



Full wwPDB EM Validation Report ⓘ

Apr 10, 2024 – 01:48 pm BST

PDB ID : 8R5H
EMDB ID : EMD-18915
Title : Ubiquitin ligation to neosubstrate by a cullin-RING E3 ligase & Cdc34: NED D8-CUL2-RBX1-ELOB/C-VHL-MZ1 with trapped UBE2R2 donor UB-BRD4 BD2
Authors : Liwocha, J.; Prabu, J.R.; Kleiger, G.; Schulman, B.A.
Deposited on : 2023-11-16
Resolution : 3.44 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:

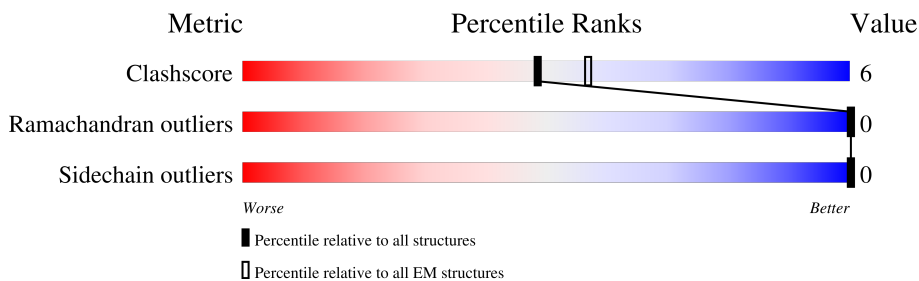
EMDB validation analysis : 0.0.1.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.44 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	745	
2	R	104	
3	C	238	
4	U	75	
5	D	112	
6	F	115	
7	G	118	
8	H	160	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 11277 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cullin-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	631	4918	3157	838	889	34	0	0

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1, N-terminally processed.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	R	79	587	376	107	95	9	0	0

- Molecule 3 is a protein called Ubiquitin-conjugating enzyme E2 R2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	203	1476	944	249	277	6	0	0

- Molecule 4 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	U	75	575	362	98	114	1	0	0

- Molecule 5 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	100	759	490	121	142	6	0	0

- Molecule 6 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	111	862	555	144	156	7	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	356	ALA	CYS	engineered mutation	UNP O60885
F	357	ALA	CYS	engineered mutation	UNP O60885
F	368	CYS	LYS	engineered mutation	UNP O60885
F	391	ALA	CYS	engineered mutation	UNP O60885
F	429	ALA	CYS	engineered mutation	UNP O60885

- Molecule 7 is a protein called Elongin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	G	105	816	519	139	154	4	0	0

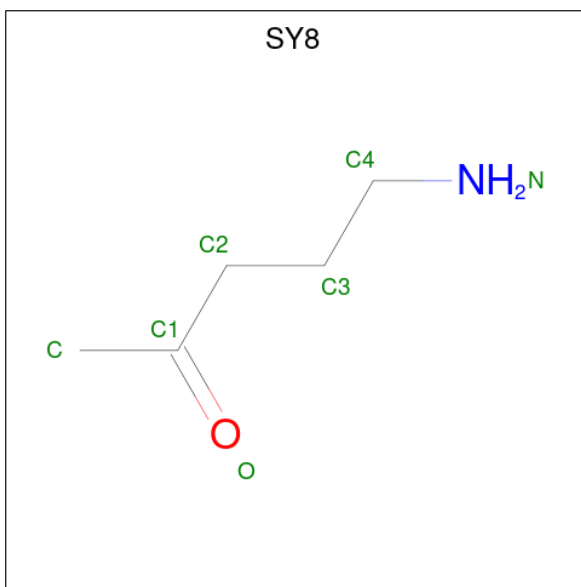
- Molecule 8 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	H	149	1205	768	220	215	2	0	0

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

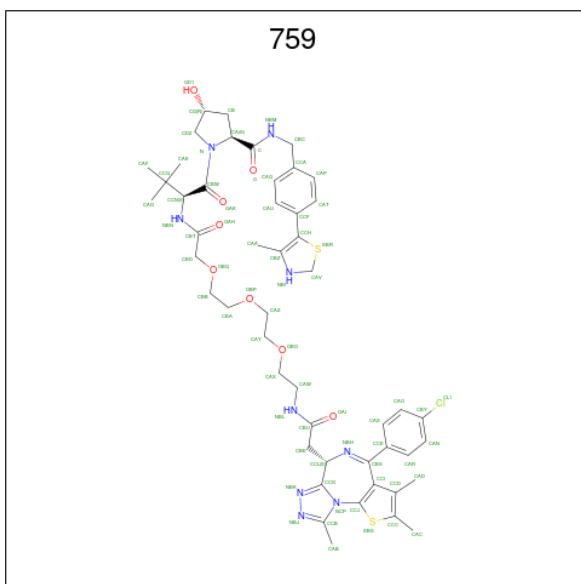
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
9	R	3	3	3	0

- Molecule 10 is 5-azanylpentan-2-one (three-letter code: SY8) (formula: C₅H₁₁NO) (labeled as "Ligand of Interest" by depositor).

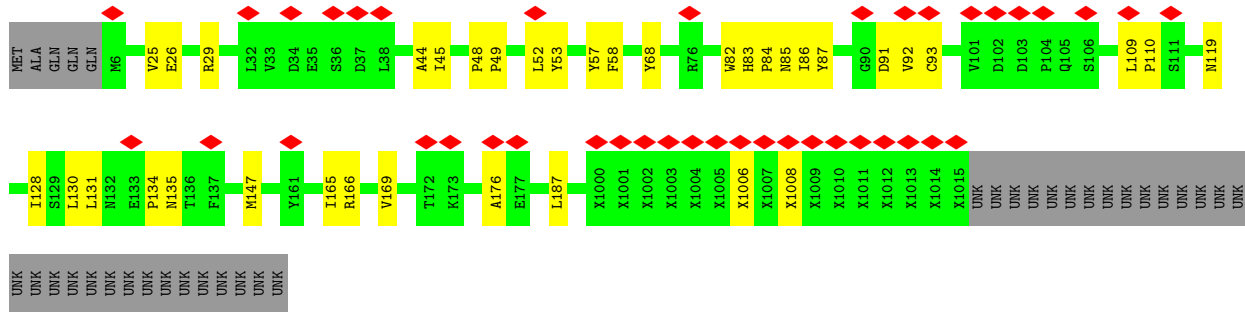


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	C	1	7	5	1	1	0

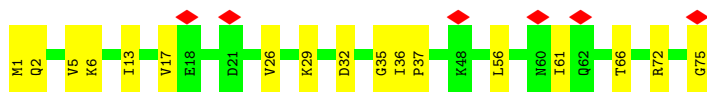
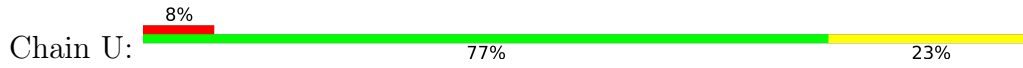
- Molecule 11 is (2 {S},4 {R})-1-[(2 {S})-2-[2-[2-[2-[2-[(9 {S})-7-(4-chlorophenyl)-4,5,13-trimethyl-3-thia-1,8,11,12-tetrazatricyclo[8.3.0.0^{2,6}]trideca-2(6),4,7,10,12-pentaen-9-yl]ethanoylamino]ethoxy]ethoxy]ethoxy]ethanoylamino]-3,3-dimethyl-butanoyl]- {N}-[[4-(4-methyl-2,3-dihydro-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (three-letter code: 759) (formula: C₄₉H₆₂ClN₉O₈S₂) (labeled as "Ligand of Interest" by depositor).



