



## Full wwPDB EM Validation Report ⓘ

May 20, 2026 – 01:20 pm BST

PDB ID : 9QRU / pdb\_00009qru  
EMDB ID : EMD-53323  
Title : Cryo-EM structure of the MMM ubiquitin ligase complex with nanobody 270 (Composite map)  
Authors : Williams, C.; Carrique, L.; Pardon, E.; Nocka, L.M.; Hedger, G.; Pusapati, G.V.; Parashara, P.; Latorraca, N.R.; Sarkar, P.; Lartey, D.; Gao, L.; Milenkovic, L.; Chalk, R.; Steyaert, J.; Bazan, F.; Rouse, S.L.; Marqusee, S.; Kong, J.H.; Rohatgi, R.; Siebold, C.  
Deposited on : 2025-04-04  
Resolution : 3.03 Å (reported)  
Based on initial models : ., 9QQS

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:

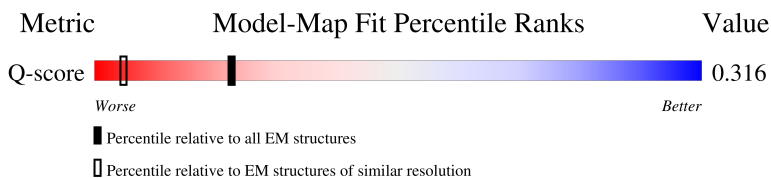
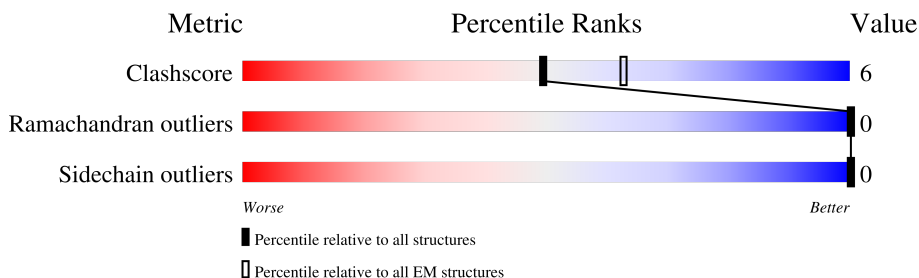
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)

# 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 3.03 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	13929 ( 2.53 - 3.53 )



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	D	539	
2	A	211	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
3	B	477	
4	C	129	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7376 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 Isoform 4 of E3 ubiquitin-protein ligase MGRN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	360	Total	C	N	O	S	0	0
			2851	1800	487	552	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	317	GLU	ARG	engineered mutation	UNP O60291
D	531	GLY	-	expression tag	UNP O60291
D	532	THR	-	expression tag	UNP O60291
D	533	LYS	-	expression tag	UNP O60291
D	534	HIS	-	expression tag	UNP O60291
D	535	HIS	-	expression tag	UNP O60291
D	536	HIS	-	expression tag	UNP O60291
D	537	HIS	-	expression tag	UNP O60291
D	538	HIS	-	expression tag	UNP O60291
D	539	HIS	-	expression tag	UNP O60291

- Molecule 2 is a protein called Modulator of smoothened protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	163	Total	C	N	O	S	0	0
			1257	832	204	212	9		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	GLY	-	linker	UNP Q8NHV5
A	169	THR	-	linker	UNP Q8NHV5
A	170	LEU	-	expression tag	UNP Q8NHV5
A	171	GLU	-	expression tag	UNP Q8NHV5
A	172	VAL	-	expression tag	UNP Q8NHV5
A	173	LEU	-	expression tag	UNP Q8NHV5
A	174	PHE	-	expression tag	UNP Q8NHV5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	175	GLN	-	expression tag	UNP Q8NHV5
A	176	GLY	-	expression tag	UNP Q8NHV5
A	177	PRO	-	expression tag	UNP Q8NHV5
A	178	GLY	-	linker	UNP Q8NHV5
A	179	GLY	-	linker	UNP Q8NHV5
A	180	SER	-	linker	UNP Q8NHV5
A	181	GLY	-	linker	UNP Q8NHV5
A	182	SER	-	expression tag	UNP Q8NHV5
A	183	ALA	-	expression tag	UNP Q8NHV5
A	184	TRP	-	expression tag	UNP Q8NHV5
A	185	SER	-	expression tag	UNP Q8NHV5
A	186	HIS	-	expression tag	UNP Q8NHV5
A	187	PRO	-	expression tag	UNP Q8NHV5
A	188	GLN	-	expression tag	UNP Q8NHV5
A	189	PHE	-	expression tag	UNP Q8NHV5
A	190	GLU	-	expression tag	UNP Q8NHV5
A	191	LYS	-	expression tag	UNP Q8NHV5
A	192	GLY	-	expression tag	UNP Q8NHV5
A	193	GLY	-	expression tag	UNP Q8NHV5
A	194	GLY	-	expression tag	UNP Q8NHV5
A	195	SER	-	expression tag	UNP Q8NHV5
A	196	GLY	-	expression tag	UNP Q8NHV5
A	197	GLY	-	expression tag	UNP Q8NHV5
A	198	GLY	-	expression tag	UNP Q8NHV5
A	199	SER	-	expression tag	UNP Q8NHV5
A	200	GLY	-	expression tag	UNP Q8NHV5
A	201	GLY	-	expression tag	UNP Q8NHV5
A	202	SER	-	expression tag	UNP Q8NHV5
A	203	ALA	-	expression tag	UNP Q8NHV5
A	204	TRP	-	expression tag	UNP Q8NHV5
A	205	SER	-	expression tag	UNP Q8NHV5
A	206	HIS	-	expression tag	UNP Q8NHV5
A	207	PRO	-	expression tag	UNP Q8NHV5
A	208	GLN	-	expression tag	UNP Q8NHV5
A	209	PHE	-	expression tag	UNP Q8NHV5
A	210	GLU	-	expression tag	UNP Q8NHV5
A	211	LYS	-	expression tag	UNP Q8NHV5

- Molecule 3 is a protein called Isoform 2 of Multiple epidermal growth factor-like domains protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	291	Total	C	N	O	S	0	0
			2271	1455	402	402	12		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2779	GLY	-	expression tag	UNP Q7Z7M0
B	2780	THR	-	expression tag	UNP Q7Z7M0
B	2781	GLU	-	expression tag	UNP Q7Z7M0
B	2782	THR	-	expression tag	UNP Q7Z7M0
B	2783	SER	-	expression tag	UNP Q7Z7M0
B	2784	GLN	-	expression tag	UNP Q7Z7M0
B	2785	VAL	-	expression tag	UNP Q7Z7M0
B	2786	ALA	-	expression tag	UNP Q7Z7M0
B	2787	PRO	-	expression tag	UNP Q7Z7M0
B	2788	ALA	-	expression tag	UNP Q7Z7M0

