Full wwPDB EM Validation Report ⓘ

Dec 31, 2024 – 01:52 AM EST

PDB ID	:	8GAM
EMDB ID	:	EMD-29900
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	:	3.46 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:

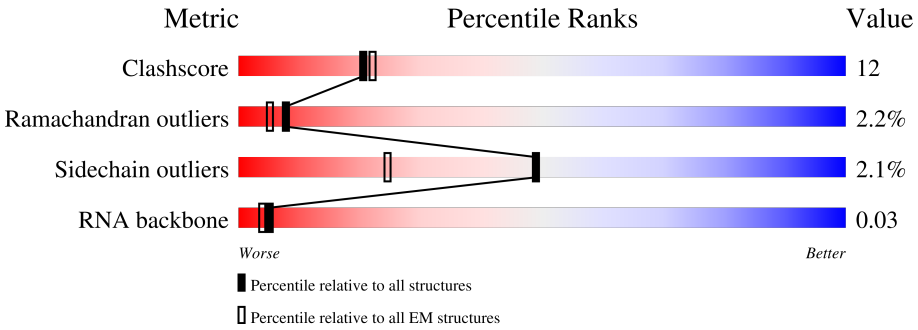
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.46 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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 <=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	16% 73% 24%
1	B	283	11% 71% 27%
1	C	283	15% 70% 28%
1	D	283	18% 73% 25%
1	E	283	25% 77% 21%
1	F	283	51% 77% 17%
1	M	283	65% 28% 7%

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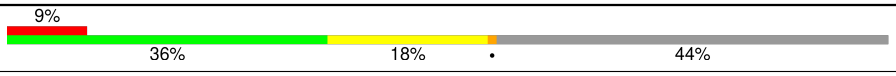
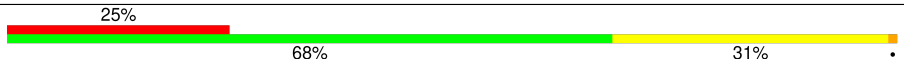
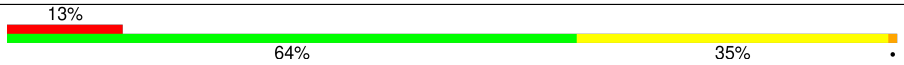
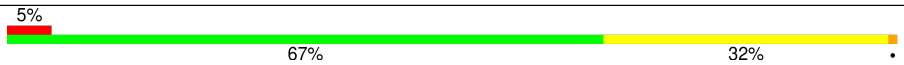
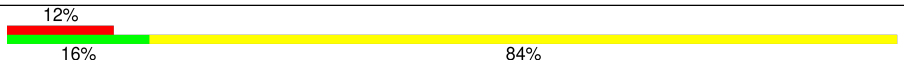
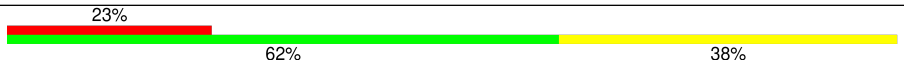
Mol	Chain	Length	Quality of chain
2	G	582	
2	H	582	
3	I	124	
3	J	124	
4	K	43	
5	N	205	
6	L	25	
7	O	13	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 25360 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 Phage associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	325	Total	C	N	O	S	0	0
			2523	1601	438	475	9		
2	H	233	Total	C	N	O	S	0	0
			1867	1189	335	336	7		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	190	ALA	VAL	conflict	UNP A0A378VF47
G	239	ALA	ILE	conflict	UNP A0A378VF47
G	242	ILE	VAL	conflict	UNP A0A378VF47
G	260	GLY	SER	conflict	UNP A0A378VF47
G	271	THR	ALA	conflict	UNP A0A378VF47
G	288	LEU	MET	conflict	UNP A0A378VF47
G	299	ALA	GLU	conflict	UNP A0A378VF47
G	306	ALA	THR	conflict	UNP A0A378VF47
G	317	CYS	GLN	conflict	UNP A0A378VF47
G	322	GLU	LYS	conflict	UNP A0A378VF47
G	323	ASP	GLU	conflict	UNP A0A378VF47
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	288	LEU	MET	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 3 is a protein called Cas11.

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

- 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 protein called Cas5.

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

- Molecule 6 is a DNA chain called Target strand DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	25	Total	C	N	O	P	0	0
			511	243	93	150	25		

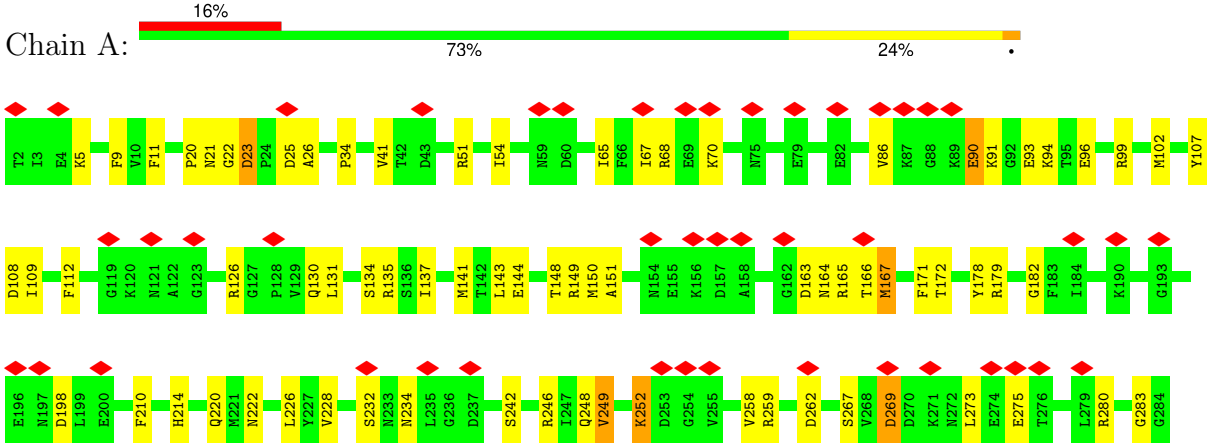
- Molecule 7 is a DNA chain called Non target strand DNA (5'-D(P*AP*TP*GP*AP*AP*C P*TP*TP*CP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	13	Total	C	N	O	P	0	0
			267	128	52	74	13		

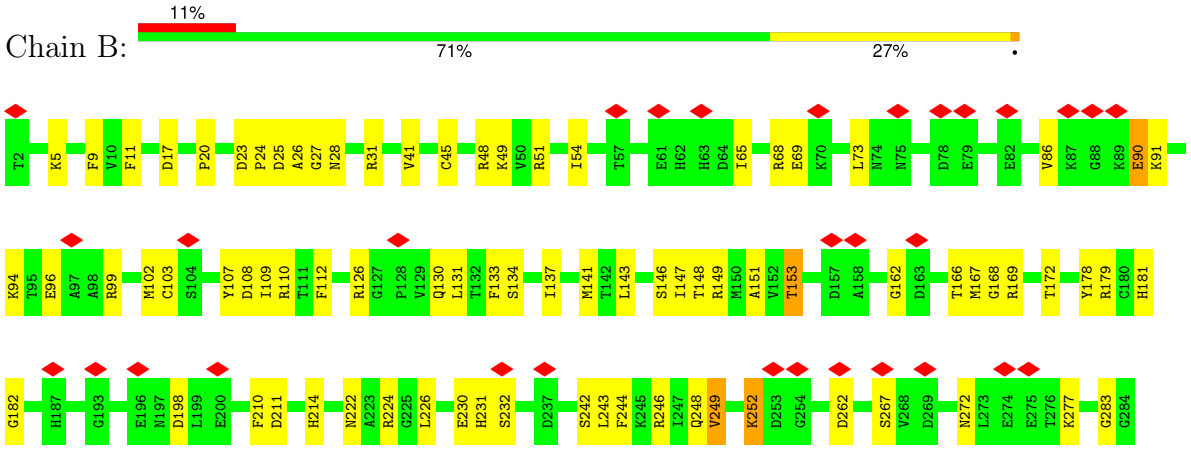
3 Residue-property plots (i)

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.

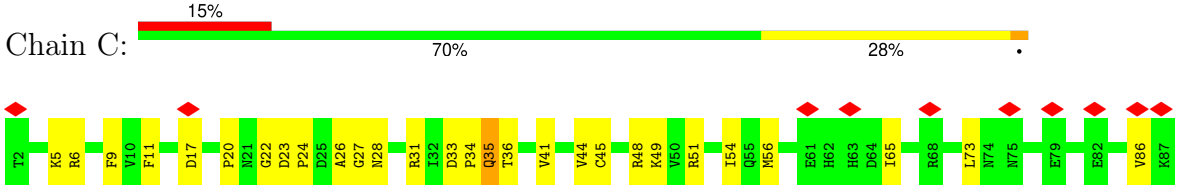
• Molecule 1: Cas7

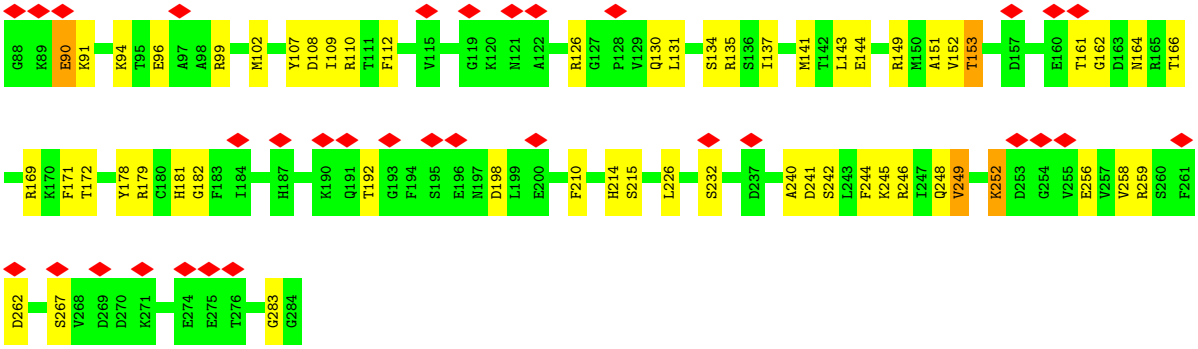


• Molecule 1: Cas7



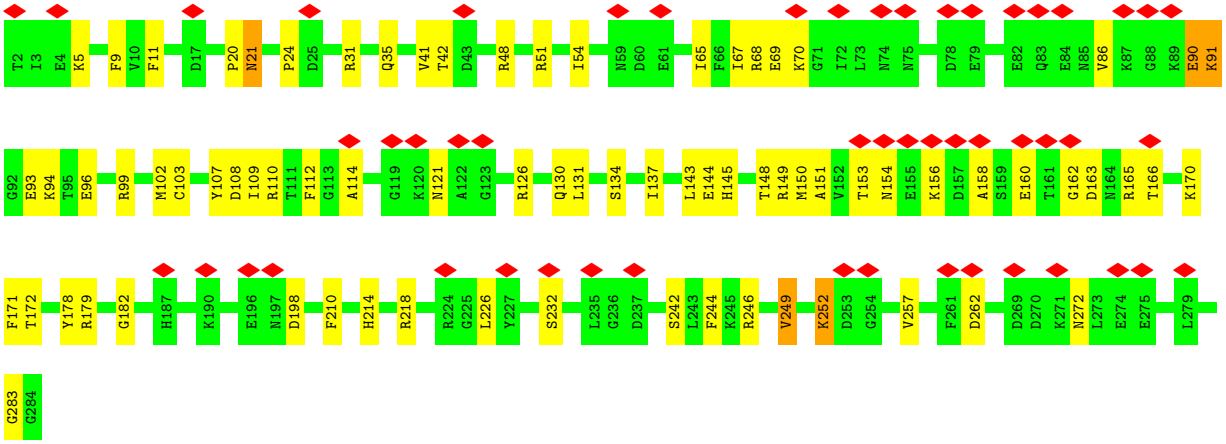
• Molecule 1: Cas7





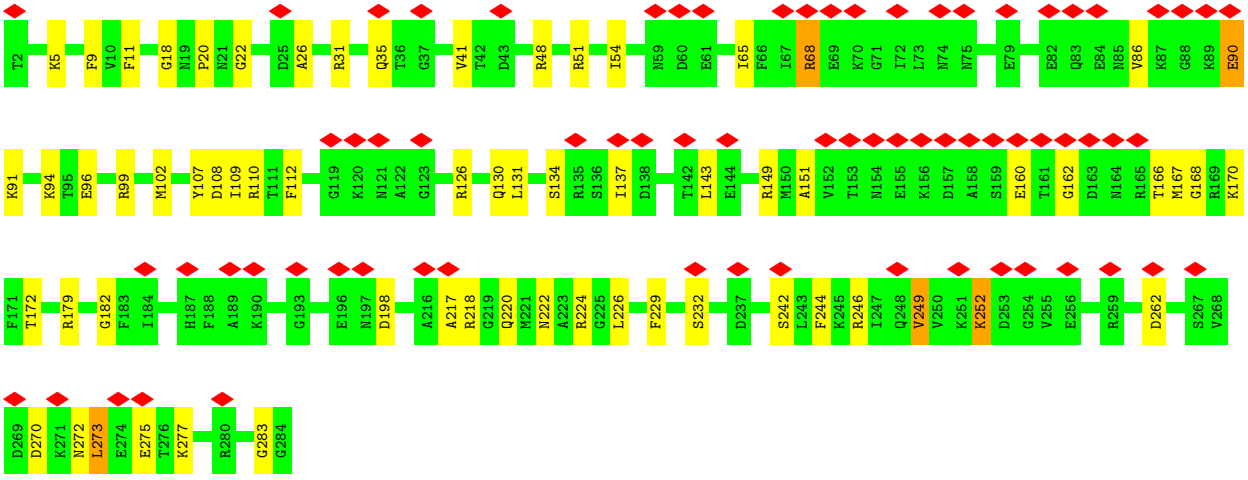
• Molecule 1: Cas7

Chain D:



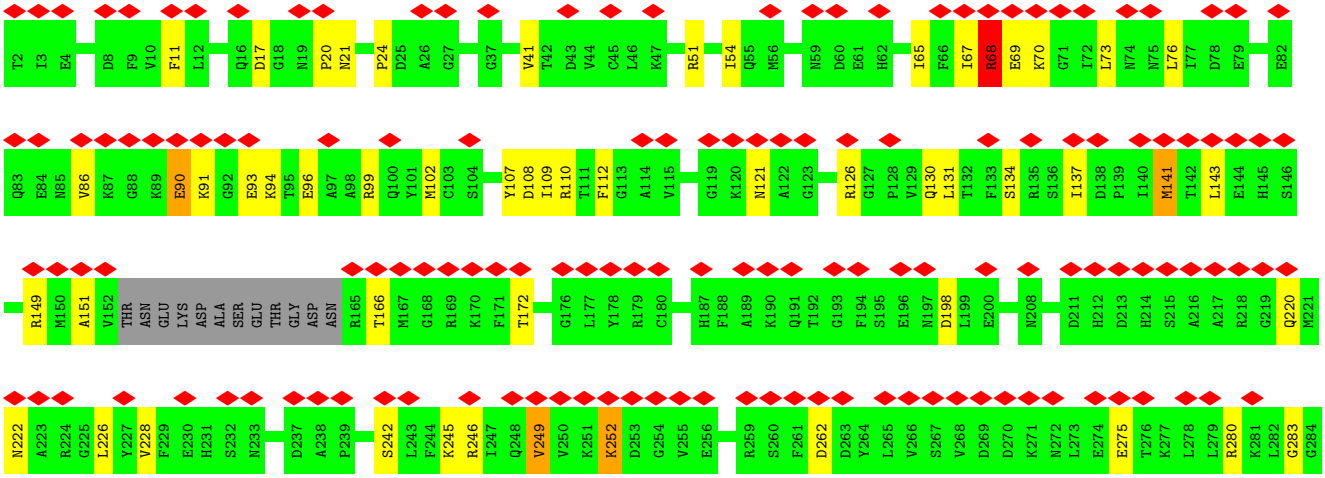
• Molecule 1: Cas7

Chain E:



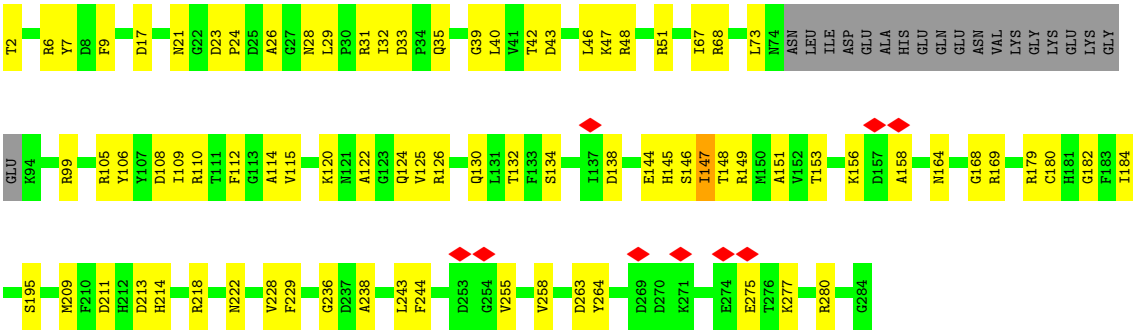
• Molecule 1: Cas7

Chain F:



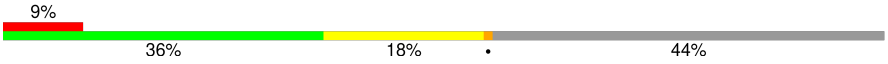
• Molecule 1: Cas7

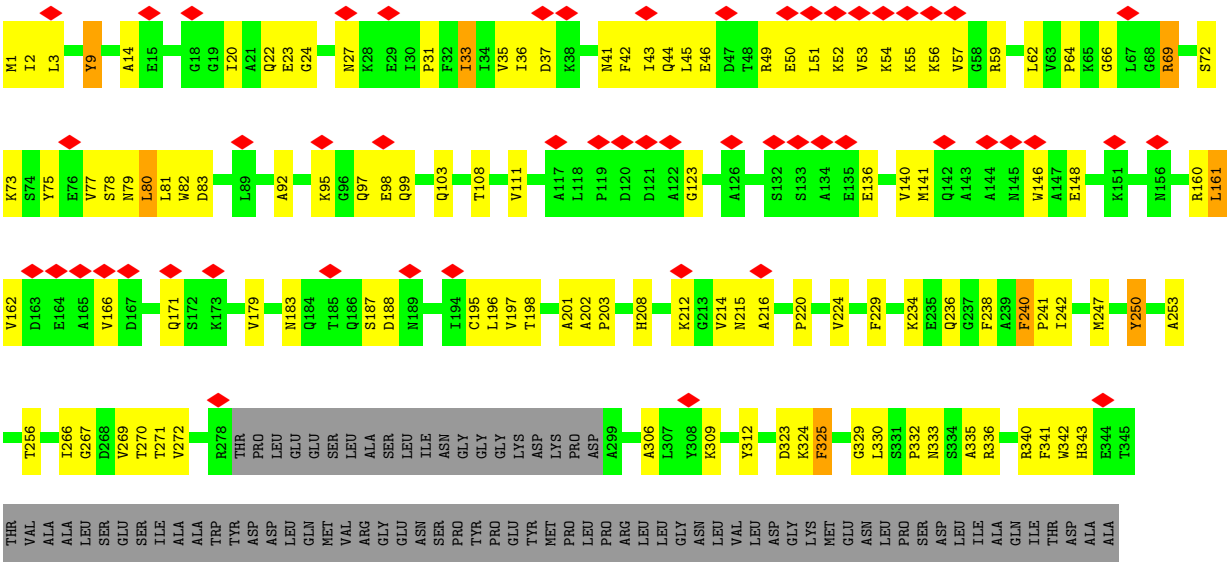
Chain M:

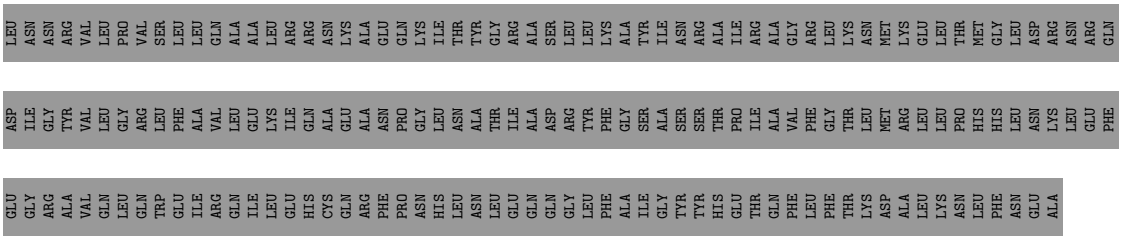


• Molecule 2: Phage associated protein

Chain G:

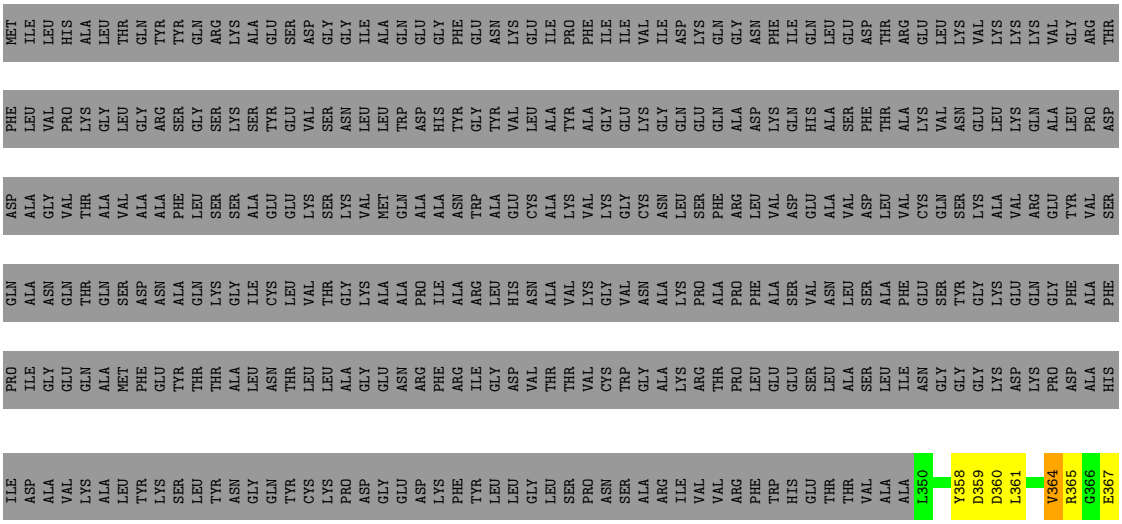






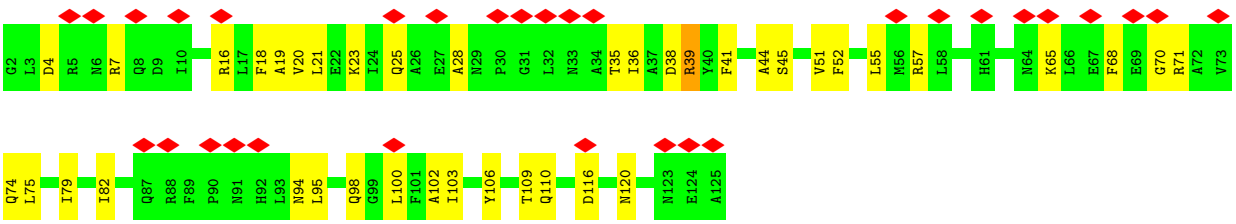
• Molecule 2: Phage associated protein

Chain H:



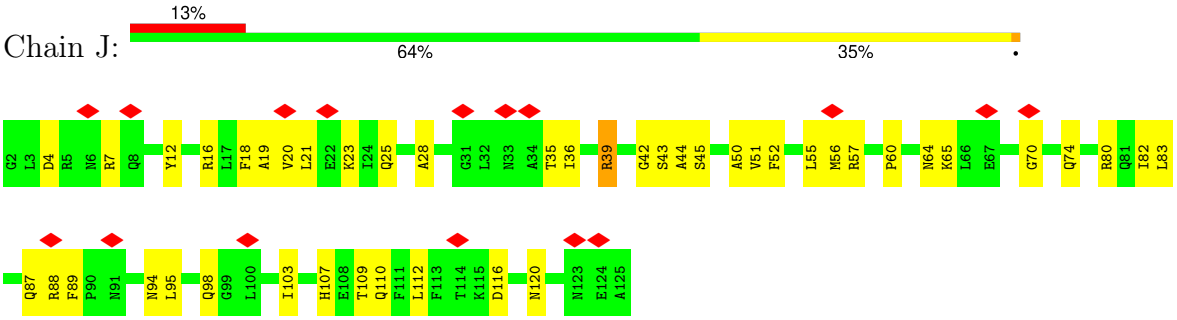
• Molecule 3: Cas11

Chain I:



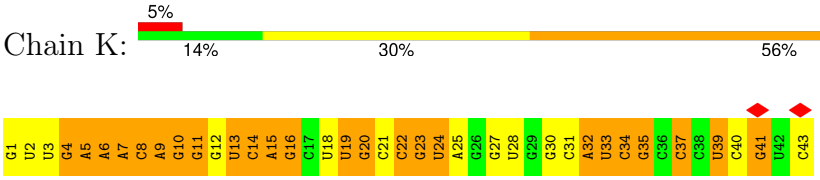
• Molecule 3: Cas11

Chain J:



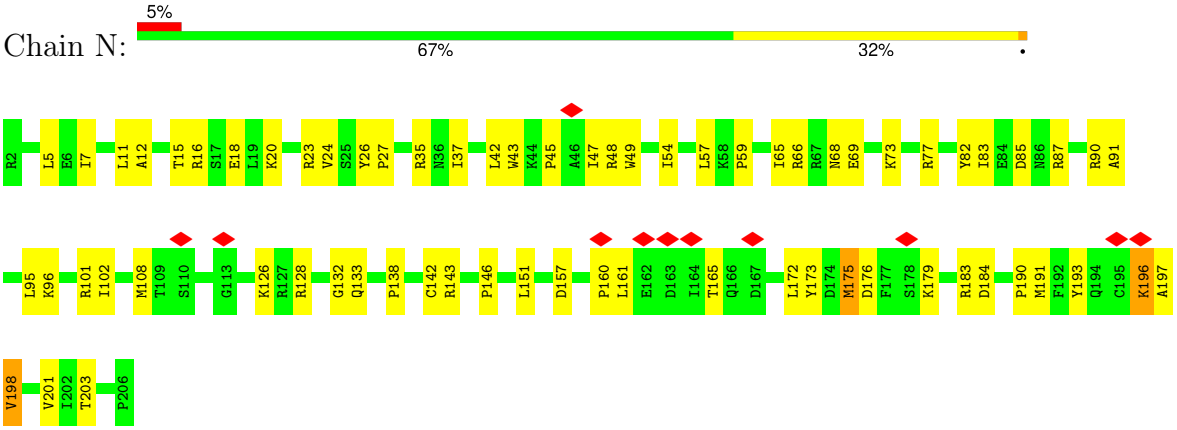
• Molecule 4: crRNA (43-MER)

Chain K:



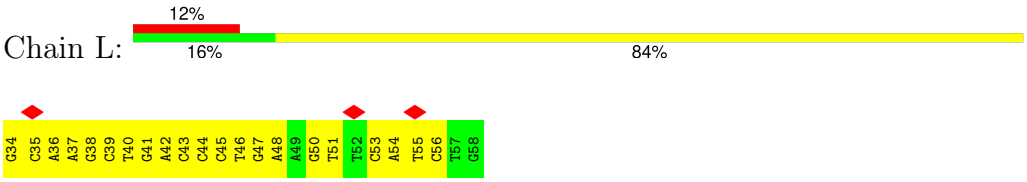
• Molecule 5: Cas5

Chain N:



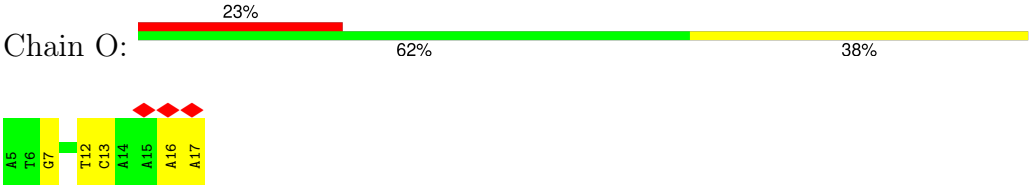
• Molecule 6: Target strand DNA (25-MER)

Chain L:



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

Chain O:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128645	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 ($e^-/Å^2$)	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	1.350	Depositor
Minimum map value	-0.565	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.035	Depositor
Recommended contour level	0.14	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	0.24	0/2303	0.48	0/3101
1	B	0.24	0/2303	0.47	0/3101
1	C	0.24	0/2303	0.48	0/3101
1	D	0.24	0/2303	0.48	0/3101
1	E	0.24	0/2303	0.48	0/3101
1	F	0.24	0/2214	0.48	0/2979
1	M	0.24	0/2150	0.49	0/2896
2	G	0.24	0/2572	0.44	0/3470
2	H	0.24	0/1903	0.47	0/2573
3	I	0.24	0/1030	0.44	0/1392
3	J	0.24	0/1030	0.44	0/1392
4	K	0.20	0/1022	0.78	1/1591 (0.1%)
5	N	0.24	0/1712	0.49	0/2307
6	L	0.52	0/572	0.90	0/880
7	O	0.53	0/300	0.85	0/460
All	All	0.25	0/26020	0.51	1/35445 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	4	G	P-O3'-C3'	5.05	125.76	119.70

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	A	2261	0	2193	48	0
1	B	2261	0	2193	61	0
1	C	2261	0	2193	62	0
1	D	2261	0	2193	55	0
1	E	2261	0	2193	40	0
1	F	2173	0	2120	30	0
1	M	2110	0	2050	65	0
2	G	2523	0	2507	65	0
2	H	1867	0	1891	73	0
3	I	1007	0	992	31	0
3	J	1007	0	992	37	0
4	K	916	0	464	49	0
5	N	1674	0	1663	49	0
6	L	511	0	282	37	0
7	O	267	0	147	7	0
All	All	25360	0	24073	579	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 12.