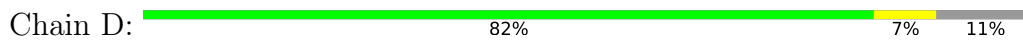
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	Cl	N	O		S
11	H	1	69	49	1	9	8	2	0



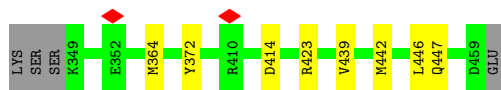
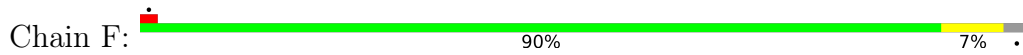
• Molecule 4: Ubiquitin



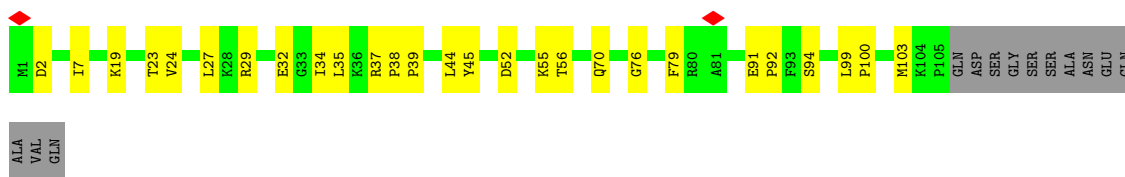
• Molecule 5: Elongin-C



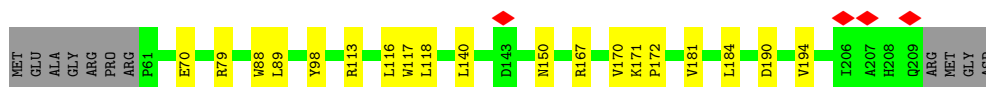
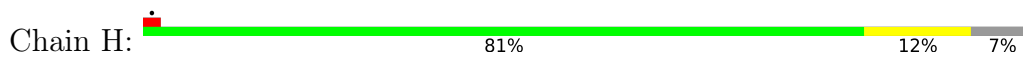
• Molecule 6: Bromodomain-containing protein 4



• Molecule 7: Elongin-B



• Molecule 8: von Hippel-Lindau disease tumor suppressor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148402	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.905	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.0319	Depositor
Map size (Å)	323.456, 323.456, 323.456	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8512, 0.8512, 0.8512	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: SY8, ZN, 759

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/5022	0.47	0/6806
2	R	0.24	0/605	0.48	0/826
3	C	0.25	0/1436	0.47	0/1973
4	U	0.24	0/581	0.49	0/787
5	D	0.27	0/777	0.44	0/1055
6	F	0.26	0/885	0.45	0/1199
7	G	0.27	0/833	0.54	0/1128
8	H	0.26	0/1237	0.53	0/1689
All	All	0.26	0/11376	0.48	0/15463

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	A	4918	0	4724	58	0
2	R	587	0	482	17	0
3	C	1476	0	1290	27	0
4	U	575	0	578	11	0
5	D	759	0	737	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	862	0	810	5	0
7	G	816	0	816	18	0
8	H	1205	0	1197	11	0
9	R	3	0	0	0	0
10	C	7	0	0	1	0
11	H	69	0	0	1	0
All	All	11277	0	10634	136	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 (136) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:GLU:HG3	1:A:576:MET:HG2	1.69	0.74
1:A:472:LYS:HG2	1:A:475:ARG:HH21	1.52	0.74
1:A:271:VAL:HG11	1:A:304:VAL:HG11	1.72	0.72
1:A:514:ALA:HB2	2:R:32:LEU:HB3	1.75	0.68
8:H:113:ARG:HD3	8:H:140:LEU:HG	1.76	0.66
2:R:98:ASN:ND2	3:C:109:LEU:O	2.29	0.66
5:D:17:MET:SD	5:D:33:ARG:NH1	2.67	0.65
3:C:45:ILE:HD12	3:C:128:ILE:HD11	1.79	0.64
1:A:589:ASN:HA	2:R:21:ARG:HD2	1.80	0.63
2:R:77:HIS:HE2	4:U:35:GLY:HA3	1.64	0.61
1:A:419:ILE:HA	1:A:422:PHE:HB3	1.83	0.61
8:H:167:ARG:NH2	8:H:190:ASP:O	2.33	0.61
1:A:71:HIS:CE1	1:A:75:ARG:HH21	2.20	0.60
1:A:155:LEU:HD13	1:A:159:LEU:HD23	1.81	0.60
1:A:151:MET:HA	1:A:155:LEU:HD23	1.84	0.60
1:A:611:THR:HG23	1:A:632:ILE:HD12	1.84	0.59
1:A:156:GLN:O	1:A:160:ILE:HB	2.02	0.59
1:A:589:ASN:O	2:R:21:ARG:NH1	2.37	0.58
3:C:48:PRO:HD2	3:C:53:TYR:HB2	1.86	0.57
3:C:93:CYS:O	10:C:1101:SY8:N	2.38	0.57
1:A:158:ILE:O	1:A:162:MET:HG3	2.05	0.56
1:A:315:LEU:HD22	1:A:364:PHE:HD2	1.71	0.55
1:A:506:SER:HB3	2:R:26:LYS:HG2	1.89	0.55
3:C:83:HIS:HB3	3:C:86:ILE:HG12	1.88	0.55
7:G:23:THR:HG22	7:G:56:THR:HG22	1.89	0.55
3:C:85:ASN:HD22	3:C:130:LEU:HD11	1.71	0.55
4:U:6:LYS:NZ	4:U:66:THR:OG1	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:MET:O	1:A:155:LEU:HB2	2.08	0.54
7:G:7:ILE:HD11	7:G:27:LEU:HD22	1.90	0.54
7:G:34:ILE:HG22	7:G:35:LEU:HD12	1.90	0.53
3:C:25:VAL:HG23	3:C:26:GLU:H	1.73	0.53
3:C:82:TRP:HE1	3:C:147:MET:HE2	1.73	0.53
5:D:91:PRO:HG2	7:G:70:GLN:HE22	1.74	0.53
1:A:72:LEU:O	1:A:76:VAL:HG23	2.09	0.53
6:F:372:TYR:HB2	6:F:442:MET:HB2	1.90	0.53
2:R:45:CYS:HB2	2:R:54:ILE:HD13	1.91	0.52
7:G:103:MET:HG2	8:H:170:VAL:HG22	1.91	0.52
1:A:510:TYR:HB2	2:R:30:VAL:HG12	1.91	0.52
4:U:17:VAL:HG11	4:U:26:VAL:HG22	1.91	0.52
2:R:77:HIS:NE2	4:U:35:GLY:HA3	2.24	0.52
7:G:45:TYR:O	7:G:76:GLY:N	2.39	0.52
8:H:171:LYS:HG3	8:H:172:PRO:HD2	1.90	0.52
3:C:29:ARG:HB2	3:C:44:ALA:HB3	1.91	0.51
3:C:86:ILE:HG22	3:C:92:VAL:HG12	1.91	0.51
3:C:166:ARG:HH21	3:C:169:VAL:HG11	1.75	0.51
1:A:573:TYR:HE1	1:A:646:SER:HB3	1.74	0.51
1:A:623:ILE:HG22	1:A:640:LEU:HA	1.92	0.50
1:A:401:LYS:HD2	1:A:449:MET:HA	1.93	0.50
1:A:620:VAL:HG23	1:A:622:MET:HG2	1.93	0.50
3:C:87:TYR:HB2	3:C:91:ASP:HB2	1.93	0.50
1:A:581:GLN:NE2	1:A:616:SER:OG	2.27	0.50
4:U:36:ILE:HD12	4:U:37:PRO:HD2	1.93	0.49
3:C:57:TYR:HB2	3:C:176:ALA:HB2	1.93	0.49
7:G:99:LEU:HD23	7:G:100:PRO:HD2	1.93	0.49
1:A:246:GLU:HA	1:A:249:ARG:HG2	1.95	0.49
1:A:255:HIS:O	1:A:257:SER:N	2.38	0.49
3:C:135:ASN:HD21	4:U:75:GLY:HA3	1.78	0.49
1:A:422:PHE:O	1:A:425:ILE:HG12	2.12	0.49
3:C:83:HIS:CD2	3:C:84:PRO:HD2	2.49	0.48
1:A:319:ILE:HD11	1:A:350:PHE:CD1	2.48	0.48
3:C:52:LEU:HB3	3:C:165:ILE:HG21	1.95	0.48
2:R:42:CYS:SG	2:R:80:HIS:HB2	2.54	0.47
1:A:49:TYR:HB3	1:A:50:PRO:HD3	1.96	0.47
7:G:32:GLU:OE2	7:G:39:PRO:HA	2.15	0.47
3:C:45:ILE:HB	3:C:58:PHE:HB2	1.96	0.47
1:A:150:LEU:O	1:A:154:PRO:HD2	2.14	0.47
1:A:633:ASP:OD1	1:A:636:SER:OG	2.25	0.47
5:D:68:HIS:ND1	7:G:94:SER:OG	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:NE	1:A:269:ARG:HA	2.29	0.47
8:H:118:LEU:HD11	8:H:194:VAL:HG13	1.97	0.47
1:A:472:LYS:HD2	1:A:516:ALA:HA	1.97	0.46
3:C:110:PRO:HB3	4:U:72:ARG:HH11	1.80	0.46
1:A:87:TYR:CZ	1:A:155:LEU:HD11	2.50	0.46
4:U:56:LEU:HD22	4:U:61:ILE:HD12	1.97	0.46
1:A:526:THR:OG1	1:A:604:GLN:O	2.33	0.46
5:D:57:THR:HG22	5:D:59:GLU:HG3	1.98	0.46
3:C:25:VAL:HG23	3:C:26:GLU:N	2.31	0.46
3:C:166:ARG:HA	3:C:169:VAL:HG12	1.97	0.45
1:A:43:TYR:O	1:A:47:VAL:HG22	2.15	0.45
1:A:354:ILE:HD13	1:A:365:MET:HG2	1.97	0.45
2:R:92:GLN:O	2:R:101:TRP:HB2	2.18	0.44
8:H:89:LEU:HD12	8:H:116:LEU:HB3	1.99	0.44
1:A:548:PHE:HB3	1:A:551:ARG:HD2	2.00	0.44
1:A:565:LYS:HZ2	2:R:25:LYS:HG2	1.81	0.44
1:A:75:ARG:HG3	1:A:90:TYR:HE2	1.83	0.44
2:R:90:THR:HG22	2:R:91:ARG:HG2	1.99	0.44
3:C:83:HIS:HE2	3:C:134:PRO:HG3	1.82	0.44
3:C:68:TYR:OH	3:C:119:ASN:HA	2.17	0.44
2:R:94:CYS:HB2	2:R:97:ASP:HB2	1.99	0.43
1:A:159:LEU:HD21	1:A:184:VAL:HG11	1.99	0.43
7:G:2:ASP:OD1	7:G:19:LYS:NZ	2.48	0.43
1:A:222:GLU:OE2	1:A:242:ARG:NE	2.52	0.43
7:G:24:VAL:HG13	7:G:44:LEU:HD12	2.01	0.43
7:G:52:ASP:HB2	7:G:55:LYS:HD3	2.00	0.43
1:A:304:VAL:HG13	1:A:304:VAL:O	2.19	0.43
4:U:29:LYS:HA	4:U:32:ASP:OD2	2.19	0.43
1:A:73:HIS:O	1:A:73:HIS:CG	2.72	0.43
3:C:83:HIS:CE1	3:C:131:LEU:HD13	2.54	0.42
3:C:1006:UNK:O	3:C:1008:UNK:N	2.51	0.42
1:A:584:VAL:HG21	1:A:613:THR:HG21	2.02	0.42
8:H:88:TRP:HB2	8:H:117:TRP:CZ3	2.54	0.42
1:A:389:GLU:OE2	1:A:389:GLU:N	2.48	0.42
1:A:537:VAL:O	1:A:541:GLU:OE1	2.38	0.42
8:H:98:TYR:HB3	11:H:301:759:SBR	2.60	0.42
1:A:376:VAL:HG11	1:A:424:TYR:HB3	2.01	0.42
6:F:439:VAL:HA	6:F:442:MET:HG2	2.02	0.42
8:H:79:ARG:HH21	8:H:150:ASN:CG	2.22	0.42
5:D:14:PRO:HG3	7:G:29:ARG:HG2	2.02	0.42
1:A:87:TYR:HE1	1:A:155:LEU:HD21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:423:ARG:NH1	6:F:447:GLN:HE22	2.18	0.41
7:G:37:ARG:HA	7:G:37:ARG:HD2	1.77	0.41
1:A:386:LYS:O	1:A:390:LEU:HD13	2.20	0.41
3:C:48:PRO:HA	3:C:49:PRO:HD3	1.86	0.41
1:A:596:TYR:N	1:A:636:SER:O	2.53	0.41
3:C:49:PRO:HB2	3:C:187:LEU:HD13	2.01	0.41
4:U:5:VAL:HG23	4:U:13:ILE:HG13	2.02	0.41
6:F:364:MET:HG3	6:F:446:LEU:HD11	2.02	0.41
1:A:476:MET:HG2	1:A:517:TRP:NE1	2.36	0.41
6:F:414:ASP:OD1	6:F:414:ASP:N	2.46	0.41
7:G:37:ARG:HB3	7:G:38:PRO:HD2	2.03	0.41
1:A:564:VAL:HG22	2:R:24:VAL:HG22	2.03	0.41
7:G:38:PRO:HA	7:G:39:PRO:HD3	1.87	0.41
3:C:83:HIS:HD2	3:C:84:PRO:HD2	1.86	0.41
5:D:33:ARG:O	5:D:37:LEU:HG	2.21	0.41
1:A:565:LYS:NZ	2:R:25:LYS:HG2	2.35	0.41
8:H:70:GLU:OE1	8:H:113:ARG:NH1	2.54	0.41
1:A:209:SER:HB2	1:A:210:PRO:HD3	2.03	0.40
1:A:565:LYS:HB3	1:A:574:VAL:HG22	2.02	0.40
2:R:79:PHE:CZ	2:R:95:PRO:HD2	2.57	0.40
7:G:91:GLU:HA	7:G:92:PRO:HD3	1.95	0.40
8:H:181:VAL:HG22	8:H:184:LEU:HD12	2.03	0.40
1:A:442:ARG:HH11	1:A:442:ARG:HB2	1.86	0.40
1:A:454:GLU:O	1:A:458:ILE:HG12	2.21	0.40
4:U:1:MET:SD	4:U:2:GLN:N	2.94	0.40
1:A:109:ASN:HA	1:A:113:ILE:HB	2.03	0.40
7:G:37:ARG:HG3	7:G:79:PHE:CE2	2.56	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	A	623/745 (84%)	567 (91%)	56 (9%)	0	100	100
2	R	75/104 (72%)	62 (83%)	13 (17%)	0	100	100
3	C	185/238 (78%)	164 (89%)	21 (11%)	0	100	100
4	U	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
5	D	98/112 (88%)	95 (97%)	3 (3%)	0	100	100
6	F	109/115 (95%)	101 (93%)	8 (7%)	0	100	100
7	G	103/118 (87%)	94 (91%)	9 (9%)	0	100	100
8	H	147/160 (92%)	140 (95%)	7 (5%)	0	100	100
All	All	1413/1667 (85%)	1294 (92%)	119 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	507/681 (74%)	507 (100%)	0	100	100
2	R	50/89 (56%)	50 (100%)	0	100	100
3	C	138/173 (80%)	138 (100%)	0	100	100
4	U	63/68 (93%)	63 (100%)	0	100	100
5	D	81/96 (84%)	81 (100%)	0	100	100
6	F	84/97 (87%)	84 (100%)	0	100	100
7	G	89/103 (86%)	89 (100%)	0	100	100
8	H	135/147 (92%)	135 (100%)	0	100	100
All	All	1147/1454 (79%)	1147 (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. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
10	SY8	C	1101	3,4,6	6,6,6	0.32	0	6,6,6	0.73	0
11	759	H	301	-	69,75,75	0.79	3 (4%)	83,107,107	0.68	2 (2%)

