



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:53 PM UTC

PDB ID : 9L7C / pdb_00009l7c
EMDB ID : EMD-62872
Title : Type III-B CRISPR-Cas effector from *Archaeoglobus fulgidus* (Form 1)
Authors : Ouchi, R.; Numata, T.
Deposited on : 2024-12-26
Resolution : 2.97 Å(reported)
Based on initial model : .

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 EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

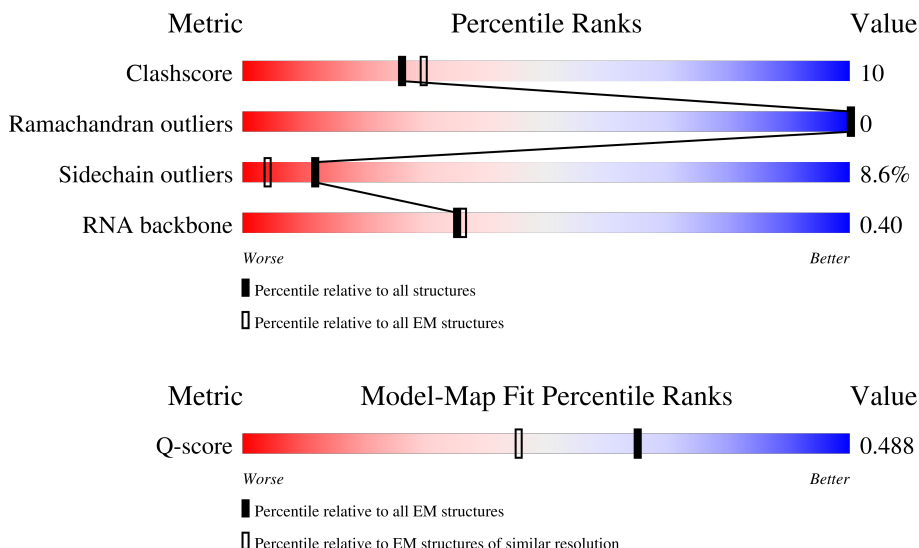
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
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 ≥ 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	369	
1	E	369	
1	F	369	

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Mol	Chain	Length	Quality of chain
2	G	155	74%23%..
2	H	155	64%30%5%.
3	I	343	5%68%28%..
4	A	329	22%76%22%..
5	B	1004	70%25%..
6	C	341	65%28%.6%
7	V	45	20%31%29%7%33%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 25745 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 Type III-B CRISPR module RAMP protein Cmr4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	337	Total	C	N	O	S	0	0
			2503	1618	431	452	2		
1	D	346	Total	C	N	O	S	0	0
			2620	1694	441	483	2		
1	E	344	Total	C	N	O		0	0
			2566	1658	439	469			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	MET	-	initiating methionine	UNP O28416
F	-12	GLY	-	expression tag	UNP O28416
F	-11	SER	-	expression tag	UNP O28416
F	-10	SER	-	expression tag	UNP O28416
F	-9	HIS	-	expression tag	UNP O28416
F	-8	HIS	-	expression tag	UNP O28416
F	-7	HIS	-	expression tag	UNP O28416
F	-6	HIS	-	expression tag	UNP O28416
F	-5	HIS	-	expression tag	UNP O28416
F	-4	HIS	-	expression tag	UNP O28416
F	-3	SER	-	expression tag	UNP O28416
F	-2	GLN	-	expression tag	UNP O28416
F	-1	ASP	-	expression tag	UNP O28416
F	0	PRO	-	expression tag	UNP O28416
F	31	ALA	ASP	engineered mutation	UNP O28416
D	-13	MET	-	initiating methionine	UNP O28416
D	-12	GLY	-	expression tag	UNP O28416
D	-11	SER	-	expression tag	UNP O28416
D	-10	SER	-	expression tag	UNP O28416
D	-9	HIS	-	expression tag	UNP O28416
D	-8	HIS	-	expression tag	UNP O28416
D	-7	HIS	-	expression tag	UNP O28416
D	-6	HIS	-	expression tag	UNP O28416
D	-5	HIS	-	expression tag	UNP O28416

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP O28416
D	-3	SER	-	expression tag	UNP O28416
D	-2	GLN	-	expression tag	UNP O28416
D	-1	ASP	-	expression tag	UNP O28416
D	0	PRO	-	expression tag	UNP O28416
D	31	ALA	ASP	engineered mutation	UNP O28416
E	-13	MET	-	initiating methionine	UNP O28416
E	-12	GLY	-	expression tag	UNP O28416
E	-11	SER	-	expression tag	UNP O28416
E	-10	SER	-	expression tag	UNP O28416
E	-9	HIS	-	expression tag	UNP O28416
E	-8	HIS	-	expression tag	UNP O28416
E	-7	HIS	-	expression tag	UNP O28416
E	-6	HIS	-	expression tag	UNP O28416
E	-5	HIS	-	expression tag	UNP O28416
E	-4	HIS	-	expression tag	UNP O28416
E	-3	SER	-	expression tag	UNP O28416
E	-2	GLN	-	expression tag	UNP O28416
E	-1	ASP	-	expression tag	UNP O28416
E	0	PRO	-	expression tag	UNP O28416
E	31	ALA	ASP	engineered mutation	UNP O28416

- Molecule 2 is a protein called CRISPR system Cmr subunit Cmr5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	153	Total	C	N	O	S	0	0
			1188	766	191	229	2		
2	G	153	Total	C	N	O	S	0	0
			1200	771	191	236	2		

- Molecule 3 is a protein called Type III-B CRISPR module RAMP protein Cmr6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	336	Total	C	N	O	S	0	0
			2583	1685	430	465	3		

- Molecule 4 is a protein called Cmr1 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	325	Total	C	N	O	S	0	0
			2245	1458	385	395	7		

- Molecule 5 is a protein called GGDEF domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	976	Total	C	N	O	S	0	0
			7612	4915	1302	1378	17		

- Molecule 6 is a protein called Type III-B CRISPR module-associated protein Cmr3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	322	Total	C	N	O	S	0	0
			2526	1649	426	443	8		

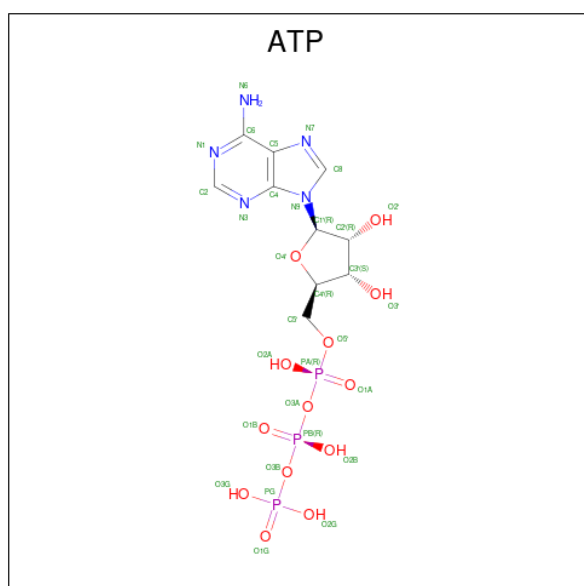
- Molecule 7 is a RNA chain called Pf7.01 crRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	30	Total	C	N	O	P	0	0
			638	287	116	207	28		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

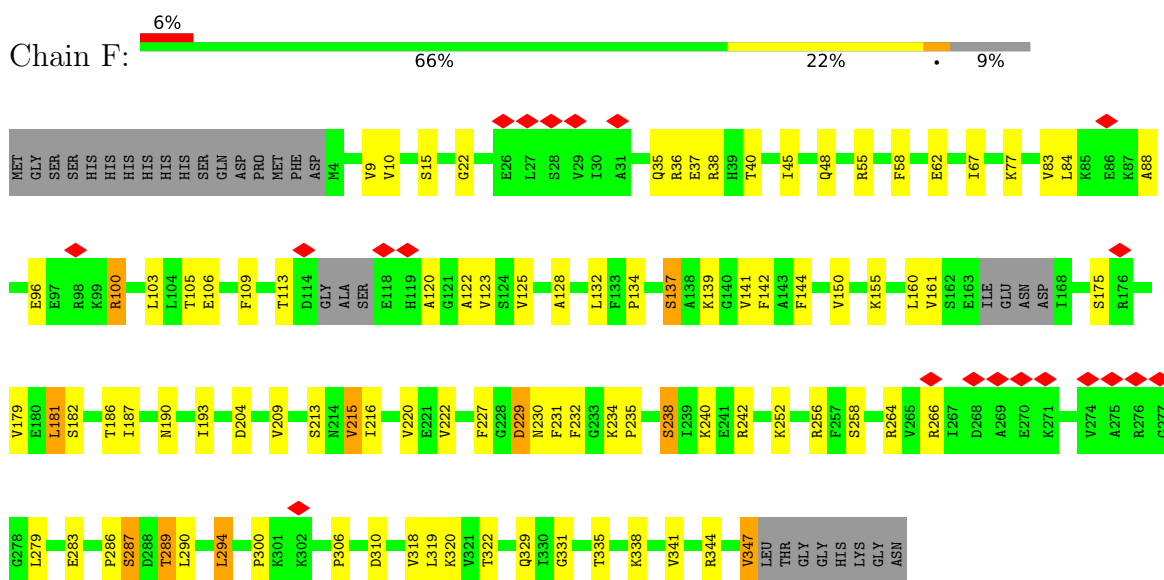
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	B	1	Total	Zn	0
			1	1	

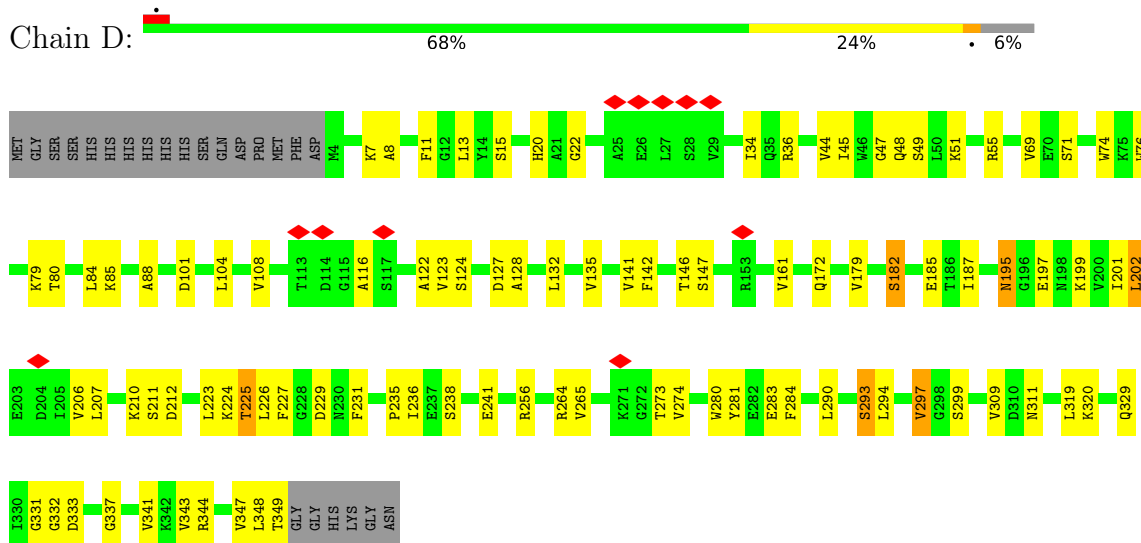
3 Residue-property plots

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.

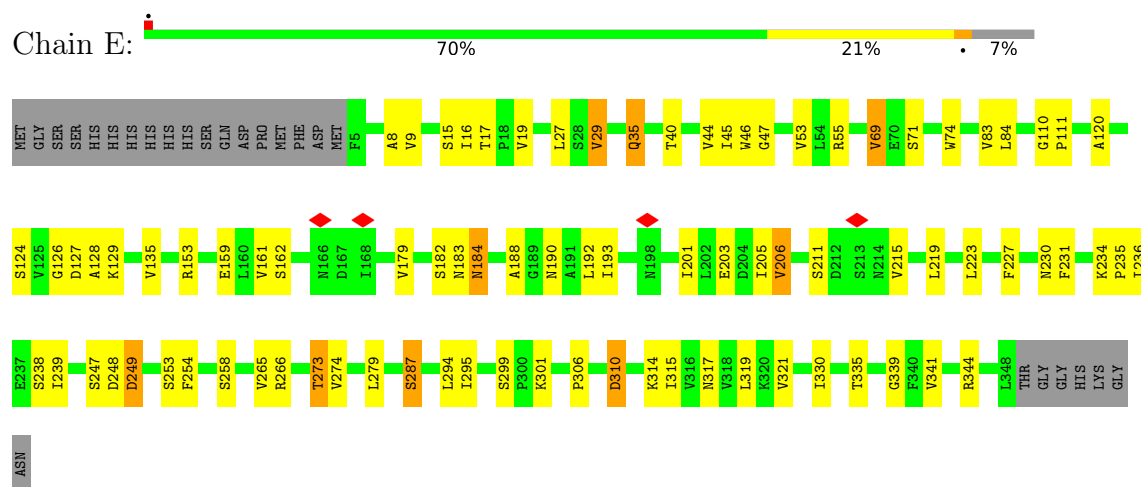
- Molecule 1: Type III-B CRISPR module RAMP protein Cmr4



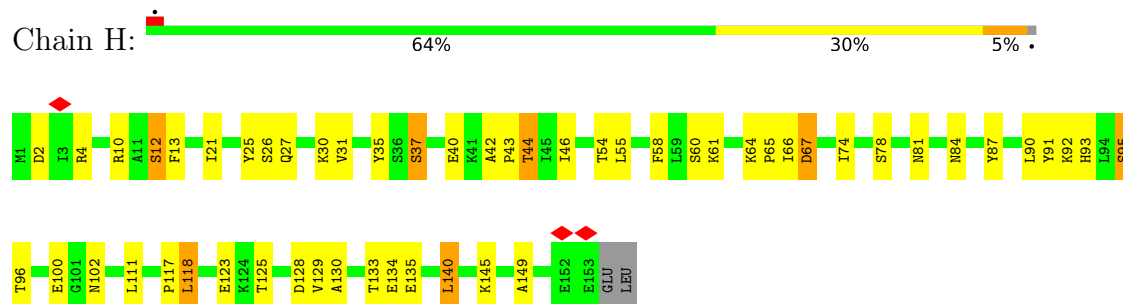
- Molecule 1: Type III-B CRISPR module RAMP protein Cmr4



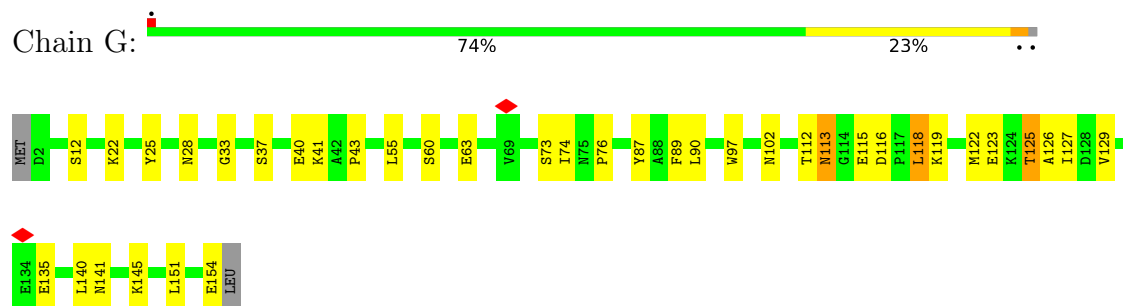
- Molecule 1: Type III-B CRISPR module RAMP protein Cmr4