All (579) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ARG:HB2	4:K:19:U:H1’	1.63	0.80
4:K:11:G:N1	6:L:44:DC:N3	2.30	0.80
4:K:16:G:N2	6:L:39:DC:C2	2.51	0.78
1:E:68:ARG:NH2	4:K:41:G:O2’	2.16	0.77
4:K:16:G:N2	6:L:39:DC:O2	2.18	0.76
1:C:45:CYS:SG	1:C:49:LYS:NZ	2.59	0.75
2:H:427:GLN:HB3	2:H:495:ASP:HA	1.66	0.75
1:B:45:CYS:SG	1:B:49:LYS:NZ	2.60	0.75
4:K:11:G:N2	6:L:44:DC:O2	2.20	0.74
1:A:228:VAL:HB	1:A:280:ARG:HG3	1.69	0.73
1:E:220:GLN:NE2	1:E:222:ASN:OD1	2.20	0.73
1:A:67:ILE:HD12	1:A:70:LYS:HG3	1.70	0.72
3:I:106:TYR:HB2	3:J:83:LEU:HD11	1.71	0.72
1:A:220:GLN:NE2	1:A:222:ASN:OD1	2.23	0.71
2:H:483:ALA:HA	6:L:35:DC:H41	1.57	0.70
6:L:45:DC:H2”	6:L:46:DT:H2’	1.72	0.70
1:A:102:MET:HG2	1:A:109:ILE:HG13	1.74	0.70
1:E:102:MET:HG2	1:E:109:ILE:HG13	1.74	0.70
1:B:102:MET:HG2	1:B:109:ILE:HG13	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:514:ARG:HB3	3:J:42:GLY:HA2	1.74	0.69
2:H:481:ILE:HG12	2:H:532:LEU:HD13	1.73	0.69
2:H:395:SER:HB3	1:M:26:ALA:HB2	1.73	0.69
1:F:102:MET:HG2	1:F:109:ILE:HG13	1.74	0.69
2:H:537:ARG:HB3	3:J:110:GLN:HB2	1.74	0.69
1:D:102:MET:HG2	1:D:109:ILE:HG13	1.74	0.69
1:F:67:ILE:HD12	1:F:70:LYS:HG3	1.75	0.69
1:M:109:ILE:HD12	1:M:114:ALA:HB2	1.75	0.68
4:K:16:G:N1	6:L:39:DC:N3	2.40	0.68
1:C:102:MET:HG2	1:C:109:ILE:HG13	1.74	0.68
4:K:16:G:C2	6:L:39:DC:C2	2.81	0.68
2:G:340:ARG:NH1	2:H:394:PRO:O	2.26	0.68
1:A:34:PRO:HB3	3:J:57:ARG:HH22	1.58	0.68
1:M:43:ASP:HA	1:M:46:LEU:HD23	1.76	0.68
1:M:130:GLN:HB2	5:N:143:ARG:HH21	1.59	0.67
1:D:160:GLU:HG2	1:D:162:GLY:H	1.59	0.66
1:C:35:GLN:HG2	1:C:36:THR:HG23	1.76	0.65
2:G:35:VAL:HB	2:G:44:GLN:HB3	1.77	0.65
2:G:188:ASP:HA	2:G:203:PRO:HG3	1.79	0.65
1:B:243:LEU:HD21	1:B:277:LYS:HZ2	1.61	0.65
2:G:73:LYS:HD3	6:L:51:DT:H5”	1.79	0.65
5:N:15:THR:OG1	5:N:23:ARG:NH1	2.29	0.65
2:H:421:ARG:HG3	1:M:144:GLU:HB2	1.78	0.64
2:H:390:MET:SD	7:O:17:DA:N6	2.70	0.64
4:K:12:G:N2	6:L:43:DC:C2	2.65	0.64
4:K:5:A:H5’	5:N:143:ARG:HD3	1.80	0.64
1:D:218:ARG:NH2	4:K:35:G:OP2	2.32	0.63
4:K:11:G:O6	6:L:44:DC:N4	2.28	0.63
1:D:156:LYS:HE3	1:D:158:ALA:HB3	1.81	0.63
1:B:133:PHE:HB2	1:M:17:ASP:HB3	1.79	0.63
1:B:5:LYS:HD2	1:B:232:SER:HA	1.81	0.63
1:B:153:THR:HA	1:C:73:LEU:HD12	1.81	0.62
1:E:90:GLU:O	1:E:94:LYS:N	2.31	0.62
2:G:212:LYS:NZ	2:G:216:ALA:O	2.31	0.62
1:C:248:GLN:HG3	1:C:267:SER:HB2	1.82	0.62
1:A:269:ASP:OD1	1:A:269:ASP:N	2.32	0.62
5:N:23:ARG:NH1	5:N:142:CYS:SG	2.72	0.62
5:N:20:LYS:O	5:N:90:ARG:NH2	2.32	0.62
1:A:246:ARG:HG3	1:A:273:LEU:HD11	1.82	0.62
1:A:248:GLN:HG3	1:A:267:SER:HB2	1.82	0.62
4:K:13:U:H1’	1:M:149:ARG:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:ARG:NH2	1:E:244:PHE:O	2.34	0.61
1:D:179:ARG:NH2	1:D:244:PHE:O	2.34	0.61
1:D:67:ILE:HD12	1:D:70:LYS:HG3	1.81	0.61
1:B:141:MET:N	1:B:141:MET:SD	2.74	0.61
1:B:248:GLN:HG3	1:B:267:SER:HB2	1.81	0.61
1:M:258:VAL:HG23	1:M:263:ASP:HB2	1.83	0.61
2:H:449:ARG:NH1	1:M:35:GLN:O	2.34	0.60
1:C:5:LYS:HD2	1:C:232:SER:HA	1.83	0.60
1:F:228:VAL:HB	1:F:280:ARG:HG2	1.82	0.60
2:H:375:MET:SD	2:H:379:ARG:NH1	2.73	0.60
1:E:5:LYS:HD2	1:E:232:SER:HA	1.82	0.60
3:I:45:SER:HB2	3:I:98:GLN:HG3	1.84	0.60
1:D:246:ARG:HH22	1:D:272:ASN:HB2	1.65	0.60
2:G:51:LEU:HD13	2:G:59:ARG:HH12	1.67	0.60
5:N:175:MET:N	5:N:175:MET:SD	2.75	0.60
1:B:90:GLU:O	1:B:94:LYS:N	2.32	0.59
2:H:473:ARG:HB3	2:H:539:ILE:HD13	1.82	0.59
2:G:240:PHE:HB3	5:N:18:GLU:HA	1.83	0.59
5:N:54:ILE:HG12	5:N:102:ILE:HG13	1.83	0.59
2:G:3:LEU:HB2	2:G:197:VAL:HG11	1.84	0.59
3:I:7:ARG:NH1	3:J:87:GLN:O	2.35	0.59
3:J:45:SER:HB2	3:J:98:GLN:HG3	1.84	0.59
1:C:90:GLU:O	1:C:94:LYS:N	2.30	0.59
1:M:228:VAL:HG11	1:M:280:ARG:HH21	1.68	0.59
1:E:41:VAL:HB	1:E:134:SER:HB2	1.85	0.58
1:M:211:ASP:OD1	1:M:222:ASN:ND2	2.36	0.58
1:B:41:VAL:HB	1:B:134:SER:HB2	1.85	0.58
1:B:252:LYS:NZ	1:B:262:ASP:O	2.36	0.58
4:K:5:A:H2'	1:M:115:VAL:HG22	1.85	0.58
5:N:66:ARG:HA	5:N:91:ALA:HA	1.84	0.58
5:N:161:LEU:HD22	5:N:165:THR:HG21	1.84	0.58
7:O:16:DA:N3	7:O:16:DA:H2'	2.19	0.58
1:A:41:VAL:HB	1:A:134:SER:HB2	1.85	0.58
1:F:252:LYS:NZ	1:F:262:ASP:O	2.37	0.58
2:G:55:LYS:NZ	2:G:148:GLU:OE2	2.36	0.58
2:G:37:ASP:HA	2:G:162:VAL:HB	1.84	0.58
2:H:509:PHE:HA	2:H:512:LEU:HB3	1.85	0.58
1:D:103:CYS:O	1:D:110:ARG:NH1	2.36	0.58
1:B:103:CYS:O	1:B:110:ARG:NH1	2.36	0.58
1:C:144:GLU:OE2	3:J:43:SER:OG	2.18	0.58
1:F:41:VAL:HB	1:F:134:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:42:LEU:O	5:N:49:TRP:NE1	2.36	0.58
1:C:23:ASP:HB3	1:C:26:ALA:HB3	1.86	0.58
1:D:5:LYS:HD2	1:D:232:SER:HA	1.86	0.58
1:F:141:MET:SD	1:F:141:MET:N	2.77	0.58
1:D:252:LYS:NZ	1:D:262:ASP:O	2.36	0.58
1:C:252:LYS:NZ	1:C:262:ASP:O	2.36	0.57
1:E:252:LYS:NZ	1:E:262:ASP:O	2.36	0.57
1:M:99:ARG:HH21	1:M:125:VAL:HG13	1.69	0.57
1:M:23:ASP:OD2	1:M:31:ARG:NH1	2.37	0.57
1:C:41:VAL:HB	1:C:134:SER:HB2	1.85	0.57
2:G:62:LEU:O	2:G:171:GLN:NE2	2.37	0.57
1:M:229:PHE:HB3	1:M:277:LYS:HD3	1.85	0.57
1:A:252:LYS:NZ	1:A:262:ASP:O	2.37	0.57
4:K:7:A:H1'	5:N:69:GLU:HA	1.86	0.57
1:B:210:PHE:O	1:B:214:HIS:NE2	2.38	0.57
6:L:47:DG:H2"	6:L:48:DA:C8	2.40	0.57
1:D:41:VAL:HB	1:D:134:SER:HB2	1.85	0.57
1:C:24:PRO:HD3	1:C:31:ARG:HH22	1.70	0.57
1:F:220:GLN:NE2	1:F:222:ASN:OD1	2.38	0.57
1:B:23:ASP:OD2	2:H:424:LYS:NZ	2.31	0.57
5:N:35:ARG:HD3	5:N:48:ARG:HH12	1.70	0.57
3:I:95:LEU:HD21	3:J:50:ALA:HA	1.87	0.56
1:M:149:ARG:NH1	1:M:151:ALA:O	2.38	0.56
5:N:69:GLU:HB2	5:N:90:ARG:HD3	1.86	0.56
2:H:392:ASN:HD22	2:H:398:ILE:HD13	1.69	0.56
4:K:5:A:H1'	1:M:124:GLN:HG3	1.86	0.56
2:G:14:ALA:HA	2:G:20:ILE:HG21	1.86	0.56
5:N:59:PRO:HD3	5:N:160:PRO:HG3	1.88	0.56
4:K:16:G:C2	6:L:39:DC:O2	2.58	0.56
2:G:49:ARG:HH22	2:G:148:GLU:HG2	1.69	0.56
3:I:38:ASP:HA	3:J:60:PRO:HB3	1.87	0.56
4:K:9:A:O2'	1:M:28:ASN:OD1	2.23	0.56
1:E:229:PHE:HB3	1:E:277:LYS:HD3	1.88	0.56
3:J:116:ASP:O	3:J:120:ASN:ND2	2.38	0.56
1:B:17:ASP:OD1	1:C:135:ARG:NH2	2.27	0.56
2:H:385:VAL:HG11	2:H:389:LYS:HD2	1.87	0.56
3:I:116:ASP:O	3:I:120:ASN:ND2	2.38	0.56
5:N:7:ILE:HD12	5:N:102:ILE:HD13	1.87	0.56
1:A:126:ARG:HH21	1:C:215:SER:HB2	1.71	0.56
2:H:376:PRO:O	2:H:380:LEU:N	2.37	0.56
2:G:36:ILE:HG22	2:G:42:PHE:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASP:O	1:C:6:ARG:NH1	2.40	0.55
1:M:32:ILE:HA	1:M:39:GLY:HA2	1.89	0.55
1:M:33:ASP:HB3	5:N:96:LYS:HZ3	1.71	0.55
2:H:424:LYS:HG3	2:H:499:GLY:HA2	1.88	0.54
2:G:64:PRO:O	2:G:82:TRP:NE1	2.40	0.54
4:K:7:A:OP1	1:M:47:LYS:NZ	2.30	0.54
1:C:22:GLY:O	1:C:31:ARG:NH2	2.41	0.54
4:K:10:G:H2'	4:K:11:G:C8	2.43	0.54
1:B:222:ASN:HD21	1:C:240:ALA:HB3	1.72	0.54
1:M:122:ALA:N	5:N:184:ASP:O	2.39	0.54
1:M:109:ILE:HG23	1:M:114:ALA:HB2	1.90	0.54
1:C:149:ARG:HB2	4:K:25:A:H1'	1.89	0.54
1:E:170:LYS:HE3	1:E:217:ALA:HA	1.90	0.54
1:M:114:ALA:H	1:M:125:VAL:HB	1.73	0.53
1:C:149:ARG:HH22	1:C:153:THR:HG23	1.72	0.53
5:N:12:ALA:HB3	5:N:95:LEU:HB2	1.90	0.53
5:N:176:ASP:OD2	5:N:179:LYS:NZ	2.41	0.53
2:H:384:LEU:HA	2:H:422:ARG:HG3	1.90	0.53
1:M:31:ARG:HD3	5:N:65:ILE:HD12	1.89	0.53
5:N:83:ILE:HD13	5:N:87:ARG:HH22	1.73	0.53
1:B:148:THR:O	4:K:19:U:O2'	2.16	0.53
1:C:144:GLU:HG3	1:C:171:PHE:HE2	1.73	0.53
2:H:551:ASN:OD1	2:H:552:LEU:N	2.42	0.53
1:D:24:PRO:HA	4:K:33:U:C5	2.44	0.53
1:F:51:ARG:NH2	1:F:112:PHE:O	2.42	0.53
2:G:270:THR:HG22	2:G:272:VAL:HG13	1.91	0.53
1:A:135:ARG:NH2	1:C:17:ASP:OD1	2.37	0.53
1:A:210:PHE:O	1:A:214:HIS:NE2	2.42	0.53
1:C:51:ARG:NH2	1:C:112:PHE:O	2.42	0.53
1:A:167:MET:SD	1:A:167:MET:N	2.82	0.53
1:B:51:ARG:NH2	1:B:112:PHE:O	2.42	0.53
1:B:147:ILE:HD12	1:C:44:VAL:HG11	1.89	0.53
1:D:51:ARG:NH2	1:D:112:PHE:O	2.42	0.53
1:D:144:GLU:HG2	1:D:171:PHE:HE2	1.74	0.53
1:D:257:VAL:HG11	1:E:35:GLN:HB3	1.91	0.53
1:C:258:VAL:O	1:C:259:ARG:NH1	2.39	0.53
2:G:27:ASN:HD21	2:G:256:THR:HA	1.73	0.53
2:G:97:GLN:O	2:G:99:GLN:N	2.40	0.53
1:C:179:ARG:HE	1:C:181:HIS:CE1	2.28	0.52
1:E:160:GLU:HG2	1:E:162:GLY:H	1.74	0.52
1:B:126:ARG:O	1:B:130:GLN:NE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PHE:O	1:D:214:HIS:NE2	2.42	0.52
1:E:126:ARG:O	1:E:130:GLN:NE2	2.42	0.52
2:G:51:LEU:HD23	2:G:56:LYS:HD2	1.92	0.52
2:G:80:LEU:HB3	2:G:81:LEU:HD22	1.91	0.52
1:A:90:GLU:O	1:A:94:LYS:N	2.38	0.52
1:M:6:ARG:HH11	1:M:236:GLY:HA3	1.74	0.52
1:B:11:PHE:HD1	1:B:226:LEU:HD13	1.75	0.52
1:E:51:ARG:NH2	1:E:112:PHE:O	2.42	0.52
1:C:11:PHE:HD1	1:C:226:LEU:HD13	1.75	0.52
1:C:210:PHE:O	1:C:214:HIS:NE2	2.42	0.52
1:E:11:PHE:HD1	1:E:226:LEU:HD13	1.75	0.52
4:K:9:A:H5"	1:M:24:PRO:HD3	1.91	0.52
6:L:54:DA:H2"	6:L:55:DT:C4	2.45	0.52
1:A:163:ASP:OD2	4:K:35:G:N2	2.43	0.52
2:G:335:ALA:HB3	6:L:47:DG:H1'	1.92	0.52
1:C:161:THR:OG1	1:C:162:GLY:N	2.41	0.52
3:J:4:ASP:HB2	3:J:7:ARG:HE	1.74	0.52
6:L:37:DA:H2'	6:L:38:DG:C8	2.45	0.52
1:A:51:ARG:NH2	1:A:112:PHE:O	2.42	0.51
3:I:4:ASP:HB2	3:I:7:ARG:HE	1.74	0.51
2:G:108:THR:HA	2:G:111:VAL:HG22	1.92	0.51
1:A:11:PHE:HD1	1:A:226:LEU:HD13	1.75	0.51
2:H:465:GLN:OE1	2:H:542:HIS:ND1	2.37	0.51
1:M:21:ASN:ND2	1:M:42:THR:H	2.09	0.51
2:H:381:LEU:HD23	2:H:398:ILE:HG22	1.91	0.51
3:I:23:LYS:HZ2	3:I:75:LEU:HD11	1.76	0.51
1:E:22:GLY:O	1:E:31:ARG:NH2	2.44	0.51
1:F:126:ARG:O	1:F:130:GLN:NE2	2.44	0.51
2:G:195:CYS:SG	2:G:196:LEU:N	2.84	0.51
1:M:255:VAL:HG11	1:M:263:ASP:HB3	1.93	0.51
6:L:50:DG:H2'	6:L:51:DT:H71	1.93	0.51
1:D:90:GLU:O	1:D:94:LYS:N	2.35	0.51
1:F:11:PHE:HD1	1:F:226:LEU:HD13	1.75	0.51
2:H:476:ALA:HB2	2:H:562:TYR:HA	1.93	0.51
5:N:37:ILE:HG23	5:N:138:PRO:HB3	1.92	0.51
1:D:11:PHE:HD1	1:D:226:LEU:HD13	1.75	0.50
4:K:6:A:C4	1:M:115:VAL:HG21	2.46	0.50
1:D:126:ARG:O	1:D:130:GLN:NE2	2.45	0.50
1:A:126:ARG:O	1:A:130:GLN:NE2	2.44	0.50
1:C:110:ARG:HG2	1:C:192:THR:HB	1.94	0.50
1:D:170:LYS:HE2	4:K:37:C:H41	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:LEU:HD12	1:E:172:THR:HG23	1.94	0.50
1:A:143:LEU:HD12	1:A:172:THR:HG23	1.94	0.50
1:B:143:LEU:HD12	1:B:172:THR:HG23	1.94	0.50
1:C:54:ILE:HD13	1:C:107:TYR:HE2	1.77	0.50
1:C:126:ARG:O	1:C:130:GLN:NE2	2.45	0.50
2:G:208:HIS:HE1	2:G:242:ILE:HD12	1.75	0.50
2:G:247:MET:HA	2:G:250:TYR:HD2	1.76	0.50
2:G:271:THR:HA	2:G:329:GLY:HA2	1.92	0.50
1:D:143:LEU:HD12	1:D:172:THR:HG23	1.94	0.50
1:F:90:GLU:O	1:F:94:LYS:N	2.39	0.50
1:M:179:ARG:NH2	1:M:244:PHE:O	2.42	0.50
5:N:57:LEU:HD13	5:N:157:ASP:HB3	1.94	0.50
1:B:54:ILE:HD13	1:B:107:TYR:HE2	1.77	0.50
1:F:54:ILE:HD13	1:F:107:TYR:HE2	1.77	0.50
2:G:33:ILE:HG23	2:G:46:GLU:HB3	1.93	0.50
1:C:143:LEU:HD12	1:C:172:THR:HG23	1.94	0.49
1:E:54:ILE:HD13	1:E:107:TYR:HE2	1.77	0.49
2:H:474:LEU:HD13	2:H:540:LEU:HD11	1.94	0.49
2:H:361:LEU:HA	2:H:438:LYS:HZ3	1.77	0.49
1:A:54:ILE:HD13	1:A:107:TYR:HE2	1.77	0.49
1:A:96:GLU:OE2	1:A:99:ARG:NH2	2.43	0.49
1:D:54:ILE:HD13	1:D:107:TYR:HE2	1.77	0.49
2:G:179:VAL:O	2:G:183:ASN:ND2	2.45	0.49
3:I:16:ARG:HB3	3:I:82:ILE:HD13	1.95	0.49
1:F:21:ASN:ND2	1:F:41:VAL:HA	2.27	0.49
1:F:143:LEU:HD12	1:F:172:THR:HG23	1.94	0.49
3:I:103:ILE:HD13	3:J:83:LEU:HD13	1.95	0.49
1:C:34:PRO:HG2	2:H:511:THR:HG22	1.94	0.49
4:K:34:C:H2'	4:K:35:G:C8	2.46	0.49
1:F:91:LYS:HA	1:F:94:LYS:HB3	1.94	0.49
2:H:403:ASP:O	2:H:407:ASN:ND2	2.37	0.49
2:H:469:TYR:OH	2:H:564:HIS:ND1	2.32	0.49
1:D:144:GLU:OE2	3:I:57:ARG:NE	2.40	0.49
1:E:218:ARG:NH2	4:K:41:G:OP1	2.46	0.49
2:H:538:GLN:OE1	3:J:110:GLN:NE2	2.46	0.49
6:L:53:DC:H5'	6:L:53:DC:C6	2.48	0.49
1:C:141:MET:SD	1:C:141:MET:N	2.86	0.49
2:G:215:ASN:OD1	2:G:216:ALA:N	2.43	0.49
3:J:44:ALA:HB2	3:J:51:VAL:HG11	1.95	0.49
4:K:15:A:OP2	1:M:147:ILE:HB	2.13	0.49
5:N:173:TYR:HE1	5:N:203:THR:HB	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:O	1:A:179:ARG:HG2	2.13	0.48
4:K:6:A:H2	5:N:73:LYS:HA	1.77	0.48
5:N:77:ARG:NH2	7:O:7:DG:O4'	2.46	0.48
1:B:69:GLU:O	1:M:164:ASN:ND2	2.43	0.48
3:I:38:ASP:O	3:J:64:ASN:ND2	2.33	0.48
2:G:161:LEU:H	2:G:161:LEU:HD23	1.79	0.48
2:G:234:LYS:HB3	2:G:238:PHE:HB2	1.94	0.48
3:J:28:ALA:HB1	3:J:65:LYS:HE3	1.96	0.48
1:C:162:GLY:O	1:C:164:ASN:ND2	2.47	0.48
4:K:8:C:H5'	1:M:48:ARG:HB2	1.96	0.48
1:M:51:ARG:NE	1:M:108:ASP:OD2	2.46	0.48
5:N:175:MET:HA	5:N:190:PRO:HD2	1.95	0.48
1:B:96:GLU:OE2	1:B:99:ARG:NH2	2.43	0.48
1:E:273:LEU:HB2	1:E:277:LYS:HZ1	1.78	0.48
1:B:25:ASP:HB3	2:H:425:ALA:HA	1.96	0.48
2:G:69:ARG:HA	2:G:77:VAL:HG21	1.96	0.48
1:M:6:ARG:NH1	5:N:132:GLY:O	2.47	0.48
1:F:96:GLU:OE2	1:F:99:ARG:NH2	2.43	0.48
3:J:16:ARG:HB3	3:J:82:ILE:HD13	1.95	0.47
6:L:55:DT:H1'	6:L:56:DC:C4	2.49	0.47
1:A:141:MET:HG3	1:D:35:GLN:HG2	1.96	0.47
1:D:91:LYS:HA	1:D:94:LYS:HB3	1.96	0.47
2:H:393:LEU:HD13	1:M:29:LEU:HD23	1.95	0.47
3:I:44:ALA:HB2	3:I:51:VAL:HG11	1.95	0.47
1:M:134:SER:HB3	1:M:180:CYS:HB2	1.96	0.47
1:E:96:GLU:OE2	1:E:99:ARG:NH2	2.43	0.47
1:B:222:ASN:ND2	1:C:240:ALA:HB3	2.29	0.47
1:F:17:ASP:N	1:F:17:ASP:OD1	2.46	0.47
2:G:240:PHE:HB2	2:G:242:ILE:HG13	1.96	0.47
1:M:2:THR:HA	1:M:195:SER:HA	1.96	0.47
2:G:266:ILE:HD13	2:H:402:THR:HG21	1.97	0.47
1:D:162:GLY:HA2	1:F:121:ASN:ND2	2.30	0.47
1:E:224:ARG:HH12	1:F:245:LYS:HE3	1.79	0.47
