



## Full wwPDB EM Validation Report ⓘ

May 2, 2026 – 03:04 PM EDT

PDB ID : 9EG8 / pdb\_00009eg8  
EMDB ID : EMD-47986  
Title : Cryo-EM structure of COP9 signalosome precatalytic state with neddylated cullin-4A  
Authors : Shi, H.; Zheng, N.  
Deposited on : 2024-11-21  
Resolution : 3.39 Å(reported)  
Based on initial model : 4D10

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

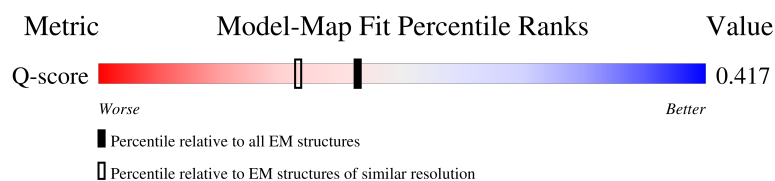
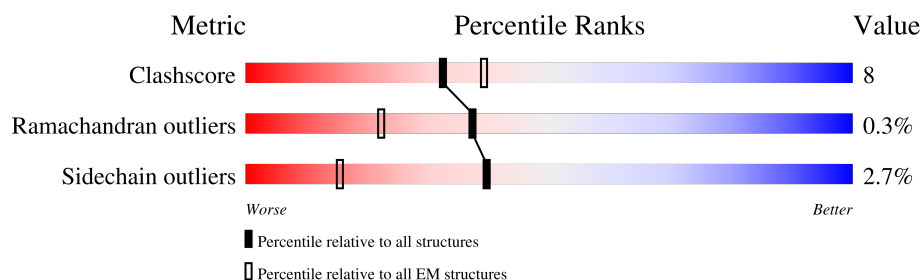
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.39 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	14220 ( 2.89 - 3.89 )

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  $\geq 3$ , 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	E	334	
2	I	81	
3	J	759	
4	A	491	

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Mol	Chain	Length	Quality of chain
5	B	443	
6	C	423	
7	D	406	
8	F	327	
9	G	264	
10	H	209	
11	K	108	

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 24745 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 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	294	Total	C	N	O	S	0	0
			2330	1489	390	437	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	76	ALA	GLU	engineered mutation	UNP Q92905
E	151	ASN	ASP	engineered mutation	UNP Q92905

- Molecule 2 is a protein called NEDD8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	76	Total	C	N	O	S	0	0
			599	378	104	115	2		

- Molecule 3 is a protein called Cullin-4A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	338	Total	C	N	O	S	0	0
			2754	1764	473	500	17		

- Molecule 4 is a protein called COP9 signalosome complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	409	Total	C	N	O	S	0	0
			3271	2066	573	610	22		

- Molecule 5 is a protein called COP9 signalosome complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	408	Total	C	N	O	S	0	0
			3342	2126	574	627	15		

- Molecule 6 is a protein called COP9 signalosome complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	405	Total	C	N	O	S	0	0
			3222	2051	541	604	26		

- Molecule 7 is a protein called COP9 signalosome complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	405	Total	C	N	O	S	0	0
			3241	2042	564	619	16		

- Molecule 8 is a protein called COP9 signalosome complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	280	Total	C	N	O	S	0	0
			2229	1422	371	423	13		

- Molecule 9 is a protein called COP9 signalosome complex subunit 7b.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	213	Total	C	N	O	S	0	0
			1687	1070	287	324	6		

- Molecule 10 is a protein called COP9 signalosome complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	172	Total	C	N	O	S	0	0
			1374	880	239	251	4		

- Molecule 11 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	82	Total	C	N	O	S	0	0
			693	443	127	114	9		

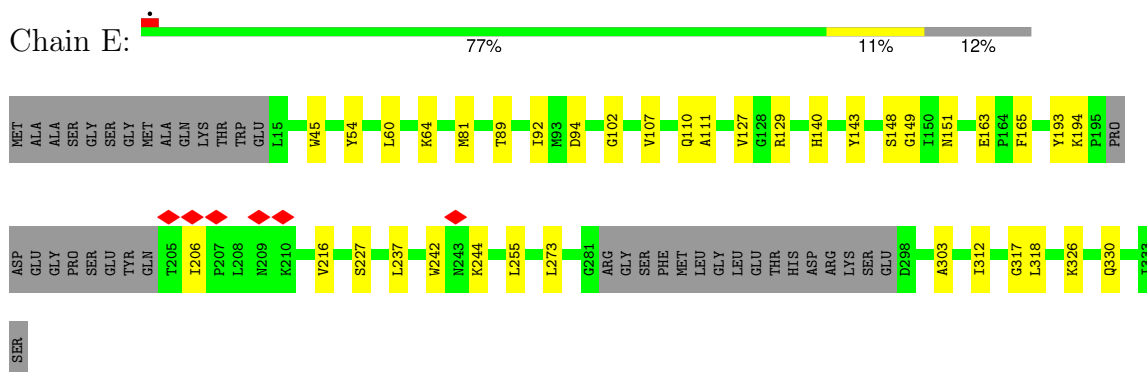
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
12	K	3	Total	Zn	0
			3	3	

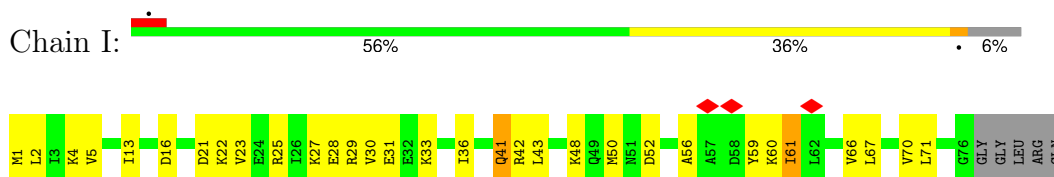
### 3 Residue-property plots

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.

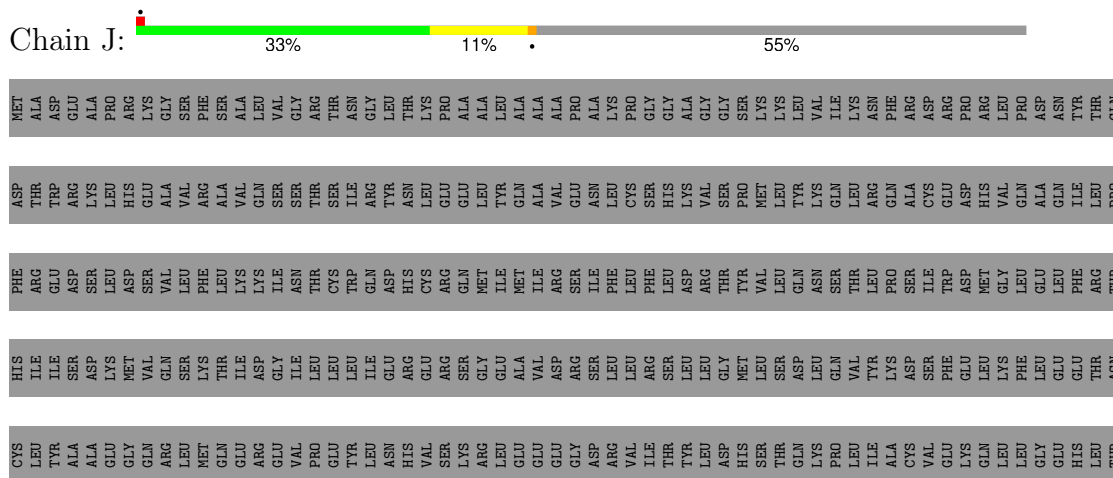
- Molecule 1: COP9 signalosome complex subunit 5