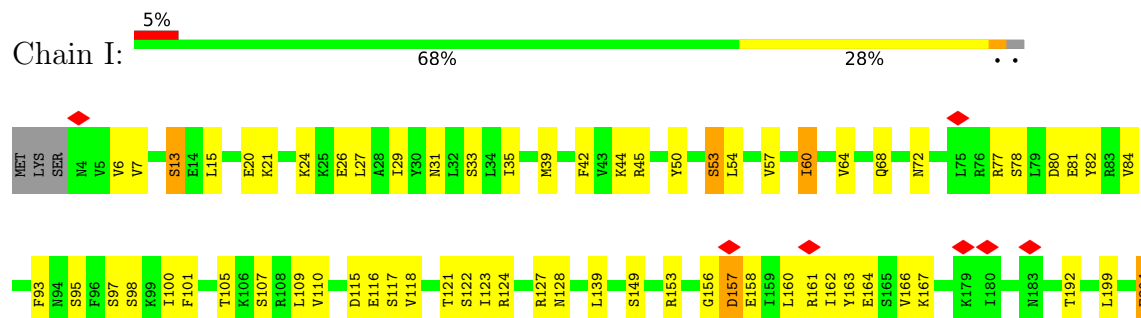
• Molecule 2: CRISPR system Cmr subunit Cmr5

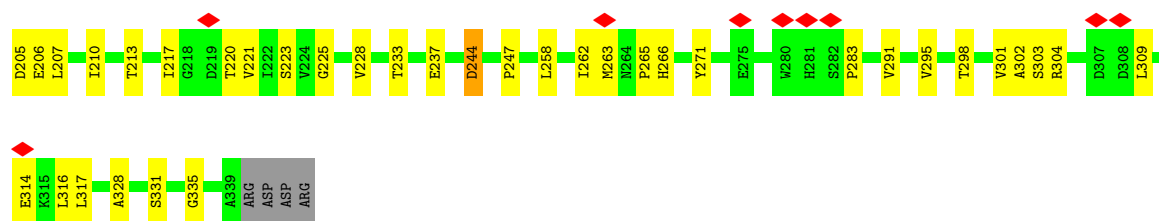


• Molecule 2: CRISPR system Cmr subunit Cmr5

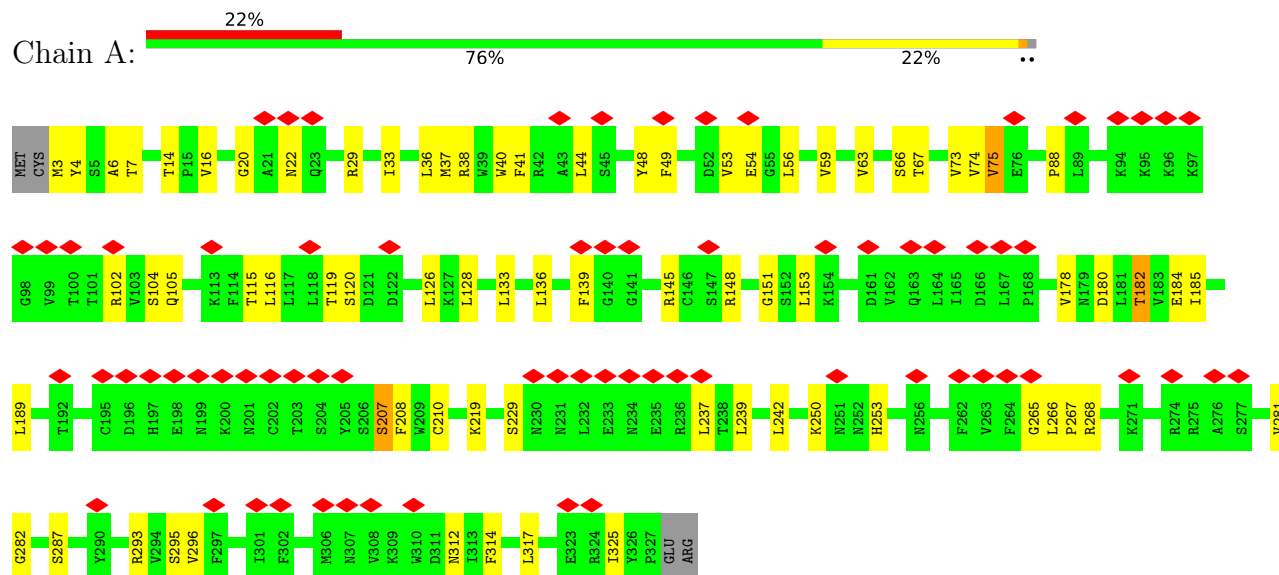


• Molecule 3: Type III-B CRISPR module RAMP protein Cmr6

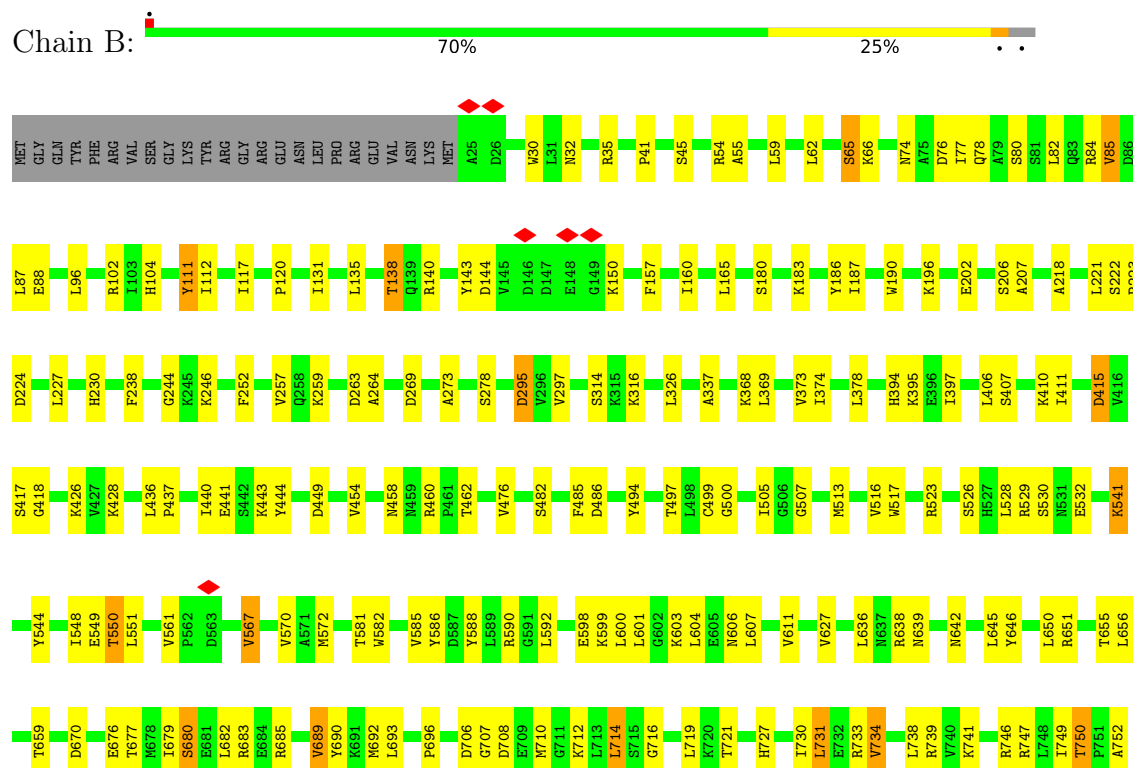


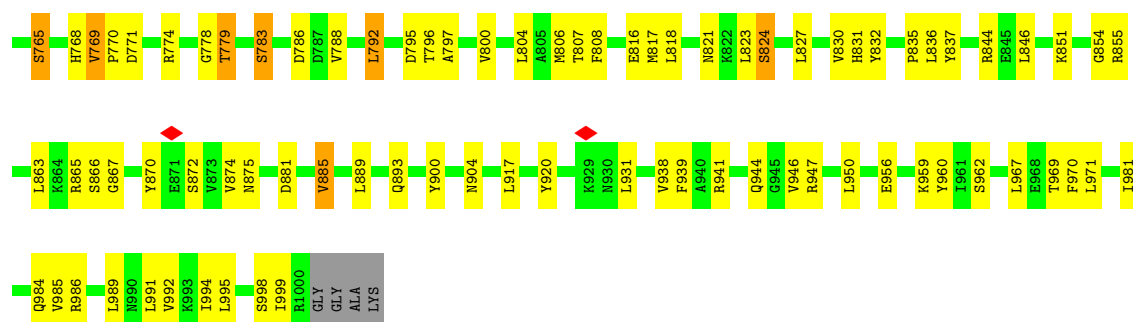


• Molecule 4: Cmr1 C-terminal domain-containing protein



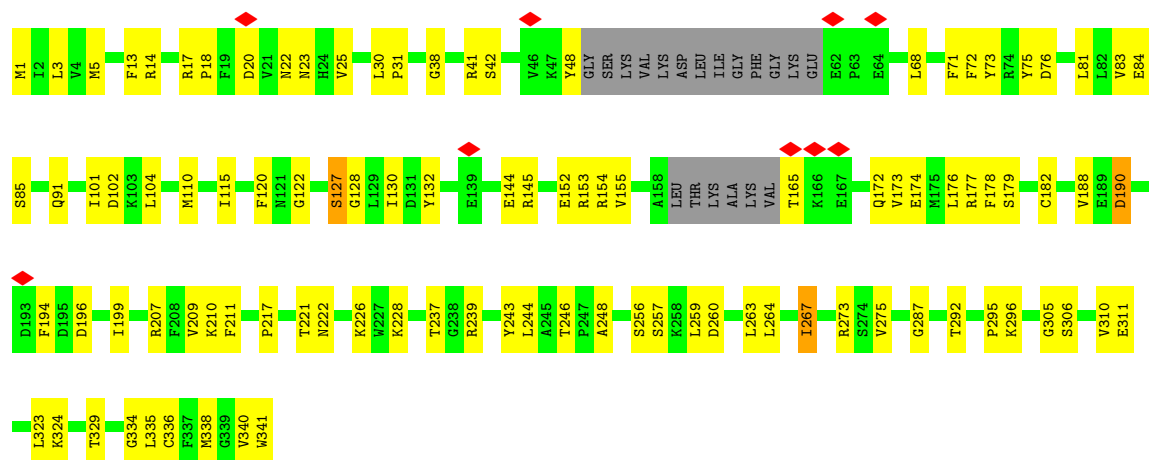
• Molecule 5: GGDEF domain-containing protein





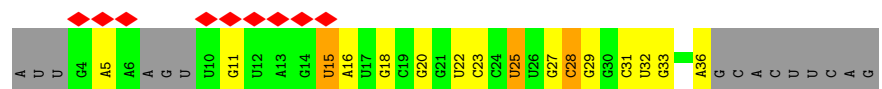
• Molecule 6: Type III-B CRISPR module-associated protein Cmr3

Chain C: 65% 28% 6%



• Molecule 7: Pf7.01 crRNA

Chain V: 20% 31% 29% 7% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80152	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.986	Depositor
Minimum map value	-0.423	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.214	Depositor
Map size (Å)	300.8, 300.8, 300.8	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.752, 0.752, 0.752	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, MG

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	0.09	0/2665	0.26	0/3613
1	E	0.09	0/2609	0.25	0/3542
1	F	0.10	0/2544	0.27	0/3450
2	G	0.14	0/1223	0.39	0/1648
2	H	0.13	0/1211	0.30	0/1634
3	I	0.10	0/2646	0.26	0/3590
4	A	0.10	0/2301	0.27	0/3151
5	B	0.11	0/7779	0.29	0/10539
6	C	0.11	0/2588	0.27	0/3500
7	V	0.08	0/713	0.15	0/1110
All	All	0.10	0/26279	0.28	0/35777

