



Full wwPDB EM Validation Report ⓘ

Jun 22, 2026 – 10:16 AM EDT

PDB ID : 9PTU / pdb_00009ptu
EMDB ID : EMD-71847
Title : Cryo-EM structure of the DCAF11 E3 ligase bound to the DDX18 helicase mediated by GSH-M12
Authors : Wachter, F.; Jin, C.Y.; Yoon, H.; Ebert, B.L.; Fischer, E.S.
Deposited on : 2025-07-29
Resolution : 2.38 Å (reported)
Based on initial models : 5FQD, .

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:

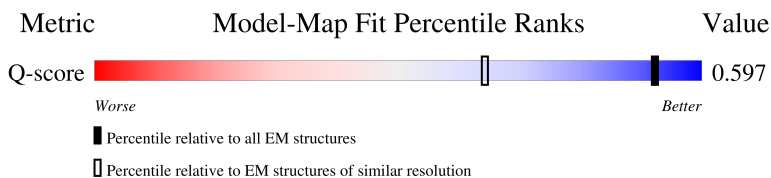
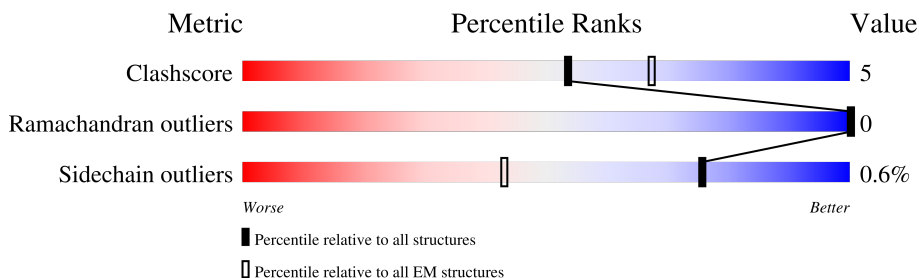
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 2.38 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	4811 (1.88 - 2.88)

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	590	 64% 8% 28%
2	C	478	 35% 9% 55%
3	B	864	 82% 9% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22803 atoms, of which 11341 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 DDB1- and CUL4-associated factor 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	427	Total	C	H	N	O	S	0	0
			6773	2162	3324	631	641	15		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-43	MET	-	initiating methionine	UNP Q8TEB1
A	-42	ASP	-	expression tag	UNP Q8TEB1
A	-41	TRP	-	expression tag	UNP Q8TEB1
A	-40	SER	-	expression tag	UNP Q8TEB1
A	-39	HIS	-	expression tag	UNP Q8TEB1
A	-38	PRO	-	expression tag	UNP Q8TEB1
A	-37	GLN	-	expression tag	UNP Q8TEB1
A	-36	PHE	-	expression tag	UNP Q8TEB1
A	-35	GLU	-	expression tag	UNP Q8TEB1
A	-34	LYS	-	expression tag	UNP Q8TEB1
A	-33	SER	-	expression tag	UNP Q8TEB1
A	-32	ALA	-	expression tag	UNP Q8TEB1
A	-31	VAL	-	expression tag	UNP Q8TEB1
A	-30	GLY	-	expression tag	UNP Q8TEB1
A	-29	LEU	-	expression tag	UNP Q8TEB1
A	-28	ASN	-	expression tag	UNP Q8TEB1
A	-27	ASP	-	expression tag	UNP Q8TEB1
A	-26	ILE	-	expression tag	UNP Q8TEB1
A	-25	PHE	-	expression tag	UNP Q8TEB1
A	-24	GLU	-	expression tag	UNP Q8TEB1
A	-23	ALA	-	expression tag	UNP Q8TEB1
A	-22	GLN	-	expression tag	UNP Q8TEB1
A	-21	LYS	-	expression tag	UNP Q8TEB1
A	-20	ILE	-	expression tag	UNP Q8TEB1
A	-19	GLU	-	expression tag	UNP Q8TEB1
A	-18	TRP	-	expression tag	UNP Q8TEB1
A	-17	HIS	-	expression tag	UNP Q8TEB1
A	-16	GLU	-	expression tag	UNP Q8TEB1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	expression tag	UNP Q8TEB1
A	-14	GLY	-	expression tag	UNP Q8TEB1
A	-13	GLY	-	expression tag	UNP Q8TEB1
A	-12	GLY	-	expression tag	UNP Q8TEB1
A	-11	SER	-	expression tag	UNP Q8TEB1
A	-10	GLY	-	expression tag	UNP Q8TEB1
A	-9	GLU	-	expression tag	UNP Q8TEB1
A	-8	ASN	-	expression tag	UNP Q8TEB1
A	-7	LEU	-	expression tag	UNP Q8TEB1
A	-6	TYR	-	expression tag	UNP Q8TEB1
A	-5	PHE	-	expression tag	UNP Q8TEB1
A	-4	GLN	-	expression tag	UNP Q8TEB1
A	-3	GLY	-	expression tag	UNP Q8TEB1
A	-2	GLY	-	expression tag	UNP Q8TEB1
A	-1	GLY	-	expression tag	UNP Q8TEB1
A	0	ARG	-	expression tag	UNP Q8TEB1

- Molecule 2 is a protein called ATP-dependent RNA helicase DDX18.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	213	Total	C	H	N	O	S	0	0
			3539	1150	1778	297	308	6		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	148	MET	-	initiating methionine	UNP Q9NVP1
C	149	ASP	-	expression tag	UNP Q9NVP1
C	150	TYR	-	expression tag	UNP Q9NVP1
C	151	LYS	-	expression tag	UNP Q9NVP1
C	152	ASP	-	expression tag	UNP Q9NVP1
C	153	ASP	-	expression tag	UNP Q9NVP1
C	154	ASP	-	expression tag	UNP Q9NVP1
C	155	ASP	-	expression tag	UNP Q9NVP1
C	156	LYS	-	expression tag	UNP Q9NVP1
C	157	SER	-	expression tag	UNP Q9NVP1
C	158	ALA	-	expression tag	UNP Q9NVP1
C	159	VAL	-	expression tag	UNP Q9NVP1
C	160	ASP	-	expression tag	UNP Q9NVP1
C	161	GLU	-	expression tag	UNP Q9NVP1
C	162	ASN	-	expression tag	UNP Q9NVP1
C	163	LEU	-	expression tag	UNP Q9NVP1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	164	TYR	-	expression tag	UNP Q9NVP1
C	165	PHE	-	expression tag	UNP Q9NVP1
C	166	GLN	-	expression tag	UNP Q9NVP1
C	167	GLY	-	expression tag	UNP Q9NVP1
C	168	GLY	-	expression tag	UNP Q9NVP1
C	169	GLY	-	expression tag	UNP Q9NVP1
C	170	ARG	-	expression tag	UNP Q9NVP1

- Molecule 3 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	B	786	Total	C	H	N	O	S	0	0
			12428	3948	6215	1049	1182	34		

There are 34 discrepancies between the modelled and reference sequences:

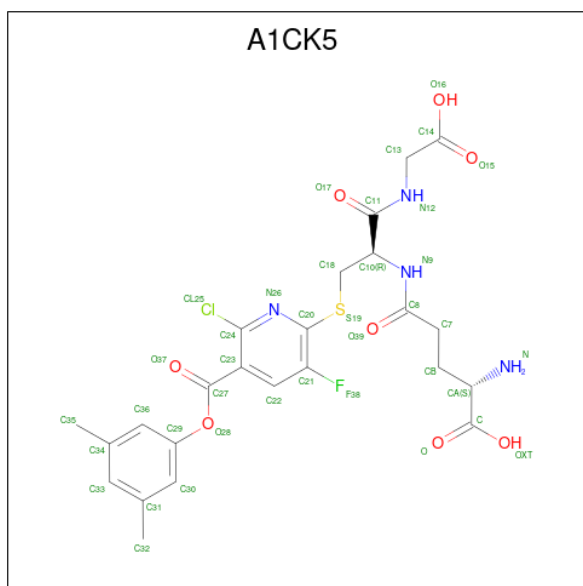
Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	MET	-	initiating methionine	UNP Q16531
B	-26	GLY	-	expression tag	UNP Q16531
B	-25	SER	-	expression tag	UNP Q16531
B	-24	SER	-	expression tag	UNP Q16531
B	-23	HIS	-	expression tag	UNP Q16531
B	-22	HIS	-	expression tag	UNP Q16531
B	-21	HIS	-	expression tag	UNP Q16531
B	-20	HIS	-	expression tag	UNP Q16531
B	-19	HIS	-	expression tag	UNP Q16531
B	-18	HIS	-	expression tag	UNP Q16531
B	-17	SER	-	expression tag	UNP Q16531
B	-16	ALA	-	expression tag	UNP Q16531
B	-15	ALA	-	expression tag	UNP Q16531
B	-14	HIS	-	expression tag	UNP Q16531
B	-13	ILE	-	expression tag	UNP Q16531
B	-12	VAL	-	expression tag	UNP Q16531
B	-11	MET	-	expression tag	UNP Q16531
B	-10	VAL	-	expression tag	UNP Q16531
B	-9	ASP	-	expression tag	UNP Q16531
B	-8	ALA	-	expression tag	UNP Q16531
B	-7	TYR	-	expression tag	UNP Q16531
B	-6	LYS	-	expression tag	UNP Q16531
B	-5	PRO	-	expression tag	UNP Q16531
B	-4	THR	-	expression tag	UNP Q16531
B	-3	LYS	-	expression tag	UNP Q16531

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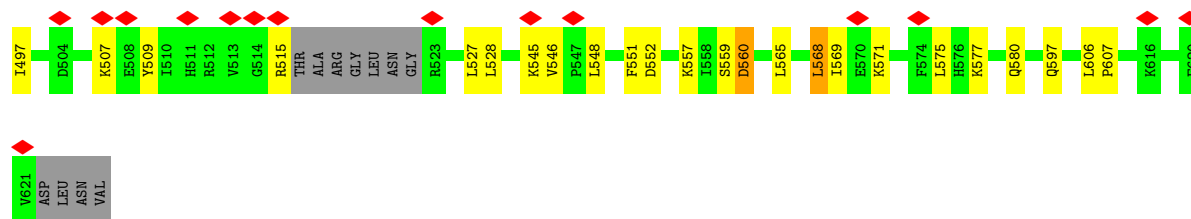
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q16531
B	-1	GLY	-	expression tag	UNP Q16531
B	0	ARG	-	expression tag	UNP Q16531
B	700	GLY	-	linker	UNP Q16531
B	701	ASN	-	linker	UNP Q16531
B	702	GLY	-	linker	UNP Q16531
B	703	ASN	-	linker	UNP Q16531
B	704	SER	-	linker	UNP Q16531
B	705	GLY	-	linker	UNP Q16531

- Molecule 4 is L-gamma-glutamyl-S-{6-chloro-5-[(3,5-dimethylphenoxy)carbonyl]-3-fluoropyridin-2-yl}-L-cysteinylglycine (CCD ID: A1CK5) (formula: C₂₄H₂₆ClFN₄O₈S) (labeled as "Ligand of Interest" by depositor).

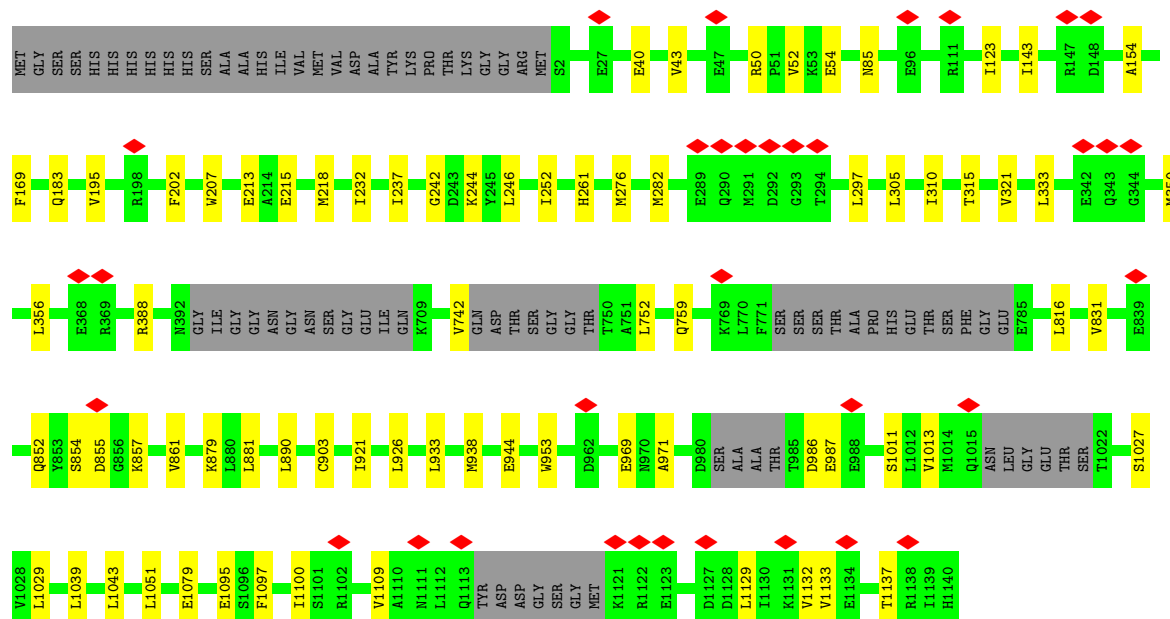


Mol	Chain	Residues	Atoms								AltConf
4	A	1	Total	C	Cl	F	H	N	O	S	0
			63	24	1	1	24	4	8	1	



• Molecule 3: DNA damage-binding protein 1

Chain B: 82% 9% 9%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	136583	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; As implemented in cryosparc live	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.004	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.256	Depositor
Minimum map value	-0.092	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (\AA)	280.32, 280.32, 280.32	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.73, 0.73, 0.73	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: A1CK5

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	0.15	0/3533	0.39	0/4770
2	C	0.20	0/1807	0.52	0/2438
3	B	0.15	0/6321	0.38	0/8540
All	All	0.16	0/11661	0.41	0/15748

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	3449	3324	3324	36	0
2	C	1761	1778	1778	35	0
3	B	6213	6215	6214	50	0
4	A	39	24	0	0	0
All	All	11462	11341	11316	119	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 5.

