



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:25 AM UTC

PDB ID : 8GAN / pdb_00008gan
EMDB ID : EMD-29901
Title : Exploiting Activation and Inactivation Mechanisms in Type I-C CRISPR-Cas3
for Genome Editing Applications
Authors : Hu, C.; Nam, K.H.; Ke, A.
Deposited on : 2023-02-23
Resolution : 3.26 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
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

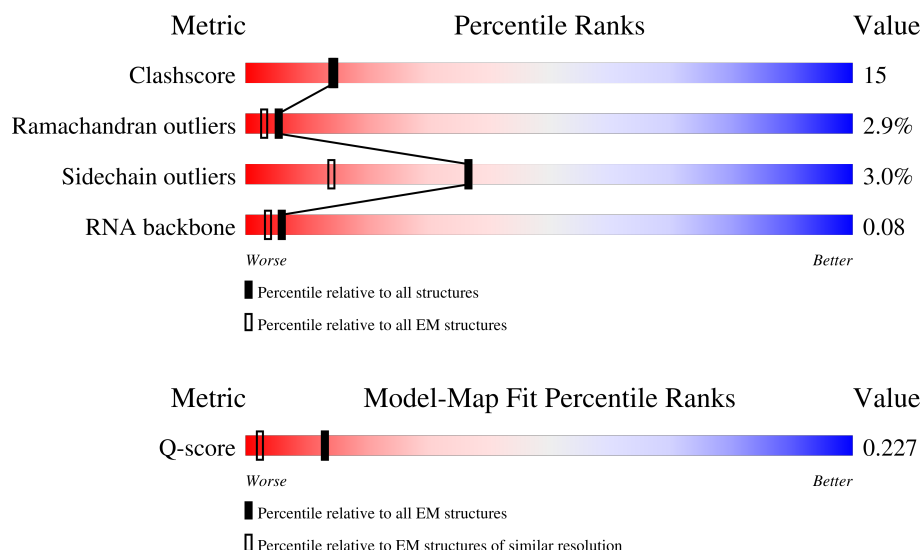
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.26 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	14557 (2.76 - 3.76)

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

Mol	Chain	Length	Quality of chain
1	A	283	8% 67% 31%
1	B	283	6% 61% 37%
1	C	283	7% 66% 31%

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Mol	Chain	Length	Quality of chain
1	D	283	
1	E	283	
1	F	283	
1	M	283	
2	G	124	
2	I	124	
2	J	124	
3	H	582	
4	K	43	
5	L	53	
6	N	205	
7	O	19	
8	Q	21	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 27669 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 Cas7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	B	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	C	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	D	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	E	283	Total	C	N	O	S	0	0
			2261	1408	406	436	11		
1	F	271	Total	C	N	O	S	0	0
			2173	1360	391	411	11		
1	M	264	Total	C	N	O	S	0	0
			2110	1318	379	402	11		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLY	-	expression tag	UNP A0A378VEU0
B	284	GLY	-	expression tag	UNP A0A378VEU0
C	284	GLY	-	expression tag	UNP A0A378VEU0
D	284	GLY	-	expression tag	UNP A0A378VEU0
E	284	GLY	-	expression tag	UNP A0A378VEU0
F	284	GLY	-	expression tag	UNP A0A378VEU0
M	284	GLY	-	expression tag	UNP A0A378VEU0

- Molecule 2 is a protein called Cas11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		
2	I	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	124	Total	C	N	O	S	0	0
			1007	646	180	179	2		

- Molecule 3 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	582	Total	C	N	O	S	0	0
			4555	2889	800	849	17		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	190	ALA	VAL	conflict	UNP A0A378VF47
H	239	ALA	ILE	conflict	UNP A0A378VF47
H	242	ILE	VAL	conflict	UNP A0A378VF47
H	260	GLY	SER	conflict	UNP A0A378VF47
H	271	THR	ALA	conflict	UNP A0A378VF47
H	296	ASN	LYS	conflict	UNP A0A378VF47
H	299	ALA	GLU	conflict	UNP A0A378VF47
H	306	ALA	THR	conflict	UNP A0A378VF47
H	317	CYS	GLN	conflict	UNP A0A378VF47
H	322	GLU	LYS	conflict	UNP A0A378VF47
H	323	ASP	GLU	conflict	UNP A0A378VF47

- Molecule 4 is a RNA chain called crRNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	43	Total	C	N	O	P	0	0
			916	408	161	304	43		

- Molecule 5 is a DNA chain called Target strand DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	53	Total	C	N	O	P	0	0
			1093	515	211	314	53		

- Molecule 6 is a protein called Cas5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	205	Total	C	N	O	S	0	0
			1674	1067	289	306	12		

- Molecule 7 is a DNA chain called Proximal Non target strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	19	Total	C	N	O	P	0	0
			393	188	82	104	19		

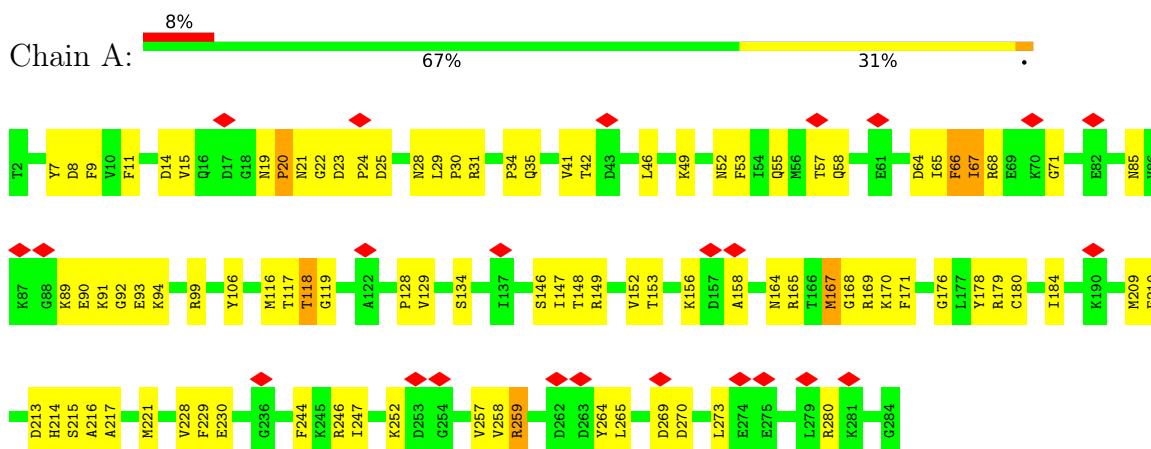
- Molecule 8 is a DNA chain called Distal Non target strand DNA (5'-D(P*AP*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*TP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	21	Total	C	N	O	P	0	0
			429	210	69	129	21		

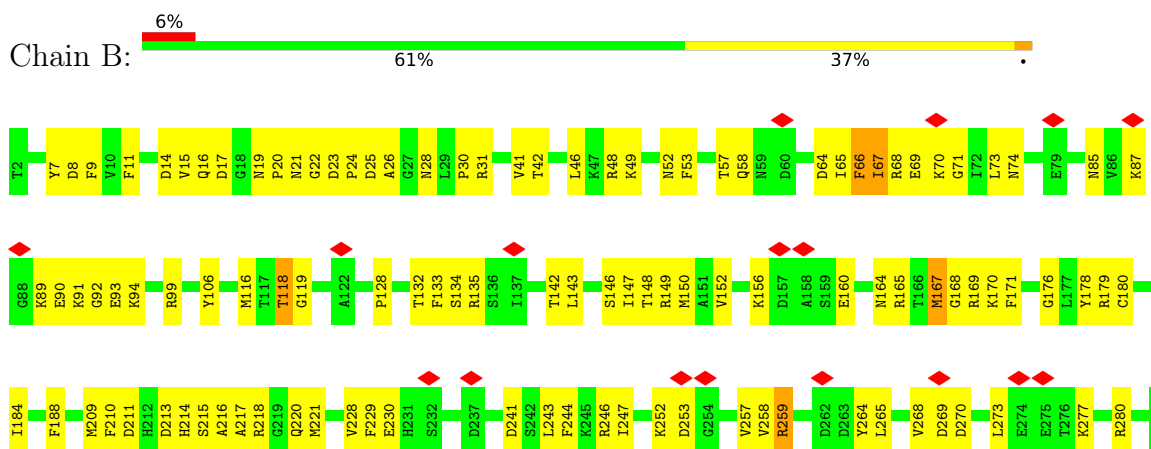
3 Residue-property plots [i](#)

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.

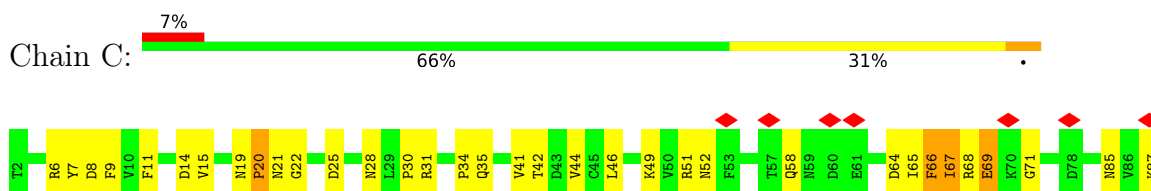
• Molecule 1: Cas7

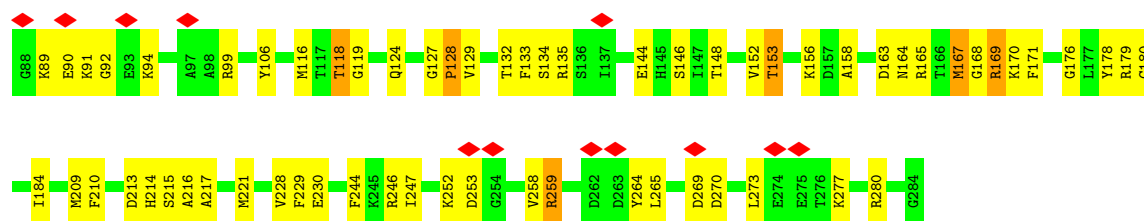


• Molecule 1: Cas7

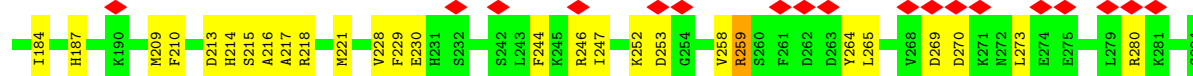
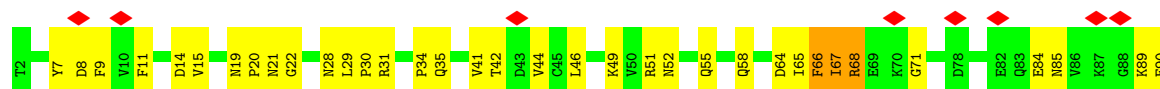


• Molecule 1: Cas7

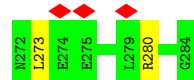
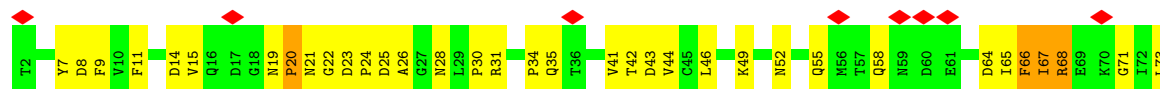




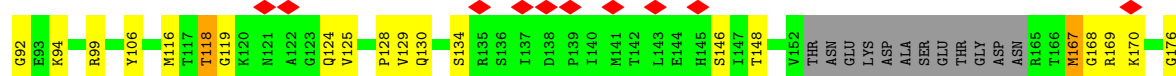
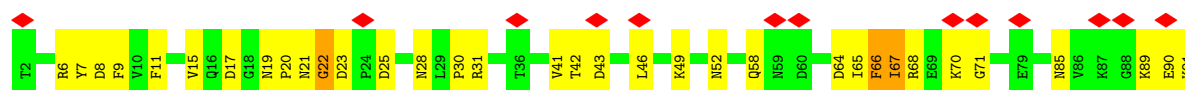
• Molecule 1: Cas7

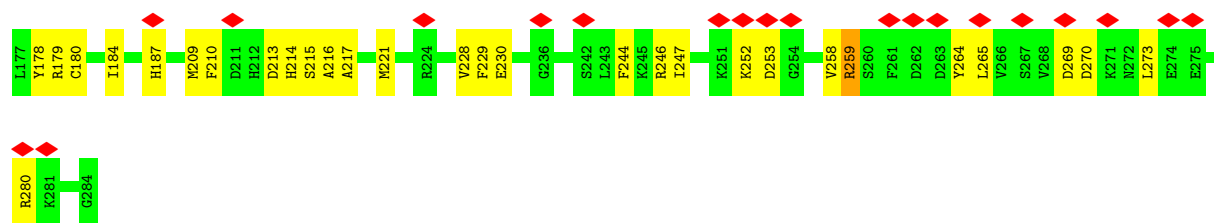


• Molecule 1: Cas7

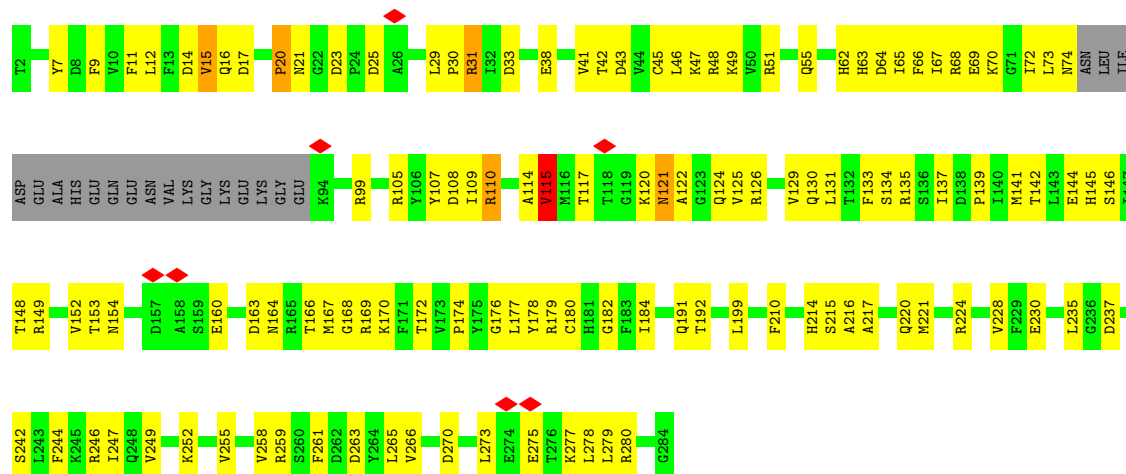


• Molecule 1: Cas7

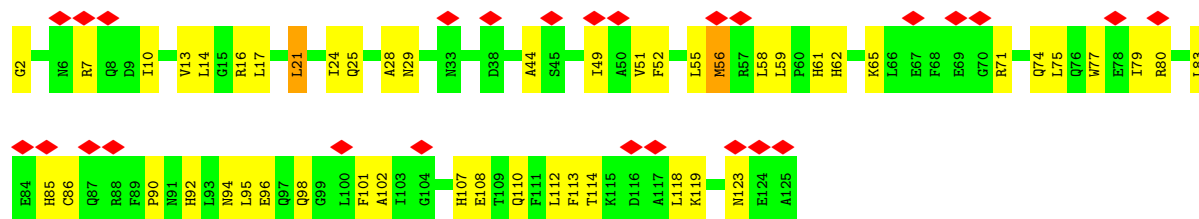




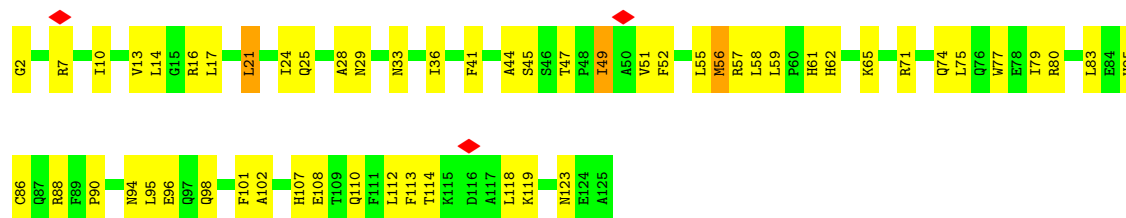
• Molecule 1: Cas7



• Molecule 2: Cas11

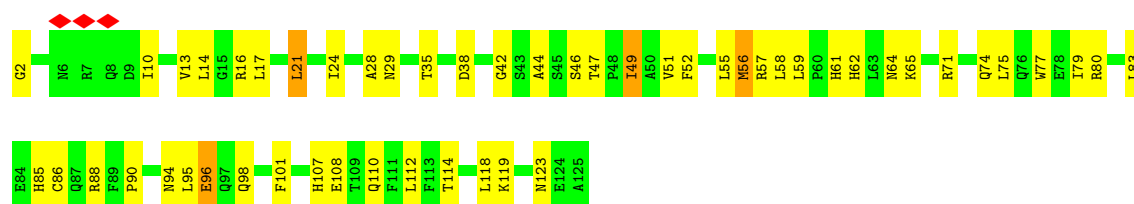


• Molecule 2: Cas11



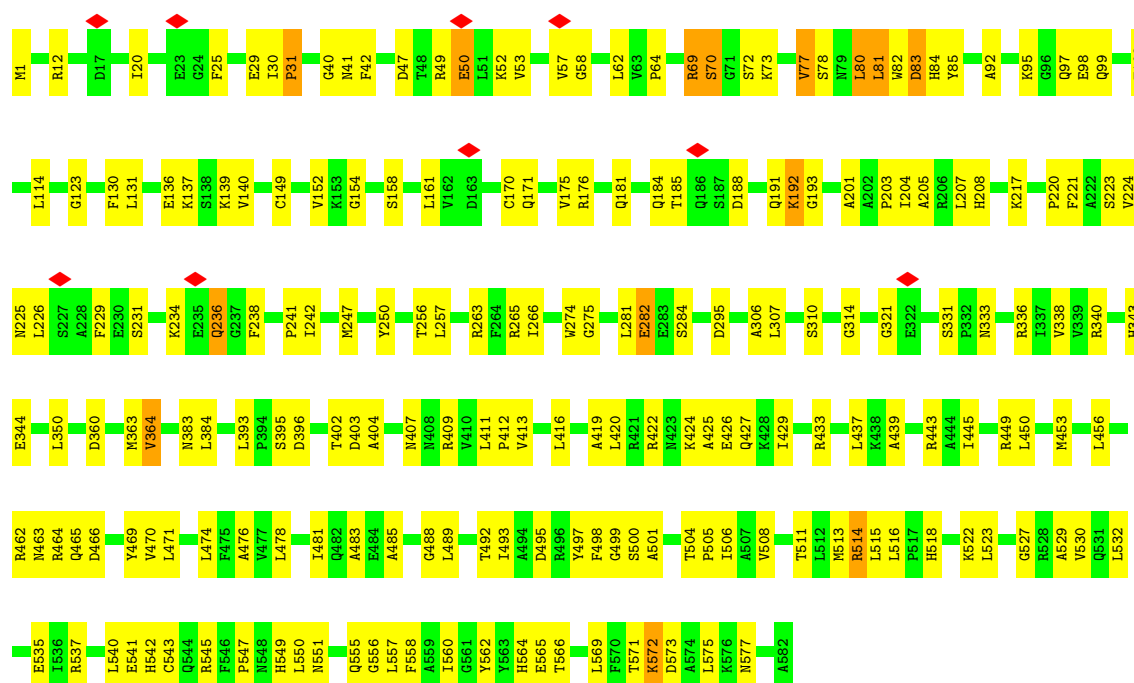
• Molecule 2: Cas11

Chain J: 