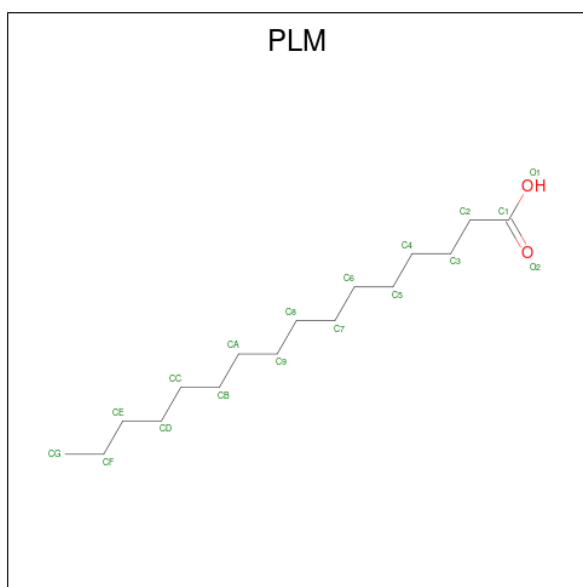
- Molecule 4 is a protein called Nanobody 270.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	119	Total	C	N	O	S	0	0
			921	575	162	179	5		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

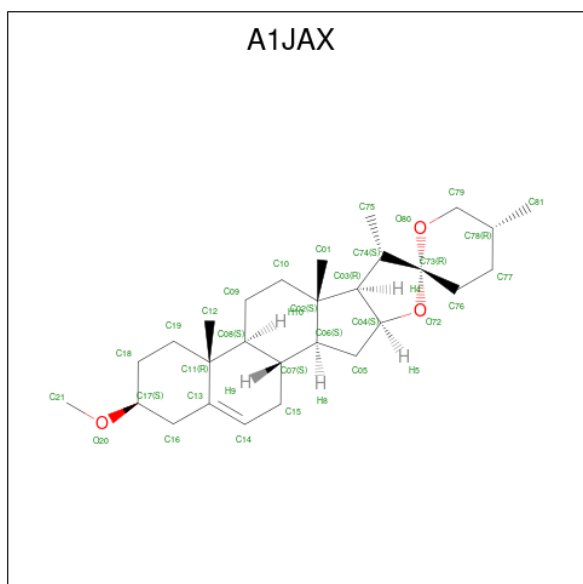
Mol	Chain	Residues	Atoms		AltConf
5	D	2	Total	Zn	0
			2	2	

- Molecule 6 is PALMITIC ACID (CCD ID: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			17	16	1	

- Molecule 7 is (1 {S},2 {S},4 {S},5' {R},6 {R},7 {S},8 {R},9 {S},12 {S},13 {R},16 {S})-16-methoxy-5',7,9,13-tetramethyl-spiro[5-oxapentacyclo[10.8.0.0<sup>2,9</sup>.0<sup>4,8</sup>.0<sup>13,18</sup>]]icos-18-ene-6,2'-oxane] (CCD ID: A1JAX) (formula: C<sub>28</sub>H<sub>44</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
7	B	1	Total	C	O	0
			31	28	3	

- Molecule 8 is water.

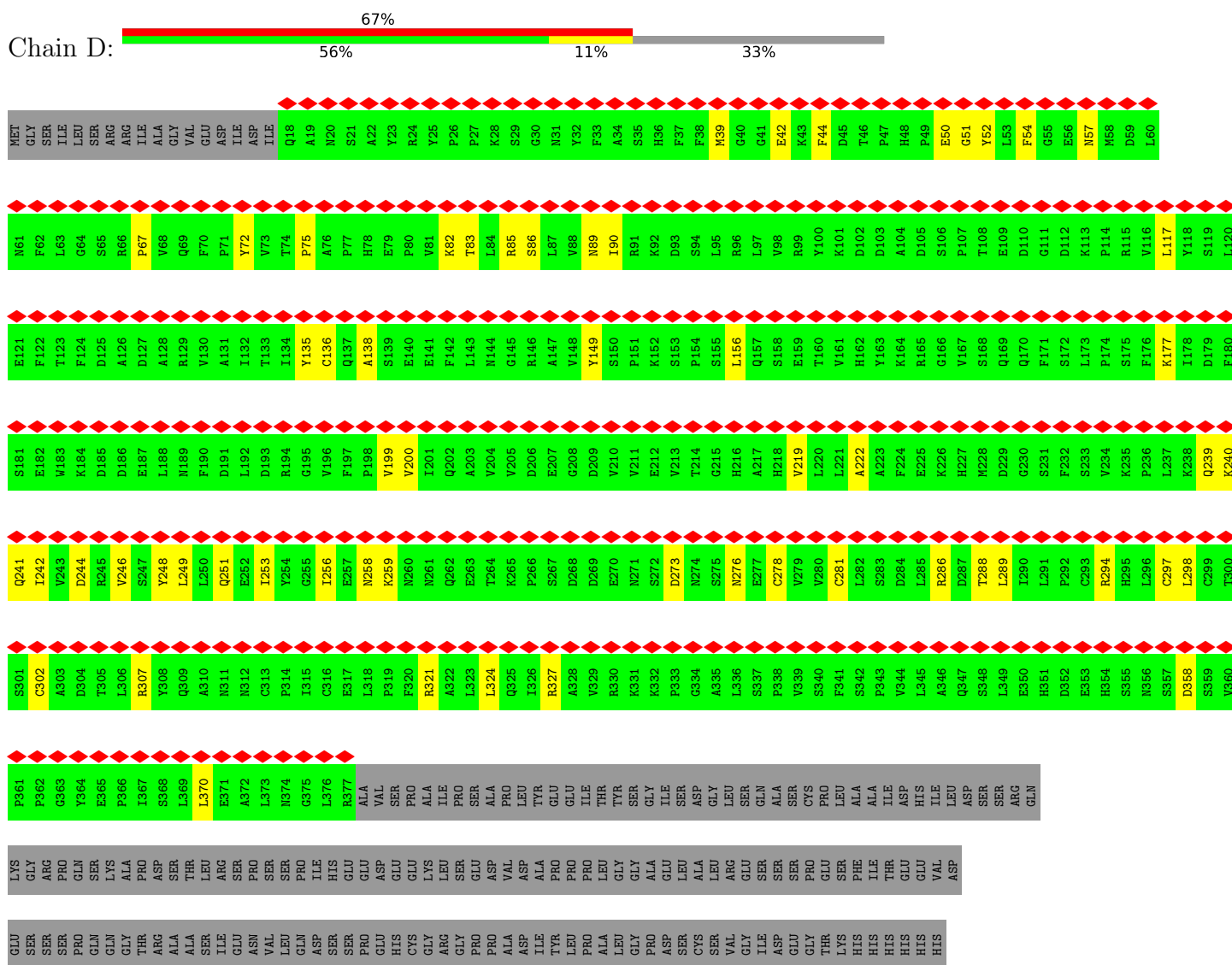
Mol	Chain	Residues	Atoms		AltConf
8	A	6	Total 6	O 6	0
8	B	17	Total 17	O 17	0
8	C	3	Total 3	O 3	0