All (119) 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)
3:B:1109:VAL:HG12	3:B:1129:LEU:HD22	1.64	0.79
2:C:491:ILE:O	2:C:491:ILE:HD12	1.85	0.76
2:C:436:MET:HA	2:C:436:MET:HE2	1.68	0.76
1:A:198:LEU:HD13	1:A:247:ILE:HG23	1.77	0.65
3:B:938:MET:H	3:B:938:MET:HE3	1.59	0.65
1:A:318:ILE:HD12	1:A:319:SER:N	2.12	0.65
2:C:461:GLN:OE1	2:C:465:THR:HG23	1.97	0.64
2:C:462:ASN:O	2:C:466:THR:HG23	1.96	0.64
2:C:405:VAL:HG11	2:C:415:LEU:HD11	1.80	0.63
3:B:232:ILE:HD12	3:B:237:ILE:HD12	1.81	0.62
2:C:515:ARG:N	2:C:515:ARG:HE	2.00	0.58
2:C:548:LEU:O	2:C:548:LEU:HD12	2.04	0.58
3:B:43:VAL:HG23	3:B:52:VAL:HG11	1.85	0.57
2:C:568:LEU:HD21	2:C:575:LEU:HD12	1.85	0.57
3:B:1095:GLU:HG2	3:B:1137:THR:HG22	1.87	0.56
3:B:232:ILE:HD13	3:B:237:ILE:HG23	1.87	0.56
1:A:350:ALA:HB3	1:A:393:MET:SD	2.46	0.56
3:B:282:MET:HB2	3:B:305:LEU:HD11	1.88	0.56
1:A:238:TRP:CD2	1:A:267:ALA:HB2	2.41	0.56
3:B:1011:SER:OG	3:B:1013:VAL:HG22	2.06	0.55
1:A:318:ILE:HD12	1:A:319:SER:H	1.73	0.54
1:A:336:ASP:HB2	1:A:348:VAL:HG21	1.90	0.54
3:B:232:ILE:CD1	3:B:237:ILE:HG23	2.38	0.54
1:A:98:THR:HG23	1:A:98:THR:O	2.08	0.53
2:C:443:GLU:HB2	2:C:575:LEU:HD21	1.90	0.52
1:A:390:ARG:NE	1:A:390:ARG:HA	2.25	0.52
3:B:742:VAL:HG13	3:B:752:LEU:HD21	1.90	0.52
2:C:475:ASP:OD1	2:C:476:SER:N	2.43	0.52
2:C:494:VAL:HG11	2:C:497:ILE:HD13	1.91	0.52
1:A:120:LEU:HD22	3:B:183:GLN:NE2	2.25	0.51
2:C:559:SER:O	2:C:560:ASP:OD1	2.27	0.51
3:B:321:VAL:HG12	3:B:333:LEU:HD22	1.92	0.51
3:B:143:ILE:HG12	3:B:154:ALA:HB2	1.94	0.50
3:B:195:VAL:HG22	3:B:202:PHE:HE1	1.76	0.50
3:B:276:MET:O	3:B:310:ILE:HD12	2.12	0.50
2:C:448:ILE:HG22	2:C:448:ILE:O	2.11	0.50
3:B:43:VAL:CG2	3:B:52:VAL:HG11	2.42	0.50
3:B:321:VAL:CG1	3:B:333:LEU:HD22	2.41	0.50
1:A:120:LEU:HD22	3:B:183:GLN:HE22	1.77	0.49
3:B:1133:VAL:O	3:B:1137:THR:HG23	2.13	0.49
2:C:402:GLN:O	2:C:402:GLN:OE1	2.29	0.49
3:B:1029:LEU:HD23	3:B:1039:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:LYS:H	2:C:507:LYS:HE2	1.78	0.48
3:B:43:VAL:HG11	3:B:50:ARG:HH21	1.78	0.48
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.77	0.48
3:B:1027:SER:OG	3:B:1039:LEU:HD11	2.13	0.48
1:A:289:LEU:HD21	1:A:310:VAL:HG11	1.94	0.48
1:A:192:GLN:HG3	1:A:220:SER:HB2	1.96	0.48
1:A:397:ARG:HG3	1:A:397:ARG:HH11	1.79	0.48
2:C:545:LYS:N	2:C:545:LYS:HD2	2.29	0.48
1:A:298:ARG:NH1	1:A:298:ARG:HB3	2.29	0.47
3:B:218:MET:HE1	3:B:261:HIS:HB3	1.96	0.47
1:A:301:LEU:HD12	1:A:342:GLU:HG3	1.97	0.47
3:B:1079:GLU:OE2	3:B:1079:GLU:O	2.33	0.47
2:C:461:GLN:OE1	2:C:461:GLN:O	2.33	0.46
3:B:933:LEU:HD23	3:B:944:GLU:HA	1.98	0.46
3:B:356:LEU:HD23	3:B:388:ARG:HD2	1.98	0.46
3:B:986:ASP:OD1	3:B:987:GLU:N	2.48	0.46
1:A:303:ILE:HD12	1:A:340:MET:HG2	1.98	0.46
2:C:495:ASP:C	2:C:495:ASP:OD2	2.58	0.46
3:B:85:ASN:O	3:B:85:ASN:OD1	2.34	0.46
1:A:173:GLN:HB3	1:A:192:GLN:HB3	1.97	0.45
2:C:439:LYS:O	2:C:443:GLU:HG3	2.15	0.45
3:B:969:GLU:OE2	3:B:971:ALA:HB3	2.17	0.45
2:C:460:LYS:CD	2:C:460:LYS:H	2.29	0.45
2:C:551:PHE:O	2:C:552:ASP:OD1	2.34	0.45
1:A:216:ASP:O	1:A:216:ASP:CG	2.59	0.45
2:C:455:ILE:HG22	2:C:467:THR:OG1	2.17	0.45
3:B:213:GLU:HG2	3:B:215:GLU:H	1.82	0.45
3:B:252:ILE:O	3:B:252:ILE:HG13	2.16	0.45
2:C:458:LYS:O	2:C:458:LYS:HG3	2.15	0.45
1:A:291:VAL:HB	1:A:301:LEU:HB3	1.98	0.45
2:C:405:VAL:HG23	2:C:527:LEU:HD11	1.99	0.45
1:A:222:LEU:HD11	1:A:238:TRP:CD1	2.52	0.45
1:A:289:LEU:HB2	1:A:303:ILE:HG23	1.99	0.45
2:C:460:LYS:H	2:C:460:LYS:HD3	1.82	0.44
3:B:123:ILE:HD12	3:B:169:PHE:CD2	2.52	0.44
1:A:317:ASP:HB3	1:A:367:ALA:HB2	1.99	0.44
2:C:509:TYR:OH	2:C:528:LEU:HB2	2.18	0.44
3:B:852:GLN:HB2	3:B:861:VAL:HG21	2.00	0.44
1:A:303:ILE:HG13	1:A:345:PRO:HB3	1.99	0.43
2:C:606:LEU:HB2	2:C:607:PRO:HD3	2.00	0.43
2:C:606:LEU:H	2:C:606:LEU:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:246:LEU:HD12	3:B:297:LEU:CD1	2.49	0.43
3:B:881:LEU:HD21	3:B:921:ILE:HG21	1.99	0.43
3:B:1129:LEU:HA	3:B:1132:VAL:HG22	2.01	0.43
3:B:207:TRP:HB3	3:B:242:GLY:HA2	2.00	0.43
1:A:216:ASP:O	1:A:216:ASP:OD1	2.36	0.43
2:C:493:GLU:O	2:C:493:GLU:HG3	2.19	0.43
3:B:855:ASP:OD1	3:B:857:LYS:HG3	2.18	0.43
3:B:1097:PHE:O	3:B:1100:ILE:HG12	2.19	0.43
3:B:926:LEU:O	3:B:953:TRP:HA	2.18	0.43
1:A:366:ASP:O	1:A:367:ALA:HB3	2.18	0.42
1:A:235:TYR:CZ	1:A:243:HIS:HB2	2.54	0.42
1:A:371:ILE:HG23	1:A:445:PHE:CZ	2.55	0.42
3:B:195:VAL:HG22	3:B:202:PHE:CE1	2.53	0.42
2:C:565:LEU:O	2:C:569:ILE:HG12	2.19	0.42
2:C:597:GLN:N	2:C:597:GLN:OE1	2.51	0.42
1:A:308:ASP:HB3	1:A:328:ASP:HB2	2.01	0.42
2:C:546:VAL:O	2:C:546:VAL:HG23	2.20	0.42
3:B:1043:LEU:HD21	3:B:1051:LEU:HD12	2.01	0.42
1:A:278:ARG:HH11	1:A:278:ARG:HB3	1.84	0.41
2:C:577:LYS:O	2:C:577:LYS:HD3	2.20	0.41
1:A:278:ARG:HB3	1:A:278:ARG:NH1	2.36	0.41
3:B:879:LYS:HB2	3:B:890:LEU:HD11	2.01	0.41
1:A:201:CYS:HA	1:A:205:ARG:O	2.20	0.41
3:B:244:LYS:CE	3:B:246:LEU:HD21	2.51	0.41
1:A:100:ASP:OD2	1:A:102:ARG:HD3	2.21	0.41
2:C:571:LYS:HD2	2:C:571:LYS:C	2.45	0.41
3:B:854:SER:O	3:B:855:ASP:OD1	2.38	0.41
3:B:857:LYS:C	3:B:857:LYS:HD2	2.46	0.41
1:A:346:LYS:HA	1:A:346:LYS:HE2	2.03	0.40
2:C:552:ASP:OD1	2:C:552:ASP:C	2.63	0.40
3:B:816:LEU:HD13	3:B:831:VAL:HG22	2.03	0.40
1:A:389:SER:O	1:A:393:MET:HG3	2.22	0.40
3:B:315:THR:O	3:B:315:THR:HG23	2.22	0.40
1:A:513:ARG:HD2	1:A:513:ARG:HA	1.96	0.40
3:B:40:GLU:HG2	3:B:54:GLU:HG2	2.03	0.40
3:B:890:LEU:HB3	3:B:903:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/590 (72%)	409 (96%)	16 (4%)	0	100	100
2	C	209/478 (44%)	205 (98%)	4 (2%)	0	100	100
3	B	772/864 (89%)	754 (98%)	18 (2%)	0	100	100
All	All	1406/1932 (73%)	1368 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/498 (74%)	368 (100%)	2 (0%)	81	90
2	C	196/419 (47%)	192 (98%)	4 (2%)	48	68
3	B	691/749 (92%)	689 (100%)	2 (0%)	86	93
All	All	1257/1666 (76%)	1249 (99%)	8 (1%)	76	88