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

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	2620	0	2631	55	0
1	E	2566	0	2552	46	0
1	F	2503	0	2472	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	1200	0	1183	24	0
2	H	1188	0	1176	34	0
3	I	2583	0	2495	57	0
4	A	2245	0	1894	44	0
5	B	7612	0	7503	166	0
6	C	2526	0	2482	63	0
7	V	638	0	323	20	0
8	B	1	0	0	0	0
9	B	62	0	24	3	0
10	B	1	0	0	0	0
All	All	25745	0	24735	510	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 (510) 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)
5:B:112:ILE:HG12	5:B:730:ILE:HG22	1.63	0.80
2:H:46:ILE:HG12	2:H:54:THR:HG21	1.64	0.78
5:B:437:PRO:HD2	5:B:440:ILE:HD11	1.66	0.76
1:F:45:ILE:HB	1:F:128:ALA:HB3	1.67	0.76
5:B:854:GLY:O	5:B:947:ARG:NH1	2.25	0.70
4:A:16:VAL:HG22	4:A:151:GLY:HA2	1.73	0.69
2:H:43:PRO:HG3	2:H:140:LEU:HB3	1.75	0.69
1:F:286:PRO:O	1:F:289:THR:OG1	2.09	0.69
2:H:111:LEU:HD11	2:H:135:GLU:HG2	1.74	0.69
5:B:443:LYS:HD3	5:B:746:ARG:HH12	1.57	0.68
1:E:29:VAL:HG13	2:G:141:ASN:HB2	1.76	0.68
1:E:258:SER:OG	3:I:127:ARG:NH1	2.27	0.68
5:B:716:GLY:HA2	5:B:719:LEU:HD12	1.76	0.68
1:E:231:PHE:HB2	1:E:236:ILE:HG13	1.74	0.67
5:B:494:TYR:HB2	5:B:513:MET:HE1	1.76	0.67
5:B:257:VAL:HB	9:B:1103:ATP:H5'1	1.77	0.66
5:B:494:TYR:HA	6:C:295:PRO:HG2	1.75	0.66
2:G:112:THR:O	2:G:113:ASN:ND2	2.28	0.66
2:H:12:SER:OG	2:H:102:ASN:ND2	2.29	0.66
5:B:394:HIS:HE1	5:B:505:ILE:HA	1.61	0.65
5:B:967:LEU:HA	5:B:970:PHE:HB3	1.79	0.65
6:C:273:ARG:HB2	6:C:311:GLU:HB2	1.79	0.64
6:C:84:GLU:O	6:C:243:TYR:OH	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:PRO:HG2	1:F:238:SER:HB3	1.79	0.64
1:E:188:ALA:HB1	1:E:192:LEU:HD12	1.78	0.64
1:F:48:GLN:OE1	6:C:207:ARG:NH1	2.30	0.64
5:B:104:HIS:CD2	5:B:111:TYR:HB3	2.33	0.63
1:E:230:ASN:OD1	1:E:344:ARG:NH2	2.31	0.63
5:B:830:VAL:HG23	5:B:863:LEU:HB3	1.81	0.62
1:F:230:ASN:O	1:F:344:ARG:NH2	2.32	0.62
5:B:867:GLY:HA3	6:C:155:VAL:HG21	1.81	0.62
3:I:244:ASP:N	3:I:244:ASP:OD1	2.31	0.62
1:D:132:LEU:HB2	1:D:290:LEU:HB3	1.82	0.61
3:I:29:ILE:O	3:I:77:ARG:NH1	2.33	0.61
5:B:572:MET:HG2	5:B:582:TRP:HB3	1.81	0.61
5:B:808:PHE:HE2	5:B:821:ASN:HB3	1.66	0.61
6:C:25:VAL:HG12	6:C:172:GLN:HB2	1.82	0.61
4:A:36:LEU:HB3	4:A:136:LEU:HD11	1.81	0.61
1:F:48:GLN:HE22	6:C:154:ARG:HH11	1.48	0.60
5:B:590:ARG:O	5:B:638:ARG:NH2	2.33	0.60
2:G:122:MET:HE2	2:G:122:MET:HA	1.83	0.60
1:F:155:LYS:HE2	1:F:175:SER:HA	1.83	0.60
4:A:265:GLY:HA3	7:V:36:A:H5'	1.82	0.60
5:B:778:GLY:HA3	5:B:792:LEU:HD23	1.83	0.60
5:B:572:MET:SD	5:B:642:ASN:ND2	2.75	0.60
1:F:55:ARG:NH1	1:F:109:PHE:O	2.35	0.60
5:B:645:LEU:O	5:B:690:TYR:OH	2.20	0.60
5:B:529:ARG:HB2	5:B:532:GLU:HG3	1.82	0.60
1:D:332:GLY:HA3	7:V:16:A:H5'	1.84	0.59
3:I:139:LEU:HD23	3:I:317:LEU:HD21	1.83	0.59
1:E:69:VAL:HG11	1:E:74:TRP:HE3	1.67	0.59
1:D:161:VAL:HG11	1:D:348:LEU:HD13	1.83	0.59
2:H:95:SER:HA	2:H:117:PRO:HG2	1.83	0.59
1:D:69:VAL:HG21	1:D:74:TRP:HE3	1.66	0.59
3:I:156:GLY:HA2	3:I:192:THR:HG21	1.84	0.59
2:H:91:TYR:O	2:H:95:SER:OG	2.20	0.58
1:F:15:SER:HA	1:F:341:VAL:HG12	1.85	0.58
1:E:45:ILE:HB	1:E:128:ALA:HB3	1.86	0.58
6:C:244:LEU:HD12	6:C:306:SER:HB2	1.86	0.58
1:E:249:ASP:OD1	1:E:249:ASP:N	2.36	0.58
5:B:186:TYR:OH	5:B:295:ASP:OD2	2.20	0.57
5:B:707:GLY:O	5:B:851:LYS:NZ	2.36	0.57
6:C:152:GLU:OE1	6:C:177:ARG:NE	2.36	0.57
5:B:80:SER:CB	5:B:752:ALA:H	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:98:SER:HB3	3:I:302:ALA:HB2	1.85	0.57
5:B:224:ASP:OD2	5:B:747:ARG:NH1	2.37	0.57
5:B:651:ARG:HD3	5:B:655:THR:HG21	1.86	0.57
5:B:394:HIS:CE1	5:B:505:ILE:HA	2.39	0.57
5:B:600:LEU:HD13	5:B:693:LEU:HD21	1.86	0.57
1:E:273:THR:OG1	1:E:274:VAL:N	2.36	0.57
2:H:149:ALA:HB2	5:B:920:TYR:HB2	1.87	0.57
3:I:42:PHE:HB3	3:I:50:TYR:HB3	1.87	0.57
5:B:995:LEU:O	5:B:999:ILE:HG12	2.04	0.57
4:A:33:ILE:HD11	4:A:75:VAL:HG21	1.87	0.57
1:E:8:ALA:HB3	1:E:161:VAL:HG23	1.87	0.56
2:H:130:ALA:O	2:H:134:GLU:HG3	2.05	0.56
4:A:145:ARG:NH2	7:V:36:A:O5'	2.38	0.56
5:B:708:ASP:OD1	5:B:824:SER:OG	2.22	0.56
1:F:181:LEU:HD21	1:F:186:THR:HA	1.88	0.56
5:B:202:GLU:HB2	5:B:207:ALA:HA	1.86	0.56
5:B:874:VAL:HG12	5:B:946:VAL:HG22	1.88	0.56
5:B:415:ASP:OD1	5:B:415:ASP:N	2.33	0.56
1:D:116:ALA:O	7:V:11:G:O2'	2.21	0.56
1:E:184:ASN:OD1	1:E:184:ASN:N	2.38	0.56
3:I:7:VAL:HG21	3:I:60:ILE:HG12	1.88	0.56
5:B:967:LEU:O	5:B:971:LEU:N	2.36	0.56
4:A:33:ILE:O	4:A:37:MET:HG3	2.07	0.55
1:E:227:PHE:O	1:E:344:ARG:NH1	2.39	0.55
2:H:55:LEU:HB3	2:H:118:LEU:HD22	1.88	0.55
3:I:266:HIS:CE1	3:I:283:PRO:HG3	2.40	0.55
6:C:237:THR:HG23	6:C:239:ARG:H	1.71	0.55
1:F:329:GLN:NE2	1:F:331:GLY:O	2.39	0.55
3:I:266:HIS:CD2	7:V:32:U:H2'	2.41	0.55
5:B:458:ASN:OD1	5:B:458:ASN:N	2.39	0.55
3:I:35:ILE:HA	3:I:39:MET:HG3	1.88	0.55
4:A:4:TYR:HB2	4:A:126:LEU:HD13	1.88	0.55
2:H:61:LYS:O	2:H:84:ASN:ND2	2.39	0.55
6:C:248:ALA:HB2	6:C:334:GLY:HA2	1.89	0.55
3:I:157:ASP:HA	3:I:160:LEU:HD12	1.88	0.55
6:C:190:ASP:N	6:C:190:ASP:OD1	2.39	0.55
1:F:227:PHE:O	1:F:344:ARG:NH2	2.40	0.54
1:E:9:VAL:O	1:E:295:ILE:N	2.33	0.54
3:I:115:ASP:OD1	3:I:124:ARG:NH1	2.40	0.54
5:B:881:ASP:O	5:B:885:VAL:HG12	2.07	0.54
3:I:164:GLU:HA	3:I:167:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:607:LEU:HD22	5:B:689:VAL:HG21	1.90	0.54
5:B:650:LEU:HD22	5:B:656:LEU:HD12	1.89	0.54
1:E:314:LYS:HA	1:E:317:ASN:HD21	1.73	0.54
3:I:93:PHE:HB3	3:I:100:ILE:HD11	1.89	0.54
1:D:76:TRP:O	1:D:80:THR:OG1	2.25	0.54
5:B:54:ARG:HG2	5:B:165:LEU:HD11	1.89	0.54
5:B:513:MET:HG2	5:B:517:TRP:HD1	1.73	0.54
5:B:939:PHE:HZ	5:B:985:VAL:HG23	1.73	0.54
1:D:36:ARG:NH2	1:D:283:GLU:OE2	2.34	0.54
1:E:19:VAL:HA	1:E:339:GLY:HA2	1.90	0.54
3:I:122:SER:OG	3:I:123:ILE:N	2.41	0.54
1:F:137:SER:OG	1:F:139:LYS:O	2.24	0.54
1:D:13:LEU:HD23	1:D:343:VAL:HG22	1.90	0.54
1:D:195:ASN:OD1	1:D:195:ASN:N	2.36	0.54
5:B:599:LYS:O	5:B:603:LYS:NZ	2.39	0.54
5:B:900:TYR:O	5:B:904:ASN:ND2	2.40	0.54
1:F:335:THR:OG1	1:D:51:LYS:NZ	2.33	0.53
2:H:35:TYR:OH	2:H:93:HIS:ND1	2.37	0.53
1:D:311:ASN:OD1	1:D:311:ASN:N	2.41	0.53
2:H:37:SER:O	2:H:40:GLU:HG3	2.09	0.53
1:D:123:VAL:HG11	1:D:319:LEU:HD11	1.90	0.53
5:B:436:LEU:HA	6:C:110:MET:HE1	1.88	0.53
4:A:207:SER:OG	4:A:208:PHE:N	2.41	0.53
1:F:204:ASP:CG	2:H:10:ARG:HH22	2.16	0.53
2:G:113:ASN:ND2	2:G:113:ASN:C	2.66	0.53
5:B:944:GLN:O	5:B:984:GLN:NE2	2.41	0.53
1:D:329:GLN:NE2	1:D:331:GLY:O	2.42	0.53
4:A:40:TRP:CE2	4:A:136:LEU:HA	2.44	0.53
5:B:765:SER:O	5:B:783:SER:OG	2.27	0.53
5:B:835:PRO:HG2	6:C:25:VAL:HG22	1.91	0.53
5:B:844:ARG:NH2	9:B:1103:ATP:O3'	2.42	0.52
5:B:440:ILE:HD12	5:B:441:GLU:N	2.24	0.52
5:B:190:TRP:NE1	5:B:295:ASP:HB3	2.25	0.52
5:B:523:ARG:O	5:B:523:ARG:NH1	2.42	0.52
1:D:235:PRO:O	1:D:238:SER:OG	2.25	0.52
1:E:111:PRO:O	7:V:18:G:O2'	2.26	0.52
5:B:41:PRO:HD3	5:B:55:ALA:HB2	1.91	0.52
1:F:84:LEU:HB3	1:F:88:ALA:HB2	1.90	0.52
1:F:338:LYS:NZ	1:D:48:GLN:OE1	2.42	0.52
2:G:41:LYS:NZ	2:G:87:TYR:OH	2.41	0.52
1:D:256:ARG:HH11	1:D:256:ARG:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:303:SER:OG	3:I:304:ARG:N	2.42	0.52
5:B:117:ILE:HA	5:B:223:PRO:HB2	1.91	0.52
6:C:73:TYR:HE2	6:C:75:TYR:HB2	1.75	0.52
1:E:40:THR:HG21	1:E:153:ARG:HH22	1.75	0.52
4:A:33:ILE:HD13	4:A:116:LEU:HD11	1.92	0.52
1:D:8:ALA:HB3	1:D:161:VAL:HG13	1.91	0.52
1:D:293:SER:OG	1:D:294:LEU:N	2.42	0.52
1:D:337:GLY:HA3	1:E:126:GLY:HA2	1.92	0.52
1:F:229:ASP:OD1	1:F:229:ASP:N	2.40	0.51
1:E:235:PRO:O	1:E:238:SER:OG	2.25	0.51
3:I:101:PHE:HZ	3:I:317:LEU:HD23	1.75	0.51
6:C:81:LEU:HD11	6:C:217:PRO:HG2	1.91	0.51
1:F:134:PRO:HG3	1:F:287:SER:O	2.10	0.51
5:B:144:ASP:O	5:B:150:LYS:NZ	2.33	0.51
5:B:986:ARG:HG3	5:B:986:ARG:HH11	1.74	0.51
1:E:83:VAL:HG21	1:E:306:PRO:HG3	1.93	0.51
3:I:271:TYR:OH	4:A:38:ARG:NH1	2.43	0.51
1:F:256:ARG:HH11	1:F:256:ARG:HB3	1.74	0.51
5:B:138:THR:OG1	5:B:140:ARG:O	2.28	0.51
1:D:49:SER:OG	7:V:15:U:OP1	2.28	0.51
1:D:108:VAL:O	1:D:122:ALA:N	2.41	0.51
1:D:146:THR:OG1	1:D:147:SER:N	2.44	0.51
1:E:266:ARG:HB2	7:V:25:U:H1'	1.92	0.51
1:F:100:ARG:NH1	1:F:106:GLU:OE2	2.44	0.51
2:H:2:ASP:OD1	2:H:4:ARG:N	2.43	0.51
1:E:15:SER:HA	1:E:341:VAL:HG12	1.93	0.51
3:I:31:ASN:ND2	3:I:128:ASN:O	2.42	0.51
5:B:418:GLY:O	5:B:460:ARG:NH2	2.44	0.51
4:A:44:LEU:HD21	4:A:185:ILE:HG21	1.92	0.50
6:C:128:GLY:O	6:C:132:TYR:N	2.34	0.50
1:D:197:GLU:HB3	1:D:199:LYS:HG3	1.93	0.50
4:A:148:ARG:NH1	7:V:36:A:O3'	2.42	0.50
5:B:246:LYS:HB2	5:B:410:LYS:HE2	1.93	0.50
1:D:201:ILE:HG12	1:D:206:VAL:HG22	1.94	0.50
3:I:262:ILE:HG12	7:V:33:G:C8	2.46	0.50
6:C:153:ARG:HA	6:C:174:GLU:HA	1.92	0.50
5:B:32:ASN:HB3	5:B:238:PHE:CZ	2.47	0.50
1:F:120:ALA:HB2	7:V:5:A:H4'	1.93	0.50
1:D:281:TYR:CE2	2:H:44:THR:HG21	2.47	0.50
5:B:721:THR:HA	5:B:746:ARG:HA	1.94	0.50
5:B:851:LYS:O	5:B:855:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:808:PHE:CG	5:B:823:LEU:HD21	2.46	0.50
5:B:273:ALA:HB2	5:B:541:LYS:HD3	1.94	0.50
1:D:123:VAL:HG12	1:D:297:VAL:HB	1.92	0.50
3:I:105:THR:OG1	3:I:295:VAL:N	2.45	0.50
6:C:101:ILE:HG22	6:C:104:LEU:H	1.77	0.50
2:H:145:LYS:HD2	5:B:920:TYR:CE2	2.47	0.49
6:C:246:THR:HG23	6:C:335:LEU:HB3	1.94	0.49
1:E:47:GLY:N	1:E:127:ASP:OD1	2.44	0.49
6:C:155:VAL:HG23	6:C:172:GLN:HG3	1.94	0.49
3:I:217:ILE:HG21	3:I:316:LEU:HA	1.95	0.49
5:B:734:VAL:HG21	5:B:738:LEU:HD11	1.94	0.49
1:F:62:GLU:HA	1:F:67:ILE:HD11	1.94	0.49
4:A:88:PRO:HA	4:A:104:SER:HA	1.95	0.49
1:D:47:GLY:N	1:D:127:ASP:OD1	2.46	0.49
5:B:252:PHE:HB2	5:B:406:LEU:HD12	1.95	0.49
1:D:274:VAL:HG23	7:V:22:U:H1'	1.94	0.49
1:D:141:VAL:HG12	1:D:142:PHE:HD1	1.77	0.49
2:H:58:PHE:HD1	2:H:87:TYR:HD2	1.61	0.49
3:I:199:LEU:HB3	3:I:207:LEU:HD21	1.95	0.49
5:B:244:GLY:O	5:B:246:LYS:NZ	2.39	0.49
1:E:45:ILE:HD13	1:E:330:ILE:HG21	1.95	0.48
5:B:499:CYS:SG	5:B:500:GLY:N	2.85	0.48
5:B:706:ASP:HB3	5:B:851:LYS:HE3	1.95	0.48
1:E:310:ASP:N	1:E:310:ASP:OD1	2.46	0.48
5:B:548:ILE:HA	5:B:551:LEU:HD23	1.96	0.48
5:B:806:MET:HE3	5:B:807:THR:N	2.28	0.48
6:C:30:LEU:HD12	6:C:72:PHE:HZ	1.79	0.48
3:I:204:PHE:HA	3:I:207:LEU:HD23	1.95	0.48
1:D:84:LEU:C	1:D:85:LYS:HD2	2.38	0.48
5:B:588:TYR:CE2	5:B:604:LEU:HB3	2.48	0.48
1:F:125:VAL:O	6:C:207:ARG:NH2	2.40	0.48
2:G:63:GLU:OE2	2:G:63:GLU:HA	2.13	0.48
4:A:266:LEU:O	4:A:268:ARG:N	2.45	0.48
2:H:81:ASN:OD1	2:H:81:ASN:N	2.47	0.48
1:F:36:ARG:NH2	1:F:283:GLU:OE2	2.45	0.48
1:F:213:SER:O	1:F:213:SER:OG	2.32	0.48
1:E:120:ALA:HB3	1:E:301:LYS:HE2	1.96	0.48
5:B:731:LEU:HD13	5:B:739:ARG:HD3	1.96	0.48
6:C:91:GLN:HA	6:C:120:PHE:HB2	1.95	0.48
1:F:134:PRO:HD3	1:F:289:THR:HG23	1.95	0.48
2:H:10:ARG:HH21	2:H:135:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:115:GLU:N	2:G:115:GLU:OE1	2.46	0.48
4:A:66:SER:O	7:V:29:G:O2'	2.31	0.48
1:D:55:ARG:NH2	1:D:101:ASP:OD2	2.47	0.47
1:D:227:PHE:HB3	1:D:344:ARG:HD3	1.96	0.47
4:A:74:VAL:HG23	4:A:119:THR:HB	1.97	0.47
6:C:76:ASP:OD1	6:C:76:ASP:N	2.47	0.47
2:G:25:TYR:HB3	2:G:28:ASN:HB2	1.96	0.47
2:G:116:ASP:OD2	2:G:118:LEU:N	2.36	0.47
5:B:374:ILE:HD11	5:B:505:ILE:HD13	1.96	0.47
6:C:68:LEU:O	6:C:324:LYS:NZ	2.47	0.47
1:D:273:THR:OG1	1:D:274:VAL:N	2.46	0.47
5:B:598:GLU:HA	5:B:601:LEU:HB2	1.96	0.47
5:B:786:ASP:N	5:B:786:ASP:OD1	2.47	0.47
6:C:48:TYR:HE2	6:C:194:PHE:HA	1.79	0.47
1:F:160:LEU:HD21	6:C:210:LYS:HG3	1.96	0.47
1:F:22:GLY:HA3	1:F:35:GLN:HE21	1.78	0.47
1:F:231:PHE:HZ	1:F:290:LEU:HD22	1.79	0.47
1:F:37:GLU:OE1	1:F:40:THR:OG1	2.33	0.47
1:E:16:ILE:O	1:E:287:SER:OG	2.33	0.47
1:E:265:VAL:O	7:V:25:U:O2'	2.32	0.47
5:B:218:ALA:HB2	5:B:227:LEU:HA	1.96	0.47
5:B:679:ILE:HG22	5:B:683:ARG:HH21	1.80	0.47
1:F:58:PHE:CE1	1:F:322:THR:HG21	2.50	0.47
3:I:163:TYR:HB3	3:I:166:VAL:HG22	1.97	0.47
5:B:956:GLU:O	5:B:960:TYR:HD1	1.97	0.47
1:E:55:ARG:NH2	1:E:110:GLY:O	2.48	0.47
5:B:507:GLY:HA2	5:B:513:MET:HB2	1.97	0.47
6:C:239:ARG:HB3	6:C:341:TRP:NE1	2.30	0.47
2:H:64:LYS:HD2	2:H:65:PRO:HD2	1.97	0.47
2:G:97:TRP:NE1	2:G:135:GLU:OE2	2.42	0.47
5:B:611:VAL:HG12	5:B:682:LEU:HD21	1.97	0.47
5:B:676:GLU:O	5:B:680:SER:OG	2.32	0.47
5:B:817:MET:HE3	5:B:817:MET:HB2	1.73	0.47
