B	501	IHP	P4-O14-C4	2.32	129.64	123.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

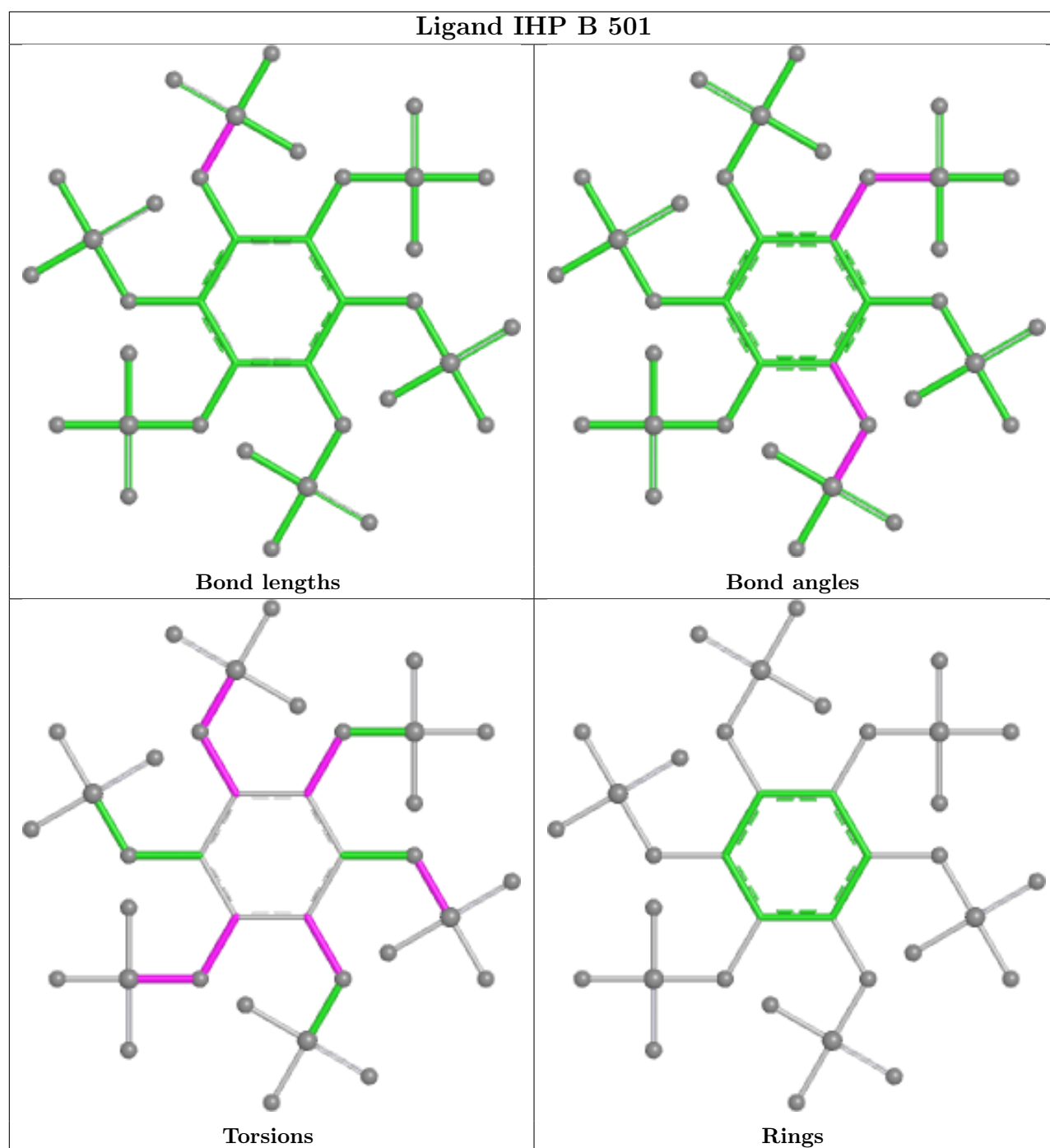
Mol	Chain	Res	Type	Atoms
15	B	501	IHP	C2-C1-O11-P1
15	B	501	IHP	C2-C3-O13-P3
15	B	501	IHP	C4-C3-O13-P3
15	B	501	IHP	C1-C6-O16-P6
15	B	501	IHP	C5-C6-O16-P6
15	B	501	IHP	C3-C4-O14-P4
15	B	501	IHP	C5-C4-O14-P4
15	B	501	IHP	C5-O15-P5-O25
15	B	501	IHP	C1-O11-P1-O21
15	B	501	IHP	C3-O13-P3-O43
15	B	501	IHP	C6-C1-O11-P1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	501	IHP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

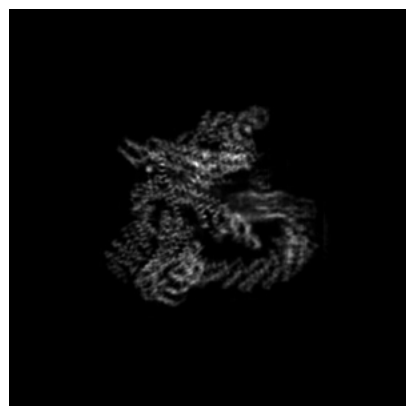
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53254. These allow visual inspection of the internal detail of the map and identification of artifacts.