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ILE
1	A	485	CYS
2	C	557	LYS
2	C	560	ASP
2	C	568	LEU

Continued on next page...

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Mol	Chain	Res	Type
2	C	580	GLN
3	B	350	MET
3	B	759	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	194	GLN
1	A	321	GLN
1	A	355	GLN
3	B	711	HIS
3	B	978	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](#)

1 ligand is modelled in this entry.

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	$\# Z > 2$
4	A1CK5	A	601	-	39,40,40	4.31	18 (46%)	49,55,55	1.42	4 (8%)

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
4	A1CK5	A	601	-	-	4/35/35/35	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	A1CK5	C20-N26	11.68	1.48	1.33
4	A	601	A1CK5	C33-C34	8.95	1.52	1.39
4	A	601	A1CK5	C30-C31	8.89	1.52	1.39
4	A	601	A1CK5	C24-C23	8.76	1.53	1.39
4	A	601	A1CK5	C36-C29	8.38	1.52	1.39
4	A	601	A1CK5	C22-C23	-7.42	1.28	1.39
4	A	601	A1CK5	C22-C21	6.53	1.48	1.37
4	A	601	A1CK5	C8-N9	5.34	1.45	1.34
4	A	601	A1CK5	C11-N12	4.76	1.44	1.33
4	A	601	A1CK5	C36-C34	-4.65	1.31	1.39
4	A	601	A1CK5	C33-C31	-4.56	1.31	1.39
4	A	601	A1CK5	C21-C20	-4.47	1.31	1.38
4	A	601	A1CK5	C30-C29	-4.28	1.31	1.39
4	A	601	A1CK5	C20-S19	3.67	1.81	1.76
4	A	601	A1CK5	C24-N26	-2.72	1.28	1.32
4	A	601	A1CK5	O17-C11	-2.49	1.18	1.23
4	A	601	A1CK5	C24-CL25	2.42	1.78	1.74
4	A	601	A1CK5	O39-C8	-2.29	1.18	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	A1CK5	C18-S19-C20	5.81	109.56	102.36
4	A	601	A1CK5	C24-N26-C20	2.78	120.12	118.03
4	A	601	A1CK5	C7-C8-N9	2.13	119.62	115.86
4	A	601	A1CK5	C22-C21-C20	-2.11	120.07	121.61

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	A1CK5	C21-C20-S19-C18

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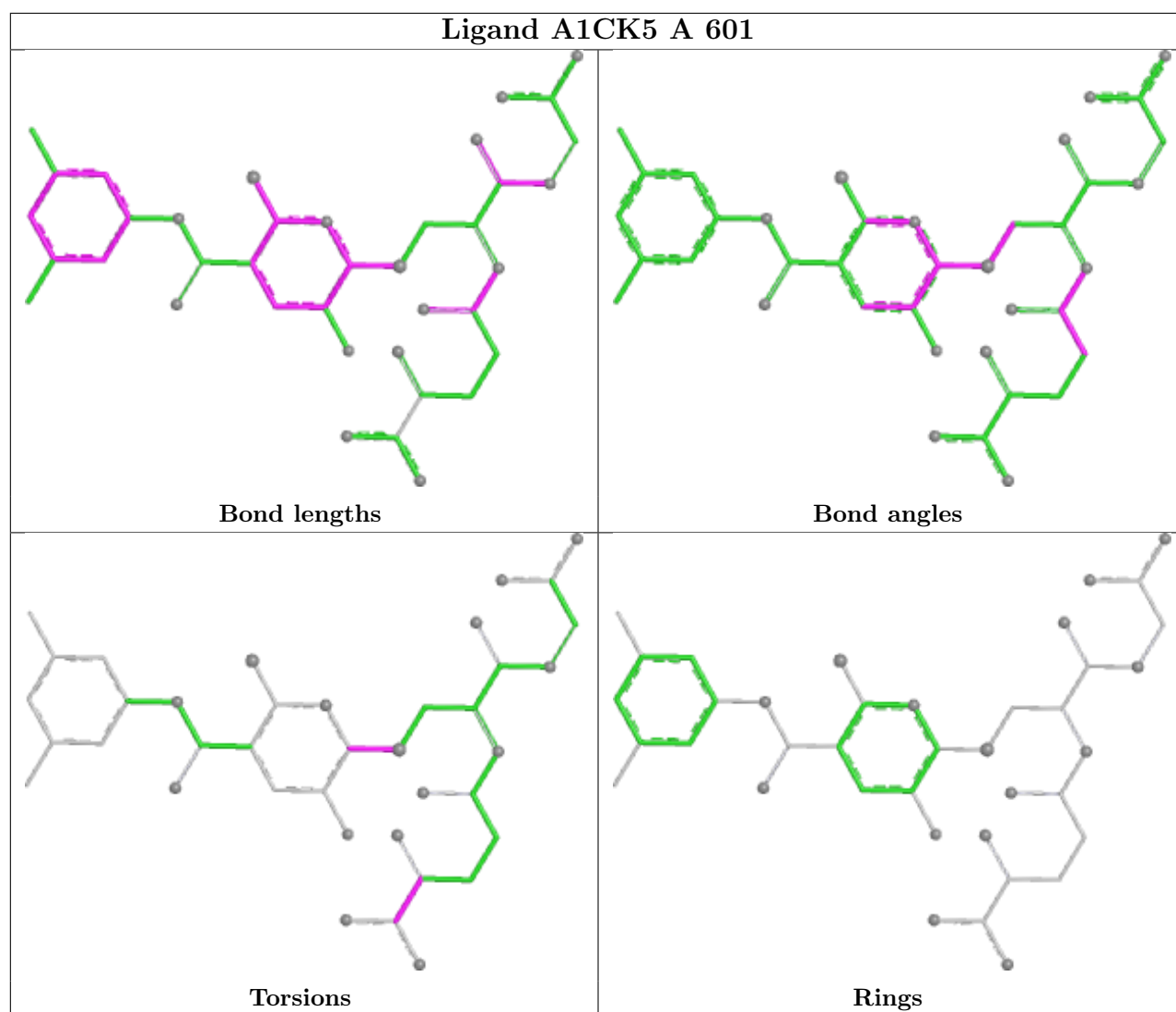
Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	601	A1CK5	N26-C20-S19-C18
4	A	601	A1CK5	OXT-C-CA-N
4	A	601	A1CK5	O-C-CA-N