6:C:323:LEU:HD22	6:C:338:MET:SD	2.55	0.47
4:A:105:GLN:N	4:A:105:GLN:OE1	2.47	0.46
5:B:590:ARG:HH21	5:B:592:LEU:HD12	1.80	0.46
5:B:797:ALA:HB1	5:B:827:LEU:HD11	1.97	0.46
6:C:18:PRO:O	6:C:23:ASN:ND2	2.40	0.46
6:C:85:SER:HB3	6:C:122:GLY:C	2.40	0.46
1:F:220:VAL:HG11	1:F:240:LYS:HE2	1.95	0.46
1:E:19:VAL:HG22	1:E:339:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:586:TYR:CZ	5:B:590:ARG:HD2	2.50	0.46
6:C:130:ILE:HD11	6:C:226:LYS:HB3	1.95	0.46
1:E:35:GLN:HE21	1:E:46:TRP:CD1	2.32	0.46
3:I:68:GLN:O	3:I:72:ASN:ND2	2.49	0.46
5:B:486:ASP:HA	6:C:256:SER:HA	1.97	0.46
5:B:505:ILE:HB	5:B:517:TRP:CZ2	2.51	0.46
6:C:196:ASP:OD1	6:C:196:ASP:N	2.49	0.46
6:C:260:ASP:HB3	6:C:263:LEU:HD12	1.98	0.46
2:G:33:GLY:HA3	2:G:154:GLU:HG2	1.98	0.46
4:A:115:THR:OG1	4:A:116:LEU:N	2.48	0.46
5:B:505:ILE:HB	5:B:517:TRP:HZ2	1.80	0.46
5:B:606:ASN:OD1	5:B:685:ARG:NH1	2.49	0.46
1:F:266:ARG:CZ	1:F:266:ARG:HB3	2.45	0.46
1:D:124:SER:O	1:D:124:SER:OG	2.31	0.46
5:B:769:VAL:HG13	5:B:770:PRO:HD3	1.98	0.46
5:B:792:LEU:HD22	5:B:800:VAL:HG11	1.97	0.46
4:A:102:ARG:NH2	4:A:229:SER:O	2.38	0.46
5:B:875:ASN:OD1	5:B:947:ARG:NE	2.45	0.46
1:D:182:SER:OG	1:D:185:GLU:OE1	2.34	0.46
2:H:96:THR:OG1	2:H:100:GLU:OE1	2.30	0.46
2:G:37:SER:HA	2:G:40:GLU:HG3	1.98	0.46
3:I:80:ASP:O	3:I:84:VAL:HG13	2.16	0.46
5:B:440:ILE:O	5:B:444:TYR:HD2	1.99	0.46
1:D:224:LYS:HD2	1:D:236:ILE:HG21	1.98	0.46
3:I:82:TYR:OH	3:I:247:PRO:O	2.30	0.46
4:A:282:GLY:O	4:A:293:ARG:N	2.43	0.46
5:B:893:GLN:HB3	5:B:931:LEU:HD13	1.98	0.46
5:B:190:TRP:HE1	5:B:295:ASP:HB3	1.81	0.45
6:C:20:ASP:OD1	6:C:20:ASP:N	2.49	0.45
6:C:275:VAL:HG22	6:C:310:VAL:HG12	1.99	0.45
3:I:6:VAL:HB	3:I:44:LYS:HD2	1.98	0.45
4:A:6:ALA:HB2	4:A:126:LEU:HD21	1.98	0.45
4:A:40:TRP:HZ2	4:A:139:PHE:HB2	1.81	0.45
4:A:182:THR:O	4:A:185:ILE:HG13	2.16	0.45
5:B:959:LYS:O	5:B:962:SER:OG	2.33	0.45
1:D:84:LEU:HB3	1:D:88:ALA:HB2	1.98	0.45
1:F:320:LYS:HD3	1:F:347:VAL:HG13	1.99	0.45
2:H:13:PHE:HZ	2:H:96:THR:HG23	1.82	0.45
5:B:84:ARG:O	5:B:88:GLU:N	2.38	0.45
5:B:544:TYR:CZ	5:B:548:ILE:HG21	2.52	0.45
6:C:287:GLY:HA3	6:C:296:LYS:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:GLN:H	1:E:35:GLN:HG2	1.53	0.45
5:B:74:ASN:O	5:B:77:ILE:HG13	2.17	0.45
5:B:646:TYR:CE1	5:B:696:PRO:HB2	2.51	0.45
5:B:714:LEU:HD12	5:B:749:ILE:HG12	1.99	0.45
5:B:836:LEU:HD23	5:B:836:LEU:HA	1.85	0.45
1:F:77:LYS:NZ	1:F:96:GLU:OE2	2.50	0.45
3:I:45:ARG:HH11	3:I:45:ARG:HA	1.82	0.45
5:B:104:HIS:NE2	5:B:111:TYR:HB3	2.31	0.45
5:B:417:SER:O	5:B:426:LYS:NZ	2.41	0.45
5:B:548:ILE:HD12	5:B:549:GLU:N	2.32	0.45
4:A:48:TYR:CE2	4:A:189:LEU:HD22	2.51	0.45
1:F:10:VAL:HG23	1:F:161:VAL:HG21	1.99	0.45
1:D:187:ILE:HG12	1:D:210:LYS:HB3	1.99	0.44
2:G:151:LEU:HD23	2:G:151:LEU:HA	1.84	0.44
5:B:485:PHE:N	6:C:257:SER:OG	2.36	0.44
5:B:670:ASP:OD1	5:B:670:ASP:N	2.42	0.44
1:D:84:LEU:HD23	1:D:88:ALA:HA	1.98	0.44
4:A:59:VAL:O	4:A:63:VAL:HG12	2.18	0.44
4:A:267:PRO:HB2	7:V:36:A:H1'	1.99	0.44
1:F:190:ASN:HA	1:F:193:ILE:HD12	2.00	0.44
1:F:264:ARG:HD3	1:D:48:GLN:HE21	1.82	0.44
1:D:320:LYS:HD2	1:D:347:VAL:HG23	1.99	0.44
1:E:258:SER:HG	3:I:127:ARG:NH1	2.15	0.44
2:H:128:ASP:OD1	2:H:128:ASP:N	2.50	0.44
5:B:818:LEU:HD23	5:B:818:LEU:HA	1.85	0.44
3:I:13:SER:O	3:I:15:LEU:N	2.47	0.44
5:B:454:VAL:HA	5:B:738:LEU:HD23	2.00	0.44
6:C:13:PHE:CZ	6:C:31:PRO:HB3	2.52	0.44
6:C:222:ASN:OD1	6:C:222:ASN:C	2.61	0.44
1:D:280:TRP:C	1:D:281:TYR:HD1	2.26	0.44
3:I:158:GLU:O	3:I:162:ILE:HG12	2.16	0.44
4:A:49:PHE:HE1	4:A:189:LEU:HD11	1.83	0.44
5:B:96:LEU:HD22	5:B:112:ILE:HD11	1.98	0.44
1:E:190:ASN:HA	1:E:193:ILE:HD12	2.00	0.44
3:I:262:ILE:HD12	3:I:263:MET:N	2.33	0.44
5:B:316:LYS:HD2	5:B:316:LYS:HA	1.79	0.44
1:D:45:ILE:HB	1:D:128:ALA:HB3	1.99	0.44
3:I:20:GLU:O	3:I:24:LYS:HG2	2.18	0.44
1:F:67:ILE:N	1:F:67:ILE:HD12	2.33	0.44
5:B:112:ILE:HG13	5:B:733:ARG:HD2	2.00	0.44
5:B:719:LEU:HD11	5:B:749:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:178:VAL:HG13	4:A:208:PHE:HE2	1.82	0.43
3:I:35:ILE:HD12	3:I:39:MET:HB2	2.01	0.43
5:B:378:LEU:HD11	5:B:516:VAL:HG13	1.99	0.43
5:B:870:TYR:HB3	5:B:994:ILE:HD11	2.00	0.43
6:C:264:LEU:O	6:C:267:ILE:HG13	2.18	0.43
1:D:223:LEU:HD22	1:D:231:PHE:HE2	1.83	0.43
4:A:20:GLY:HA2	4:A:29:ARG:HD2	1.99	0.43
5:B:35:ARG:HH21	5:B:62:LEU:HA	1.83	0.43
5:B:259:LYS:HE2	5:B:259:LYS:HB3	1.63	0.43
5:B:779:THR:O	5:B:779:THR:OG1	2.36	0.43
1:D:22:GLY:O	7:V:15:U:H3'	2.19	0.43
1:D:225:THR:HG22	1:D:226:LEU:HD23	1.99	0.43
3:I:328:ALA:HA	7:V:28:C:H5'	1.99	0.43
5:B:65:SER:OG	5:B:66:LYS:N	2.52	0.43
2:G:12:SER:OG	2:G:102:ASN:OD1	2.35	0.43
2:G:41:LYS:HB2	3:I:116:GLU:HG3	2.00	0.43
5:B:831:HIS:ND1	5:B:865:ARG:HD3	2.34	0.43
1:F:294:LEU:HD23	1:F:294:LEU:HA	1.88	0.43
3:I:210:ILE:O	3:I:213:THR:OG1	2.28	0.43
6:C:153:ARG:HB3	6:C:174:GLU:HG2	1.99	0.43
7:V:15:U:H1'	7:V:16:A:C8	2.54	0.43
1:D:329:GLN:HE22	1:D:332:GLY:HA2	1.83	0.43
3:I:54:LEU:HA	3:I:57:VAL:HG22	2.01	0.43
4:A:49:PHE:CE1	4:A:189:LEU:HD11	2.54	0.43
5:B:710:MET:HG2	9:B:1102:ATP:C8	2.53	0.43
5:B:981:ILE:O	5:B:985:VAL:HG12	2.19	0.43
3:I:163:TYR:OH	3:I:206:GLU:O	2.36	0.43
4:A:178:VAL:O	4:A:182:THR:OG1	2.34	0.43
6:C:22:ASN:OD1	6:C:22:ASN:N	2.43	0.43
4:A:54:GLU:OE2	4:A:54:GLU:HA	2.19	0.43
5:B:76:ASP:OD2	5:B:230:HIS:NE2	2.48	0.43
1:E:239:ILE:HD12	1:E:239:ILE:C	2.44	0.43
1:E:319:LEU:HD23	1:E:319:LEU:HA	1.83	0.43
5:B:78:GLN:HA	5:B:462:THR:HG21	2.00	0.43
5:B:476:VAL:HG21	6:C:115:ILE:HB	2.00	0.43
1:F:132:LEU:HD22	1:F:144:PHE:HB3	2.00	0.42
1:D:7:LYS:HA	1:D:7:LYS:HD3	1.87	0.42
5:B:59:LEU:HD23	5:B:59:LEU:HA	1.93	0.42
6:C:127:SER:O	6:C:130:ILE:HG22	2.19	0.42
1:E:129:LYS:HE2	1:E:129:LYS:HB2	1.83	0.42
2:G:115:GLU:HG3	2:G:119:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:118:LEU:O	2:G:122:MET:HG2	2.19	0.42
5:B:102:ARG:O	5:B:143:TYR:HB2	2.19	0.42
5:B:889:LEU:HD23	5:B:889:LEU:HA	1.89	0.42
1:D:20:HIS:HB2	1:D:284:PHE:CD2	2.54	0.42
1:D:224:LYS:NZ	1:D:229:ASP:OD1	2.45	0.42
2:H:74:ILE:HG21	2:H:92:LYS:HB2	2.01	0.42
2:H:129:VAL:O	2:H:133:THR:OG1	2.35	0.42
3:I:164:GLU:O	3:I:167:LYS:HG2	2.20	0.42
5:B:832:TYR:CD1	5:B:832:TYR:C	2.96	0.42
1:E:201:ILE:HA	1:E:205:ILE:O	2.19	0.42
3:I:162:ILE:HG21	3:I:210:ILE:HD11	2.01	0.42
4:A:312:ASN:OD1	4:A:312:ASN:N	2.51	0.42
1:F:38:ARG:HB2	6:C:152:GLU:HB2	2.00	0.42
5:B:222:SER:O	5:B:222:SER:OG	2.29	0.42
2:G:55:LEU:HD23	2:G:55:LEU:HA	1.88	0.42
2:G:125:THR:O	2:G:129:VAL:HG13	2.20	0.42
3:I:309:LEU:HD12	3:I:309:LEU:HA	1.89	0.42
3:I:331:SER:HA	4:A:74:VAL:HG12	2.00	0.42
4:A:219:LYS:HG3	4:A:239:LEU:HB2	2.02	0.42
5:B:82:LEU:HA	5:B:85:VAL:HG12	2.00	0.42
1:F:122:ALA:HB2	1:F:300:PRO:HB3	2.02	0.42
1:E:315:ILE:HD13	1:E:315:ILE:HA	1.90	0.42
5:B:196:LYS:HD3	5:B:196:LYS:HA	1.84	0.42
5:B:795:ASP:OD2	5:B:795:ASP:C	2.62	0.42
1:E:201:ILE:HG12	1:E:206:VAL:HG13	2.02	0.42
4:A:22:ASN:OD1	4:A:22:ASN:C	2.63	0.42
6:C:243:TYR:CE1	6:C:305:GLY:HA2	2.54	0.42
1:E:182:SER:OG	1:E:183:ASN:N	2.53	0.42
2:H:2:ASP:OD1	2:H:2:ASP:C	2.62	0.42
2:H:42:ALA:O	2:H:46:ILE:HG13	2.20	0.42
2:G:76:PRO:HB2	2:G:89:PHE:CD1	2.55	0.42
5:B:769:VAL:HA	5:B:804:LEU:HD21	2.00	0.42
2:H:67:ASP:OD1	2:H:67:ASP:N	2.53	0.41
3:I:21:LYS:HB3	3:I:27:LEU:HD13	2.02	0.41
3:I:153:ARG:NH2	4:A:3:MET:O	2.53	0.41
6:C:239:ARG:HB3	6:C:341:TRP:CE2	2.55	0.41
2:G:43:PRO:HG3	2:G:140:LEU:HB3	2.02	0.41
1:F:204:ASP:OD1	2:H:10:ARG:NH2	2.40	0.41
1:E:314:LYS:HA	1:E:317:ASN:ND2	2.35	0.41
2:H:30:LYS:HA	2:H:30:LYS:HD2	1.92	0.41
4:A:314:PHE:HA	4:A:317:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:551:LEU:HD13	5:B:551:LEU:HA	1.92	0.41
6:C:176:LEU:HD23	6:C:178:PHE:HE1	1.85	0.41
2:G:126:ALA:O	2:G:129:VAL:HG22	2.20	0.41
3:I:265:PRO:HB3	7:V:31:C:H1'	2.02	0.41
4:A:250:LYS:HA	4:A:253:HIS:NE2	2.36	0.41
5:B:120:PRO:O	5:B:747:ARG:NH2	2.54	0.41
5:B:157:PHE:O	5:B:160:ILE:HG13	2.20	0.41
5:B:586:TYR:O	5:B:590:ARG:HD3	2.20	0.41
6:C:1:MET:N	6:C:188:VAL:O	2.41	0.41
6:C:14:ARG:NH2	6:C:17:ARG:O	2.42	0.41
3:I:53:SER:O	3:I:57:VAL:HG13	2.20	0.41
5:B:30:TRP:NE1	5:B:183:LYS:HB2	2.35	0.41
5:B:297:VAL:HA	5:B:337:ALA:HA	2.02	0.41
6:C:228:LYS:HD2	6:C:228:LYS:HA	1.81	0.41
6:C:323:LEU:HD23	6:C:336:CYS:HB2	2.03	0.41
1:D:264:ARG:HE	1:D:264:ARG:HB3	1.61	0.41
5:B:30:TRP:CD1	5:B:183:LYS:HB2	2.56	0.41
5:B:846:LEU:HD23	5:B:846:LEU:HA	1.91	0.41
1:F:83:VAL:HG11	1:F:306:PRO:HG3	2.02	0.41
1:F:187:ILE:HD13	1:F:215:VAL:HG11	2.02	0.41
3:I:24:LYS:HB2	3:I:26:GLU:HG3	2.01	0.41
4:A:237:LEU:HB3	4:A:242:LEU:HG	2.02	0.41
5:B:84:ARG:HA	5:B:87:LEU:HB3	2.02	0.41
5:B:548:ILE:HD11	5:B:561:VAL:HG23	2.03	0.41
5:B:771:ASP:O	5:B:774:ARG:NH2	2.54	0.41
3:I:157:ASP:OD1	3:I:157:ASP:N	2.54	0.41
5:B:598:GLU:OE1	5:B:598:GLU:N	2.54	0.41
6:C:38:GLY:HA2	6:C:41:ARG:HE	1.86	0.41
1:F:142:PHE:HE1	1:F:242:ARG:HH21	1.69	0.41
1:F:187:ILE:HG22	1:F:216:ILE:HD11	2.02	0.41
1:F:319:LEU:HD12	1:F:319:LEU:HA	1.85	0.41
1:D:141:VAL:HG23	1:E:248:ASP:HB3	2.03	0.41
2:H:66:ILE:O	2:G:22:LYS:NZ	2.53	0.41
2:G:90:LEU:HD12	2:G:90:LEU:HA	1.91	0.41
3:I:109:LEU:HD12	3:I:335:GLY:HA2	2.03	0.41
3:I:225:GLY:HA2	3:I:228:VAL:HG12	2.03	0.41
4:A:41:PHE:CD1	4:A:128:LEU:HD21	2.55	0.41
5:B:440:ILE:HG22	5:B:443:LYS:HE3	2.02	0.41
5:B:567:VAL:O	5:B:570:VAL:HG22	2.21	0.41
5:B:706:ASP:OD1	5:B:707:GLY:N	2.53	0.41
6:C:3:LEU:HD12	6:C:3:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:144:GLU:OE1	6:C:145:ARG:N	2.54	0.41
6:C:259:LEU:HG	6:C:264:LEU:HD11	2.03	0.41
1:D:79:LYS:HA	1:D:79:LYS:HD3	1.74	0.41
3:I:157:ASP:O	3:I:161:ARG:HG3	2.21	0.41
5:B:264:ALA:HB1	5:B:269:ASP:HB2	2.03	0.41
5:B:768:HIS:NE2	5:B:816:GLU:OE2	2.45	0.41
1:F:232:PHE:O	1:F:234:LYS:NZ	2.54	0.40
1:F:252:LYS:O	1:F:256:ARG:HG3	2.21	0.40
1:D:256:ARG:O	1:D:256:ARG:NH1	2.53	0.40
5:B:428:LYS:NZ	5:B:449:ASP:OD1	2.39	0.40
1:E:83:VAL:HG12	1:E:84:LEU:HG	2.03	0.40
2:H:27:GLN:HA	2:H:27:GLN:OE1	2.21	0.40
2:H:125:THR:OG1	2:H:128:ASP:OD1	2.36	0.40
3:I:237:GLU:HG3	7:V:23:C:H5"	2.03	0.40
5:B:80:SER:CB	5:B:750:THR:HB	2.50	0.40
5:B:550:THR:O	5:B:550:THR:OG1	2.35	0.40
5:B:872:SER:CB	5:B:991:LEU:HB2	2.52	0.40
1:D:202:LEU:HD23	1:D:207:LEU:HD12	2.02	0.40
2:H:25:TYR:CD2	2:H:31:VAL:HG11	2.55	0.40
3:I:81:GLU:OE1	3:I:81:GLU:N	2.49	0.40
4:A:180:ASP:O	4:A:184:GLU:HG2	2.21	0.40
5:B:692:MET:HE3	5:B:692:MET:N	2.36	0.40
5:B:727:HIS:HB3	5:B:730:ILE:HG23	2.03	0.40
5:B:837:TYR:OH	6:C:25:VAL:HG23	2.21	0.40
5:B:938:VAL:HG12	5:B:941:ARG:NH2	2.37	0.40
5:B:989:LEU:HA	5:B:992:VAL:HG12	2.03	0.40
1:E:219:LEU:O	1:E:223:LEU:HG	2.21	0.40
4:A:148:ARG:HA	4:A:281:VAL:HB	2.03	0.40
5:B:183:LYS:O	5:B:187:ILE:HG13	2.22	0.40
5:B:263:ASP:OD1	6:C:17:ARG:NH1	2.53	0.40
5:B:368:LYS:HE2	5:B:368:LYS:HB2	1.84	0.40
5:B:639:ASN:OD1	5:B:639:ASN:N	2.55	0.40
5:B:738:LEU:HA	5:B:741:LYS:HB2	2.03	0.40
6:C:5:MET:HG2	6:C:211:PHE:HB2	2.03	0.40
1:E:135:VAL:HG21	1:E:254:PHE:CD2	2.57	0.40
6:C:179:SER:HB2	6:C:182: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	D	344/369 (93%)	332 (96%)	12 (4%)	0	100	100
1	E	342/369 (93%)	330 (96%)	12 (4%)	0	100	100
1	F	331/369 (90%)	313 (95%)	18 (5%)	0	100	100
2	G	151/155 (97%)	145 (96%)	6 (4%)	0	100	100
2	H	151/155 (97%)	148 (98%)	3 (2%)	0	100	100
3	I	334/343 (97%)	311 (93%)	23 (7%)	0	100	100
4	A	323/329 (98%)	307 (95%)	16 (5%)	0	100	100
5	B	974/1004 (97%)	929 (95%)	45 (5%)	0	100	100
6	C	316/341 (93%)	306 (97%)	10 (3%)	0	100	100
All	All	3266/3434 (95%)	3121 (96%)	145 (4%)	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	D	274/320 (86%)	250 (91%)	24 (9%)	9	33
1	E	260/320 (81%)	231 (89%)	29 (11%)	6	23
1	F	249/320 (78%)	224 (90%)	25 (10%)	7	27
2	G	126/131 (96%)	117 (93%)	9 (7%)	13	41
2	H	123/131 (94%)	110 (89%)	13 (11%)	6	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	258/303 (85%)	231 (90%)	27 (10%)	6	26
4	A	176/292 (60%)	159 (90%)	17 (10%)	8	29
5	B	786/885 (89%)	730 (93%)	56 (7%)	13	41
6	C	257/295 (87%)	242 (94%)	15 (6%)	18	49
All	All	2509/2997 (84%)	2294 (91%)	215 (9%)	12	34