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
10	SY8	C	1101	3,4,6	-	0/4/4/4	-
11	759	H	301	-	-	17/53/91/91	0/6/7/7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	301	759	CCI-CBX	-3.94	1.43	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	301	759	CCI-CCD	3.02	1.44	1.39
11	H	301	759	CCI-CCJ	-2.97	1.36	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	301	759	SBR-CAV-NBI	-3.52	103.42	105.41
11	H	301	759	CCQ-CCN-NBN	2.25	114.66	111.84

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	H	301	759	NBN-CCN-CCQ-CAF
11	H	301	759	NBN-CCN-CCQ-CAG
11	H	301	759	NBN-CCN-CCQ-CAE
11	H	301	759	CCQ-CCN-NBN-CBT
11	H	301	759	CCL-CBE-CBU-NBL
11	H	301	759	CCL-CBE-CBU-OAI
11	H	301	759	O-C-CA-CB
11	H	301	759	NBM-C-CA-CB
11	H	301	759	CBW-CCN-CCQ-CAE
11	H	301	759	CBW-CCN-CCQ-CAF
11	H	301	759	O-C-CA-N
11	H	301	759	CBW-CCN-CCQ-CAG
11	H	301	759	CBA-CBB-OBQ-CBD
11	H	301	759	NBM-C-CA-N
11	H	301	759	OBQ-CBD-CBT-OAH
11	H	301	759	OBQ-CBD-CBT-NBN
11	H	301	759	OBO-CAY-CAZ-OBP