There are no ring outliers.

No monomer is involved in short contacts.

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.

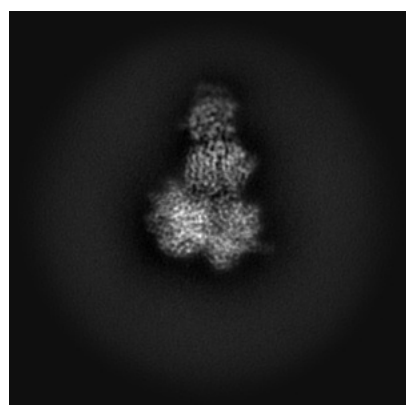
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71847. These allow visual inspection of the internal detail of the map and identification of artifacts.

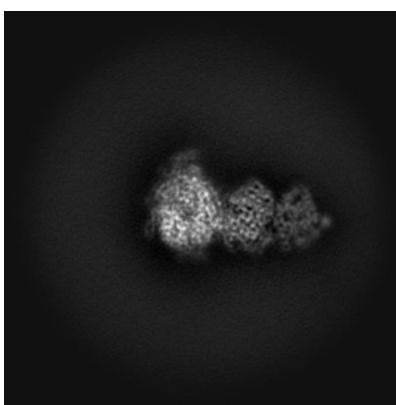
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

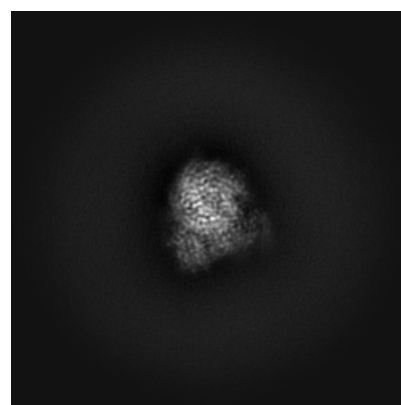
6.1.1 Primary map



X



Y

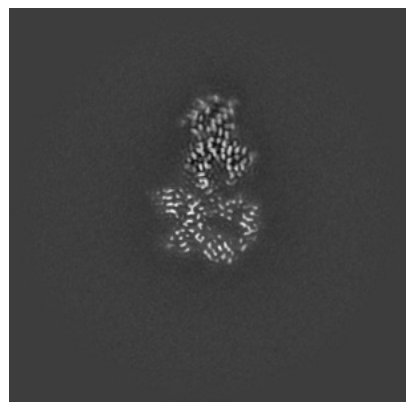


Z

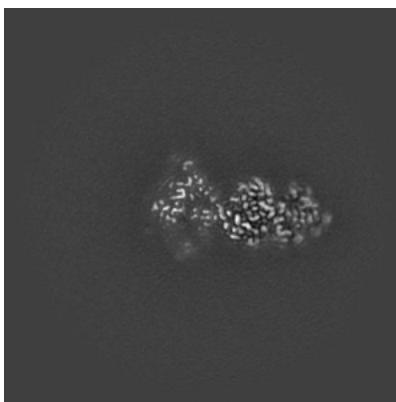
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

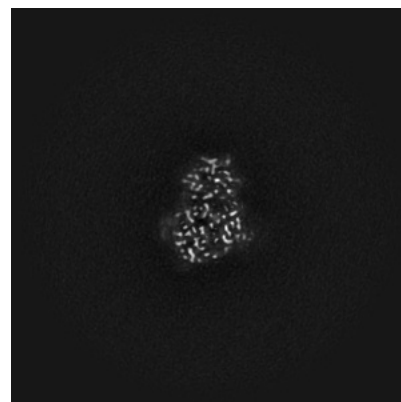
6.2.1 Primary map



X Index: 192



Y Index: 192

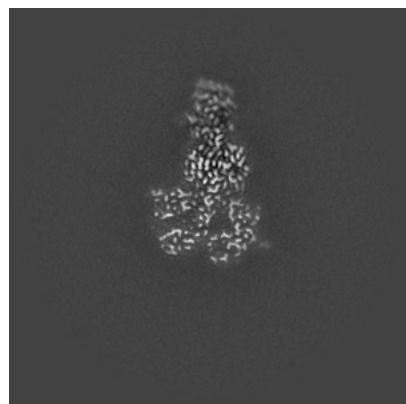


Z Index: 192

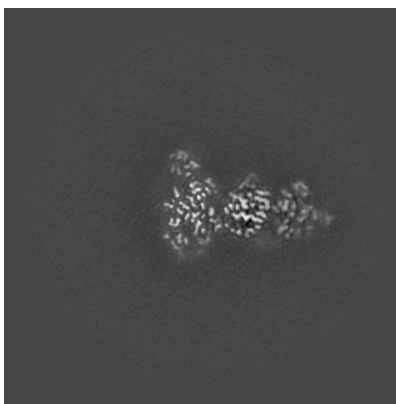
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

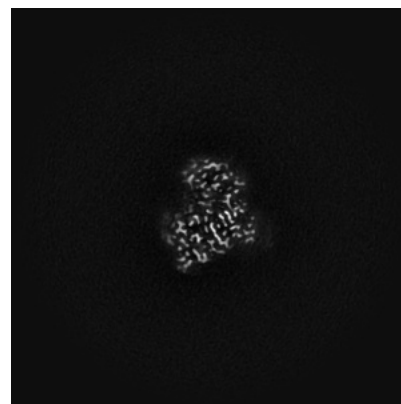
6.3.1 Primary map



X Index: 183



Y Index: 183

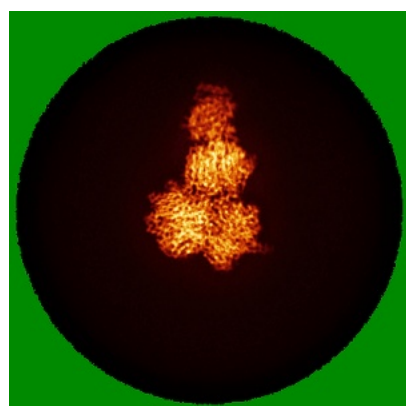


Z Index: 187

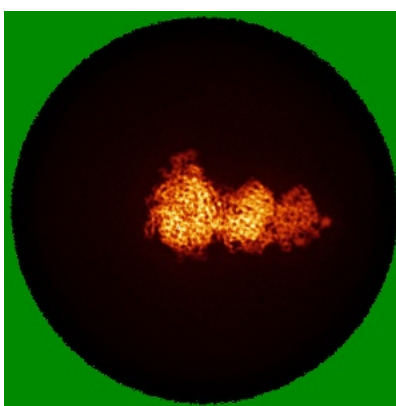
The images above show the largest variance slices of the map in three orthogonal directions.