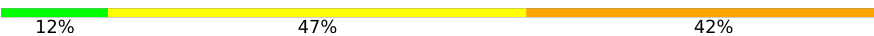


• Molecule 3: Cas8

Chain H: 



• Molecule 4: crRNA (43-MER)

Chain K: 



• Molecule 5: Target strand DNA (53-MER)

Chain L: 



• Molecule 6: Cas5

Chain N: 



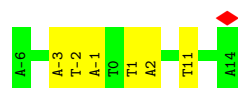
- Molecule 7: Proximal Non target strand DNA (5'-D(P*AP*TP*GP*AP*AP*CP*TP*TP*CP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3')

Chain O: 58% 42%



- Molecule 8: Distal Non target strand DNA (5'-D(P*AP*TP*TP*AP*TP*AP*TP*TP*AP*AP*TP*AP*TP*TP*AP*TP*AP*TP*TP*A)-3')

Chain Q: 5% 71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108723	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	67000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.168	Depositor
Minimum map value	-0.578	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.131	Depositor
Map size (Å)	393.59598, 393.59598, 393.59598	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4057, 1.4057, 1.4057	Depositor

5 Model quality

5.1 Standard geometry

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	0.09	0/2303	0.25	0/3101
1	B	0.09	0/2303	0.23	0/3101
1	C	0.09	0/2303	0.25	0/3101
1	D	0.09	0/2303	0.23	0/3101
1	E	0.09	0/2303	0.24	0/3101
1	F	0.09	0/2214	0.24	0/2979
1	M	0.08	0/2150	0.20	0/2896
2	G	0.09	0/1030	0.21	0/1392
2	I	0.09	0/1030	0.21	0/1392
2	J	0.09	0/1030	0.21	0/1392
3	H	0.09	0/4644	0.25	0/6277
4	K	0.26	0/1022	0.44	0/1591
5	L	0.19	0/1228	0.36	0/1894
6	N	0.08	0/1712	0.21	0/2307
7	O	0.13	0/444	0.26	0/682
8	Q	0.15	0/479	0.38	0/737
All	All	0.11	0/28498	0.26	0/39044

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	22	GLY	Peptide

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	A	2261	0	2193	58	0
1	B	2261	0	2193	84	0
1	C	2261	0	2193	80	0
1	D	2261	0	2193	69	0
1	E	2261	0	2193	68	0
1	F	2173	0	2120	49	0
1	M	2110	0	2050	104	0
2	G	1007	0	992	36	0
2	I	1007	0	992	52	0
2	J	1007	0	992	50	0
3	H	4555	0	4558	149	0
4	K	916	0	464	56	0
5	L	1093	0	592	64	0
6	N	1674	0	1663	71	0
7	O	393	0	213	9	0
8	Q	429	0	244	6	0
All	All	27669	0	25845	810	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 15.