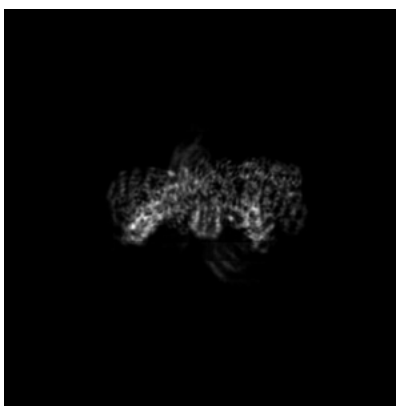
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

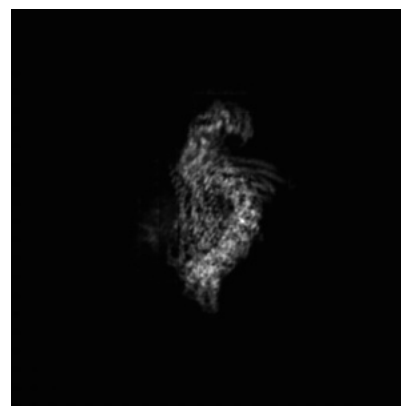
6.1.1 Primary map



X

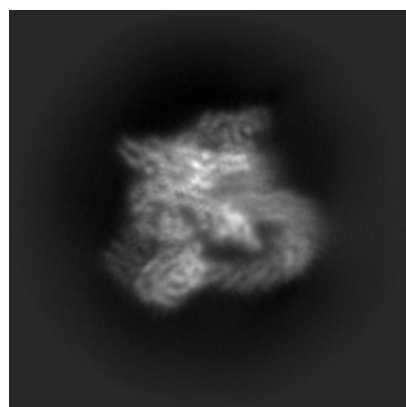


Y

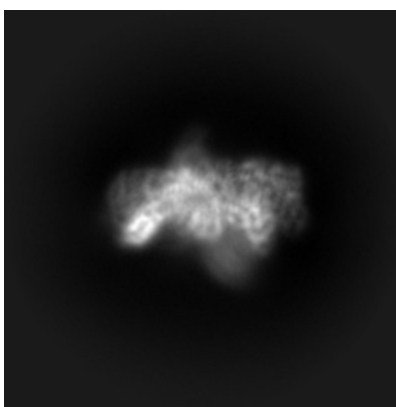


Z

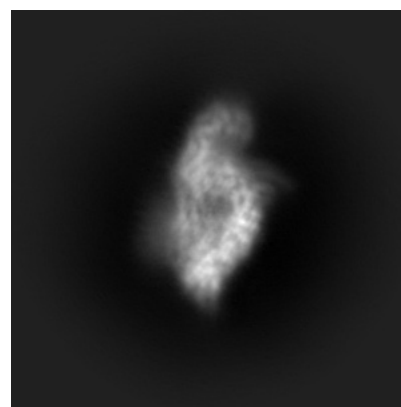
6.1.2 Raw map



X



Y



Z

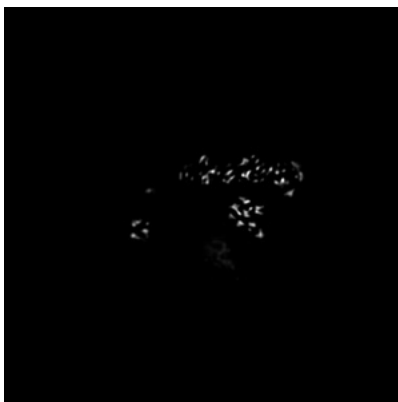
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160

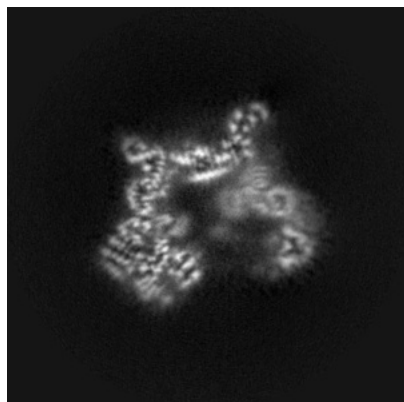


Y Index: 160



Z Index: 160

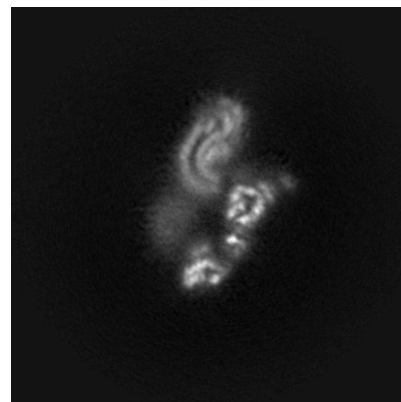
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