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

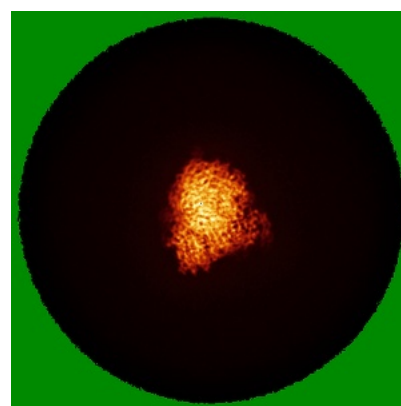
6.4.1 Primary map



X



Y



Z

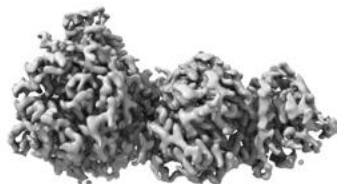
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

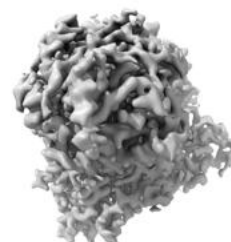
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

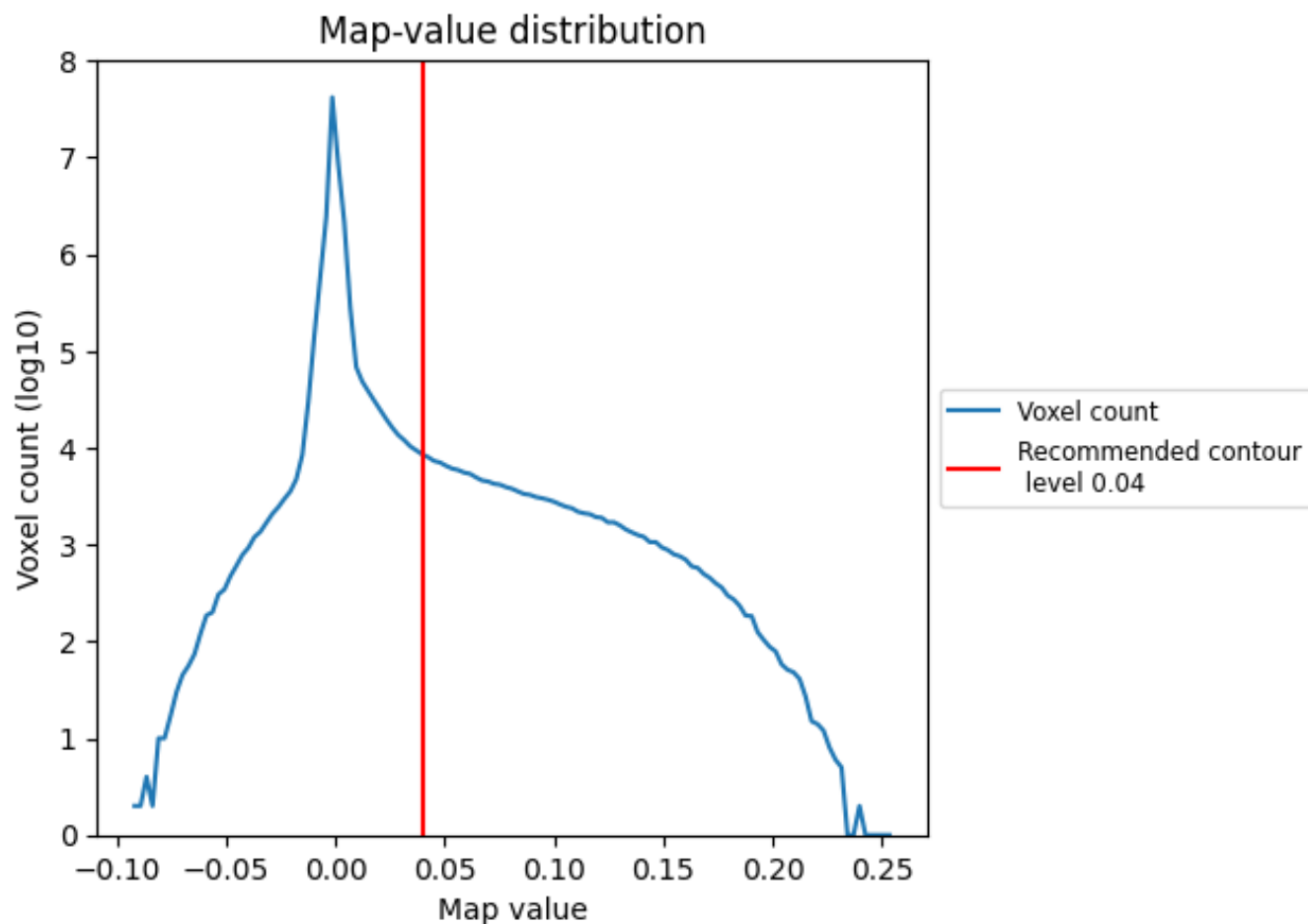
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

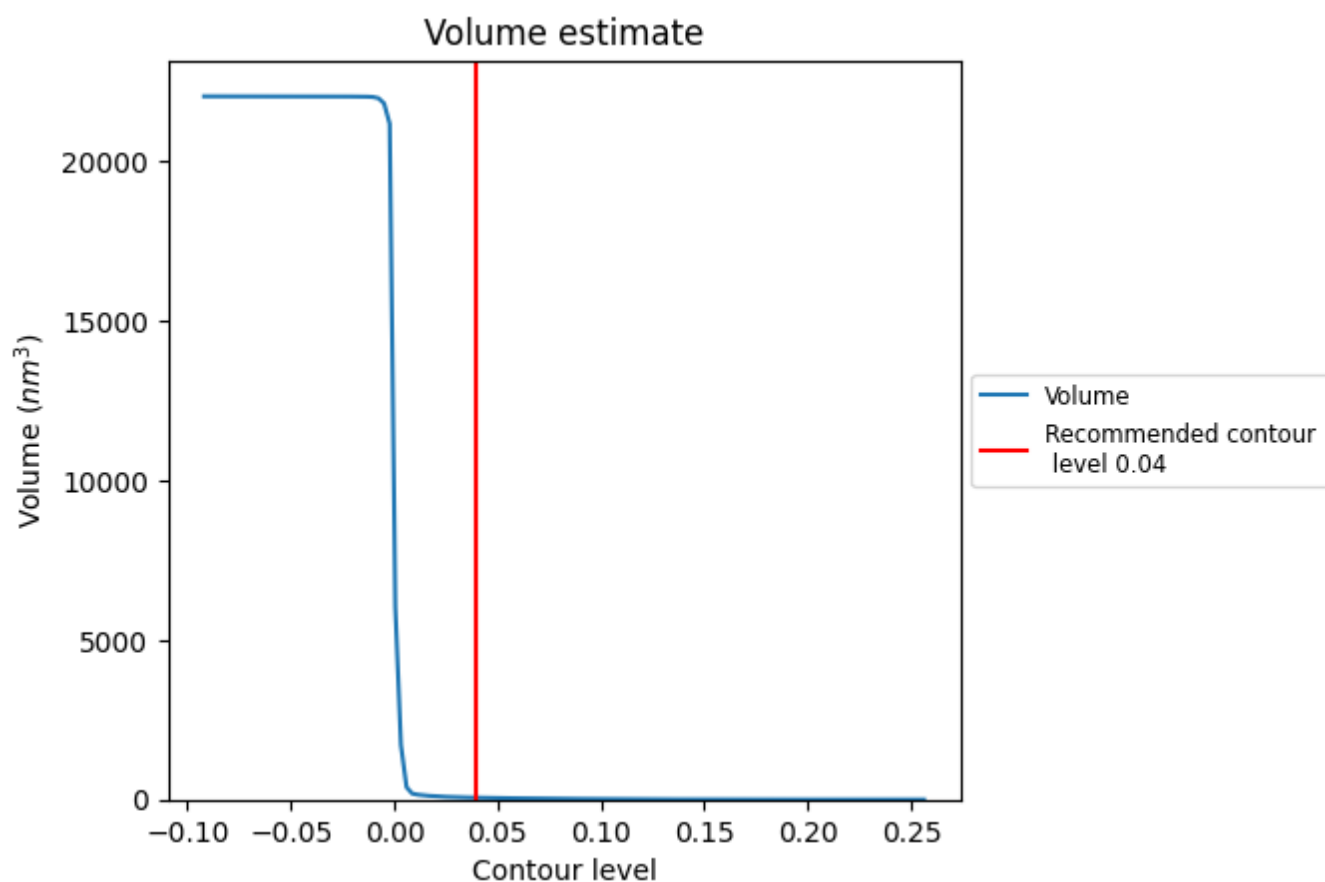
This section contains the results of statistical analysis of the map.

