



## Full wwPDB EM Validation Report ⓘ

Nov 18, 2025 – 04:28 PM JST

PDB ID : 9LQ5 / pdb\_00009lq5  
EMDB ID : EMD-63293  
Title : Cryo-EM structure of Apo type III-B CRISPR-Cas effector complex  
Authors : Jin, X.; Chen, Z.; Zhao, B.  
Deposited on : 2025-01-27  
Resolution : 2.97 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](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.dev129  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

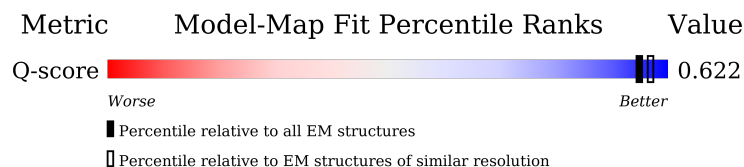
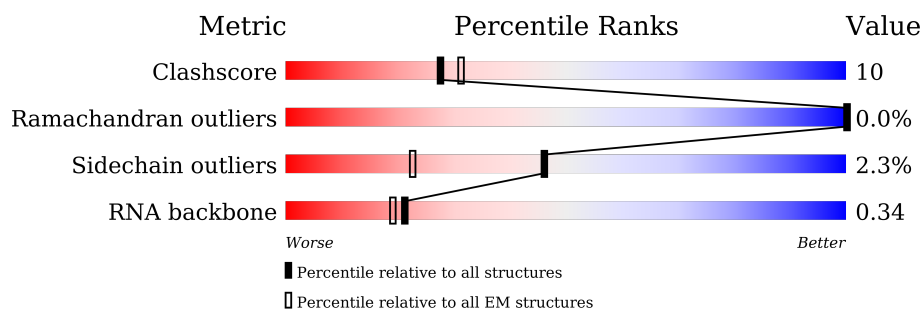
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	13205 ( 2.47 - 3.47 )

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	A	469	<div> <div>71%</div> <div>26%</div> <div>.</div> </div>
2	B	600	<div> <div>73%</div> <div>25%</div> <div>..</div> </div>
3	C	423	<div> <div>66%</div> <div>21%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	279	 82% 18% .
4	E	279	 81% 19%
4	F	279	 84% 16%
5	G	136	 65% 33% .
5	H	136	 71% 28% .
6	I	314	 81% 18%
7	J	49	 37% 35% 12% 16%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23974 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 Cmr1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	468	Total	C	N	O	S	0	0
			3895	2509	662	711	13		

- Molecule 2 is a protein called Type III-B CRISPR-associated protein Cas10/Cmr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	595	Total	C	N	O	S	0	0
			4828	3094	795	913	26		

- Molecule 3 is a protein called CRISPR-associated protein Cmr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	370	Total	C	N	O	S	0	0
			3044	1957	497	576	14		

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP A0A9X9IKM4
C	2	SER	-	expression tag	UNP A0A9X9IKM4
C	3	HIS	-	expression tag	UNP A0A9X9IKM4
C	4	HIS	-	expression tag	UNP A0A9X9IKM4
C	5	HIS	-	expression tag	UNP A0A9X9IKM4
C	6	HIS	-	expression tag	UNP A0A9X9IKM4
C	7	HIS	-	expression tag	UNP A0A9X9IKM4
C	8	HIS	-	expression tag	UNP A0A9X9IKM4
C	9	HIS	-	expression tag	UNP A0A9X9IKM4
C	10	HIS	-	expression tag	UNP A0A9X9IKM4
C	11	ASP	-	expression tag	UNP A0A9X9IKM4
C	12	GLY	-	expression tag	UNP A0A9X9IKM4
C	13	LYS	-	expression tag	UNP A0A9X9IKM4
C	14	PRO	-	expression tag	UNP A0A9X9IKM4
C	15	ILE	-	expression tag	UNP A0A9X9IKM4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	PRO	-	expression tag	UNP A0A9X9IKM4
C	17	ASN	-	expression tag	UNP A0A9X9IKM4
C	18	PRO	-	expression tag	UNP A0A9X9IKM4
C	19	LEU	-	expression tag	UNP A0A9X9IKM4
C	20	LEU	-	expression tag	UNP A0A9X9IKM4
C	21	GLY	-	expression tag	UNP A0A9X9IKM4
C	22	LEU	-	expression tag	UNP A0A9X9IKM4
C	23	ASP	-	expression tag	UNP A0A9X9IKM4
C	24	SER	-	expression tag	UNP A0A9X9IKM4
C	25	THR	-	expression tag	UNP A0A9X9IKM4
C	26	GLY	-	expression tag	UNP A0A9X9IKM4
C	27	SER	-	expression tag	UNP A0A9X9IKM4
C	28	ASP	-	expression tag	UNP A0A9X9IKM4
C	29	GLN	-	expression tag	UNP A0A9X9IKM4
C	30	THR	-	expression tag	UNP A0A9X9IKM4
C	31	GLU	-	expression tag	UNP A0A9X9IKM4
C	32	ASN	-	expression tag	UNP A0A9X9IKM4
C	33	SER	-	expression tag	UNP A0A9X9IKM4
C	34	GLY	-	expression tag	UNP A0A9X9IKM4
C	35	GLU	-	expression tag	UNP A0A9X9IKM4
C	36	ASN	-	expression tag	UNP A0A9X9IKM4
C	37	LEU	-	expression tag	UNP A0A9X9IKM4
C	38	TYR	-	expression tag	UNP A0A9X9IKM4
C	39	PHE	-	expression tag	UNP A0A9X9IKM4
C	40	GLN	-	expression tag	UNP A0A9X9IKM4
C	41	GLY	-	expression tag	UNP A0A9X9IKM4
C	42	ALA	-	expression tag	UNP A0A9X9IKM4
C	43	ASN	-	expression tag	UNP A0A9X9IKM4
C	44	ALA	-	expression tag	UNP A0A9X9IKM4
C	279	TYR	CYS	conflict	UNP A0A9X9IKM4

- Molecule 4 is a protein called Type III-B CRISPR module RAMP protein Cmr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	279	Total	C	N	O	S	0	0
			2218	1411	372	423	12		
4	E	279	Total	C	N	O	S	0	0
			2218	1411	372	423	12		
4	F	279	Total	C	N	O	S	0	0
			2218	1411	372	423	12		

- Molecule 5 is a protein called CRISPR type III-B/RAMP module-associated protein Cmr5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	136	Total	C	N	O	S	0	0
			1072	681	180	206	5		
5	H	136	Total	C	N	O	S	0	0
			1072	681	180	206	5		

- Molecule 6 is a protein called RAMP superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	314	Total	C	N	O	S	0	0
			2535	1630	414	483	8		

- Molecule 7 is a RNA chain called crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	41	Total	C	N	O	P	0	0
			873	390	150	292	41		

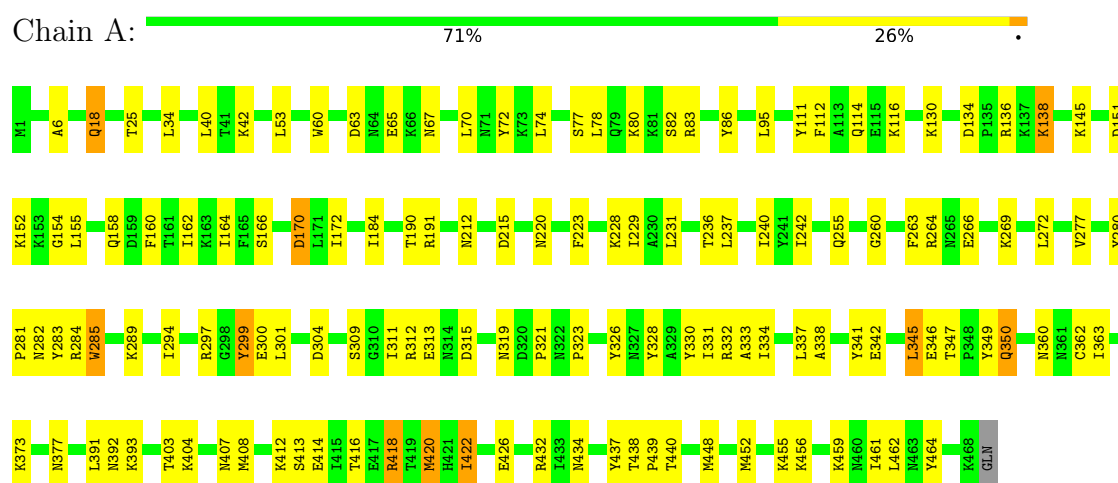
- Molecule 8 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
8	B	1	Total	Mn	0
			1	1	

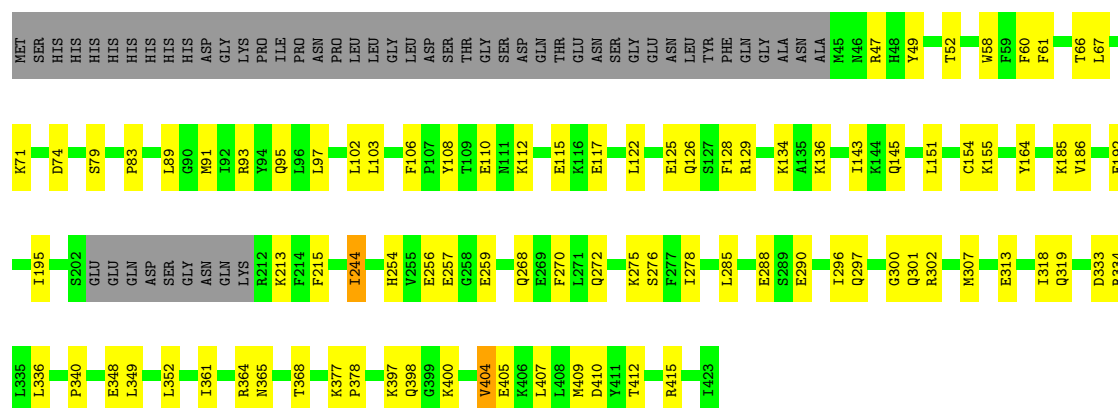
### 3 Residue-property plots [i](#)

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: Cmr1

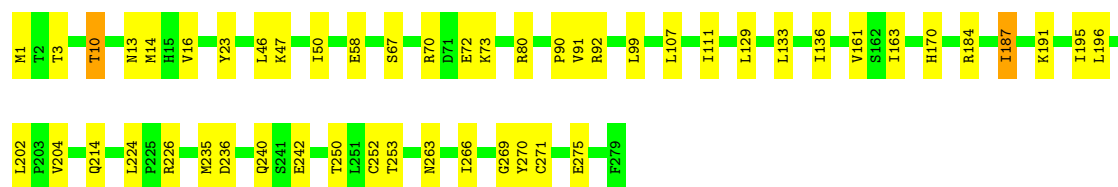


Chain C:  66% 21% 13%




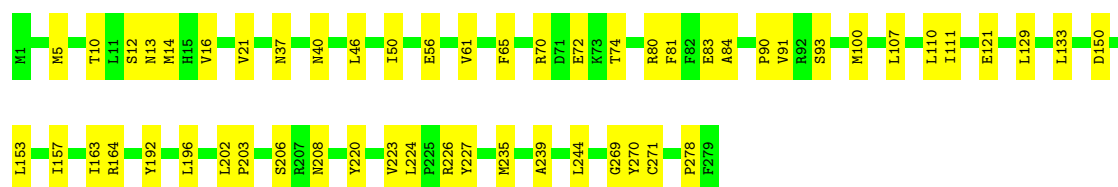
- Molecule 4: Type III-B CRISPR module RAMP protein Cmr4

Chain D:  82% 18%




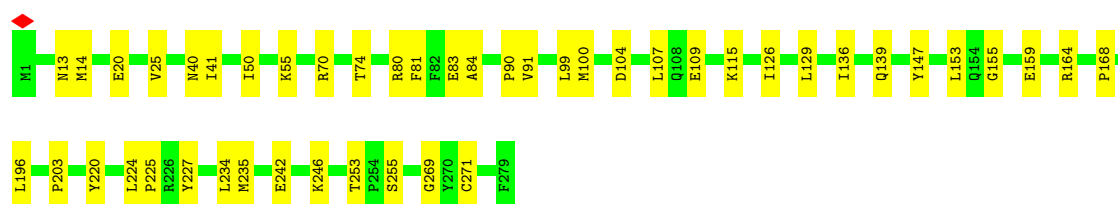
- Molecule 4: Type III-B CRISPR module RAMP protein Cmr4