3:I:28:ALA:HB1	3:I:65:LYS:HE3	1.96	0.47
1:M:31:ARG:NH2	5:N:66:ARG:O	2.38	0.47
1:M:48:ARG:HH22	1:M:67:ILE:HG22	1.80	0.47
1:M:106:TYR:O	1:M:110:ARG:NH1	2.47	0.47
1:A:65:ILE:HA	1:A:108:ASP:HB2	1.97	0.47
1:B:48:ARG:HG2	4:K:14:C:C2	2.50	0.47
1:B:65:ILE:HA	1:B:108:ASP:HB2	1.97	0.47
1:D:90:GLU:OE1	1:D:93:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:THR:HG21	4:K:39:U:H3	1.78	0.47
1:F:90:GLU:OE1	1:F:93:GLU:N	2.46	0.47
3:I:35:THR:O	3:I:39:ARG:NH1	2.46	0.47
5:N:68:ASN:HD22	5:N:87:ARG:HD2	1.79	0.47
1:B:149:ARG:HH22	1:B:153:THR:HG23	1.80	0.47
1:C:149:ARG:NH2	1:C:166:THR:OG1	2.48	0.47
1:B:73:LEU:HD12	1:M:153:THR:HG22	1.97	0.46
1:B:179:ARG:HH21	1:B:244:PHE:HB3	1.79	0.46
2:G:35:VAL:HG21	2:G:160:ARG:HH21	1.80	0.46
2:G:216:ALA:HB2	7:O:16:DA:C8	2.50	0.46
4:K:15:A:H5"	1:M:148:THR:HG22	1.97	0.46
1:A:90:GLU:OE1	1:A:93:GLU:N	2.48	0.46
1:C:65:ILE:HA	1:C:108:ASP:HB2	1.97	0.46
3:J:19:ALA:HB1	3:J:109:THR:HG23	1.98	0.46
1:E:65:ILE:HA	1:E:108:ASP:HB2	1.97	0.46
2:G:9:TYR:HE1	2:G:253:ALA:HB1	1.79	0.46
3:I:100:LEU:HD21	3:J:88:ARG:HD2	1.98	0.46
1:B:246:ARG:HH22	1:B:272:ASN:HB3	1.80	0.46
1:C:169:ARG:HH12	2:H:521:ASN:ND2	2.13	0.46
1:F:65:ILE:HA	1:F:108:ASP:HB2	1.97	0.46
2:G:336:ARG:HG3	6:L:47:DG:H4'	1.96	0.46
5:N:172:LEU:HA	5:N:191:MET:HG2	1.96	0.46
1:E:149:ARG:NH2	1:E:166:THR:OG1	2.48	0.46
2:H:520:LEU:HD22	2:H:529:ALA:HA	1.98	0.46
3:I:102:ALA:HB1	3:J:56:MET:HG2	1.97	0.46
1:D:153:THR:HG23	1:D:154:ASN:HD22	1.81	0.46
5:N:16:ARG:HG2	5:N:26:TYR:CZ	2.50	0.46
1:B:149:ARG:NH2	1:B:166:THR:OG1	2.48	0.46
1:C:179:ARG:HH21	1:C:244:PHE:HB3	1.81	0.46
1:D:145:HIS:CD2	1:E:31:ARG:HD3	2.50	0.46
4:K:20:G:C2	4:K:22:C:H4'	2.50	0.46
1:A:23:ASP:HB2	1:A:26:ALA:HB3	1.98	0.46
1:E:91:LYS:HA	1:E:94:LYS:HB3	1.97	0.46
3:I:19:ALA:HB1	3:I:109:THR:HG23	1.98	0.46
1:A:149:ARG:NH2	1:A:166:THR:OG1	2.48	0.46
1:F:149:ARG:NH2	1:F:166:THR:OG1	2.48	0.46
2:G:312:TYR:CZ	2:H:376:PRO:HB3	2.51	0.46
2:H:358:TYR:HA	2:H:361:LEU:HB2	1.96	0.46
2:H:544:GLN:OE1	3:J:7:ARG:NH2	2.49	0.46
1:D:149:ARG:NH2	1:D:166:THR:OG1	2.48	0.45
1:M:68:ARG:HE	1:M:73:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:48:DA:C8	6:L:48:DA:H5'	2.51	0.45
1:D:163:ASP:OD1	1:D:163:ASP:N	2.49	0.45
1:E:270:ASP:HA	1:E:273:LEU:HD21	1.99	0.45
2:H:532:LEU:HA	2:H:535:GLU:HG2	1.97	0.45
1:B:146:SER:OG	2:H:496:ARG:NH1	2.44	0.45
1:B:148:THR:HG22	1:B:167:MET:HG2	1.98	0.45
1:D:24:PRO:HG3	4:K:33:U:H5"	1.98	0.45
2:H:471:LEU:HB3	2:H:558:PHE:CE1	2.51	0.45
1:B:231:HIS:NE2	1:B:277:LYS:HE2	2.32	0.45
2:G:220:PRO:HG2	6:L:48:DA:H4'	1.98	0.45
2:H:505:PRO:O	2:H:509:PHE:HB2	2.15	0.45
1:M:238:ALA:HB3	1:M:277:LYS:HZ2	1.81	0.45
1:B:169:ARG:NH1	2:H:496:ARG:HB2	2.31	0.45
2:G:20:ILE:HG13	2:G:256:THR:HG21	1.97	0.45
2:G:36:ILE:HA	2:G:43:ILE:HG12	1.99	0.45
2:H:421:ARG:HH12	2:H:422:ARG:HH11	1.64	0.45
5:N:108:MET:SD	5:N:108:MET:N	2.90	0.45
1:D:65:ILE:HA	1:D:108:ASP:HB2	1.97	0.45
2:G:22:GLN:O	2:G:24:GLY:N	2.50	0.45
3:J:25:GLN:HG2	3:J:36:ILE:H	1.82	0.45
2:G:214:VAL:HG12	2:G:332:PRO:HB3	1.99	0.45
1:M:146:SER:HA	1:M:169:ARG:HA	1.99	0.45
1:C:137:ILE:HG13	1:C:249:VAL:HG23	1.99	0.45
1:D:137:ILE:HG13	1:D:249:VAL:HG23	1.99	0.45
1:E:246:ARG:HH22	1:E:272:ASN:HB2	1.81	0.45
2:G:224:VAL:HG22	2:G:229:PHE:HB3	1.98	0.45
2:G:247:MET:HG2	2:G:250:TYR:HE2	1.82	0.45
2:H:525:PHE:HD1	2:H:528:ARG:H	1.63	0.45
3:J:21:LEU:HD13	3:J:55:LEU:HB3	1.99	0.45
1:M:213:ASP:O	1:M:218:ARG:NH1	2.48	0.45
7:O:12:DT:H2'	7:O:13:DC:C6	2.52	0.45
1:A:91:LYS:HA	1:A:94:LYS:HB3	1.98	0.44
1:A:165:ARG:HH22	4:K:32:A:H62	1.65	0.44
1:C:91:LYS:HA	1:C:94:LYS:HB3	1.99	0.44
3:I:41:PHE:HB3	3:J:60:PRO:HG2	1.99	0.44
2:H:425:ALA:HB1	6:L:41:DG:H22	1.83	0.44
3:I:25:GLN:HG2	3:I:36:ILE:H	1.82	0.44
1:M:9:PHE:CZ	1:M:182:GLY:HA3	2.52	0.44
1:C:161:THR:HG21	1:D:121:ASN:HD22	1.81	0.44
2:H:463:ASN:O	2:H:465:GLN:N	2.42	0.44
2:H:482:GLN:HE21	2:H:482:GLN:HB3	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:497:TYR:CZ	2:H:512:LEU:HD13	2.53	0.44
1:A:258:VAL:O	1:A:259:ARG:NE	2.50	0.44
2:G:42:PHE:HZ	2:G:45:LEU:HB2	1.83	0.44
2:H:359:ASP:OD1	2:H:360:ASP:N	2.51	0.44
1:F:68:ARG:HB3	1:F:69:GLU:H	1.50	0.44
1:A:137:ILE:HG13	1:A:249:VAL:HG23	1.99	0.44
1:B:222:ASN:CB	1:C:241:ASP:HB2	2.48	0.44
1:A:144:GLU:HG2	1:A:171:PHE:CE2	2.53	0.44
1:B:107:TYR:HE1	1:B:198:ASP:HB3	1.83	0.44
1:B:137:ILE:HG13	1:B:249:VAL:HG23	1.99	0.44
1:B:226:LEU:HB3	1:B:283:GLY:H	1.83	0.44
1:C:96:GLU:OE2	1:C:99:ARG:NH2	2.43	0.44
2:G:323:ASP:OD1	2:G:324:LYS:N	2.51	0.44
1:C:226:LEU:HB3	1:C:283:GLY:H	1.83	0.44
5:N:126:LYS:HZ2	5:N:151:LEU:HD21	1.83	0.44
5:N:196:LYS:HB3	5:N:197:ALA:H	1.53	0.44
1:A:5:LYS:HG2	1:A:232:SER:HA	2.00	0.43
1:E:107:TYR:HE1	1:E:198:ASP:HB3	1.83	0.43
2:G:66:GLY:HA2	2:G:79:ASN:HD21	1.83	0.43
2:H:424:LYS:O	2:H:427:GLN:NE2	2.49	0.43
1:B:179:ARG:NH2	1:B:244:PHE:O	2.51	0.43
2:G:183:ASN:HA	2:G:187:SER:HB2	1.99	0.43
2:G:329:GLY:H	2:G:341:PHE:HB2	1.82	0.43
2:H:364:VAL:HG21	2:H:564:HIS:HA	2.00	0.43
3:J:18:PHE:HB2	3:J:52:PHE:CZ	2.54	0.43
4:K:24:U:O2'	4:K:25:A:N7	2.48	0.43
1:D:96:GLU:OE2	1:D:99:ARG:NH2	2.43	0.43
1:F:137:ILE:HG13	1:F:249:VAL:HG23	1.99	0.43
1:A:107:TYR:HE1	1:A:198:ASP:HB3	1.83	0.43
1:D:114:ALA:HA	4:K:30:G:H4'	1.99	0.43
2:H:512:LEU:HD12	2:H:515:LEU:HD22	2.00	0.43
2:H:531:GLN:HE22	2:H:576:LYS:HG2	1.83	0.43
4:K:22:C:H2'	4:K:23:G:C8	2.54	0.43
4:K:23:G:H3'	4:K:24:U:H5'	1.99	0.43
1:M:48:ARG:NH1	1:M:67:ILE:O	2.47	0.43
5:N:16:ARG:HH21	5:N:27:PRO:HD3	1.82	0.43
1:F:107:TYR:HE1	1:F:198:ASP:HB3	1.83	0.43
2:G:1:MET:HG3	2:G:342:TRP:HZ2	1.83	0.43
4:K:16:G:N1	6:L:39:DC:C2	2.87	0.43
1:E:137:ILE:HG13	1:E:249:VAL:HG23	1.99	0.43
2:G:42:PHE:CG	2:G:140:VAL:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:ASP:OD1	1:M:264:TYR:OH	2.37	0.43
1:M:158:ALA:HB1	6:L:40:DT:H4'	2.01	0.43
1:B:31:ARG:HD3	1:M:145:HIS:CE1	2.54	0.43
1:B:224:ARG:HH22	1:C:245:LYS:HE2	1.82	0.43
1:D:107:TYR:HE1	1:D:198:ASP:HB3	1.83	0.43
1:E:18:GLY:N	1:E:172:THR:OG1	2.52	0.43
1:E:167:MET:HG2	1:E:168:GLY:H	1.82	0.43
2:G:92:ALA:HB1	2:G:95:LYS:HB2	2.01	0.43
3:I:94:ASN:O	3:I:98:GLN:N	2.48	0.43
1:A:25:ASP:OD2	3:J:39:ARG:NH2	2.52	0.43
1:B:179:ARG:HE	1:B:181:HIS:CE1	2.37	0.43
1:C:107:TYR:HE1	1:C:198:ASP:HB3	1.83	0.43
1:C:144:GLU:HG3	1:C:171:PHE:CE2	2.54	0.43
1:D:21:ASN:OD1	1:D:42:THR:OG1	2.34	0.43
3:I:18:PHE:HB2	3:I:52:PHE:CZ	2.53	0.43
1:B:24:PRO:HB3	4:K:15:A:C5	2.54	0.43
1:B:242:SER:O	1:B:246:ARG:HG2	2.19	0.43
2:G:2:ILE:HD13	2:G:342:TRP:CH2	2.54	0.43
1:M:47:LYS:HE3	1:M:112:PHE:CD1	2.53	0.43
1:B:26:ALA:O	1:B:28:ASN:N	2.49	0.43
1:D:226:LEU:HB3	1:D:283:GLY:H	1.83	0.43
1:E:226:LEU:HB3	1:E:283:GLY:H	1.83	0.43
2:H:367:GLU:HG3	2:H:572:LYS:HG3	2.01	0.43
3:I:23:LYS:HZ2	3:I:75:LEU:HD21	1.83	0.43
1:M:153:THR:OG1	1:M:156:LYS:NZ	2.48	0.43
1:M:214:HIS:HA	1:M:218:ARG:HH12	1.84	0.43
5:N:5:LEU:O	5:N:101:ARG:HA	2.18	0.43
5:N:11:LEU:HD23	5:N:96:LYS:HA	1.99	0.43
5:N:42:LEU:HD22	5:N:128:ARG:HD2	2.01	0.43
5:N:77:ARG:HA	6:L:56:DC:H5'	2.01	0.43
1:C:152:VAL:HB	1:C:164:ASN:HB3	2.01	0.42
1:F:226:LEU:HB3	1:F:283:GLY:H	1.83	0.42
2:G:75:TYR:HB3	2:G:103:GLN:HG2	2.00	0.42
3:I:21:LEU:HD13	3:I:55:LEU:HB3	1.99	0.42
6:L:47:DG:H8	6:L:47:DG:OP2	2.02	0.42
1:C:33:ASP:OD2	1:C:35:GLN:NE2	2.52	0.42
1:B:167:MET:HB3	1:B:168:GLY:H	1.57	0.42
2:H:371:TYR:HD1	2:H:379:ARG:HH12	1.65	0.42
1:E:112:PHE:HE1	1:E:131:LEU:HD13	1.85	0.42
1:A:226:LEU:HB3	1:A:283:GLY:H	1.83	0.42
1:D:242:SER:O	1:D:246:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:PHE:HD1	1:E:277:LYS:HZ3	1.66	0.42
1:M:105:ARG:HG3	1:M:106:TYR:CD2	2.55	0.42
1:M:120:LYS:HB3	5:N:183:ARG:HG2	2.02	0.42
6:L:53:DC:H5'	6:L:53:DC:H6	1.84	0.42
1:B:112:PHE:HE1	1:B:131:LEU:HD13	1.85	0.42
2:G:141:MET:HA	2:G:146:TRP:CD1	2.54	0.42
3:J:35:THR:O	3:J:39:ARG:NH1	2.46	0.42
1:C:242:SER:O	1:C:246:ARG:HG2	2.19	0.42
1:F:242:SER:O	1:F:246:ARG:HG2	2.19	0.42
2:G:306:ALA:HB1	2:G:309:LYS:HE3	2.01	0.42
2:H:386:LEU:HD12	2:H:386:LEU:H	1.84	0.42
2:H:386:LEU:HA	2:H:422:ARG:NH1	2.35	0.42
3:I:110:GLN:HB2	3:J:80:ARG:HB3	2.01	0.42
1:A:150:MET:SD	1:D:48:ARG:NH2	2.93	0.42
1:A:242:SER:O	1:A:246:ARG:HG2	2.19	0.42
1:D:21:ASN:ND2	1:D:31:ARG:HH21	2.17	0.42
3:J:16:ARG:CZ	3:J:82:ILE:HG12	2.50	0.42
1:M:7:TYR:HB2	1:M:184:ILE:HB	2.01	0.42
1:B:148:THR:HA	1:B:167:MET:HA	2.02	0.42
1:C:112:PHE:HE1	1:C:131:LEU:HD13	1.85	0.42
1:D:21:ASN:HD21	1:D:31:ARG:HH21	1.66	0.42
2:G:54:LYS:NZ	7:O:17:DA:OP2	2.46	0.42
2:H:421:ARG:NH1	2:H:422:ARG:HH11	2.17	0.42
1:M:33:ASP:HB3	5:N:96:LYS:NZ	2.34	0.42
1:B:153:THR:HG21	6:L:37:DA:H1'	2.02	0.42
1:C:26:ALA:O	1:C:28:ASN:N	2.52	0.42
1:F:112:PHE:HE1	1:F:131:LEU:HD13	1.85	0.42
2:H:473:ARG:NH2	2:H:539:ILE:HG12	2.35	0.42
2:H:503:SER:HA	2:H:550:LEU:HB2	2.02	0.42
3:J:94:ASN:O	3:J:98:GLN:N	2.48	0.42
4:K:1:G:N2	5:N:43:TRP:HB3	2.34	0.42
1:A:234:ASN:HD21	1:C:56:MET:HG2	1.85	0.41
1:D:112:PHE:HE1	1:D:131:LEU:HD13	1.85	0.41
1:D:170:LYS:HD3	1:D:170:LYS:HA	1.94	0.41
1:E:242:SER:O	1:E:246:ARG:HG2	2.19	0.41
2:H:489:LEU:HA	6:L:34:DG:H2'	2.02	0.41
2:H:516:LEU:HG	2:H:517:PRO:HD3	2.02	0.41
3:I:16:ARG:O	3:I:20:VAL:HG23	2.20	0.41
3:J:23:LYS:HE3	3:J:112:LEU:HB3	2.02	0.41
1:M:132:THR:HG23	5:N:146:PRO:HD3	2.02	0.41
1:M:168:GLY:HA2	6:L:42:DA:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:489:LEU:HB3	6:L:35:DC:C2	2.55	0.41
1:A:21:ASN:HD22	1:A:22:GLY:H	1.68	0.41
1:C:256:GLU:OE2	3:I:94:ASN:ND2	2.53	0.41
1:F:73:LEU:HD23	1:F:76:LEU:HD21	2.03	0.41
2:H:429:ILE:HG13	2:H:433:ARG:HB2	2.02	0.41
4:K:6:A:N1	5:N:73:LYS:HD3	2.36	0.41
1:B:9:PHE:CZ	1:B:182:GLY:HA3	2.56	0.41
1:E:273:LEU:HD22	1:E:277:LYS:HZ1	1.85	0.41
2:G:136:GLU:O	2:G:140:VAL:HG23	2.20	0.41
2:G:195:CYS:HG	2:G:198:THR:HG1	1.66	0.41
1:M:21:ASN:HD22	1:M:42:THR:H	1.66	0.41
1:B:134:SER:HB3	1:B:178:TYR:HB3	2.03	0.41
1:D:165:ARG:HE	4:K:41:G:N2	2.19	0.41
1:B:149:ARG:NH2	1:B:153:THR:HG23	2.36	0.41
1:C:48:ARG:HH11	1:C:51:ARG:HD3	1.86	0.41
1:D:150:MET:SD	1:E:48:ARG:NH2	2.94	0.41
2:H:531:GLN:HG2	2:H:579:PHE:CG	2.55	0.41
3:I:16:ARG:CZ	3:I:82:ILE:HG12	2.50	0.41
3:I:70:GLY:O	3:I:74:GLN:HG2	2.20	0.41
3:J:16:ARG:O	3:J:20:VAL:HG23	2.20	0.41
3:J:70:GLY:O	3:J:74:GLN:HG2	2.20	0.41
5:N:54:ILE:HB	5:N:201:VAL:HG13	2.02	0.41
5:N:128:ARG:HA	5:N:133:GLN:HB2	2.02	0.41
6:L:55:DT:H1'	6:L:56:DC:N4	2.35	0.41
1:A:9:PHE:CZ	1:A:182:GLY:HA3	2.56	0.41
1:A:112:PHE:HE1	1:A:131:LEU:HD13	1.85	0.41
1:D:143:LEU:HB3	1:D:145:HIS:CE1	2.55	0.41
1:F:149:ARG:HG2	1:F:151:ALA:H	1.86	0.41
2:H:393:LEU:HB3	1:M:26:ALA:HB1	2.02	0.41
1:M:243:LEU:HD11	1:M:277:LYS:HZ3	1.84	0.41
1:A:148:THR:HA	1:A:167:MET:HA	2.03	0.41
1:A:149:ARG:HG2	1:A:151:ALA:H	1.86	0.41
1:B:149:ARG:HG2	1:B:151:ALA:H	1.86	0.41
1:C:9:PHE:CZ	1:C:182:GLY:HA3	2.56	0.41
1:C:149:ARG:HG2	1:C:151:ALA:H	1.86	0.41
2:G:196:LEU:HD12	2:G:241:PRO:HD2	2.02	0.41
6:L:43:DC:H2'	6:L:44:DC:C5	2.55	0.41
7:O:16:DA:H2"	7:O:17:DA:C5	2.56	0.41
1:A:134:SER:HB3	1:A:178:TYR:HB3	2.03	0.41
1:E:9:PHE:CZ	1:E:182:GLY:HA3	2.56	0.41
2:H:509:PHE:O	2:H:513:MET:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:16:G:C2	6:L:39:DC:N3	2.89	0.41
1:D:153:THR:HG23	1:D:154:ASN:ND2	2.36	0.40
1:A:23:ASP:OD1	1:A:23:ASP:N	2.54	0.40
1:C:134:SER:HB3	1:C:178:TYR:HB3	2.03	0.40
1:D:149:ARG:HG2	1:D:151:ALA:H	1.86	0.40
2:G:267:GLY:O	2:G:269:VAL:HG12	2.21	0.40
2:H:510:GLY:HA3	3:J:95:LEU:HD11	2.03	0.40
2:H:546:PHE:CE1	3:J:103:ILE:HD11	2.57	0.40
3:I:20:VAL:HG11	3:I:79:ILE:HG13	2.03	0.40
3:I:68:PHE:HD2	3:I:71:ARG:H	1.70	0.40
3:J:89:PHE:HD1	3:J:89:PHE:HA	1.76	0.40
1:A:164:ASN:ND2	1:D:69:GLU:O	2.55	0.40
1:B:91:LYS:HA	1:B:94:LYS:HB3	2.03	0.40
1:C:48:ARG:HD2	1:C:48:ARG:HA	1.85	0.40
1:D:9:PHE:CZ	1:D:182:GLY:HA3	2.56	0.40
2:H:533:GLN:HG2	2:H:537:ARG:HD3	2.04	0.40
2:H:539:ILE:HD11	2:H:565:GLU:OE2	2.21	0.40
6:L:50:DG:C2'	6:L:51:DT:H71	2.50	0.40
1:D:134:SER:HB3	1:D:178:TYR:HB3	2.03	0.40
1:B:168:GLY:HA2	6:L:36:DA:N6	2.37	0.40
1:C:44:VAL:HB	4:K:20:G:H5'	2.02	0.40
1:E:149:ARG:HG2	1:E:151:ALA:H	1.86	0.40
2:G:52:LYS:HG3	2:G:53:VAL:H	1.85	0.40
2:G:343:HIS:CE1	2:H:407:ASN:HD21	2.39	0.40
2:H:404:ALA:HB3	2:H:411:LEU:HD13	2.04	0.40
3:J:12:TYR:OH	3:J:107:HIS:ND1	2.45	0.40
5:N:184:ASP:N	5:N:184:ASP:OD1	2.54	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%)	234 (83%)	42 (15%)	5 (2%)	7 35
1	B	281/283 (99%)	232 (83%)	42 (15%)	7 (2%)	4 29
1	C	281/283 (99%)	236 (84%)	40 (14%)	5 (2%)	7 35
1	D	281/283 (99%)	232 (83%)	45 (16%)	4 (1%)	9 40
1	E	281/283 (99%)	232 (83%)	43 (15%)	6 (2%)	5 32
1	F	267/283 (94%)	221 (83%)	40 (15%)	6 (2%)	5 32
1	M	260/283 (92%)	209 (80%)	48 (18%)	3 (1%)	11 43
2	G	321/582 (55%)	240 (75%)	64 (20%)	17 (5%)	1 15
2	H	231/582 (40%)	198 (86%)	25 (11%)	8 (4%)	3 24
3	I	122/124 (98%)	109 (89%)	13 (11%)	0	100 100
3	J	122/124 (98%)	109 (89%)	13 (11%)	0	100 100
5	N	203/205 (99%)	167 (82%)	32 (16%)	4 (2%)	6 33
All	All	2931/3598 (82%)	2419 (82%)	447 (15%)	65 (2%)	8 32