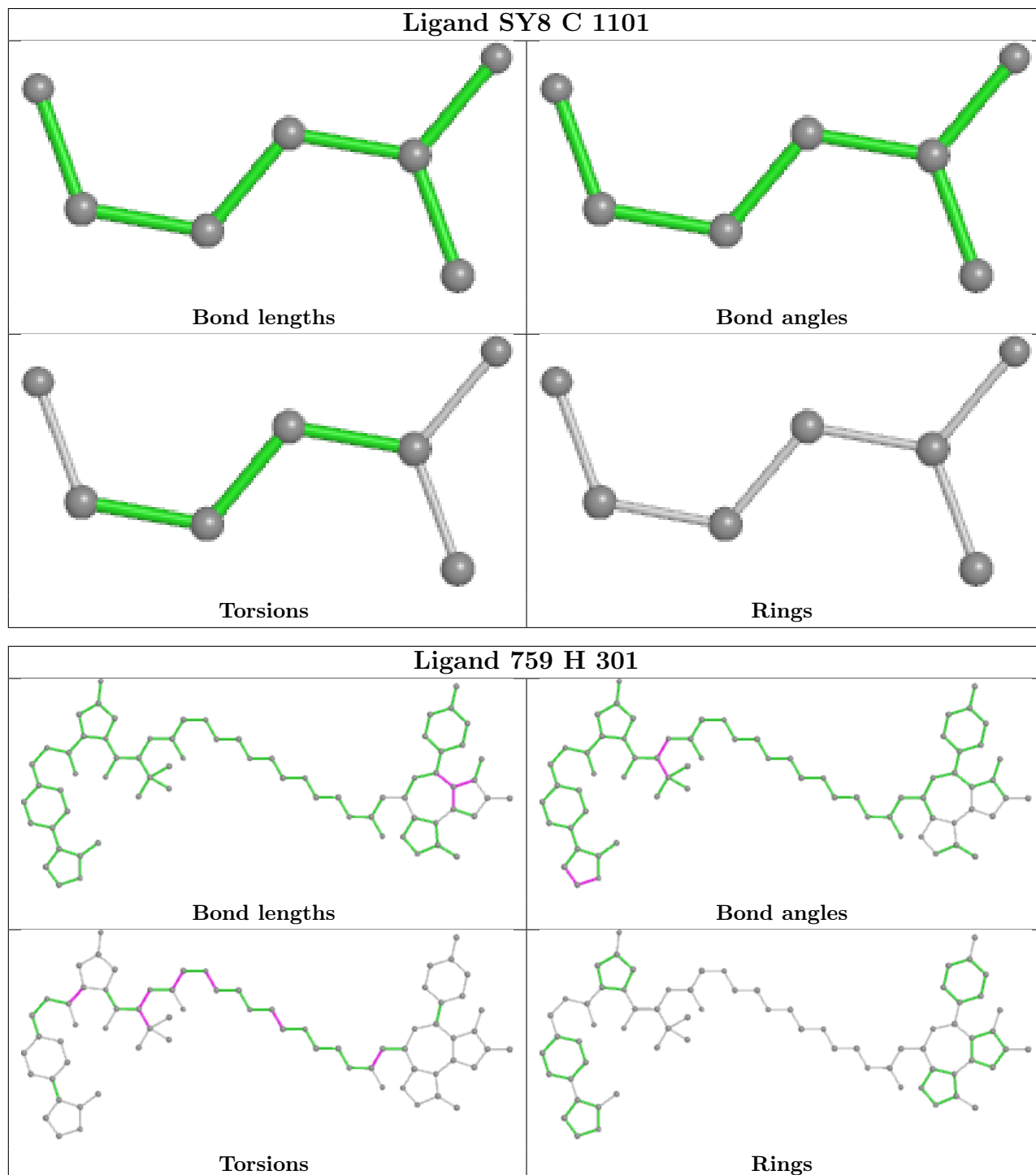
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1101	SY8	1	0
11	H	301	759	1	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	192:ILE	C	1000:UNK	N	27.05

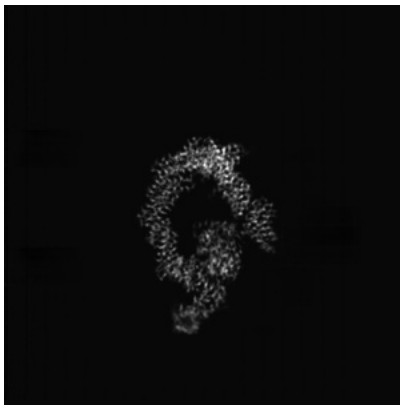
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18915. These allow visual inspection of the internal detail of the map and identification of artifacts.

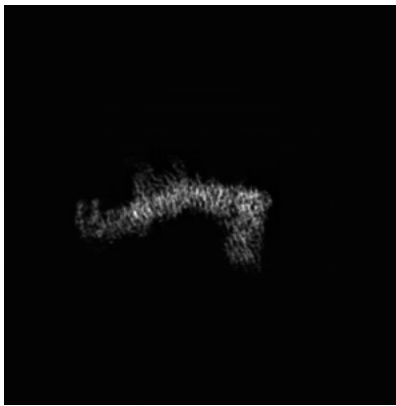
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

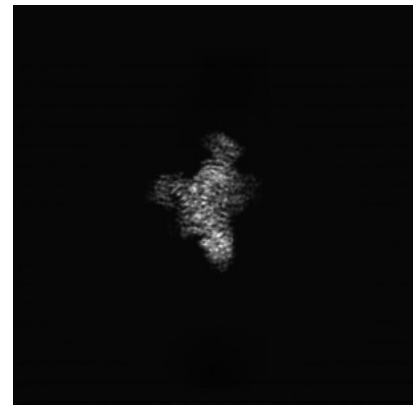
6.1.1 Primary map



X

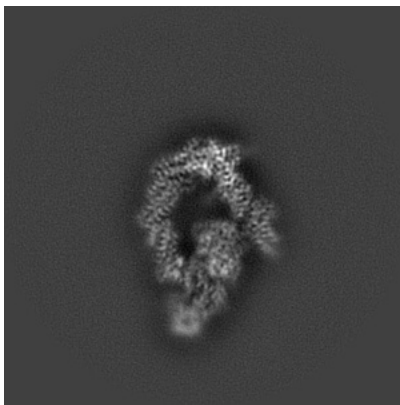


Y

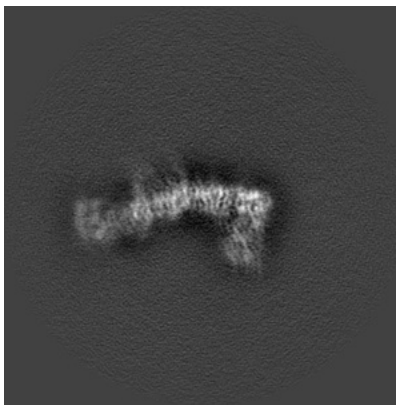


Z

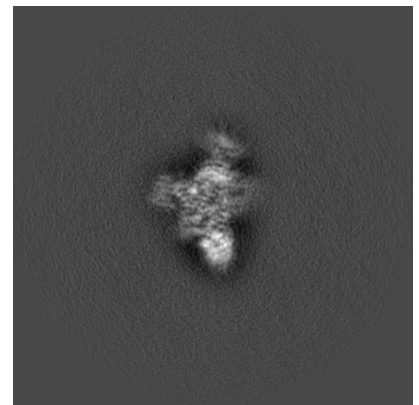
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