Chain E:  81% 19%



- Molecule 4: Type III-B CRISPR module RAMP protein Cmr4

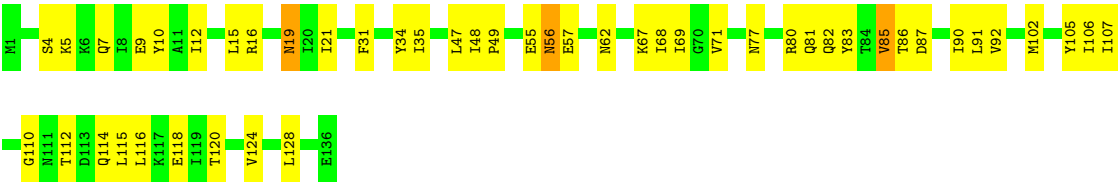
Chain F:  84% 16%



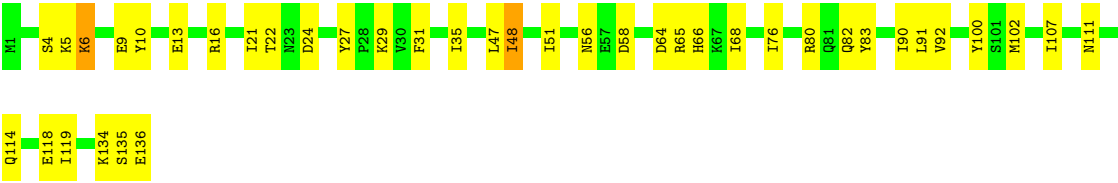
- Molecule 5: CRISPR type III-B/RAMP module-associated protein Cmr5

Chain G:  65% 33%

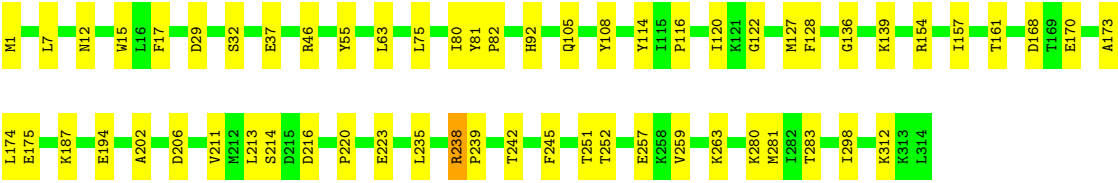
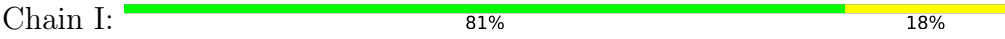




• Molecule 5: CRISPR type III-B/RAMP module-associated protein Cmr5



• Molecule 6: RAMP superfamily protein



• Molecule 7: crRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	95862	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	31.097	Depositor
Minimum map value	-0.154	Depositor
Average map value	-0.017	Depositor
Map value standard deviation	0.470	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	372.8, 372.8, 372.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.932, 0.932, 0.932	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: MN

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	0.16	0/3986	0.40	0/5369
2	B	0.17	0/4926	0.34	0/6645
3	C	0.17	0/3114	0.38	0/4192
4	D	0.15	0/2262	0.30	0/3062
4	E	0.15	0/2262	0.28	0/3062
4	F	0.16	0/2262	0.31	0/3062
5	G	0.17	0/1087	0.42	0/1466
5	H	0.15	0/1087	0.30	0/1466
6	I	0.16	0/2594	0.32	0/3500
7	J	0.16	0/975	0.38	0/1515
All	All	0.16	0/24555	0.35	0/33339

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	3895	0	3916	101	0
2	B	4828	0	4822	96	0
3	C	3044	0	3006	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	2218	0	2217	31	0
4	E	2218	0	2217	37	0
4	F	2218	0	2217	31	0
5	G	1072	0	1091	36	0
5	H	1072	0	1091	26	0
6	I	2535	0	2529	38	0
7	J	873	0	437	22	0
8	B	1	0	0	0	0
All	All	23974	0	23543	453	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 10.