6.3 Largest variance slices [i](#)

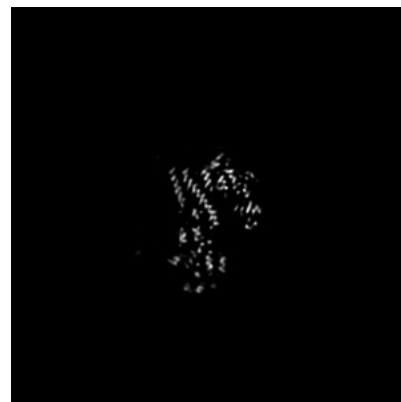
6.3.1 Primary map



X Index: 159

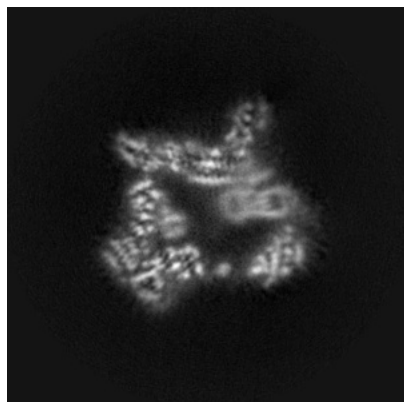


Y Index: 150

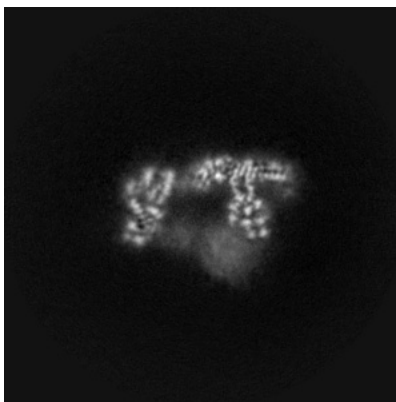


Z Index: 202

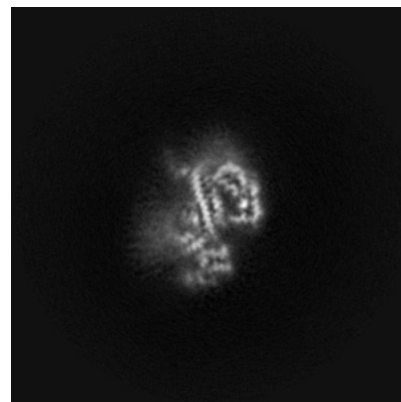
6.3.2 Raw map



X Index: 153



Y Index: 150

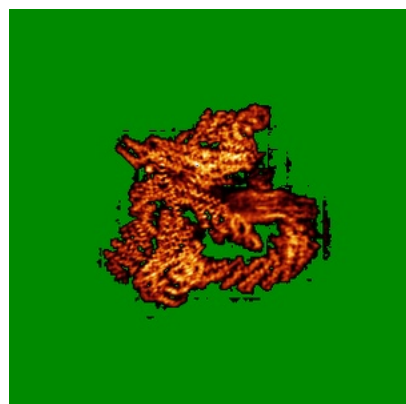


Z Index: 194

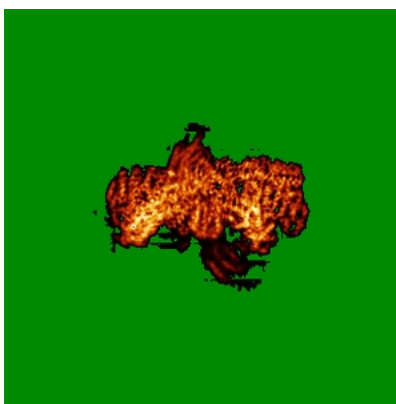
The images above show the largest variance slices of the map in three orthogonal directions.