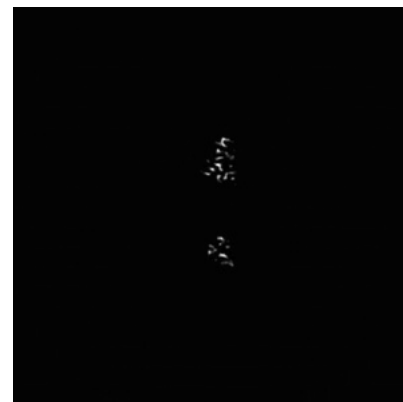
6.2.1 Primary map



X Index: 190

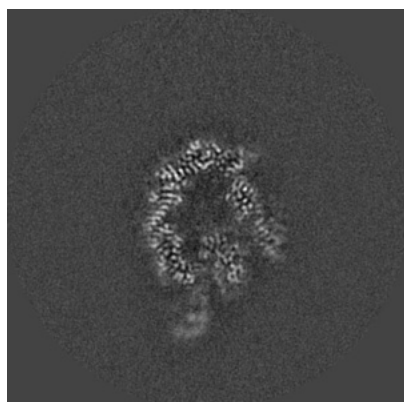


Y Index: 190

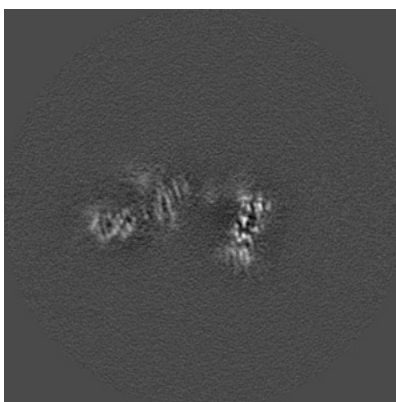


Z Index: 190

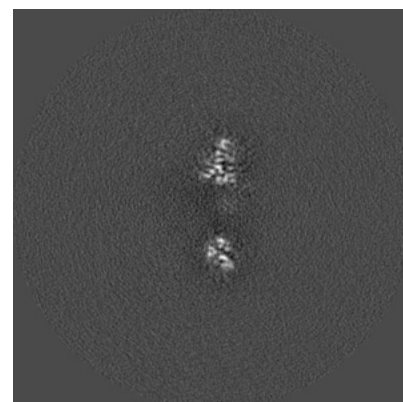
6.2.2 Raw map



X Index: 190



Y Index: 190



Z Index: 190

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: 193

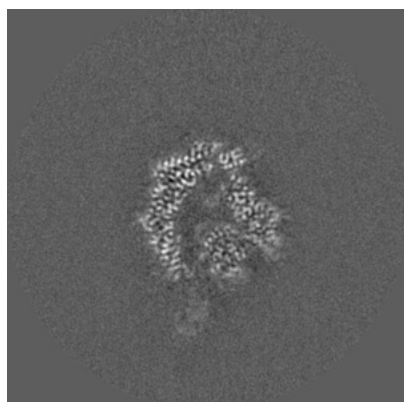


Y Index: 208

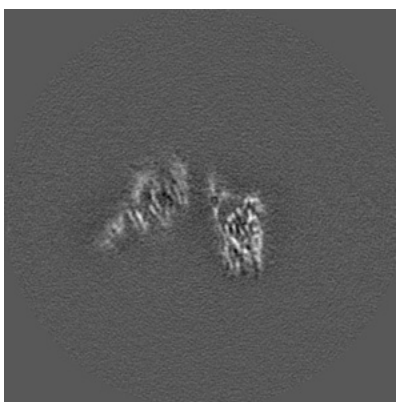


Z Index: 228

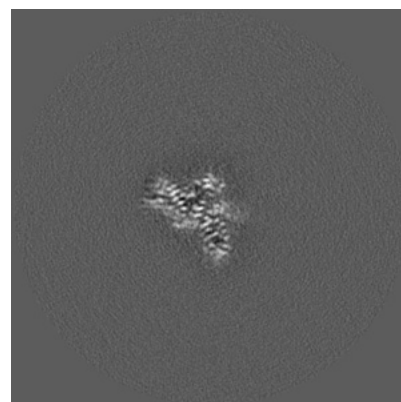
6.3.2 Raw map



X Index: 197



Y Index: 208

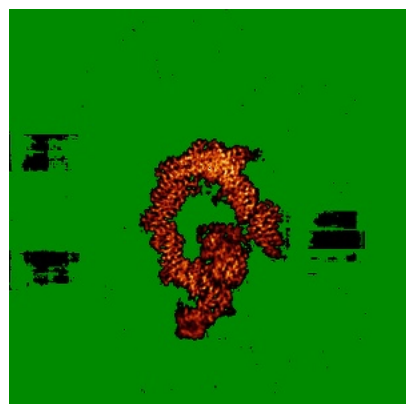


Z Index: 228

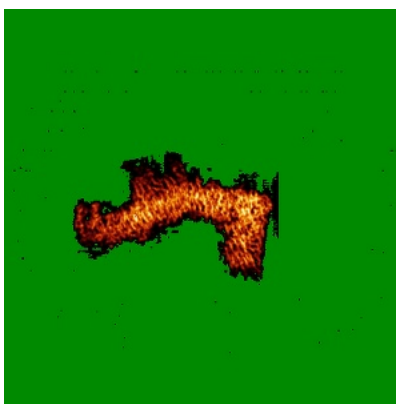
The images above show the largest variance slices of the map in three orthogonal directions.

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

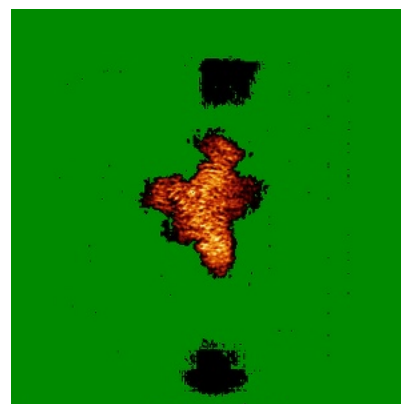
6.4.1 Primary map



X

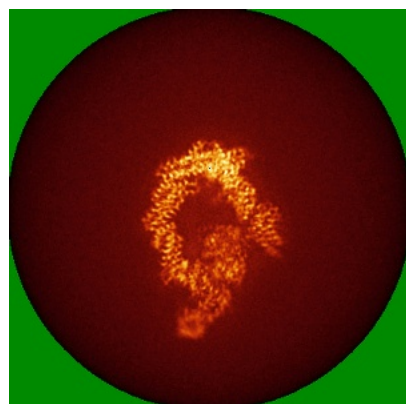


Y

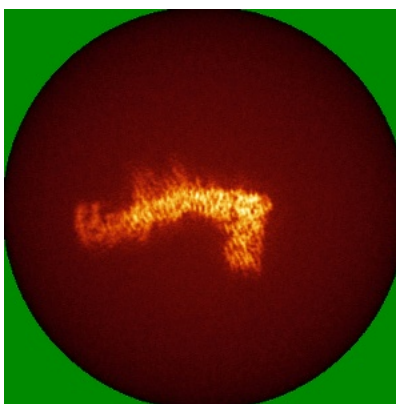


Z

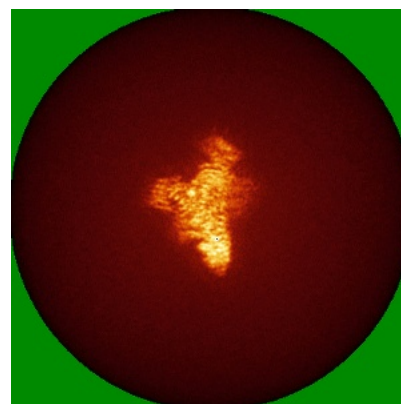
6.4.2 Raw map



X



Y

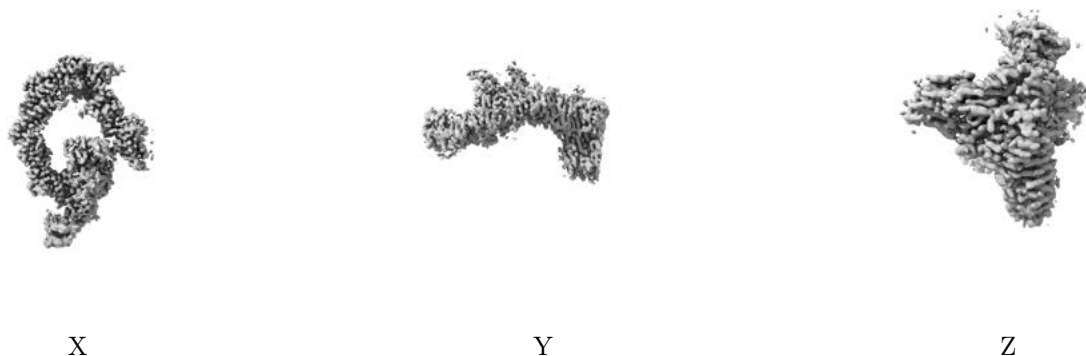


Z

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.

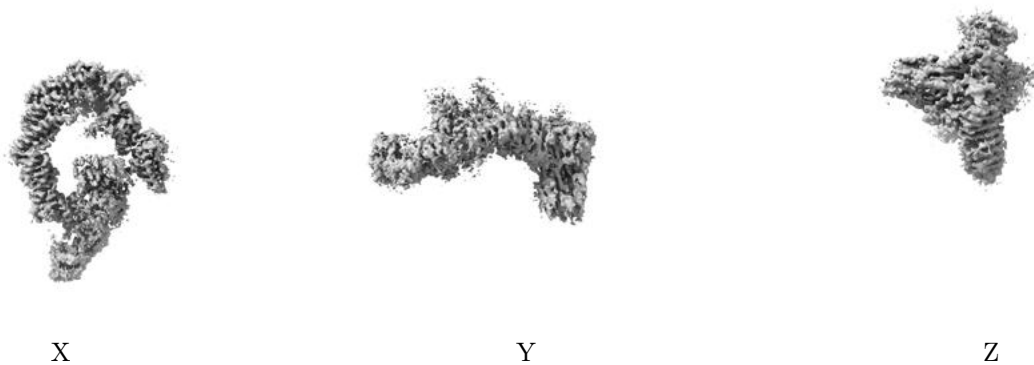
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0319. 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.