All (453) 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)
2:B:295:ILE:HD12	2:B:296:PRO:HD2	1.53	0.88
2:B:260:ASN:O	2:B:263:LYS:NZ	2.16	0.76
4:D:58:GLU:OE1	4:D:58:GLU:N	2.20	0.74
6:I:194:GLU:N	6:I:194:GLU:OE1	2.20	0.74
2:B:267:ARG:HD2	2:B:473:LYS:HB2	1.70	0.73
2:B:132:GLU:OE1	2:B:132:GLU:N	2.22	0.73
2:B:423:ASN:O	2:B:426:MET:N	2.23	0.71
5:G:57:GLU:OE1	5:G:57:GLU:N	2.24	0.71
2:B:290:MET:HE1	2:B:300:LEU:HB2	1.71	0.71
3:C:117:GLU:OE1	3:C:117:GLU:N	2.19	0.71
2:B:434:LYS:NZ	2:B:551:TYR:OH	2.24	0.70
2:B:162:THR:OG1	3:C:364:ARG:NH2	2.24	0.70
3:C:296:ILE:HG21	3:C:307:MET:HE2	1.73	0.70
5:G:15:LEU:HB3	5:G:21:ILE:HD11	1.75	0.68
1:A:170:ASP:OD1	1:A:170:ASP:N	2.22	0.68
2:B:409:ASP:OD2	2:B:554:ARG:NH1	2.25	0.68
3:C:125:GLU:OE1	3:C:125:GLU:N	2.21	0.67
4:E:72:GLU:OE1	4:E:72:GLU:N	2.20	0.67
3:C:112:LYS:HB3	3:C:115:GLU:HG2	1.77	0.67
1:A:301:LEU:HA	1:A:345:LEU:HA	1.77	0.67
6:I:37:GLU:OE1	6:I:37:GLU:N	2.28	0.67
2:B:228:ILE:HG23	2:B:258:ILE:HD11	1.78	0.66
3:C:256:GLU:HB2	4:D:70:ARG:HH12	1.59	0.66
2:B:15:ILE:HG23	2:B:24:LEU:HD11	1.78	0.66
4:E:14:MET:HB3	4:E:224:LEU:HB3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:GLU:OE2	3:C:110:GLU:N	2.29	0.65
5:H:10:TYR:OH	5:H:82:GLN:OE1	2.12	0.64
3:C:128:PHE:O	3:C:365:ASN:ND2	2.30	0.64
5:H:29:LYS:HZ3	5:H:29:LYS:HB2	1.62	0.64
1:A:65:GLU:OE2	1:A:65:GLU:N	2.28	0.64
1:A:311:ILE:HD12	1:A:311:ILE:O	1.97	0.64
1:A:391:LEU:HB3	1:A:440:THR:HA	1.80	0.64
4:D:91:VAL:HG11	4:D:196:LEU:HD13	1.80	0.63
5:H:56:ASN:ND2	5:H:58:ASP:OD1	2.32	0.63
2:B:185:ARG:HH22	2:B:192:PRO:HG3	1.62	0.63
2:B:220:SER:HA	2:B:335:PRO:HB3	1.79	0.63
3:C:213:LYS:HE3	3:C:213:LYS:HA	1.80	0.63
3:C:313:GLU:N	3:C:313:GLU:OE1	2.32	0.63
3:C:377:LYS:HA	3:C:377:LYS:HE3	1.81	0.62
3:C:47:ARG:NH1	3:C:288:GLU:OE1	2.32	0.62
3:C:60:PHE:HD2	3:C:300:GLY:HA2	1.64	0.62
1:A:95:LEU:HD23	1:A:95:LEU:H	1.64	0.62
5:H:16:ARG:HH11	5:H:16:ARG:HG2	1.64	0.62
6:I:220:PRO:HB3	7:J:31:U:H1'	1.81	0.62
6:I:127:MET:HE2	6:I:127:MET:HA	1.82	0.62
1:A:42:LYS:NZ	1:A:220:ASN:OD1	2.27	0.61
2:B:477:LYS:N	2:B:477:LYS:HE2	2.16	0.61
4:D:67:SER:O	7:J:6:G:O2'	2.19	0.61
5:H:114:GLN:O	5:H:118:GLU:HG3	2.00	0.61
2:B:319:GLY:O	2:B:335:PRO:HD2	2.01	0.61
4:F:253:THR:HG22	4:F:255:SER:H	1.65	0.60
6:I:213:LEU:HD13	6:I:235:LEU:HD21	1.83	0.60
5:G:19:ASN:C	5:G:19:ASN:HD22	2.08	0.60
2:B:52:PRO:HG3	2:B:72:TYR:HD1	1.66	0.60
4:F:70:ARG:NH1	4:F:70:ARG:HB2	2.16	0.60
6:I:7:LEU:HD21	6:I:63:LEU:HD21	1.84	0.60
1:A:404:LYS:HE2	1:A:404:LYS:HA	1.82	0.60
2:B:224:LEU:HB2	2:B:226:ILE:HG13	1.84	0.60
4:F:104:ASP:N	4:F:104:ASP:OD1	2.35	0.60
1:A:432:ARG:NH1	1:A:437:TYR:OH	2.35	0.59
1:A:321:PRO:HB2	1:A:323:PRO:HD2	1.83	0.59
5:H:21:ILE:HD13	5:H:27:TYR:HB3	1.84	0.59
6:I:1:MET:N	6:I:55:TYR:OH	2.33	0.59
6:I:136:GLY:HA2	6:I:139:LYS:HG2	1.84	0.59
2:B:1:MET:SD	2:B:1:MET:N	2.66	0.59
3:C:134:LYS:NZ	3:C:410:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:565:THR:OG1	2:B:568:GLU:OE2	2.21	0.58
5:H:90:ILE:HG22	5:H:92:VAL:H	1.68	0.58
3:C:275:LYS:HE3	3:C:275:LYS:HA	1.84	0.58
2:B:515:ASN:O	2:B:519:ASN:ND2	2.35	0.58
4:D:204:VAL:HB	4:E:21:VAL:HG21	1.86	0.57
1:A:231:LEU:HD11	1:A:242:ILE:HG12	1.86	0.57
2:B:215:SER:OG	2:B:255:GLU:OE1	2.23	0.57
2:B:362:LEU:HD22	2:B:365:TYR:HB3	1.86	0.57
4:D:236:ASP:OD1	4:D:236:ASP:N	2.33	0.57
1:A:82:SER:OG	1:A:158:GLN:NE2	2.37	0.57
2:B:293:TYR:O	2:B:295:ILE:HG22	2.05	0.57
3:C:398:GLN:OE1	3:C:398:GLN:N	2.38	0.57
6:I:105:GLN:HG2	6:I:116:PRO:HD3	1.86	0.57
2:B:290:MET:HE3	2:B:362:LEU:HD21	1.86	0.57
4:E:150:ASP:HB3	4:E:153:LEU:HG	1.87	0.57
4:F:13:ASN:O	4:F:269:GLY:N	2.38	0.56
1:A:300:GLU:N	1:A:346:GLU:OE1	2.39	0.56
1:A:426:GLU:O	1:A:434:ASN:ND2	2.37	0.56
1:A:300:GLU:O	1:A:346:GLU:N	2.37	0.56
3:C:67:LEU:HD13	7:J:7:A:H62	1.70	0.56
4:F:41:ILE:HB	4:F:84:ALA:HB3	1.87	0.56
2:B:503:LEU:HD21	2:B:540:LEU:HD22	1.86	0.56
4:D:90:PRO:HG3	4:D:226:ARG:O	2.05	0.56
5:G:47:LEU:HD12	5:G:116:LEU:HD23	1.87	0.56
5:H:4:SER:HB2	5:H:6:LYS:HZ3	1.71	0.56
4:F:203:PRO:HG3	4:F:225:PRO:HG3	1.85	0.56
5:H:76:ILE:HG22	5:H:80:ARG:HD2	1.87	0.56
4:E:13:ASN:O	4:E:269:GLY:N	2.37	0.56
3:C:145:GLN:HB3	3:C:318:ILE:HD11	1.88	0.55
1:A:392:ASN:N	1:A:438:THR:OG1	2.39	0.55
2:B:161:GLU:H	2:B:169:SER:HB3	1.71	0.55
2:B:185:ARG:HG3	2:B:186:LYS:O	2.06	0.55
4:F:220:TYR:OH	7:J:27:U:O4	2.15	0.55
5:G:16:ARG:HG3	5:G:16:ARG:HH11	1.71	0.55
5:H:31:PHE:O	5:H:35:ILE:HG13	2.06	0.55
5:H:29:LYS:NZ	5:H:135:SER:OG	2.39	0.55
2:B:249:ASP:OD1	2:B:249:ASP:N	2.39	0.55
1:A:116:LYS:HA	1:A:116:LYS:HE2	1.88	0.55
3:C:290:GLU:OE1	3:C:290:GLU:N	2.40	0.55
1:A:231:LEU:HD23	1:A:236:THR:HG22	1.89	0.55
1:A:455:LYS:HB3	1:A:459:LYS:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:GLN:HG2	2:B:573:ILE:HD11	1.88	0.55
3:C:97:LEU:HD23	3:C:122:LEU:HD23	1.87	0.55
1:A:74:LEU:HD12	1:A:164:ILE:HG12	1.89	0.55
1:A:283:TYR:HB3	1:A:331:ILE:HD11	1.89	0.54
5:G:102:MET:O	5:G:106:ILE:HG13	2.06	0.54
4:E:91:VAL:HG11	4:E:196:LEU:HD13	1.90	0.54
3:C:244:ILE:HG13	3:C:272:GLN:HB3	1.89	0.54
3:C:368:THR:OG1	7:J:2:U:OP2	2.27	0.54
2:B:536:ILE:HD11	2:B:588:LEU:HD21	1.89	0.53
1:A:228:LYS:HG2	1:A:464:TYR:CE2	2.42	0.53
1:A:456:LYS:HE3	1:A:456:LYS:O	2.08	0.53
7:J:23:U:O4	7:J:24:A:N6	2.41	0.53
2:B:8:LEU:HD21	2:B:38:ILE:HD12	1.89	0.53
3:C:58:TRP:HB3	3:C:270:PHE:HB3	1.90	0.53
1:A:86:TYR:N	1:A:154:GLY:O	2.42	0.53
4:F:40:ASN:ND2	4:F:83:GLU:OE2	2.40	0.53
6:I:187:LYS:HB3	6:I:187:LYS:NZ	2.22	0.53
1:A:18:GLN:NE2	6:I:216:ASP:OD1	2.41	0.53
1:A:83:ARG:HD2	1:A:155:LEU:HD13	1.90	0.52
4:D:214:GLN:NE2	4:F:74:THR:HG23	2.24	0.52
6:I:281:MET:HE3	6:I:283:THR:HG22	1.91	0.52
4:E:157:ILE:HD13	4:E:164:ARG:HG2	1.92	0.52
7:J:37:G:H2'	7:J:38:G:C8	2.45	0.52
3:C:397:LYS:HG3	3:C:400:LYS:HD3	1.92	0.52
4:F:50:ILE:HD12	4:F:81:PHE:HE2	1.75	0.52
1:A:345:LEU:HD11	1:A:350:GLN:HG3	1.92	0.52
2:B:4:ILE:HG13	2:B:76:SER:HB2	1.91	0.52
2:B:184:TYR:HE1	2:B:193:ARG:HH11	1.56	0.52
3:C:67:LEU:HD13	7:J:7:A:N6	2.25	0.52
3:C:115:GLU:OE1	3:C:115:GLU:N	2.43	0.52
4:F:20:GLU:OE1	4:F:20:GLU:HA	2.10	0.52
1:A:294:ILE:HG23	1:A:301:LEU:HD21	1.92	0.52
6:I:170:GLU:HG3	6:I:257:GLU:HG2	1.92	0.52
1:A:272:LEU:HD11	1:A:334:ILE:HD11	1.91	0.52
5:H:22:THR:OG1	5:H:24:ASP:OD1	2.23	0.51
6:I:120:ILE:HD11	6:I:202:ALA:HB2	1.91	0.51
1:A:6:ALA:HB3	1:A:162:ILE:HG23	1.92	0.51
1:A:60:TRP:HZ2	1:A:170:ASP:HB2	1.75	0.51
4:D:10:THR:HA	4:D:271:CYS:HB3	1.92	0.51
5:H:135:SER:OG	5:H:136:GLU:N	2.42	0.51
6:I:194:GLU:H	6:I:194:GLU:CD	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:136:LYS:HE2	3:C:136:LYS:HA	1.92	0.51
4:E:208:ASN:O	7:J:20:A:H5'	2.10	0.51
1:A:284:ARG:NH1	1:A:309:SER:O	2.43	0.51
1:A:190:THR:OG1	7:J:34:A:OP2	2.28	0.51
1:A:312:ARG:NH2	1:A:313:GLU:O	2.43	0.51
3:C:52:THR:HB	3:C:278:ILE:HD12	1.93	0.51
2:B:226:ILE:HD13	2:B:262:ASN:ND2	2.26	0.50
3:C:185:LYS:NZ	3:C:192:GLU:OE2	2.33	0.50
7:J:15:G:O2'	7:J:16:A:OP2	2.29	0.50
2:B:281:ASP:OD2	2:B:380:SER:OG	2.25	0.50
1:A:408:MET:SD	1:A:412:LYS:N	2.84	0.50
3:C:254:HIS:ND1	3:C:256:GLU:OE1	2.45	0.50
3:C:106:PHE:O	3:C:108:TYR:N	2.37	0.50
2:B:276:ILE:HG12	2:B:383:ILE:HD12	1.93	0.50
3:C:91:MET:HE2	3:C:296:ILE:HD13	1.94	0.50
1:A:34:LEU:HD11	7:J:32:G:C2	2.47	0.50
4:D:136:ILE:HD11	4:D:187:ILE:HD12	1.94	0.50
4:F:203:PRO:HB3	6:I:108:TYR:CD1	2.47	0.50
5:H:83:TYR:HB3	5:H:90:ILE:HD12	1.93	0.50
5:G:5:LYS:O	5:G:9:GLU:HG3	2.12	0.50
5:G:114:GLN:NE2	5:G:118:GLU:OE2	2.45	0.50
2:B:425:ASN:OD1	2:B:428:ARG:NH2	2.45	0.49
2:B:474:ASP:OD1	2:B:474:ASP:N	2.34	0.49
4:D:46:LEU:O	4:D:50:ILE:HG12	2.12	0.49
6:I:238:ARG:HG2	6:I:239:PRO:HD2	1.94	0.49
1:A:332:ARG:HH12	7:J:38:G:H5''	1.76	0.49
4:D:72:GLU:OE1	4:D:72:GLU:HA	2.11	0.49
1:A:452:MET:HG3	1:A:461:ILE:HB	1.93	0.49
2:B:5:ALA:HB1	2:B:147:LEU:HD11	1.93	0.49
2:B:149:ILE:HG22	3:C:215:PHE:CD2	2.47	0.49
5:G:56:ASN:ND2	5:G:56:ASN:C	2.69	0.49
6:I:81:TYR:O	6:I:239:PRO:HG3	2.13	0.49
4:E:56:GLU:HA	4:E:56:GLU:OE1	2.12	0.49
1:A:350:GLN:HB3	1:A:403:THR:HG22	1.94	0.49
6:I:128:PHE:HB3	6:I:175:GLU:CD	2.38	0.49
1:A:346:GLU:OE2	1:A:347:THR:HG22	2.12	0.49
3:C:348:GLU:HG2	3:C:407:LEU:HD11	1.95	0.49
3:C:352:LEU:HD22	3:C:407:LEU:HD12	1.93	0.49
4:D:111:ILE:HD12	4:D:133:LEU:HD12	1.94	0.49
6:I:46:ARG:HB2	6:I:46:ARG:CZ	2.43	0.49
1:A:407:ASN:HB2	1:A:412:LYS:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:19:ASN:C	5:G:19:ASN:ND2	2.71	0.49
5:G:56:ASN:ND2	5:G:56:ASN:O	2.46	0.49
1:A:40:LEU:HD21	1:A:70:LEU:HD21	1.95	0.48
3:C:145:GLN:OE1	3:C:319:GLN:NE2	2.46	0.48
4:F:99:LEU:HD21	4:F:153:LEU:HD13	1.94	0.48
1:A:114:GLN:OE1	1:A:152:LYS:N	2.46	0.48
6:I:206:ASP:HB3	6:I:242:THR:HB	1.95	0.48
4:E:14:MET:HE1	4:E:271:CYS:SG	2.53	0.48
4:E:90:PRO:HG2	4:E:226:ARG:O	2.12	0.48
2:B:469:ILE:HD12	2:B:594:ILE:HG21	1.95	0.48
6:I:29:ASP:OD2	6:I:32:SER:OG	2.26	0.48
1:A:130:LYS:HA	1:A:138:LYS:NZ	2.29	0.48
4:F:136:ILE:HD13	4:F:147:TYR:HD2	1.79	0.48
5:G:55:GLU:HG3	5:G:69:ILE:HG21	1.95	0.48
1:A:228:LYS:HD2	1:A:462:LEU:HD22	1.96	0.48
3:C:268:GLN:HE22	3:C:301:GLN:HG3	1.78	0.48
1:A:312:ARG:HB3	1:A:315:ASP:HB2	1.95	0.48
5:H:65:ARG:O	5:H:68:ILE:HG22	2.14	0.48
1:A:145:LYS:NZ	1:A:145:LYS:HB3	2.28	0.48
1:A:297:ARG:HH12	1:A:422:ILE:HD12	1.78	0.48
2:B:1:MET:N	2:B:131:LEU:O	2.46	0.48
1:A:112:PHE:CD1	1:A:112:PHE:C	2.92	0.48
2:B:60:LYS:HE2	2:B:61:PRO:HD2	1.95	0.48
3:C:405:GLU:O	3:C:409:MET:HG3	2.14	0.47
2:B:480:GLU:OE1	2:B:480:GLU:HA	2.14	0.47
5:G:77:ASN:O	5:G:81:GLN:HG2	2.14	0.47
5:H:29:LYS:HB2	5:H:29:LYS:NZ	2.25	0.47
4:D:14:MET:HB3	4:D:224:LEU:HB3	1.96	0.47
4:F:80:ARG:HB2	4:F:235:MET:HB2	1.94	0.47
4:F:107:LEU:HD22	4:F:129:LEU:HD22	1.97	0.47
5:G:107:ILE:O	5:H:5:LYS:NZ	2.45	0.47
1:A:304:ASP:OD1	1:A:304:ASP:N	2.38	0.47
5:G:9:GLU:HA	5:G:12:ILE:HD12	1.97	0.47
2:B:286:THR:HG21	2:B:377:PRO:HD3	1.97	0.47
4:D:92:ARG:HD2	4:E:37:ASN:HB2	1.96	0.47
4:E:107:LEU:HD22	4:E:129:LEU:HD22	1.97	0.47
6:I:12:ASN:HB3	6:I:15:TRP:HB3	1.97	0.47
3:C:334:ARG:NH1	3:C:336:LEU:HB2	2.30	0.47
4:E:203:PRO:HB2	4:E:223:VAL:HG23	1.97	0.47
5:H:83:TYR:HD2	5:H:90:ILE:HG23	1.80	0.47
1:A:404:LYS:NZ	1:A:413:SER:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLY:HA2	2:B:123:LYS:H	1.80	0.46
2:B:65:ALA:HB2	2:B:322:PRO:HB2	1.96	0.46
2:B:180:ASN:ND2	2:B:214:GLU:OE1	2.39	0.46