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	31	PRO
5	N	198	VAL
1	A	275	GLU
1	B	153	THR
1	C	153	THR
1	E	68	ARG
1	F	24	PRO
1	F	275	GLU
2	G	23	GLU
2	G	80	LEU
2	G	201	ALA
1	A	68	ARG
1	A	90	GLU
1	B	68	ARG
1	B	90	GLU
1	B	162	GLY
1	C	27	GLY
1	C	86	VAL
1	C	90	GLU
1	D	86	VAL
1	D	90	GLU
1	E	86	VAL

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Mol	Chain	Res	Type
1	E	90	GLU
1	F	68	ARG
1	F	86	VAL
1	F	90	GLU
2	G	50	GLU
2	G	69	ARG
2	G	83	ASP
2	G	123	GLY
2	G	236	GLN
2	G	333	ASN
2	H	395	SER
2	H	489	LEU
2	H	503	SER
1	M	126	ARG
1	M	275	GLU
5	N	196	LYS
1	A	86	VAL
1	B	86	VAL
1	D	68	ARG
1	E	275	GLU
2	G	72	SER
2	G	325	PHE
2	H	365	ARG
5	N	82	TYR
1	E	26	ALA
2	G	41	ASN
2	G	78	SER
2	G	98	GLU
2	G	166	VAL
2	G	202	ALA
2	H	450	LEU
2	H	490	ASN
1	A	20	PRO
1	B	27	GLY
2	H	432	GLY
1	B	20	PRO
1	C	20	PRO
1	D	20	PRO
1	F	20	PRO
1	E	20	PRO
2	H	448	GLY
1	M	147	ILE