All (810) 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)
4:K:30:G:N2	5:L:25:DC:O2	2.06	0.87
2:G:113:PHE:HB2	2:I:80:ARG:HH12	1.40	0.87
2:I:113:PHE:HB2	2:J:80:ARG:HH12	1.43	0.84
2:I:110:GLN:HB2	2:J:80:ARG:HB3	1.60	0.83
1:B:133:PHE:HB2	1:M:17:ASP:HB3	1.61	0.81
4:K:27:G:N2	5:L:28:DC:O2	2.16	0.77
1:A:148:THR:HG22	1:A:167:MET:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:235:LEU:HB3	6:N:133:GLN:HB3	1.67	0.75
1:B:149:ARG:HB2	4:K:19:U:H1'	1.69	0.74
2:G:110:GLN:HB2	2:I:80:ARG:HB3	1.69	0.73
3:H:52:LYS:NZ	7:O:19:DA:OP1	2.19	0.73
4:K:27:G:N1	5:L:28:DC:N3	2.36	0.73
4:K:32:A:N6	4:K:34:C:O2'	2.22	0.73
2:G:7:ARG:HH22	2:I:88:ARG:HD2	1.54	0.72
1:C:153:THR:HG21	5:L:31:DA:H2''	1.71	0.72
1:M:146:SER:HB3	1:M:167:MET:HE2	1.72	0.71
2:I:7:ARG:HH22	2:J:88:ARG:HD2	1.55	0.71
3:H:306:ALA:O	3:H:310:SER:N	2.23	0.71
4:K:43:C:O2	5:L:12:DG:N2	2.18	0.70
3:H:188:ASP:HA	3:H:203:PRO:HG3	1.73	0.70
3:H:416:LEU:HD23	3:H:437:LEU:HD22	1.73	0.70
5:L:50:DG:H2'	5:L:51:DT:H71	1.75	0.68
1:M:69:GLU:HG3	1:M:72:ILE:HD12	1.75	0.68
1:D:152:VAL:HB	1:D:164:ASN:HB3	1.74	0.68
1:B:135:ARG:NH2	1:M:16:GLN:O	2.25	0.68
1:M:210:PHE:O	1:M:214:HIS:NE2	2.28	0.67
1:B:169:ARG:NH2	3:H:424:LYS:O	2.29	0.66
2:J:24:ILE:HG12	2:J:75:LEU:HD13	1.77	0.66
1:D:168:GLY:HA3	5:L:18:DG:C6	2.31	0.66
1:B:90:GLU:O	1:B:92:GLY:N	2.29	0.66
8:Q:1:DT:OP2	8:Q:2:DA:N6	2.29	0.66
2:I:24:ILE:HG12	2:I:75:LEU:HD13	1.77	0.66
1:D:51:ARG:NH2	4:K:31:C:OP1	2.22	0.66
3:H:1:MET:SD	6:N:166:GLN:NE2	2.69	0.66
1:F:90:GLU:O	1:F:92:GLY:N	2.29	0.66
1:B:148:THR:O	4:K:19:U:O2'	2.14	0.65
1:D:90:GLU:O	1:D:92:GLY:N	2.29	0.65
1:E:90:GLU:O	1:E:92:GLY:N	2.29	0.65
6:N:44:LYS:HG3	6:N:45:PRO:HD2	1.78	0.65
4:K:15:A:H5''	1:M:148:THR:H	1.60	0.65
1:M:43:ASP:HB2	1:M:131:LEU:HB3	1.78	0.65
1:A:90:GLU:O	1:A:92:GLY:N	2.29	0.65
1:A:148:THR:O	4:K:31:C:O2'	2.13	0.65
1:C:90:GLU:O	1:C:92:GLY:N	2.29	0.65
3:H:481:ILE:HG12	3:H:532:LEU:HD13	1.79	0.65
1:C:25:ASP:HB3	3:H:500:SER:HB2	1.79	0.64
1:E:156:LYS:HG3	1:E:158:ALA:H	1.61	0.64
1:E:149:ARG:HD3	4:K:43:C:H1'	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:ILE:HG12	2:G:75:LEU:HD13	1.78	0.64
1:B:211:ASP:O	1:C:6:ARG:NH1	2.30	0.64
3:H:474:LEU:HD21	3:H:513:MET:HE2	1.80	0.64
5:L:41:DG:H21	1:M:169:ARG:HH21	1.44	0.64
1:M:179:ARG:NH2	1:M:244:PHE:O	2.31	0.64
1:D:259:ARG:HH21	1:E:35:GLN:HG3	1.63	0.63
1:M:11:PHE:HB3	1:M:180:CYS:HB3	1.80	0.63
3:H:333:ASN:HD21	6:N:89:GLN:HB2	1.63	0.63
1:B:73:LEU:HD12	1:M:153:THR:HG22	1.80	0.63
1:B:241:ASP:OD2	1:M:224:ARG:NH1	2.31	0.63
3:H:72:SER:HB2	5:L:50:DG:H21	1.64	0.62
1:D:156:LYS:HE3	1:D:158:ALA:HB3	1.80	0.62
2:I:62:HIS:NE2	5:L:18:DG:OP1	2.28	0.62
1:M:126:ARG:O	6:N:143:ARG:NH1	2.33	0.62
1:M:99:ARG:HH12	1:M:191:GLN:HB3	1.64	0.62
1:C:144:GLU:OE1	1:C:169:ARG:NH1	2.33	0.61
1:C:152:VAL:HB	1:C:164:ASN:HB3	1.82	0.61
3:H:29:GLU:HB3	3:H:57:VAL:HG23	1.81	0.61
2:I:80:ARG:NH2	8:Q:11:DT:O2	2.34	0.61
1:C:165:ARG:NH2	4:K:26:G:N7	2.48	0.61
6:N:14:PHE:HB2	6:N:26:TYR:HB2	1.80	0.61
1:C:169:ARG:HH22	3:H:511:THR:HB	1.66	0.61
1:F:130:GLN:NE2	4:K:42:U:OP1	2.34	0.61
3:H:501:ALA:HB2	3:H:508:VAL:HG11	1.82	0.61
1:C:229:PHE:HB3	1:C:277:LYS:HD2	1.81	0.61
1:E:21:ASN:ND2	1:E:42:THR:OG1	2.34	0.61
3:H:411:LEU:HD13	3:H:443:ARG:HD2	1.82	0.61
1:A:21:ASN:ND2	1:A:42:THR:OG1	2.34	0.60
1:B:165:ARG:NH2	4:K:20:G:N7	2.47	0.60
1:B:17:ASP:HB3	1:C:133:PHE:HB2	1.83	0.60
1:A:25:ASP:HB3	2:J:42:GLY:HA3	1.82	0.60
1:M:23:ASP:N	1:M:29:LEU:O	2.33	0.60
1:M:134:SER:HB3	1:M:178:TYR:HB3	1.83	0.60
1:F:21:ASN:ND2	1:F:42:THR:OG1	2.34	0.59
6:N:55:GLU:HB3	6:N:101:ARG:HG3	1.84	0.59
1:C:21:ASN:ND2	1:C:42:THR:OG1	2.34	0.59
1:M:258:VAL:O	1:M:259:ARG:NH1	2.35	0.59
6:N:184:ASP:OD1	6:N:184:ASP:N	2.34	0.59
1:M:255:VAL:HG11	1:M:263:ASP:HB3	1.84	0.59
1:B:21:ASN:ND2	1:B:42:THR:OG1	2.34	0.59
1:C:68:ARG:HD3	1:C:69:GLU:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:109:ILE:HD12	1:M:114:ALA:HB2	1.85	0.59
1:C:19:ASN:ND2	1:C:28:ASN:O	2.36	0.59
3:H:108:THR:HG22	3:H:131:LEU:HB3	1.84	0.59
2:I:95:LEU:HB3	2:J:49:ILE:HD12	1.85	0.59
1:A:214:HIS:HE1	1:A:221:MET:H	1.51	0.58
5:L:48:DA:H5'	5:L:48:DA:H8	1.68	0.58
1:D:21:ASN:ND2	1:D:42:THR:OG1	2.34	0.58
6:N:172:LEU:HA	6:N:191:MET:HG2	1.85	0.58
1:M:48:ARG:HH22	1:M:67:ILE:HG22	1.69	0.58
5:L:47:DG:H5''	6:N:88:GLN:HE22	1.69	0.58
1:A:149:ARG:HB2	4:K:31:C:H1'	1.83	0.58
1:C:148:THR:HG22	1:C:167:MET:HE3	1.86	0.58
1:F:19:ASN:ND2	1:F:28:ASN:O	2.36	0.58
1:B:48:ARG:HG2	4:K:14:C:C2	2.39	0.58
1:E:19:ASN:ND2	1:E:28:ASN:O	2.36	0.58
1:B:135:ARG:NH2	1:M:174:PRO:O	2.33	0.58
3:H:360:ASP:HB3	3:H:439:ALA:HA	1.84	0.58
1:B:19:ASN:ND2	1:B:28:ASN:O	2.36	0.58
1:D:55:GLN:HG2	1:E:187:HIS:HE1	1.68	0.58
3:H:225:ASN:ND2	3:H:236:GLN:OE1	2.36	0.58
4:K:30:G:N1	5:L:25:DC:N3	2.41	0.58
1:E:214:HIS:HE1	1:E:221:MET:H	1.51	0.58
1:B:25:ASP:OD1	5:L:41:DG:N2	2.30	0.57
1:F:214:HIS:HE1	1:F:221:MET:H	1.51	0.57
1:M:121:ASN:HB2	1:M:124:GLN:HG2	1.85	0.57
1:D:19:ASN:ND2	1:D:28:ASN:O	2.36	0.57
5:L:57:DT:H2''	5:L:58:DG:N7	2.18	0.57
1:B:214:HIS:HE1	1:B:221:MET:H	1.51	0.57
3:H:437:LEU:HD13	3:H:556:GLY:HA2	1.85	0.57
1:A:19:ASN:ND2	1:A:28:ASN:O	2.36	0.57
3:H:427:GLN:HB3	3:H:495:ASP:HA	1.86	0.57
1:M:228:VAL:HB	1:M:280:ARG:HB2	1.86	0.57
1:C:214:HIS:HE1	1:C:221:MET:H	1.51	0.57
6:N:180:SER:OG	6:N:186:ASN:O	2.22	0.57
1:F:269:ASP:OD1	1:F:269:ASP:N	2.38	0.57
3:H:485:ALA:HB1	3:H:522:LYS:HD3	1.87	0.57
1:D:269:ASP:OD1	1:D:269:ASP:N	2.38	0.57
1:E:270:ASP:OD1	1:E:270:ASP:N	2.38	0.57
1:M:179:ARG:NH2	1:M:247:ILE:O	2.38	0.57
3:H:537:ARG:NH1	8:Q:1:DT:O2	2.28	0.56
1:A:270:ASP:OD1	1:A:270:ASP:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASP:HB2	1:B:229:PHE:HB2	1.88	0.56
1:A:269:ASP:OD1	1:A:269:ASP:N	2.38	0.56
3:H:263:ARG:NH1	7:O:18:DA:OP1	2.38	0.56
2:J:77:TRP:HA	2:J:80:ARG:HH21	1.71	0.56
6:N:20:LYS:O	6:N:90:ARG:NH2	2.38	0.56
1:F:148:THR:HA	1:F:167:MET:HA	1.88	0.56
1:A:148:THR:HA	1:A:167:MET:HA	1.88	0.56
1:D:148:THR:HA	1:D:167:MET:HA	1.88	0.56
1:D:156:LYS:NZ	5:L:17:DG:OP1	2.35	0.56
2:G:107:HIS:NE2	2:I:86:CYS:O	2.38	0.56
2:I:33:ASN:O	2:J:64:ASN:ND2	2.33	0.56
1:D:8:ASP:HB2	1:D:229:PHE:HB2	1.88	0.56
1:D:214:HIS:HE1	1:D:221:MET:H	1.51	0.56
1:E:25:ASP:OD1	5:L:17:DG:N2	2.38	0.56
3:H:470:VAL:HG11	3:H:542:HIS:HB2	1.86	0.56
6:N:69:GLU:HG3	6:N:90:ARG:HB2	1.88	0.56
6:N:175:MET:SD	6:N:187:ASN:ND2	2.79	0.56
1:C:8:ASP:HB2	1:C:229:PHE:HB2	1.88	0.56
6:N:22:GLU:O	6:N:24:VAL:N	2.39	0.56
6:N:6:GLU:HA	6:N:101:ARG:HA	1.87	0.55
3:H:64:PRO:O	3:H:82:TRP:NE1	2.35	0.55
1:A:156:LYS:HG3	1:A:158:ALA:H	1.71	0.55
1:B:269:ASP:N	1:B:269:ASP:OD1	2.38	0.55
1:E:8:ASP:HB2	1:E:229:PHE:HB2	1.88	0.55
1:E:269:ASP:OD1	1:E:269:ASP:N	2.38	0.55
3:H:505:PRO:HG2	3:H:547:PRO:HG2	1.87	0.55
5:L:43:DC:O2	1:M:149:ARG:NH2	2.38	0.55
6:N:57:LEU:HD13	6:N:157:ASP:HB3	1.88	0.55
3:H:463:ASN:O	3:H:465:GLN:N	2.38	0.55
6:N:128:ARG:HG2	6:N:133:GLN:HB2	1.88	0.55
1:C:269:ASP:OD1	1:C:269:ASP:N	2.38	0.55
1:D:218:ARG:NH1	4:K:35:G:OP1	2.40	0.55
2:G:94:ASN:O	2:G:98:GLN:N	2.36	0.55
1:A:8:ASP:HB2	1:A:229:PHE:HB2	1.88	0.55
2:G:77:TRP:HA	2:G:80:ARG:HH21	1.70	0.55
2:I:77:TRP:HA	2:I:80:ARG:HH21	1.71	0.55
1:B:148:THR:HA	1:B:167:MET:HA	1.88	0.54
1:F:8:ASP:HB2	1:F:229:PHE:HB2	1.88	0.54
3:H:97:GLN:O	3:H:99:GLN:N	2.39	0.54
4:K:13:U:H1'	1:M:149:ARG:HB2	1.88	0.54
6:N:161:LEU:HD22	6:N:165:THR:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:16:ARG:HG2	2:J:108:GLU:HB2	1.90	0.54
1:M:21:ASN:ND2	1:M:42:THR:OG1	2.39	0.54
1:M:215:SER:OG	1:M:216:ALA:N	2.40	0.54
1:D:21:ASN:OD1	1:D:31:ARG:NE	2.38	0.54
1:M:7:TYR:HB2	1:M:184:ILE:HB	1.89	0.54
1:B:16:GLN:O	1:C:135:ARG:NH2	2.40	0.54
2:I:16:ARG:HG2	2:I:108:GLU:HB2	1.90	0.54
4:K:8:C:OP2	1:M:48:ARG:NH2	2.39	0.54
1:B:270:ASP:OD1	1:B:270:ASP:N	2.38	0.54
3:H:478:LEU:HD23	3:H:516:LEU:HD13	1.90	0.54
2:I:113:PHE:HB2	2:J:80:ARG:NH1	2.20	0.54
1:C:270:ASP:N	1:C:270:ASP:OD1	2.38	0.54
2:I:41:PHE:HD1	2:J:57:ARG:HA	1.71	0.54
4:K:8:C:OP1	6:N:87:ARG:NH1	2.40	0.54
1:B:22:GLY:HA2	1:B:30:PRO:HA	1.90	0.54
1:B:52:ASN:ND2	1:B:213:ASP:OD2	2.38	0.54
1:C:167:MET:SD	4:K:27:G:N1	2.80	0.54
1:E:55:GLN:HG2	1:F:187:HIS:HE1	1.72	0.54
1:F:21:ASN:OD1	1:F:31:ARG:NE	2.38	0.54
1:D:22:GLY:HA2	1:D:30:PRO:HA	1.90	0.54
2:I:94:ASN:O	2:I:98:GLN:N	2.36	0.54
8:Q:-3:DA:H2''	8:Q:-2:DT:H5'	1.90	0.54
1:A:21:ASN:OD1	1:A:31:ARG:NE	2.38	0.54
1:B:152:VAL:HB	1:B:164:ASN:HB3	1.90	0.54
1:D:152:VAL:HG21	1:D:159:SER:HB3	1.90	0.54
2:G:16:ARG:HG2	2:G:108:GLU:HB2	1.90	0.54
2:G:25:GLN:NE2	5:L:12:DG:OP1	2.41	0.54
6:N:37:ILE:HG12	6:N:138:PRO:HB3	1.90	0.54
1:A:22:GLY:HA2	1:A:30:PRO:HA	1.90	0.53
1:A:35:GLN:HG3	1:C:259:ARG:HH21	1.72	0.53
1:C:146:SER:HB2	1:C:169:ARG:HD3	1.89	0.53
3:H:569:LEU:HD22	3:H:575:LEU:HD22	1.90	0.53
1:F:17:ASP:N	1:F:17:ASP:OD1	2.40	0.53
3:H:225:ASN:HD21	5:L:49:DA:H2'	1.72	0.53
1:B:220:GLN:HB2	1:C:132:THR:HG21	1.90	0.53
1:E:68:ARG:NH2	1:F:124:GLN:HE21	2.07	0.53
3:H:363:MET:HE1	3:H:560:ILE:HG23	1.90	0.53
3:H:217:LYS:HB3	7:O:14:DA:C8	2.43	0.53
2:J:58:LEU:HA	2:J:61:HIS:CD2	2.44	0.53
3:H:527:GLY:HA3	8:Q:-1:DA:H2''	1.91	0.53
1:B:21:ASN:OD1	1:B:31:ARG:NE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:8:SER:O	6:N:148:ASP:N	2.40	0.53
2:J:112:LEU:HD22	2:J:118:LEU:HD22	1.91	0.53
5:L:37:DA:H2"	5:L:38:DG:H8	1.74	0.53
1:M:63:HIS:HA	1:M:107:TYR:HB2	1.90	0.53
2:G:58:LEU:HA	2:G:61:HIS:CD2	2.44	0.53
3:H:20:ILE:HG13	3:H:256:THR:HG21	1.90	0.52
5:L:48:DA:H5'	5:L:48:DA:C8	2.43	0.52
1:C:148:THR:HA	1:C:167:MET:HA	1.90	0.52
1:C:22:GLY:HA2	1:C:30:PRO:HA	1.90	0.52
1:F:22:GLY:HA2	1:F:30:PRO:HA	1.90	0.52
2:I:58:LEU:HA	2:I:61:HIS:CD2	2.44	0.52
5:L:43:DC:H2"	1:M:153:THR:HG21	1.91	0.52
1:M:133:PHE:HZ	6:N:67:ARG:HD3	1.74	0.52
1:E:22:GLY:HA2	1:E:30:PRO:HA	1.90	0.52
1:A:11:PHE:HB3	1:A:180:CYS:HB3	1.92	0.52
1:E:23:ASP:HB3	1:E:26:ALA:HB3	1.92	0.52
1:B:132:THR:HG21	1:M:220:GLN:HB2	1.90	0.52
3:H:208:HIS:HE1	3:H:242:ILE:HD12	1.73	0.52
3:H:422:ARG:NH2	3:H:426:GLU:OE2	2.42	0.52
6:N:138:PRO:HB2	6:N:147:CYS:HB2	1.92	0.52
2:G:58:LEU:HA	2:G:61:HIS:HD2	1.75	0.52
1:A:146:SER:OG	1:A:168:GLY:O	2.27	0.52
1:C:68:ARG:NH2	4:K:20:G:O6	2.43	0.52
2:I:112:LEU:HD22	2:I:118:LEU:HD22	1.91	0.52
5:L:37:DA:H2"	5:L:38:DG:C8	2.45	0.52
1:C:11:PHE:HB3	1:C:180:CYS:HB3	1.92	0.52
1:E:11:PHE:HB3	1:E:180:CYS:HB3	1.92	0.52
2:G:112:LEU:HD22	2:G:118:LEU:HD22	1.91	0.52
1:M:62:HIS:HD2	1:M:105:ARG:HA	1.75	0.52
1:B:150:MET:HE2	1:C:68:ARG:HG3	1.91	0.52
1:C:210:PHE:O	1:C:214:HIS:NE2	2.37	0.52
1:D:11:PHE:HB3	1:D:180:CYS:HB3	1.92	0.52
1:F:11:PHE:HB3	1:F:180:CYS:HB3	1.92	0.52
2:I:58:LEU:HA	2:I:61:HIS:HD2	1.75	0.52
1:M:55:GLN:HG2	1:M:73:LEU:HD13	1.91	0.52
1:B:11:PHE:HB3	1:B:180:CYS:HB3	1.92	0.51
2:J:52:PHE:HA	2:J:55:LEU:HB2	1.92	0.51
1:B:69:GLU:HG3	1:M:163:ASP:HA	1.92	0.51
1:E:156:LYS:NZ	5:L:11:DG:OP1	2.43	0.51
1:F:146:SER:OG	1:F:168:GLY:O	2.27	0.51
3:H:47:ASP:OD1	3:H:47:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:LEU:HA	2:J:61:HIS:HD2	1.75	0.51
2:J:94:ASN:O	2:J:98:GLN:N	2.36	0.51
4:K:3:U:OP1	1:M:121:ASN:ND2	2.43	0.51
5:L:38:DG:C8	5:L:38:DG:H5'	2.45	0.51
1:B:16:GLN:OE1	1:C:135:ARG:NH1	2.44	0.51
1:M:43:ASP:OD2	1:M:47:LYS:NZ	2.43	0.51
1:M:242:SER:OG	1:M:246:ARG:NH1	2.43	0.51
3:H:295:ASP:N	3:H:295:ASP:OD1	2.37	0.51
1:M:70:LYS:O	1:M:74:ASN:ND2	2.43	0.51
3:H:514:ARG:HG2	2:J:42:GLY:HA2	1.93	0.51
6:N:23:ARG:NH1	6:N:142:CYS:SG	2.84	0.51
3:H:30:ILE:HD13	3:H:158:SER:HB2	1.92	0.51
3:H:532:LEU:HA	3:H:535:GLU:HG2	1.92	0.51
1:M:249:VAL:HG13	1:M:266:VAL:HG22	1.91	0.51
1:E:148:THR:HA	1:E:167:MET:HA	1.92	0.51
3:H:220:PRO:HB2	3:H:223:SER:HB3	1.92	0.51
3:H:424:LYS:HB2	3:H:499:GLY:HA2	1.93	0.51
4:K:3:U:O2'	6:N:36:ASN:OD1	2.24	0.51
2:I:110:GLN:HA	2:J:80:ARG:NH1	2.27	0.50
1:E:21:ASN:OD1	1:E:31:ARG:NE	2.38	0.50
3:H:383:ASN:HB3	3:H:433:ARG:HG3	1.93	0.50
1:M:99:ARG:HE	1:M:125:VAL:HG22	1.76	0.50
1:E:52:ASN:ND2	1:E:213:ASP:OD2	2.38	0.50
2:I:13:VAL:HG11	2:I:85:HIS:HB2	1.93	0.50
1:F:52:ASN:ND2	1:F:213:ASP:OD2	2.38	0.50
1:E:153:THR:HG21	5:L:13:DG:H2''	1.92	0.50
1:B:23:ASP:HB3	1:B:26:ALA:HB3	1.94	0.50
1:B:257:VAL:HG11	1:C:35:GLN:HG2	1.93	0.50
1:E:64:ASP:HB2	1:E:106:TYR:HA	1.94	0.50
1:A:179:ARG:NH2	1:A:244:PHE:O	2.45	0.50
1:D:31:ARG:NH2	4:K:33:U:OP2	2.45	0.50
2:G:119:LYS:O	2:G:123:ASN:ND2	2.45	0.50
3:H:234:LYS:HB3	3:H:238:PHE:HB2	1.94	0.50
2:J:13:VAL:HG11	2:J:85:HIS:HB2	1.93	0.50
1:B:142:THR:H	3:H:549:HIS:CE1	2.30	0.50
1:D:179:ARG:NH2	1:D:244:PHE:O	2.45	0.50
1:F:64:ASP:HB2	1:F:106:TYR:HA	1.94	0.50
2:G:13:VAL:HG11	2:G:85:HIS:HB2	1.93	0.50
2:G:52:PHE:HA	2:G:55:LEU:HB2	1.92	0.50
5:L:43:DC:H2'	5:L:44:DC:C5	2.47	0.50
5:L:47:DG:H2''	5:L:48:DA:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:51:DT:H2'	5:L:52:DT:H71	1.93	0.50
1:B:64:ASP:HB2	1:B:106:TYR:HA	1.94	0.50
1:D:210:PHE:O	1:D:214:HIS:NE2	2.37	0.50
1:E:24:PRO:HA	4:K:39:U:C5	2.46	0.50
3:H:481:ILE:HD13	3:H:516:LEU:HD11	1.94	0.49
6:N:173:TYR:HB2	6:N:192:PHE:CD1	2.47	0.49
2:I:52:PHE:HA	2:I:55:LEU:HB2	1.92	0.49
1:C:21:ASN:OD1	1:C:31:ARG:NE	2.38	0.49
1:F:41:VAL:HB	1:F:134:SER:HB2	1.94	0.49
2:I:44:ALA:HA	2:I:51:VAL:HG21	1.95	0.49
1:B:179:ARG:NH2	1:B:244:PHE:O	2.45	0.49
3:H:85:TYR:HE2	3:H:154:GLY:H	1.59	0.49
3:H:340:ARG:O	6:N:64:ASN:ND2	2.45	0.49
1:M:110:ARG:HA	1:M:192:THR:HB	1.95	0.49
6:N:37:ILE:HG23	6:N:138:PRO:HB3	1.94	0.49
1:A:215:SER:OG	1:A:216:ALA:N	2.45	0.49
1:B:215:SER:OG	1:B:216:ALA:N	2.45	0.49
1:A:64:ASP:HB2	1:A:106:TYR:HA	1.94	0.49
1:B:168:GLY:HA3	5:L:36:DA:N6	2.28	0.49
1:C:215:SER:OG	1:C:216:ALA:N	2.45	0.49
1:D:153:THR:HG23	1:E:73:LEU:HD12	1.94	0.49
3:H:403:ASP:O	3:H:407:ASN:ND2	2.44	0.49
1:M:135:ARG:HH12	6:N:11:LEU:HD13	1.78	0.49
1:M:146:SER:HA	1:M:169:ARG:HA	1.95	0.49
1:M:252:LYS:HG2	1:M:265:LEU:HG	1.95	0.49
1:A:41:VAL:HB	1:A:134:SER:HB2	1.94	0.49
1:D:41:VAL:HB	1:D:134:SER:HB2	1.95	0.49
1:F:210:PHE:O	1:F:214:HIS:NE2	2.37	0.49
3:H:420:LEU:HD21	3:H:555:GLN:HB2	1.95	0.49
3:H:537:ARG:HB3	2:J:110:GLN:HB2	1.94	0.49
2:I:119:LYS:O	2:I:123:ASN:ND2	2.45	0.49
2:J:119:LYS:O	2:J:123:ASN:ND2	2.45	0.49
1:C:146:SER:OG	1:C:168:GLY:O	2.27	0.49
1:D:215:SER:OG	1:D:216:ALA:N	2.45	0.49
3:H:224:VAL:HG13	3:H:229:PHE:HB3	1.95	0.49
1:M:15:VAL:HG11	1:M:20:PRO:HG3	1.94	0.49
1:M:214:HIS:HE1	1:M:221:MET:H	1.60	0.49
1:B:156:LYS:NZ	5:L:35:DC:OP1	2.46	0.49
1:B:210:PHE:O	1:B:214:HIS:NE2	2.37	0.49
1:E:179:ARG:NH2	1:E:244:PHE:O	2.45	0.49
6:N:56:ILE:HD13	6:N:161:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PRO:HG3	1:A:31:ARG:HG2	1.95	0.48
1:A:52:ASN:ND2	1:A:213:ASP:OD2	2.38	0.48
1:E:215:SER:OG	1:E:216:ALA:N	2.45	0.48
1:F:179:ARG:NH2	1:F:244:PHE:O	2.45	0.48
1:M:45:CYS:SG	1:M:49:LYS:NZ	2.81	0.48
1:A:165:ARG:HB2	5:L:22:DA:H1'	1.95	0.48
1:B:146:SER:OG	1:B:168:GLY:O	2.27	0.48
1:C:64:ASP:HB2	1:C:106:TYR:HA	1.94	0.48
1:E:146:SER:OG	1:E:168:GLY:O	2.27	0.48
3:H:25:PHE:HA	3:H:64:PRO:HA	1.94	0.48
3:H:573:ASP:O	3:H:577:ASN:ND2	2.46	0.48
3:H:395:SER:OG	1:M:169:ARG:NH2	2.46	0.48
1:D:52:ASN:ND2	1:D:213:ASP:OD2	2.38	0.48
1:E:41:VAL:HB	1:E:134:SER:HB2	1.94	0.48
4:K:33:U:H1'	4:K:34:C:C6	2.48	0.48
1:A:210:PHE:O	1:A:214:HIS:NE2	2.37	0.48
1:A:214:HIS:CE1	1:A:221:MET:H	2.32	0.48
2:G:59:LEU:HD21	2:G:79:ILE:HD13	1.96	0.48
2:J:44:ALA:HA	2:J:51:VAL:HG21	1.95	0.48
1:C:179:ARG:NH2	1:C:244:PHE:O	2.45	0.48
1:D:49:LYS:HB3	1:D:209:MET:HB2	1.96	0.48
1:E:152:VAL:HB	1:E:164:ASN:HB3	1.95	0.48
1:E:214:HIS:CE1	1:E:221:MET:H	2.32	0.48
1:F:49:LYS:HB3	1:F:209:MET:HB2	1.96	0.48
1:B:252:LYS:HB3	1:B:253:ASP:H	1.52	0.48
2:G:28:ALA:HB1	2:G:65:LYS:HD3	1.96	0.48
2:I:24:ILE:HD13	2:I:59:LEU:HD11	1.95	0.48
1:M:145:HIS:ND1	1:M:172:THR:OG1	2.42	0.48
1:A:34:PRO:HB3	2:J:47:THR:HG23	1.96	0.48
2:G:24:ILE:HD13	2:G:59:LEU:HD11	1.95	0.48
2:J:28:ALA:HB1	2:J:65:LYS:HD3	1.96	0.48
1:A:49:LYS:HB3	1:A:209:MET:HB2	1.96	0.48
1:D:85:ASN:OD1	1:D:85:ASN:N	2.47	0.48
1:E:99:ARG:HG3	1:E:116:MET:HE1	1.96	0.48
1:F:99:ARG:HG3	1:F:116:MET:HE1	1.96	0.48
1:F:270:ASP:OD1	1:F:270:ASP:N	2.38	0.48
2:G:44:ALA:HA	2:G:51:VAL:HG21	1.95	0.48
4:K:6:A:N1	6:N:73:LYS:HG2	2.29	0.48
1:M:64:ASP:OD2	1:M:105:ARG:NH2	2.47	0.48
1:M:137:ILE:HD11	1:M:179:ARG:HD2	1.96	0.48
7:O:20:DA:H5''	7:O:21:DA:H4'	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:HG3	1:C:116:MET:HE1	1.96	0.48
2:J:59:LEU:HD21	2:J:79:ILE:HD13	1.96	0.48
6:N:27:PRO:HG2	6:N:168:PHE:HB3	1.96	0.48
1:D:64:ASP:HB2	1:D:106:TYR:HA	1.94	0.47
1:E:85:ASN:OD1	1:E:85:ASN:N	2.47	0.47
2:I:28:ALA:HB1	2:I:65:LYS:HD3	1.96	0.47
1:B:41:VAL:HB	1:B:134:SER:HB2	1.94	0.47
1:B:49:LYS:HB3	1:B:209:MET:HB2	1.96	0.47
4:K:1:G:C2	6:N:43:TRP:HB3	2.49	0.47
3:H:506:ILE:HD12	2:J:95:LEU:HB3	1.96	0.47
1:A:147:ILE:HD11	4:K:31:C:C5	2.49	0.47
3:H:514:ARG:HH22	2:J:46:SER:HB3	1.79	0.47
1:C:41:VAL:HB	1:C:134:SER:HB2	1.94	0.47
1:C:52:ASN:ND2	1:C:213:ASP:OD2	2.38	0.47
1:F:215:SER:OG	1:F:216:ALA:N	2.45	0.47
3:H:69:ARG:NH1	3:H:83:ASP:OD1	2.47	0.47
3:H:226:LEU:HD13	6:N:71:GLY:HA3	1.97	0.47
3:H:483:ALA:HA	3:H:489:LEU:HD12	1.96	0.47
1:M:120:LYS:HB3	6:N:183:ARG:HG2	1.97	0.47
1:E:49:LYS:HB3	1:E:209:MET:HB2	1.96	0.47
1:M:51:ARG:NE	1:M:108:ASP:OD1	2.47	0.47
1:B:85:ASN:OD1	1:B:85:ASN:N	2.47	0.47
1:B:99:ARG:HG3	1:B:116:MET:HE1	1.96	0.47
1:B:168:GLY:HA3	5:L:36:DA:C6	2.49	0.47
1:C:214:HIS:CE1	1:C:221:MET:H	2.31	0.47
1:D:99:ARG:HG3	1:D:116:MET:HE1	1.96	0.47
3:H:12:ARG:NH2	3:H:275:GLY:O	2.43	0.47
2:I:59:LEU:HD21	2:I:79:ILE:HD13	1.96	0.47
1:D:270:ASP:OD1	1:D:270:ASP:N	2.38	0.47
3:H:331:SER:N	3:H:338:VAL:O	2.46	0.47
3:H:429:ILE:HD11	3:H:498:PHE:CZ	2.50	0.47
3:H:522:LYS:HG3	5:L:28:DC:P	2.55	0.47
6:N:165:THR:OG1	6:N:197:ALA:O	2.29	0.47
3:H:469:TYR:HE1	3:H:560:ILE:HG22	1.80	0.47
2:J:24:ILE:HD13	2:J:59:LEU:HD11	1.95	0.47
1:M:62:HIS:O	1:M:63:HIS:ND1	2.47	0.47
1:C:14:ASP:OD1	1:C:14:ASP:N	2.48	0.47
1:C:49:LYS:HB3	1:C:209:MET:HB2	1.96	0.47
1:D:146:SER:OG	1:D:168:GLY:O	2.27	0.47
1:F:70:LYS:HA	1:F:70:LYS:HD3	1.63	0.47