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	9	VAL
1	F	100	ARG
1	F	103	LEU
1	F	105	THR
1	F	113	THR
1	F	123	VAL
1	F	137	SER
1	F	141	VAL
1	F	150	VAL
1	F	179	VAL
1	F	181	LEU
1	F	182	SER
1	F	209	VAL
1	F	215	VAL
1	F	222	VAL
1	F	229	ASP
1	F	238	SER
1	F	258	SER
1	F	279	LEU
1	F	287	SER
1	F	289	THR
1	F	294	LEU
1	F	310	ASP
1	F	318	VAL
1	F	347	VAL
1	D	11	PHE
1	D	15	SER
1	D	34	ILE
1	D	44	VAL
1	D	71	SER
1	D	104	LEU
1	D	135	VAL

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Mol	Chain	Res	Type
1	D	172	GLN
1	D	179	VAL
1	D	182	SER
1	D	195	ASN
1	D	202	LEU
1	D	211	SER
1	D	212	ASP
1	D	225	THR
1	D	241	GLU
1	D	265	VAL
1	D	293	SER
1	D	297	VAL
1	D	299	SER
1	D	309	VAL
1	D	333	ASP
1	D	341	VAL
1	D	349	THR
1	E	17	THR
1	E	27	LEU
1	E	29	VAL
1	E	35	GLN
1	E	44	VAL
1	E	53	VAL
1	E	69	VAL
1	E	71	SER
1	E	124	SER
1	E	159	GLU
1	E	162	SER
1	E	179	VAL
1	E	184	ASN
1	E	203	GLU
1	E	206	VAL
1	E	211	SER
1	E	215	VAL
1	E	234	LYS
1	E	247	SER
1	E	249	ASP
1	E	253	SER
1	E	273	THR
1	E	279	LEU
1	E	287	SER
1	E	294	LEU

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Mol	Chain	Res	Type
1	E	299	SER
1	E	310	ASP
1	E	321	VAL
1	E	335	THR
2	H	12	SER
2	H	21	ILE
2	H	26	SER
2	H	37	SER
2	H	44	THR
2	H	60	SER
2	H	67	ASP
2	H	78	SER
2	H	90	LEU
2	H	95	SER
2	H	118	LEU
2	H	123	GLU
2	H	140	LEU
2	G	60	SER
2	G	73	SER
2	G	74	ILE
2	G	113	ASN
2	G	118	LEU
2	G	123	GLU
2	G	125	THR
2	G	127	ILE
2	G	145	LYS
3	I	13	SER
3	I	33	SER
3	I	53	SER
3	I	60	ILE
3	I	64	VAL
3	I	78	SER
3	I	95	SER
3	I	97	SER
3	I	107	SER
3	I	110	VAL
3	I	117	SER
3	I	118	VAL
3	I	121	THR
3	I	149	SER
3	I	157	ASP
3	I	204	PHE

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Mol	Chain	Res	Type
3	I	205	ASP
3	I	220	THR
3	I	221	VAL
3	I	223	SER
3	I	233	THR
3	I	244	ASP
3	I	258	LEU
3	I	291	VAL
3	I	298	THR
3	I	301	VAL
3	I	314	GLU
4	A	7	THR
4	A	14	THR
4	A	53	VAL
4	A	56	LEU
4	A	67	THR
4	A	73	VAL
4	A	75	VAL
4	A	120	SER
4	A	133	LEU
4	A	153	LEU
4	A	182	THR
4	A	207	SER
4	A	210	CYS
4	A	287	SER
4	A	295	SER
4	A	296	VAL
4	A	325	ILE
5	B	45	SER
5	B	65	SER
5	B	85	VAL
5	B	111	TYR
5	B	131	ILE
5	B	135	LEU
5	B	138	THR
5	B	180	SER
5	B	206	SER
5	B	221	LEU
5	B	278	SER
5	B	295	ASP
5	B	314	SER
5	B	326	LEU

Continued on next page...

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Mol	Chain	Res	Type
5	B	369	LEU
5	B	373	VAL
5	B	395	LYS
5	B	397	ILE
5	B	407	SER
5	B	411	ILE
5	B	415	ASP
5	B	482	SER
5	B	497	THR
5	B	526	SER
5	B	528	LEU
5	B	530	SER
5	B	541	LYS
5	B	550	THR
5	B	567	VAL
5	B	581	THR
5	B	585	VAL
5	B	627	VAL
5	B	636	LEU
5	B	659	THR
5	B	677	THR
5	B	680	SER
5	B	689	VAL
5	B	712	LYS
5	B	714	LEU
5	B	731	LEU
5	B	734	VAL
5	B	750	THR
5	B	765	SER
5	B	769	VAL
5	B	779	THR
5	B	783	SER
5	B	788	VAL
5	B	792	LEU
5	B	796	THR
5	B	824	SER
5	B	866	SER
5	B	885	VAL
5	B	917	LEU
5	B	950	LEU
5	B	969	THR
5	B	998	SER

Continued on next page...

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Mol	Chain	Res	Type
6	C	42	SER
6	C	71	PHE
6	C	83	VAL
6	C	102	ASP
6	C	127	SER
6	C	165	THR
6	C	173	VAL
6	C	190	ASP
6	C	199	ILE
6	C	209	VAL
6	C	221	THR
6	C	267	ILE
6	C	292	THR
6	C	329	THR
6	C	340	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	325	ASN
1	D	39	HIS
1	D	60	GLN
1	D	317	ASN
2	H	49	ASN
2	H	75	ASN
2	H	102	ASN
3	I	72	ASN
3	I	266	HIS
4	A	252	ASN
5	B	114	GLN
5	B	301	HIS
5	B	333	ASN
5	B	394	HIS
5	B	446	GLN
5	B	609	HIS
5	B	813	ASN
6	C	146	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	V	28/45 (62%)	5 (17%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	V	15	U
7	V	20	G
7	V	25	U
7	V	27	G
7	V	28	C

There are no RNA pucker outliers to report.

