



Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 08:34 PM JST

PDB ID : 9JMK / pdb_00009jmk
EMDB ID : EMD-61605
Title : 50S Ribosomal Subunit precursor state III
Authors : Sengupta, S.; Mukherjee, R.; Pilsl, M.; Bagale, S.; Adhikary, A.D.; Borkar, A.;
Pradeepkumar, P.I.; Engel, C.; Chowdhury, A.; Kaushal, P.S.; Anand, R.
Deposited on : 2024-09-20
Resolution : 4.00 Å(reported)
Based on initial model : 6GC8

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.dev129
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

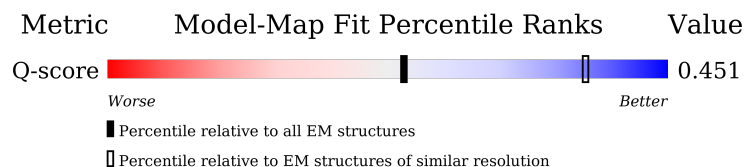
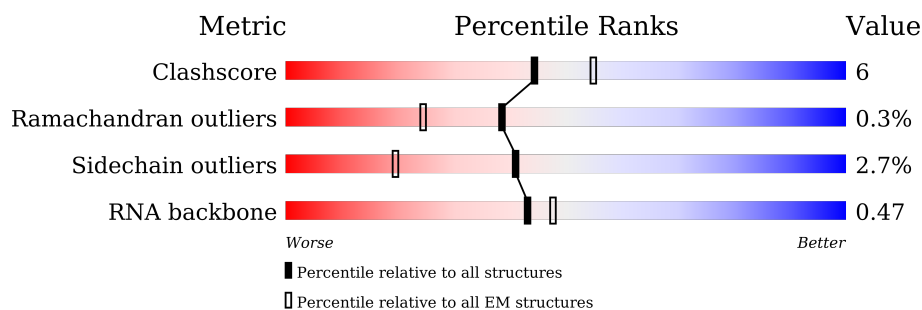
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.









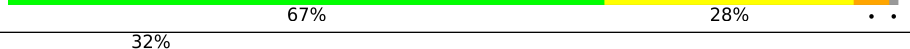
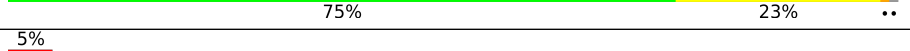
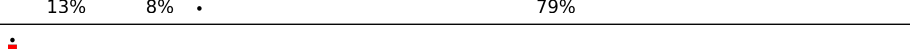
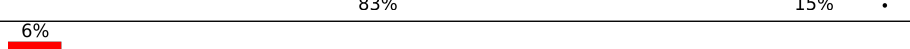
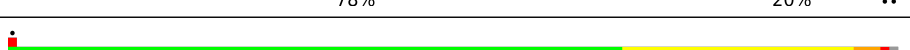

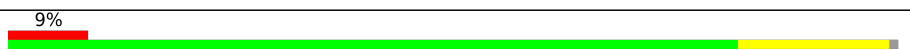

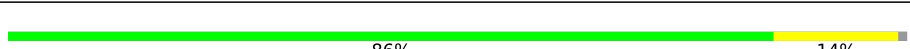





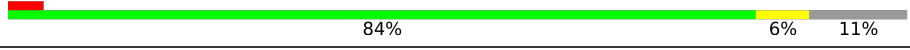
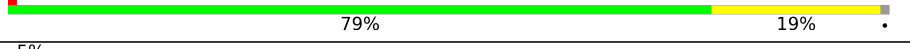



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
RNA backbone	6643	2191	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	0	57	 5% 77% 21% .
2	1	55	 75% 13% 13%
3	2	46	 83% 17%

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Mol	Chain	Length	Quality of chain
4	3	65	
5	A	2904	
6	B	120	
7	C	273	
8	D	209	
9	E	201	
10	F	179	
11	G	177	
12	H	149	
13	J	142	
14	K	123	
15	L	144	
16	N	127	
17	O	117	
18	P	115	
19	Q	118	
20	R	103	
21	S	110	
22	T	100	
23	U	104	
24	V	94	
25	W	85	
26	X	78	
27	Y	63	
28	Z	59	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 76537 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 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	48	Total	C	N	O	0	0
			395	254	72	69		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2390	Total	C	N	O	P	0	0
			51353	22907	9498	16558	2390		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	119	Total	C	N	O	P	0	0
			2548	1135	466	829	118		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	175	Total	C	N	O	S	0	0
			1317	829	242	244	2		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	32	Total	C	N	O	S	0	0
			241	155	42	43	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	98	Total	C	N	O	S	0	0
			783	494	148	140	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	87	Total	C	N	O	S	0	0
			686	434	128	123	1		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	76	Total	C	N	O	S	0	0
			581	360	117	103	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

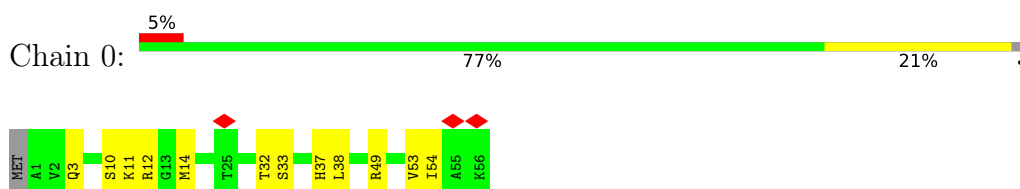
- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

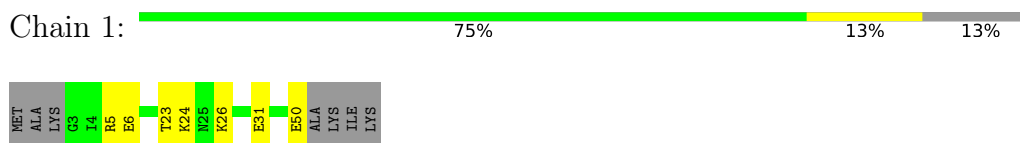
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