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Mol	Chain	Res	Type
5	N	45	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	245/245 (100%)	240 (98%)	5 (2%)	50 73
1	B	245/245 (100%)	242 (99%)	3 (1%)	67 82
1	C	245/245 (100%)	242 (99%)	3 (1%)	67 82
1	D	245/245 (100%)	241 (98%)	4 (2%)	58 76
1	E	245/245 (100%)	241 (98%)	4 (2%)	58 76
1	F	235/245 (96%)	230 (98%)	5 (2%)	48 72
1	M	229/245 (94%)	227 (99%)	2 (1%)	75 86
2	G	261/475 (55%)	253 (97%)	8 (3%)	35 64
2	H	196/475 (41%)	186 (95%)	10 (5%)	20 49
3	I	104/104 (100%)	103 (99%)	1 (1%)	73 84
3	J	104/104 (100%)	103 (99%)	1 (1%)	73 84
5	N	182/182 (100%)	176 (97%)	6 (3%)	33 62
All	All	2536/3055 (83%)	2484 (98%)	52 (2%)	49 72

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	167	MET
1	A	249	VAL
1	A	252	LYS
1	A	269	ASP
1	B	230	GLU
1	B	249	VAL
1	B	252	LYS
1	C	35	GLN

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Mol	Chain	Res	Type
1	C	249	VAL
1	C	252	LYS
1	D	21	ASN
1	D	91	LYS
1	D	249	VAL
1	D	252	LYS
1	E	110	ARG
1	E	249	VAL
1	E	252	LYS
1	E	273	LEU
1	F	68	ARG
1	F	110	ARG
1	F	141	MET
1	F	249	VAL
1	F	252	LYS
2	G	9	TYR
2	G	33	ILE
2	G	57	VAL
2	G	161	LEU
2	G	240	PHE
2	G	250	TYR
2	G	325	PHE
2	G	330	LEU
2	H	364	VAL
2	H	394	PRO
2	H	416	LEU
2	H	431	TYR
2	H	438	LYS
2	H	467	ILE
2	H	482	GLN
2	H	498	PHE
2	H	514	ARG
2	H	516	LEU
3	I	39	ARG
3	J	39	ARG
1	M	40	LEU
1	M	209	MET
5	N	24	VAL
5	N	47	ILE
5	N	85	ASP
5	N	175	MET
5	N	193	TYR

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Mol	Chain	Res	Type
5	N	198	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	154	ASN
1	A	248	GLN
1	B	58	GLN
1	B	204	GLN
1	B	222	ASN
1	B	248	GLN
1	C	58	GLN
1	C	83	GLN
1	C	164	ASN
1	C	220	GLN
1	D	35	GLN
1	D	58	GLN
1	E	35	GLN
1	E	58	GLN
1	E	100	GLN
1	E	234	ASN
1	E	248	GLN
1	F	16	GLN
1	F	58	GLN
1	F	83	GLN
2	G	97	GLN
2	G	142	GLN
2	G	183	ASN
2	H	383	ASN
2	H	392	ASN
2	H	407	ASN
2	H	482	GLN
2	H	486	ASN
2	H	521	ASN
3	I	8	GLN
3	I	97	GLN
3	I	120	ASN
3	J	8	GLN
3	J	97	GLN
3	J	120	ASN
1	M	16	GLN

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Mol	Chain	Res	Type
1	M	21	ASN
1	M	58	GLN
1	M	62	HIS
1	M	124	GLN
1	M	204	GLN
1	M	220	GLN
1	M	248	GLN
5	N	133	GLN
5	N	137	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	K	42/43 (97%)	32 (76%)	3 (7%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	K	2	U
4	K	3	U
4	K	4	G
4	K	5	A
4	K	6	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	14	C
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	24	U
4	K	27	G
4	K	28	U

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Mol	Chain	Res	Type
4	K	31	C
4	K	32	A
4	K	33	U
4	K	35	G
4	K	37	C
4	K	39	U
4	K	40	C
4	K	41	G
4	K	43	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	K	4	G
4	K	9	A
4	K	34	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 (i)

There are no ligands in this entry.

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.

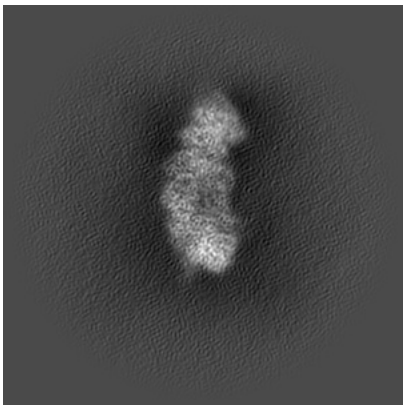
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29900. These allow visual inspection of the internal detail of the map and identification of artifacts.

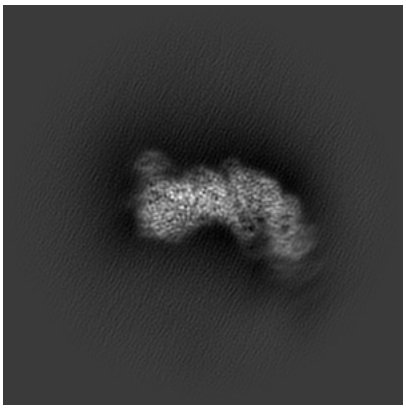
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

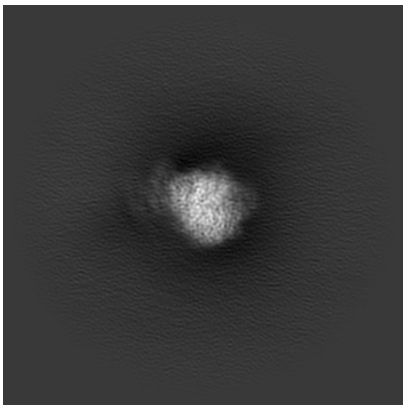
6.1.1 Primary map



X

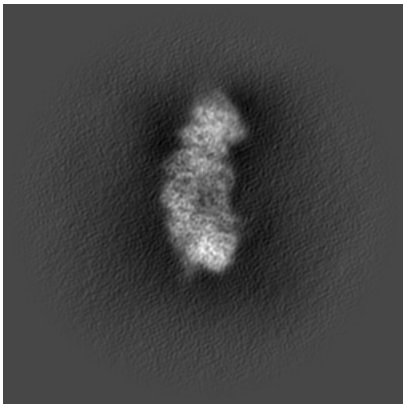


Y

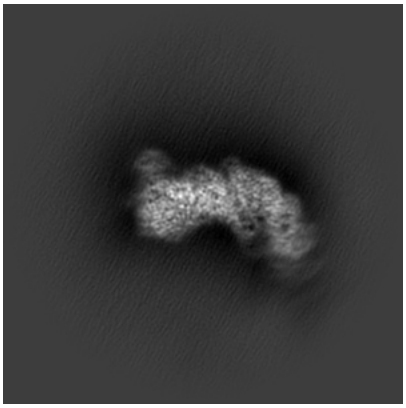


Z

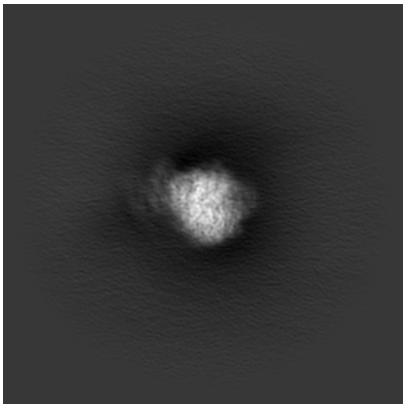
6.1.2 Raw map



X



Y

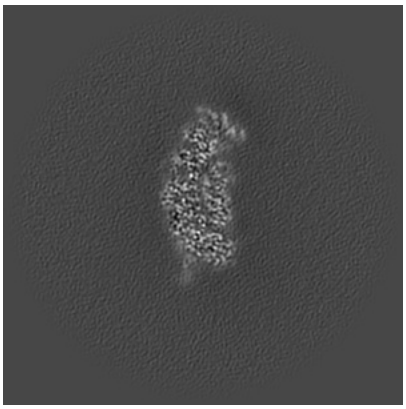


Z

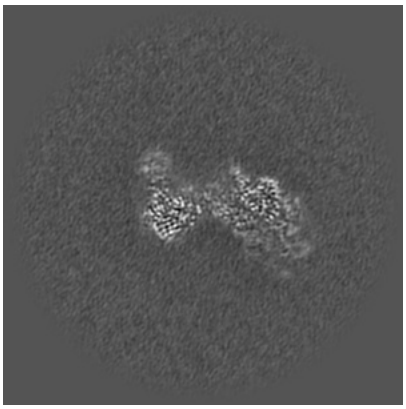
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

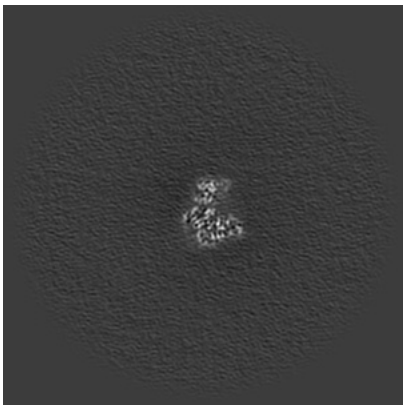
6.2.1 Primary map



X Index: 140

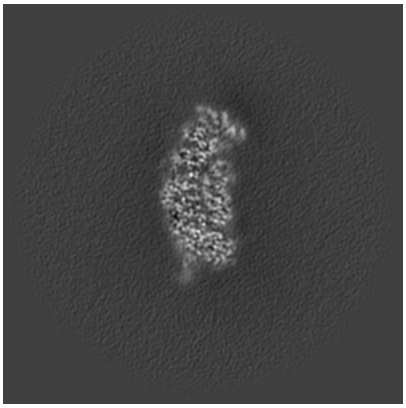


Y Index: 140

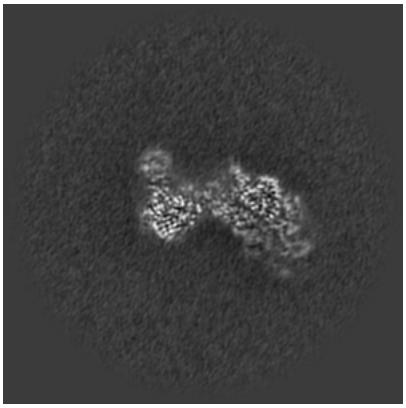


Z Index: 140

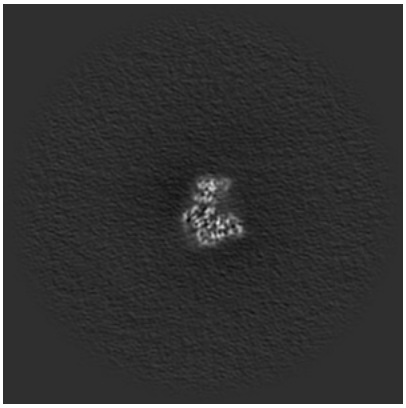
6.2.2 Raw map



X Index: 140



Y Index: 140

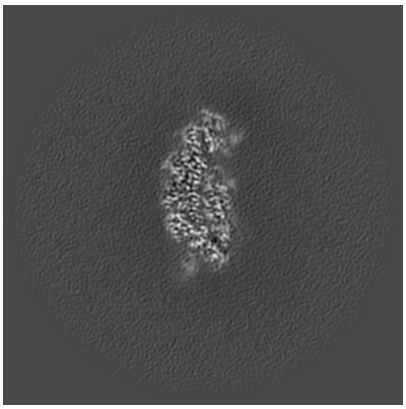


Z Index: 140

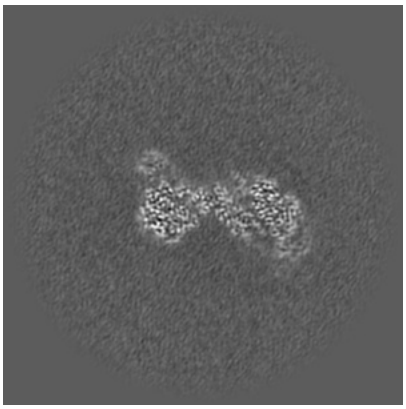
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