### 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: Isoform 4 of E3 ubiquitin-protein ligase MGRN1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	223808	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF estimation was performed in cryoSPARC live pre-processing.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	70.960	Depositor
Minimum map value	-55.130	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.934	Depositor
Recommended contour level	5.9	Depositor
Map size ( $\text{\AA}$ )	350.544, 350.544, 350.544	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.7303, 0.7303, 0.7303	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: A1JAX, ZN, PLM

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	D	0.10	0/2921	0.29	0/3968
2	A	0.24	0/1290	0.36	0/1760
3	B	0.24	0/2330	0.36	0/3171
4	C	0.22	0/939	0.39	0/1269
All	All	0.20	0/7480	0.34	0/10168

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	D	2851	0	2755	39	0
2	A	1257	0	1291	13	0
3	B	2271	0	2265	35	0
4	C	921	0	889	13	0
5	D	2	0	0	0	0
6	A	17	0	31	0	0
7	B	31	0	0	0	0
8	A	6	0	0	0	0
8	B	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	3	0	0	0	0
All	All	7376	0	7231	83	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 (83) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:VAL:HB	1:D:240:LYS:HB2	1.65	0.78
1:D:138:ALA:HB1	1:D:149:TYR:HB3	1.65	0.77
4:C:82:MET:HB2	4:C:85:LEU:HD21	1.66	0.76
2:A:47:GLN:HE21	3:B:2507:LEU:HD23	1.54	0.71
1:D:136:CYS:HB2	1:D:156:LEU:HB3	1.76	0.68
1:D:288:THR:HB	1:D:298:LEU:HB2	1.77	0.67
1:D:278:CYS:HB3	1:D:281:CYS:SG	2.36	0.66
3:B:2523:ARG:NH2	4:C:54:VAL:O	2.29	0.65
1:D:258:ASN:ND2	3:B:2724:PRO:O	2.29	0.65
2:A:25:ASN:ND2	2:A:141:SER:OG	2.32	0.63
1:D:286:ARG:HD3	1:D:297:CYS:HA	1.79	0.63
1:D:259:LYS:NZ	1:D:273:ASP:O	2.32	0.63
2:A:82:THR:HG21	2:A:103:ALA:HB2	1.82	0.61
1:D:281:CYS:HB3	1:D:302:CYS:SG	2.41	0.60
4:C:13:GLN:HE22	4:C:119:SER:HA	1.67	0.58
1:D:72:TYR:OH	1:D:244:ASP:OD2	2.22	0.58
3:B:2397:GLU:OE1	3:B:2400:ARG:NH2	2.37	0.57
3:B:2704:GLU:HB2	3:B:2713:VAL:HB	1.85	0.57
3:B:2421:ASP:OD1	3:B:2535:HIS:ND1	2.30	0.57
1:D:307:ARG:NH2	3:B:2626:ALA:O	2.38	0.56
4:C:81:GLN:OE1	4:C:83:ASN:ND2	2.40	0.54
3:B:2407:ARG:NH1	3:B:2453:GLY:O	2.40	0.53
4:C:32:ASP:OD2	4:C:101:ARG:NH2	2.38	0.53
1:D:117:LEU:HB3	1:D:177:LYS:HB3	1.89	0.53
1:D:135:TYR:HB2	1:D:200:VAL:HB	1.90	0.53
3:B:2700:PRO:HA	3:B:2716:LEU:HG	1.90	0.53
2:A:47:GLN:NE2	3:B:2507:LEU:HD23	2.23	0.53
1:D:50:GLU:O	1:D:57:ASN:ND2	2.42	0.52
4:C:24:ALA:HB1	4:C:28:ILE:HG21	1.92	0.52
1:D:85:ARG:NH2	3:B:2640:ASP:OD1	2.42	0.51
1:D:82:LYS:HB3	3:B:2698:ALA:HB2	1.93	0.51
3:B:2437:VAL:HG13	3:B:2547:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2440:SER:OG	3:B:2442:ASP:OD1	2.29	0.51
1:D:251:GLN:HB2	3:B:2732:LEU:HB2	1.93	0.50
4:C:6:GLU:HG3	4:C:113:THR:HG23	1.94	0.49
1:D:89:ASN:HB2	3:B:2721:PRO:HD2	1.93	0.49
4:C:63:VAL:HG13	4:C:67:PHE:CD1	2.46	0.49
4:C:63:VAL:HG13	4:C:67:PHE:HB2	1.93	0.49
1:D:289:LEU:HD21	3:B:2732:LEU:HD11	1.95	0.49
1:D:39:MET:HG3	3:B:2702:THR:HG22	1.94	0.49
1:D:199:VAL:HB	1:D:222:ALA:HB3	1.94	0.49
2:A:62:PRO:HB2	2:A:64:GLU:OE1	2.13	0.48
1:D:138:ALA:HB3	1:D:200:VAL:HG21	1.95	0.48
3:B:2706:THR:OG1	3:B:2708:ASP:OD1	2.28	0.48
3:B:2386:LEU:HD22	3:B:2549:LEU:HD22	1.96	0.47
3:B:2446:VAL:HG11	3:B:2455:HIS:HD2	1.79	0.47
1:D:83:THR:HG22	3:B:2717:LEU:HB3	1.96	0.47
2:A:31:THR:HG21	2:A:35:ALA:HB3	1.97	0.47
4:C:48:VAL:HG13	4:C:63:VAL:HG21	1.95	0.47
2:A:112:MET:O	2:A:116:ILE:HG13	2.16	0.46
1:D:67:PRO:HB3	3:B:2736:LEU:HG	1.97	0.46
1:D:86:SER:OG	1:D:241:GLN:NE2	2.48	0.46
2:A:108:ILE:HG22	2:A:112:MET:HE2	1.97	0.45
2:A:122:TYR:HA	2:A:128:GLY:O	2.16	0.45
2:A:43:VAL:O	2:A:59:PRO:HD3	2.17	0.45
4:C:66:ARG:HD2	4:C:84:SER:HB3	1.99	0.45
2:A:110:PHE:HB3	2:A:150:ILE:HG12	1.99	0.44
1:D:289:LEU:HD23	1:D:324:LEU:HD23	1.99	0.44
3:B:2396:HIS:ND1	3:B:2398:PRO:HD2	2.32	0.44
3:B:2744:HIS:ND1	3:B:2744:HIS:O	2.50	0.44
1:D:75:PRO:HB3	3:B:2697:ARG:HB2	1.99	0.44
1:D:90:ILE:O	1:D:239:GLN:NE2	2.50	0.44
4:C:20:LEU:HD11	4:C:82:MET:HE3	2.00	0.44
1:D:51:GLY:HA3	1:D:321:ARG:HH12	1.83	0.43
3:B:2426:LEU:HD13	3:B:2570:LEU:HD12	2.00	0.43
3:B:2624:LYS:O	3:B:2627:SER:OG	2.28	0.43
2:A:122:TYR:HB3	2:A:130:PRO:HD3	1.99	0.43
3:B:2700:PRO:HB3	3:B:2714:ALA:HB1	2.00	0.43
1:D:52:TYR:CZ	1:D:54:PHE:HB2	2.54	0.43
1:D:249:LEU:O	3:B:2733:GLY:HA2	2.18	0.43
1:D:42:GLU:HB3	1:D:44:PHE:CE2	2.54	0.43
1:D:248:TYR:HE1	3:B:2716:LEU:HD13	1.84	0.43
2:A:42:LEU:HA	2:A:61:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2451:ASP:OD1	3:B:2451:ASP:N	2.51	0.42
1:D:242:ILE:HA	1:D:246:VAL:O	2.19	0.42
4:C:52:THR:N	4:C:56:SER:O	2.35	0.42
1:D:294:ARG:HD2	3:B:2732:LEU:HD12	2.02	0.42
3:B:2706:THR:OG1	3:B:2711:ALA:O	2.38	0.42
1:D:327:ARG:NH1	1:D:358:ASP:OD2	2.53	0.41
1:D:276:ASN:HB3	1:D:370:LEU:HD13	2.03	0.41
3:B:2438:SER:CB	3:B:2443:THR:HG21	2.51	0.41
1:D:253:ILE:O	1:D:256:ILE:HG12	2.21	0.41
1:D:289:LEU:N	1:D:324:LEU:O	2.42	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	D	358/539 (66%)	354 (99%)	4 (1%)	0	100	100
2	A	161/211 (76%)	160 (99%)	1 (1%)	0	100	100
3	B	285/477 (60%)	278 (98%)	7 (2%)	0	100	100
4	C	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
All	All	921/1356 (68%)	904 (98%)	17 (2%)	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	D	322/473 (68%)	322 (100%)	0	100	100
2	A	135/167 (81%)	135 (100%)	0	100	100
3	B	249/377 (66%)	249 (100%)	0	100	100
4	C	98/107 (92%)	98 (100%)	0	100	100
All	All	804/1124 (72%)	804 (100%)	0	100	100