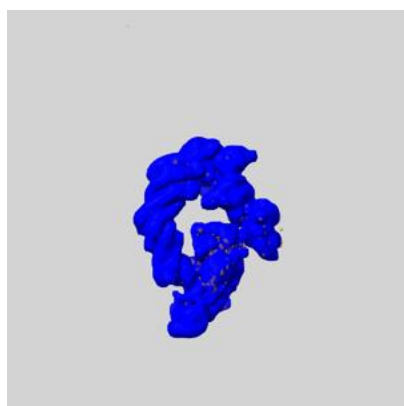
6.6 Mask visualisation [i](#)

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

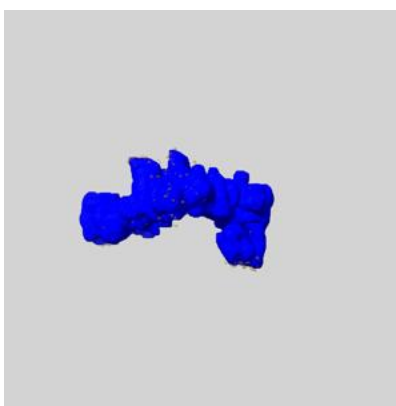
A mask typically either:

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

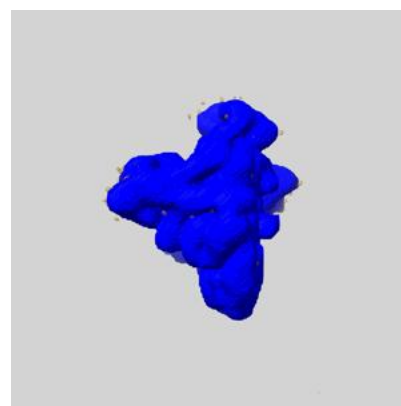
6.6.1 emd_18915_msk_1.map [i](#)



X



Y

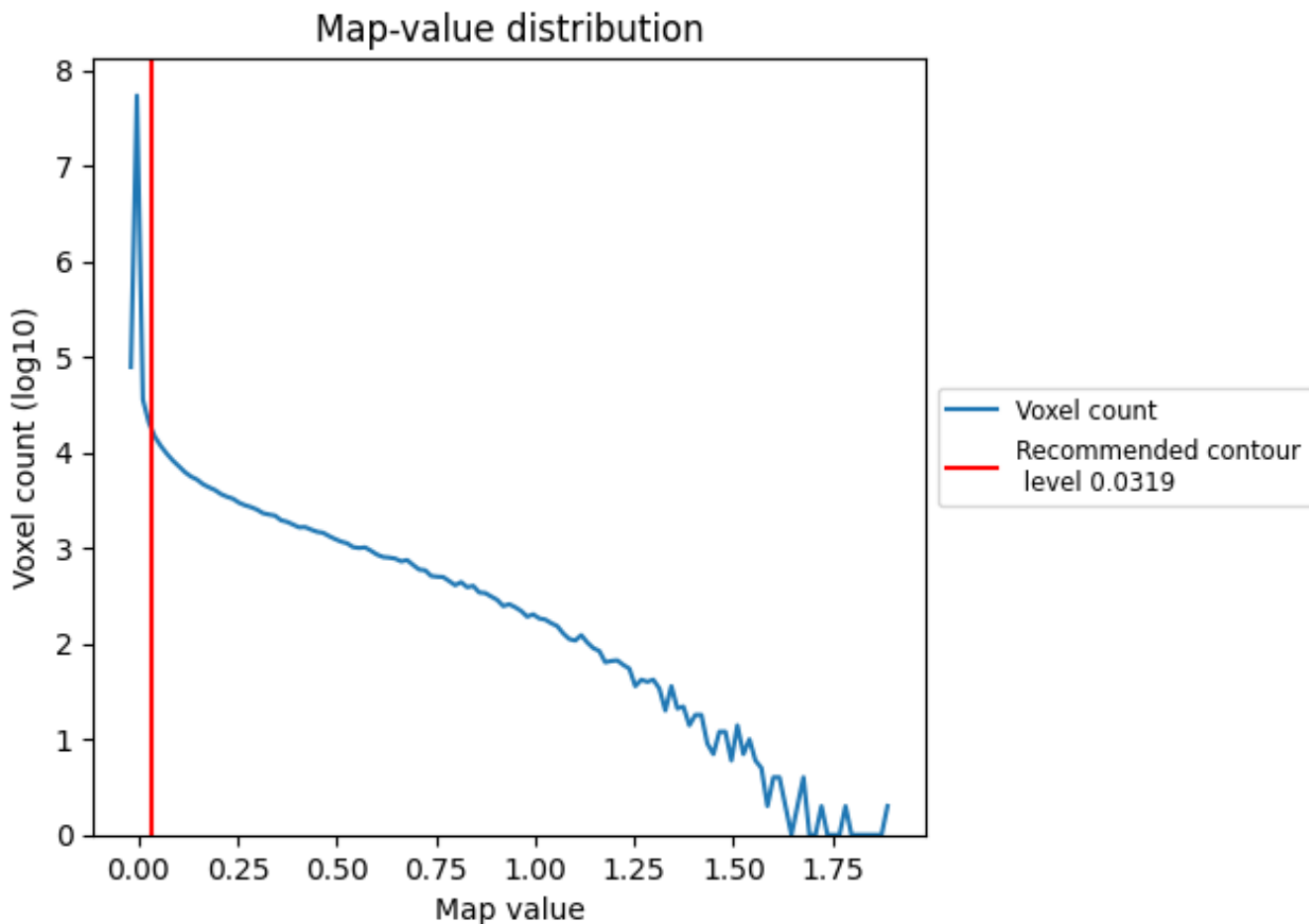


Z

7 Map analysis [i](#)

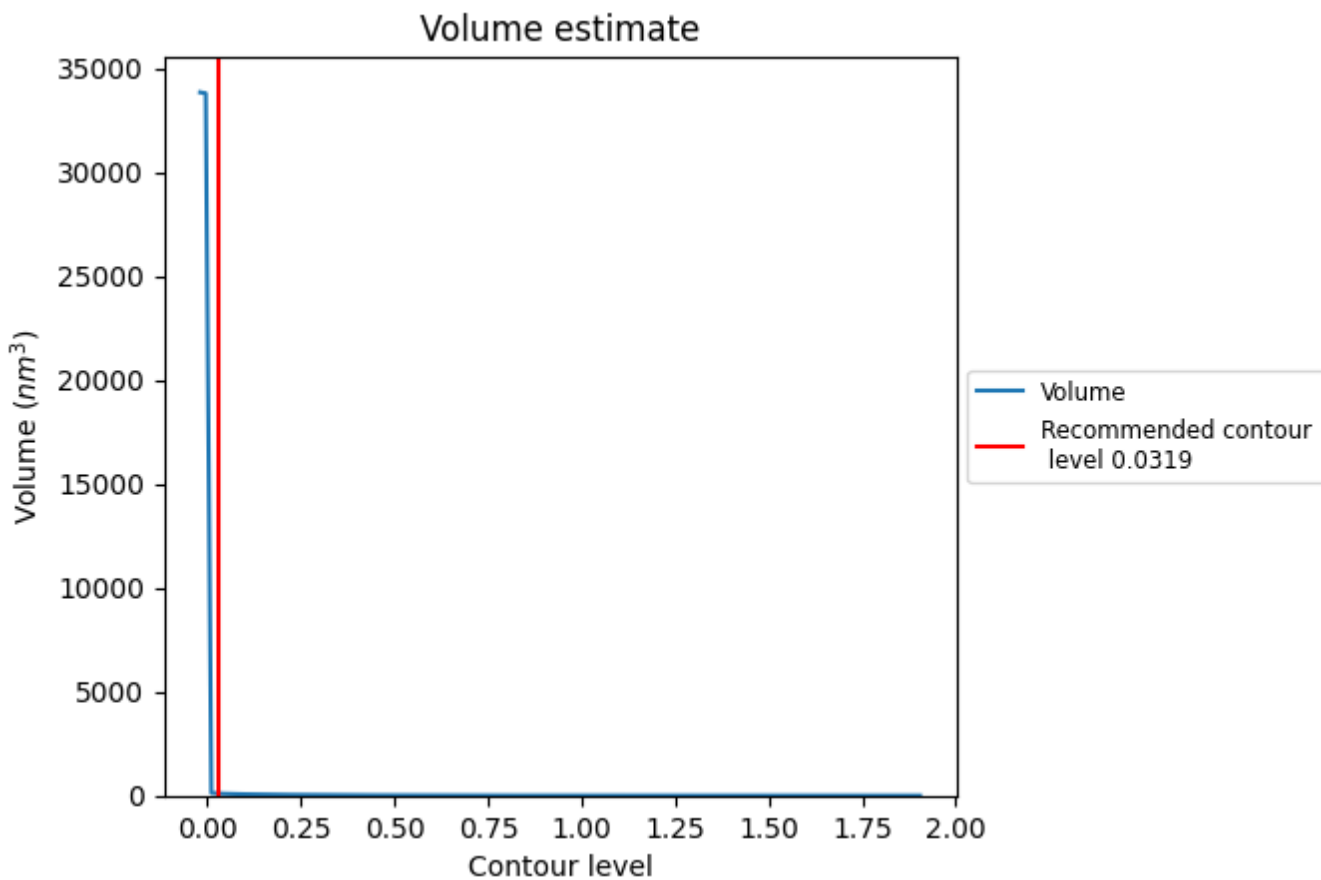
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