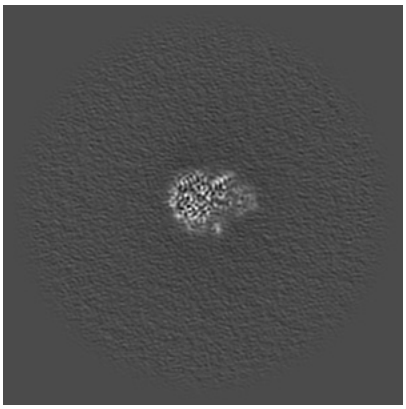
6.3.1 Primary map



X Index: 144

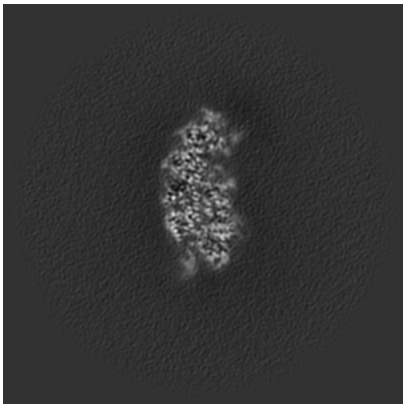


Y Index: 144

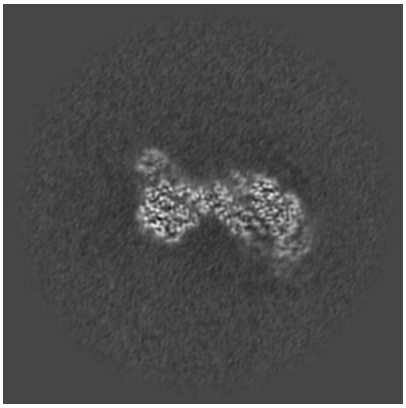


Z Index: 110

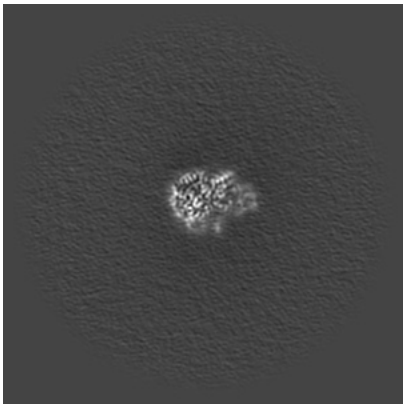
6.3.2 Raw map



X Index: 145



Y Index: 144

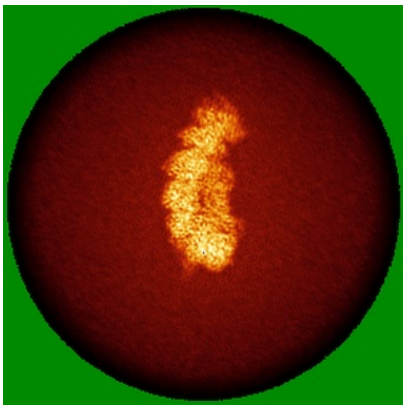


Z Index: 109

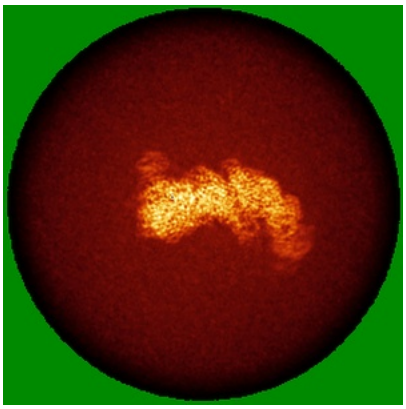
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

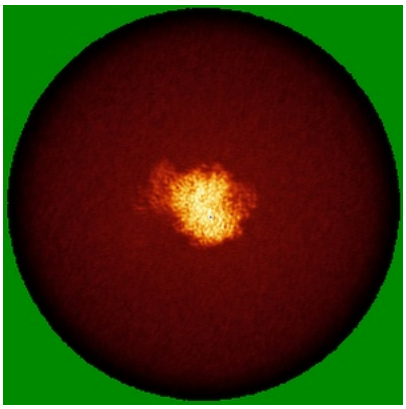
6.4.1 Primary map



X

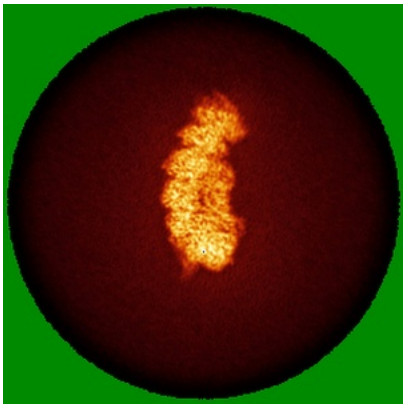


Y

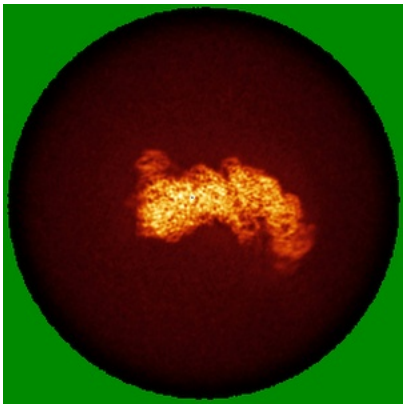


Z

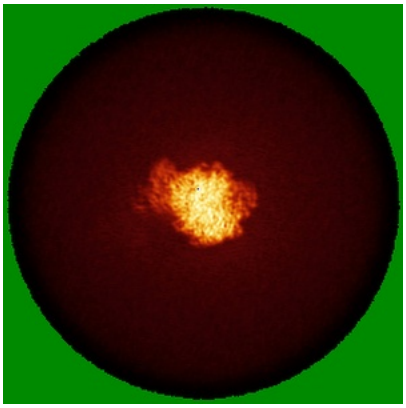
6.4.2 Raw map



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 0.14. 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.

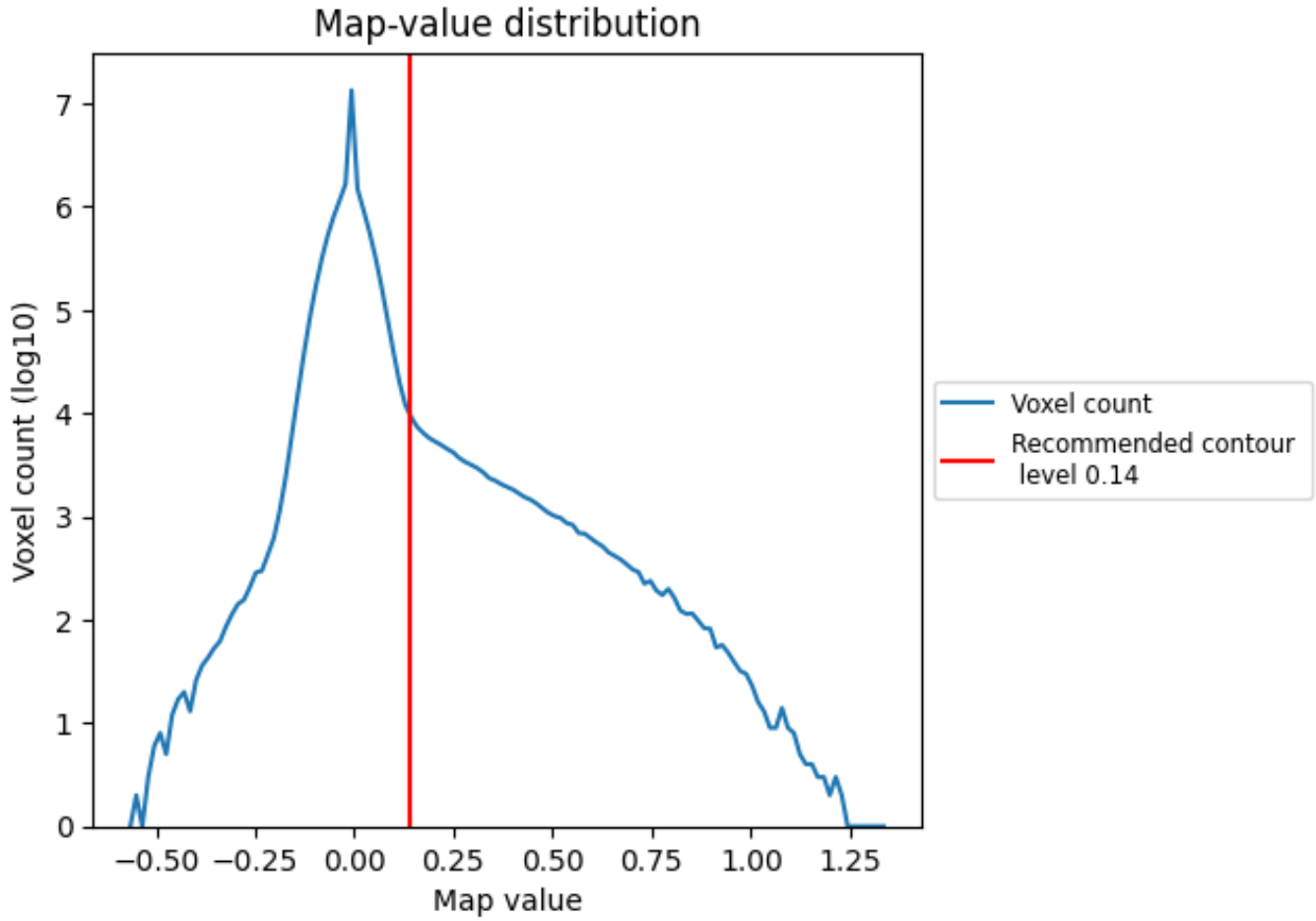
6.6 Mask visualisation (i)

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

7 Map analysis

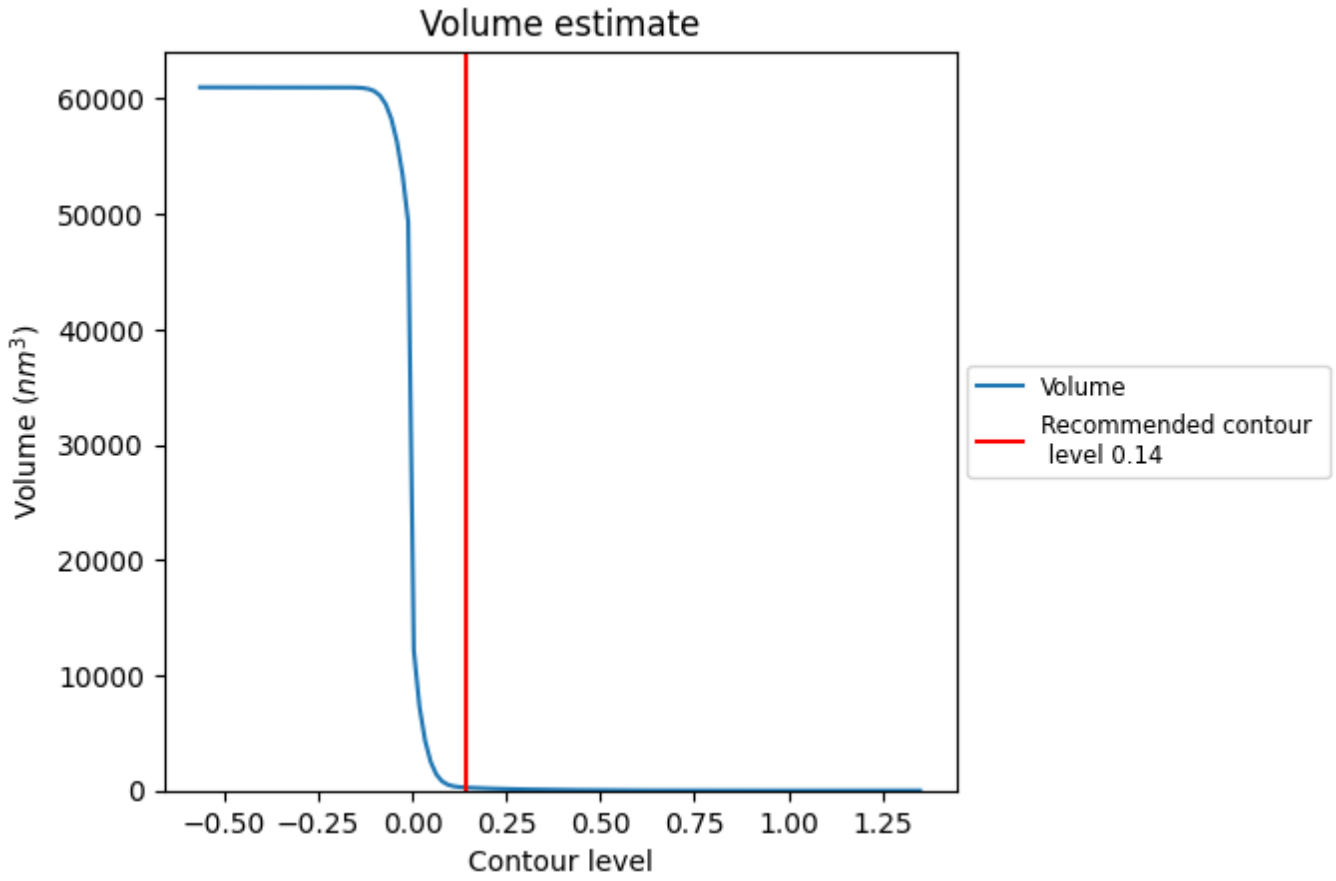
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