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

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

Mol	Chain	Res	Type
1	D	89	ASN
2	A	25	ASN
3	B	2458	HIS
3	B	2728	ASN
4	C	13	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 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
6	PLM	A	301	2	16,16,17	0.40	0	15,15,17	0.50	0
7	A1JAX	B	2801	-	36,36,36	0.52	0	59,59,59	0.62	0

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
6	PLM	A	301	2	-	5/13/14/15	-
7	A1JAX	B	2801	-	-	0/2/90/90	0/6/6/6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

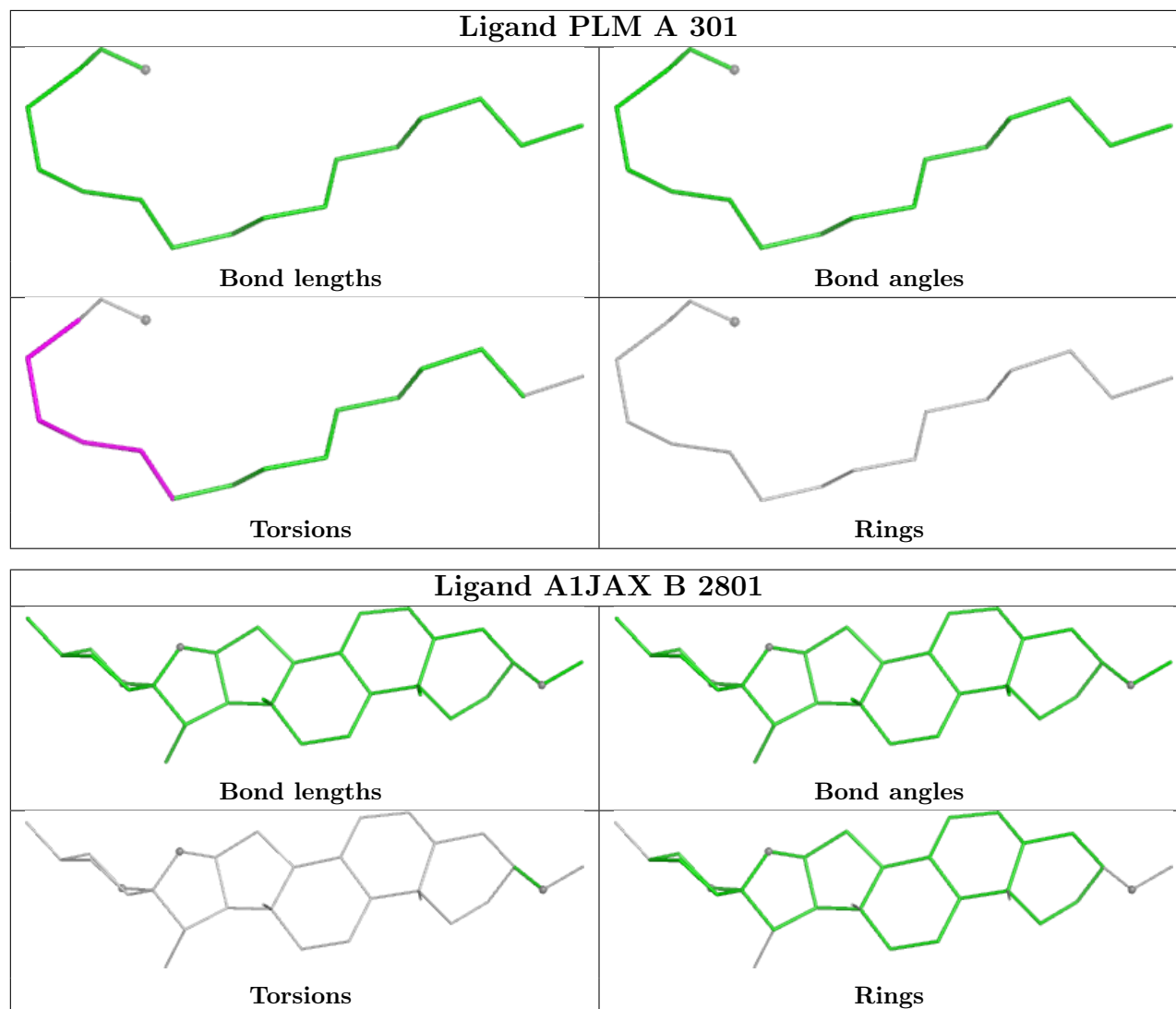
Mol	Chain	Res	Type	Atoms
6	A	301	PLM	C1-C2-C3-C4
6	A	301	PLM	C3-C4-C5-C6
6	A	301	PLM	C5-C6-C7-C8
6	A	301	PLM	C4-C5-C6-C7
6	A	301	PLM	C2-C3-C4-C5

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.

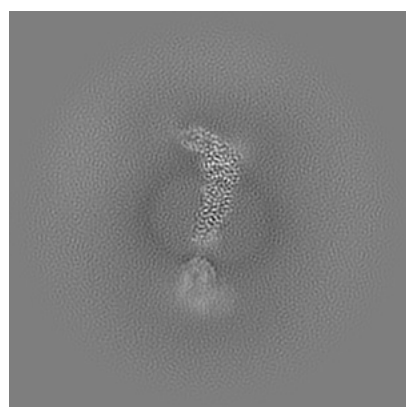
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53323. These allow visual inspection of the internal detail of the map and identification of artifacts.