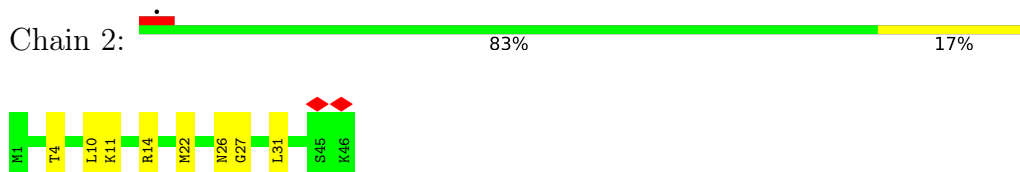
- Molecule 1: 50S ribosomal protein L32



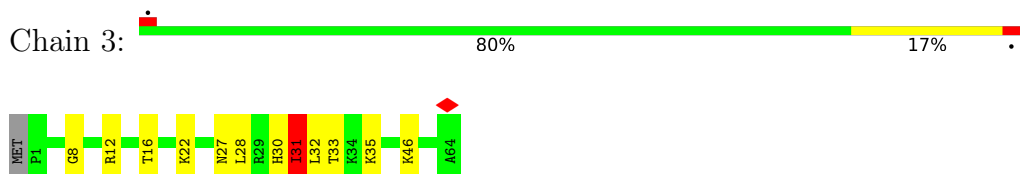
- Molecule 2: 50S ribosomal protein L33



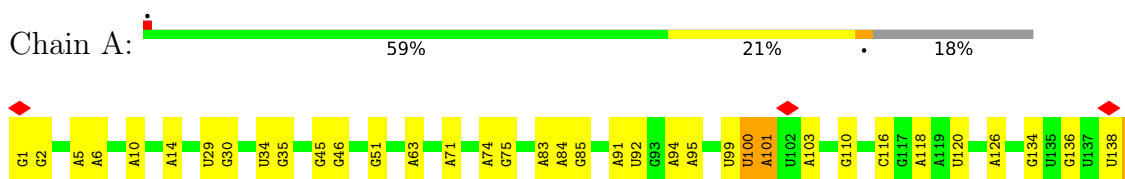
- Molecule 3: 50S ribosomal protein L34



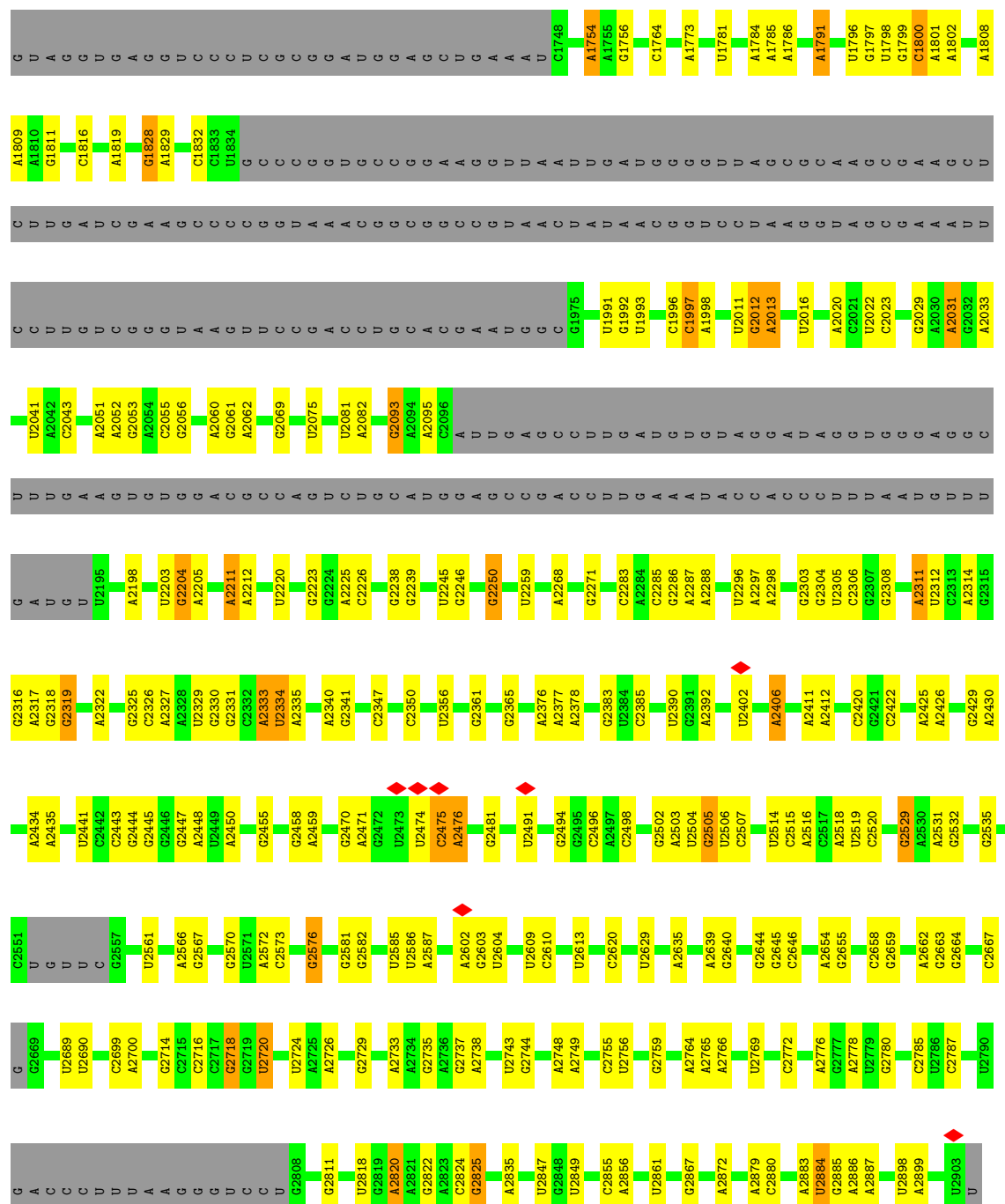
- Molecule 4: 50S ribosomal protein L35



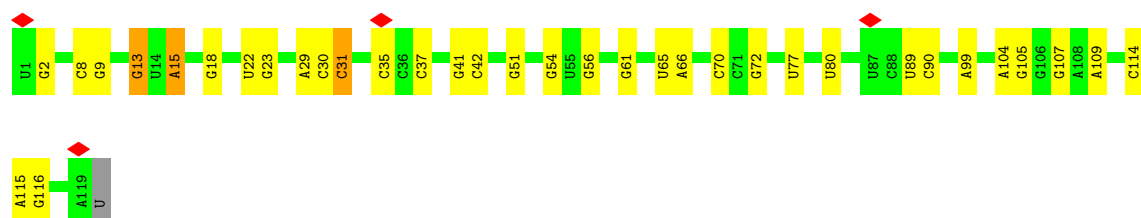
- Molecule 5: 23S ribosomal RNA



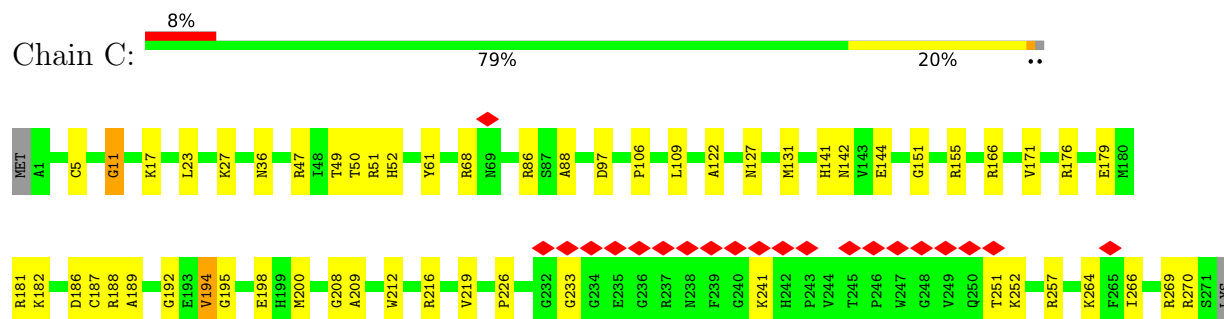




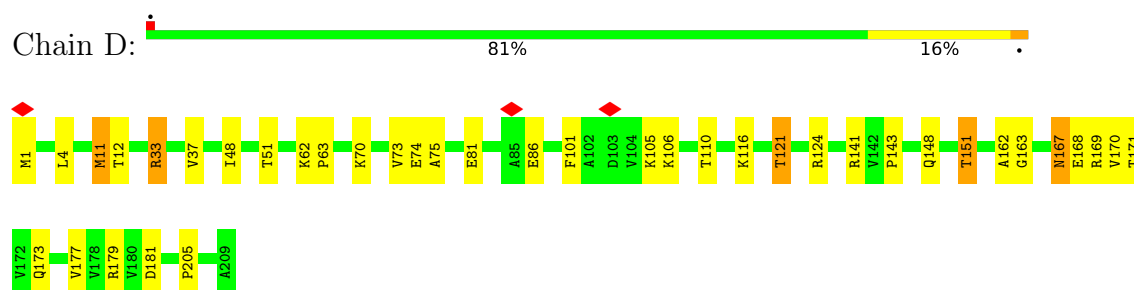
Chain B: 70% 27%



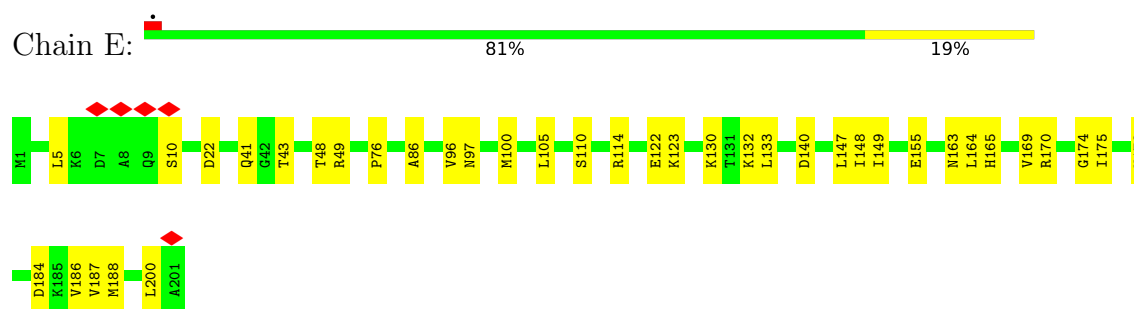
- Molecule 7: 50S ribosomal protein L2



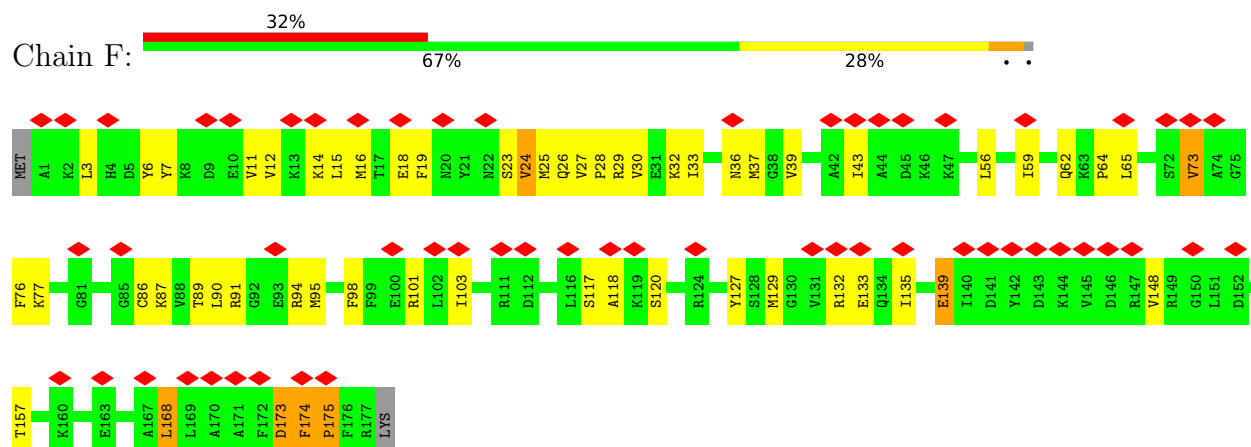
- Molecule 8: 50S ribosomal protein L3



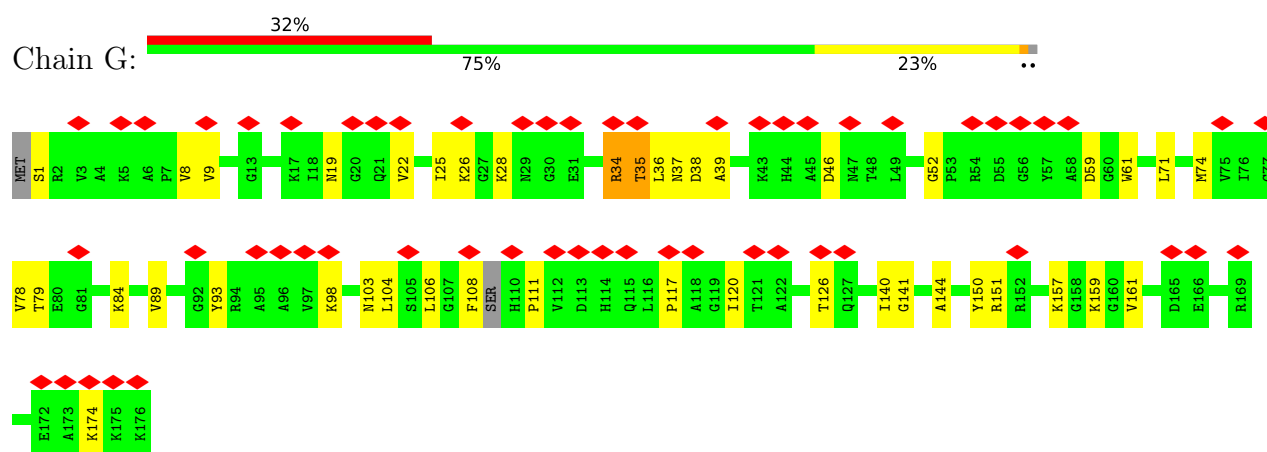
- Molecule 9: 50S ribosomal protein L4



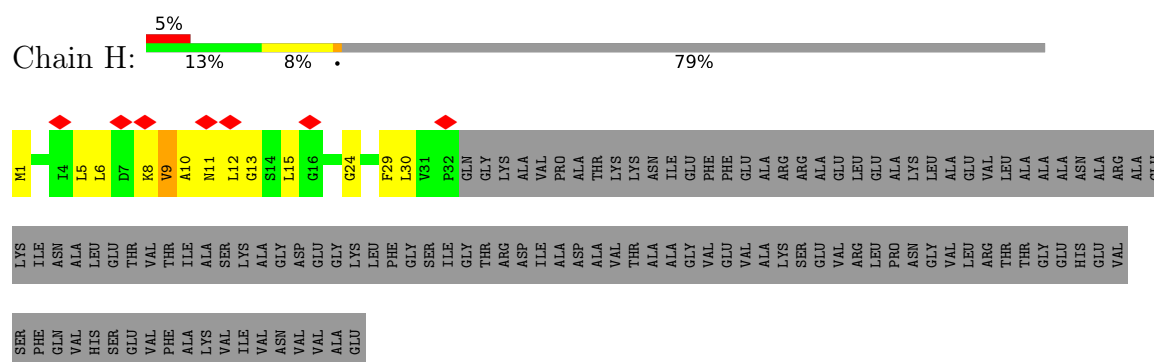
- Molecule 10: 50S ribosomal protein L5



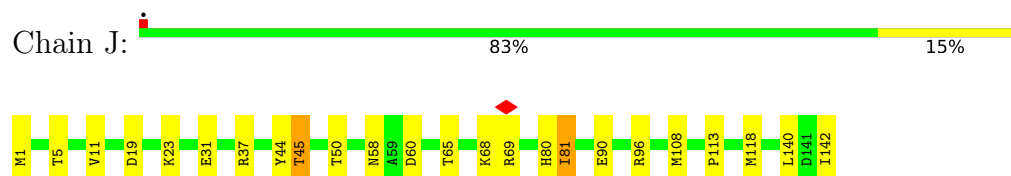
- Molecule 11: 50S ribosomal protein L6