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	$\# Z > 2$
9	ATP	B	1103	-	32,33,33	0.27	0	48,52,52	0.29	0
9	ATP	B	1102	8	32,33,33	0.32	0	48,52,52	0.31	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
9	ATP	B	1103	-	-	12/22/38/38	0/3/3/3
9	ATP	B	1102	8	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	1103	ATP	C5'-O5'-PA-O1A
9	B	1103	ATP	C5'-O5'-PA-O2A
9	B	1103	ATP	C5'-O5'-PA-O3A
9	B	1103	ATP	O4'-C4'-C5'-O5'
9	B	1103	ATP	C3'-C4'-C5'-O5'
9	B	1103	ATP	C2'-C1'-N9-C8
9	B	1103	ATP	PG-O3B-PB-O3A
9	B	1102	ATP	PG-O3B-PB-O3A
9	B	1103	ATP	PB-O3A-PA-O5'
9	B	1102	ATP	C2'-C1'-N9-C8
9	B	1102	ATP	C2'-C1'-N9-C4
9	B	1103	ATP	C2'-C1'-N9-C4
9	B	1102	ATP	O4'-C4'-C5'-O5'
9	B	1102	ATP	O4'-C1'-N9-C8
9	B	1103	ATP	O4'-C1'-N9-C8
9	B	1102	ATP	PA-O3A-PB-O1B
9	B	1102	ATP	PA-O3A-PB-O2B
9	B	1103	ATP	PA-O3A-PB-O1B
9	B	1103	ATP	PA-O3A-PB-O2B

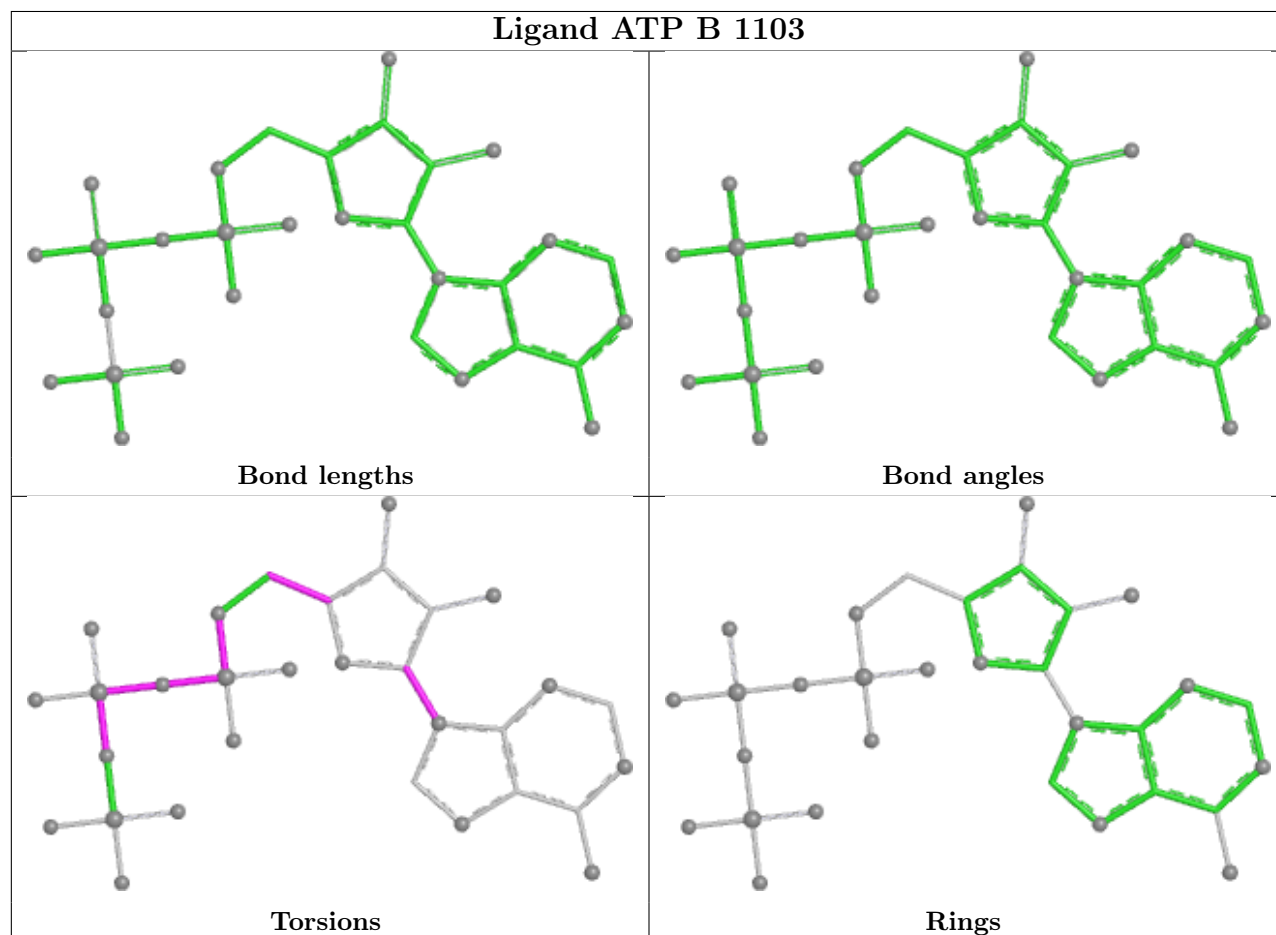
There are no ring outliers.

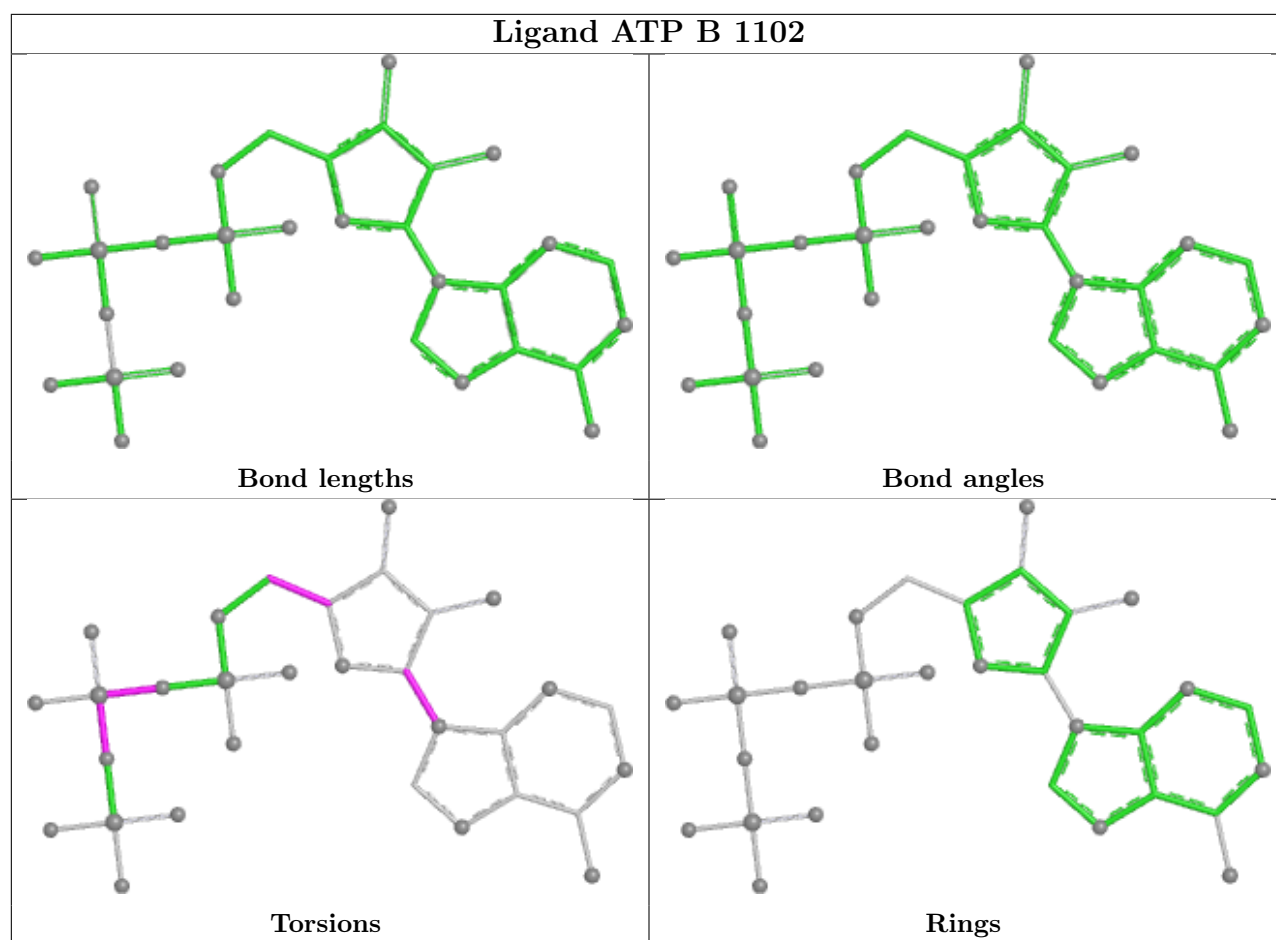
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1103	ATP	2	0
9	B	1102	ATP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

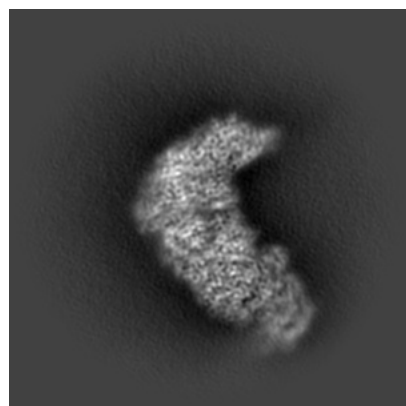
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62872. These allow visual inspection of the internal detail of the map and identification of artifacts.

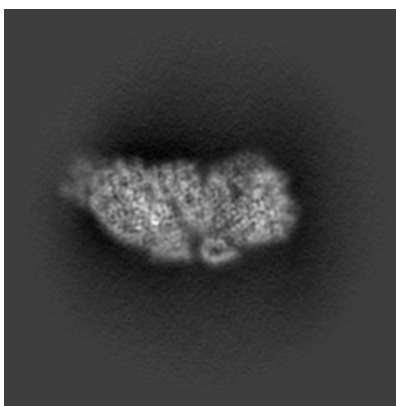
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

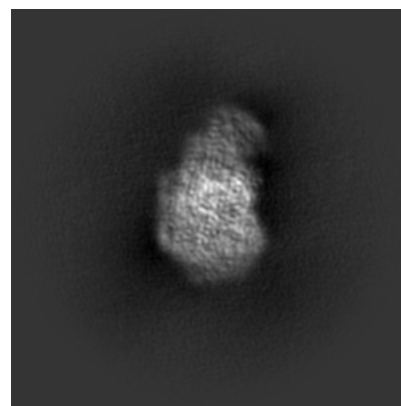
6.1.1 Primary map



X

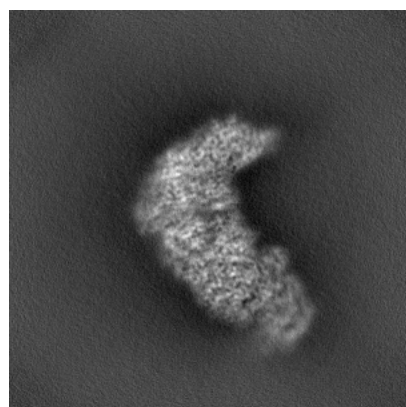


Y

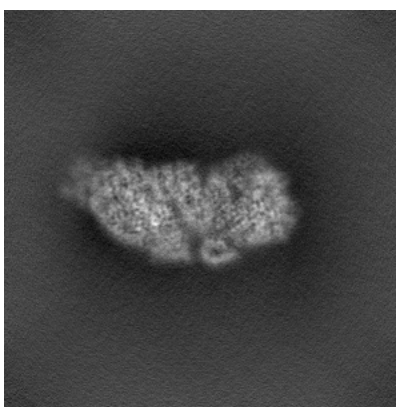


Z

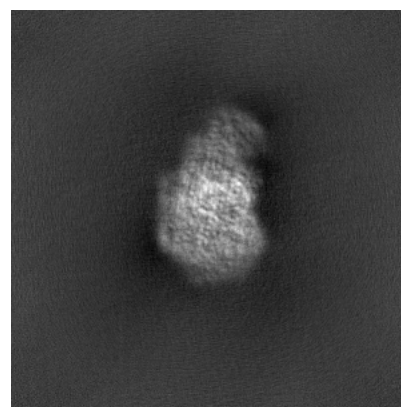
6.1.2 Raw map



X



Y

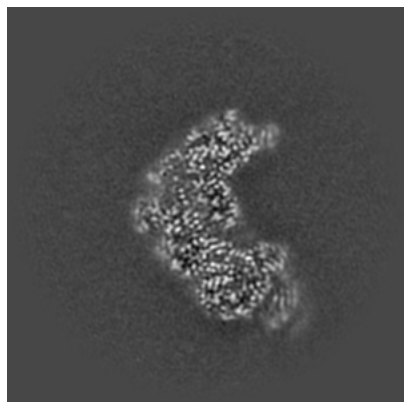


Z

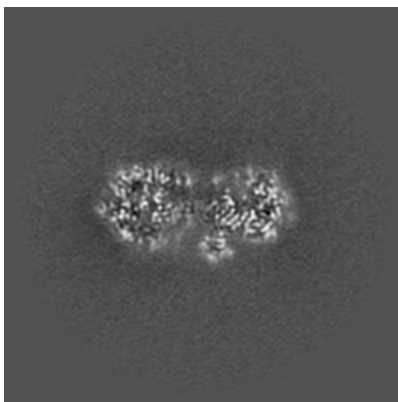
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

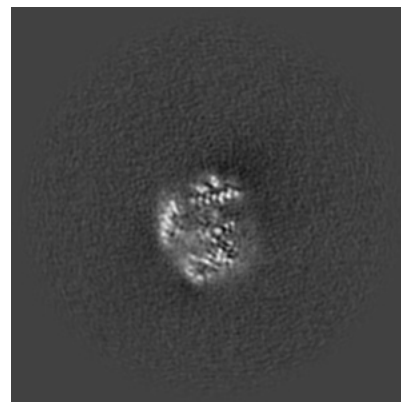
6.2.1 Primary map



X Index: 200

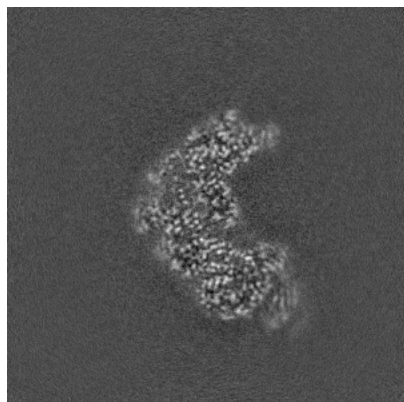


Y Index: 200

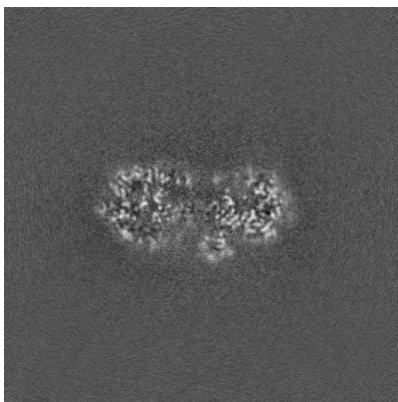


Z Index: 200

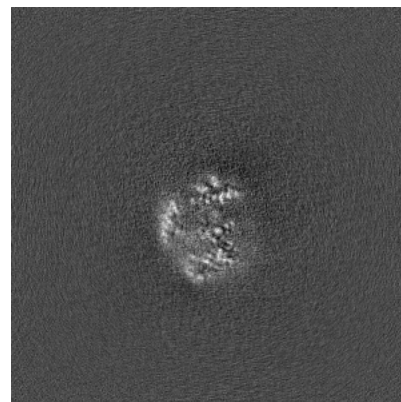
6.2.2 Raw map



X Index: 200



Y Index: 200

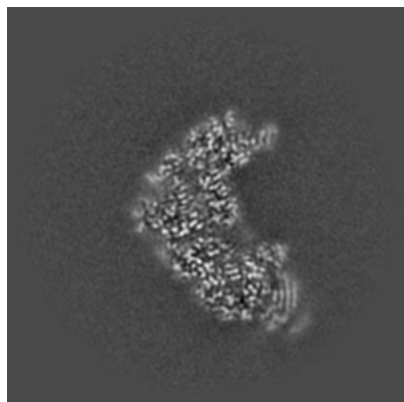


Z Index: 200

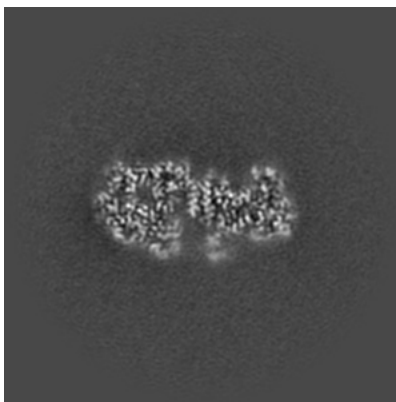
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