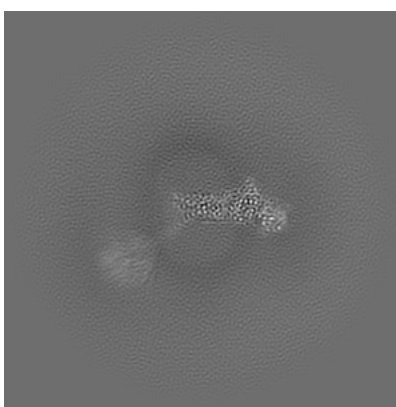
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

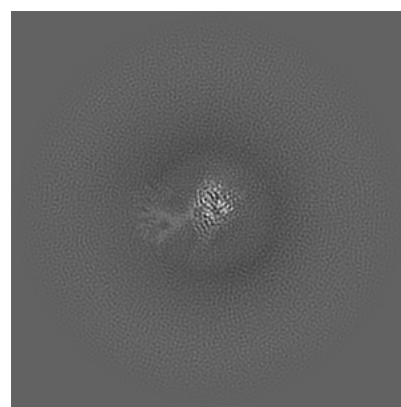
#### 6.1.1 Primary map



X



Y

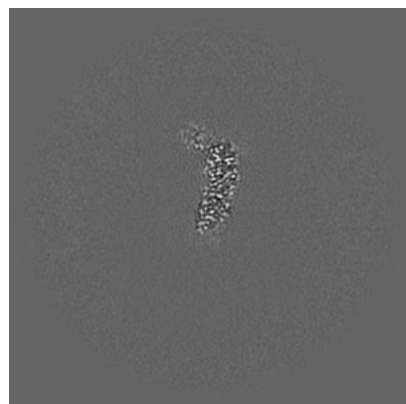


Z

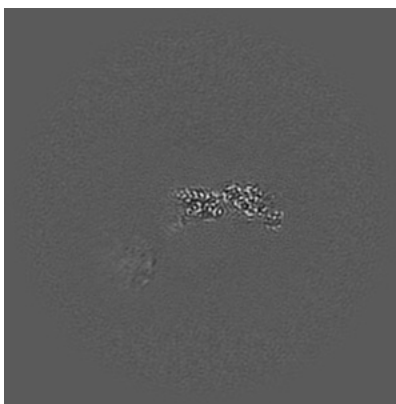
The images above show the map projected in three orthogonal directions.

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

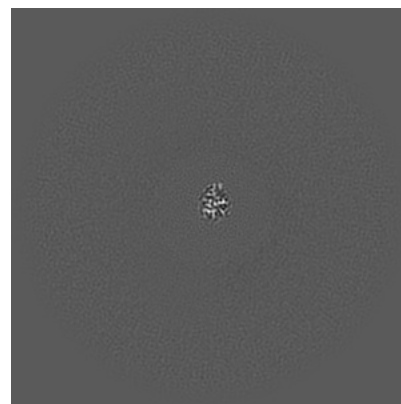
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

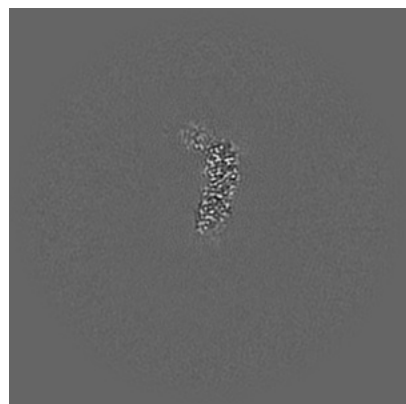


Z Index: 240

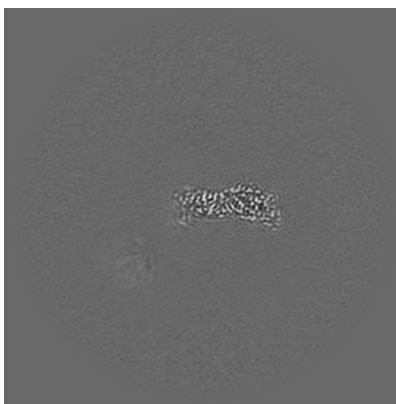
The images above show central slices of the map in three orthogonal directions.

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

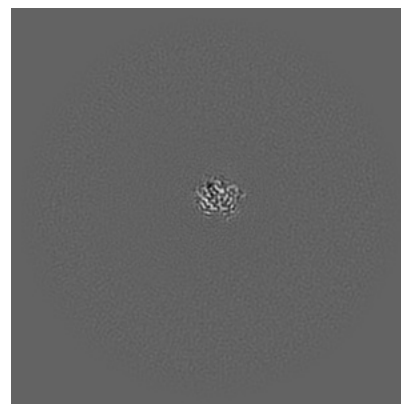
### 6.3.1 Primary map



X Index: 240



Y Index: 246

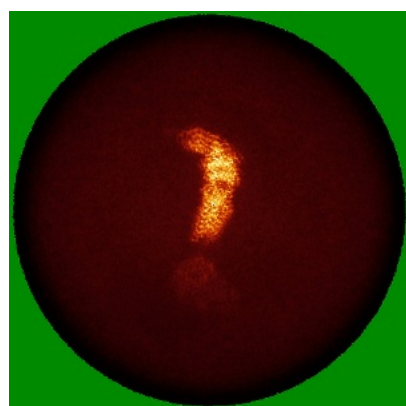


Z Index: 295

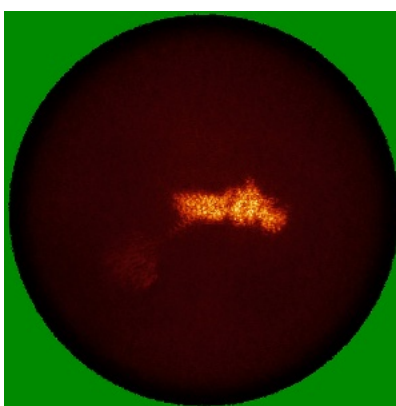
The images above show the largest variance slices of the map in three orthogonal directions.