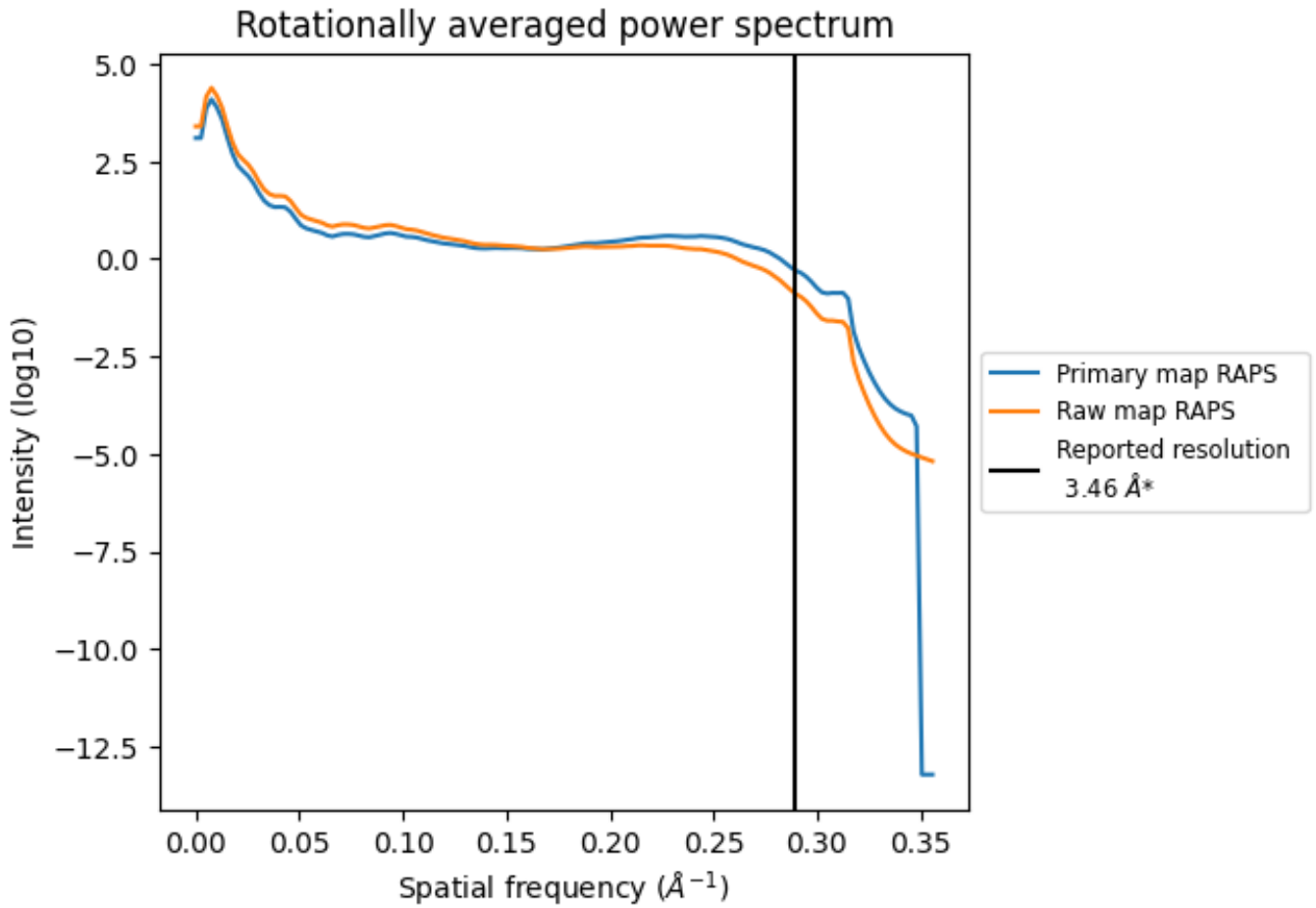
7.2 Volume estimate



The volume at the recommended contour level is 267 nm^3; this corresponds to an approximate mass of 241 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)

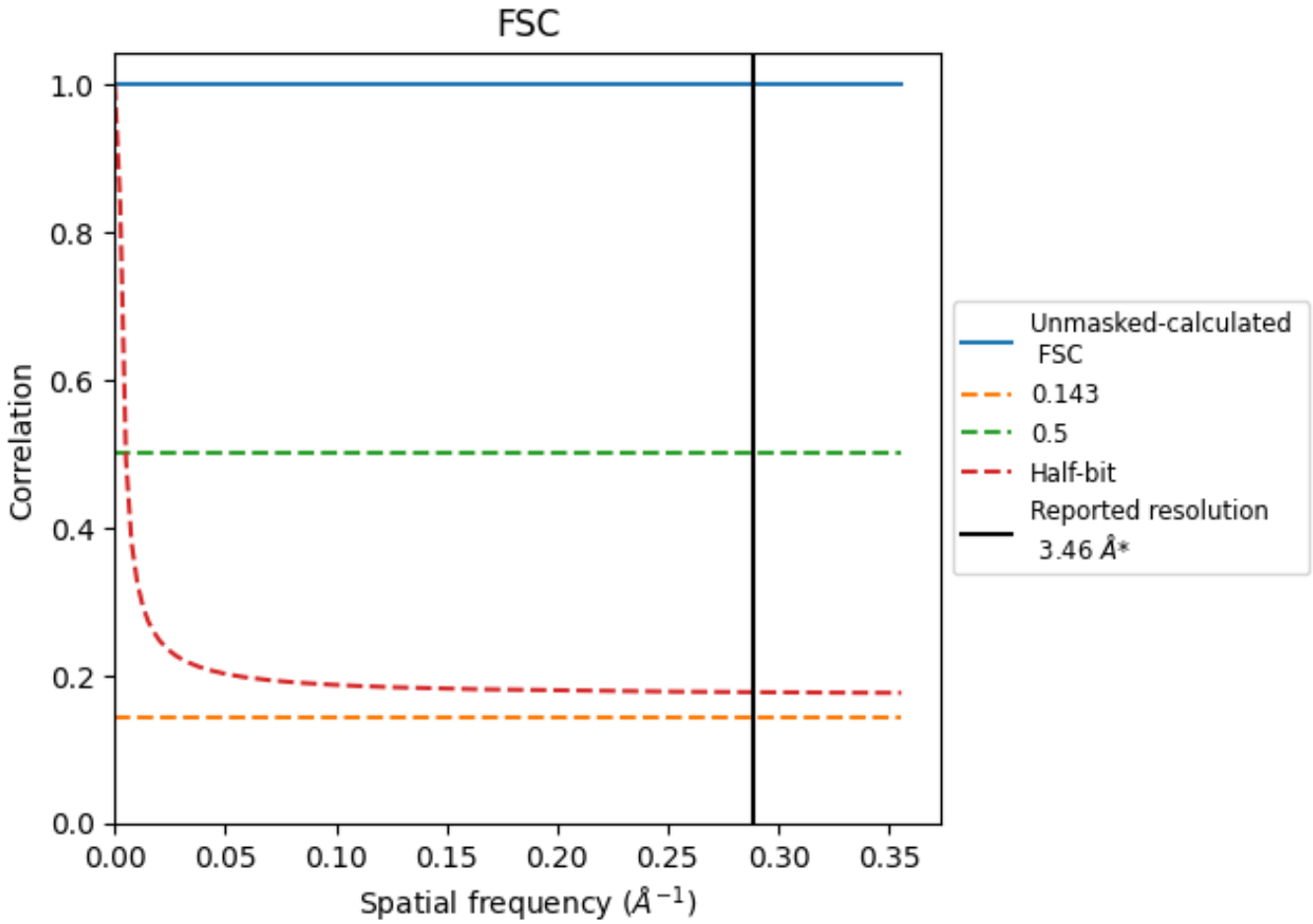


*Reported resolution corresponds to spatial frequency of 0.289 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.289 Å^{-1}

8.2 Resolution estimates (i)

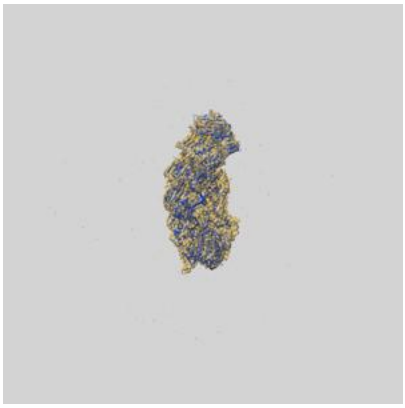
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	-	-	-

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

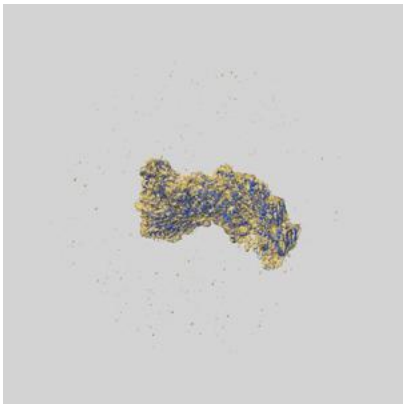
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29900 and PDB model 8GAM. Per-residue inclusion information can be found in section 3 on page 7.

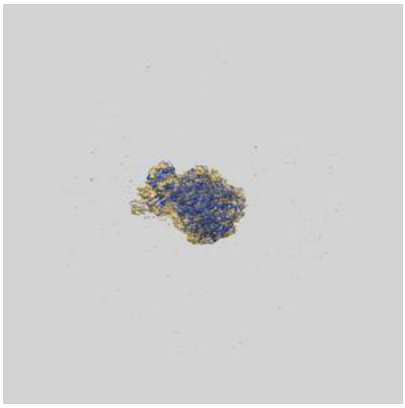
9.1 Map-model overlay



X



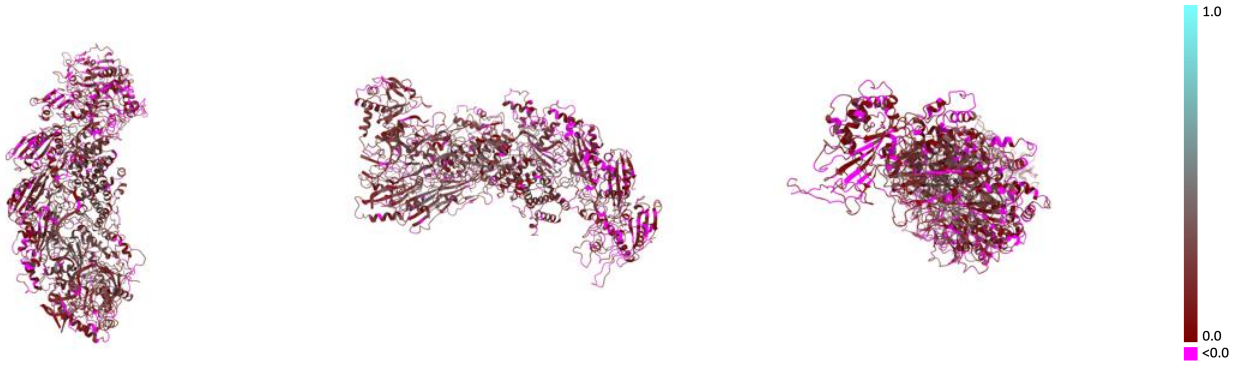
Y



Z

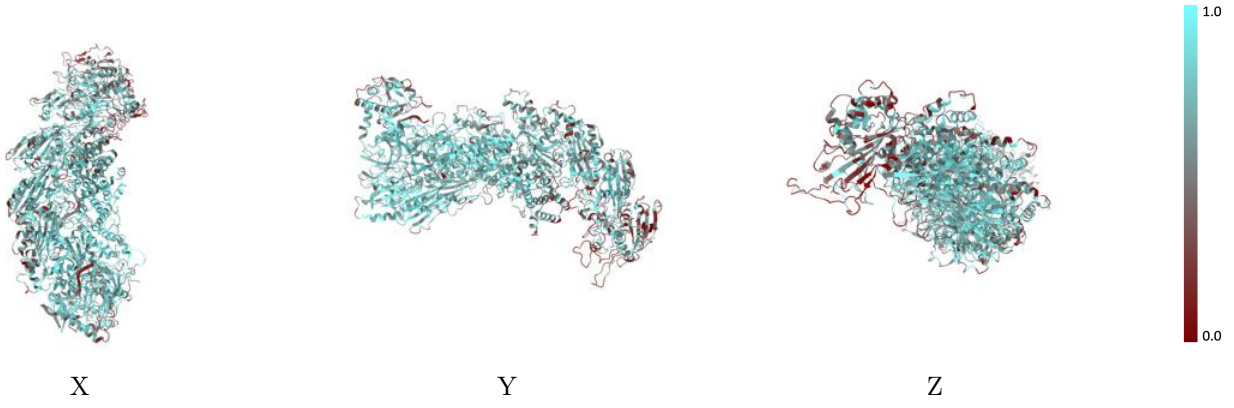
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



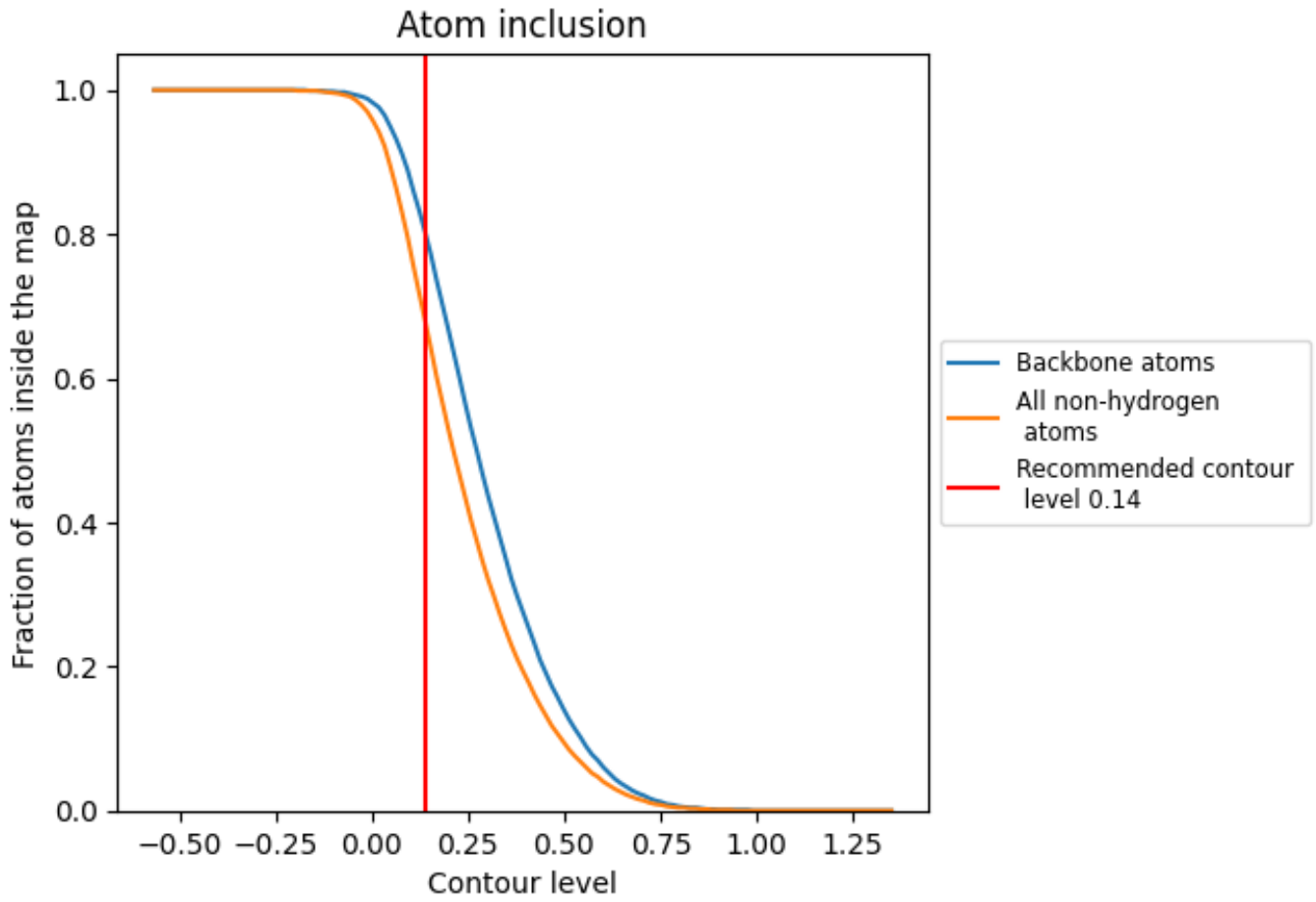
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 80% of all backbone atoms, 68% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6760	0.1600
A	0.6630	0.1240
B	0.7000	0.1530
C	0.6880	0.1700
D	0.6480	0.1060
E	0.5930	0.0950
F	0.4310	0.0720
G	0.6530	0.1730
H	0.8320	0.2300
I	0.5870	0.1860
J	0.7390	0.2040
K	0.8180	0.2190
L	0.6440	0.1780
M	0.8040	0.2320
N	0.7760	0.2220
O	0.5690	0.1340