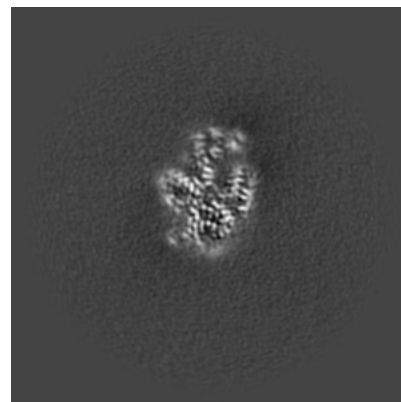
6.3.1 Primary map



X Index: 203

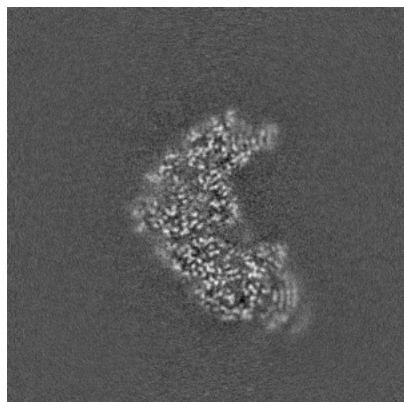


Y Index: 210

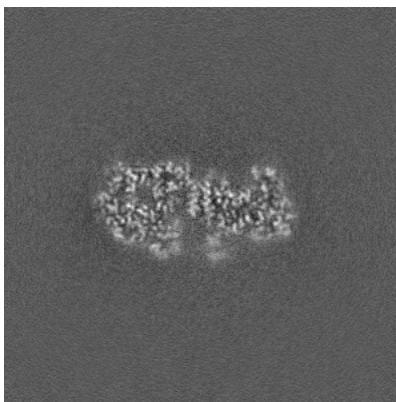


Z Index: 152

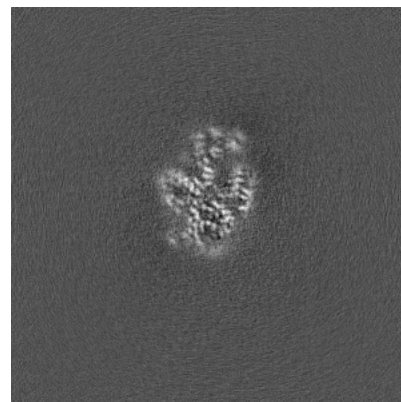
6.3.2 Raw map



X Index: 202



Y Index: 210

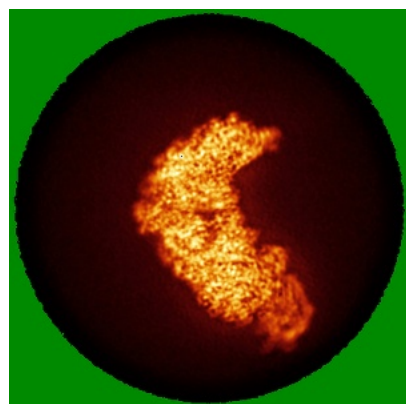


Z Index: 152

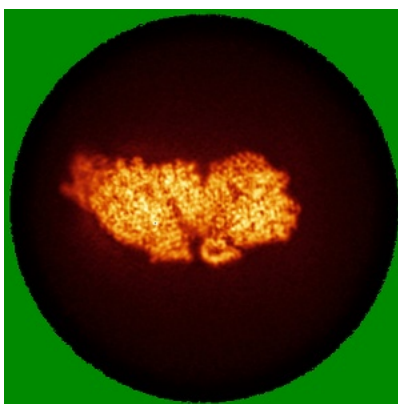
The images above show the largest variance slices of the map in three orthogonal directions.

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

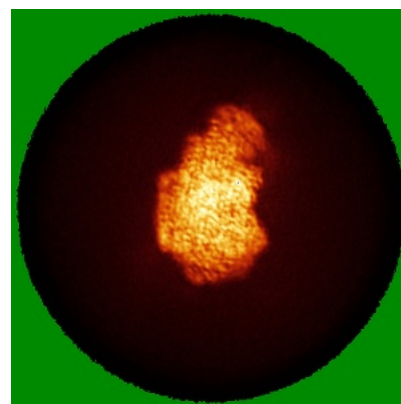
6.4.1 Primary map



X

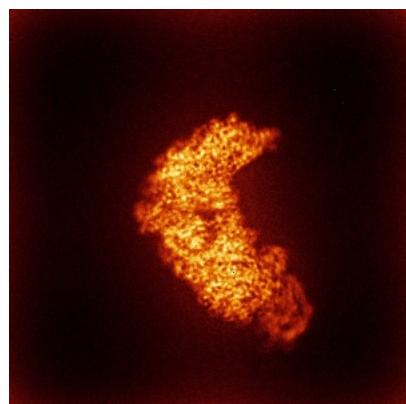


Y

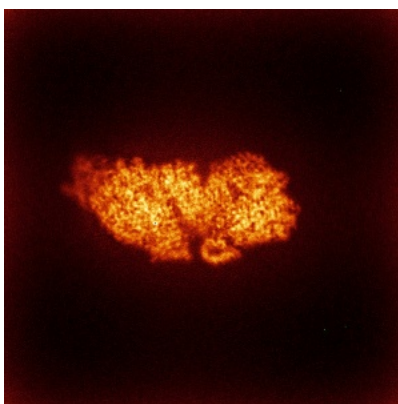


Z

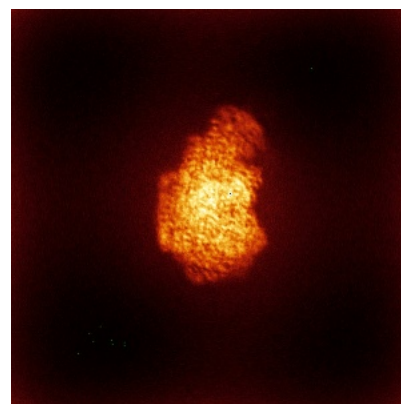
6.4.2 Raw map



X



Y

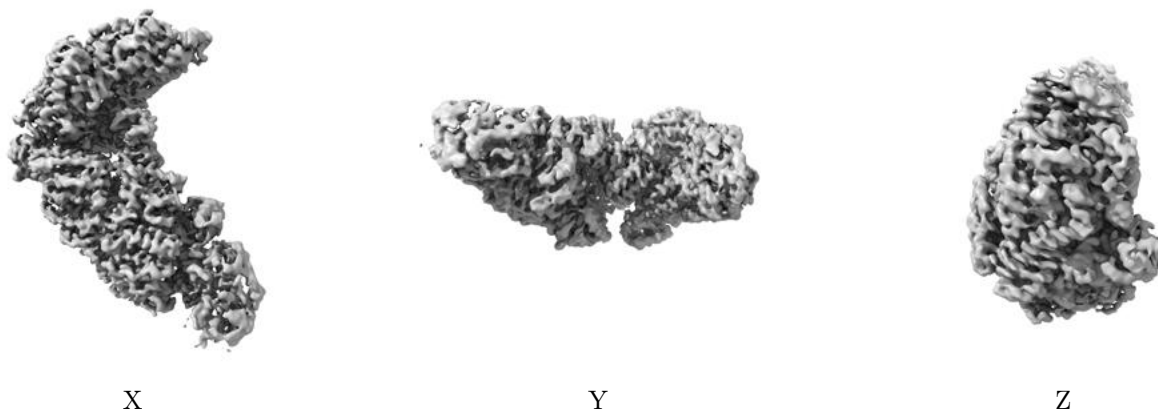


Z

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.

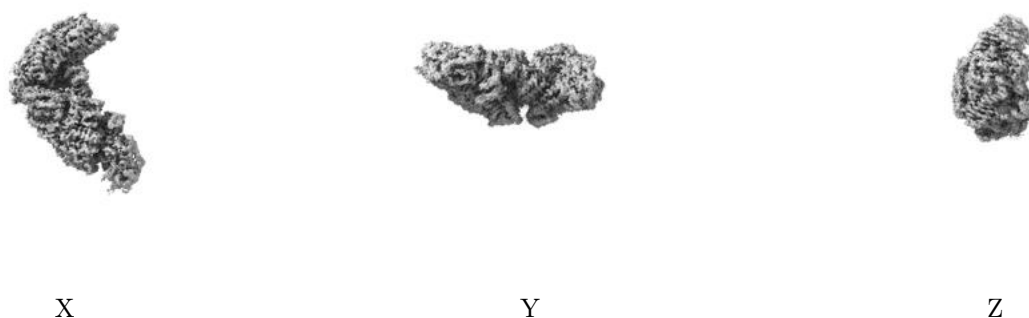
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.214. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

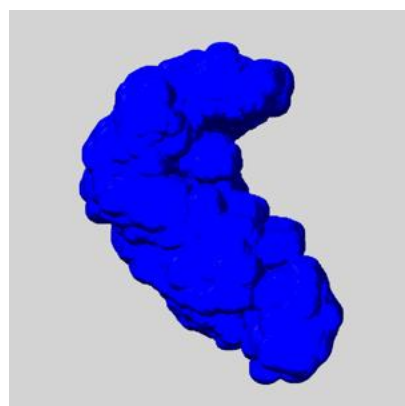
6.6 Mask visualisation [i](#)

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

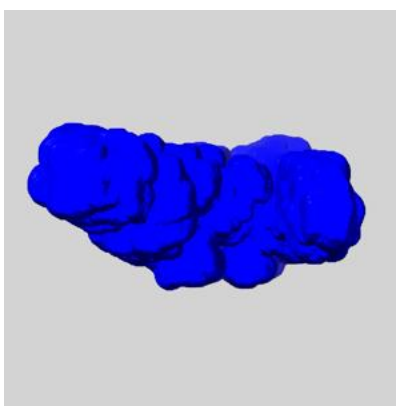
A mask typically either:

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

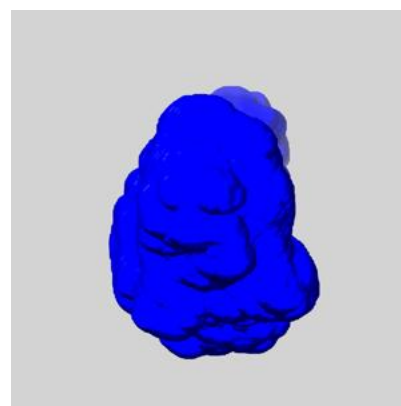
6.6.1 emd_62872_msk_1.map [i](#)



X



Y

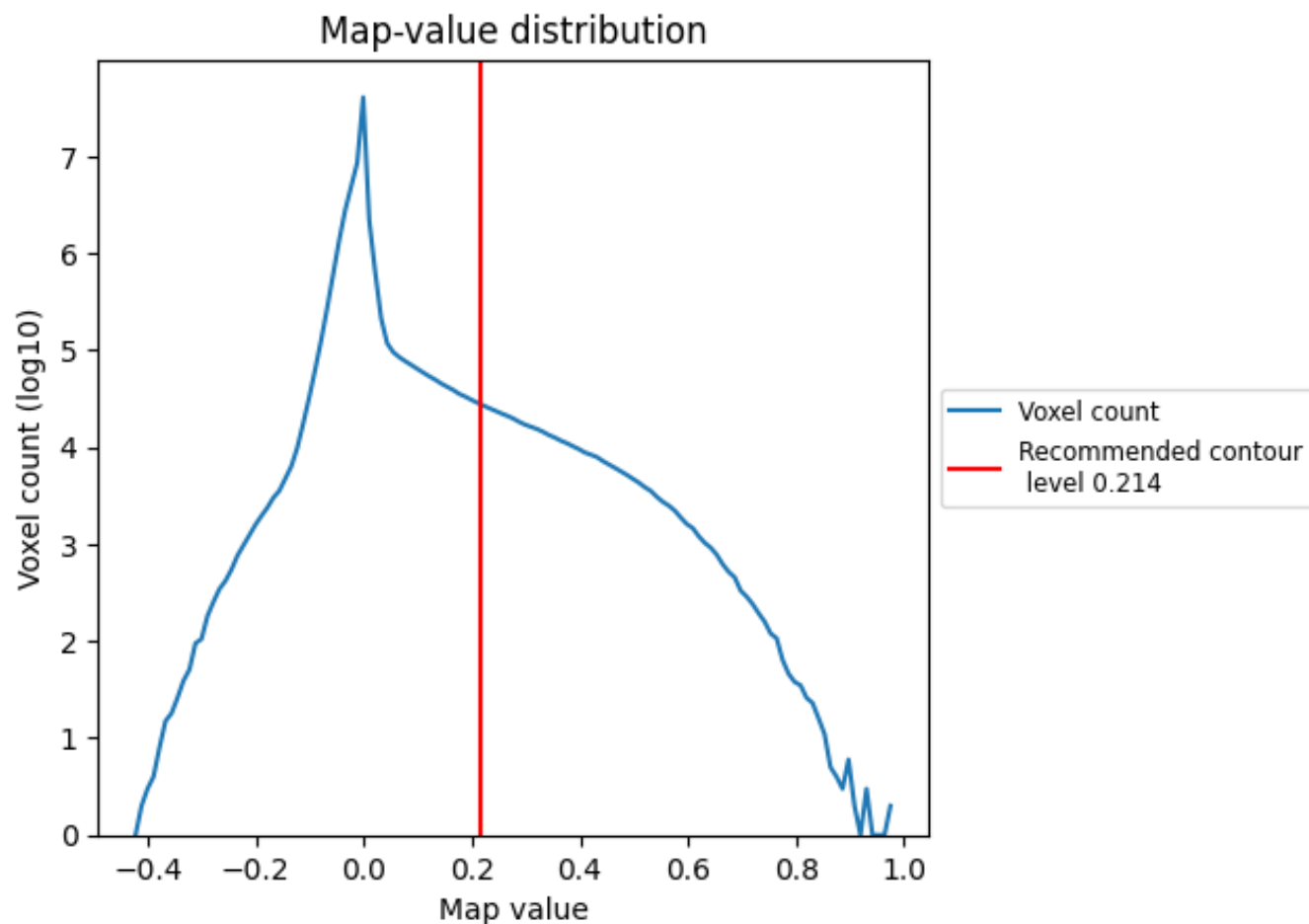


Z

7 Map analysis [i](#)

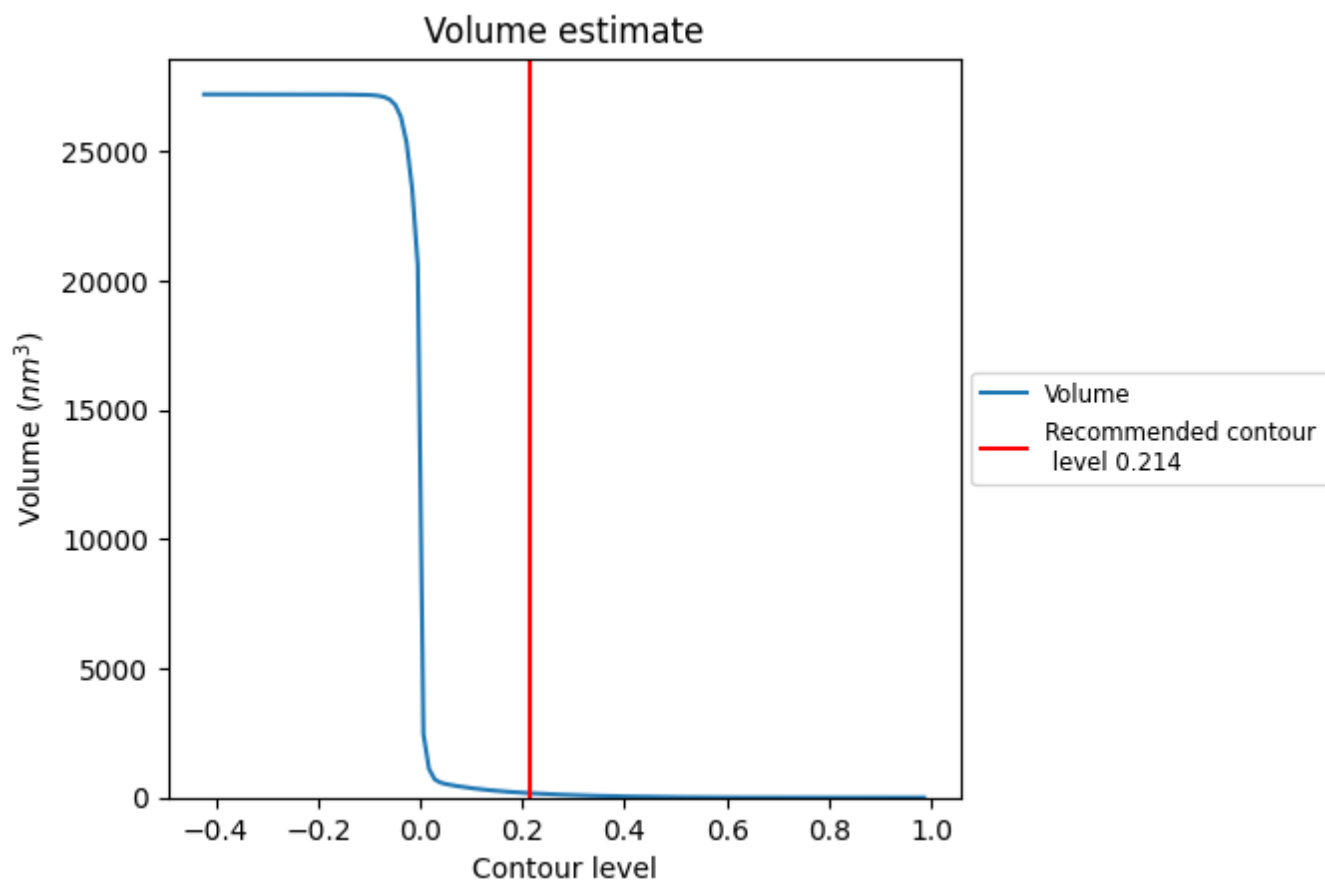
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