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

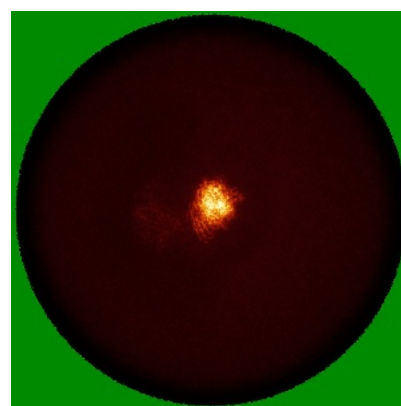
### 6.4.1 Primary map



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

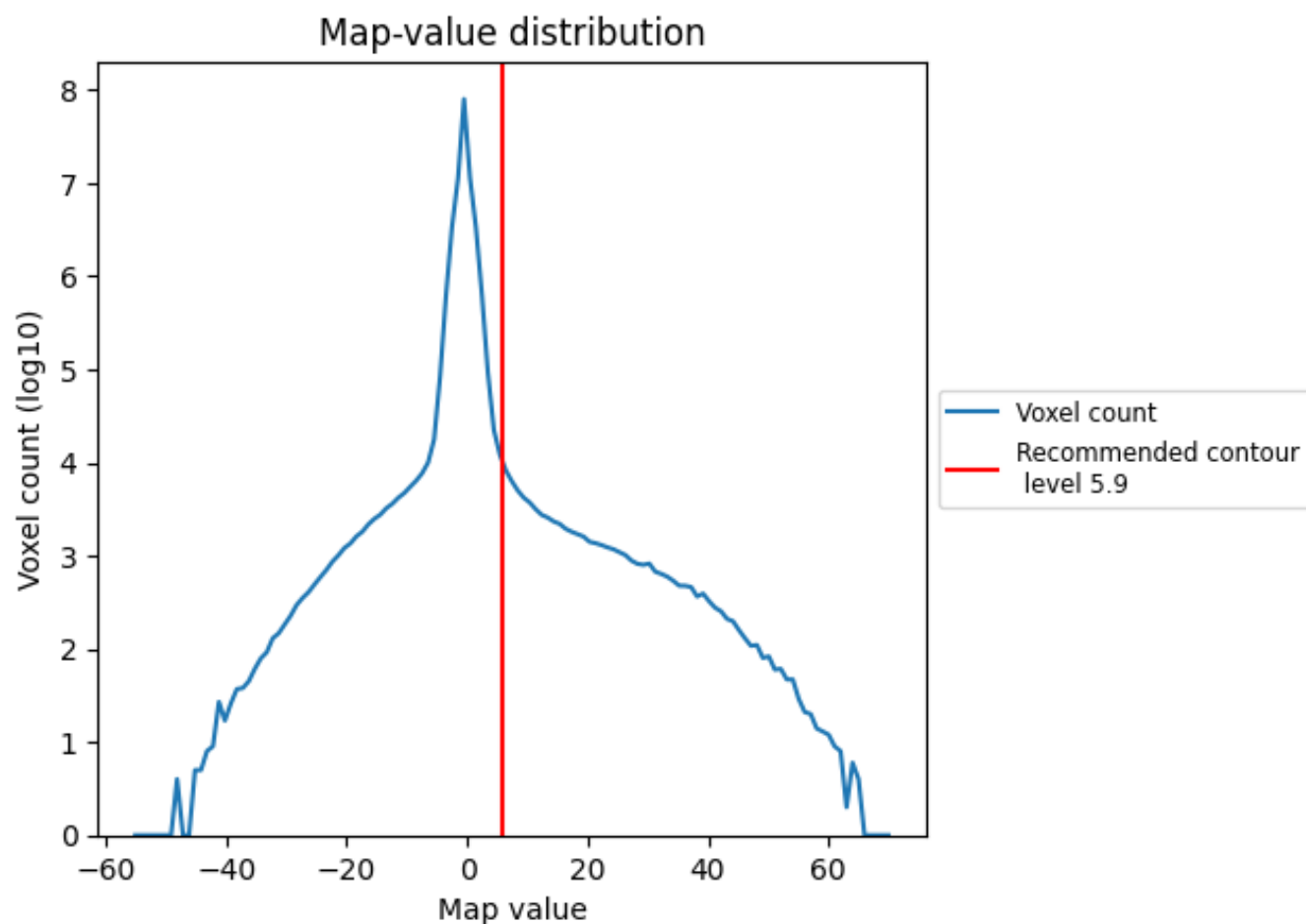
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

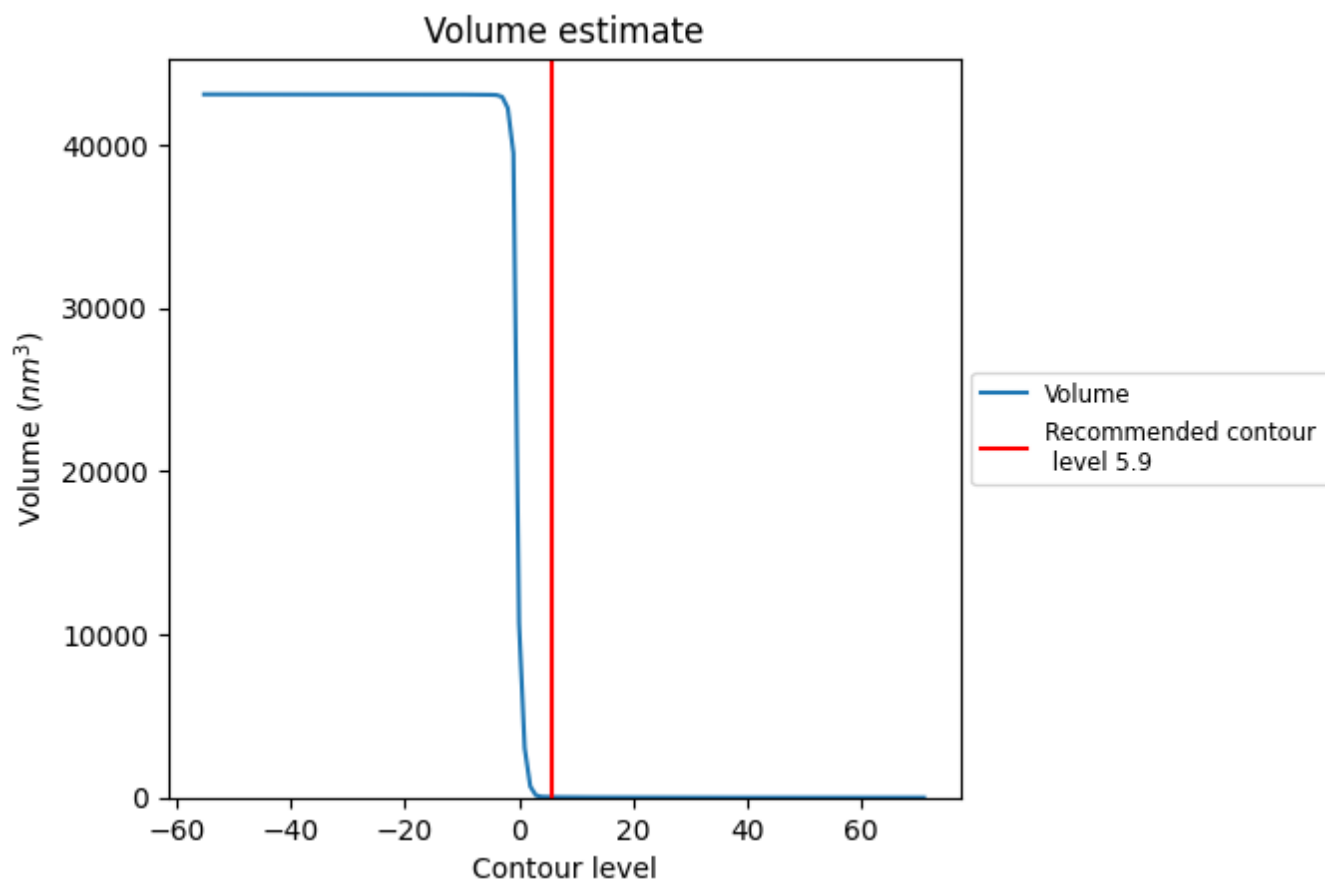
This section contains the results of statistical analysis of the map.