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.

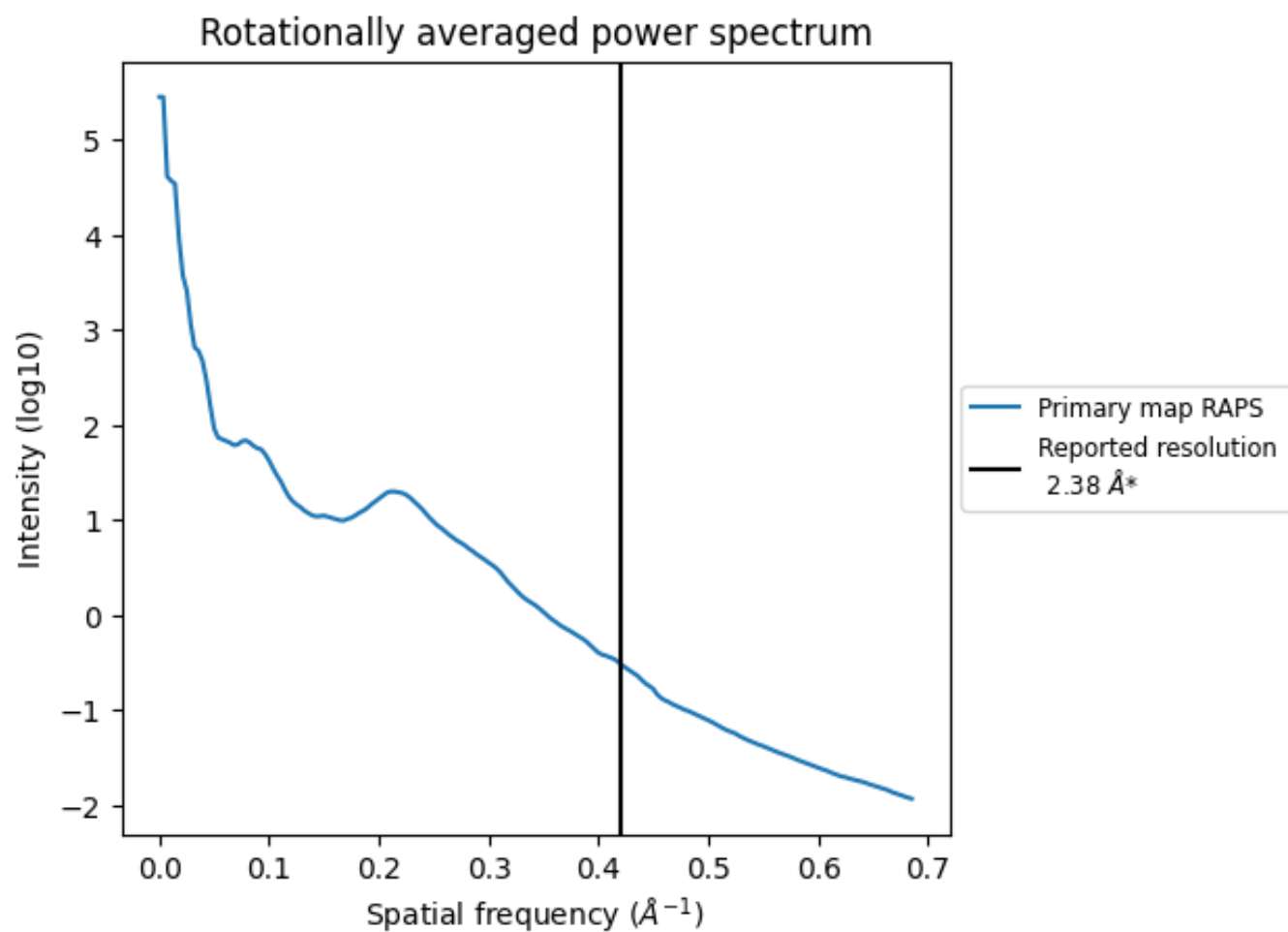
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 59 nm^3 ; this corresponds to an approximate mass of 53 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 0.420 Å⁻¹

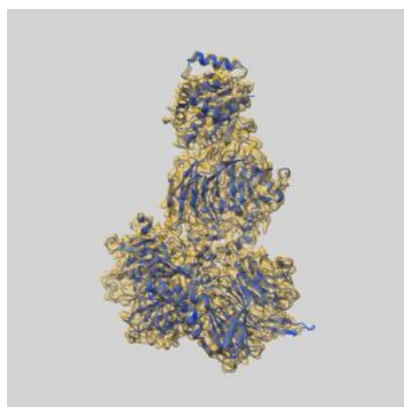
8 Fourier-Shell correlation

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

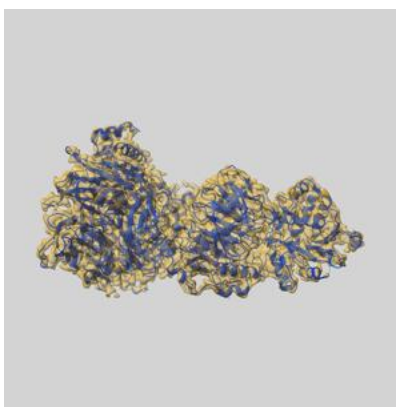
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71847 and PDB model 9PTU. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

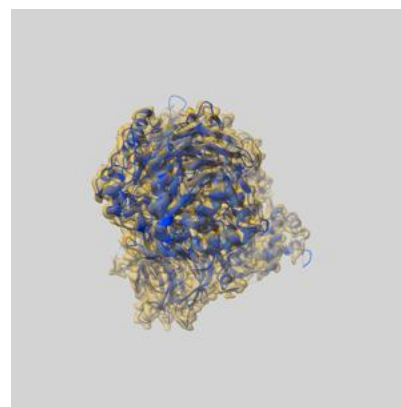
9.1 Map-model overlay [i](#)