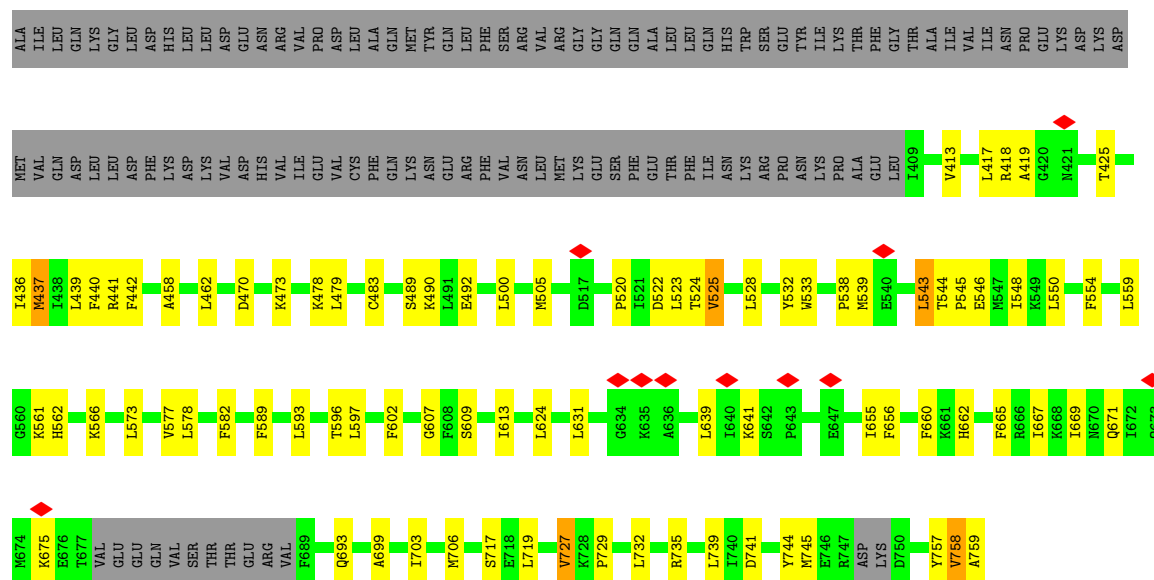


- Molecule 2: NEDD8

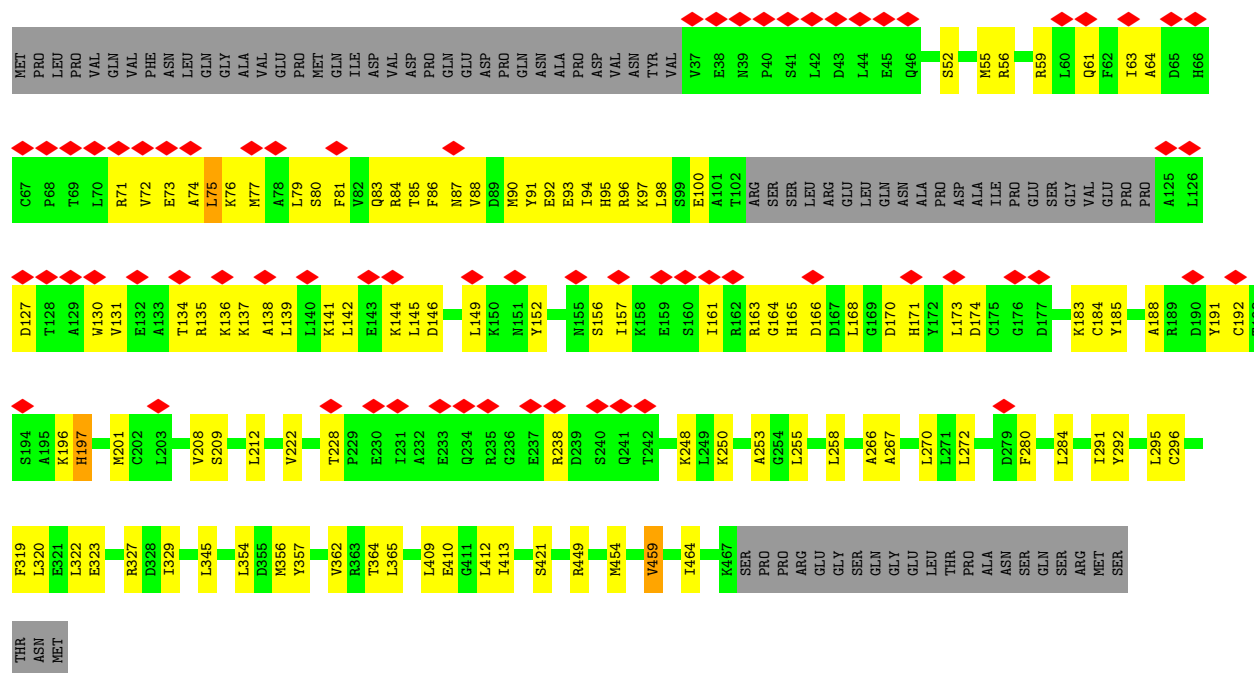


- Molecule 3: Cullin-4A

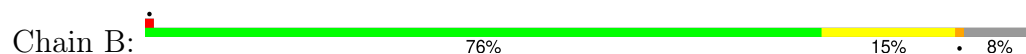


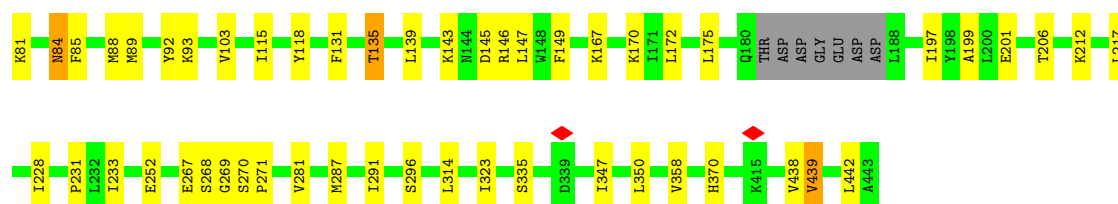


• Molecule 4: COP9 signalosome complex subunit 1

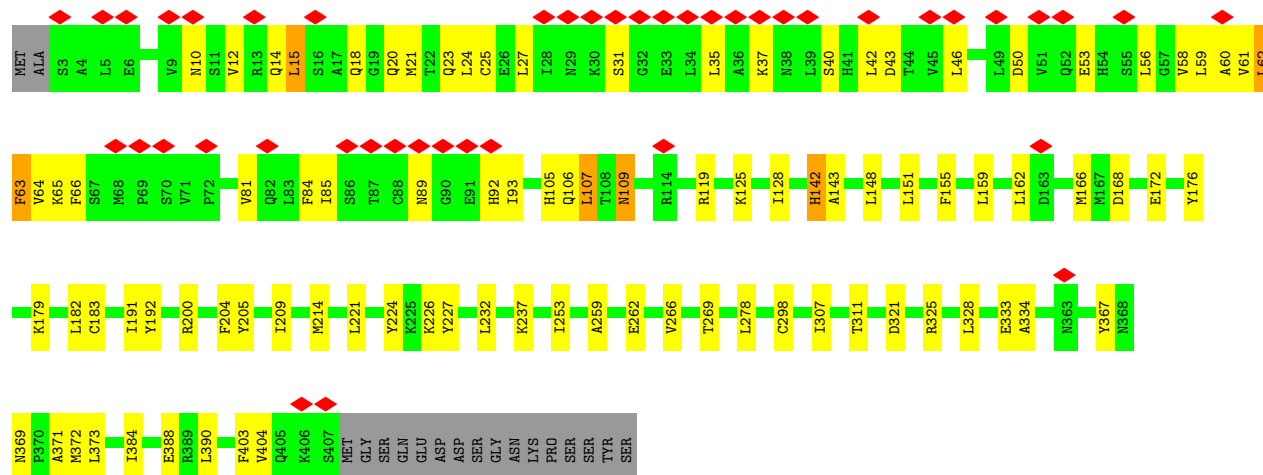
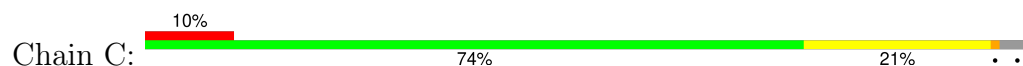


• Molecule 5: COP9 signalosome complex subunit 2

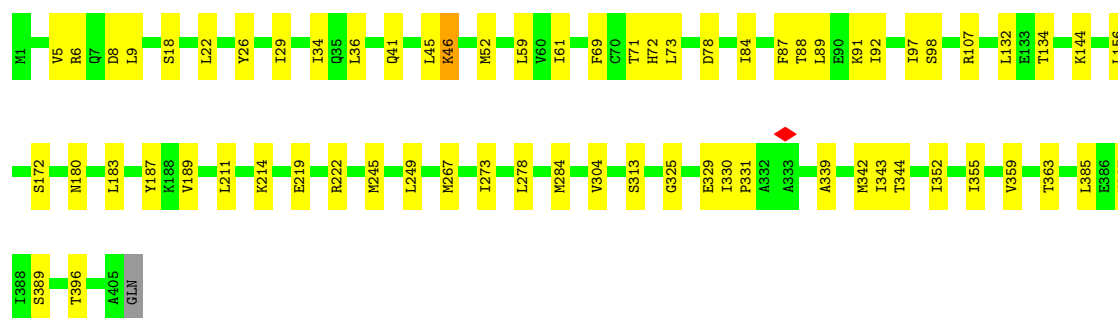
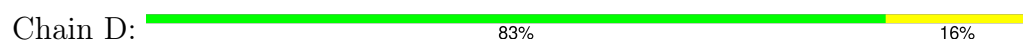




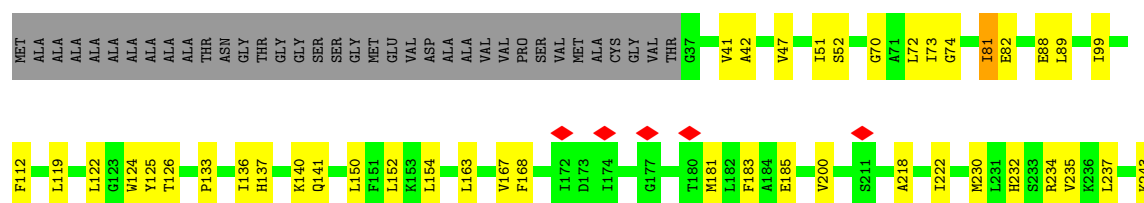
• Molecule 6: COP9 signalosome complex subunit 3



• Molecule 7: COP9 signalosome complex subunit 4



• Molecule 8: COP9 signalosome complex subunit 6







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	163795	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 ( $e^-/\text{\AA}^2$ )	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.416	Depositor
Minimum map value	-0.391	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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	E	0.11	0/2377	0.25	0/3210
2	I	0.16	0/604	0.39	0/808
3	J	0.13	0/2804	0.36	0/3745
4	A	0.15	0/3324	0.41	0/4478
5	B	0.21	0/3399	0.38	0/4571
6	C	0.13	0/3281	0.33	0/4431
7	D	0.13	0/3293	0.28	0/4448
8	F	0.12	0/2276	0.28	0/3085
9	G	0.13	0/1707	0.30	0/2309
10	H	0.15	0/1407	0.39	0/1912
11	K	0.11	0/713	0.34	0/965
All	All	0.14	0/25185	0.34	0/33962

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	E	2330	0	2322	25	0
2	I	599	0	638	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	2754	0	2806	56	0
4	A	3271	0	3309	81	0
5	B	3342	0	3397	52	0
6	C	3222	0	3243	62	0
7	D	3241	0	3245	48	0
8	F	2229	0	2211	35	0
9	G	1687	0	1730	23	0
10	H	1374	0	1360	28	0
11	K	693	0	656	17	0
12	K	3	0	0	0	0
All	All	24745	0	24917	421	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 8.