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

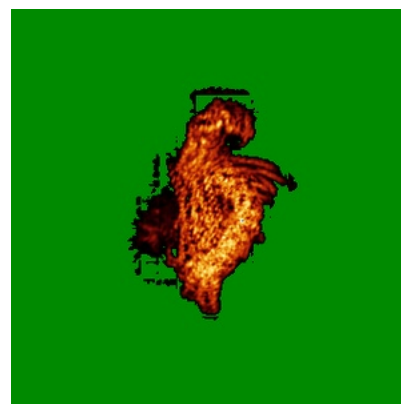
6.4.1 Primary map



X

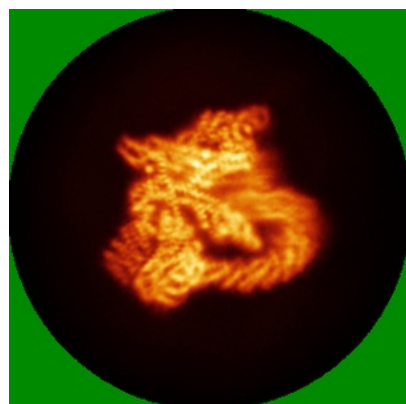


Y



Z

6.4.2 Raw map



X



Y

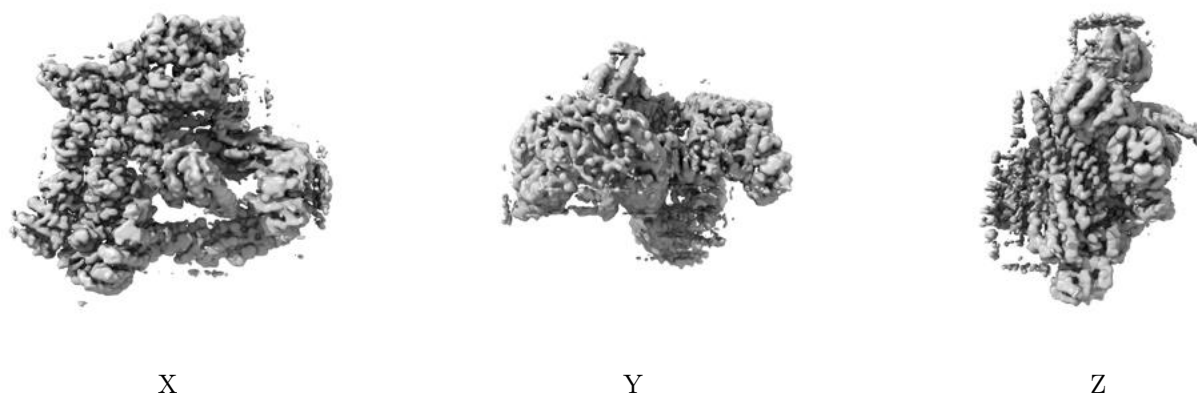


Z

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.

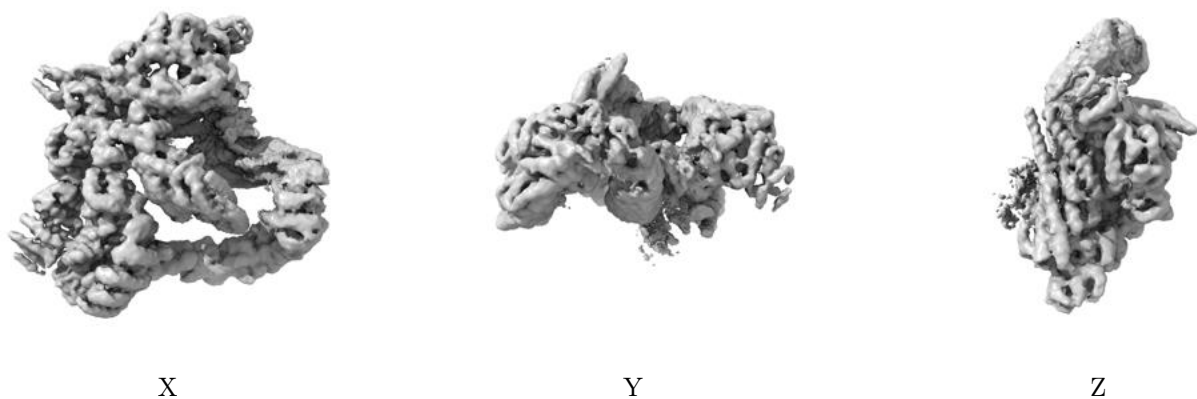
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0094. 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.

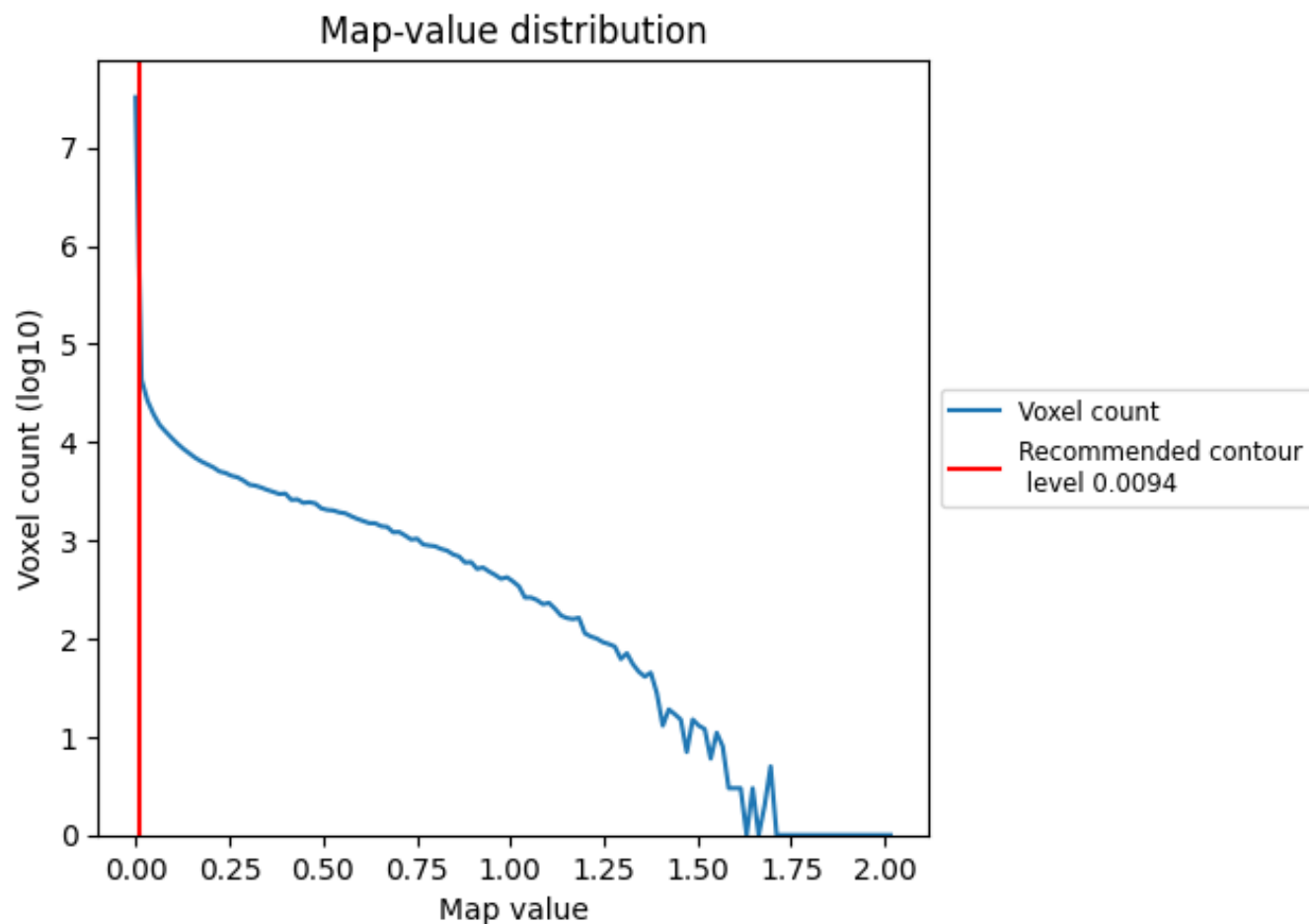
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