### 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.

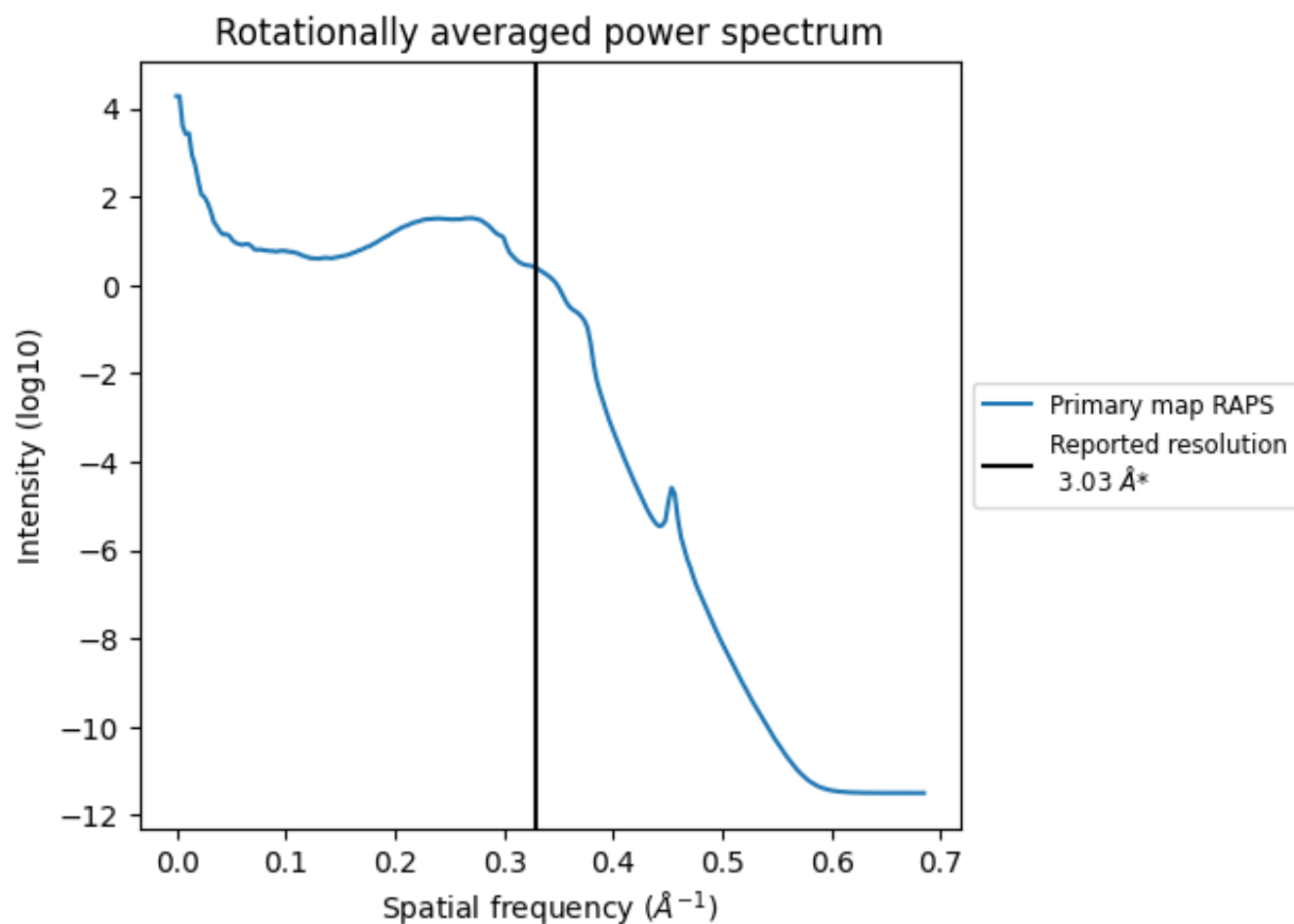
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 28 nm<sup>3</sup>; this corresponds to an approximate mass of 25 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 0.330  $\text{\AA}^{-1}$