1:M:9:PHE:CE1	1:M:11:PHE:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ARG:HG3	1:A:116:MET:HE1	1.96	0.46
1:C:169:ARG:HH21	3:H:515:LEU:HG	1.79	0.46
1:F:230:GLU:OE1	1:F:280:ARG:NH2	2.46	0.46
1:M:33:ASP:N	1:M:38:GLU:O	2.47	0.46
1:M:109:ILE:HG23	1:M:114:ALA:HB2	1.97	0.46
1:E:147:ILE:HD11	4:K:43:C:C5	2.50	0.46
1:F:214:HIS:CE1	1:F:221:MET:H	2.32	0.46
4:K:27:G:O6	5:L:28:DC:N4	2.47	0.46
6:N:14:PHE:O	6:N:26:TYR:N	2.46	0.46
1:A:7:TYR:HB2	1:A:184:ILE:HD12	1.98	0.46
1:B:243:LEU:HD21	1:B:277:LYS:HE3	1.98	0.46
2:I:17:LEU:HD21	2:I:56:MET:HE1	1.97	0.46
6:N:129:ALA:HB3	6:N:151:LEU:HD22	1.98	0.46
6:N:168:PHE:HD2	6:N:194:GLN:HE21	1.64	0.46
1:B:7:TYR:HB2	1:B:184:ILE:HD12	1.98	0.46
1:B:143:LEU:HD21	1:C:34:PRO:HD3	1.97	0.46
1:B:214:HIS:CE1	1:B:221:MET:H	2.32	0.46
1:C:146:SER:HA	1:C:169:ARG:HA	1.97	0.46
1:D:214:HIS:CE1	1:D:221:MET:H	2.32	0.46
1:D:252:LYS:HB3	1:D:253:ASP:H	1.52	0.46
1:E:7:TYR:HB2	1:E:184:ILE:HD12	1.98	0.46
3:H:407:ASN:O	3:H:409:ARG:NH1	2.48	0.46
3:H:420:LEU:O	3:H:424:LYS:HG2	2.15	0.46
2:I:29:ASN:N	2:I:29:ASN:OD1	2.49	0.46
2:J:17:LEU:HD21	2:J:56:MET:HE1	1.98	0.46
5:L:42:DA:C6	1:M:168:GLY:HA2	2.50	0.46
1:A:53:PHE:O	1:A:57:THR:OG1	2.26	0.46
1:D:166:THR:HB	5:L:18:DG:H21	1.80	0.46
2:I:107:HIS:NE2	2:J:86:CYS:O	2.49	0.46
1:A:257:VAL:HG21	1:D:35:GLN:HG2	1.97	0.46
1:C:34:PRO:HA	2:J:95:LEU:HD23	1.97	0.46
1:D:14:ASP:OD1	1:D:14:ASP:N	2.48	0.46
1:D:68:ARG:HH12	1:E:124:GLN:NE2	2.14	0.46
1:D:149:ARG:CZ	5:L:19:DG:H21	2.28	0.46
1:D:258:VAL:O	1:D:259:ARG:NH1	2.49	0.46
1:E:211:ASP:O	1:F:6:ARG:NH1	2.48	0.46
3:H:70:SER:HB3	5:L:48:DA:C2	2.50	0.46
3:H:445:ILE:HG12	3:H:450:LEU:HD23	1.98	0.46
1:F:125:VAL:O	4:K:41:G:O2'	2.27	0.46
3:H:474:LEU:HD13	3:H:540:LEU:HD13	1.97	0.46
1:B:24:PRO:HG3	4:K:15:A:H2'	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:VAL:O	1:B:259:ARG:NH1	2.49	0.46
1:F:7:TYR:HB2	1:F:184:ILE:HD12	1.98	0.46
3:H:40:GLY:HA2	3:H:130:PHE:HB2	1.97	0.46
3:H:205:ALA:HB1	3:H:247:MET:HE3	1.98	0.46
3:H:338:VAL:HA	6:N:22:GLU:HG3	1.97	0.46
3:H:541:GLU:HG3	2:J:2:GLY:HA3	1.98	0.46
4:K:4:G:H1	1:M:122:ALA:HB3	1.81	0.46
4:K:6:A:C2	1:M:115:VAL:HG21	2.51	0.46
1:C:7:TYR:HB2	1:C:184:ILE:HD12	1.98	0.46
3:H:523:LEU:HD12	3:H:529:ALA:HB2	1.97	0.46
4:K:4:G:OP2	6:N:36:ASN:ND2	2.49	0.46
1:C:118:THR:OG1	1:C:119:GLY:N	2.49	0.45
1:C:165:ARG:HH11	4:K:27:G:H21	1.64	0.45
1:E:14:ASP:OD1	1:E:14:ASP:N	2.48	0.45
1:E:252:LYS:HB3	1:E:253:ASP:H	1.52	0.45
3:H:42:PHE:CG	3:H:140:VAL:HG22	2.52	0.45
3:H:229:PHE:CE1	6:N:90:ARG:HD2	2.50	0.45
3:H:404:ALA:O	3:H:443:ARG:NH1	2.44	0.45
1:A:230:GLU:OE1	1:A:280:ARG:NH2	2.46	0.45
1:C:156:LYS:HD3	3:H:488:GLY:HA3	1.98	0.45
1:E:118:THR:OG1	1:E:119:GLY:N	2.49	0.45
3:H:310:SER:O	3:H:314:GLY:N	2.47	0.45
3:H:424:LYS:O	3:H:427:GLN:NE2	2.48	0.45
3:H:515:LEU:HA	3:H:518:HIS:HD2	1.81	0.45
1:M:9:PHE:CE2	1:M:182:GLY:HA3	2.51	0.45
1:A:85:ASN:OD1	1:A:85:ASN:N	2.47	0.45
1:B:118:THR:OG1	1:B:119:GLY:N	2.49	0.45
1:C:144:GLU:HG2	1:C:171:PHE:CE2	2.51	0.45
1:C:258:VAL:O	1:C:259:ARG:NH1	2.49	0.45
2:G:113:PHE:HB2	2:I:80:ARG:NH1	2.21	0.45
3:H:464:ARG:HH21	3:H:557:LEU:HD21	1.82	0.45
3:H:515:LEU:HD22	5:L:29:DC:H2"	1.97	0.45
1:M:237:ASP:OD1	1:M:237:ASP:N	2.50	0.45
1:F:258:VAL:O	1:F:259:ARG:NH1	2.49	0.45
2:J:14:LEU:HB3	2:J:101:PHE:CE2	2.52	0.45
5:L:42:DA:N1	1:M:168:GLY:HA2	2.31	0.45
1:A:258:VAL:O	1:A:259:ARG:NH1	2.49	0.45
1:B:46:LEU:HB3	1:B:209:MET:HE1	1.99	0.45
1:B:211:ASP:HB3	1:C:6:ARG:NH2	2.32	0.45
1:C:85:ASN:OD1	1:C:85:ASN:N	2.47	0.45
3:H:31:PRO:HA	3:H:58:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:489:LEU:HB3	3:H:492:THR:HG22	1.97	0.45
1:F:85:ASN:OD1	1:F:85:ASN:N	2.47	0.45
5:L:52:DT:H2''	5:L:53:DC:C5	2.52	0.45
6:N:16:ARG:HG2	6:N:26:TYR:CD1	2.52	0.45
6:N:205:PRO:HA	6:N:206:PRO:HD3	1.89	0.45
1:D:7:TYR:HB2	1:D:184:ILE:HD12	1.98	0.45
1:E:258:VAL:O	1:E:259:ARG:NH1	2.49	0.45
1:M:41:VAL:HB	1:M:134:SER:HB2	1.98	0.45
1:B:74:ASN:ND2	1:M:154:ASN:OD1	2.49	0.45
3:H:225:ASN:ND2	5:L:49:DA:H2'	2.32	0.45
5:L:38:DG:H2''	5:L:39:DC:C5	2.51	0.45
6:N:23:ARG:N	6:N:91:ALA:O	2.49	0.45
6:N:53:LYS:HB2	6:N:202:ILE:HG22	1.98	0.45
1:A:146:SER:HA	1:A:169:ARG:HA	1.99	0.45
1:B:277:LYS:HB2	1:B:277:LYS:HE2	1.71	0.45
1:D:46:LEU:HB3	1:D:209:MET:HE1	1.99	0.45
1:E:168:GLY:HA3	5:L:12:DG:C5	2.51	0.45
1:F:118:THR:OG1	1:F:119:GLY:N	2.49	0.45
2:G:77:TRP:HA	2:G:80:ARG:HE	1.82	0.45
2:G:95:LEU:HB3	2:I:49:ILE:HD12	1.99	0.45
3:H:449:ARG:HD3	1:M:141:MET:HG3	1.98	0.45
2:I:14:LEU:HB3	2:I:101:PHE:CE2	2.52	0.45
5:L:12:DG:H2''	5:L:13:DG:C8	2.51	0.45
1:M:115:VAL:HB	6:N:73:LYS:HD3	1.99	0.45
1:A:20:PRO:HB2	1:A:21:ASN:H	1.67	0.45
1:A:153:THR:HG21	5:L:25:DC:H2''	1.98	0.45
1:D:118:THR:OG1	1:D:119:GLY:N	2.49	0.45
1:D:148:THR:HG22	1:D:167:MET:HE3	1.98	0.45
2:G:14:LEU:HB3	2:G:101:PHE:CE2	2.52	0.45
3:H:476:ALA:HB2	3:H:562:TYR:HA	1.98	0.45
1:M:12:LEU:HD23	1:M:177:LEU:HD21	2.00	0.45
1:C:46:LEU:HB3	1:C:209:MET:HE1	1.99	0.44
1:E:146:SER:HA	1:E:169:ARG:HA	2.00	0.44
1:E:210:PHE:O	1:E:214:HIS:NE2	2.37	0.44
1:E:218:ARG:NH2	4:K:38:C:H1'	2.33	0.44
2:G:17:LEU:HD21	2:G:56:MET:HE1	1.97	0.44
2:I:77:TRP:HA	2:I:80:ARG:HE	1.82	0.44
1:D:252:LYS:HG3	1:D:265:LEU:HB2	2.00	0.44
3:H:241:PRO:HG2	6:N:189:GLU:HB2	2.00	0.44
3:H:340:ARG:NH1	1:M:25:ASP:OD1	2.51	0.44
3:H:396:ASP:HB2	1:M:169:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:130:GLN:HB2	6:N:143:ARG:HH21	1.82	0.44
1:M:270:ASP:HB3	1:M:279:LEU:HD13	2.00	0.44
1:B:252:LYS:HG3	1:B:265:LEU:HB2	2.00	0.44
1:C:163:ASP:OD2	1:D:121:ASN:ND2	2.47	0.44
1:E:20:PRO:HB2	1:E:21:ASN:H	1.67	0.44
1:F:252:LYS:HG3	1:F:265:LEU:HB2	2.00	0.44
1:M:170:LYS:HD3	1:M:217:ALA:HA	2.00	0.44
1:A:252:LYS:HG3	1:A:265:LEU:HB2	2.00	0.44
1:B:188:PHE:HE1	1:M:72:ILE:HG23	1.82	0.44
3:H:83:ASP:HB3	3:H:84:HIS:H	1.55	0.44
3:H:130:PHE:O	3:H:137:LYS:NZ	2.41	0.44
3:H:344:GLU:OE1	6:N:166:GLN:NE2	2.51	0.44
1:A:46:LEU:HB3	1:A:209:MET:HE1	1.99	0.44
1:A:118:THR:OG1	1:A:119:GLY:N	2.49	0.44
1:E:46:LEU:HB3	1:E:209:MET:HE1	1.99	0.44
1:F:46:LEU:HB3	1:F:209:MET:HE1	1.99	0.44
3:H:384:LEU:HA	3:H:422:ARG:HG3	1.99	0.44
3:H:419:ALA:HB3	3:H:437:LEU:HD21	1.99	0.44
2:I:102:ALA:HB1	2:J:56:MET:HE2	1.99	0.44
2:J:58:LEU:HB3	2:J:62:HIS:CE1	2.53	0.44
5:L:20:DC:H2''	5:L:21:DG:C8	2.53	0.44
1:B:147:ILE:HD12	1:C:44:VAL:HG11	1.98	0.44
1:C:152:VAL:HG21	1:C:158:ALA:HA	1.99	0.44
1:D:125:VAL:O	4:K:29:G:H4'	2.18	0.44
1:E:230:GLU:OE1	1:E:280:ARG:NH2	2.46	0.44
3:H:220:PRO:HD2	5:L:48:DA:H4'	2.00	0.44
3:H:336:ARG:HD2	6:N:21:VAL:HB	1.99	0.44
4:K:6:A:C4	1:M:115:VAL:HG21	2.52	0.44
1:B:259:ARG:NH2	1:C:35:GLN:HE21	2.15	0.44
1:D:142:THR:HG22	1:D:144:GLU:HG3	2.00	0.44
1:D:154:ASN:OD1	1:E:74:ASN:ND2	2.51	0.44
2:G:2:GLY:O	2:G:107:HIS:ND1	2.51	0.44
3:H:403:ASP:OD1	3:H:407:ASN:ND2	2.51	0.44
2:I:2:GLY:O	2:I:107:HIS:ND1	2.51	0.44
2:J:29:ASN:OD1	2:J:29:ASN:N	2.49	0.44
2:J:74:GLN:HE22	2:J:119:LYS:HG3	1.83	0.44
5:L:45:DC:O3'	5:L:46:DT:H2'	2.18	0.44
5:L:47:DG:H2''	5:L:48:DA:N7	2.33	0.44
1:M:55:GLN:HE22	1:M:68:ARG:HB2	1.83	0.44
1:B:258:VAL:HG11	1:B:264:TYR:CE1	2.53	0.44
1:E:44:VAL:HG11	4:K:37:C:H2'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:58:LEU:HB3	2:G:62:HIS:CE1	2.53	0.44
1:M:47:LYS:HG3	1:M:131:LEU:HD22	1.99	0.44
6:N:10:ASP:O	6:N:97:ASP:N	2.46	0.44
1:F:252:LYS:HB3	1:F:253:ASP:H	1.53	0.43
3:H:181:GLN:HE21	3:H:185:THR:HG21	1.82	0.43
3:H:257:LEU:HD21	3:H:274:TRP:HB3	2.00	0.43
1:M:130:GLN:OE1	6:N:136:HIS:NE2	2.50	0.43
3:H:52:LYS:HG3	3:H:53:VAL:H	1.82	0.43
2:I:45:SER:HB3	2:J:57:ARG:NH2	2.31	0.43
1:M:9:PHE:HE1	1:M:11:PHE:HB2	1.83	0.43
1:M:25:ASP:HA	6:N:66:ARG:HD3	1.99	0.43
1:E:9:PHE:HA	1:E:228:VAL:HA	2.01	0.43
1:E:258:VAL:HG11	1:E:264:TYR:CE1	2.53	0.43
3:H:191:GLN:HB3	3:H:204:ILE:HB	1.99	0.43
2:J:77:TRP:HA	2:J:80:ARG:HE	1.82	0.43
5:L:57:DT:H2''	5:L:58:DG:C8	2.52	0.43
1:B:14:ASP:OD1	1:B:14:ASP:N	2.48	0.43
1:C:9:PHE:HA	1:C:228:VAL:HA	2.01	0.43
1:C:51:ARG:NH2	4:K:19:U:OP1	2.48	0.43
1:C:252:LYS:HB3	1:C:253:ASP:H	1.52	0.43
1:C:252:LYS:HG3	1:C:265:LEU:HB2	2.00	0.43
1:D:130:GLN:NE2	4:K:30:G:OP1	2.46	0.43
1:E:252:LYS:HG3	1:E:265:LEU:HB2	2.00	0.43
5:L:53:DC:H2''	5:L:54:DA:C5	2.54	0.43
1:A:14:ASP:OD1	1:A:14:ASP:N	2.48	0.43
1:C:258:VAL:HG11	1:C:264:TYR:CE1	2.53	0.43
1:E:134:SER:HB3	1:E:178:TYR:HB3	2.01	0.43
2:G:29:ASN:N	2:G:29:ASN:OD1	2.49	0.43
3:H:462:ARG:O	3:H:542:HIS:NE2	2.52	0.43
3:H:481:ILE:HD11	3:H:532:LEU:HB3	2.00	0.43
2:I:58:LEU:HB3	2:I:62:HIS:CE1	2.53	0.43
1:M:62:HIS:HA	1:M:105:ARG:HA	1.99	0.43
1:A:152:VAL:HB	1:A:164:ASN:HB3	1.99	0.43
1:B:89:LYS:HB3	1:B:94:LYS:HB2	2.01	0.43
3:H:49:ARG:C	3:H:50:GLU:HG3	2.43	0.43
4:K:38:C:H2'	4:K:39:U:H4'	2.00	0.43
6:N:55:GLU:OE2	6:N:101:ARG:NH1	2.48	0.43
1:A:179:ARG:NH2	1:A:247:ILE:O	2.52	0.43
2:G:83:LEU:HD23	2:G:86:CYS:HB3	2.01	0.43
3:H:217:LYS:HD3	5:L:47:DG:H22	1.84	0.43
1:M:14:ASP:OD2	1:M:224:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:181:ASP:OD1	6:N:181:ASP:N	2.52	0.43
1:C:89:LYS:HB3	1:C:94:LYS:HB2	2.01	0.43
1:C:127:GLY:HA2	1:C:128:PRO:HD3	1.91	0.43
1:F:9:PHE:HA	1:F:228:VAL:HA	2.01	0.43
6:N:175:MET:HA	6:N:190:PRO:HD2	2.01	0.43
1:A:134:SER:HB3	1:A:178:TYR:HB3	2.01	0.43
1:B:179:ARG:NH2	1:B:247:ILE:O	2.52	0.43
1:C:179:ARG:NH2	1:C:247:ILE:O	2.52	0.43
1:E:246:ARG:HD2	1:E:273:LEU:HD23	2.01	0.43
2:G:74:GLN:HE22	2:G:119:LYS:HG3	1.83	0.43
2:G:102:ALA:HB1	2:I:56:MET:HE2	2.01	0.43
3:H:136:GLU:O	3:H:140:VAL:HG23	2.19	0.43
1:A:89:LYS:HB3	1:A:94:LYS:HB2	2.01	0.43
1:A:258:VAL:HG11	1:A:264:TYR:CE1	2.53	0.43
1:C:87:LYS:HB3	1:C:87:LYS:HE3	1.63	0.43
1:D:179:ARG:NH2	1:D:247:ILE:O	2.52	0.43
1:F:258:VAL:HG11	1:F:264:TYR:CE1	2.53	0.43
2:I:102:ALA:HB1	2:J:56:MET:HG2	2.01	0.43
4:K:6:A:N6	6:N:73:LYS:HE2	2.33	0.43
1:M:152:VAL:HG22	1:M:164:ASN:HB3	2.00	0.43
1:C:170:LYS:HE2	1:C:217:ALA:HA	2.01	0.42
3:H:383:ASN:O	3:H:433:ARG:NH1	2.42	0.42
2:I:10:ILE:HD11	2:I:90:PRO:HD3	2.01	0.42
2:I:74:GLN:HE22	2:I:119:LYS:HG3	1.83	0.42
2:J:2:GLY:O	2:J:107:HIS:ND1	2.51	0.42
2:J:83:LEU:HD23	2:J:86:CYS:HB3	2.01	0.42
1:M:38:GLU:HA	1:M:139:PRO:HA	2.00	0.42
1:A:246:ARG:HD2	1:A:273:LEU:HD23	2.01	0.42
1:B:9:PHE:HA	1:B:228:VAL:HA	2.01	0.42
1:D:170:LYS:HE2	1:D:217:ALA:HA	2.01	0.42
1:D:246:ARG:HD2	1:D:273:LEU:HD23	2.01	0.42
1:E:170:LYS:HE2	1:E:217:ALA:HA	2.01	0.42
1:F:179:ARG:NH2	1:F:247:ILE:O	2.52	0.42
5:L:9:DG:H2'	5:L:10:DA:C4	2.54	0.42
6:N:95:LEU:HD23	6:N:95:LEU:HA	1.89	0.42
1:D:44:VAL:HG12	4:K:31:C:OP2	2.18	0.42
1:D:89:LYS:HB3	1:D:94:LYS:HB2	2.01	0.42
1:D:258:VAL:HG11	1:D:264:TYR:CE1	2.53	0.42
1:E:67:ILE:HG13	1:E:71:GLY:HA3	2.02	0.42
1:E:89:LYS:HB3	1:E:94:LYS:HB2	2.01	0.42
3:H:62:LEU:O	3:H:171:GLN:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:425:ALA:HB1	5:L:35:DC:H2''	2.02	0.42
2:I:83:LEU:HD23	2:I:86:CYS:HB3	2.01	0.42
7:O:18:DA:H2''	7:O:19:DA:C5	2.54	0.42
1:B:67:ILE:HG13	1:B:71:GLY:HA3	2.01	0.42
1:C:67:ILE:HG13	1:C:71:GLY:HA3	2.01	0.42
1:E:179:ARG:NH2	1:E:247:ILE:O	2.52	0.42
1:M:65:ILE:O	1:M:67:ILE:N	2.52	0.42
1:M:163:ASP:OD1	1:M:163:ASP:N	2.41	0.42
1:M:167:MET:HE3	1:M:168:GLY:H	1.85	0.42
1:M:230:GLU:HB3	1:M:278:LEU:HB2	2.01	0.42
1:E:167:MET:HE1	1:F:25:ASP:OD2	2.19	0.42
2:J:21:LEU:HD23	2:J:59:LEU:HD13	2.02	0.42
1:M:255:VAL:HG21	1:M:263:ASP:HA	2.02	0.42
1:D:146:SER:HA	1:D:169:ARG:HA	2.01	0.42
1:E:149:ARG:NH2	5:L:12:DG:H21	2.17	0.42
3:H:192:LYS:HB3	3:H:193:GLY:H	1.62	0.42
3:H:265:ARG:NH2	7:O:17:DA:O3'	2.53	0.42
1:M:31:ARG:HD3	6:N:65:ILE:HG23	2.01	0.42
1:A:170:LYS:HE2	1:A:217:ALA:HA	2.01	0.42
1:D:127:GLY:HA2	1:D:128:PRO:HD3	1.91	0.42
1:D:134:SER:HB3	1:D:178:TYR:HB3	2.01	0.42
3:H:92:ALA:HB1	3:H:95:LYS:HB2	2.02	0.42
3:H:282:GLU:OE1	3:H:284:SER:OG	2.30	0.42
3:H:364:VAL:HG21	3:H:564:HIS:HA	2.01	0.42
2:J:10:ILE:HD11	2:J:90:PRO:HD3	2.01	0.42
4:K:6:A:C5	1:M:115:VAL:HG11	2.55	0.42
1:B:147:ILE:HD12	1:C:44:VAL:HG21	2.00	0.42
1:C:20:PRO:HB2	1:C:21:ASN:H	1.67	0.42
1:C:134:SER:HB3	1:C:178:TYR:HB3	2.01	0.42
3:H:500:SER:O	3:H:504:THR:N	2.52	0.42
5:L:18:DG:H1'	5:L:19:DG:C8	2.55	0.42
1:B:134:SER:HB3	1:B:178:TYR:HB3	2.01	0.42
1:C:148:THR:HG21	4:K:27:G:C2	2.55	0.42
1:F:89:LYS:HB3	1:F:94:LYS:HB2	2.01	0.42
2:G:10:ILE:HD11	2:G:90:PRO:HD3	2.01	0.42
3:H:136:GLU:HA	3:H:139:LYS:HD3	2.01	0.42
3:H:469:TYR:OH	3:H:564:HIS:ND1	2.36	0.42
5:L:51:DT:C2'	5:L:52:DT:H71	2.50	0.42
6:N:29:ILE:HD13	6:N:102:ILE:HD11	2.02	0.42
7:O:17:DA:H2''	7:O:18:DA:C8	2.54	0.42
1:A:9:PHE:HA	1:A:228:VAL:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ARG:HG2	1:B:69:GLU:N	2.33	0.42
1:F:134:SER:HB3	1:F:178:TYR:HB3	2.01	0.42
3:H:217:LYS:HD2	7:O:14:DA:C5	2.55	0.42
3:H:476:ALA:HB3	3:H:565:GLU:HB3	2.01	0.42
3:H:551:ASN:O	3:H:555:GLN:HG3	2.20	0.42
4:K:11:G:O6	4:K:12:G:N1	2.52	0.42
4:K:40:C:H2'	4:K:41:G:C4	2.55	0.42
1:M:273:LEU:HD21	1:M:279:LEU:HD12	2.02	0.42
6:N:171:MET:HE3	6:N:171:MET:HB3	1.72	0.42
1:B:68:ARG:O	1:B:70:LYS:N	2.53	0.41
1:C:148:THR:HG21	4:K:27:G:N3	2.35	0.41
1:C:246:ARG:HD2	1:C:273:LEU:HD23	2.01	0.41
1:E:34:PRO:HG2	2:G:92:HIS:HD2	1.83	0.41
2:I:21:LEU:HD23	2:I:59:LEU:HD13	2.02	0.41
1:M:273:LEU:HB2	1:M:277:LYS:HB2	2.01	0.41
6:N:168:PHE:HB2	6:N:194:GLN:HG3	2.02	0.41
3:H:407:ASN:HB2	3:H:409:ARG:HG2	2.01	0.41
3:H:572:LYS:HA	3:H:572:LYS:HD2	1.90	0.41
5:L:32:DC:H2''	5:L:33:DG:C8	2.54	0.41
7:O:12:DT:H2'	7:O:13:DC:C6	2.55	0.41
1:A:55:GLN:HG2	1:D:187:HIS:HE1	1.86	0.41
1:B:215:SER:HB3	1:B:218:ARG:HG2	2.03	0.41
1:B:230:GLU:OE1	1:B:280:ARG:NH2	2.46	0.41
1:D:67:ILE:HG13	1:D:71:GLY:HA3	2.01	0.41
2:G:98:GLN:OE1	2:I:57:ARG:NH2	2.43	0.41
3:H:52:LYS:HD2	3:H:52:LYS:HA	1.94	0.41
3:H:343:HIS:HB2	3:H:350:LEU:HD21	2.02	0.41
2:I:71:ARG:HH12	2:I:118:LEU:HD23	1.85	0.41
2:J:71:ARG:HH12	2:J:118:LEU:HD23	1.85	0.41
1:M:259:ARG:HA	1:M:259:ARG:HD3	1.74	0.41
1:D:9:PHE:HA	1:D:228:VAL:HA	2.01	0.41
1:F:129:VAL:HG13	1:F:184:ILE:HG12	2.03	0.41
3:H:69:ARG:HA	3:H:77:VAL:HG21	2.02	0.41
3:H:489:LEU:HD13	3:H:492:THR:HG22	2.03	0.41
1:A:67:ILE:HG13	1:A:71:GLY:HA3	2.02	0.41
1:B:246:ARG:HD2	1:B:273:LEU:HD23	2.01	0.41
1:E:127:GLY:HA2	1:E:128:PRO:HD3	1.91	0.41
1:F:246:ARG:HD2	1:F:273:LEU:HD23	2.01	0.41
1:M:55:GLN:HE21	1:M:73:LEU:HD22	1.85	0.41
1:A:117:THR:OG1	5:L:32:DC:O2	2.35	0.41
1:C:230:GLU:OE1	1:C:280:ARG:NH2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:73:LYS:HD3	5:L:51:DT:H5''	2.02	0.41
6:N:140:LEU:HG	6:N:147:CYS:SG	2.60	0.41
1:B:68:ARG:HH21	1:C:124:GLN:HE21	1.69	0.41
1:B:69:GLU:HG2	1:B:70:LYS:HE2	2.02	0.41
1:D:129:VAL:HG13	1:D:184:ILE:HG12	2.02	0.41
1:E:206:LEU:HD23	1:E:206:LEU:HA	1.92	0.41
1:F:146:SER:HA	1:F:169:ARG:HA	2.01	0.41
3:H:493:ILE:O	3:H:497:TYR:HB2	2.21	0.41
1:B:53:PHE:O	1:B:57:THR:OG1	2.26	0.41
1:B:170:LYS:HE2	1:B:217:ALA:HA	2.01	0.41
1:C:19:ASN:HD22	1:C:171:PHE:HB2	1.86	0.41
1:D:19:ASN:HD22	1:D:171:PHE:HB2	1.86	0.41
1:D:34:PRO:HB3	2:I:47:THR:HG23	2.03	0.41
1:D:84:GLU:H	1:D:84:GLU:HG3	1.77	0.41
1:F:67:ILE:HG13	1:F:71:GLY:HA3	2.02	0.41
2:G:21:LEU:HD23	2:G:59:LEU:HD13	2.02	0.41
2:G:21:LEU:HD22	2:G:55:LEU:HD22	2.02	0.41
2:G:71:ARG:HH12	2:G:118:LEU:HD23	1.85	0.41
3:H:471:LEU:HB3	3:H:558:PHE:CE2	2.56	0.41
3:H:530:VAL:HG13	8:Q:1:DT:C4	2.55	0.41
3:H:545:ARG:NH2	2:J:96:GLU:OE1	2.54	0.41
2:I:21:LEU:HD22	2:I:55:LEU:HD22	2.02	0.41
4:K:5:A:OP1	6:N:143:ARG:N	2.34	0.41
6:N:126:LYS:HE2	6:N:126:LYS:HB2	1.89	0.41
1:D:230:GLU:OE1	1:D:280:ARG:NH2	2.46	0.41
3:H:247:MET:HA	3:H:250:TYR:CD1	2.56	0.41
3:H:412:PRO:HB3	1:M:144:GLU:CD	2.46	0.41
3:H:429:ILE:HD12	3:H:562:TYR:CD2	2.56	0.41
3:H:505:PRO:HG3	3:H:550:LEU:HG	2.02	0.41
2:I:41:PHE:HE1	2:J:56:MET:HB3	1.85	0.41
2:J:52:PHE:HA	2:J:55:LEU:HD12	2.03	0.41
1:A:129:VAL:HG13	1:A:184:ILE:HG12	2.02	0.40
1:F:170:LYS:HE2	1:F:217:ALA:HA	2.01	0.40
3:H:393:LEU:HD22	5:L:41:DG:C6	2.56	0.40
1:B:87:LYS:HE3	1:B:87:LYS:HB3	1.90	0.40
1:C:129:VAL:HG13	1:C:184:ILE:HG12	2.02	0.40
1:E:43:ASP:N	1:E:43:ASP:OD1	2.54	0.40
1:F:43:ASP:N	1:F:43:ASP:OD1	2.54	0.40
3:H:422:ARG:HA	3:H:422:ARG:HD2	1.91	0.40
4:K:7:A:O2'	6:N:69:GLU:HA	2.21	0.40
1:M:69:GLU:HB2	1:M:72:ILE:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:MET:HE3	1:A:116:MET:HB2	2.00	0.40
1:B:169:ARG:HH12	3:H:499:GLY:HA2	1.87	0.40
1:E:125:VAL:O	4:K:35:G:O2'	2.36	0.40
3:H:25:PHE:CZ	3:H:176:ARG:HG3	2.56	0.40
3:H:470:VAL:HG21	3:H:543:CYS:HB2	2.04	0.40
2:I:25:GLN:OE1	2:I:36:ILE:HG12	2.21	0.40
2:I:52:PHE:HA	2:I:55:LEU:HD12	2.03	0.40
1:M:129:VAL:O	6:N:143:ARG:NH2	2.55	0.40
1:M:224:ARG:NH1	1:M:261:PHE:HB2	2.37	0.40
6:N:68:ASN:HB3	6:N:87:ARG:HD2	2.03	0.40
1:B:19:ASN:HD22	1:B:171:PHE:HB2	1.86	0.40
3:H:80:LEU:HB3	3:H:81:LEU:H	1.71	0.40
3:H:170:CYS:HA	3:H:175:VAL:HG11	2.03	0.40
3:H:450:LEU:HD21	3:H:453:MET:HE2	2.02	0.40
2:J:35:THR:N	2:J:38:ASP:OD2	2.49	0.40
1:A:29:LEU:HB3	1:A:171:PHE:CE2	2.57	0.40
1:B:247:ILE:HG23	1:B:268:VAL:HG22	2.04	0.40
1:D:29:LEU:HB3	1:D:171:PHE:CE2	2.57	0.40
1:D:149:ARG:NH2	1:D:153:THR:OG1	2.54	0.40
1:E:177:LEU:HD23	1:E:249:VAL:HG11	2.04	0.40
1:F:67:ILE:H	1:F:67:ILE:HG12	1.67	0.40
2:J:21:LEU:HD22	2:J:55:LEU:HD22	2.02	0.40
1:M:30:PRO:HD2	1:M:142:THR:HG23	2.03	0.40
6:N:12:ALA:HB2	6:N:98:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	281/283 (99%)	224 (80%)	47 (17%)	10 (4%)	2 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/283 (99%)	225 (80%)	47 (17%)	9 (3%)	3	18
1	C	281/283 (99%)	230 (82%)	42 (15%)	9 (3%)	3	18
1	D	281/283 (99%)	226 (80%)	46 (16%)	9 (3%)	3	18
1	E	281/283 (99%)	224 (80%)	47 (17%)	10 (4%)	2	16
1	F	267/283 (94%)	215 (80%)	42 (16%)	10 (4%)	2	15
1	M	260/283 (92%)	209 (80%)	44 (17%)	7 (3%)	4	21
2	G	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
2	I	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
2	J	122/124 (98%)	118 (97%)	4 (3%)	0	100	100
3	H	580/582 (100%)	486 (84%)	74 (13%)	20 (3%)	3	17
6	N	203/205 (99%)	179 (88%)	19 (9%)	5 (2%)	4	22
All	All	3081/3140 (98%)	2572 (84%)	420 (14%)	89 (3%)	5	20