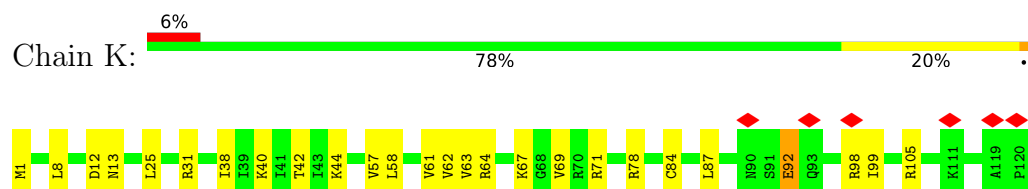
• Molecule 12: 50S ribosomal protein L9



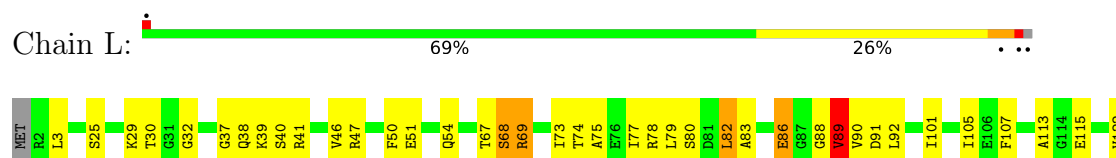
• Molecule 13: 50S ribosomal protein L13

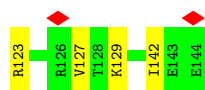


• Molecule 14: 50S ribosomal protein L14



• Molecule 15: 50S ribosomal protein L15





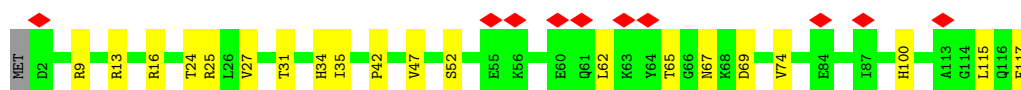
- Molecule 16: 50S ribosomal protein L17

Chain N: 80% 14% 6%



- Molecule 17: 50S ribosomal protein L18

Chain O: 9% 82% 17%



- Molecule 18: 50S ribosomal protein L19

Chain P: 66% 17% 15%



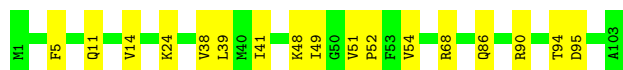
- Molecule 19: 50S ribosomal protein L20

Chain Q: 86% 14%



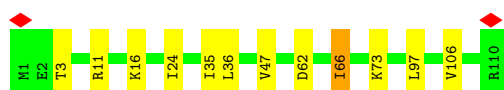
- Molecule 20: 50S ribosomal protein L21

Chain R: 83% 17%

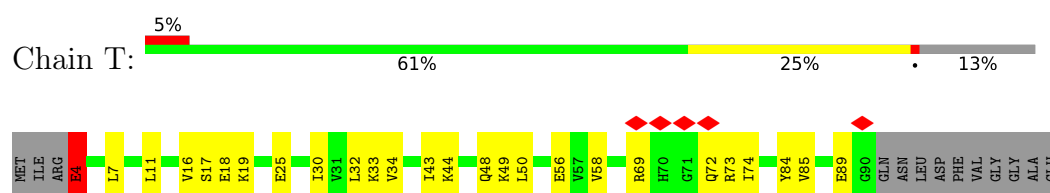


- Molecule 21: 50S ribosomal protein L22

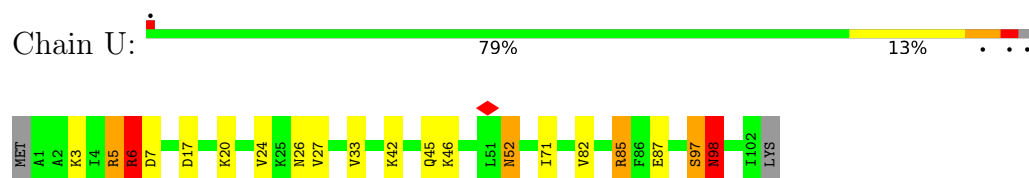
Chain S: 89% 10%



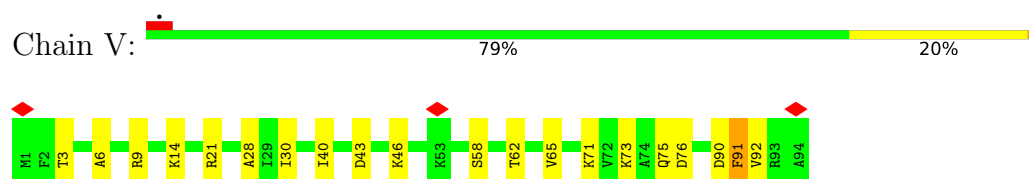
- Molecule 22: 50S ribosomal protein L23