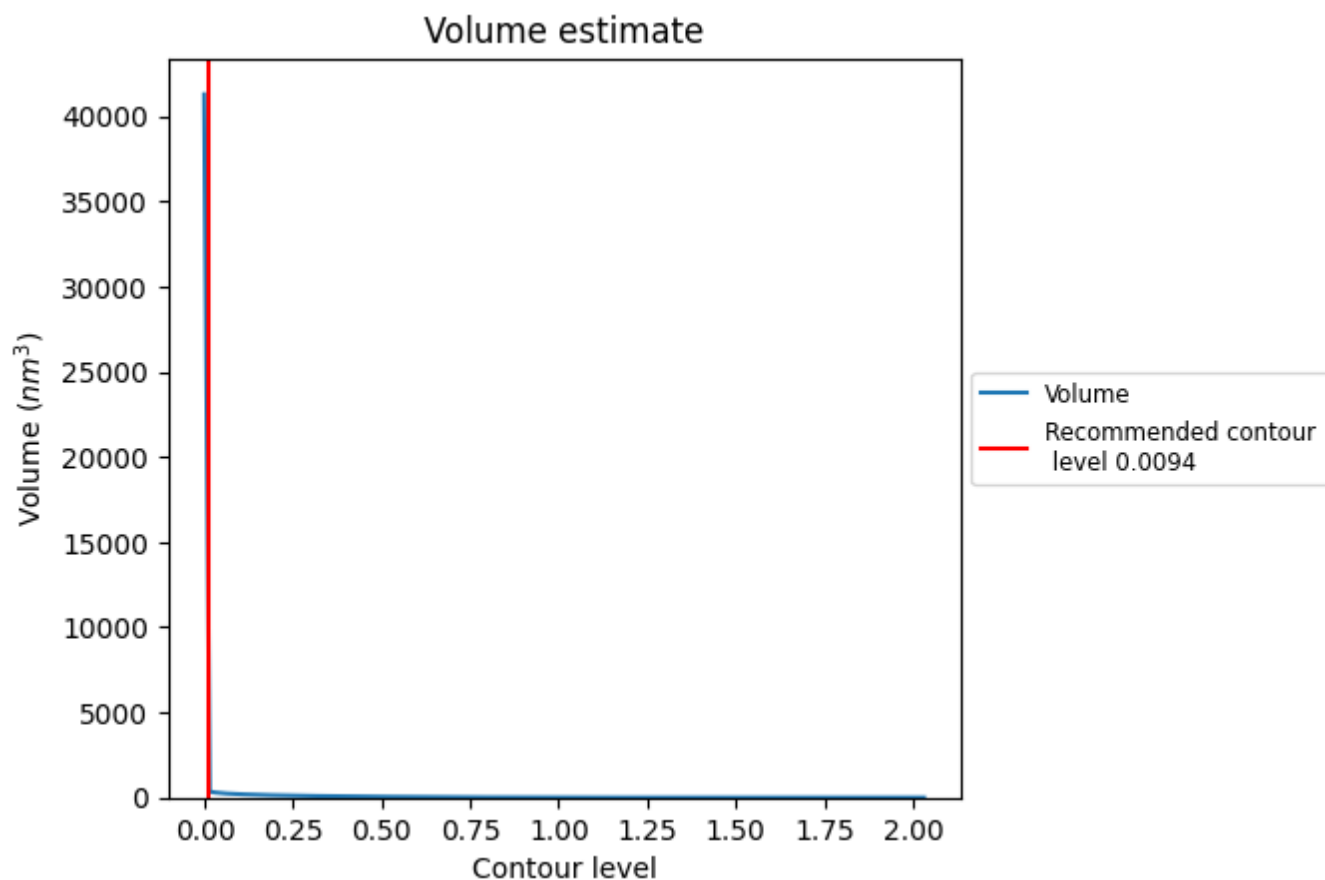
This section contains the results of statistical analysis of the map.

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.