All (421) 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)
4:A:91:TYR:O	4:A:95:HIS:HB3	1.59	1.02
11:K:53:CYS:SG	11:K:56:CYS:HB2	2.12	0.88
6:C:15:LEU:HA	6:C:23:GLN:HE22	1.43	0.84
4:A:94:ILE:HA	4:A:97:LYS:HD2	1.59	0.81
3:J:739:LEU:HD23	3:J:745:MET:HE2	1.60	0.81
3:J:578:LEU:HD21	3:J:596:THR:HG23	1.65	0.77
5:B:72:LEU:HD13	5:B:75:MET:HE3	1.66	0.77
11:K:42:CYS:SG	11:K:80:HIS:CE1	2.78	0.76
1:E:54:TYR:HB2	1:E:89:THR:HG22	1.69	0.74
8:F:181:MET:HE3	8:F:181:MET:HA	1.70	0.73
4:A:61:GLN:HG2	4:A:71:ARG:HH22	1.55	0.71
4:A:454:MET:HE2	6:C:390:LEU:HG	1.74	0.69
7:D:69:PHE:O	7:D:73:LEU:HB2	1.93	0.69
5:B:172:LEU:HG	5:B:197:ILE:HD11	1.75	0.68
5:B:287:MET:HE1	11:K:98:ASN:HD21	1.58	0.68
4:A:171:HIS:HA	4:A:174:ASP:HB3	1.76	0.67
6:C:20:GLN:HB3	6:C:23:GLN:HE21	1.60	0.67
1:E:312:ILE:HG12	10:H:204:VAL:HG23	1.76	0.67
6:C:66:PHE:HD2	6:C:106:GLN:HG3	1.60	0.66
7:D:132:LEU:HD12	7:D:144:LYS:HG2	1.76	0.66
7:D:325:GLY:HA3	7:D:331:PRO:HA	1.77	0.66
6:C:62:LEU:HA	6:C:65:LYS:HD3	1.77	0.65
3:J:639:LEU:HD21	3:J:656:PHE:HA	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:137:LYS:O	4:A:141:LYS:HG2	1.97	0.65
6:C:84:PHE:HE1	6:C:93:ILE:HD12	1.62	0.65
4:A:76:LYS:HA	4:A:79:LEU:HD12	1.78	0.65
4:A:90:MET:H	4:A:90:MET:HE3	1.62	0.64
4:A:449:ARG:HG2	5:B:439:VAL:HG21	1.79	0.64
5:B:71:ALA:O	5:B:75:MET:HG2	1.98	0.64
4:A:131:VAL:O	4:A:135:ARG:HB2	1.98	0.64
8:F:47:VAL:O	8:F:51:ILE:HG12	1.98	0.64
10:H:155:ALA:HB2	10:H:163:LEU:HB2	1.80	0.64
3:J:492:GLU:HG3	5:B:228:ILE:HG23	1.78	0.63
1:E:242:TRP:HE1	1:E:244:LYS:HB2	1.63	0.63
5:B:172:LEU:HD11	5:B:201:GLU:HG3	1.80	0.63
4:A:72:VAL:HG13	4:A:74:ALA:H	1.65	0.62
5:B:89:MET:HE3	5:B:89:MET:O	2.00	0.62
10:H:70:GLU:HG3	10:H:98:TRP:HD1	1.65	0.62
2:I:30:VAL:HG21	2:I:41:GLN:HE22	1.65	0.61
9:G:69:LEU:HD21	9:G:78:TYR:HB2	1.82	0.61
7:D:278:LEU:HD11	7:D:304:VAL:HG21	1.82	0.61
4:A:88:VAL:HG21	4:A:135:ARG:HG2	1.82	0.61
10:H:61:PRO:HD2	10:H:64:ILE:HD12	1.82	0.61
3:J:418:ARG:HD2	3:J:419:ALA:H	1.66	0.60
3:J:602:PHE:HD1	3:J:602:PHE:O	1.84	0.60
6:C:18:GLN:HE22	6:C:20:GLN:HB2	1.66	0.60
7:D:89:LEU:HD21	7:D:107:ARG:HG2	1.84	0.60
8:F:136:ILE:HD11	8:F:181:MET:HB2	1.83	0.60
10:H:77:VAL:HG22	10:H:92:THR:HG23	1.83	0.60
4:A:95:HIS:HA	4:A:98:LEU:HG	1.83	0.60
9:G:146:ASP:HB3	9:G:151:LEU:HD23	1.83	0.60
6:C:105:HIS:O	6:C:109:ASN:HB2	2.01	0.60
6:C:128:ILE:HG12	6:C:142:HIS:CE1	2.36	0.60
3:J:520:PRO:HG2	3:J:550:LEU:HD21	1.84	0.60
5:B:80:PHE:HD2	5:B:88:MET:HE3	1.67	0.60
5:B:252:GLU:HA	5:B:287:MET:HE3	1.82	0.59
9:G:149:ASN:HB2	9:G:151:LEU:HD22	1.84	0.59
4:A:222:VAL:HG11	4:A:253:ALA:HB2	1.84	0.59
5:B:88:MET:HE1	5:B:131:PHE:HZ	1.66	0.59
1:E:140:HIS:HB3	1:E:143:TYR:HB2	1.84	0.59
1:E:148:SER:H	1:E:151:ASN:HD22	1.50	0.59
4:A:87:ASN:HA	4:A:90:MET:HE1	1.84	0.58
4:A:209:SER:HA	4:A:212:LEU:HB2	1.84	0.58
7:D:389:SER:HA	7:D:396:THR:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:50:ASP:HA	6:C:53:GLU:HG2	1.85	0.58
2:I:50:MET:HG2	2:I:59:TYR:OH	2.03	0.58
4:A:410:GLU:HG3	4:A:412:LEU:HD23	1.84	0.58
9:G:210:GLU:O	9:G:213:VAL:HG12	2.04	0.57
4:A:136:LYS:HA	4:A:139:LEU:HD12	1.85	0.57
4:A:165:HIS:CE1	4:A:188:ALA:HB2	2.39	0.57
4:A:88:VAL:O	4:A:92:GLU:HG3	2.04	0.57
6:C:328:LEU:HD23	6:C:334:ALA:HA	1.87	0.57
7:D:385:LEU:HD22	8:F:234:ARG:HG2	1.86	0.56
1:E:102:GLY:HA3	1:E:107:VAL:HG12	1.87	0.56
5:B:370:HIS:NE2	7:D:355:ILE:HG22	2.20	0.56
2:I:56:ALA:HB1	2:I:61:ILE:HD11	1.87	0.56
6:C:12:VAL:HA	6:C:15:LEU:HG	1.88	0.56
1:E:148:SER:H	1:E:151:ASN:ND2	2.04	0.55
8:F:74:GLY:HA3	8:F:82:GLU:O	2.07	0.55
3:J:505:MET:HE3	3:J:505:MET:O	2.07	0.55
4:A:164:GLY:O	4:A:168:LEU:HB2	2.06	0.55
7:D:5:VAL:O	7:D:8:ASP:HB2	2.07	0.55
10:H:141:VAL:HG11	10:H:160:ARG:HH21	1.72	0.55
5:B:139:LEU:HD21	5:B:147:LEU:HD22	1.90	0.54
4:A:85:THR:HB	4:A:174:ASP:OD1	2.08	0.54
2:I:21:ASP:OD2	2:I:25:ARG:HG3	2.07	0.54
7:D:6:ARG:O	7:D:9:LEU:HB2	2.08	0.54
8:F:81:ILE:HG23	8:F:122:LEU:HD13	1.89	0.54
4:A:56:ARG:HA	4:A:59:ARG:HG2	1.90	0.54
3:J:505:MET:SD	3:J:524:THR:HA	2.48	0.53
5:B:291:ILE:HD13	11:K:95:PRO:HB3	1.90	0.53
6:C:40:SER:HB2	6:C:43:ASP:HB2	1.91	0.53
8:F:261:TYR:HA	9:G:170:ILE:HD12	1.90	0.53
9:G:110:CYS:SG	9:G:151:LEU:HD12	2.47	0.53
5:B:88:MET:HE1	5:B:131:PHE:CZ	2.43	0.53
3:J:719:LEU:HD13	3:J:732:LEU:HD11	1.90	0.53
5:B:58:LEU:HD11	5:B:75:MET:HE1	1.90	0.53
4:A:192:CYS:HA	4:A:197:HIS:CE1	2.42	0.53
6:C:61:VAL:O	6:C:64:VAL:HG22	2.07	0.53
6:C:128:ILE:HG12	6:C:142:HIS:HE1	1.73	0.53
9:G:99:LEU:HB3	9:G:160:ARG:HE	1.74	0.53
4:A:319:PHE:HA	4:A:322:LEU:HD12	1.91	0.53
5:B:201:GLU:HB3	5:B:217:LEU:HD13	1.90	0.53
6:C:307:ILE:O	6:C:311:THR:HG23	2.09	0.53
11:K:94:CYS:HB3	11:K:97:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:245:MET:O	7:D:249:LEU:HD12	2.09	0.53
9:G:163:ARG:HG3	9:G:166:ASP:HB2	1.91	0.53
4:A:266:ALA:O	4:A:270:LEU:HB2	2.09	0.53
9:G:166:ASP:O	9:G:169:ASN:HB3	2.07	0.53
5:B:53:SER:O	5:B:57:VAL:HG23	2.09	0.52
4:A:449:ARG:HD3	5:B:439:VAL:HG11	1.91	0.52
7:D:59:LEU:HD21	7:D:98:SER:HB3	1.92	0.52
6:C:209:ILE:HD11	6:C:224:TYR:HA	1.90	0.52
3:J:609:SER:O	3:J:613:ILE:HG12	2.09	0.52
4:A:139:LEU:HD23	4:A:142:LEU:HD12	1.90	0.52
4:A:165:HIS:HD2	4:A:184:CYS:HB3	1.75	0.52
4:A:272:LEU:HD23	4:A:272:LEU:H	1.75	0.52
10:H:32:ALA:HB3	10:H:37:TYR:CZ	2.45	0.52
8:F:41:VAL:HG21	8:F:167:VAL:HG11	1.90	0.52
3:J:470:ASP:HA	3:J:473:LYS:NZ	2.25	0.52
5:B:50:ALA:O	5:B:54:PHE:HD1	1.92	0.52
9:G:111:ILE:HD12	9:G:152:LEU:HD23	1.92	0.52
1:E:242:TRP:HD1	1:E:244:LYS:H	1.58	0.52
1:E:273:LEU:HD22	1:E:303:ALA:HB1	1.92	0.52
9:G:213:VAL:HA	9:G:216:ILE:HD12	1.91	0.52
4:A:59:ARG:HB3	4:A:356:MET:HE1	1.91	0.51
4:A:197:HIS:O	4:A:201:MET:HG2	2.11	0.51
9:G:97:LYS:HB3	9:G:131:LEU:HD21	1.91	0.51
2:I:43:LEU:HD23	2:I:67:LEU:HD23	1.91	0.51
4:A:329:ILE:HD12	4:A:345:LEU:HG	1.93	0.51
3:J:602:PHE:HZ	3:J:655:ILE:HG13	1.75	0.51
10:H:146:LYS:O	10:H:150:GLU:HG2	2.11	0.51
6:C:266:VAL:O	6:C:269:THR:HG22	2.11	0.51
9:G:18:LEU:HD11	9:G:30:LEU:HD11	1.91	0.51
6:C:12:VAL:HA	6:C:15:LEU:CG	2.42	0.50
1:E:149:GLY:H	3:J:759:ALA:HB3	1.76	0.50
4:A:72:VAL:HG22	4:A:73:GLU:H	1.76	0.50
10:H:16:LEU:HB3	10:H:43:LEU:HD11	1.93	0.50
2:I:27:LYS:O	2:I:31:GLU:HG2	2.10	0.50
7:D:46:LYS:HD2	7:D:87:PHE:CD2	2.46	0.50
1:E:110:GLN:HG2	1:E:111:ALA:H	1.77	0.50
4:A:90:MET:HA	4:A:93:GLU:OE1	2.12	0.50
7:D:189:VAL:HG22	7:D:211:LEU:HD21	1.94	0.49
3:J:437:MET:SD	3:J:478:LYS:HB3	2.51	0.49
4:A:165:HIS:HB2	4:A:191:TYR:HE2	1.76	0.49
4:A:459:VAL:HG22	4:A:464:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:133:PRO:O	8:F:136:ILE:HG22	2.12	0.49
9:G:211:ALA:O	9:G:214:THR:HB	2.12	0.49
9:G:140:ILE:HG13	9:G:141:ILE:HG23	1.92	0.49
3:J:528:LEU:HD22	3:J:533:TRP:CE2	2.48	0.49
3:J:577:VAL:HG22	11:K:26:LYS:HG2	1.95	0.49
5:B:438:VAL:HG11	8:F:302:MET:HB3	1.94	0.49
6:C:369:ASN:HD22	6:C:371:ALA:HB3	1.78	0.49
3:J:739:LEU:O	3:J:744:TYR:HB2	2.13	0.48
7:D:88:THR:O	7:D:92:ILE:HG13	2.13	0.48
3:J:729:PRO:HG2	11:K:104:GLN:HA	1.95	0.48
3:J:462:LEU:HD21	3:J:573:LEU:HD13	1.95	0.48
4:A:86:PHE:HB3	4:A:174:ASP:O	2.13	0.48
5:B:85:PHE:O	5:B:88:MET:HG3	2.13	0.48
7:D:329:GLU:C	7:D:330:ILE:HG13	2.38	0.48
3:J:578:LEU:HD11	3:J:596:THR:HA	1.95	0.48
4:A:96:ARG:O	4:A:100:GLU:HG3	2.13	0.48
5:B:296:SER:HB3	11:K:96:LEU:HD22	1.95	0.48
6:C:59:LEU:HD11	6:C:84:PHE:HD2	1.78	0.48
7:D:36:LEU:HB3	7:D:41:GLN:HB2	1.95	0.48
7:D:219:GLU:HA	7:D:222:ARG:HE	1.79	0.48
2:I:36:ILE:HG21	2:I:71:LEU:HD22	1.96	0.48
3:J:561:LYS:HG2	3:J:562:HIS:CD2	2.49	0.48
6:C:367:TYR:CE1	6:C:372:MET:HE3	2.48	0.48
8:F:41:VAL:HA	8:F:81:ILE:O	2.14	0.48
5:B:199:ALA:HB2	5:B:233:ILE:HG23	1.95	0.48
6:C:21:MET:HA	6:C:24:LEU:HG	1.95	0.48
8:F:168:PHE:CD2	8:F:183:PHE:HB2	2.49	0.48
1:E:45:TRP:CD1	1:E:163:GLU:HG2	2.48	0.48
1:E:216:VAL:HG21	3:J:758:VAL:HG22	1.95	0.48
3:J:745:MET:HA	3:J:757:TYR:O	2.13	0.48
4:A:77:MET:HA	4:A:81:PHE:CD2	2.49	0.48
9:G:20:LYS:HB2	9:G:20:LYS:HE2	1.73	0.48
10:H:37:TYR:CD1	10:H:60:ILE:HD11	2.49	0.48
3:J:607:GLY:HA2	3:J:655:ILE:HB	1.96	0.48
4:A:185:TYR:HE2	4:A:208:VAL:HG11	1.79	0.47
3:J:665:PHE:H	5:B:34:ASN:HD22	1.61	0.47
2:I:13:ILE:HG23	2:I:33:LYS:HG2	1.96	0.47
6:C:24:LEU:HD12	6:C:25:CYS:N	2.29	0.47
6:C:56:LEU:O	6:C:59:LEU:HD23	2.13	0.47
3:J:548:ILE:HD11	7:D:97:ILE:HB	1.95	0.47
6:C:18:GLN:NE2	6:C:20:GLN:HB2	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:115:ILE:HD12	5:B:118:TYR:HD2	1.80	0.47
3:J:525:VAL:HG21	3:J:554:PHE:CZ	2.50	0.47
2:I:1:MET:HB3	2:I:16:ASP:HA	1.97	0.47
3:J:500:LEU:HD11	5:B:231:PRO:HG3	1.97	0.47
5:B:323:ILE:HD11	5:B:358:VAL:HG11	1.97	0.47
7:D:245:MET:HE2	7:D:245:MET:HA	1.96	0.47
2:I:22:LYS:HD2	2:I:22:LYS:HA	1.68	0.47
6:C:321:ASP:O	6:C:325:ARG:HG3	2.15	0.47
3:J:544:THR:HB	3:J:546:GLU:OE2	2.15	0.47
3:J:671:GLN:O	3:J:675:LYS:HG2	2.14	0.47
6:C:179:LYS:HA	6:C:182:LEU:HD12	1.96	0.47
6:C:259:ALA:O	6:C:262:GLU:HG2	2.15	0.47
7:D:180:ASN:HB3	7:D:183:LEU:HB2	1.96	0.47
7:D:284:MET:HE2	7:D:284:MET:HB3	1.84	0.47
7:D:385:LEU:HD11	8:F:237:LEU:HD23	1.95	0.46
8:F:73:ILE:HB	8:F:119:LEU:HD12	1.98	0.46
9:G:217:LYS:O	9:G:220:LEU:HB2	2.16	0.46
6:C:221:LEU:HD12	6:C:253:ILE:HG23	1.97	0.46
9:G:99:LEU:HB3	9:G:160:ARG:HH21	1.81	0.46
4:A:165:HIS:CD2	4:A:184:CYS:HB3	2.51	0.46
7:D:26:TYR:HD2	7:D:61:ILE:HD11	1.79	0.46
4:A:144:LYS:HE3	4:A:144:LYS:HB3	1.69	0.46
3:J:589:PHE:HE2	3:J:669:ILE:HD13	1.81	0.46
6:C:404:VAL:HG12	6:C:404:VAL:O	2.15	0.46
8:F:70:GLY:HA3	8:F:125:TYR:CZ	2.51	0.46
1:E:242:TRP:NE1	1:E:244:LYS:HB2	2.28	0.46
2:I:48:LYS:HE2	2:I:48:LYS:HB2	1.63	0.46
4:A:52:SER:HA	4:A:56:ARG:HE	1.80	0.46
4:A:149:LEU:HA	4:A:152:TYR:CD2	2.50	0.46
5:B:92:TYR:OH	5:B:135:THR:HG23	2.16	0.46
11:K:72:TRP:CD2	11:K:78:ALA:HB2	2.51	0.46
10:H:20:CYS:SG	10:H:40:LEU:HD13	2.55	0.46