3:C:377:LYS:HD3	3:C:378:PRO:HD2	1.97	0.46
5:G:34:TYR:OH	5:G:62:ASN:ND2	2.48	0.46
4:E:61:VAL:HA	4:E:65:PHE:HD1	1.81	0.46
5:G:114:GLN:O	5:G:118:GLU:HG3	2.14	0.46
3:C:186:VAL:HB	3:C:195:ILE:HD12	1.98	0.46
4:D:99:LEU:HD23	4:D:184:ARG:HB3	1.98	0.46
6:I:127:MET:SD	6:I:298:ILE:HG21	2.56	0.46
6:I:157:ILE:O	6:I:161:THR:OG1	2.30	0.46
3:C:61:PHE:CE1	3:C:83:PRO:HB3	2.51	0.46
5:H:64:ASP:HB2	5:H:66:HIS:CE1	2.51	0.46
6:I:17:PHE:O	6:I:92:HIS:NE2	2.46	0.46
1:A:231:LEU:HD21	1:A:242:ILE:HD11	1.98	0.46
1:A:338:ALA:HB3	1:A:341:TYR:HE1	1.80	0.46
2:B:402:LEU:HD21	2:B:438:SER:HB2	1.98	0.45
4:D:161:VAL:O	4:D:163:ILE:N	2.46	0.45
2:B:295:ILE:HD11	2:B:299:GLN:CD	2.41	0.45
1:A:338:ALA:HA	7:J:36:U:O2'	2.16	0.45
2:B:188:LYS:N	2:B:188:LYS:HE2	2.32	0.45
4:D:263:ASN:HB3	4:D:266:ILE:HG12	1.98	0.45
4:E:80:ARG:HB2	4:E:235:MET:HB2	1.97	0.45
4:F:14:MET:HB3	4:F:224:LEU:HB3	1.97	0.45
1:A:285:TRP:HZ3	7:J:41:U:H3	1.64	0.45
1:A:301:LEU:H	1:A:301:LEU:HD22	1.82	0.45
4:F:155:GLY:O	4:F:164:ARG:NH1	2.50	0.45
6:I:174:LEU:HD12	6:I:252:THR:HG21	1.98	0.45
1:A:112:PHE:HE2	7:J:37:G:H5''	1.82	0.45
1:A:289:LYS:HB2	1:A:328:TYR:CD2	2.52	0.45
1:A:404:LYS:NZ	1:A:414:GLU:HA	2.31	0.45
2:B:60:LYS:HZ3	2:B:61:PRO:HD2	1.81	0.45
5:G:110:GLY:O	5:G:115:LEU:HD23	2.16	0.45
5:H:51:ILE:HD13	5:H:102:MET:HG2	1.99	0.45
4:D:202:LEU:HD23	4:D:202:LEU:HA	1.85	0.45
2:B:280:GLY:N	2:B:328:ASP:HB2	2.32	0.45
3:C:89:LEU:O	3:C:93:ARG:HG3	2.17	0.45
2:B:280:GLY:H	2:B:328:ASP:HB2	1.82	0.45
2:B:362:LEU:HD23	2:B:362:LEU:HA	1.71	0.45
4:F:14:MET:HB2	4:F:14:MET:HE3	1.79	0.45
1:A:78:LEU:HD23	1:A:160:PHE:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:MET:H	1:A:408:MET:CE	2.30	0.44
1:A:416:THR:HA	1:A:418:ARG:HH12	1.81	0.44
4:D:47:LYS:NZ	7:J:7:A:OP1	2.50	0.44
1:A:112:PHE:HZ	7:J:36:U:C2	2.36	0.44
1:A:448:MET:HE3	1:A:448:MET:HA	1.99	0.44
2:B:329:ASP:OD1	2:B:329:ASP:N	2.51	0.44
3:C:349:LEU:HD11	3:C:404:VAL:HG23	1.98	0.44
5:H:16:ARG:HG2	5:H:16:ARG:NH1	2.32	0.44
5:H:102:MET:HE2	5:H:119:ILE:HD11	1.98	0.44
6:I:75:LEU:HB3	6:I:245:PHE:HB2	2.00	0.44
1:A:297:ARG:NH2	1:A:422:ILE:O	2.51	0.44
1:A:299:TYR:HB2	1:A:345:LEU:HD22	2.00	0.44
2:B:275:ILE:HG12	2:B:333:PHE:HE2	1.82	0.44
4:F:14:MET:HE1	4:F:271:CYS:SG	2.57	0.44
5:G:10:TYR:OH	5:G:82:GLN:OE1	2.34	0.44
6:I:80:ILE:HG22	6:I:82:PRO:HD2	1.99	0.44
6:I:170:GLU:OE2	6:I:280:LYS:NZ	2.40	0.44
1:A:25:THR:HB	1:A:78:LEU:HG	1.99	0.44
2:B:162:THR:HG1	3:C:364:ARG:HH22	1.63	0.44
2:B:469:ILE:HD13	2:B:469:ILE:HA	1.87	0.44
4:E:70:ARG:HG2	4:E:70:ARG:NH1	2.33	0.44
1:A:330:TYR:CD2	1:A:333:ALA:HB2	2.53	0.44
2:B:77:GLU:O	2:B:80:ASP:HB2	2.18	0.44
4:F:91:VAL:HG11	4:F:196:LEU:HD13	1.99	0.44
2:B:104:LEU:HD21	2:B:197:SER:HB3	2.00	0.44
2:B:490:GLN:O	2:B:493:ARG:HG3	2.18	0.44
3:C:151:LEU:HD23	3:C:164:TYR:HB2	1.99	0.44
4:E:72:GLU:H	4:E:72:GLU:CD	2.16	0.44
4:E:133:LEU:HD23	4:E:133:LEU:HA	1.86	0.44
6:I:214:SER:HB2	6:I:238:ARG:HG3	2.00	0.44
1:A:319:ASN:C	1:A:319:ASN:OD1	2.60	0.44
3:C:257:GLU:HB3	3:C:259:GLU:OE1	2.17	0.44
4:D:252:CYS:SG	4:D:275:GLU:HB2	2.57	0.44
5:G:87:ASP:N	5:G:87:ASP:OD1	2.51	0.44
3:C:95:GLN:HG3	3:C:307:MET:HE1	1.99	0.44
2:B:211:ARG:HD2	2:B:229:GLN:CD	2.43	0.43
4:E:70:ARG:HG2	4:E:70:ARG:HH11	1.82	0.43
6:I:251:THR:HG23	6:I:283:THR:HA	1.99	0.43
1:A:264:ARG:O	1:A:266:GLU:N	2.50	0.43
1:A:277:VAL:O	1:A:282:ASN:ND2	2.51	0.43
1:A:363:ILE:HD11	1:A:393:LYS:HZ3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:LYS:HB3	3:C:71:LYS:HE3	1.87	0.43
4:F:55:LYS:HB3	4:F:55:LYS:NZ	2.33	0.43
5:G:21:ILE:HD12	5:G:21:ILE:H	1.84	0.43
5:G:80:ARG:NH2	5:G:83:TYR:O	2.51	0.43
5:G:90:ILE:O	5:G:91:LEU:HD13	2.18	0.43
5:H:47:LEU:HD21	5:H:119:ILE:HD12	1.98	0.43
1:A:240:ILE:HD13	1:A:240:ILE:HA	1.80	0.43
2:B:482:GLU:OE2	2:B:595:ASN:HB3	2.19	0.43
5:G:48:ILE:HB	5:G:49:PRO:HD3	2.00	0.43
1:A:263:PHE:O	1:A:264:ARG:HB2	2.18	0.43
3:C:126:GLN:HB2	3:C:129:ARG:NH1	2.33	0.43
1:A:172:ILE:HD13	1:A:172:ILE:HA	1.91	0.43
1:A:166:SER:HB3	1:A:172:ILE:HG12	2.00	0.43
1:A:212:ASN:HB3	1:A:215:ASP:HB2	2.01	0.43
1:A:280:TYR:O	1:A:281:PRO:C	2.61	0.43
2:B:142:ALA:HA	2:B:145:LYS:HE2	2.00	0.43
3:C:333:ASP:N	3:C:333:ASP:OD1	2.51	0.43
5:G:115:LEU:HD13	5:G:115:LEU:HA	1.87	0.43
2:B:53:LEU:O	2:B:53:LEU:HD23	2.19	0.43
2:B:374:ARG:HG2	2:B:374:ARG:HH11	1.83	0.43
1:A:111:TYR:HD1	1:A:191:ARG:HG3	1.84	0.43
1:A:134:ASP:OD2	1:A:136:ARG:NE	2.51	0.43
2:B:336:VAL:HG11	2:B:594:ILE:HD11	2.00	0.43
4:D:73:LYS:HE2	4:D:73:LYS:HB2	1.88	0.43
4:E:40:ASN:ND2	4:E:83:GLU:OE1	2.52	0.43
1:A:77:SER:O	1:A:160:PHE:HB2	2.19	0.42
2:B:182:LYS:O	2:B:195:THR:HG23	2.19	0.42
2:B:459:VAL:O	2:B:463:MET:HG3	2.19	0.42
3:C:268:GLN:NE2	3:C:301:GLN:HG3	2.34	0.42
6:I:122:GLY:HA3	7:J:26:U:O4'	2.19	0.42
1:A:439:PRO:O	1:A:440:THR:HG22	2.19	0.42
2:B:13:ARG:NH1	2:B:154:GLU:OE2	2.35	0.42
2:B:283:MET:HG2	2:B:377:PRO:HB3	2.01	0.42
4:E:206:SER:HB3	4:E:220:TYR:CE1	2.54	0.42
5:H:48:ILE:HG21	5:H:107:ILE:HD11	2.01	0.42
1:A:269:LYS:NZ	1:A:311:ILE:HA	2.34	0.42
1:A:420:MET:HE3	1:A:420:MET:HB3	1.88	0.42
2:B:421:ILE:HD11	2:B:563:ILE:HG21	2.01	0.42
5:H:9:GLU:O	5:H:13:GLU:HG3	2.20	0.42
1:A:114:GLN:OE1	1:A:151:ASP:HB2	2.18	0.42
1:A:184:ILE:O	1:A:373:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:LEU:HD12	2:B:259:LEU:HA	1.93	0.42
2:B:194:PHE:HE2	2:B:229:GLN:HE21	1.67	0.42
4:F:70:ARG:HB2	4:F:70:ARG:HH11	1.83	0.42
1:A:321:PRO:HD3	1:A:326:TYR:OH	2.20	0.42
2:B:476:SER:C	2:B:477:LYS:HE2	2.44	0.42
4:D:250:THR:O	4:D:253:THR:HG22	2.20	0.42
4:E:5:MET:HE1	4:E:110:LEU:HD11	2.00	0.42
4:F:40:ASN:HD22	4:F:83:GLU:CD	2.27	0.42
1:A:223:PHE:CZ	1:A:448:MET:HG3	2.55	0.42
4:D:270:TYR:OH	4:E:80:ARG:HG2	2.19	0.42
7:J:29:C:N3	7:J:30:A:N6	2.68	0.42
2:B:254:ALA:O	2:B:258:ILE:HG23	2.19	0.42
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.91	0.42
4:F:139:GLN:HG2	4:F:168:PRO:HB3	2.02	0.42
6:I:211:VAL:HG23	6:I:238:ARG:HD3	2.02	0.42
3:C:102:LEU:HD21	3:C:115:GLU:HB2	2.02	0.42
5:G:31:PHE:O	5:G:35:ILE:HG13	2.20	0.42
7:J:12:C:N4	7:J:13:G:O6	2.53	0.42
2:B:196:GLY:O	2:B:201:ARG:NH1	2.53	0.41
2:B:507:ASP:OD1	2:B:508:LYS:N	2.53	0.41
3:C:154:CYS:O	3:C:276:SER:HB2	2.20	0.41
4:E:46:LEU:HD11	4:E:84:ALA:HB2	2.02	0.41
4:F:100:MET:HE1	4:F:227:TYR:O	2.20	0.41
4:F:159:GLU:O	4:F:159:GLU:HG3	2.20	0.41
5:G:80:ARG:HA	5:G:80:ARG:NE	2.34	0.41
6:I:173:ALA:HB1	6:I:259:VAL:HG23	2.01	0.41
1:A:63:ASP:OD2	1:A:67:ASN:N	2.48	0.41
1:A:294:ILE:HD11	1:A:299:TYR:HE1	1.84	0.41
3:C:60:PHE:CD1	3:C:79:SER:HB2	2.55	0.41
4:D:3:THR:HG23	4:D:235:MET:HG3	2.02	0.41
1:A:432:ARG:CZ	1:A:432:ARG:HB3	2.51	0.41
2:B:53:LEU:HD13	2:B:301:SER:HB2	2.03	0.41
2:B:63:CYS:O	2:B:65:ALA:N	2.53	0.41
3:C:67:LEU:O	3:C:74:ASP:HB2	2.21	0.41
3:C:297:GLN:O	7:J:2:U:H5	2.03	0.41
4:D:107:LEU:HD22	4:D:129:LEU:HD22	2.02	0.41
1:A:242:ILE:HD13	1:A:377:ASN:ND2	2.35	0.41
2:B:6:ILE:HD11	2:B:74:PHE:HE1	1.85	0.41
2:B:185:ARG:NH2	2:B:237:THR:HG21	2.36	0.41
4:E:10:THR:HG22	4:E:12:SER:O	2.20	0.41
4:E:100:MET:HE1	4:E:227:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:110:GLY:C	5:G:112:THR:H	2.29	0.41
5:H:134:LYS:NZ	5:H:134:LYS:HB3	2.35	0.41
1:A:63:ASP:O	1:A:65:GLU:N	2.53	0.41
1:A:72:TYR:HE2	1:A:74:LEU:HD13	1.86	0.41
2:B:56:GLU:HA	2:B:56:GLU:OE1	2.21	0.41
3:C:155:LYS:HD3	3:C:155:LYS:HA	1.84	0.41
4:D:240:GLN:NE2	4:D:242:GLU:OE2	2.53	0.41
4:E:157:ILE:HD12	4:E:157:ILE:HA	1.84	0.41
5:G:4:SER:OG	5:G:7:GLN:HG3	2.20	0.41
5:G:105:TYR:HE2	5:G:115:LEU:HD21	1.86	0.41
3:C:340:PRO:HB3	3:C:361:ILE:HD11	2.03	0.41
4:E:121:GLU:HG2	4:E:278:PRO:HA	2.01	0.41
4:D:191:LYS:O	4:D:195:ILE:HG13	2.20	0.41
4:E:202:LEU:HD23	4:E:202:LEU:HA	1.88	0.41
5:G:56:ASN:C	5:G:56:ASN:HD22	2.28	0.41
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.89	0.41
1:A:408:MET:SD	1:A:408:MET:N	2.80	0.41
2:B:233:LEU:HA	2:B:236:ILE:HG22	2.02	0.41
2:B:358:ILE:O	2:B:362:LEU:HB2	2.20	0.41
3:C:143:ILE:H	3:C:143:ILE:HG13	1.65	0.41
4:F:90:PRO:HA	4:F:99:LEU:O	2.20	0.41
5:G:80:ARG:HH22	5:G:83:TYR:HD2	1.67	0.41
5:G:83:TYR:CD1	5:G:86:THR:HG21	2.55	0.41
1:A:229:ILE:HA	1:A:229:ILE:HD12	1.84	0.41
1:A:282:ASN:OD1	1:A:282:ASN:N	2.54	0.41
2:B:347:VAL:HG12	2:B:458:TYR:OH	2.21	0.41
3:C:302:ARG:O	4:D:80:ARG:NH1	2.54	0.41
4:E:111:ILE:HD12	4:E:133:LEU:HD12	2.03	0.41
4:E:270:TYR:OH	4:F:80:ARG:HG2	2.20	0.41
5:G:67:LYS:O	5:G:71:VAL:HG23	2.21	0.41
5:G:85:VAL:HG23	5:G:86:THR:H	1.86	0.41
2:B:9:GLY:N	2:B:123:LYS:O	2.49	0.41
2:B:410:ASN:HB3	2:B:414:TYR:CE1	2.56	0.41
3:C:49:TYR:CE2	3:C:285:LEU:HD12	2.56	0.41
4:E:50:ILE:HD12	4:E:81:PHE:HE2	1.85	0.41
4:E:93:SER:HA	4:E:157:ILE:O	2.20	0.41
4:F:115:LYS:HG3	4:F:126:ILE:HD13	2.03	0.41
1:A:360:ASN:O	1:A:362:CYS:N	2.53	0.40
2:B:21:THR:HG23	2:B:333:PHE:CD1	2.56	0.40
3:C:125:GLU:H	3:C:125:GLU:CD	2.21	0.40
3:C:334:ARG:HH12	3:C:336:LEU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:412:THR:HA	3:C:415:ARG:HB2	2.02	0.40
1:A:416:THR:HA	1:A:418:ARG:NH1	2.37	0.40
2:B:367:ASN:OD1	2:B:368:ALA:N	2.55	0.40
2:B:404:GLU:O	2:B:410:ASN:HB2	2.21	0.40
4:D:13:ASN:O	4:D:269:GLY:N	2.51	0.40
6:I:223:GLU:C	6:I:223:GLU:OE1	2.64	0.40
2:B:437:PHE:HB3	2:B:449:THR:HG22	2.03	0.40
4:E:163:ILE:HD13	4:E:192:TYR:CE2	2.57	0.40
1:A:255:GLN:O	1:A:260:GLY:N	2.54	0.40
2:B:158:GLU:H	2:B:158:GLU:CD	2.30	0.40
2:B:447:TYR:HA	4:D:23:TYR:OH	2.21	0.40
2:B:558:ILE:HD13	2:B:558:ILE:HA	1.93	0.40
3:C:66:THR:CG2	3:C:67:LEU:H	2.35	0.40
6:I:80:ILE:HD11	6:I:312:LYS:HB2	2.02	0.40
4:E:227:TYR:OH	4:F:109:GLU:OE2	2.26	0.40
4:E:239:ALA:HB3	4:E:244:LEU:HD11	2.04	0.40
5:G:120:THR:O	5:G:124:VAL:HG23	2.20	0.40
6:I:154:ARG:NH2	6:I:168:ASP:OD1	2.52	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	466/469 (99%)	431 (92%)	35 (8%)	0	100	100
2	B	591/600 (98%)	548 (93%)	42 (7%)	1 (0%)	44	74
3	C	366/423 (86%)	341 (93%)	25 (7%)	0	100	100
4	D	277/279 (99%)	271 (98%)	6 (2%)	0	100	100
4	E	277/279 (99%)	266 (96%)	11 (4%)	0	100	100
4	F	277/279 (99%)	272 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	G	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
5	H	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
6	I	312/314 (99%)	299 (96%)	13 (4%)	0	100	100
All	All	2834/2915 (97%)	2679 (94%)	154 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	376	LEU