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	PRO
1	A	91	LYS
1	B	20	PRO
1	B	91	LYS
1	C	20	PRO
1	C	91	LYS
1	C	167	MET
1	D	20	PRO
1	D	91	LYS
1	E	20	PRO
1	E	91	LYS
1	F	20	PRO
1	F	91	LYS
6	N	23	ARG
1	A	68	ARG
1	A	167	MET
1	B	167	MET
1	C	69	GLU
1	E	68	ARG
1	F	68	ARG
1	F	167	MET
3	H	31	PRO

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Mol	Chain	Res	Type
3	H	69	ARG
3	H	192	LYS
3	H	201	ALA
3	H	266	ILE
1	A	118	THR
1	A	128	PRO
1	B	118	THR
1	B	128	PRO
1	B	160	GLU
1	C	118	THR
1	C	128	PRO
1	D	68	ARG
1	D	118	THR
1	D	128	PRO
1	D	167	MET
1	E	118	THR
1	E	128	PRO
1	F	118	THR
1	F	128	PRO
3	H	41	ASN
3	H	77	VAL
3	H	78	SER
3	H	83	ASP
3	H	221	PHE
3	H	231	SER
3	H	236	GLN
3	H	281	LEU
3	H	572	LYS
1	M	121	ASN
6	N	195	CYS
1	A	58	GLN
1	A	66	PHE
1	B	58	GLN
1	B	66	PHE
1	C	58	GLN
1	C	66	PHE
1	D	58	GLN
1	D	66	PHE
1	E	58	GLN
1	E	66	PHE
1	E	167	MET
1	F	58	GLN