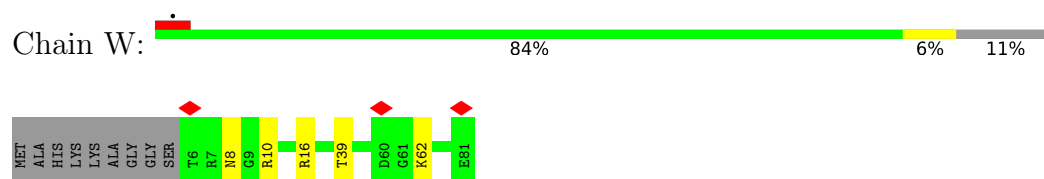
- Molecule 23: 50S ribosomal protein L24



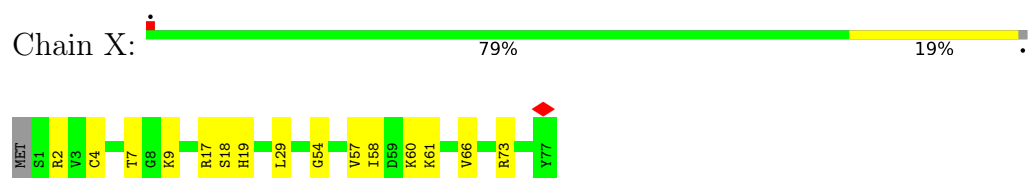
- Molecule 24: 50S ribosomal protein L25



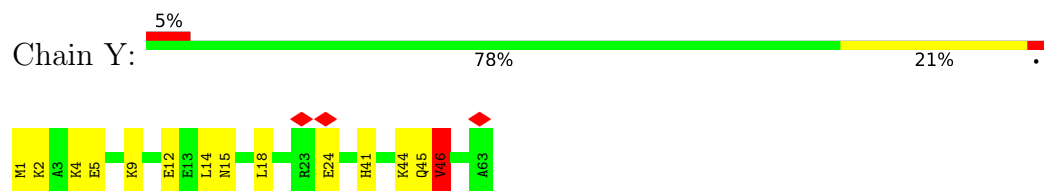
- Molecule 25: 50S ribosomal protein L27



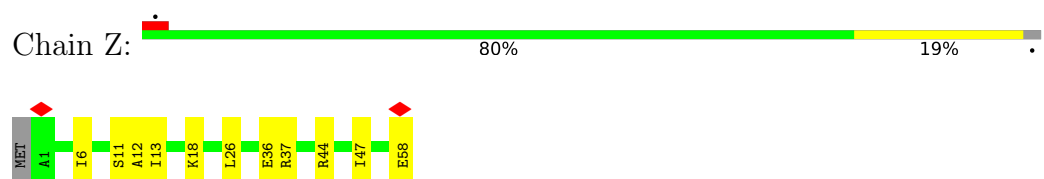
- Molecule 26: 50S ribosomal protein L28



- Molecule 27: 50S ribosomal protein L29



- Molecule 28: 50S ribosomal protein L30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	6081	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.25	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0033	Depositor
Map size (Å)	331.2, 331.2, 331.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.69, 0.69, 0.69	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	0	0.36	0/450	0.63	0/599
2	1	0.24	0/402	0.56	0/536
3	2	0.26	0/380	0.43	0/498
4	3	0.35	0/513	0.75	1/676 (0.1%)
5	A	0.26	0/57514	0.39	6/89699 (0.0%)
6	B	0.18	0/2847	0.31	0/4440
7	C	0.27	0/2121	0.57	2/2852 (0.1%)
8	D	0.36	0/1586	0.66	3/2134 (0.1%)
9	E	0.25	0/1571	0.51	0/2113
10	F	0.27	0/1434	0.68	0/1926
11	G	0.33	0/1336	0.72	3/1805 (0.2%)
12	H	0.57	0/243	0.80	0/328
13	J	0.30	0/1152	0.66	2/1551 (0.1%)
14	K	0.28	0/947	0.75	2/1268 (0.2%)
15	L	0.36	0/1054	1.18	11/1403 (0.8%)
16	N	0.31	0/973	0.68	0/1301
17	O	0.26	0/902	0.56	0/1209
18	P	0.32	0/795	0.63	1/1067 (0.1%)
19	Q	0.30	0/960	0.51	0/1278
20	R	0.30	0/829	0.57	0/1107
21	S	0.37	0/864	0.62	0/1156
22	T	0.33	0/692	1.00	5/925 (0.5%)
23	U	0.44	0/787	0.83	5/1051 (0.5%)
24	V	0.27	0/766	0.70	0/1025
25	W	0.32	0/588	0.46	0/779
26	X	0.21	0/635	0.49	0/848
27	Y	0.37	0/510	0.80	0/677
28	Z	0.24	0/453	0.51	0/605
All	All	0.27	0/83304	0.47	41/124856 (0.0%)

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
4	3	0	1
7	C	0	1
8	D	0	1
11	G	0	1
14	K	0	1
15	L	0	1
18	P	0	2
22	T	0	1
23	U	0	4
All	All	0	13

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	69	ARG	N-CA-C	15.91	128.09	111.07
15	L	68	SER	N-CA-C	-13.10	90.11	109.63
4	3	31	ILE	N-CA-C	12.93	136.24	109.34
13	J	81	ILE	N-CA-C	11.80	122.75	110.36
22	T	4	GLU	N-CA-C	-11.52	78.74	111.00
22	T	4	GLU	CA-C-N	11.20	142.92	121.54
22	T	4	GLU	C-N-CA	11.20	142.92	121.54
15	L	115	GLU	N-CA-C	10.04	125.30	111.74
5	A	1545	A	P-O3'-C3'	8.91	133.56	120.20
15	L	83	ALA	N-CA-C	-8.86	100.25	112.30
15	L	69	ARG	N-CA-CB	-8.80	97.24	110.01
11	G	35	THR	N-CA-C	-8.79	97.32	110.24
23	U	97	SER	CA-C-N	7.99	134.01	122.35
23	U	97	SER	C-N-CA	7.99	134.01	122.35
11	G	35	THR	CB-CA-C	7.35	120.87	109.84
15	L	29	LYS	CA-C-N	6.86	134.65	121.54
15	L	29	LYS	C-N-CA	6.86	134.65	121.54
5	A	1546	G	C5'-C4'-C3'	6.79	126.19	116.00
23	U	98	ASN	CA-C-N	6.55	132.74	122.78
23	U	98	ASN	C-N-CA	6.55	132.74	122.78
22	T	4	GLU	CB-CA-C	-6.50	97.75	110.10
23	U	52	ASN	N-CA-C	6.50	120.85	111.56
8	D	86	GLU	N-CA-C	6.35	124.33	110.80
5	A	1546	G	P-O3'-C3'	6.26	129.58	120.20
18	P	95	LYS	O-C-N	-6.21	116.00	123.27
11	G	36	LEU	N-CA-C	-5.99	100.52	110.17
13	J	81	ILE	N-CA-CB	-5.89	103.97	110.51
14	K	92	GLU	N-CA-C	5.82	120.97	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	L	82	LEU	CB-CA-C	-5.69	103.81	111.89
22	T	56	GLU	CA-CB-CG	5.58	125.26	114.10
8	D	168	GLU	N-CA-CB	-5.52	101.42	110.52
15	L	86	GLU	CA-CB-CG	5.49	125.08	114.10
5	A	1545	A	C4'-C3'-O3'	5.43	121.14	113.00
15	L	88	GLY	N-CA-C	5.29	117.55	111.36
5	A	1545	A	O3'-P-O5'	5.24	111.87	104.00
7	C	11	GLY	CA-C-N	5.21	131.50	121.54
7	C	11	GLY	C-N-CA	5.21	131.50	121.54
8	D	167	ASN	N-CA-C	5.20	119.57	113.23
5	A	1546	G	P-O5'-C5'	5.09	128.53	120.90
14	K	92	GLU	CB-CA-C	-5.07	102.33	110.74
15	L	82	LEU	N-CA-C	-5.03	104.45	111.39