5:B:92:TYR:CE2	5:B:131:PHE:CD1	3.03	0.46
6:C:172:GLU:HG3	6:C:176:TYR:HB2	1.98	0.46
10:H:201:THR:HA	10:H:204:VAL:HG12	1.98	0.46
11:K:88:LEU:HD11	11:K:101:TRP:CD1	2.50	0.46
4:A:196:LYS:HD3	4:A:196:LYS:N	2.31	0.46
7:D:52:MET:HA	7:D:52:MET:HE2	1.98	0.46
7:D:267:MET:HE2	7:D:273:ILE:HD13	1.98	0.46
7:D:342:MET:HE2	7:D:342:MET:HB3	1.82	0.46
1:E:318:LEU:HD22	8:F:286:VAL:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:VAL:HB	2:I:13:ILE:HB	1.99	0.45
3:J:593:LEU:HD11	11:K:27:TRP:HE1	1.81	0.45
8:F:72:LEU:HD21	8:F:152:LEU:HD13	1.98	0.45
1:E:110:GLN:HG2	1:E:111:ALA:N	2.29	0.45
6:C:125:LYS:O	6:C:128:ILE:HG22	2.17	0.45
8:F:124:TRP:HZ3	8:F:126:THR:HB	1.80	0.45
10:H:128:ILE:HG23	10:H:162:VAL:HG13	1.98	0.45
5:B:167:LYS:O	5:B:170:LYS:HG3	2.16	0.45
6:C:58:VAL:O	6:C:61:VAL:HB	2.16	0.45
3:J:462:LEU:HD11	3:J:573:LEU:HD13	1.97	0.45
1:E:318:LEU:HD23	10:H:200:LEU:HD21	1.98	0.45
3:J:413:VAL:HG23	3:J:436:ILE:HD13	1.99	0.45
3:J:582:PHE:HD2	3:J:660:PHE:HB2	1.81	0.45
4:A:90:MET:O	4:A:94:ILE:HG12	2.17	0.45
4:A:156:SER:HA	4:A:161:ILE:HD11	1.98	0.45
10:H:46:LEU:HA	10:H:109:LEU:HD13	1.98	0.45
2:I:1:MET:HE3	2:I:1:MET:HA	1.98	0.45
4:A:55:MET:HB2	4:A:356:MET:SD	2.57	0.45
5:B:146:ARG:HE	5:B:146:ARG:HB3	1.53	0.45
5:B:314:LEU:HD23	5:B:314:LEU:HA	1.88	0.45
9:G:213:VAL:O	9:G:216:ILE:HB	2.17	0.45
5:B:143:LYS:HG3	5:B:145:ASP:OD1	2.17	0.45
10:H:60:ILE:HD13	10:H:60:ILE:HA	1.77	0.45
4:A:170:ASP:O	4:A:174:ASP:HB2	2.17	0.45
6:C:10:ASN:O	6:C:14:GLN:HG2	2.17	0.45
7:D:329:GLU:O	7:D:330:ILE:HG13	2.17	0.45
10:H:128:ILE:HG22	10:H:164:PRO:HD3	1.99	0.45
4:A:320:LEU:HB3	4:A:327:ARG:HG3	1.98	0.45
7:D:34:ILE:HG21	7:D:72:HIS:CE1	2.52	0.45
4:A:157:ILE:O	4:A:161:ILE:HG13	2.17	0.45
8:F:136:ILE:O	8:F:140:LYS:HG2	2.17	0.45
7:D:387:LYS:HD2	8:F:256:ILE:HG12	2.00	0.44
5:B:64:LYS:HD3	5:B:64:LYS:HA	1.76	0.44
8:F:112:PHE:HE2	8:F:119:LEU:HB3	1.81	0.44
4:A:84:ARG:HA	4:A:84:ARG:HH11	1.81	0.44
4:A:185:TYR:CZ	4:A:208:VAL:HG21	2.52	0.44
5:B:93:LYS:HA	5:B:93:LYS:HD2	1.87	0.44
5:B:370:HIS:CD2	7:D:355:ILE:HG22	2.52	0.44
6:C:192:TYR:CZ	6:C:200:ARG:HD3	2.53	0.44
7:D:343:ILE:HG22	7:D:344:THR:H	1.82	0.44
10:H:111:ASP:HB3	10:H:115:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:252:PHE:HE1	8:F:257:LEU:HG	1.82	0.44
4:A:59:ARG:O	4:A:63:ILE:HG13	2.17	0.44
8:F:70:GLY:HA2	8:F:89:LEU:HB2	1.99	0.44
3:J:490:LYS:H	3:J:490:LYS:HG2	1.64	0.44
3:J:545:PRO:O	3:J:548:ILE:HG22	2.18	0.44
4:A:127:ASP:HB3	4:A:131:VAL:HG23	1.99	0.44
4:A:138:ALA:O	4:A:142:LEU:HG	2.18	0.44
4:A:238:ARG:HD2	4:A:238:ARG:HA	1.85	0.44
5:B:175:LEU:HD13	5:B:197:ILE:HD13	2.00	0.44
5:B:442:LEU:HD12	5:B:442:LEU:HA	1.85	0.44
7:D:352:ILE:HG12	7:D:359:VAL:HG13	1.99	0.44
8:F:51:ILE:HB	8:F:154:LEU:HD13	2.00	0.44
9:G:208:GLN:OE1	9:G:208:GLN:HA	2.17	0.44
10:H:148:ILE:HG12	10:H:154:GLN:HB2	1.98	0.44
4:A:142:LEU:O	4:A:146:ASP:HB2	2.18	0.44
11:K:84:ILE:HD12	11:K:84:ILE:HA	1.83	0.44
6:C:31:SER:HA	6:C:35:LEU:HB2	2.00	0.43
7:D:59:LEU:HD23	7:D:59:LEU:HA	1.87	0.43
8:F:42:ALA:HB3	8:F:82:GLU:HG3	2.00	0.43
10:H:78:GLY:HA2	10:H:81:ILE:HG22	1.98	0.43
7:D:18:SER:HA	7:D:22:LEU:HD11	2.00	0.43
5:B:66:GLU:HA	5:B:103:VAL:HG12	2.00	0.43
5:B:84:ASN:C	5:B:84:ASN:ND2	2.76	0.43
8:F:140:LYS:NZ	8:F:181:MET:HG3	2.33	0.43
6:C:205:TYR:HB3	6:C:227:TYR:HB2	2.00	0.43
6:C:384:ILE:O	6:C:388:GLU:HG2	2.18	0.43
6:C:403:PHE:HD1	6:C:404:VAL:H	1.66	0.43
7:D:330:ILE:HD12	7:D:330:ILE:O	2.19	0.43
5:B:267:GLU:C	5:B:269:GLY:H	2.25	0.43
6:C:42:LEU:O	6:C:46:LEU:HB2	2.18	0.43
7:D:267:MET:HG2	7:D:273:ILE:HD11	1.99	0.43
2:I:23:VAL:HG11	2:I:52:ASP:HA	2.01	0.43
2:I:42:ARG:HB2	2:I:70:VAL:HG23	2.01	0.43
3:J:667:ILE:HD13	3:J:667:ILE:HA	1.87	0.43
8:F:232:HIS:HA	8:F:235:VAL:HG12	2.01	0.43
10:H:141:VAL:HG11	10:H:160:ARG:NH2	2.33	0.43
7:D:339:ALA:O	7:D:343:ILE:HG13	2.19	0.43
8:F:218:ALA:O	8:F:222:ILE:HG12	2.19	0.43
9:G:215:ASN:O	9:G:218:LYS:HB2	2.19	0.43
6:C:59:LEU:HG	6:C:84:PHE:HE2	1.82	0.43
6:C:205:TYR:CE2	6:C:226:LYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:326:LYS:HA	1:E:330:GLN:HG3	2.01	0.43
3:J:538:PRO:C	3:J:539:MET:HE2	2.44	0.43
4:A:267:ALA:HB2	4:A:296:CYS:SG	2.59	0.43
5:B:35:GLN:NE2	5:B:57:VAL:HG22	2.33	0.43
5:B:72:LEU:HD13	5:B:72:LEU:HA	1.82	0.43
5:B:149:PHE:CZ	5:B:175:LEU:HD21	2.54	0.43
7:D:69:PHE:HA	7:D:72:HIS:CD2	2.54	0.43
1:E:60:LEU:HG	1:E:64:LYS:HE2	2.01	0.43
1:E:94:ASP:HB2	1:E:129:ARG:NH2	2.34	0.43
4:A:63:ILE:HG12	4:A:354:LEU:HD11	1.99	0.43
4:A:173:LEU:HD11	4:A:208:VAL:HG22	2.01	0.43
11:K:54:ILE:HG23	11:K:55:GLU:N	2.34	0.43
1:E:255:LEU:HD11	1:E:317:GLY:C	2.44	0.42
3:J:458:ALA:O	3:J:462:LEU:HB3	2.19	0.42
5:B:73:LYS:O	5:B:74:GLN:C	2.60	0.42
6:C:119:ARG:NH2	10:H:30:GLY:HA3	2.34	0.42
6:C:159:LEU:HD23	6:C:159:LEU:HA	1.79	0.42
1:E:237:LEU:HD12	8:F:52:SER:HB3	2.02	0.42
4:A:163:ARG:HD2	4:A:163:ARG:HA	1.75	0.42
6:C:81:VAL:O	6:C:85:ILE:HG13	2.19	0.42
4:A:95:HIS:HA	4:A:98:LEU:CD2	2.49	0.42
4:A:409:LEU:HD23	4:A:409:LEU:HA	1.92	0.42
5:B:81:LYS:HE3	5:B:81:LYS:HB3	1.69	0.42
6:C:155:PHE:CE2	6:C:191:ILE:HA	2.54	0.42
2:I:60:LYS:HD3	2:I:60:LYS:HA	1.74	0.42
3:J:559:LEU:HA	3:J:559:LEU:HD23	1.79	0.42
3:J:639:LEU:HD22	3:J:641:LYS:NZ	2.34	0.42
4:A:145:LEU:HD13	4:A:171:HIS:CE1	2.54	0.42
4:A:255:LEU:HD22	4:A:284:LEU:HD22	2.00	0.42
6:C:89:ASN:HD21	6:C:92:HIS:HB2	1.84	0.42
6:C:232:LEU:HB3	6:C:298:CYS:SG	2.59	0.42
6:C:328:LEU:HD12	6:C:328:LEU:HA	1.81	0.42
3:J:441:ARG:HH11	3:J:442:PHE:HB3	1.85	0.42
3:J:532:TYR:CD1	3:J:532:TYR:N	2.88	0.42
3:J:624:LEU:HD12	3:J:624:LEU:O	2.20	0.42
3:J:699:ALA:O	3:J:703:ILE:HG12	2.19	0.42
4:A:137:LYS:HE2	4:A:141:LYS:HD3	2.01	0.42
6:C:166:MET:HE3	6:C:166:MET:HB3	1.78	0.42
10:H:147:GLY:O	10:H:151:GLN:HG2	2.19	0.42
7:D:9:LEU:HD21	7:D:29:ILE:HG21	2.02	0.42
8:F:163:LEU:HD12	8:F:163:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:323:ILE:H	5:B:323:ILE:HG13	1.63	0.42
5:B:347:ILE:HD12	5:B:350:LEU:HD12	2.02	0.42
4:A:183:LYS:HA	4:A:183:LYS:HD3	1.81	0.42
4:A:250:LYS:HD2	4:A:272:LEU:HG	2.02	0.42
5:B:212:LYS:HD2	5:B:212:LYS:HA	1.69	0.42
7:D:156:LEU:HD23	7:D:156:LEU:HA	1.88	0.42
8:F:168:PHE:CE1	8:F:185:GLU:HG2	2.55	0.42
4:A:248:LYS:HG3	4:A:280:PHE:CE1	2.55	0.41
5:B:32:LEU:HD21	5:B:61:GLU:HA	2.00	0.41
1:E:81:MET:SD	1:E:92:ILE:HD13	2.60	0.41
2:I:2:LEU:O	2:I:4:LYS:HD3	2.20	0.41
3:J:523:LEU:HD13	3:J:550:LEU:HB3	2.01	0.41
4:A:258:LEU:HD13	4:A:292:TYR:CD2	2.55	0.41
9:G:51:ASN:O	9:G:54:GLU:HG3	2.20	0.41
3:J:436:ILE:HA	3:J:439:LEU:HD12	2.02	0.41
3:J:543:LEU:HA	3:J:597:LEU:HD21	2.02	0.41
4:A:163:ARG:HH11	4:A:166:ASP:HB2	1.85	0.41
4:A:365:LEU:HD23	4:A:365:LEU:HA	1.89	0.41
6:C:328:LEU:HG	6:C:333:GLU:HG2	2.02	0.41
7:D:183:LEU:HD23	7:D:183:LEU:HA	1.85	0.41
8:F:88:GLU:H	8:F:88:GLU:HG3	1.66	0.41
11:K:53:CYS:O	11:K:55:GLU:N	2.54	0.41
1:E:110:GLN:H	1:E:110:GLN:CD	2.29	0.41
4:A:185:TYR:CE2	4:A:208:VAL:HG21	2.56	0.41
4:A:291:ILE:HG12	4:A:323:GLU:OE2	2.21	0.41
6:C:148:LEU:HD23	6:C:148:LEU:HA	1.85	0.41
6:C:162:LEU:HD22	6:C:204:PHE:HE2	1.86	0.41
11:K:49:ILE:HG22	11:K:50:MET:HG2	2.02	0.41
11:K:88:LEU:HD11	11:K:101:TRP:HD1	1.86	0.41
6:C:37:LYS:HD3	6:C:37:LYS:HA	1.95	0.41
8:F:243:LYS:O	8:F:246:GLU:HG3	2.20	0.41
10:H:60:ILE:CG2	10:H:65:LYS:HG3	2.50	0.41
2:I:29:ARG:HA	2:I:29:ARG:NE	2.36	0.41
3:J:546:GLU:H	3:J:546:GLU:CD	2.29	0.41
6:C:143:ALA:HB1	6:C:183:CYS:SG	2.60	0.41
7:D:34:ILE:HG21	7:D:72:HIS:HE1	1.85	0.41
3:J:719:LEU:HD22	3:J:732:LEU:HD21	2.03	0.41
4:A:64:ALA:HB3	4:A:75:LEU:HG	2.02	0.41
4:A:130:TRP:CE2	4:A:134:THR:HG21	2.56	0.41
6:C:66:PHE:CE2	6:C:107:LEU:HA	2.56	0.41
6:C:266:VAL:HG21	6:C:278:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:133:PHE:O	10:H:137:VAL:HG22	2.20	0.41
2:I:25:ARG:HD2	2:I:28:GLU:OE2	2.21	0.41
3:J:693:GLN:HG2	3:J:735:ARG:HD3	2.02	0.41
6:C:373:LEU:HD12	6:C:373:LEU:HA	1.90	0.41
8:F:99:ILE:HG23	8:F:141:GLN:HE22	1.85	0.41
10:H:154:GLN:NE2	10:H:156:ASP:N	2.69	0.41
1:E:45:TRP:NE1	1:E:163:GLU:HG2	2.36	0.40
4:A:161:ILE:HG22	4:A:191:TYR:CZ	2.56	0.40
8:F:230:MET:HE3	8:F:230:MET:HB3	1.97	0.40
9:G:116:LEU:HB3	9:G:128:LEU:HD11	2.03	0.40
2:I:4:LYS:HE2	2:I:4:LYS:HB2	1.82	0.40
2:I:22:LYS:HZ2	2:I:23:VAL:HG12	1.86	0.40
3:J:522:ASP:HB2	11:K:26:LYS:HB2	2.02	0.40
4:A:55:MET:HE2	4:A:55:MET:HB3	1.95	0.40
4:A:80:SER:O	4:A:83:GLN:HB3	2.21	0.40
7:D:91:LYS:HA	7:D:91:LYS:HD3	1.88	0.40
3:J:441:ARG:HD2	3:J:442:PHE:N	2.36	0.40
5:B:36:TYR:CE1	5:B:54:PHE:HE2	2.40	0.40
6:C:200:ARG:HH21	6:C:204:PHE:HE1	1.68	0.40
7:D:69:PHE:CE1	7:D:73:LEU:HD13	2.56	0.40
10:H:64:ILE:H	10:H:64:ILE:HG13	1.64	0.40
10:H:209:ASN:OD1	10:H:209:ASN:C	2.65	0.40
2:I:43:LEU:HB3	2:I:50:MET:CE	2.51	0.40
6:C:151:LEU:HD12	6:C:151:LEU:HA	1.82	0.40
7:D:84:ILE:O	7:D:88:THR:HG22	2.22	0.40
3:J:631:LEU:HG	3:J:669:ILE:HD12	2.03	0.40
6:C:60:ALA:O	6:C:63:PHE:HB2	2.22	0.40
7:D:172:SER:HB3	7:D:187:TYR:CE1	2.56	0.40
7:D:214:LYS:HA	7:D:214:LYS:HD2	1.83	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	E	288/334 (86%)	272 (94%)	16 (6%)	0	100	100
2	I	74/81 (91%)	72 (97%)	2 (3%)	0	100	100
3	J	332/759 (44%)	303 (91%)	24 (7%)	5 (2%)	8	30
4	A	405/491 (82%)	373 (92%)	32 (8%)	0	100	100
5	B	404/443 (91%)	370 (92%)	32 (8%)	2 (0%)	24	54
6	C	403/423 (95%)	385 (96%)	17 (4%)	1 (0%)	43	71
7	D	403/406 (99%)	388 (96%)	15 (4%)	0	100	100
8	F	278/327 (85%)	270 (97%)	8 (3%)	0	100	100
9	G	211/264 (80%)	204 (97%)	7 (3%)	0	100	100
10	H	168/209 (80%)	162 (96%)	6 (4%)	0	100	100
11	K	78/108 (72%)	66 (85%)	11 (14%)	1 (1%)	9	33
All	All	3044/3845 (79%)	2865 (94%)	170 (6%)	9 (0%)	37	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	J	706	MET
3	J	727	VAL
3	J	489	SER
3	J	566	LYS
3	J	758	VAL
5	B	271	PRO
5	B	270	SER
6	C	168	ASP
11	K	54	ILE