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Mol	Chain	Res	Type
1	F	66	PHE
3	H	50	GLU
3	H	70	SER
3	H	80	LEU
1	M	20	PRO
6	N	77	ARG
6	N	183	ARG
1	A	23	ASP
1	F	23	ASP
3	H	98	GLU
1	M	31	ARG
1	M	66	PHE
1	M	115	VAL
1	M	160	GLU
6	N	82	TYR
3	H	321	GLY
1	E	162	GLY
1	A	176	GLY
1	B	176	GLY
1	C	176	GLY
1	D	176	GLY
1	E	176	GLY
1	F	176	GLY
1	M	176	GLY
3	H	123	GLY

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	245/245 (100%)	239 (98%)	6 (2%)	43	64
1	B	245/245 (100%)	239 (98%)	6 (2%)	43	64
1	C	245/245 (100%)	238 (97%)	7 (3%)	37	60
1	D	245/245 (100%)	239 (98%)	6 (2%)	43	64
1	E	245/245 (100%)	240 (98%)	5 (2%)	48	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	235/245 (96%)	230 (98%)	5 (2%)	47	66
1	M	229/245 (94%)	221 (96%)	8 (4%)	32	56
2	G	104/104 (100%)	99 (95%)	5 (5%)	23	50
2	I	104/104 (100%)	99 (95%)	5 (5%)	23	50
2	J	104/104 (100%)	99 (95%)	5 (5%)	23	50
3	H	475/475 (100%)	458 (96%)	17 (4%)	31	56
6	N	182/182 (100%)	176 (97%)	6 (3%)	33	57
All	All	2658/2684 (99%)	2577 (97%)	81 (3%)	37	59

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	65	ILE
1	A	66	PHE
1	A	67	ILE
1	A	93	GLU
1	A	259	ARG
1	B	15	VAL
1	B	65	ILE
1	B	66	PHE
1	B	67	ILE
1	B	93	GLU
1	B	259	ARG
1	C	15	VAL
1	C	65	ILE
1	C	66	PHE
1	C	67	ILE
1	C	153	THR
1	C	169	ARG
1	C	259	ARG
1	D	15	VAL
1	D	65	ILE
1	D	66	PHE
1	D	67	ILE
1	D	153	THR
1	D	259	ARG
1	E	15	VAL
1	E	65	ILE
1	E	66	PHE

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Mol	Chain	Res	Type
1	E	67	ILE
1	E	259	ARG
1	F	15	VAL
1	F	65	ILE
1	F	66	PHE
1	F	67	ILE
1	F	259	ARG
2	G	21	LEU
2	G	49	ILE
2	G	56	MET
2	G	96	GLU
2	G	114	THR
3	H	81	LEU
3	H	114	LEU
3	H	149	CYS
3	H	152	VAL
3	H	161	LEU
3	H	184	GLN
3	H	207	LEU
3	H	282	GLU
3	H	307	LEU
3	H	364	VAL
3	H	402	THR
3	H	413	VAL
3	H	456	LEU
3	H	466	ASP
3	H	514	ARG
3	H	566	THR
3	H	571	THR
2	I	21	LEU
2	I	49	ILE
2	I	56	MET
2	I	96	GLU
2	I	114	THR
2	J	21	LEU
2	J	49	ILE
2	J	56	MET
2	J	96	GLU
2	J	114	THR
1	M	15	VAL
1	M	46	LEU
1	M	110	ARG

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Mol	Chain	Res	Type
1	M	115	VAL
1	M	117	THR
1	M	166	THR
1	M	199	LEU
1	M	275	GLU
6	N	44	LYS
6	N	159	LEU
6	N	166	GLN
6	N	171	MET
6	N	193	TYR
6	N	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	74	ASN
1	A	83	GLN
1	A	187	HIS
1	B	74	ASN
1	B	83	GLN
1	B	187	HIS
1	C	83	GLN
1	C	124	GLN
1	C	130	GLN
1	C	181	HIS
1	D	21	ASN
1	D	74	ASN
1	D	83	GLN
1	D	187	HIS
1	D	212	HIS
1	D	231	HIS
1	E	35	GLN
1	E	74	ASN
1	E	83	GLN
1	E	124	GLN
1	E	187	HIS
1	E	220	GLN
1	E	231	HIS
1	F	21	ASN
1	F	74	ASN
1	F	83	GLN

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Mol	Chain	Res	Type
1	F	124	GLN
1	F	187	HIS
2	G	97	GLN
2	G	110	GLN
3	H	79	ASN
3	H	181	GLN
3	H	209	ASN
3	H	225	ASN
3	H	300	HIS
3	H	400	GLN
3	H	407	ASN
3	H	518	HIS
3	H	531	GLN
3	H	544	GLN
3	H	548	ASN
3	H	549	HIS
2	I	87	GLN
2	I	97	GLN
2	I	110	GLN
2	J	87	GLN
2	J	97	GLN
1	M	55	GLN
1	M	58	GLN
1	M	59	ASN
1	M	62	HIS
1	M	121	ASN
1	M	220	GLN
1	M	233	ASN
1	M	248	GLN
6	N	61	GLN
6	N	88	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	K	42/43 (97%)	25 (59%)	3 (7%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	K	2	U

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Mol	Chain	Res	Type
4	K	3	U
4	K	5	A
4	K	7	A
4	K	8	C
4	K	9	A
4	K	10	G
4	K	11	G
4	K	13	U
4	K	15	A
4	K	16	G
4	K	18	U
4	K	19	U
4	K	20	G
4	K	21	C
4	K	22	C
4	K	23	G
4	K	27	G
4	K	29	G
4	K	31	C
4	K	33	U
4	K	35	G
4	K	37	C
4	K	39	U
4	K	41	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	K	4	G
4	K	9	A
4	K	22	C

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

There are no ligands in this entry.

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.

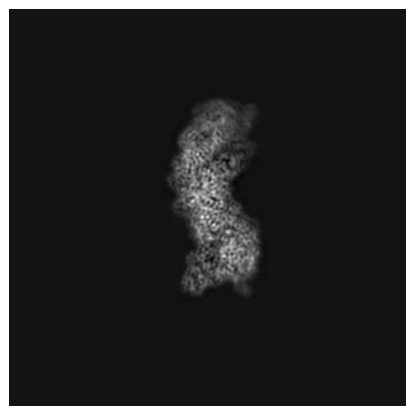
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29901. These allow visual inspection of the internal detail of the map and identification of artifacts.

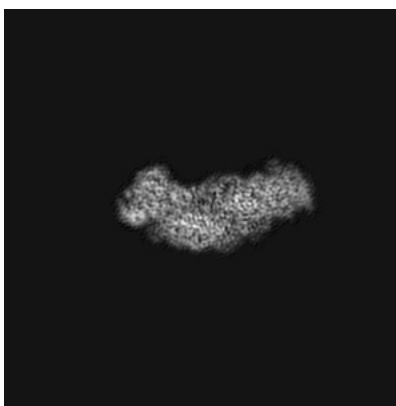
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

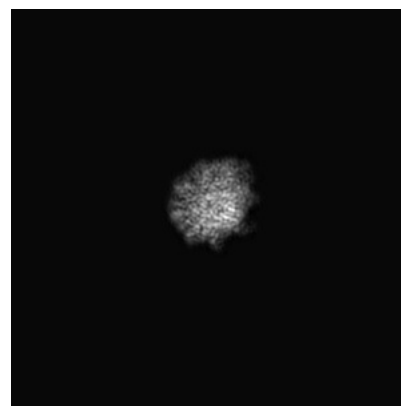
6.1.1 Primary map



X

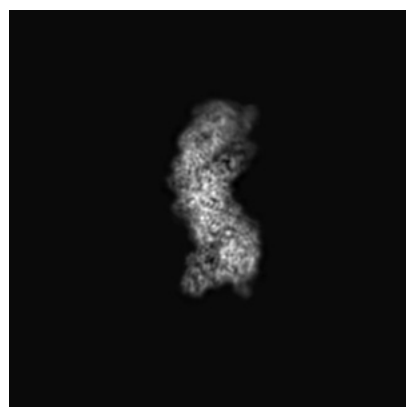


Y

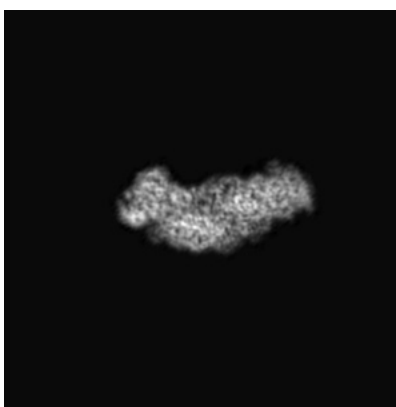


Z

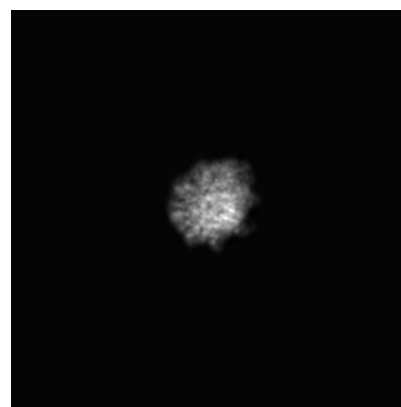
6.1.2 Raw map



X



Y

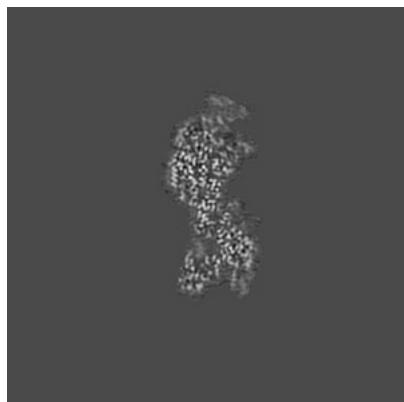


Z

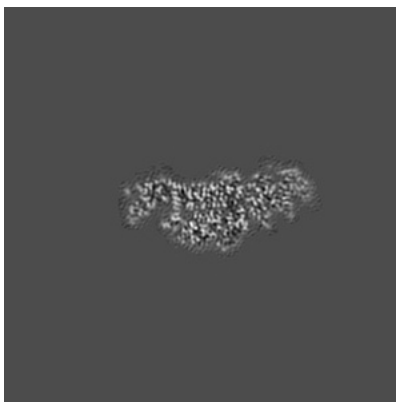
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