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	31	ILE	Peptide
7	C	11	GLY	Peptide
8	D	33	ARG	Sidechain
11	G	34	ARG	Sidechain
14	K	92	GLU	Peptide
15	L	69	ARG	Peptide
18	P	61	ARG	Sidechain
18	P	95	LYS	Mainchain
22	T	4	GLU	Peptide
23	U	5	ARG	Sidechain
23	U	6	ARG	Sidechain
23	U	85	ARG	Sidechain
23	U	98	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	1	395	0	422	13	0
3	2	377	0	418	5	0
4	3	504	0	574	33	0
5	A	51353	0	25840	247	0
6	B	2548	0	1292	15	0
7	C	2082	0	2157	67	0
8	D	1565	0	1616	38	0
9	E	1552	0	1619	23	0
10	F	1410	0	1447	70	0
11	G	1317	0	1368	50	0
12	H	241	0	257	12	0
13	J	1129	0	1162	31	0
14	K	938	0	1012	22	0
15	L	1045	0	1117	31	0
16	N	960	0	999	18	0
17	O	892	0	923	15	0
18	P	783	0	816	12	0
19	Q	947	0	1022	30	0
20	R	816	0	839	49	0
21	S	857	0	922	6	0
22	T	686	0	746	15	0
23	U	779	0	834	18	0
24	V	753	0	780	12	0
25	W	581	0	599	4	0
26	X	625	0	655	21	0
27	Y	509	0	543	11	0
28	Z	449	0	491	6	0
All	All	76537	0	50931	776	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (776) 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)
8:D:33:ARG:HH21	8:D:51:THR:CG2	1.08	1.67
4:3:22:LYS:CE	4:3:46:LYS:HZ1	1.30	1.43
11:G:84:LYS:NZ	11:G:144:ALA:HB2	1.31	1.43
10:F:64:PRO:HB2	10:F:86:CYS:SG	1.59	1.42
4:3:22:LYS:CE	4:3:46:LYS:NZ	1.82	1.40
4:3:22:LYS:HD2	4:3:46:LYS:CE	1.51	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:108:LEU:HD11	20:R:48:LYS:NZ	1.29	1.40
10:F:64:PRO:CB	10:F:86:CYS:SG	2.12	1.36
8:D:33:ARG:NH2	8:D:51:THR:CG2	1.88	1.36
11:G:84:LYS:NZ	11:G:144:ALA:CB	1.90	1.32
20:R:49:ILE:CG2	20:R:52:PRO:HA	1.62	1.30
8:D:4:LEU:HD13	8:D:101:PHE:CZ	1.66	1.30
11:G:28:LYS:CE	11:G:79:THR:HA	1.65	1.26
4:3:22:LYS:NZ	4:3:46:LYS:HZ1	1.32	1.25
20:R:49:ILE:HD13	20:R:54:VAL:CG2	1.64	1.25
7:C:51:ARG:CD	7:C:52:HIS:CE1	2.21	1.24
10:F:94:ARG:O	10:F:98:PHE:HD2	1.14	1.24
4:3:22:LYS:CD	4:3:46:LYS:NZ	1.99	1.24
4:3:22:LYS:HD2	4:3:46:LYS:NZ	1.54	1.23
7:C:209:ALA:HA	7:C:212:TRP:CZ2	1.74	1.23
13:J:37:ARG:HA	13:J:118:MET:CE	1.69	1.23
11:G:93:TYR:OH	11:G:104:LEU:HD13	1.38	1.22
5:A:371:A:O2'	26:X:60:LYS:NZ	1.72	1.22
16:N:86:ARG:HH22	16:N:118:ARG:N	1.36	1.20
11:G:28:LYS:HE2	11:G:79:THR:HA	1.24	1.20
20:R:49:ILE:HG21	20:R:52:PRO:CA	1.70	1.20
20:R:49:ILE:CD1	20:R:54:VAL:HG23	1.72	1.19
10:F:94:ARG:O	10:F:98:PHE:CD2	1.96	1.18
7:C:51:ARG:HD3	7:C:52:HIS:CE1	1.76	1.18
8:D:33:ARG:NH2	8:D:51:THR:HG23	1.48	1.17
20:R:49:ILE:CD1	20:R:54:VAL:H	1.57	1.17
2:1:5:ARG:HG3	2:1:23:THR:CG2	1.74	1.17
10:F:37:MET:HE2	10:F:39:VAL:CG1	1.75	1.16
11:G:84:LYS:HZ3	11:G:144:ALA:CB	1.53	1.16
19:Q:108:LEU:CD1	20:R:48:LYS:NZ	2.09	1.15
5:A:449:A:H4'	19:Q:2:ARG:HH12	1.06	1.14
10:F:37:MET:CE	10:F:39:VAL:CG1	2.28	1.11
5:A:559:G:H21	19:Q:51:GLN:CD	1.57	1.11
10:F:37:MET:HE2	10:F:39:VAL:HG11	1.29	1.11
10:F:32:LYS:CE	10:F:91:ARG:HH21	1.65	1.10
10:F:32:LYS:NZ	10:F:91:ARG:HH21	1.50	1.10
4:3:22:LYS:CD	4:3:46:LYS:HZ1	1.58	1.09
12:H:29:PHE:HD2	12:H:30:LEU:HD22	1.16	1.08
4:3:31:ILE:CG1	4:3:31:ILE:O	1.96	1.08
20:R:49:ILE:CG2	20:R:51:VAL:O	2.02	1.08
26:X:58:ILE:HD13	26:X:66:VAL:HG21	1.24	1.07
11:G:84:LYS:HD2	11:G:140:ILE:HD12	1.29	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:31:ILE:O	4:3:31:ILE:HG13	1.26	1.07
13:J:37:ARG:HA	13:J:118:MET:HE3	1.11	1.06
23:U:27:VAL:HG12	23:U:33:VAL:HG12	1.31	1.06
20:R:49:ILE:HD12	20:R:54:VAL:H	1.18	1.05
10:F:64:PRO:HB3	10:F:86:CYS:SG	1.88	1.05
4:3:22:LYS:HD2	4:3:46:LYS:HE3	1.34	1.04
7:C:209:ALA:HA	7:C:212:TRP:CH2	1.92	1.04
2:1:5:ARG:HG3	2:1:23:THR:HG22	1.35	1.04
20:R:49:ILE:HD12	20:R:54:VAL:N	1.70	1.04
4:3:22:LYS:HE3	4:3:46:LYS:HZ2	1.21	1.04
10:F:32:LYS:HG3	10:F:90:LEU:O	1.58	1.03
10:F:32:LYS:HD3	10:F:91:ARG:HE	1.18	1.03
16:N:86:ARG:NH2	16:N:118:ARG:N	2.05	1.03
4:3:22:LYS:HE3	4:3:46:LYS:NZ	1.70	1.02
2:1:5:ARG:CG	2:1:23:THR:CG2	2.35	1.02
20:R:49:ILE:HG23	20:R:51:VAL:O	1.59	1.02
10:F:12:VAL:O	10:F:16:MET:HG2	1.60	1.01
26:X:58:ILE:CD1	26:X:66:VAL:HG21	1.90	1.01
10:F:37:MET:CE	10:F:39:VAL:HG11	1.91	1.00
12:H:29:PHE:CD2	12:H:30:LEU:HD22	1.96	1.00
7:C:209:ALA:CA	7:C:212:TRP:CH2	2.44	1.00
11:G:84:LYS:HZ1	11:G:144:ALA:CB	1.61	1.00
8:D:33:ARG:NH2	8:D:51:THR:HG21	1.60	0.99
7:C:251:THR:HG22	7:C:252:LYS:H	1.25	0.99
5:A:291:G:H1	5:A:349:U:H3	1.08	0.99
12:H:29:PHE:HD2	12:H:30:LEU:CD2	1.73	0.99
10:F:32:LYS:CE	10:F:91:ARG:NH2	2.25	0.98
5:A:559:G:H21	19:Q:51:GLN:NE2	1.61	0.97
5:A:449:A:H4'	19:Q:2:ARG:NH1	1.80	0.96
15:L:82:LEU:O	15:L:82:LEU:HD23	1.65	0.96
10:F:32:LYS:HD3	10:F:91:ARG:NE	1.80	0.96
11:G:28:LYS:NZ	11:G:78:VAL:O	1.96	0.96