### 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	E	250/282 (89%)	244 (98%)	6 (2%)	43	62
2	I	66/69 (96%)	63 (96%)	3 (4%)	24	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	300/679 (44%)	288 (96%)	12 (4%)	28	53
4	A	356/429 (83%)	346 (97%)	10 (3%)	38	60
5	B	371/405 (92%)	360 (97%)	11 (3%)	36	59
6	C	362/377 (96%)	353 (98%)	9 (2%)	42	62
7	D	346/347 (100%)	339 (98%)	7 (2%)	48	65
8	F	249/276 (90%)	244 (98%)	5 (2%)	48	65
9	G	185/229 (81%)	180 (97%)	5 (3%)	39	60
10	H	143/173 (83%)	140 (98%)	3 (2%)	47	64
11	K	74/90 (82%)	73 (99%)	1 (1%)	59	70
All	All	2702/3356 (80%)	2630 (97%)	72 (3%)	40	60

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	127	VAL
1	E	165	PHE
1	E	193	TYR
1	E	194	LYS
1	E	206	ILE
1	E	227	SER
2	I	41	GLN
2	I	61	ILE
2	I	66	VAL
3	J	417	LEU
3	J	425	THR
3	J	437	MET
3	J	440	PHE
3	J	479	LEU
3	J	483	CYS
3	J	525	VAL
3	J	543	LEU
3	J	662	HIS
3	J	717	SER
3	J	727	VAL
3	J	741	ASP
4	A	75	LEU
4	A	197	HIS
4	A	228	THR
4	A	295	LEU