### 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	432/433 (100%)	417 (96%)	15 (4%)	31	63
2	B	540/544 (99%)	523 (97%)	17 (3%)	35	66
3	C	342/387 (88%)	340 (99%)	2 (1%)	84	92
4	D	251/251 (100%)	246 (98%)	5 (2%)	50	76
4	E	251/251 (100%)	249 (99%)	2 (1%)	79	90
4	F	251/251 (100%)	247 (98%)	4 (2%)	58	81
5	G	115/115 (100%)	109 (95%)	6 (5%)	19	50
5	H	115/115 (100%)	110 (96%)	5 (4%)	25	56
6	I	283/283 (100%)	280 (99%)	3 (1%)	70	86
All	All	2580/2630 (98%)	2521 (98%)	59 (2%)	46	73

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	53	LEU
1	A	80	LYS

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Mol	Chain	Res	Type
1	A	138	LYS
1	A	170	ASP
1	A	237	LEU
1	A	285	TRP
1	A	299	TYR
1	A	342	GLU
1	A	345	LEU
1	A	349	TYR
1	A	350	GLN
1	A	418	ARG
1	A	420	MET
1	A	422	ILE
2	B	15	ILE
2	B	59	GLN
2	B	80	ASP
2	B	127	ILE
2	B	172	LEU
2	B	191	ILE
2	B	236	ILE
2	B	250	GLN
2	B	258	ILE
2	B	329	ASP
2	B	330	LEU
2	B	342	ASN
2	B	397	HIS
2	B	459	VAL
2	B	561	ASN
2	B	562	THR
2	B	579	ASP
3	C	244	ILE
3	C	404	VAL
4	D	1	MET
4	D	10	THR
4	D	16	VAL
4	D	170	HIS
4	D	187	ILE
4	E	16	VAL
4	E	74	THR
4	F	25	VAL
4	F	234	LEU
4	F	242	GLU
4	F	246	LYS

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Mol	Chain	Res	Type
5	G	19	ASN
5	G	56	ASN
5	G	68	ILE
5	G	85	VAL
5	G	92	VAL
5	G	128	LEU
5	H	6	LYS
5	H	48	ILE
5	H	91	LEU
5	H	100	TYR
5	H	111	ASN
6	I	114	TYR
6	I	238	ARG
6	I	263	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	186	HIS
1	A	192	ASN
1	A	407	ASN
2	B	55	ASN
2	B	137	HIS
2	B	294	ASN
2	B	526	HIS
3	C	105	GLN
3	C	248	GLN
3	C	268	GLN
3	C	272	GLN
3	C	319	GLN
3	C	386	HIS
4	D	13	ASN
4	D	40	ASN
4	D	85	ASN
4	D	209	ASN
4	D	222	GLN
4	E	40	ASN
4	E	190	HIS
4	F	85	ASN
4	F	124	GLN
4	F	170	HIS

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Mol	Chain	Res	Type
4	F	200	ASN
4	F	209	ASN
5	G	111	ASN
6	I	181	ASN
6	I	264	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	J	40/49 (81%)	8 (20%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	J	2	U
7	J	3	U
7	J	15	G
7	J	28	C
7	J	29	C
7	J	32	G
7	J	37	G
7	J	41	U

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

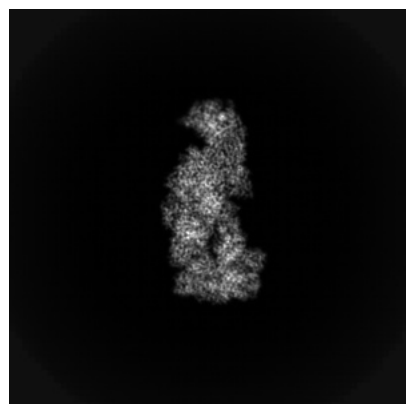
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63293. These allow visual inspection of the internal detail of the map and identification of artifacts.

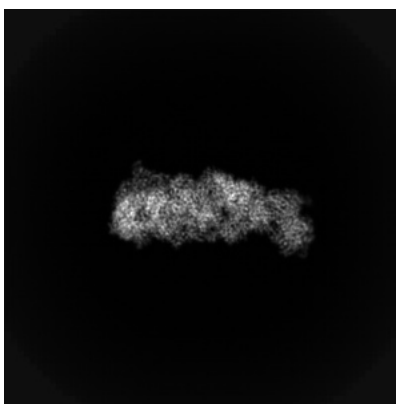
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

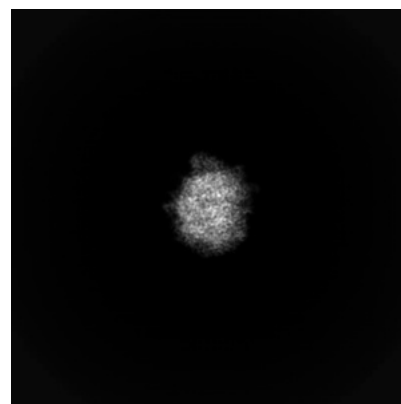
#### 6.1.1 Primary map



X

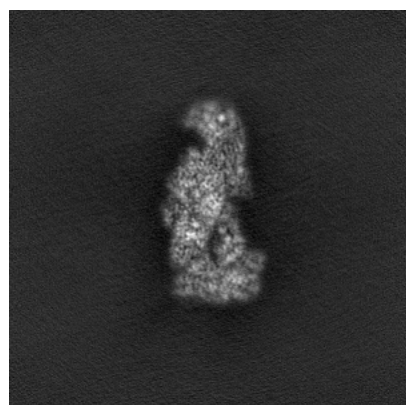


Y

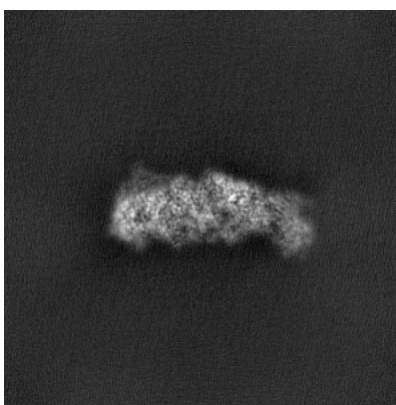


Z

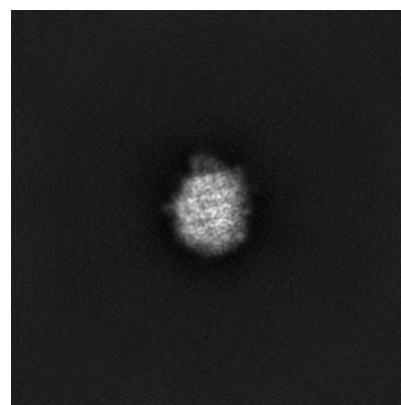
#### 6.1.2 Raw map



X



Y

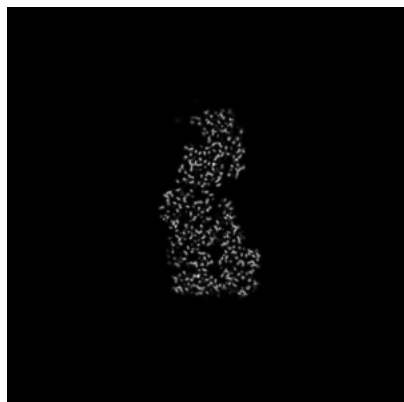


Z

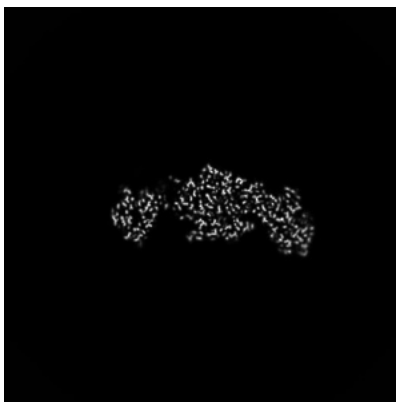
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