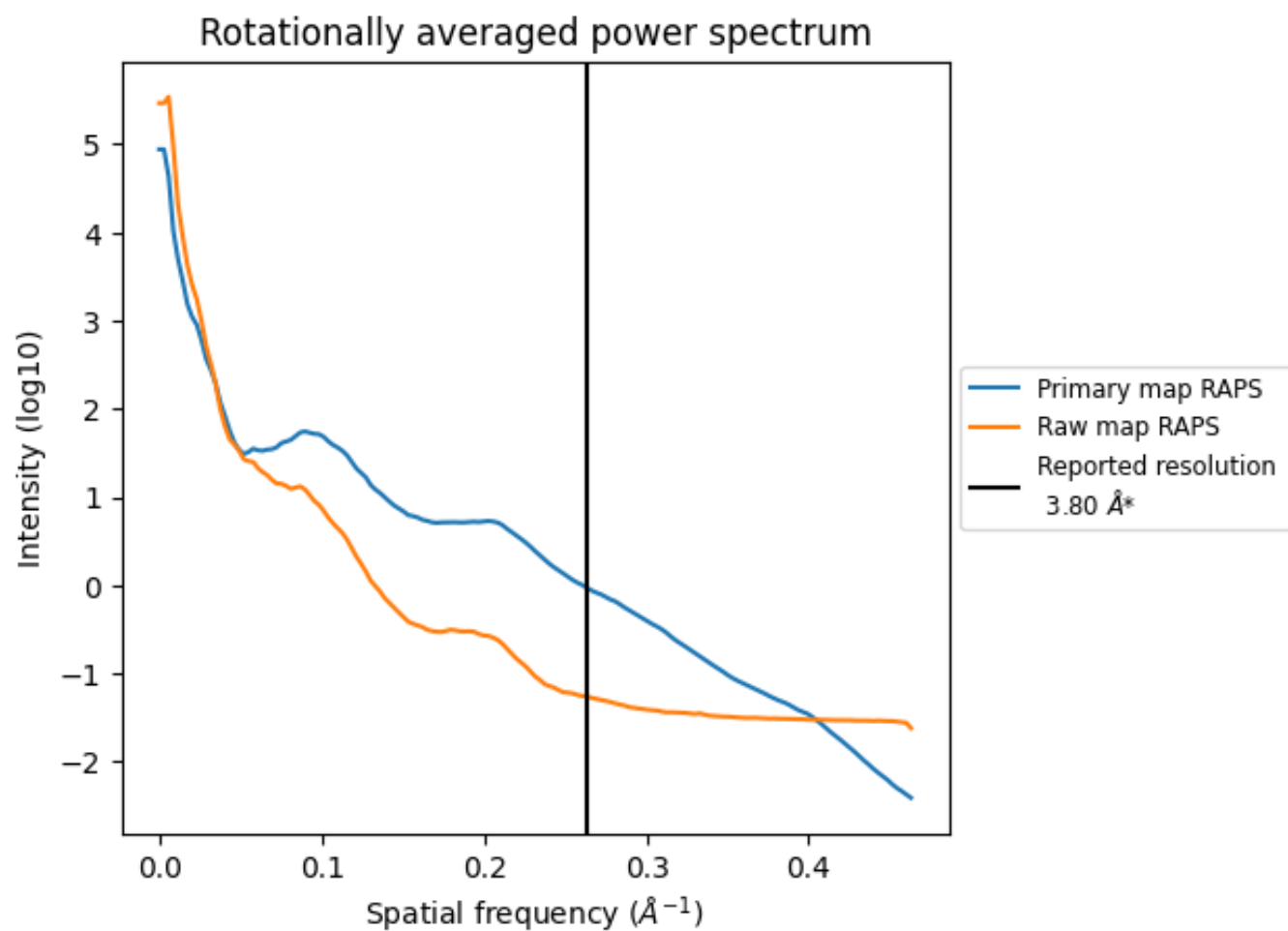
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 12845 nm³; this corresponds to an approximate mass of 11603 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 ⓘ