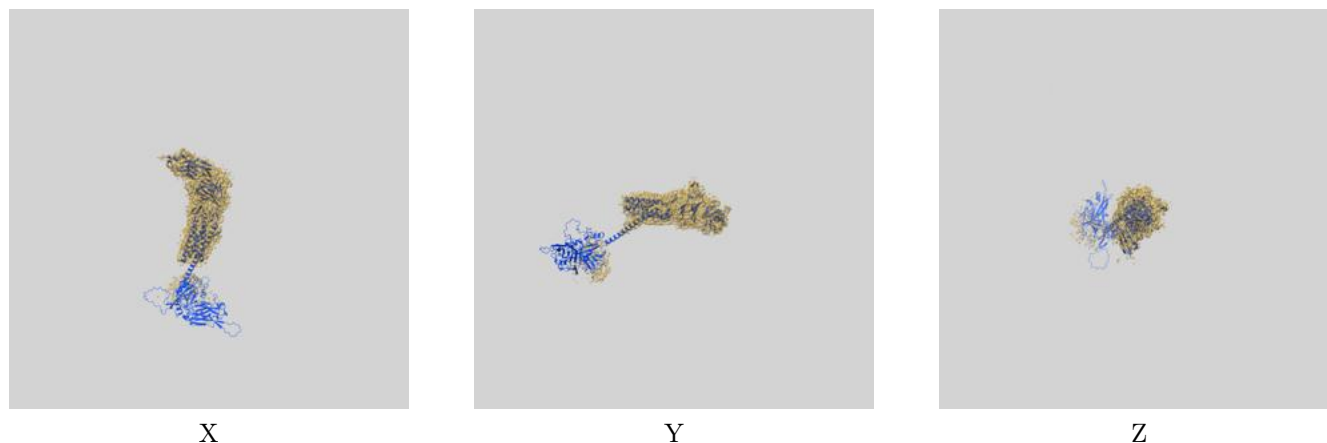
## 8 Fourier-Shell correlation

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

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

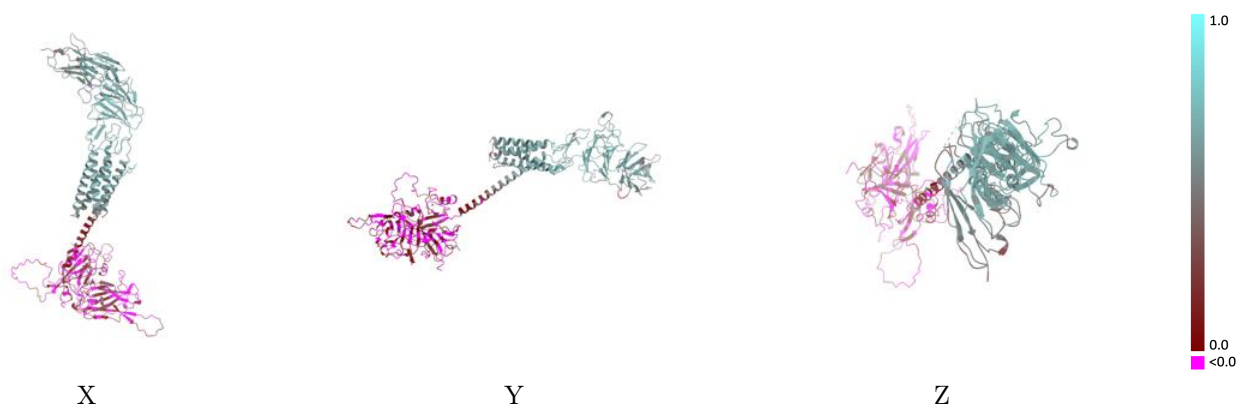
This section contains information regarding the fit between EMDB map EMD-53323 and PDB model 9QRU. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

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



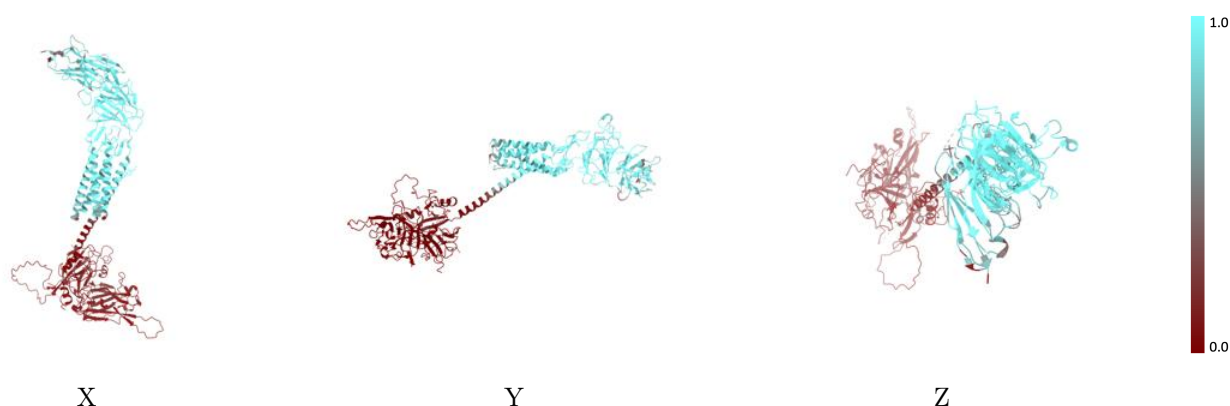
The images above show the 3D surface view of the map at the recommended contour level 5.9 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



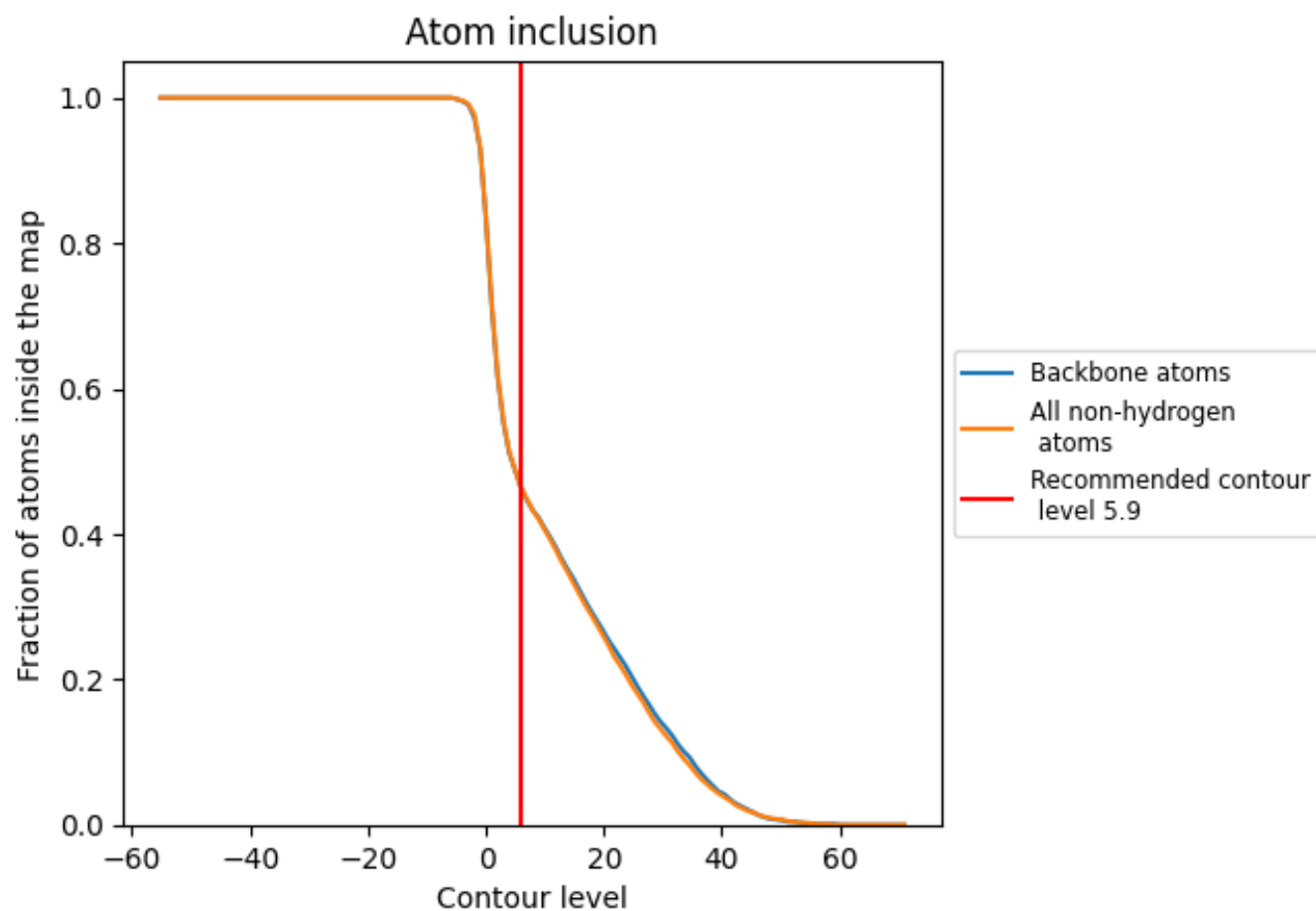
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.9).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 46% of all backbone atoms, 46% 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 (5.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4650	<div></div> 0.3160
A	<div></div> 0.9030	<div></div> 0.5990
B	<div></div> 0.6680	<div></div> 0.4440
C	<div></div> 0.7940	<div></div> 0.5270
D	<div></div> 0.0060	<div></div> 0.0190