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Mol	Chain	Res	Type
4	A	357	TYR
4	A	362	VAL
4	A	364	THR
4	A	413	ILE
4	A	421	SER
4	A	459	VAL
5	B	33	GLU
5	B	42	LEU
5	B	72	LEU
5	B	75	MET
5	B	84	ASN
5	B	135	THR
5	B	206	THR
5	B	268	SER
5	B	281	VAL
5	B	335	SER
5	B	439	VAL
6	C	15	LEU
6	C	27	LEU
6	C	62	LEU
6	C	63	PHE
6	C	107	LEU
6	C	109	ASN
6	C	142	HIS
6	C	214	MET
6	C	237	LYS
7	D	45	LEU
7	D	46	LYS
7	D	71	THR
7	D	78	ASP
7	D	134	THR
7	D	313	SER
7	D	363	THR
8	F	81	ILE
8	F	137	HIS
8	F	150	LEU
8	F	200	VAL
8	F	302	MET
9	G	30	LEU
9	G	43	PHE
9	G	79	ILE
9	G	96	LEU

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Mol	Chain	Res	Type
9	G	170	ILE
10	H	40	LEU
10	H	162	VAL
10	H	163	LEU
11	K	56	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	140	HIS
1	E	160	GLN
1	E	182	ASN
1	E	209	ASN
3	J	481	HIS
3	J	507	HIS
4	A	95	HIS
4	A	213	GLN
5	B	35	GLN
5	B	129	GLN
5	B	174	GLN
5	B	176	HIS
5	B	255	HIS
5	B	346	HIS
6	C	109	ASN
6	C	126	GLN
6	C	142	HIS
6	C	239	GLN
6	C	297	GLN
6	C	327	GLN
6	C	363	ASN
6	C	369	ASN
6	C	402	GLN
7	D	72	HIS
7	D	180	ASN
7	D	380	GLN
8	F	114	GLN
8	F	141	GLN
9	G	33	GLN
9	G	81	ASN
9	G	190	GLN
9	G	215	ASN
10	H	22	ASN

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Mol	Chain	Res	Type
10	H	151	GLN
11	K	98	ASN
11	K	104	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

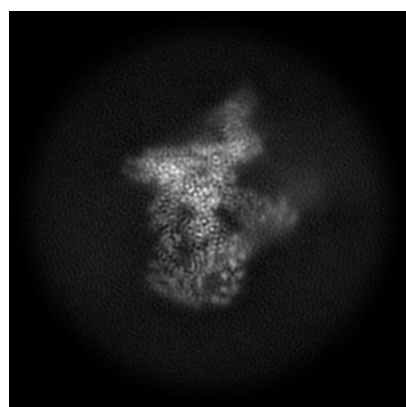
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47986. These allow visual inspection of the internal detail of the map and identification of artifacts.

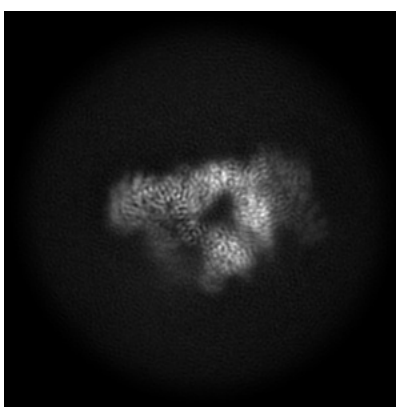
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

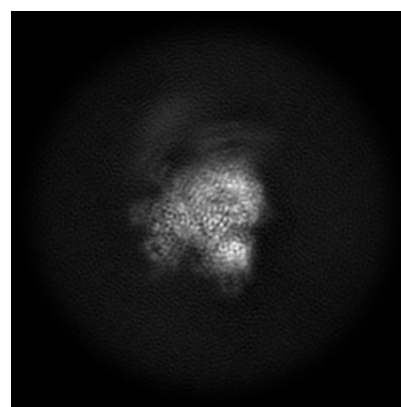
#### 6.1.1 Primary map



X



Y

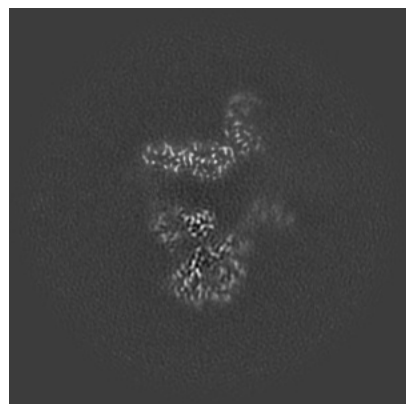


Z

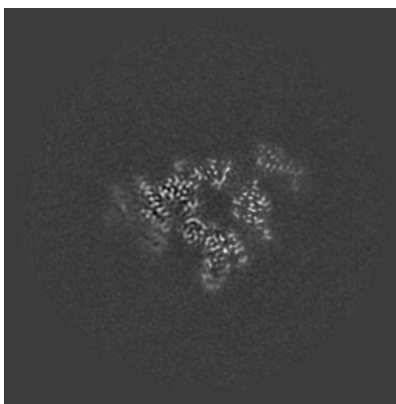
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

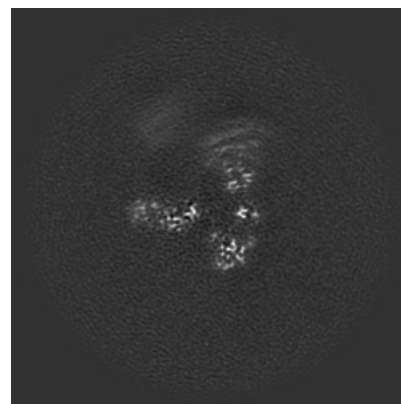
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

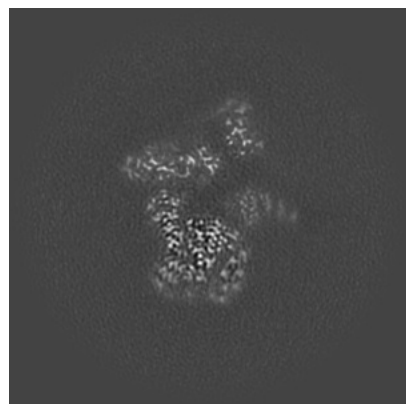


Z Index: 200

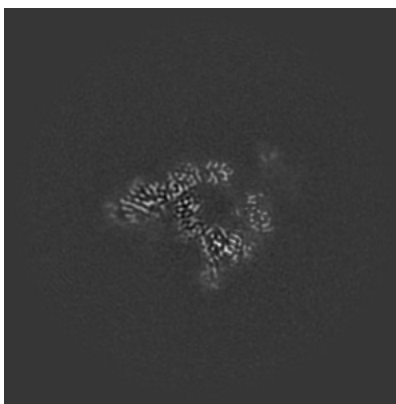
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

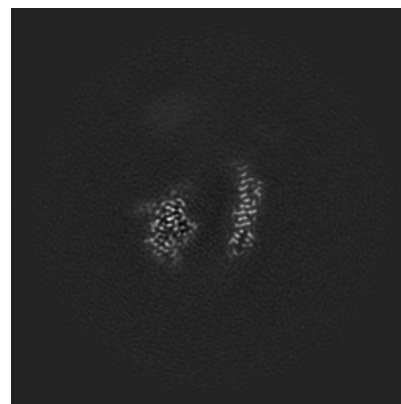
### 6.3.1 Primary map



X Index: 214



Y Index: 189

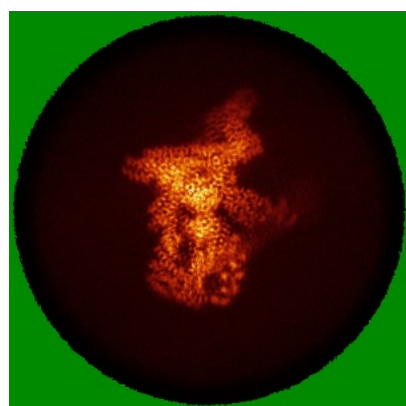


Z Index: 221

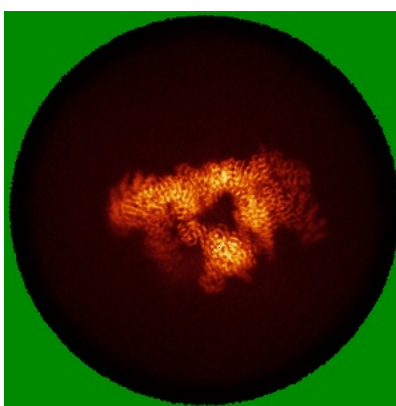
The images above show the largest variance slices of the map in three orthogonal directions.