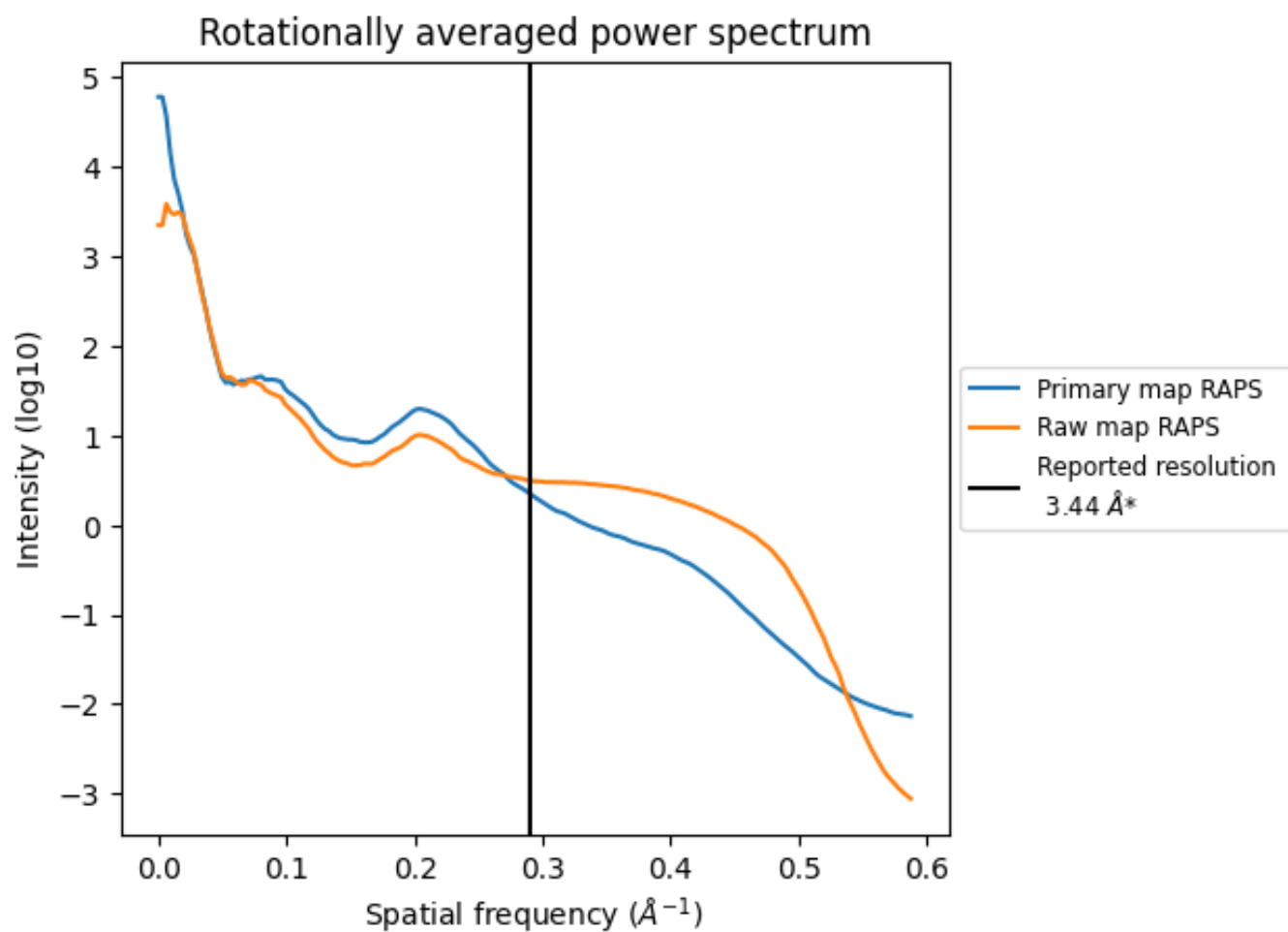
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 98 nm³; this corresponds to an approximate mass of 89 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 i

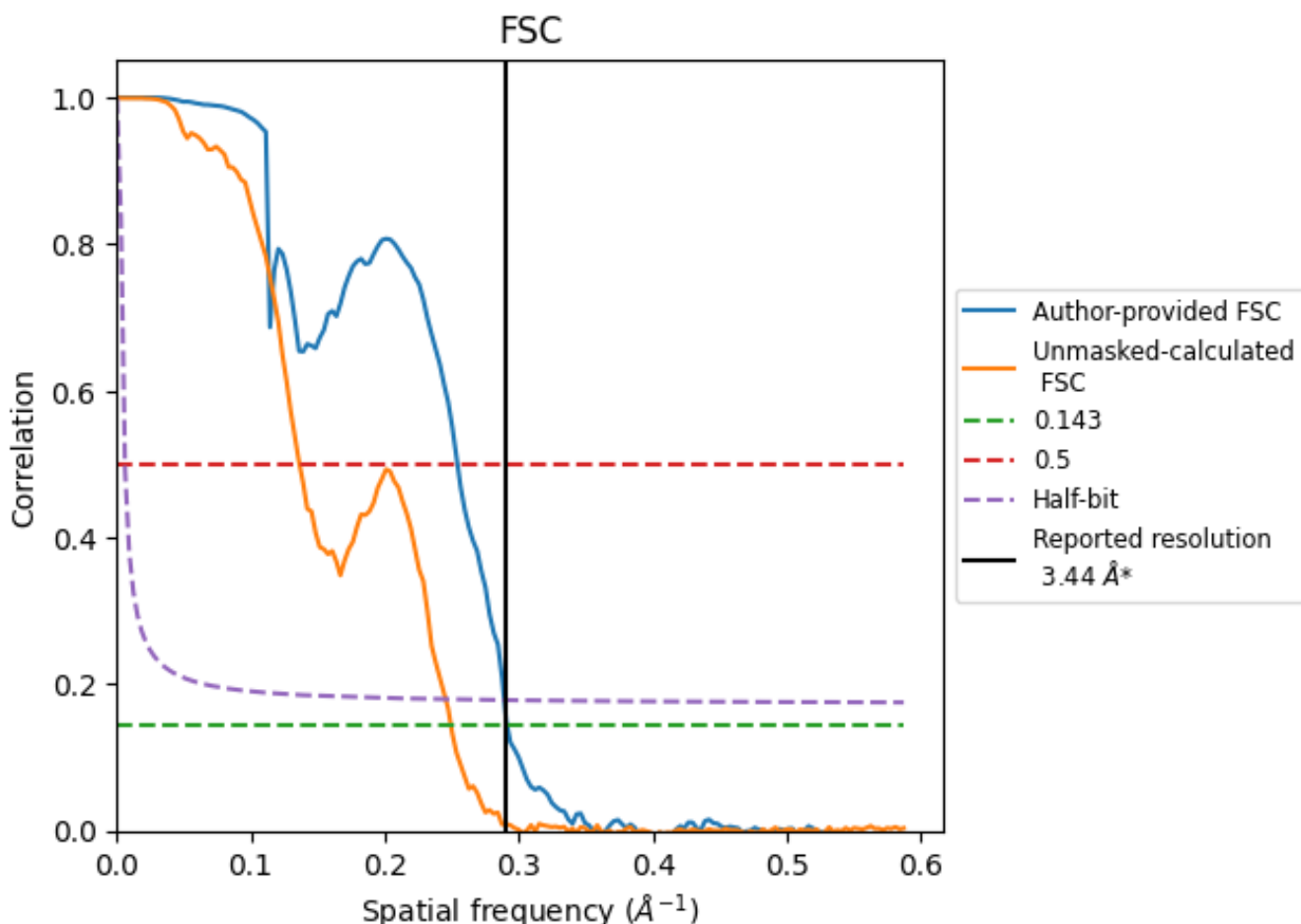


*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.291 Å⁻¹

8.2 Resolution estimates [i](#)

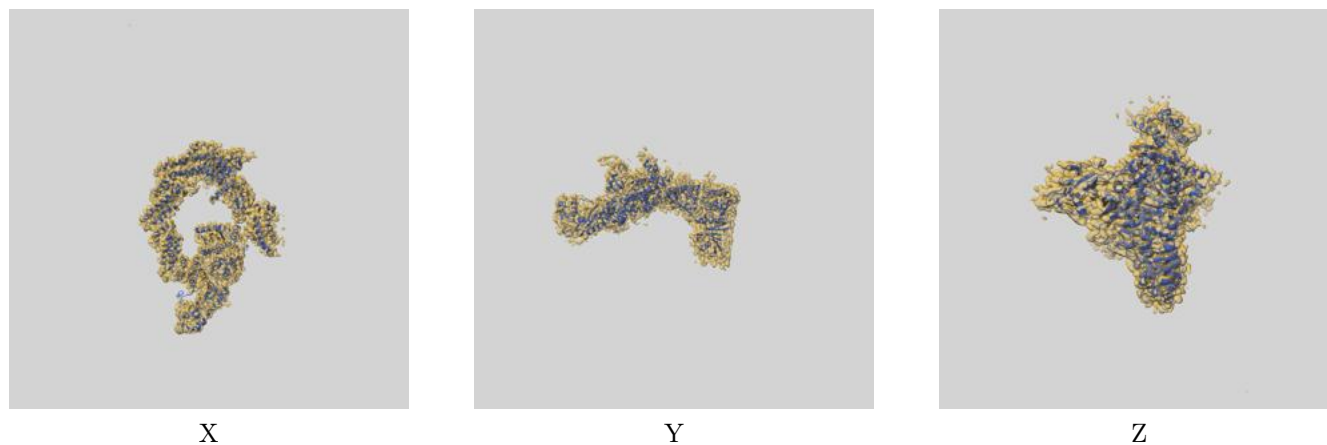
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.44	-	-
Author-provided FSC curve	3.43	3.93	3.46
Unmasked-calculated*	4.01	7.33	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.44 by more than 10 %