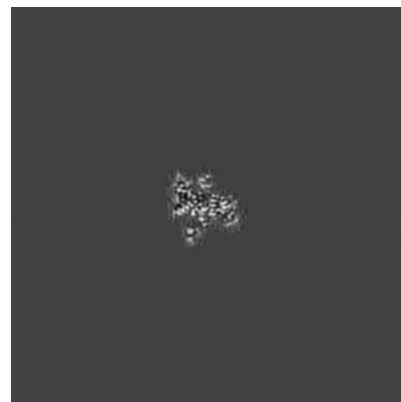
6.2.1 Primary map



X Index: 140

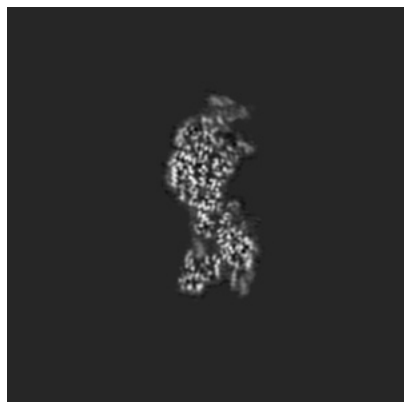


Y Index: 140

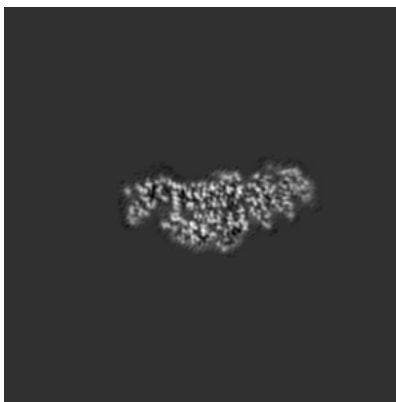


Z Index: 140

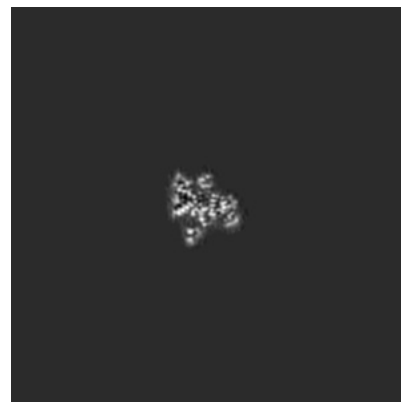
6.2.2 Raw map



X Index: 140



Y Index: 140



Z Index: 140

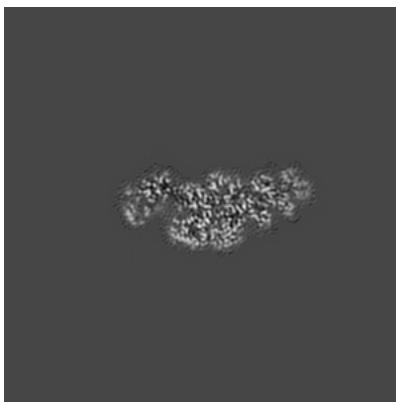
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

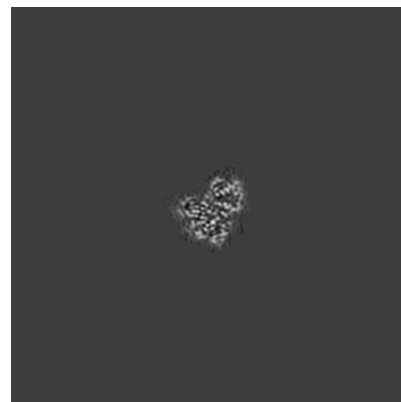
6.3.1 Primary map



X Index: 149

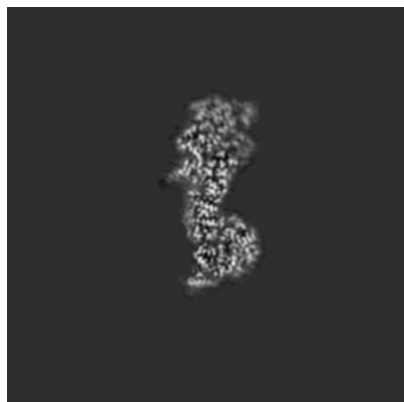


Y Index: 137

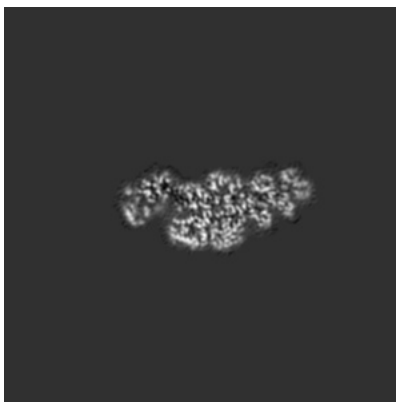


Z Index: 164

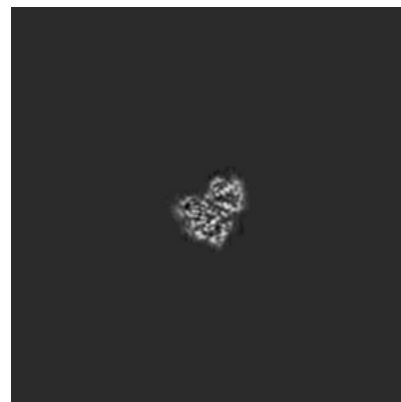
6.3.2 Raw map



X Index: 149



Y Index: 137

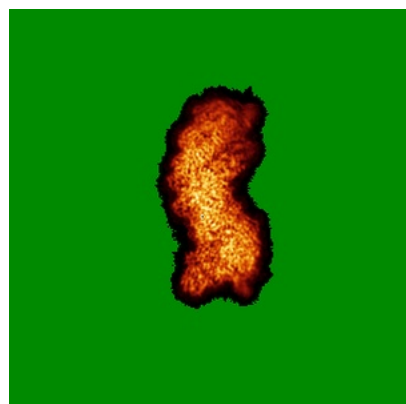


Z Index: 164

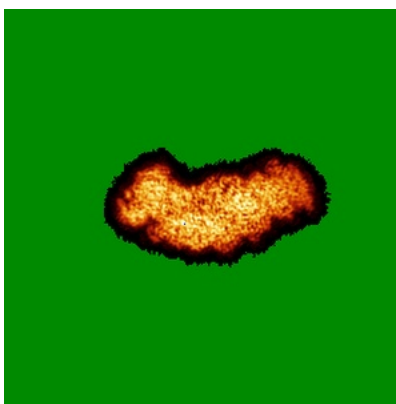
The images above show the largest variance slices of the map in three orthogonal directions.

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

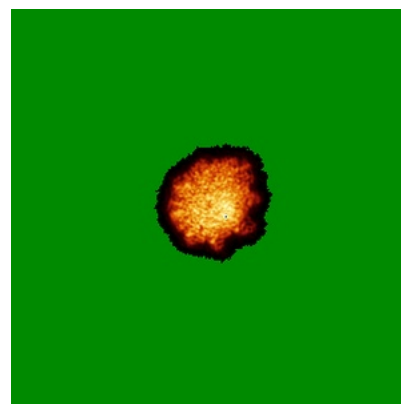
6.4.1 Primary map



X

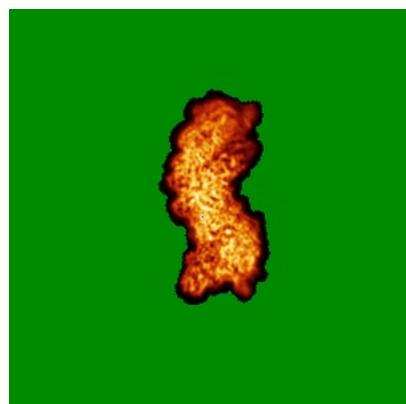


Y

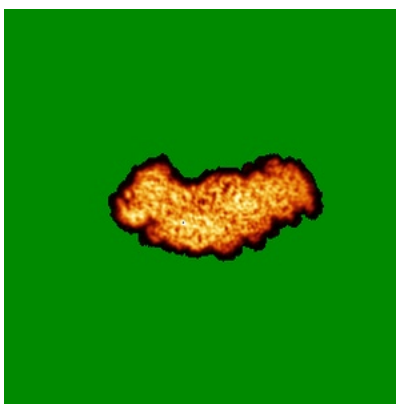


Z

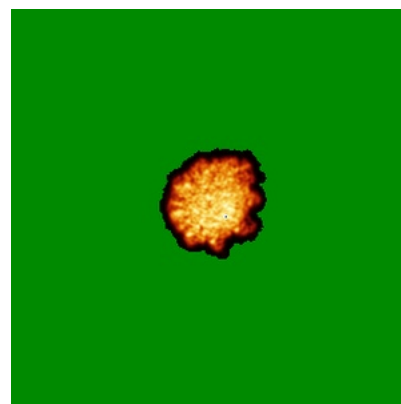
6.4.2 Raw map



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](#)

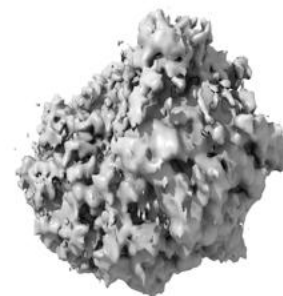
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.131. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

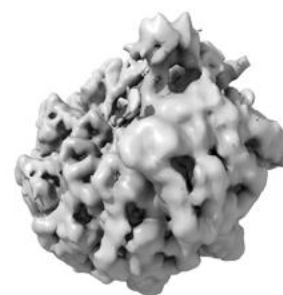
6.5.2 Raw map



X



Y



Z

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.

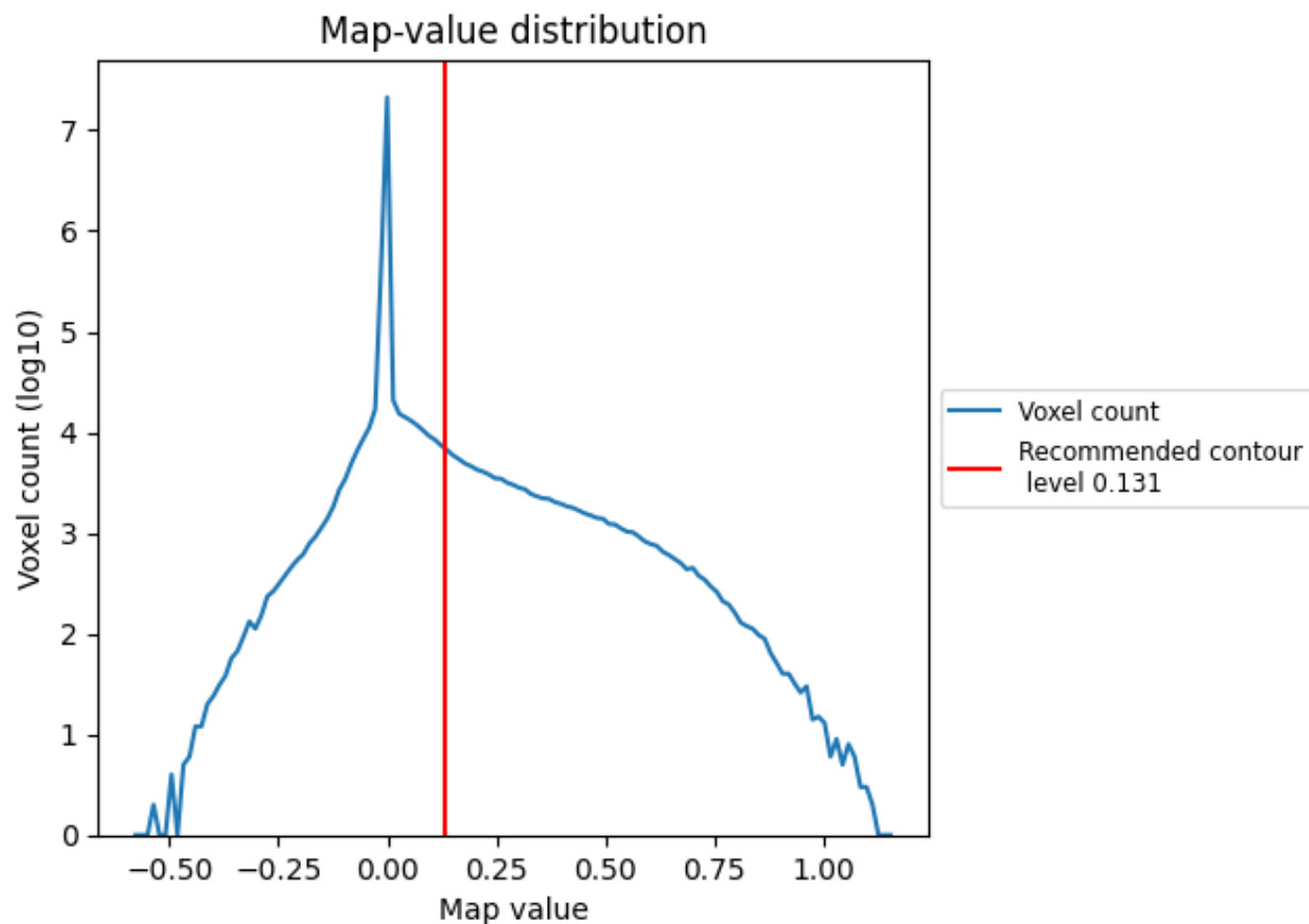
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

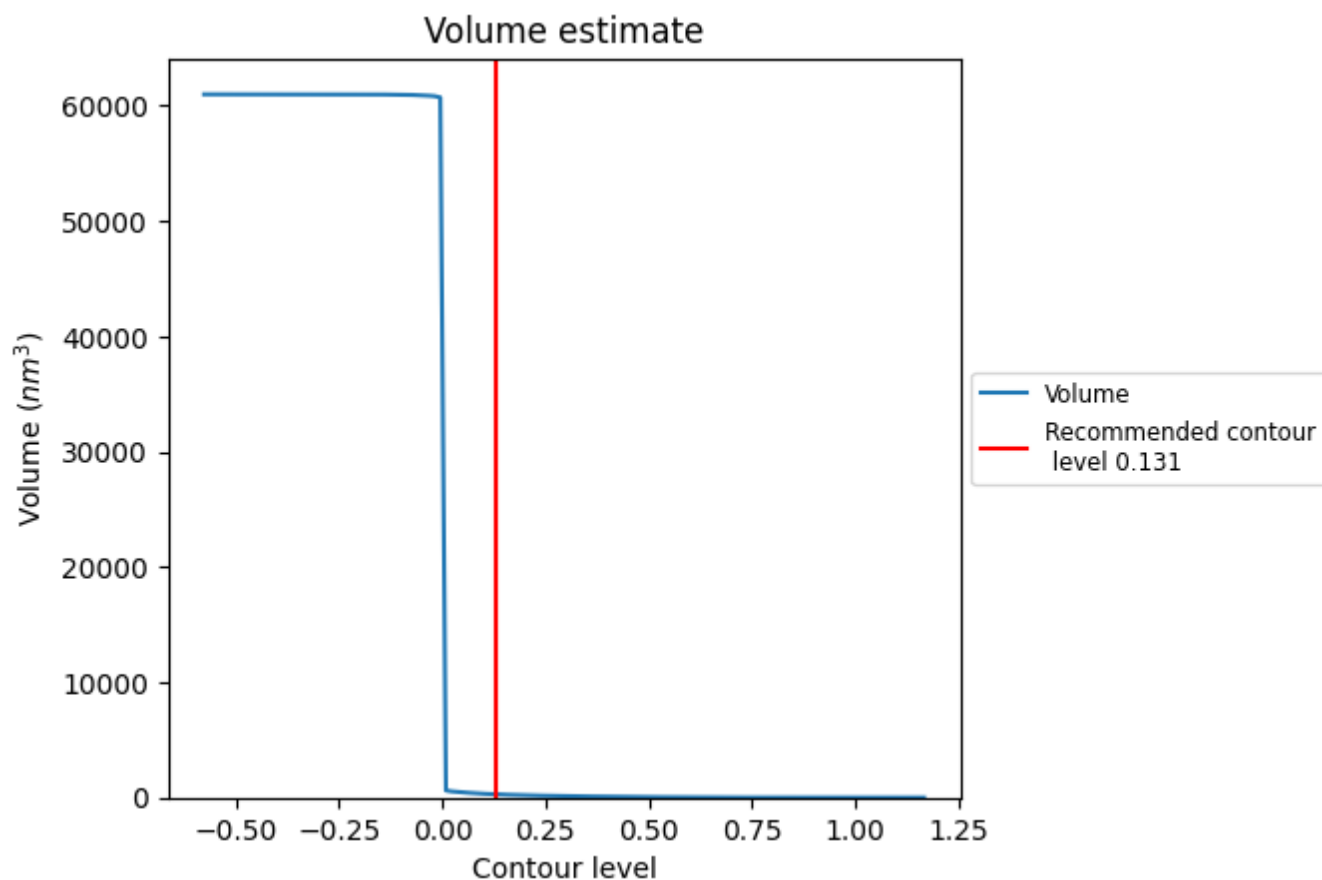
This section contains the results of statistical analysis of the map.

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.