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

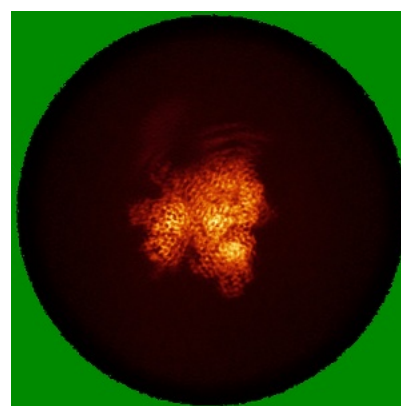
### 6.4.1 Primary map



X



Y

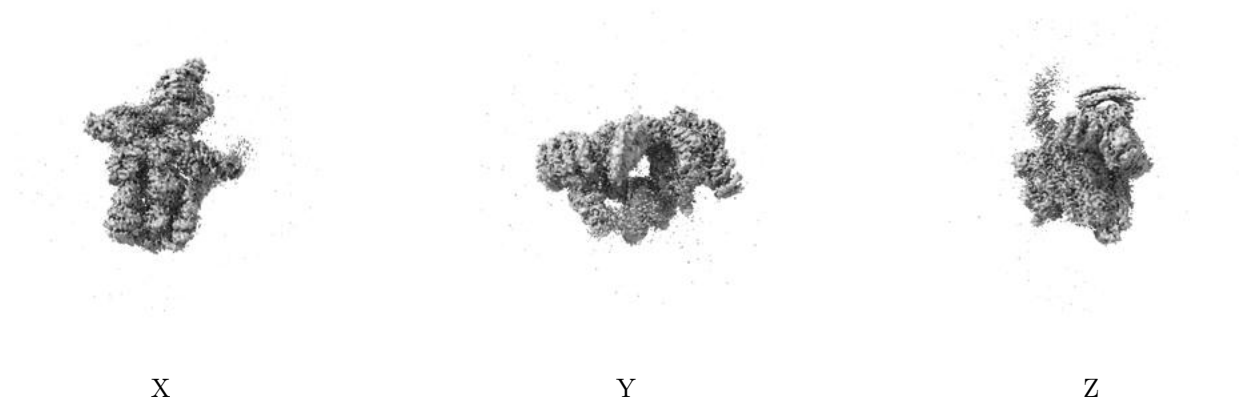


Z

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

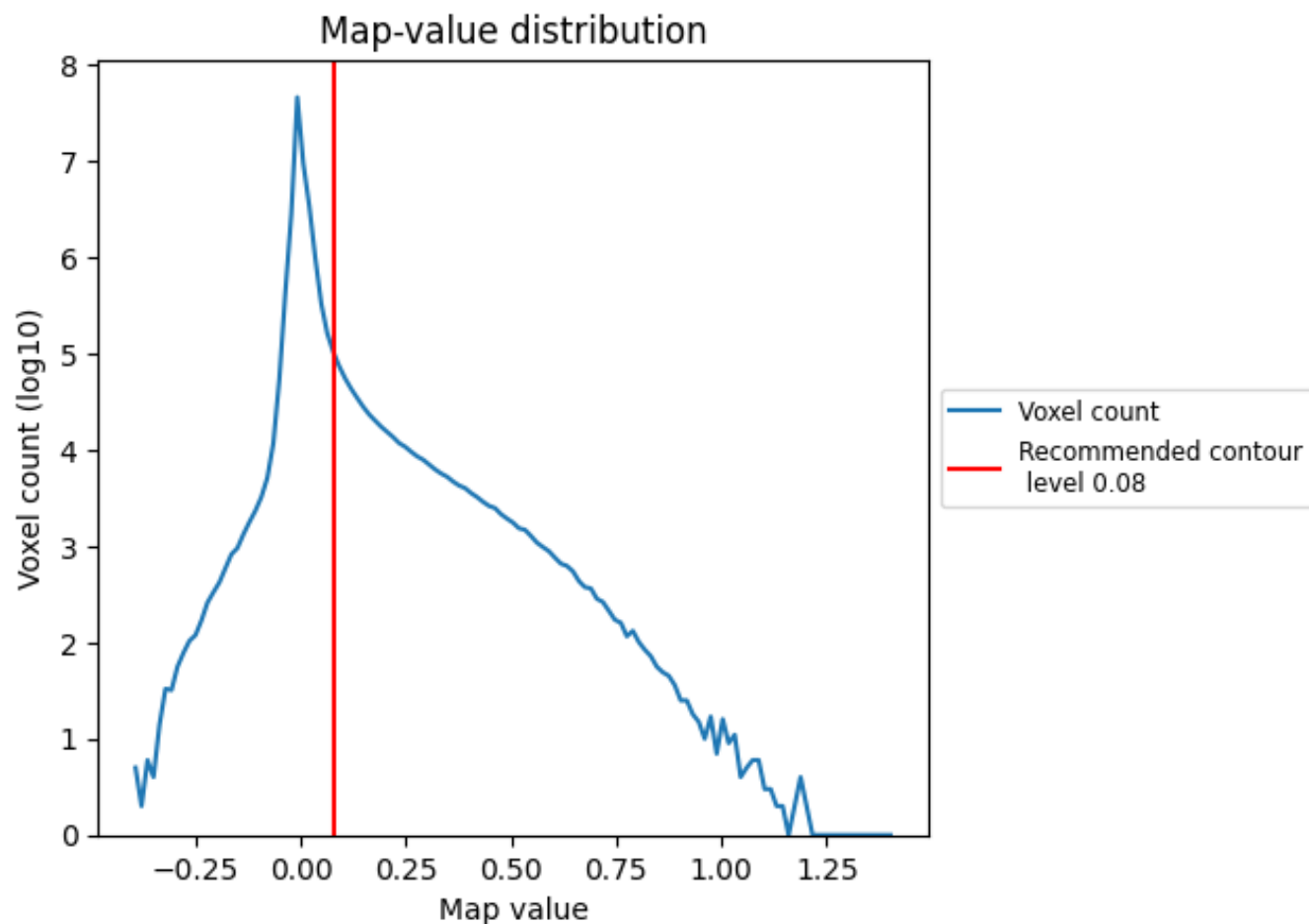
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

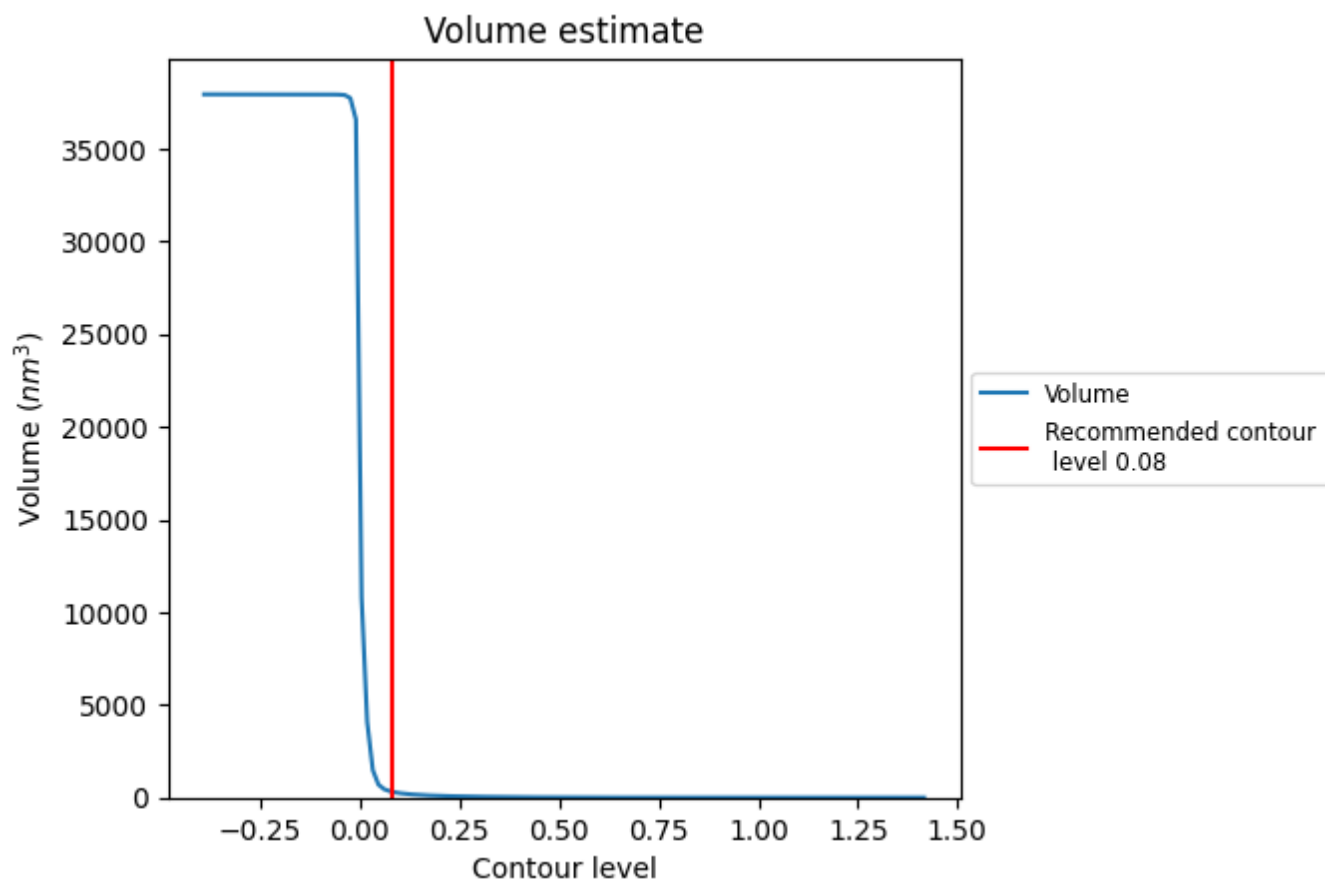
This section contains the results of statistical analysis of the map.

### 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](#)

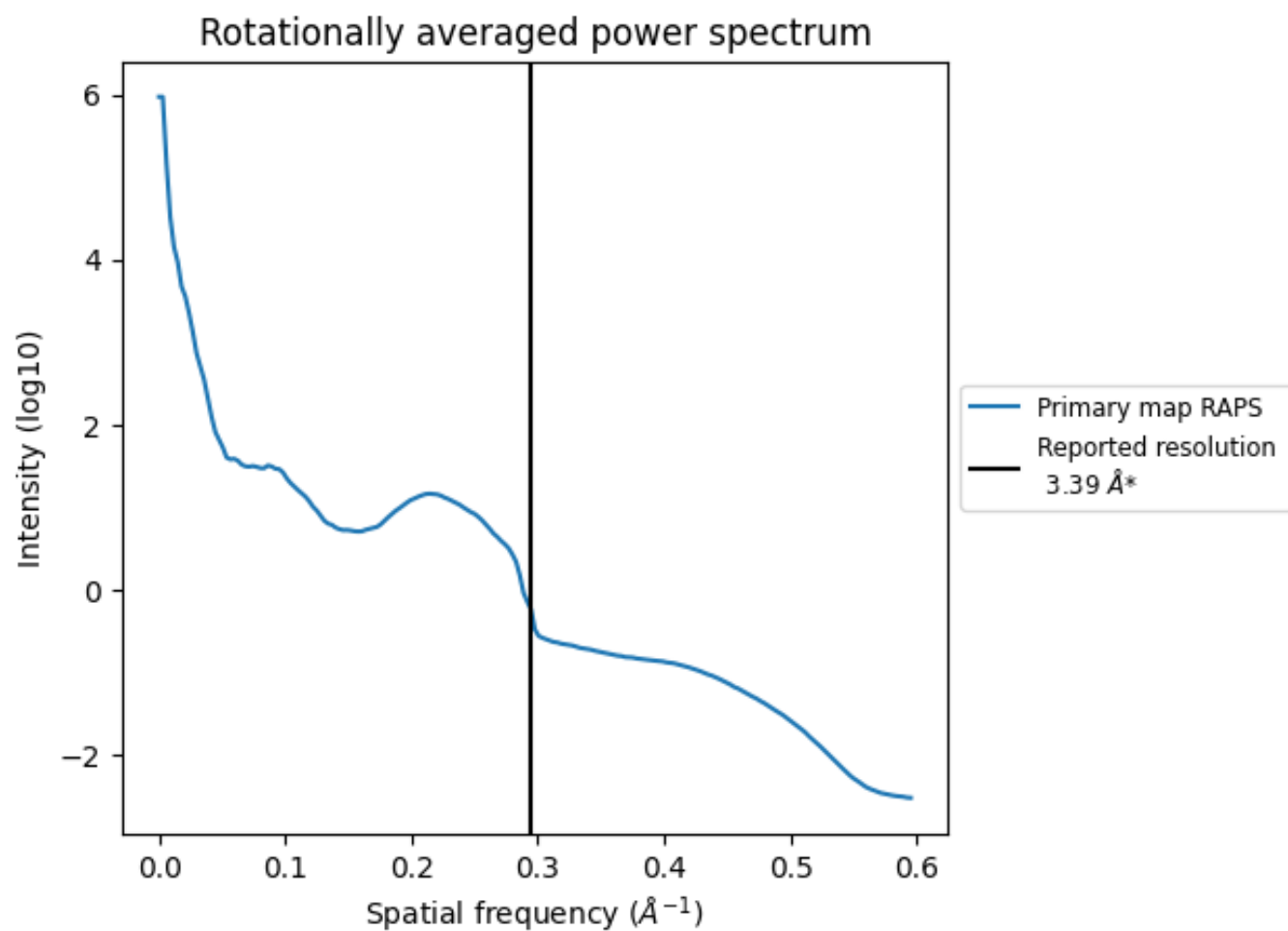


The volume at the recommended contour level is 318  $\text{nm}^3$ ; this corresponds to an approximate mass of 287 kDa.