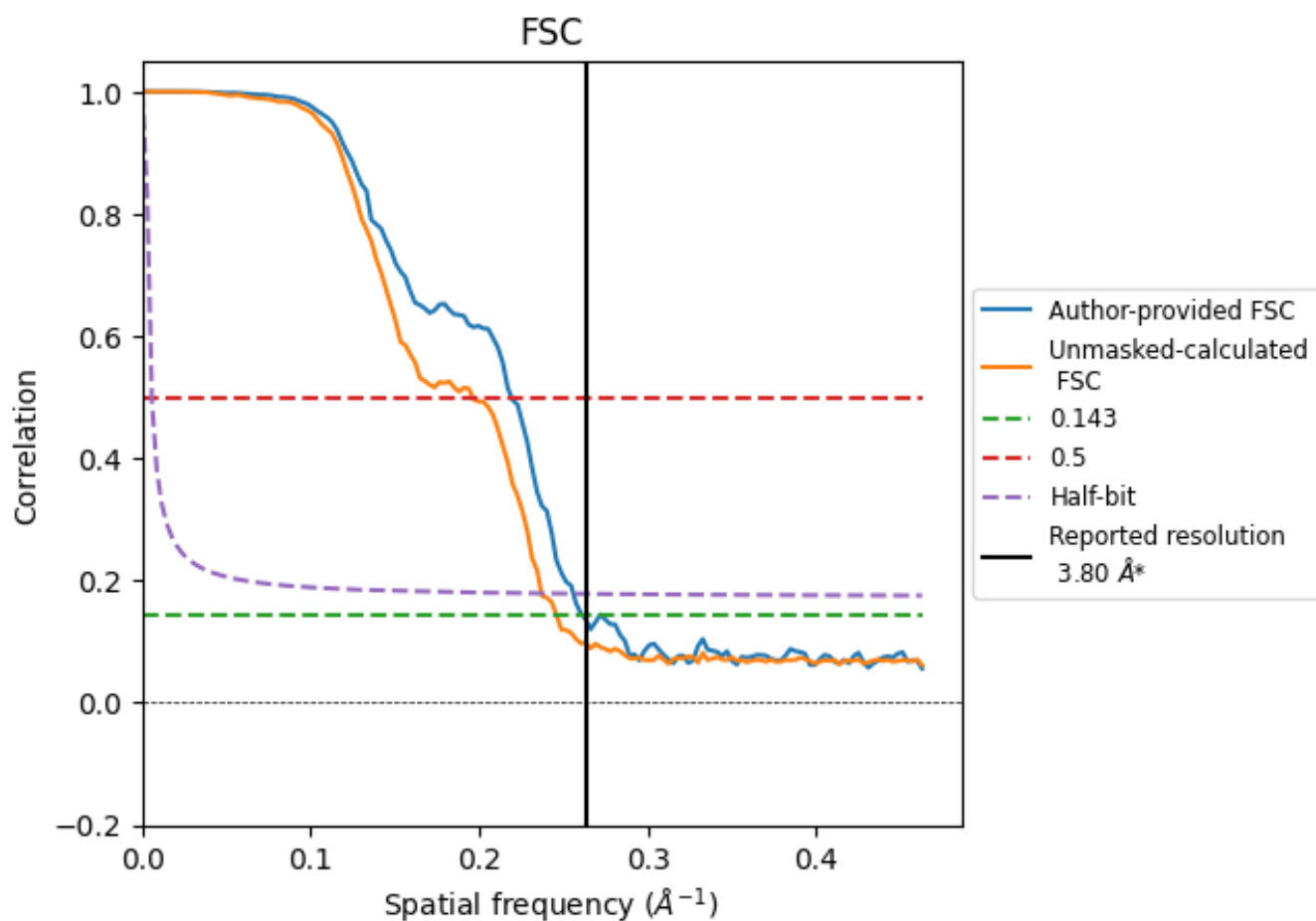


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

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 0.263 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.83	4.56	3.91
Unmasked-calculated*	4.07	5.10	4.22

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

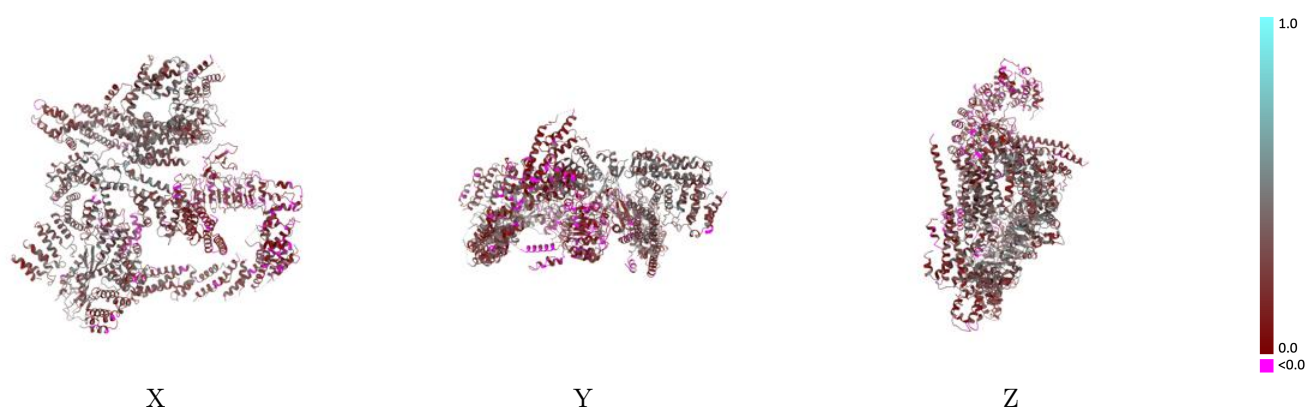
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53254 and PDB model 9QO2. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

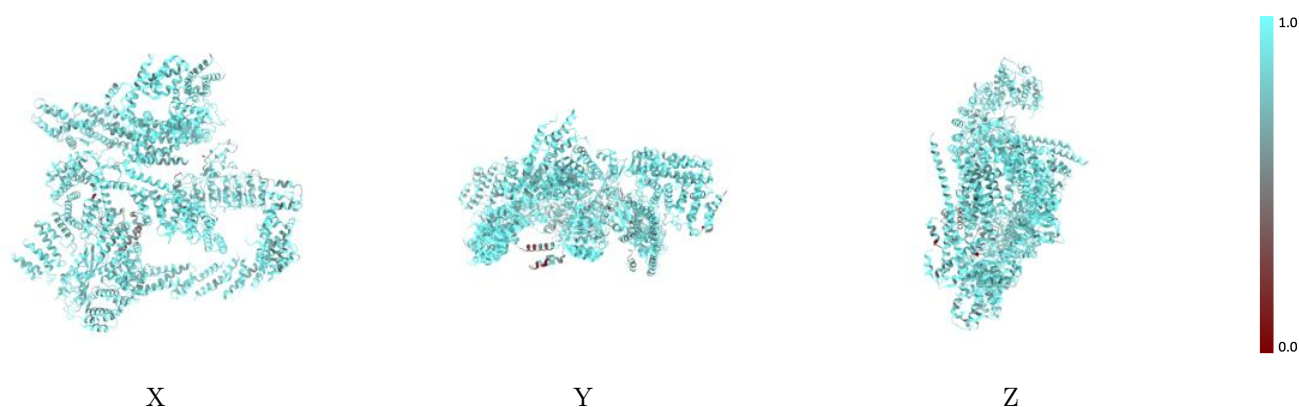
This section was not generated.