7:C:51:ARG:HD2	7:C:52:HIS:CE1	1.97	0.96
8:D:33:ARG:HH21	8:D:51:THR:HG21	0.80	0.95
4:3:22:LYS:CE	4:3:46:LYS:HZ2	1.71	0.95
26:X:4:CYS:SG	26:X:7:THR:HG22	2.07	0.95
20:R:49:ILE:CD1	20:R:54:VAL:N	2.29	0.94
10:F:32:LYS:NZ	10:F:91:ARG:NH2	2.16	0.94
19:Q:108:LEU:CD1	20:R:48:LYS:HZ2	1.74	0.93
7:C:209:ALA:N	7:C:212:TRP:CH2	2.36	0.93
4:3:22:LYS:NZ	4:3:46:LYS:NZ	2.00	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2724:U:OP1	8:D:116:LYS:HE2	1.68	0.92
10:F:64:PRO:HB2	10:F:86:CYS:HG	1.24	0.92
7:C:51:ARG:HD2	7:C:52:HIS:NE2	1.86	0.91
4:3:22:LYS:CD	4:3:46:LYS:CE	2.45	0.90
11:G:84:LYS:HD2	11:G:140:ILE:CD1	2.02	0.90
19:Q:108:LEU:CD1	20:R:48:LYS:HZ3	1.74	0.90
13:J:37:ARG:CA	13:J:118:MET:CE	2.51	0.89
10:F:32:LYS:HZ3	10:F:91:ARG:HH21	1.19	0.89
14:K:8:LEU:HD13	14:K:84:CYS:SG	2.12	0.89
14:K:13:ASN:ND2	14:K:98:ARG:HG2	1.88	0.89
5:A:290:U:H3	5:A:350:G:H1	0.93	0.89
5:A:2075:U:OP1	7:C:241:LYS:NZ	2.06	0.89
20:R:49:ILE:CG2	20:R:52:PRO:CA	2.38	0.89
2:1:5:ARG:CG	2:1:23:THR:HG21	2.02	0.88
16:N:86:ARG:NH2	16:N:118:ARG:H	1.72	0.87
5:A:1268:A:H62	5:A:2012:G:H21	1.16	0.87
19:Q:108:LEU:CD2	20:R:48:LYS:HZ2	1.88	0.87
7:C:251:THR:HG22	7:C:252:LYS:N	1.87	0.87
15:L:89:VAL:HB	15:L:123:ARG:HH22	1.40	0.86
5:A:1390:U:H3	5:A:1395:A:H62	1.24	0.86
8:D:33:ARG:HD2	8:D:73:VAL:HB	1.58	0.85
20:R:48:LYS:HG2	20:R:49:ILE:H	1.40	0.85
8:D:167:ASN:OD1	8:D:167:ASN:O	1.94	0.85
20:R:49:ILE:HD11	20:R:54:VAL:H	1.39	0.85
11:G:84:LYS:HZ3	11:G:144:ALA:HB2	0.74	0.85
5:A:2724:U:OP1	8:D:116:LYS:CE	2.24	0.85
11:G:84:LYS:NZ	11:G:144:ALA:HB3	1.90	0.85
7:C:209:ALA:HA	7:C:212:TRP:CE2	2.13	0.84
2:1:5:ARG:HG2	2:1:23:THR:HG21	1.58	0.84
10:F:37:MET:HE3	10:F:39:VAL:HG12	1.58	0.84
5:A:2223:G:O3'	7:C:264:LYS:NZ	2.10	0.84
20:R:49:ILE:HG22	20:R:51:VAL:O	1.77	0.84
8:D:4:LEU:HD13	8:D:101:PHE:CE2	2.13	0.83
17:O:24:THR:HG22	17:O:42:PRO:HD3	1.59	0.83
4:3:30:HIS:O	4:3:32:LEU:HD12	1.79	0.82
26:X:58:ILE:CD1	26:X:66:VAL:HG11	2.09	0.82
26:X:7:THR:CG2	26:X:9:LYS:HG3	2.09	0.82
7:C:251:THR:CG2	7:C:252:LYS:H	1.93	0.82
7:C:209:ALA:N	7:C:212:TRP:CZ3	2.23	0.81
16:N:86:ARG:NE	16:N:117:ASP:OD2	1.92	0.81
10:F:37:MET:HE3	10:F:39:VAL:CG1	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2223:G:H4'	7:C:264:LYS:HZ1	1.46	0.80
11:G:93:TYR:HH	11:G:104:LEU:HD13	1.46	0.80
1:0:10:SER:O	1:0:14:MET:HG2	1.81	0.80
2:1:5:ARG:CG	2:1:23:THR:HG22	2.03	0.80
2:1:6:GLU:O	2:1:23:THR:HG23	1.81	0.80
10:F:32:LYS:HE2	10:F:91:ARG:NH2	1.97	0.79
13:J:37:ARG:CB	13:J:118:MET:HE1	2.12	0.79
7:C:209:ALA:CA	7:C:212:TRP:CZ2	2.59	0.78
11:G:28:LYS:HE3	11:G:79:THR:HA	1.60	0.78
4:3:30:HIS:O	4:3:32:LEU:CD1	2.31	0.78
5:A:559:G:N2	19:Q:51:GLN:CD	2.40	0.78
19:Q:108:LEU:HD21	20:R:48:LYS:HZ2	1.48	0.78
7:C:208:GLY:HA3	7:C:212:TRP:HZ3	1.48	0.77
16:N:22:ARG:HG3	16:N:70:THR:HA	1.67	0.77
11:G:28:LYS:HE2	11:G:79:THR:CA	2.12	0.76
20:R:49:ILE:HG21	20:R:52:PRO:HA	0.80	0.76
4:3:22:LYS:HZ2	4:3:46:LYS:HZ1	1.32	0.76
26:X:7:THR:HG23	26:X:9:LYS:HG3	1.68	0.76
14:K:71:ARG:NH1	14:K:105:ARG:HH21	1.84	0.75
13:J:69:ARG:CZ	13:J:90:GLU:HG2	2.17	0.74
20:R:39:LEU:O	20:R:49:ILE:HG12	1.87	0.74
11:G:93:TYR:CD1	11:G:106:LEU:HB3	2.21	0.74
27:Y:12:GLU:O	27:Y:15:ASN:OD1	2.05	0.74
7:C:51:ARG:HG3	7:C:52:HIS:CG	2.23	0.74
5:A:1408:G:H1	5:A:1594:U:H3	1.36	0.73
10:F:32:LYS:CD	10:F:91:ARG:HH21	2.01	0.73
20:R:49:ILE:CD1	20:R:54:VAL:CB	2.66	0.73
5:A:499:U:C5'	23:U:42:LYS:HD2	2.18	0.73
4:3:22:LYS:HZ1	4:3:46:LYS:NZ	1.88	0.72
20:R:49:ILE:HG22	20:R:51:VAL:C	2.14	0.72
5:A:559:G:N2	19:Q:51:GLN:NE2	2.38	0.71
20:R:49:ILE:HD13	20:R:54:VAL:HG23	0.81	0.71
10:F:11:VAL:HA	10:F:14:LYS:HG2	1.73	0.71
20:R:49:ILE:CD1	20:R:54:VAL:CG2	2.47	0.70
5:A:559:G:N2	19:Q:51:GLN:OE1	2.25	0.70
26:X:54:GLY:O	26:X:58:ILE:HG12	1.91	0.70
11:G:84:LYS:HZ1	11:G:144:ALA:HB3	1.49	0.70
13:J:37:ARG:HA	13:J:118:MET:HE1	1.72	0.70
10:F:174:PHE:O	10:F:175:PRO:C	2.33	0.70
5:A:1798:U:OP2	7:C:270:ARG:NH2	2.25	0.69
11:G:84:LYS:CE	11:G:144:ALA:HB2	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:T:72:GLN:O	22:T:73:ARG:HG3	1.91	0.69
14:K:13:ASN:ND2	14:K:98:ARG:CG	2.55	0.69
5:A:2296:U:C5	17:O:9:ARG:NH2	2.60	0.69
14:K:13:ASN:HD21	14:K:98:ARG:HG2	1.55	0.69
5:A:572:A:H61	5:A:2029:G:H21	1.41	0.69
19:Q:108:LEU:HD21	20:R:48:LYS:NZ	2.07	0.68
15:L:73:ILE:HG22	15:L:73:ILE:O	1.93	0.68
20:R:49:ILE:CG2	20:R:51:VAL:C	2.66	0.68
15:L:90:VAL:HB	15:L:122:VAL:HG22	1.74	0.68
4:3:22:LYS:HD2	4:3:46:LYS:CD	2.23	0.67
14:K:8:LEU:CD1	14:K:84:CYS:SG	2.82	0.67
5:A:1268:A:H62	5:A:2012:G:N2	1.92	0.67
7:C:51:ARG:HD3	7:C:52:HIS:HE1	1.54	0.67