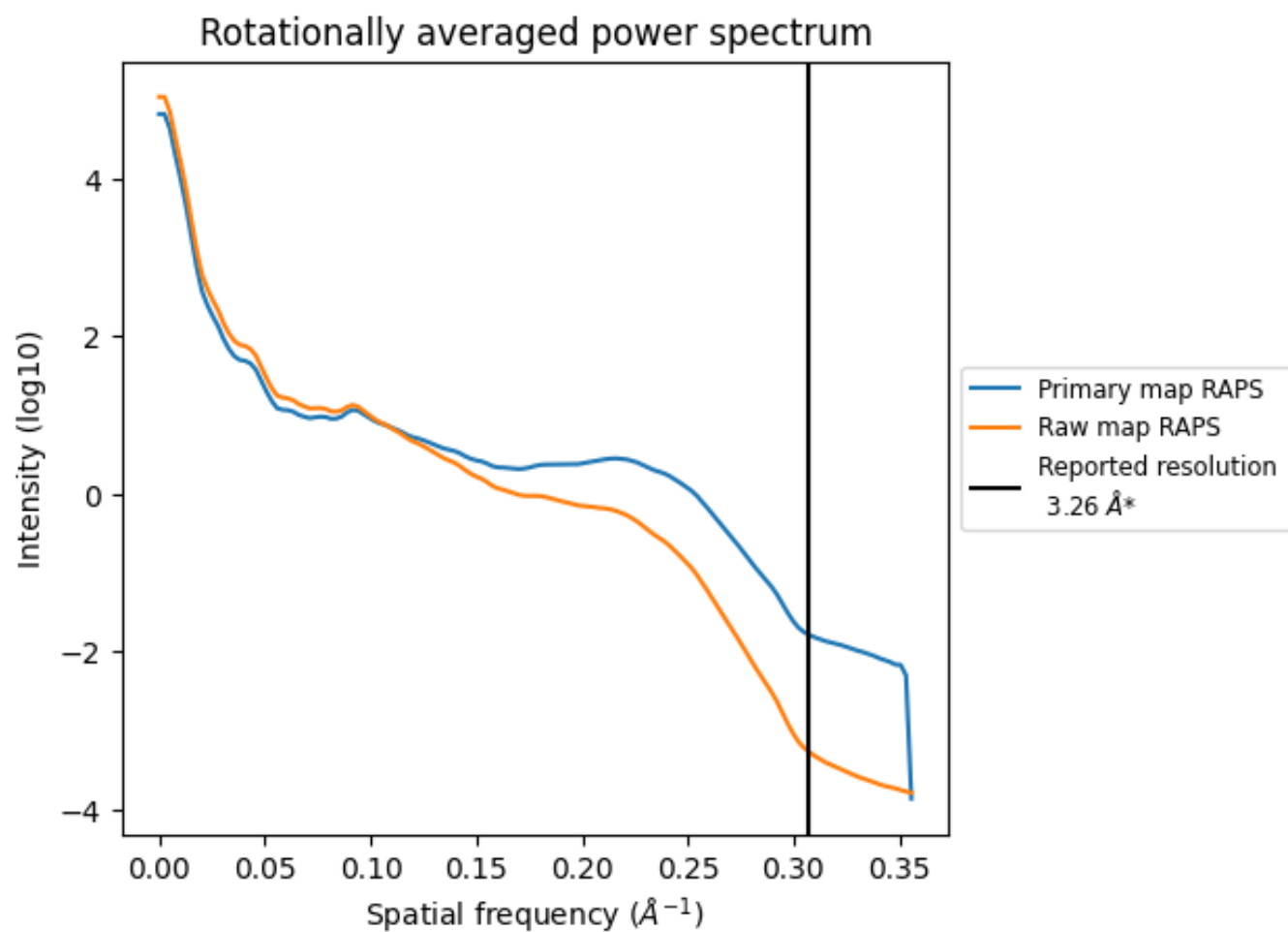
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 279 nm³; this corresponds to an approximate mass of 252 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 ⓘ

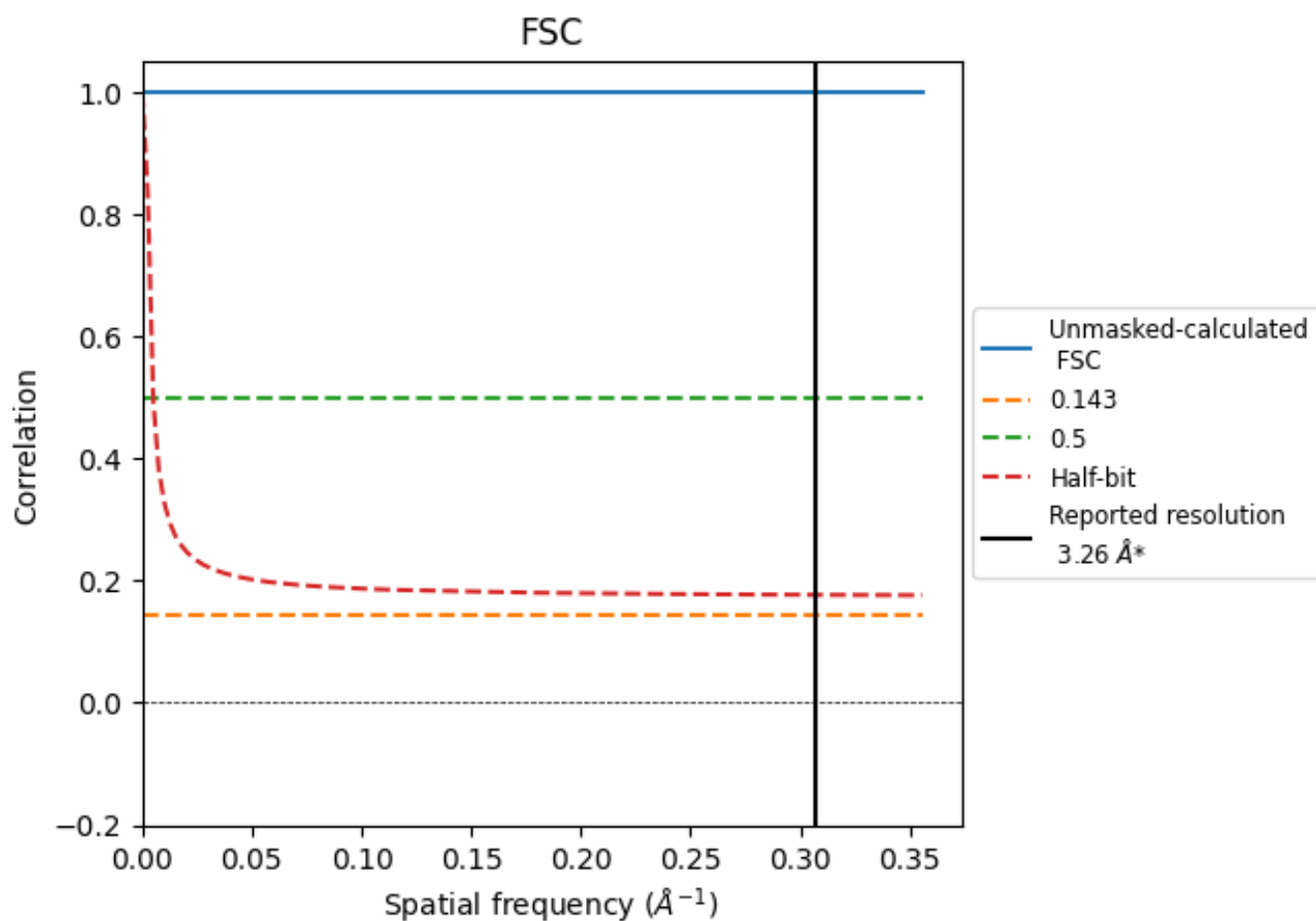


*Reported resolution corresponds to spatial frequency of 0.307 Å⁻¹

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 0.307 Å⁻¹

8.2 Resolution estimates [i](#)

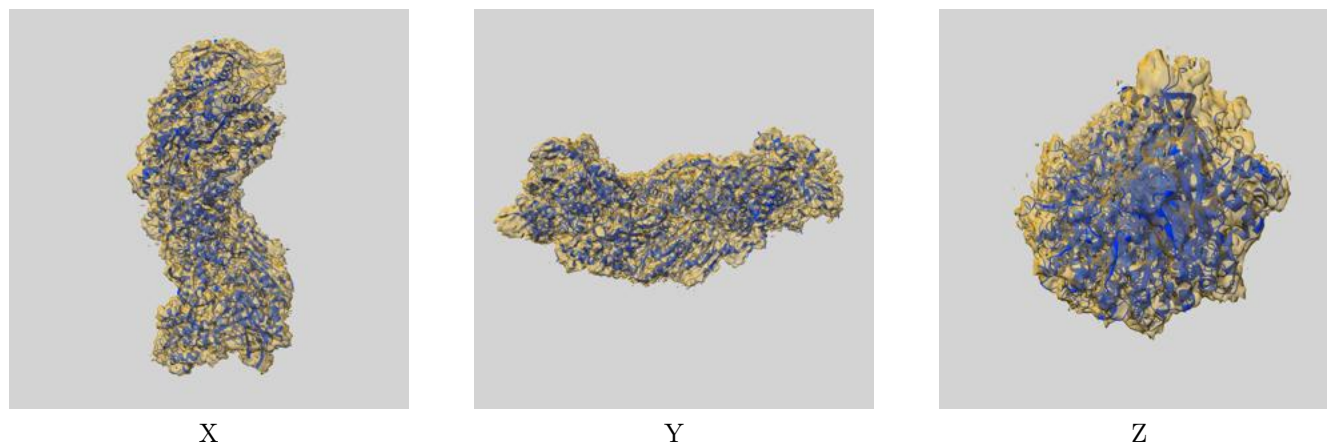
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.26	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

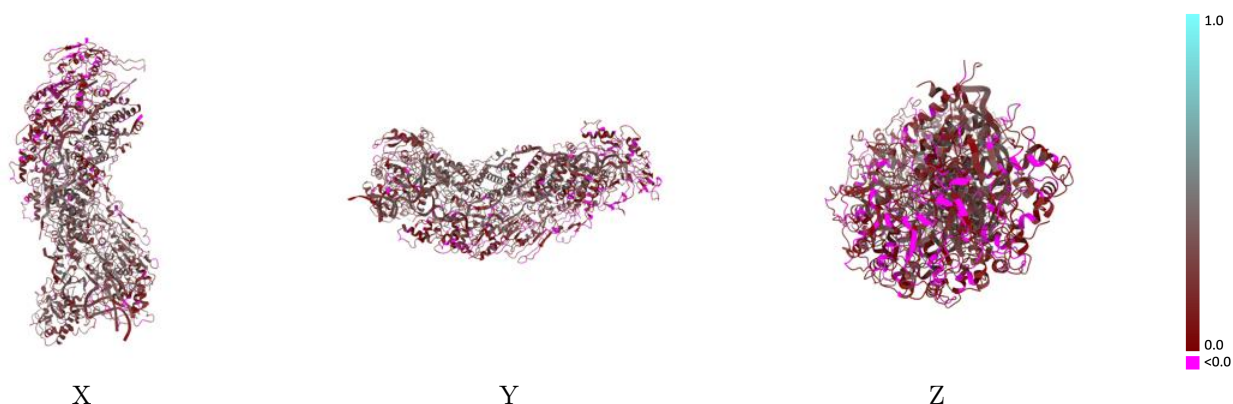
This section contains information regarding the fit between EMDB map EMD-29901 and PDB model 8GAN. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



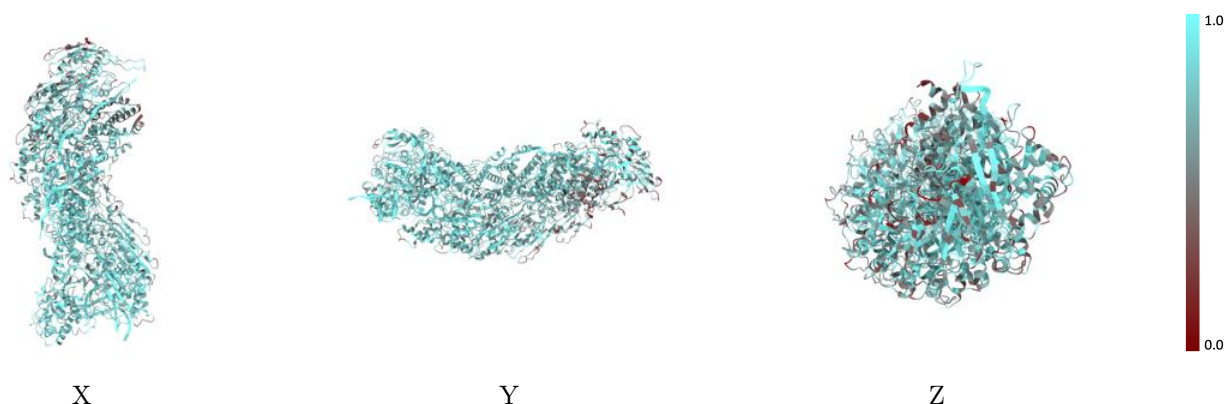
The images above show the 3D surface view of the map at the recommended contour level 0.131 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



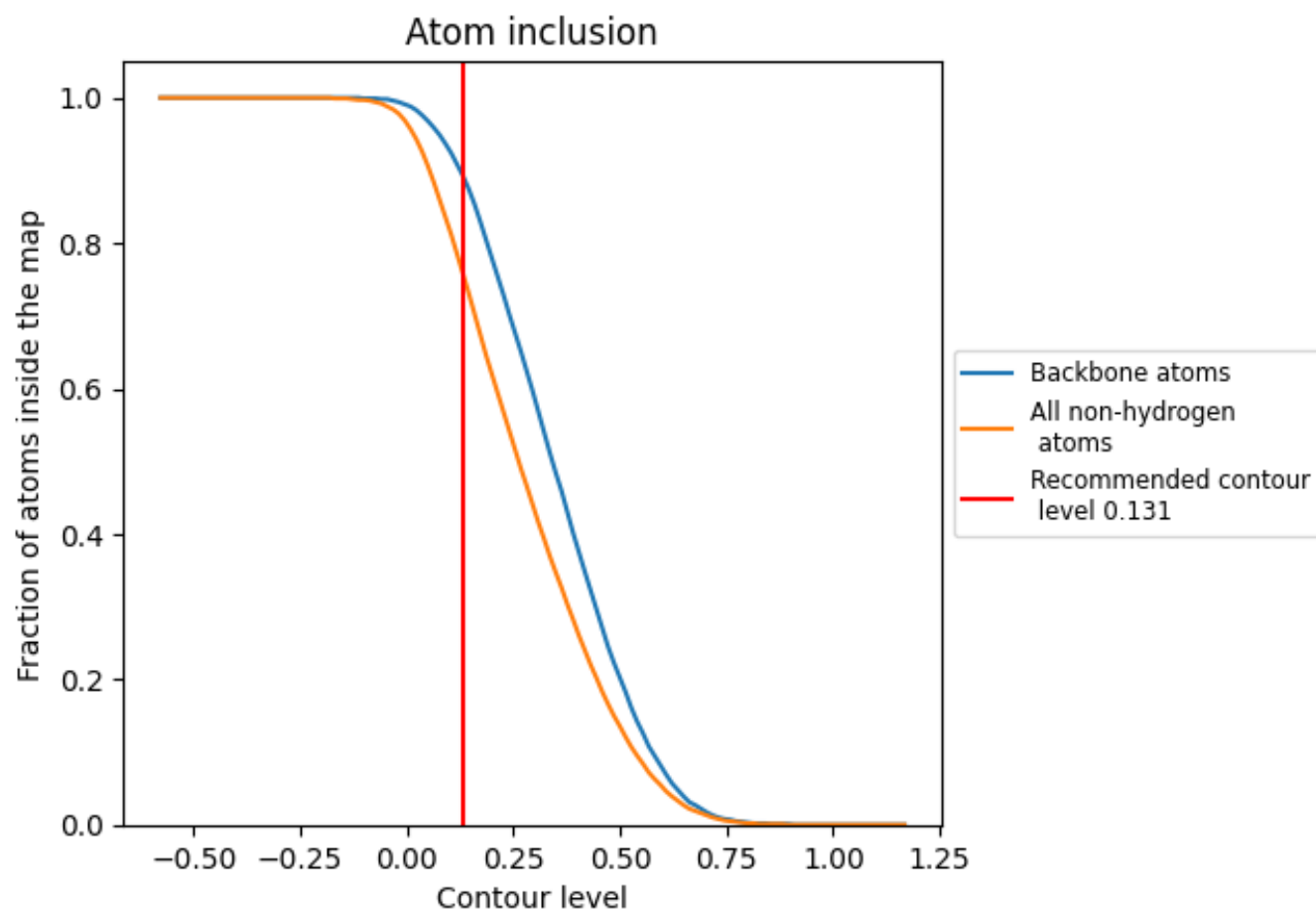
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.131).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 76% 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 (0.131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7600	 0.2270
A	 0.7180	 0.1640
B	 0.7560	 0.2040
C	 0.7520	 0.1950
D	 0.7100	 0.1500
E	 0.6810	 0.1250
F	 0.6650	 0.1080
G	 0.5700	 0.2220
H	 0.8000	 0.3130
I	 0.7700	 0.2890
J	 0.7970	 0.2680
K	 0.9130	 0.2930
L	 0.9340	 0.3280
M	 0.8230	 0.3030
N	 0.7910	 0.2680
O	 0.8400	 0.2690
Q	 0.8300	 0.3060