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



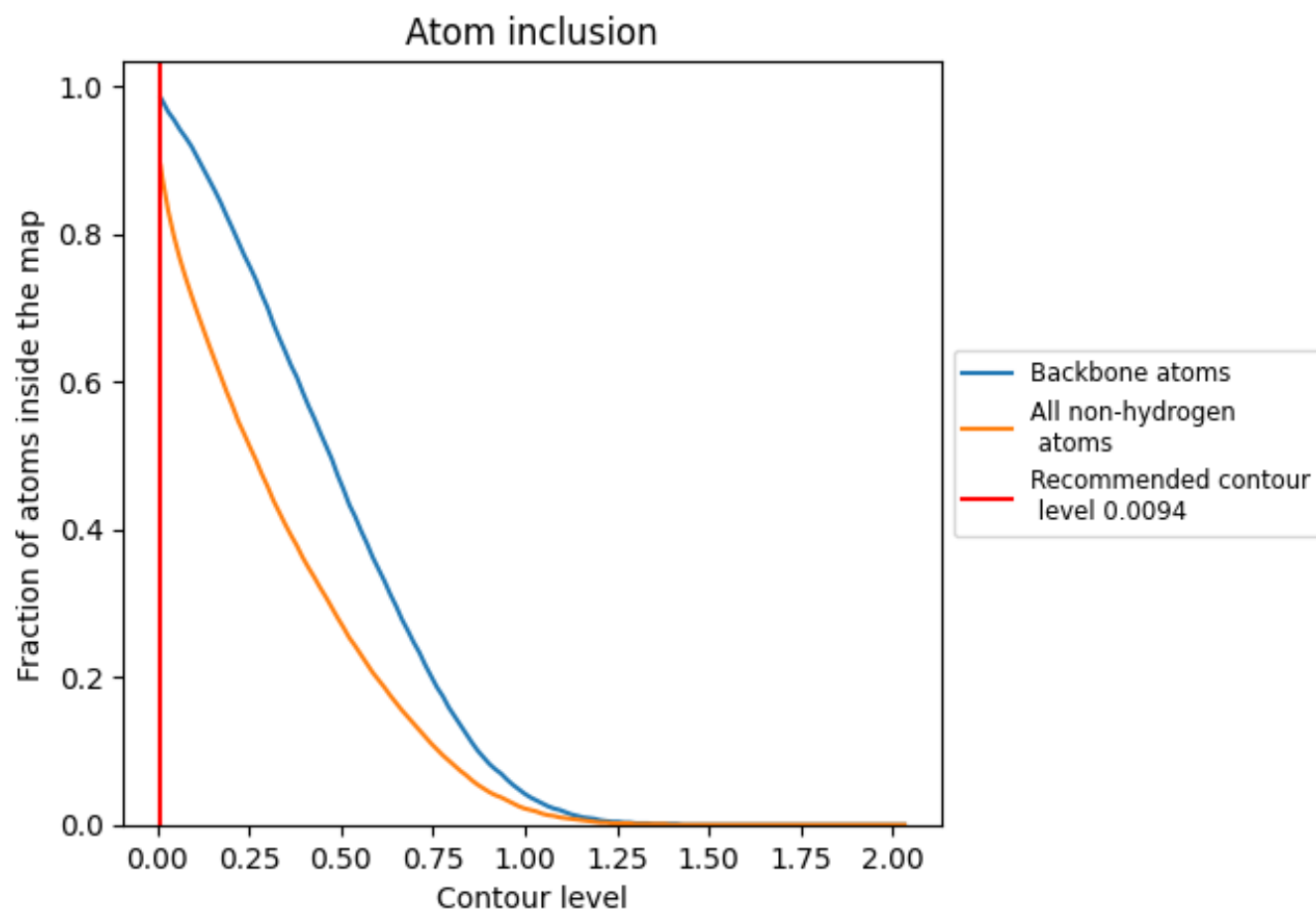
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0094).































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 89% 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 (0.0094) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.2800
A	 0.9330	 0.2910
B	 0.8930	 0.3150
C	 0.9350	 0.3650
D	 0.9080	 0.3270
E	 0.8410	 0.2320
F	 0.9260	 0.3140
G	 0.8650	 0.2640
H	 0.9220	 0.3390
I	 0.8920	 0.2790
J	 0.7210	 0.1600
L	 0.8230	 0.1370
M	 0.8850	 0.1640
N	 0.7700	 0.1650
P	 0.9110	 0.3580