5:A:1566:A:O4'	7:C:212:TRP:CD1	2.48	0.67
26:X:58:ILE:HD11	26:X:66:VAL:HG11	1.74	0.67
2:1:5:ARG:HG2	2:1:23:THR:CG2	2.17	0.66
8:D:4:LEU:CD1	8:D:101:PHE:CZ	2.62	0.66
26:X:58:ILE:HD12	26:X:66:VAL:HG11	1.75	0.66
11:G:93:TYR:HD1	11:G:106:LEU:CB	2.08	0.66
4:3:28:LEU:HG	4:3:28:LEU:O	1.95	0.66
5:A:2204:G:H1	5:A:2220:U:H3	1.42	0.66
12:H:29:PHE:CD2	12:H:30:LEU:CD2	2.64	0.66
15:L:51:GLU:HG2	15:L:54:GLN:HE21	1.60	0.65
27:Y:12:GLU:OE1	27:Y:15:ASN:ND2	2.28	0.65
5:A:2658:C:H5''	11:G:157:LYS:HE2	1.79	0.65
16:N:22:ARG:CG	16:N:70:THR:HA	2.26	0.65
7:C:208:GLY:CA	7:C:212:TRP:HZ3	1.91	0.65
26:X:7:THR:HG21	26:X:9:LYS:HG3	1.78	0.65
10:F:32:LYS:HD3	10:F:91:ARG:CZ	2.26	0.65
8:D:4:LEU:HD13	8:D:101:PHE:HZ	1.52	0.64
6:B:22:U:H3	6:B:61:G:H1	1.45	0.64
13:J:69:ARG:NH2	13:J:90:GLU:HG2	2.11	0.64
5:A:1282:U:H3	5:A:1286:A:H62	1.45	0.64
11:G:93:TYR:CE1	11:G:106:LEU:HB3	2.33	0.64
8:D:33:ARG:HE	8:D:73:VAL:CG2	2.11	0.64
10:F:37:MET:HE2	10:F:39:VAL:HG13	1.78	0.64
20:R:48:LYS:HG2	20:R:49:ILE:N	2.11	0.63
16:N:97:ILE:CD1	16:N:113:ILE:HD12	2.28	0.63
5:A:2529:G:H4'	11:G:174:LYS:HG3	1.80	0.63
18:P:1:SER:OG	18:P:2:ASN:N	2.32	0.63
12:H:1:MET:SD	12:H:1:MET:N	2.71	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:49:ILE:HD11	20:R:54:VAL:HB	1.81	0.62
9:E:170:ARG:HH22	9:E:175:ILE:HG22	1.65	0.62
14:K:13:ASN:HD21	14:K:98:ARG:H	1.48	0.62
16:N:86:ARG:NH2	16:N:117:ASP:C	2.57	0.62
5:A:95:A:HO2'	27:Y:41:HIS:HD1	1.45	0.62
5:A:2316:G:H2'	5:A:2317:A:H8	1.65	0.62
5:A:1270:C:H5''	5:A:1271:G:H5'	1.82	0.62
5:A:320:A:N3	9:E:163:ASN:ND2	2.48	0.62
4:3:22:LYS:CD	4:3:46:LYS:HE3	2.20	0.61
15:L:82:LEU:O	15:L:82:LEU:CD2	2.45	0.61
19:Q:108:LEU:HD11	20:R:48:LYS:HZ3	0.78	0.61
5:A:917:A:H5''	5:A:2268:A:H61	1.65	0.61
21:S:36:LEU:HD21	21:S:47:VAL:HG13	1.82	0.61
5:A:320:A:N7	9:E:132:LYS:NZ	2.48	0.61
5:A:2824:C:OP2	5:A:2825:G:N2	2.33	0.61
18:P:4:ILE:HD13	18:P:7:LEU:HD12	1.81	0.61
5:A:1597:A:H5''	5:A:1598:A:H5'	1.80	0.61
13:J:44:TYR:O	19:Q:63:ARG:NH2	2.34	0.61
6:B:70:C:N3	6:B:107:G:N2	2.49	0.61
20:R:5:PHE:CZ	20:R:14:VAL:HG21	2.36	0.61
5:A:1154:G:OP2	19:Q:57:ARG:NH1	2.33	0.61
10:F:32:LYS:HZ3	10:F:91:ARG:NH2	1.87	0.60
5:A:2331:G:HO2'	25:W:39:THR:HG1	1.49	0.60
10:F:94:ARG:C	10:F:98:PHE:HD2	2.01	0.60
5:A:372:G:OP2	26:X:61:LYS:NZ	2.34	0.60
5:A:1442:U:O4	5:A:1548:A:N6	2.35	0.60
10:F:18:GLU:HG3	10:F:19:PHE:HD1	1.66	0.60
16:N:86:ARG:HH22	16:N:118:ARG:CA	2.13	0.60
19:Q:108:LEU:CG	20:R:48:LYS:HZ2	2.15	0.60
15:L:89:VAL:C	15:L:123:ARG:HH12	2.08	0.60
7:C:122:ALA:O	7:C:127:ASN:ND2	2.34	0.60
2:1:6:GLU:OE1	2:1:26:LYS:NZ	2.35	0.60
8:D:33:ARG:CD	8:D:73:VAL:HB	2.31	0.60
10:F:173:ASP:O	10:F:174:PHE:C	2.45	0.59
5:A:499:U:H5'	23:U:42:LYS:HD2	1.82	0.59
8:D:121:THR:HG21	8:D:143:PRO:HG3	1.84	0.59
5:A:585:G:H21	5:A:1254:A:H62	1.50	0.59
10:F:103:ILE:HD12	10:F:175:PRO:HD3	1.83	0.59
5:A:2514:U:H5''	13:J:81:ILE:HD11	1.85	0.59
13:J:37:ARG:CA	13:J:118:MET:HE1	2.25	0.59
26:X:2:ARG:NH1	26:X:29:LEU:HD13	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:26:ASN:OD1	3:2:27:GLY:N	2.36	0.59
4:3:31:ILE:O	4:3:31:ILE:CD1	2.51	0.59
5:A:1251:C:OP2	19:Q:5:ARG:NH1	2.35	0.59
27:Y:14:LEU:HD23	27:Y:18:LEU:CD2	2.32	0.59
4:3:22:LYS:CD	4:3:46:LYS:HZ2	1.97	0.59
16:N:86:ARG:HH22	16:N:117:ASP:C	2.08	0.58
5:A:589:U:H2'	5:A:590:A:H8	1.68	0.58
13:J:37:ARG:CG	13:J:118:MET:HE1	2.32	0.58
5:A:848:C:H2'	5:A:849:A:H8	1.69	0.58
16:N:97:ILE:HD13	16:N:113:ILE:HG13	1.85	0.58
7:C:208:GLY:CA	7:C:212:TRP:CZ3	2.57	0.58
10:F:32:LYS:HD3	10:F:91:ARG:NH2	2.18	0.58
10:F:36:ASN:ND2	10:F:86:CYS:O	2.36	0.58
15:L:51:GLU:O	15:L:54:GLN:HG2	2.04	0.58
5:A:2735:G:H1	5:A:2769:U:H3	1.51	0.58
5:A:500:G:H21	5:A:505:A:H62	1.52	0.58
9:E:170:ARG:NH1	9:E:174:GLY:O	2.36	0.58
1:0:49:ARG:HE	5:A:2884:U:H1'	1.68	0.57
5:A:2659:G:N2	5:A:2662:A:OP2	2.36	0.57
26:X:18:SER:OG	26:X:19:HIS:N	2.37	0.57
5:A:2724:U:OP1	8:D:116:LYS:HE3	2.01	0.57
11:G:28:LYS:CE	11:G:78:VAL:O	2.52	0.57
27:Y:1:MET:HA	27:Y:4:LYS:HG2	1.85	0.57
24:V:76:ASP:HB3	24:V:90:ASP:HB2	1.87	0.57
5:A:2081:U:H2'	5:A:2082:A:H8	1.70	0.57
7:C:251:THR:CG2	7:C:252:LYS:N	2.57	0.57
4:3:8:GLY:O	4:3:12:ARG:NH1	2.38	0.57
5:A:1222:U:H3	5:A:1227:G:H1	1.52	0.57
5:A:1799:G:OP2	7:C:269:ARG:NH2	2.36	0.57
9:E:5:LEU:HD13	9:E:10:SER:HB3	1.87	0.57
7:C:131:MET:HE3	7:C:189:ALA:HB2	1.87	0.57
13:J:69:ARG:NH1	13:J:90:GLU:HG2	2.19	0.57
4:3:27:ASN:O	4:3:35:LYS:NZ	2.39	0.56
5:A:1153:C:OP1	19:Q:91:ARG:NH2	2.38	0.56
5:A:1582:C:O2'	5:A:1585:C:N3	2.34	0.56
5:A:2515:C:H2'	5:A:2516:A:H8	1.70	0.56
9:E:22:ASP:OD1	9:E:22:ASP:N	2.34	0.56