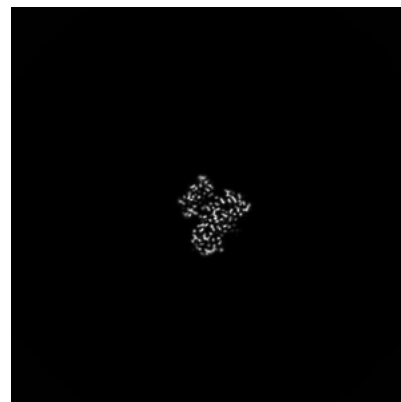
### 6.2.1 Primary map



X Index: 200

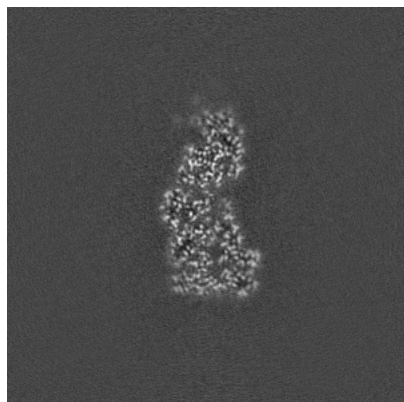


Y Index: 200

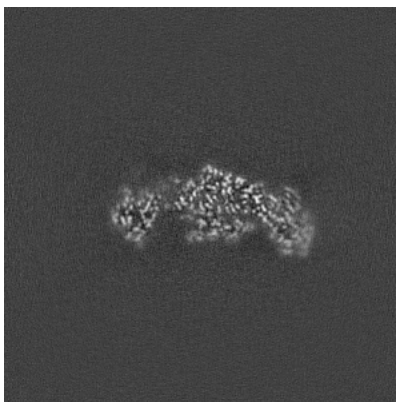


Z Index: 200

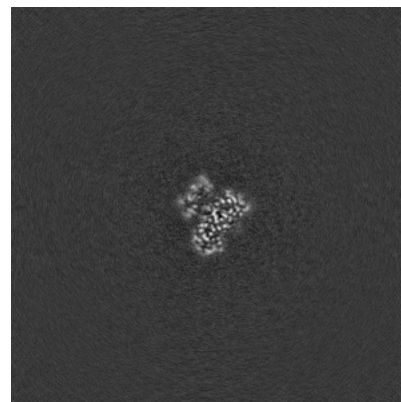
### 6.2.2 Raw map



X Index: 200



Y Index: 200



Z Index: 200

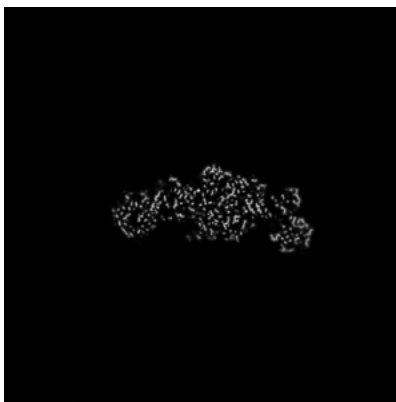
The images above show central slices of the map in three orthogonal directions.

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

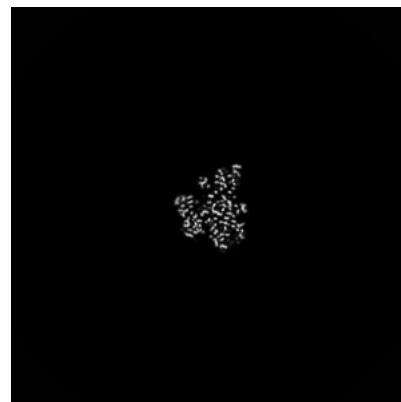
### 6.3.1 Primary map



X Index: 206

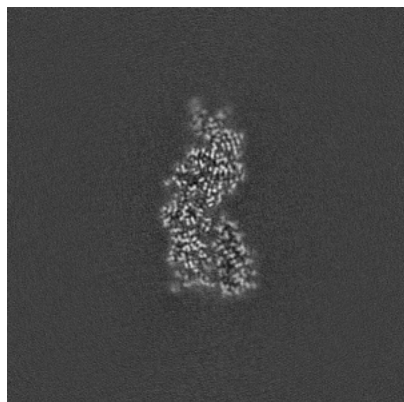


Y Index: 197

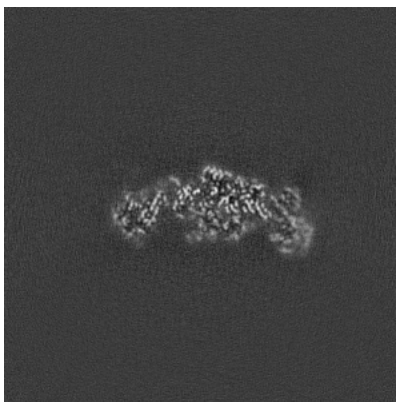


Z Index: 226

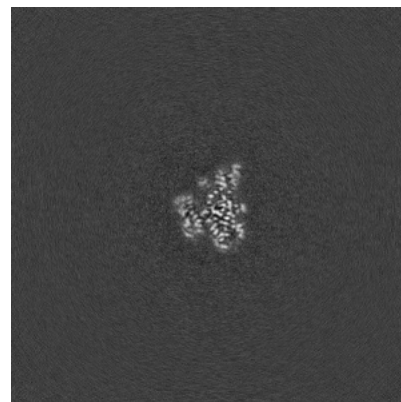
### 6.3.2 Raw map



X Index: 207



Y Index: 198

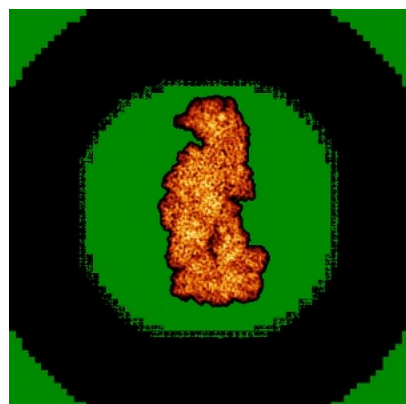


Z Index: 226

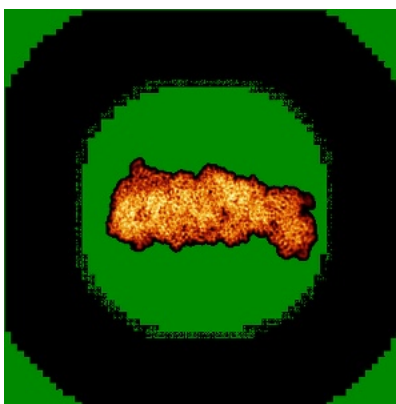
The images above show the largest variance slices of the map in three orthogonal directions.

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

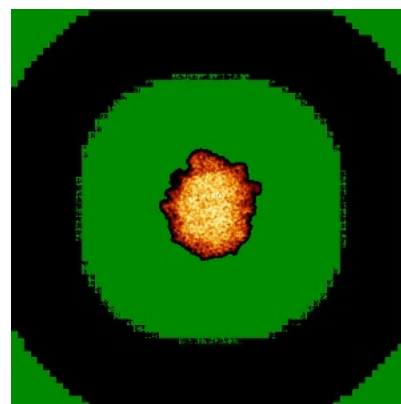
### 6.4.1 Primary map



X

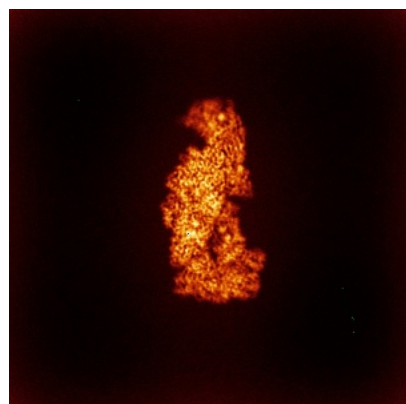


Y

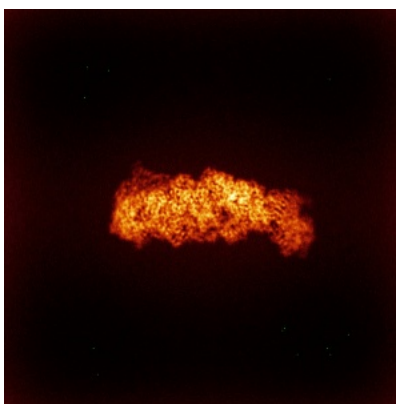


Z

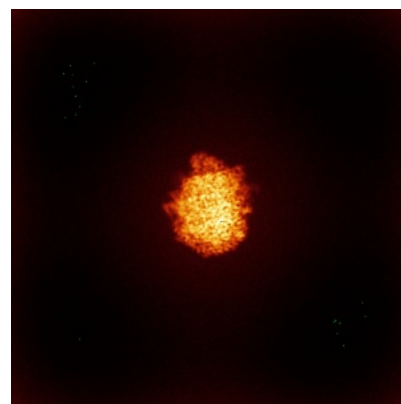
### 6.4.2 Raw map



X



Y



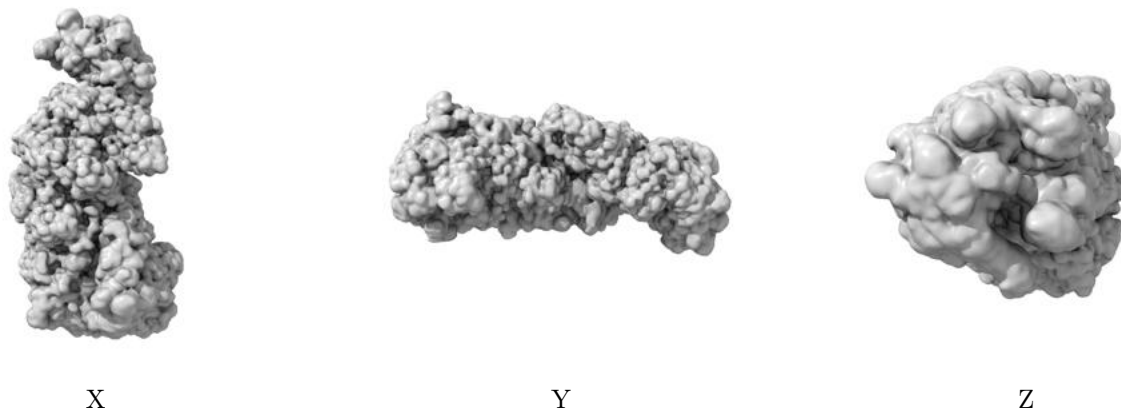
Z

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.



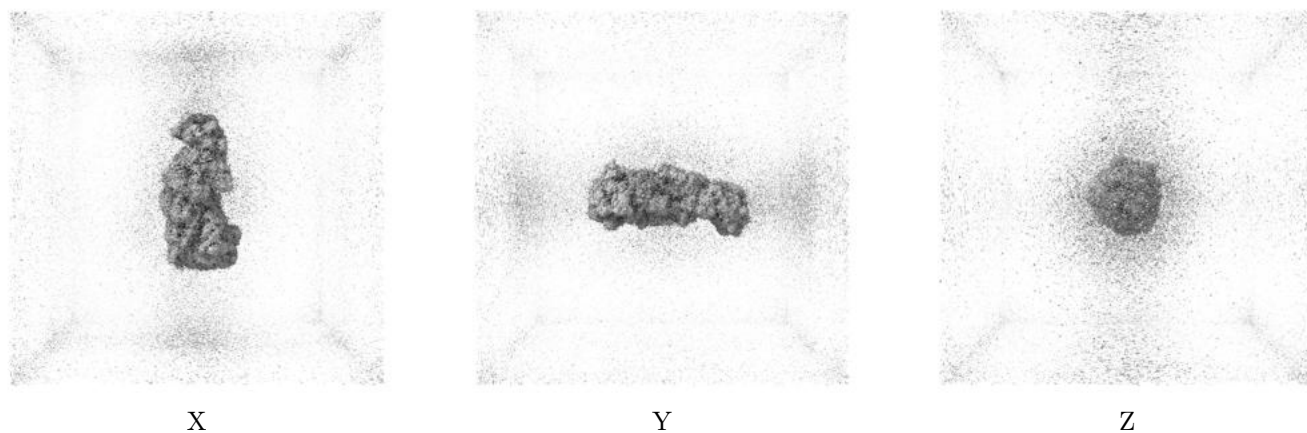
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