X



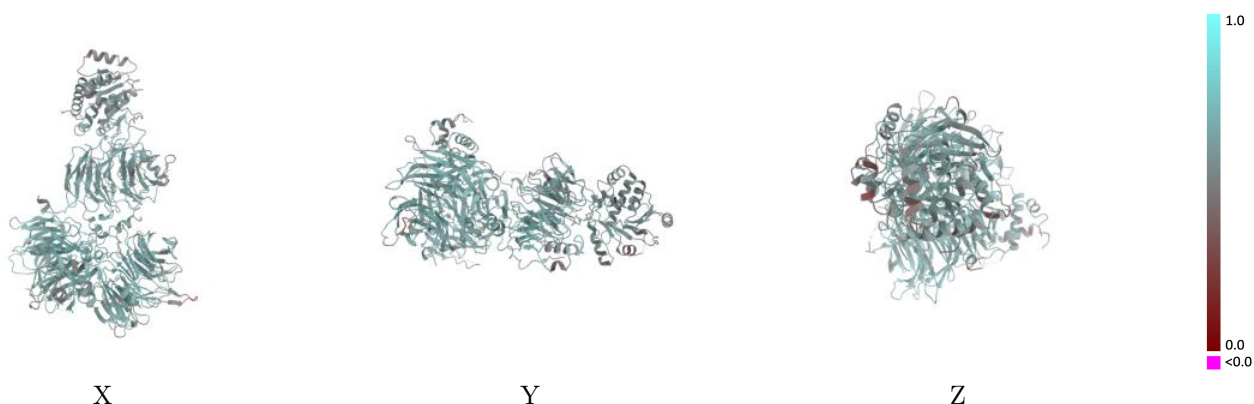
Y



Z

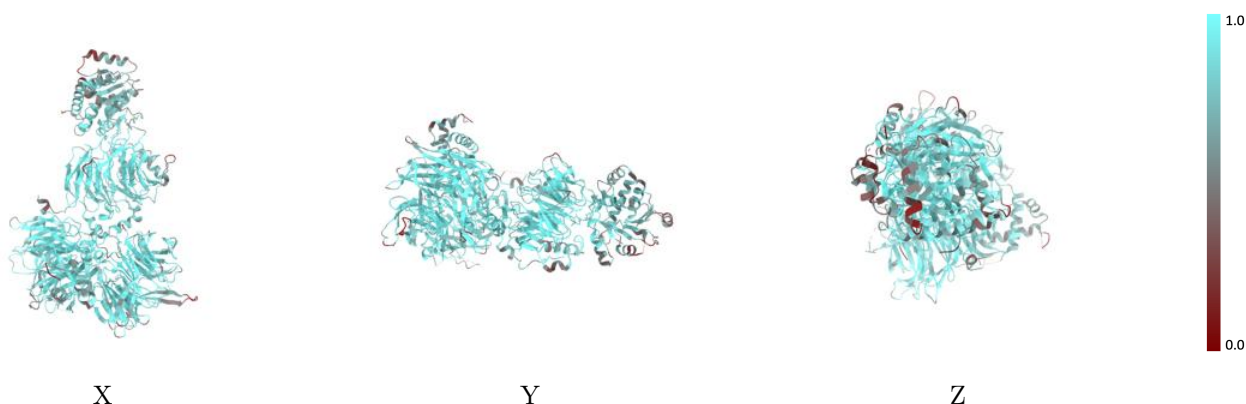
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



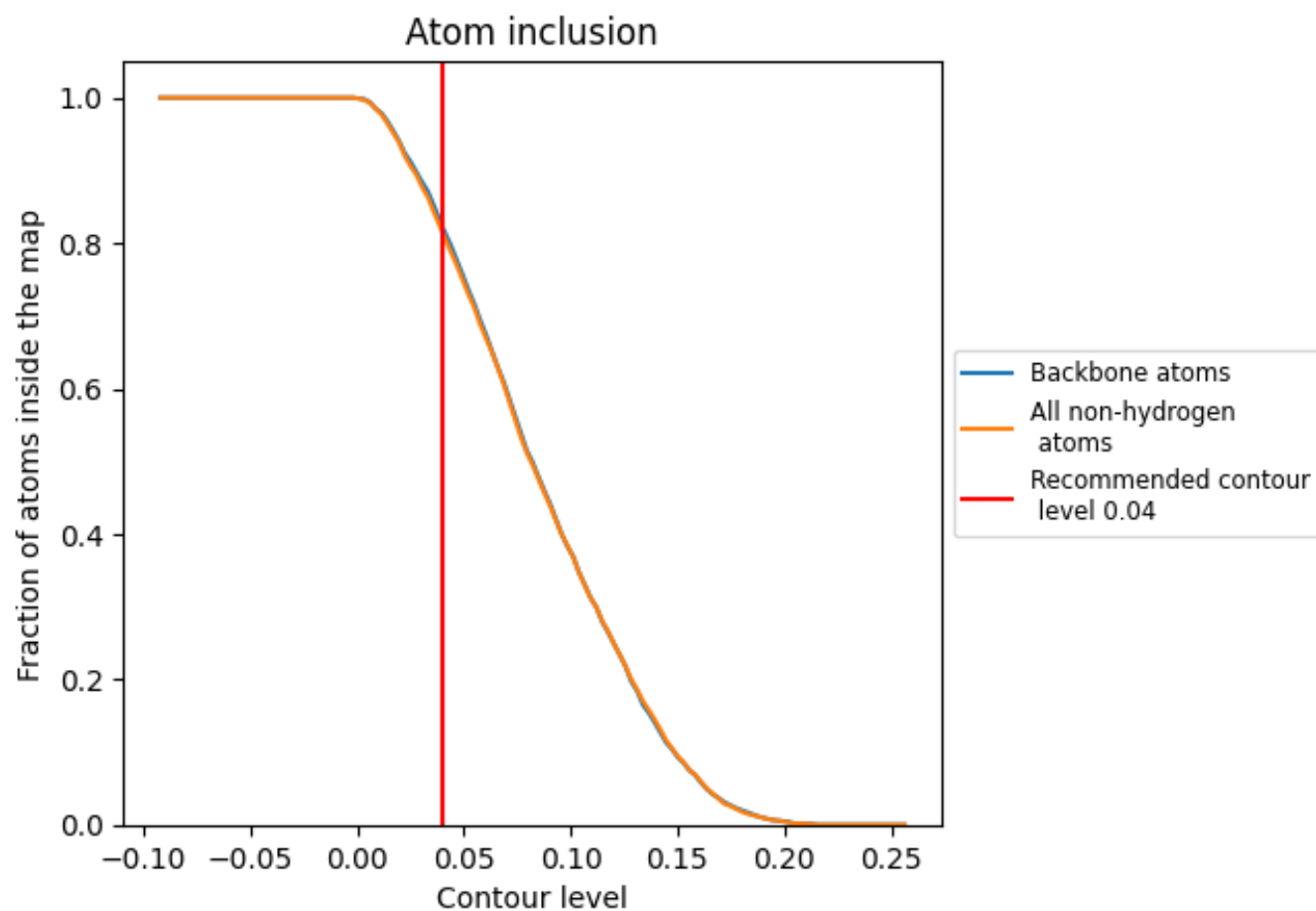
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 82% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8150	<div><div></div></div> 0.5970
A	<div><div></div></div> 0.8750	<div><div></div></div> 0.6040
B	<div><div></div></div> 0.8510	<div><div></div></div> 0.6130
C	<div><div></div></div> 0.6590	<div><div></div></div> 0.5270