9 Map-model fit [i](#)

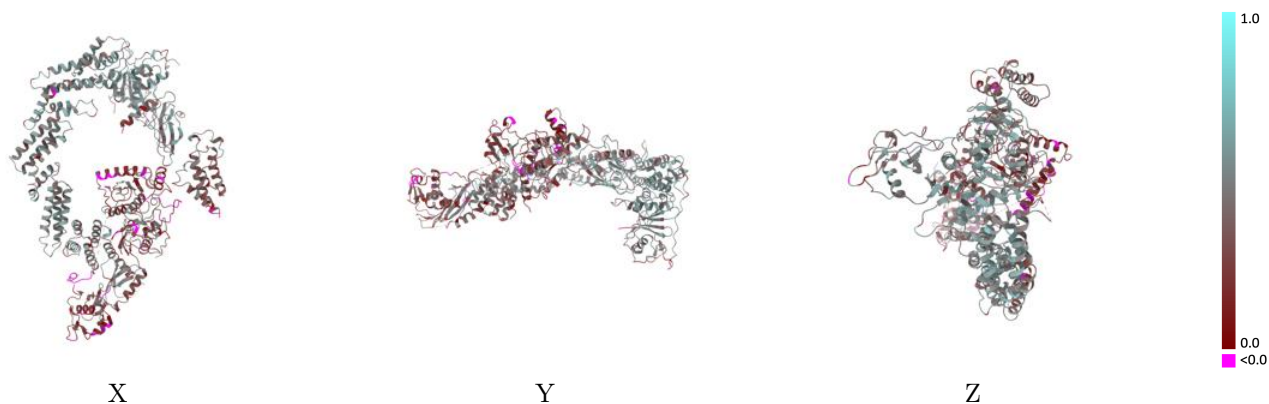
This section contains information regarding the fit between EMDB map EMD-18915 and PDB model 8R5H. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



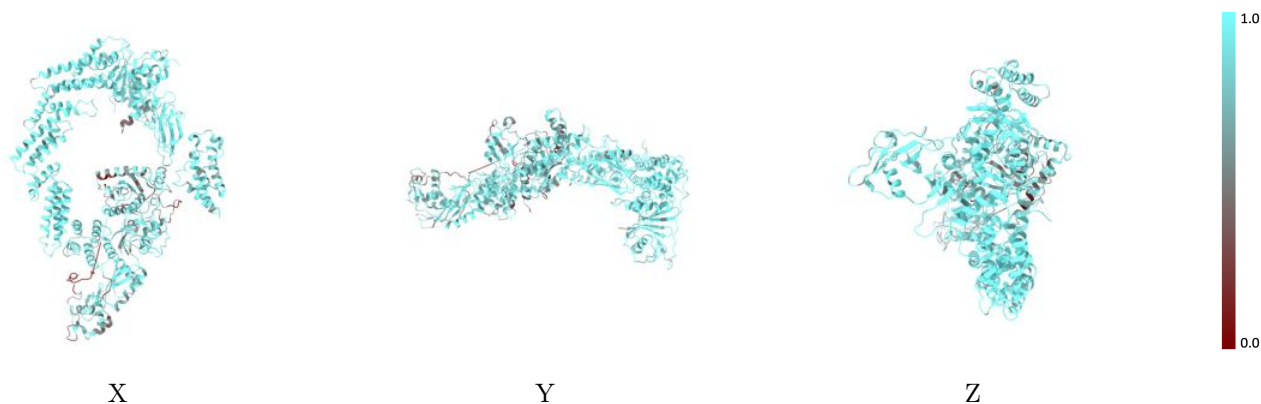
The images above show the 3D surface view of the map at the recommended contour level 0.0319 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



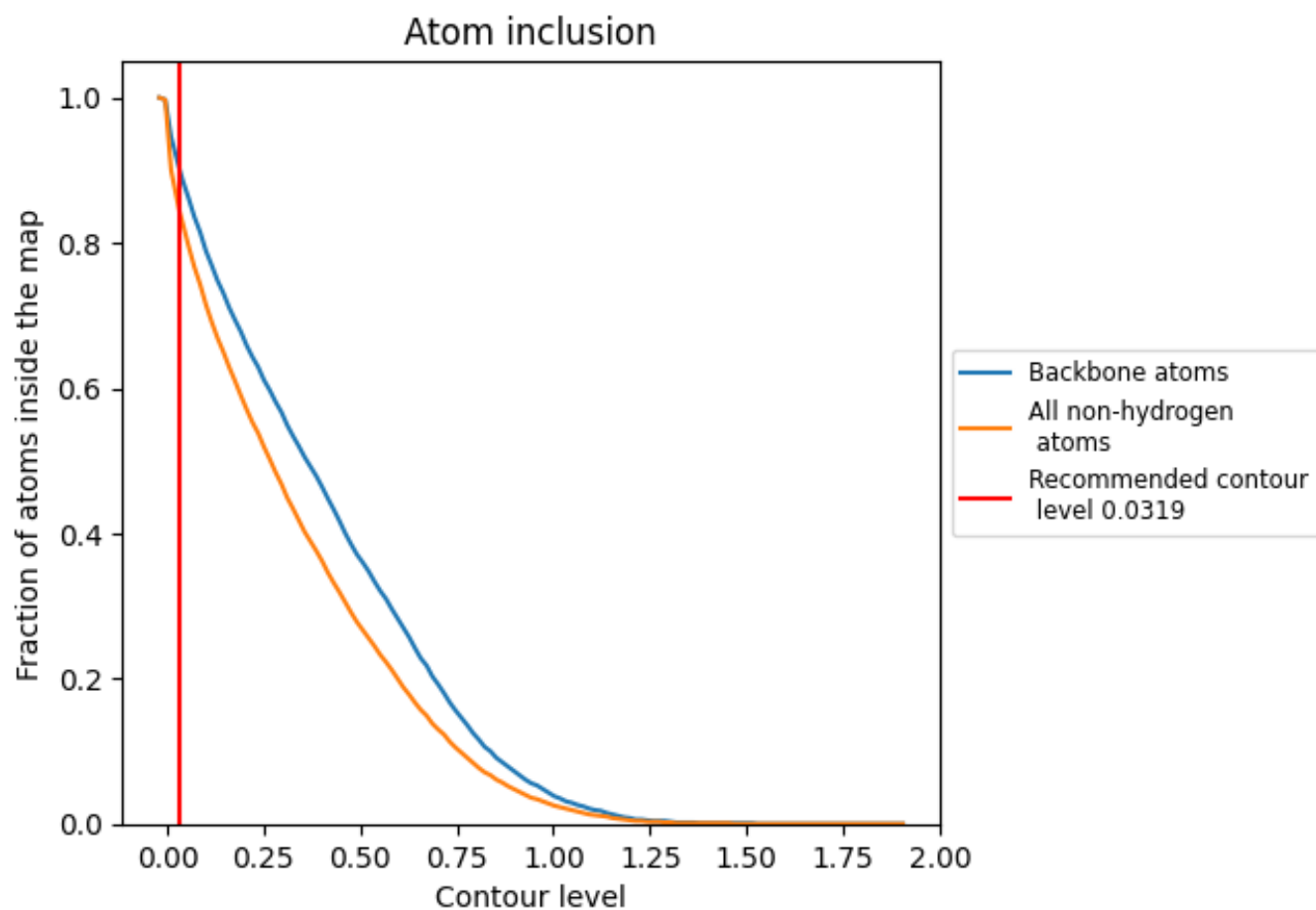
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0319).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0319) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8440	 0.3940
A	 0.8760	 0.4220
C	 0.6680	 0.2540
D	 0.9280	 0.5020
F	 0.8410	 0.3550
G	 0.8710	 0.4190
H	 0.9030	 0.4720
R	 0.8430	 0.3530
U	 0.7480	 0.2590