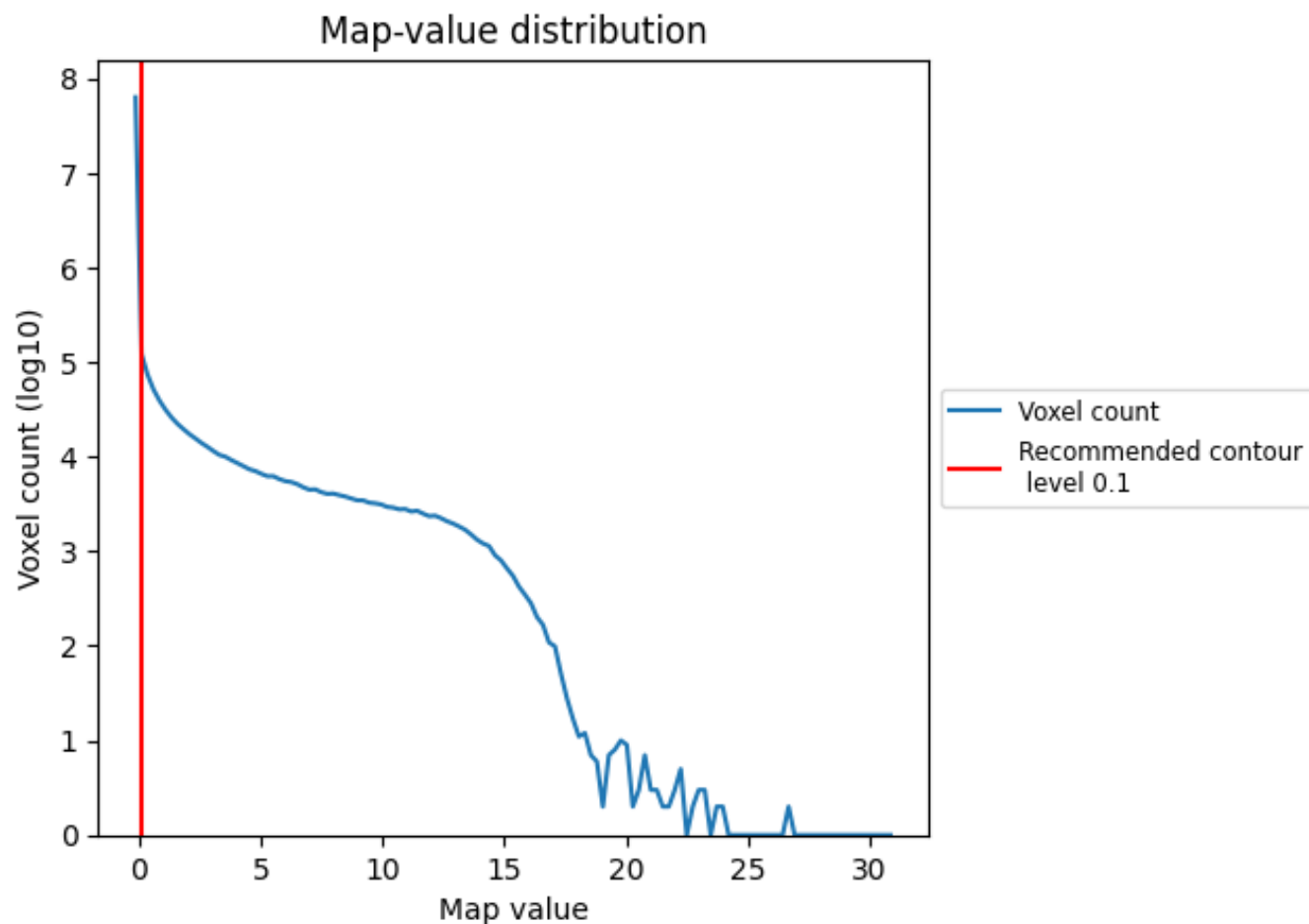
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

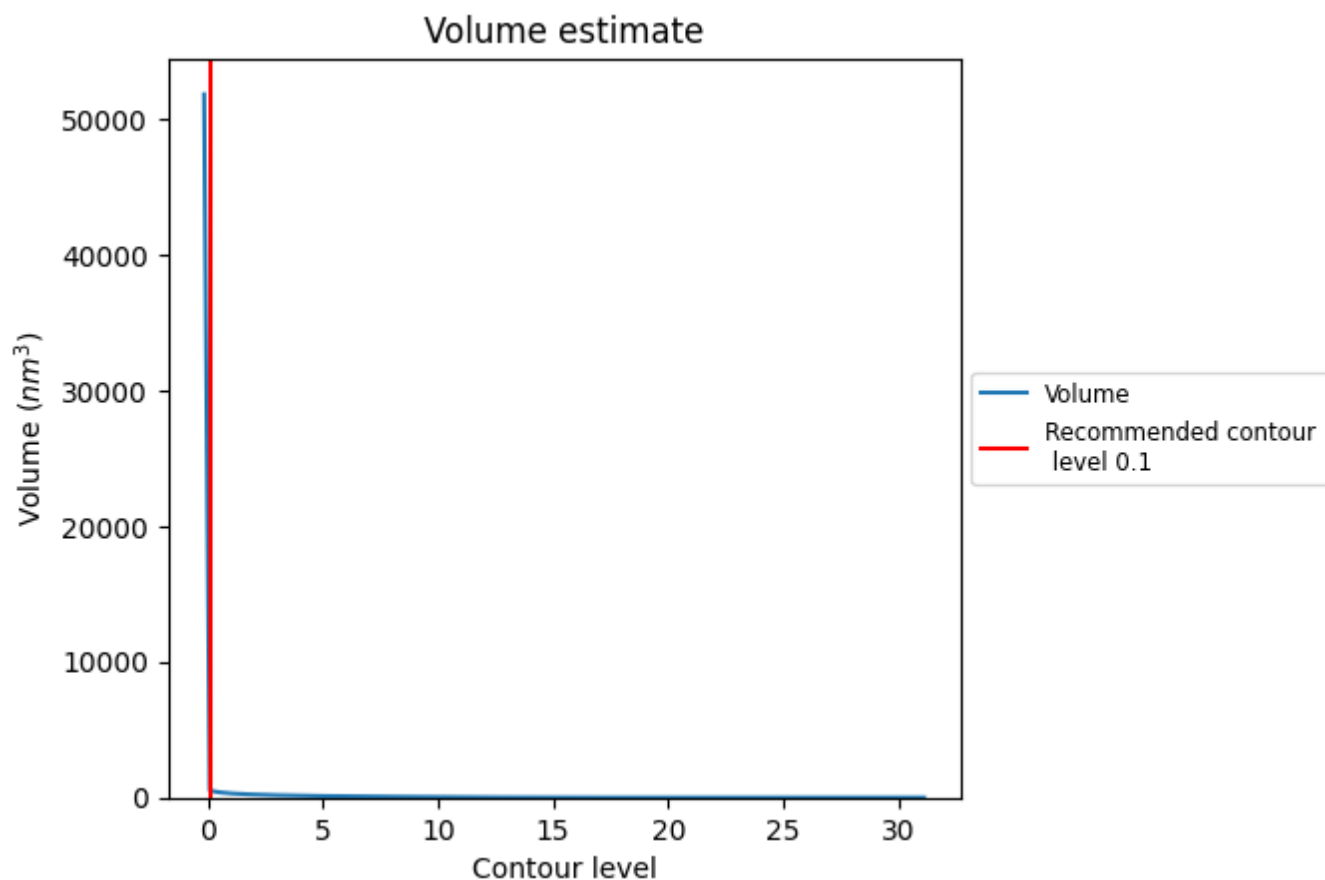
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

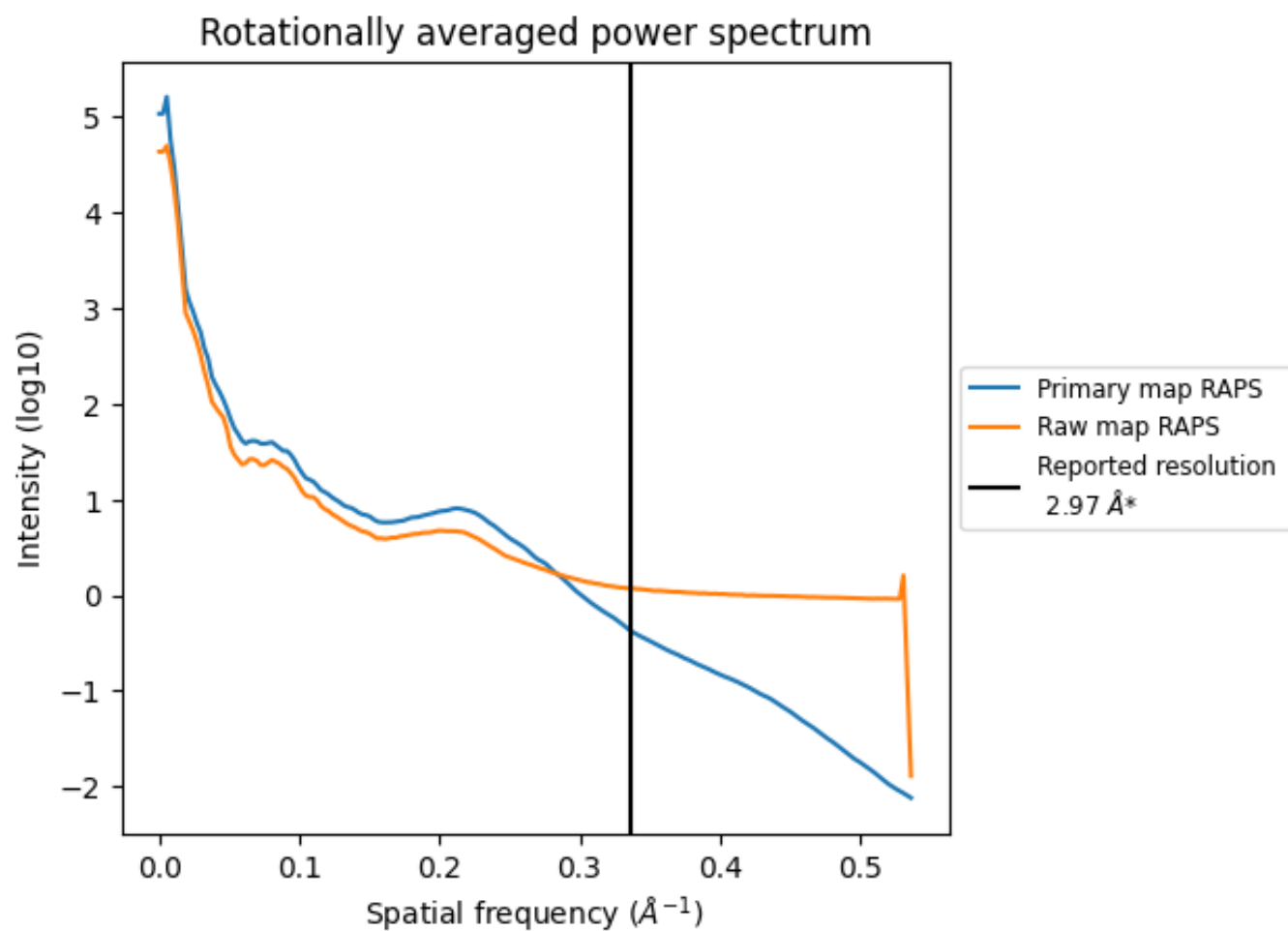
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 529 nm<sup>3</sup>; this corresponds to an approximate mass of 478 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 ⓘ