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  $0.295 \text{ Å}^{-1}$

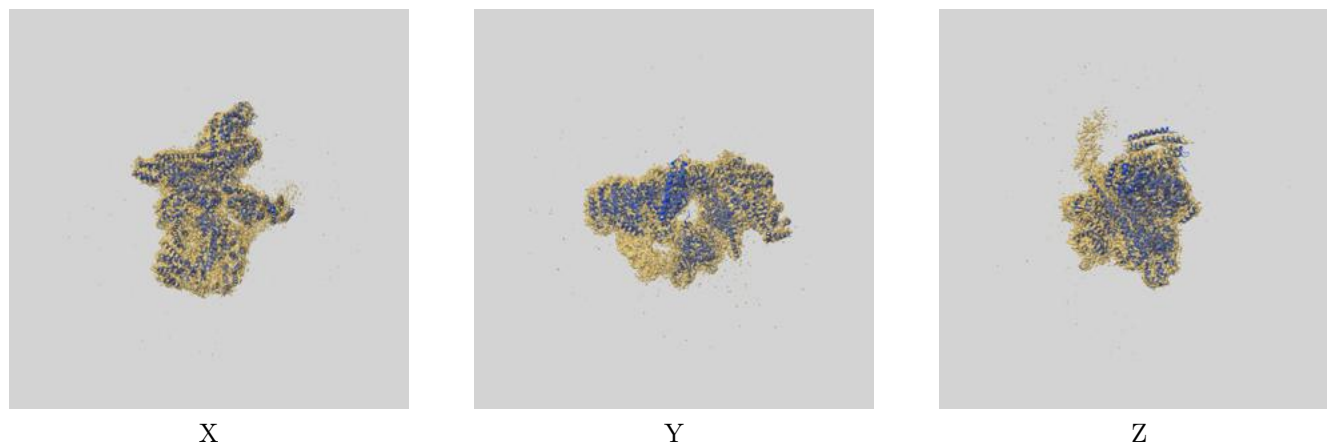
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

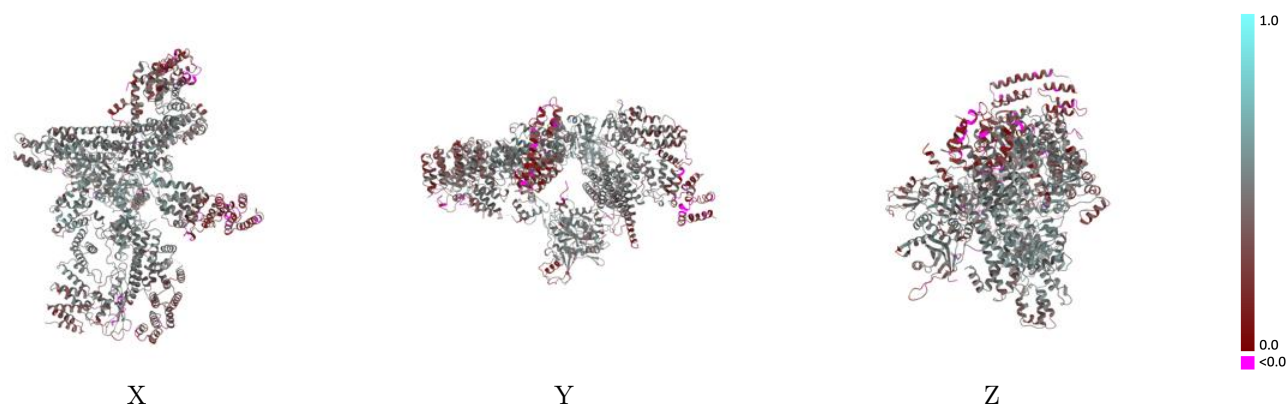
This section contains information regarding the fit between EMDB map EMD-47986 and PDB model 9EG8. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



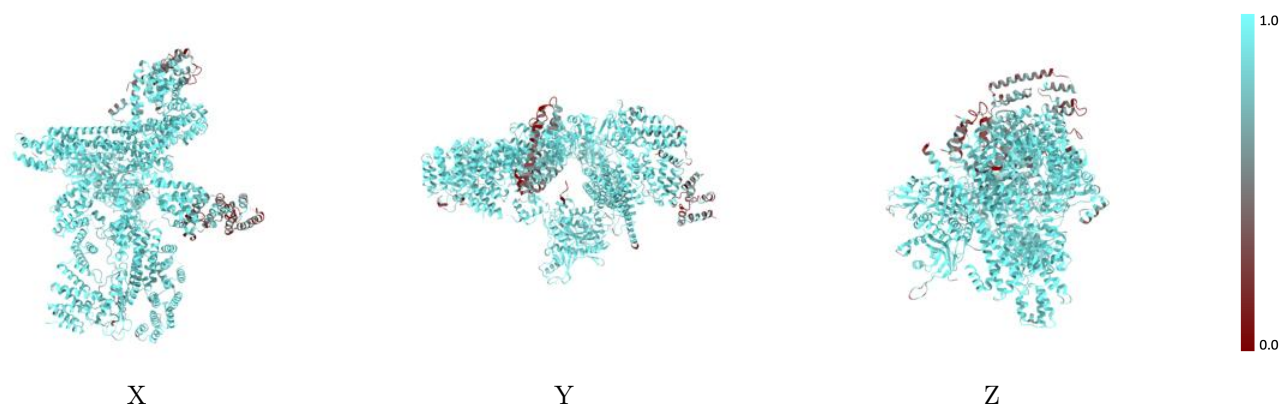
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



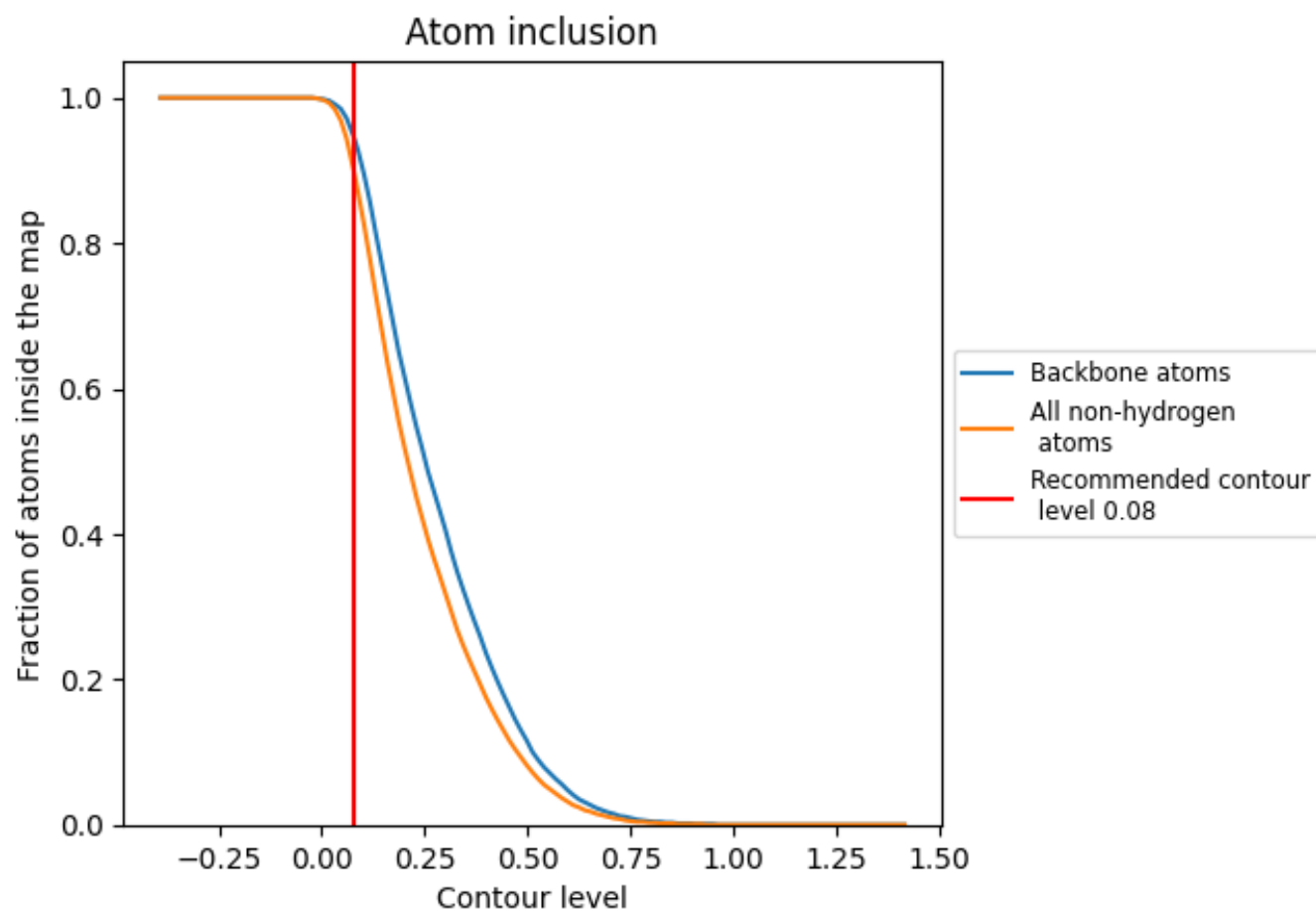
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8940	 0.4170
A	 0.7410	 0.3440
B	 0.9540	 0.4380
C	 0.8200	 0.3760
D	 0.9580	 0.4730
E	 0.9550	 0.4600
F	 0.9470	 0.4350
G	 0.9490	 0.4530
H	 0.8370	 0.3660
I	 0.8980	 0.3580
J	 0.8970	 0.4060
K	 0.9630	 0.5020