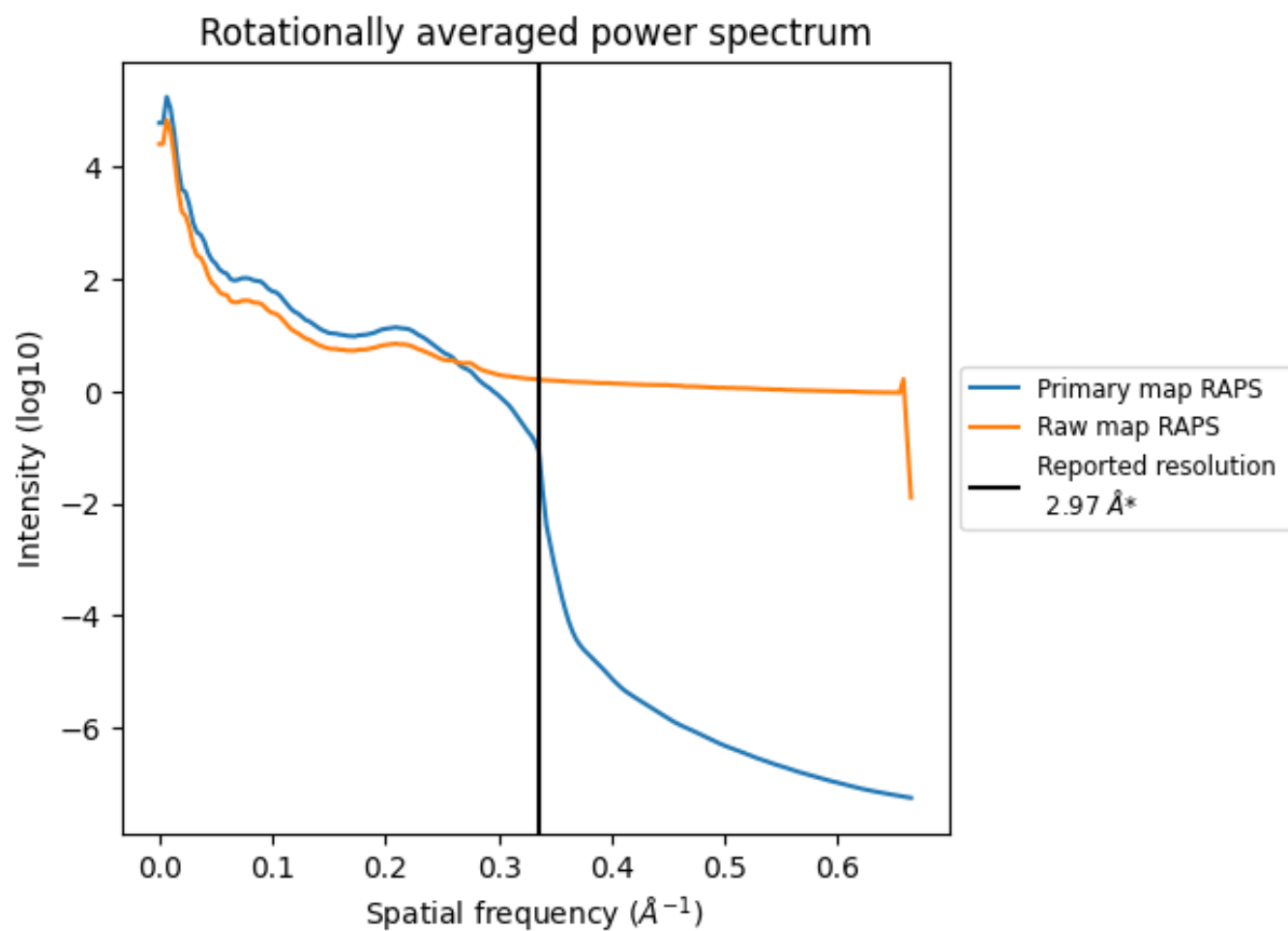
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm³; this corresponds to an approximate mass of 154 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

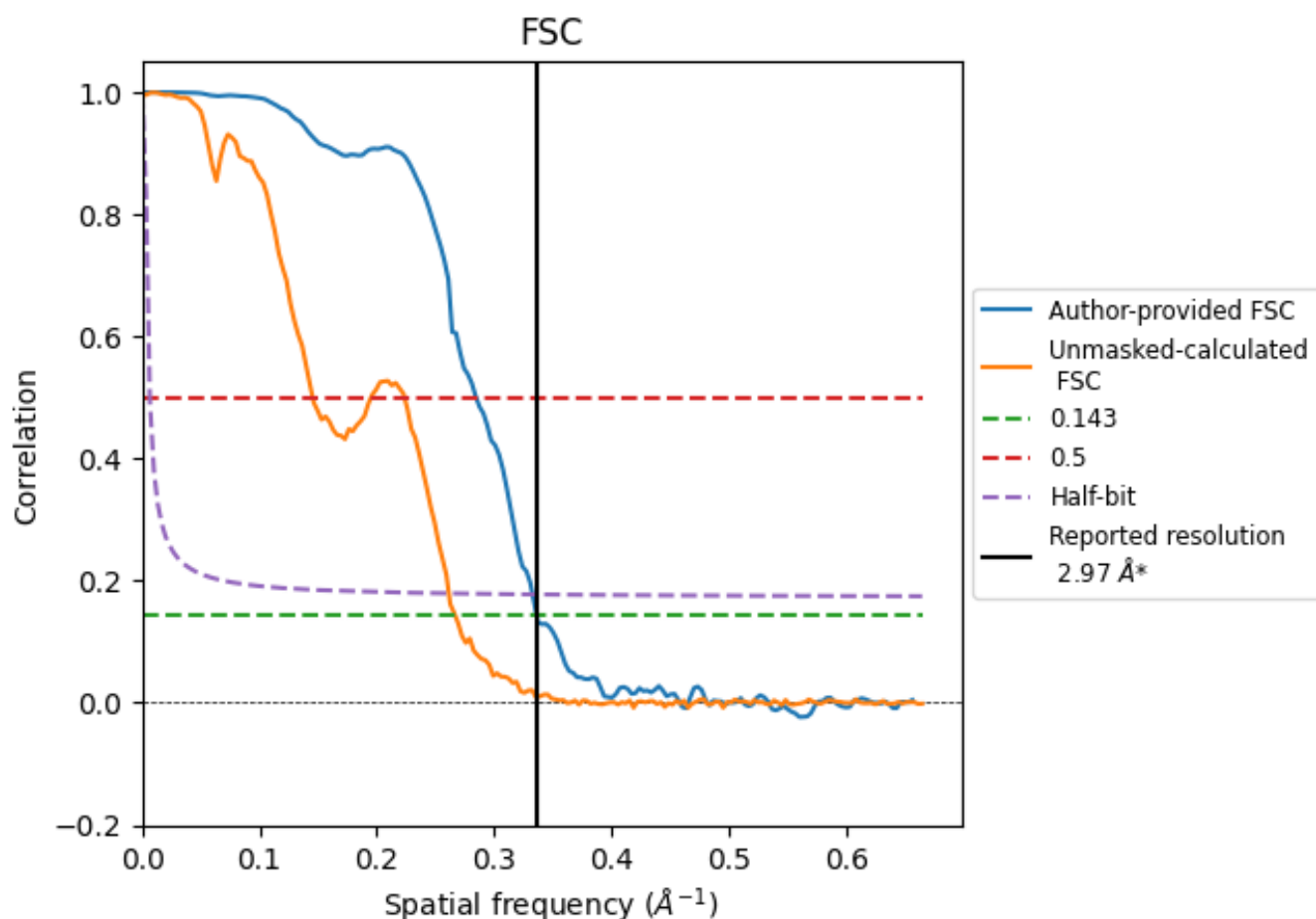


*Reported resolution corresponds to spatial frequency of 0.337 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.337 $\text{\AA}^{-1}$

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	2.97	3.51	3.00
Unmasked-calculated*	3.75	6.88	3.83

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

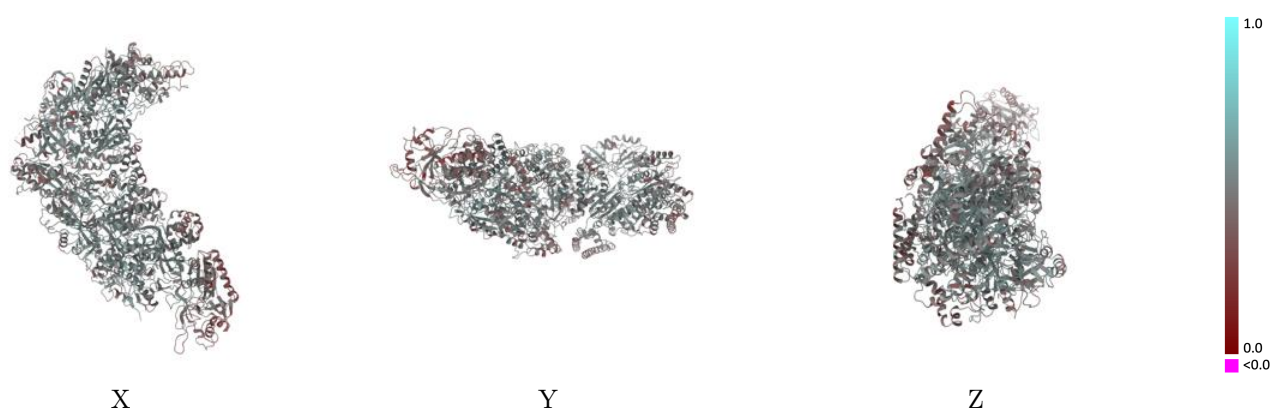
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62872 and PDB model 9L7C. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

This section was not generated.

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

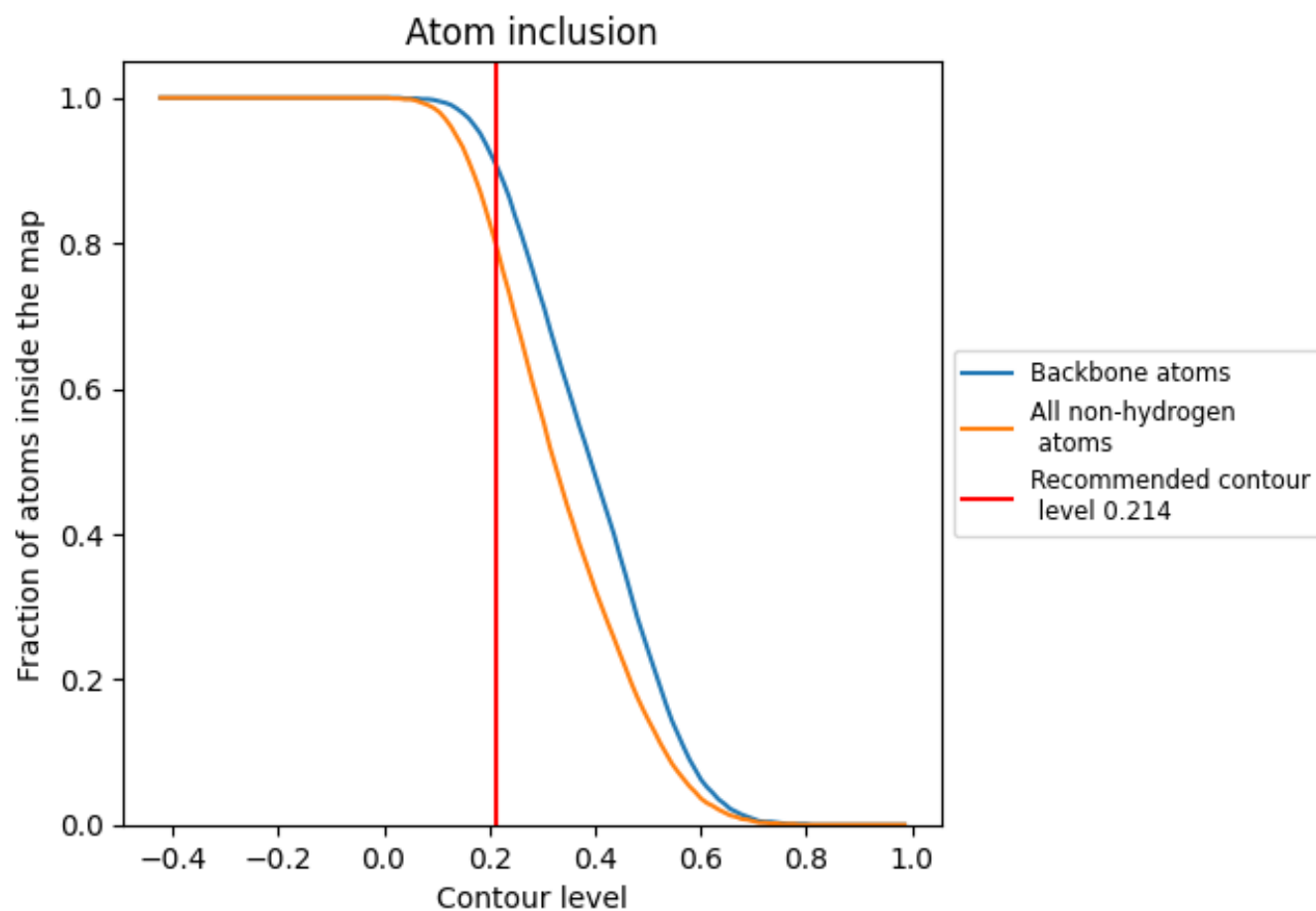


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 79% 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 (0.214) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.4880
A	 0.5860	 0.4130
B	 0.8450	 0.4910
C	 0.8280	 0.4970
D	 0.8130	 0.4990
E	 0.8200	 0.5000
F	 0.7870	 0.4910
G	 0.7990	 0.5070
H	 0.8260	 0.4920
I	 0.7670	 0.4940
V	 0.6710	 0.4910