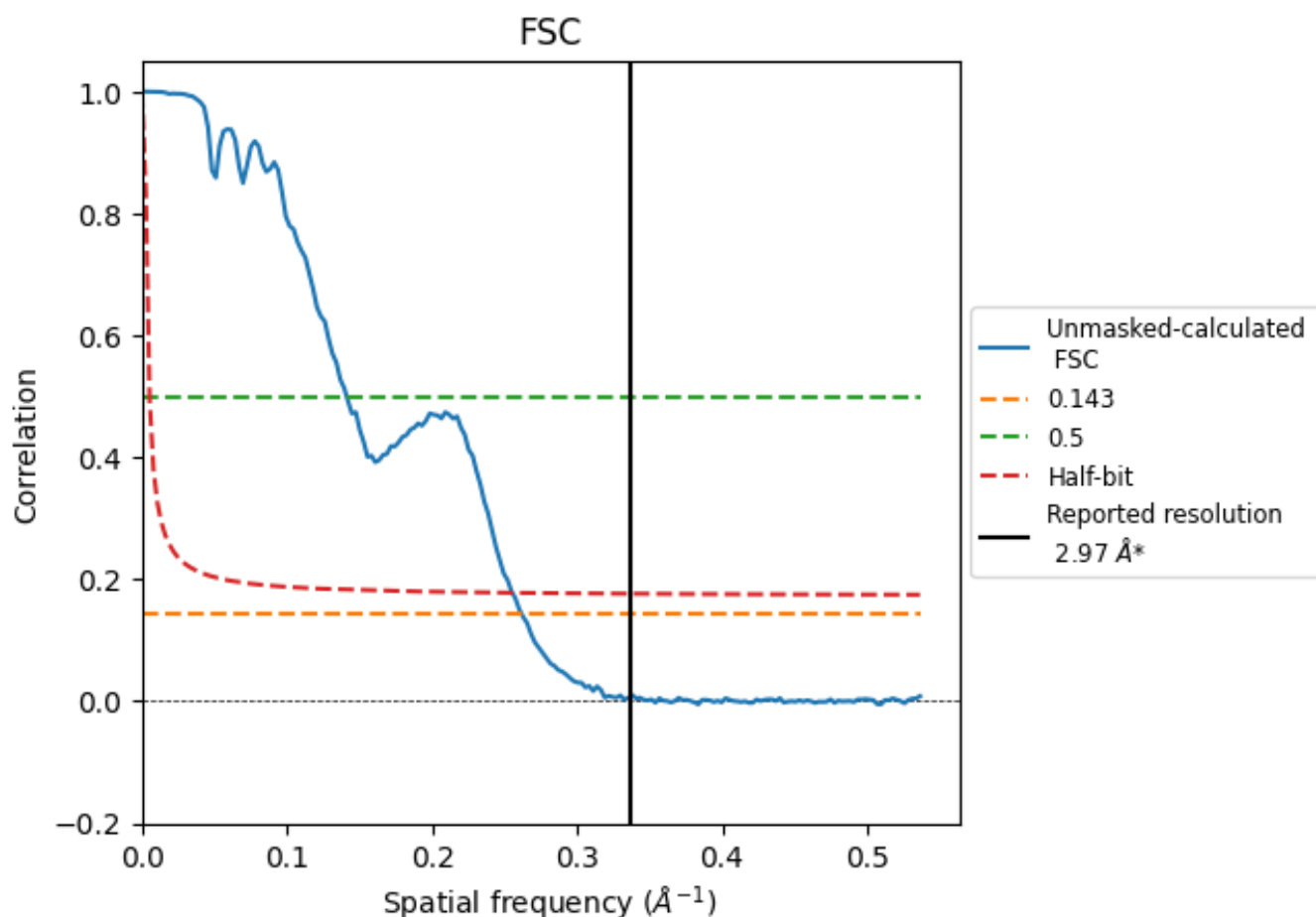


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 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 0.337 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

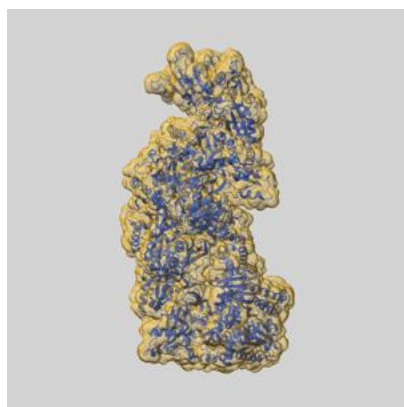
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.82	7.09	3.92

\*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 3.82 differs from the reported value 2.97 by more than 10 %

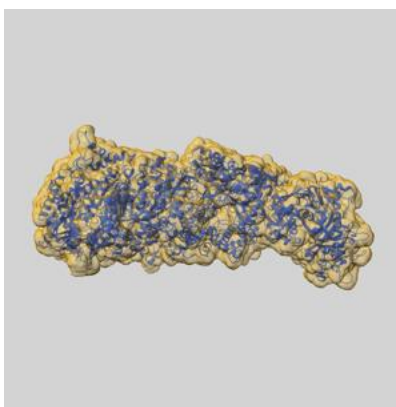
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63293 and PDB model 9LQ5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

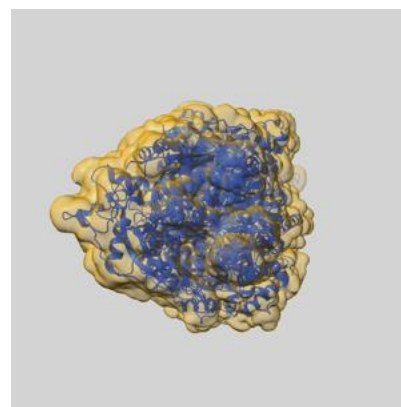
### 9.1 Map-model overlay [i](#)



X



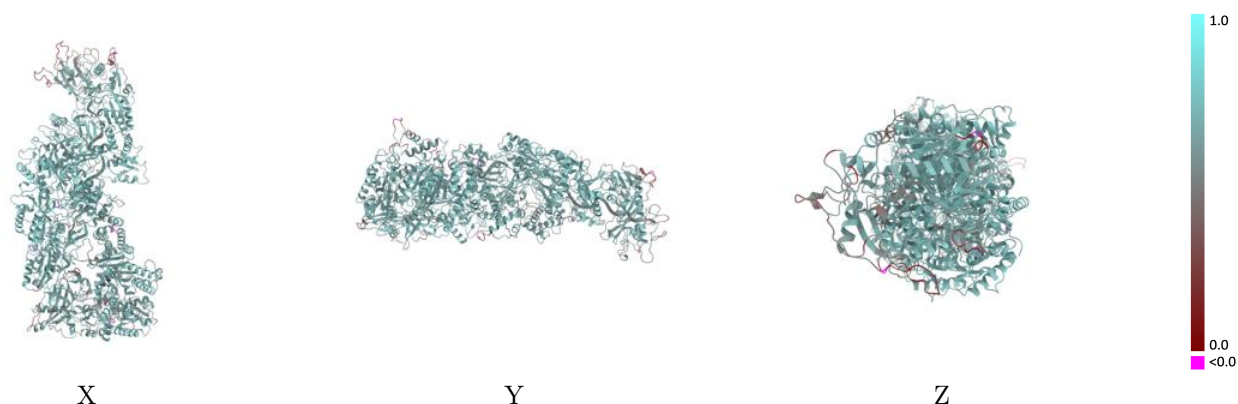
Y



Z

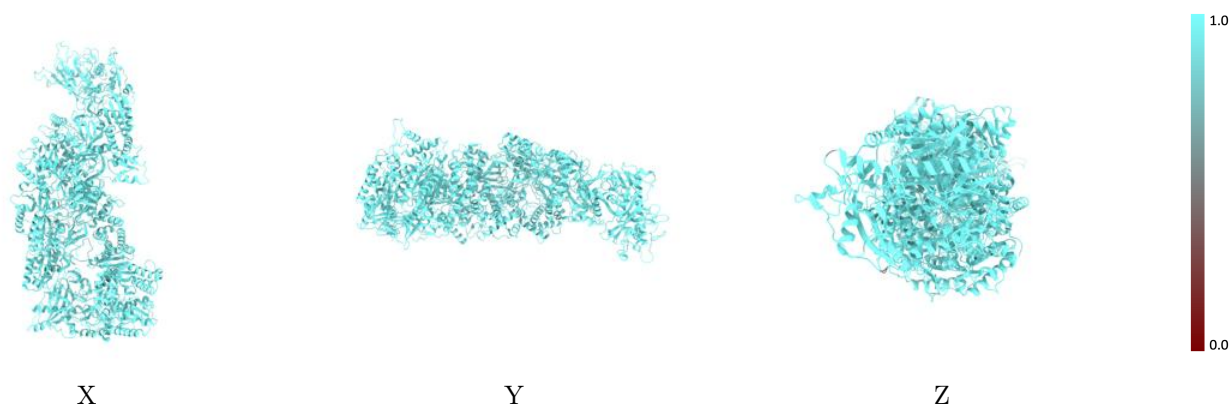
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

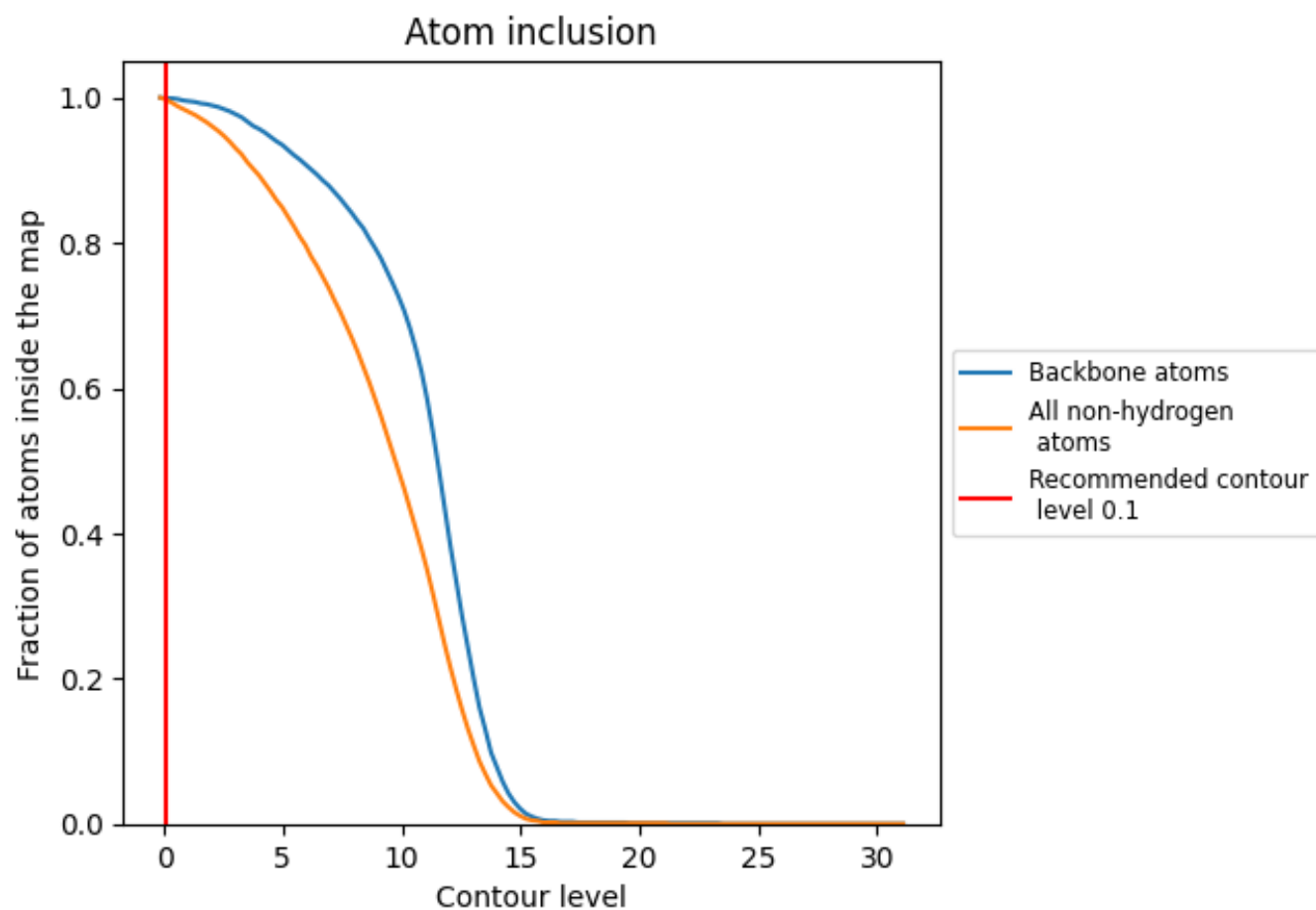
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.1).



## 9.4 Atom inclusion ⓘ



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9970	<div><div></div></div> 0.6220
A	<div><div></div></div> 0.9910	<div><div></div></div> 0.5630
B	<div><div></div></div> 0.9970	<div><div></div></div> 0.6210
C	<div><div></div></div> 0.9970	<div><div></div></div> 0.5970
D	<div><div></div></div> 0.9980	<div><div></div></div> 0.6560
E	<div><div></div></div> 0.9990	<div><div></div></div> 0.6740
F	<div><div></div></div> 0.9970	<div><div></div></div> 0.6730
G	<div><div></div></div> 0.9970	<div><div></div></div> 0.5870
H	<div><div></div></div> 0.9960	<div><div></div></div> 0.6060
I	<div><div></div></div> 0.9980	<div><div></div></div> 0.6610
J	<div><div></div></div> 1.0000	<div><div></div></div> 0.5800

1.0

0.0

<0.0