10:F:28:PRO:HB2	10:F:168:LEU:HD13	1.88	0.56
19:Q:101:ASP:OD1	19:Q:101:ASP:N	2.38	0.56
6:B:54:G:H21	10:F:25:MET:HE1	1.70	0.56
13:J:69:ARG:NH1	13:J:90:GLU:CG	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:5:PHE:CE1	20:R:14:VAL:HG21	2.39	0.56
19:Q:89:ILE:HD12	20:R:48:LYS:HE3	1.87	0.56
23:U:27:VAL:HG12	23:U:33:VAL:CG1	2.21	0.56
5:A:2356:U:H4'	25:W:16:ARG:HG3	1.88	0.56
13:J:23:LYS:NZ	13:J:142:ILE:OXT	2.38	0.56
20:R:48:LYS:CG	20:R:49:ILE:H	2.16	0.56
20:R:68:ARG:HH21	20:R:90:ARG:HB2	1.70	0.56
5:A:1019:U:OP1	5:A:1035:U:O2'	2.22	0.56
5:A:1190:G:H5''	15:L:32:GLY:HA2	1.87	0.56
11:G:59:ASP:OD1	11:G:59:ASP:N	2.38	0.56
10:F:32:LYS:CD	10:F:91:ARG:NH2	2.65	0.56
23:U:52:ASN:CG	23:U:52:ASN:O	2.49	0.55
13:J:5:THR:HG23	13:J:45:THR:HG21	1.87	0.55
26:X:58:ILE:CD1	26:X:66:VAL:CG2	2.77	0.55
5:A:2640:G:OP1	13:J:96:ARG:NH2	2.39	0.55
11:G:89:VAL:O	11:G:159:LYS:HA	2.07	0.55
15:L:75:ALA:HB2	15:L:105:ILE:HG21	1.88	0.55
10:F:7:TYR:HA	10:F:11:VAL:HG22	1.89	0.55
5:A:2311:A:H62	10:F:77:LYS:HE2	1.70	0.55
10:F:32:LYS:HD3	10:F:91:ARG:HH21	1.72	0.55
5:A:1668:A:N3	5:A:1670:C:N4	2.55	0.55
7:C:36:ASN:OD1	7:C:36:ASN:O	2.25	0.55
5:A:2644:G:H3'	5:A:2645:G:H21	1.72	0.55
5:A:1140:C:OP2	13:J:68:LYS:NZ	2.39	0.54
10:F:32:LYS:HG3	10:F:90:LEU:C	2.29	0.54
5:A:2296:U:H5	17:O:9:ARG:NH2	2.03	0.54
5:A:2011:U:OP2	21:S:16:LYS:NZ	2.41	0.54
5:A:2785:C:O3'	8:D:70:LYS:NZ	2.40	0.54
12:H:6:LEU:O	12:H:6:LEU:HG	2.06	0.54
5:A:1796:U:H2'	5:A:1797:G:H8	1.72	0.54
5:A:805:G:O4'	15:L:38:GLN:NE2	2.41	0.54
5:A:1463:C:H2'	5:A:1464:G:C8	2.42	0.54
5:A:1138:G:H21	13:J:108:MET:HE2	1.71	0.54
13:J:37:ARG:HG3	13:J:118:MET:HE1	1.89	0.54
5:A:370:G:O2'	5:A:424:G:OP1	2.24	0.54
7:C:106:PRO:HD2	7:C:109:LEU:HD22	1.90	0.54
9:E:140:ASP:OD1	9:E:140:ASP:N	2.41	0.54
11:G:104:LEU:O	11:G:111:PRO:HA	2.07	0.54
23:U:17:ASP:HB3	23:U:20:LYS:HD3	1.90	0.54
5:A:99:U:H5''	5:A:100:U:H5'	1.88	0.54
5:A:1217:U:OP2	19:Q:14:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:51:GLU:CG	15:L:54:GLN:HE21	2.21	0.54
11:G:93:TYR:CD1	11:G:106:LEU:CB	2.86	0.53
20:R:38:VAL:HG11	20:R:41:ILE:HD11	1.91	0.53
20:R:49:ILE:HG21	20:R:52:PRO:C	2.33	0.53
6:B:13:G:O2'	6:B:15:A:OP2	2.27	0.53
6:B:77:U:OP1	24:V:21:ARG:NH1	2.41	0.53
7:C:51:ARG:CG	7:C:52:HIS:CE1	2.90	0.53
9:E:149:ILE:HG23	9:E:188:MET:HA	1.90	0.53
5:A:83:A:N7	5:A:101:A:N6	2.56	0.53
15:L:77:ILE:HD11	15:L:101:ILE:HD11	1.90	0.53
4:3:22:LYS:HZ1	4:3:46:LYS:HZ3	1.55	0.53
5:A:1444:G:H2'	5:A:1445:G:C8	2.43	0.53
5:A:465:G:H21	5:A:684:G:H1'	1.73	0.53
5:A:2654:A:H61	5:A:2667:C:H42	1.56	0.53
11:G:117:PRO:HG2	11:G:120:ILE:HD12	1.90	0.53
28:Z:11:SER:OG	28:Z:12:ALA:N	2.42	0.53
5:A:463:G:N2	5:A:466:A:OP2	2.40	0.53
5:A:1589:U:H2'	5:A:1590:A:H8	1.74	0.53
23:U:98:ASN:OD1	23:U:98:ASN:O	2.27	0.53
24:V:58:SER:O	24:V:73:LYS:NZ	2.42	0.53
5:A:29:U:H2'	5:A:30:G:H8	1.74	0.53
5:A:393:C:N3	5:A:394:C:C4	2.77	0.53
5:A:1754:A:N1	5:A:2716:C:O2'	2.41	0.53
7:C:144:GLU:HB3	7:C:187:CYS:HB3	1.90	0.52
22:T:49:LYS:HG3	22:T:50:LEU:HD12	1.90	0.52
8:D:33:ARG:NH1	8:D:75:ALA:O	2.43	0.52
10:F:37:MET:SD	10:F:56:LEU:HD21	2.50	0.52
24:V:43:ASP:HB3	24:V:46:LYS:HE2	1.90	0.52
5:A:2334:U:O2	17:O:13:ARG:NH1	2.43	0.52
5:A:1433:A:H2'	5:A:1434:A:H8	1.74	0.52
25:W:8:ASN:HA	25:W:10:ARG:HH21	1.75	0.52
5:A:1429:G:H2'	5:A:1430:G:H8	1.74	0.52
5:A:1998:A:OP2	8:D:141:ARG:NH2	2.34	0.52
5:A:1444:G:H2'	5:A:1445:G:H8	1.73	0.52
5:A:1997:C:H2'	5:A:1998:A:H8	1.74	0.52
6:B:31:C:N4	6:B:51:G:O6	2.42	0.52
7:C:166:ARG:HA	7:C:171:VAL:HG12	1.91	0.52
11:G:84:LYS:CD	11:G:140:ILE:CD1	2.83	0.51
5:A:478:A:N7	5:A:480:A:N6	2.58	0.51
7:C:194:VAL:HG22	7:C:195:GLY:H	1.75	0.51
15:L:91:ASP:OD1	15:L:92:LEU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1326:U:H2'	5:A:1327:A:H8	1.74	0.51
5:A:2223:G:H4'	7:C:264:LYS:NZ	2.22	0.51
6:B:72:G:H21	6:B:104:A:H62	1.57	0.51
5:A:1440:U:H2'	5:A:1441:G:H8	1.75	0.51
12:H:9:VAL:HB	12:H:12:LEU:HB3	1.92	0.51
13:J:19:ASP:OD1	13:J:58:ASN:ND2	2.44	0.51
8:D:4:LEU:HD22	8:D:101:PHE:CE2	2.46	0.51
10:F:101:ARG:NH1	10:F:139:GLU:OE2	2.43	0.51
22:T:17:SER:OG	22:T:18:GLU:N	2.44	0.51
17:O:62:LEU:HD13	17:O:65:THR:HA	1.93	0.51
5:A:781:A:OP1	7:C:216:ARG:NH2	2.44	0.51
5:A:2311:A:N7	10:F:77:LYS:NZ	2.48	0.51
11:G:93:TYR:CD2	11:G:151:ARG:HG3	2.45	0.51
13:J:37:ARG:HB2	13:J:118:MET:HE1	1.89	0.51
15:L:37:GLY:H	15:L:40:SER:HG	1.57	0.51
5:A:1996:C:OP1	14:K:31:ARG:NH1	2.43	0.51
5:A:2377:A:H2'	5:A:2378:A:H8	1.76	0.51
10:F:15:LEU:HG	10:F:27:VAL:HG13	1.93	0.51
7:C:5:CYS:SG	7:C:17:LYS:NZ	2.79	0.50
5:A:742:A:H2'	5:A:743:A:H8	1.76	0.50
10:F:56:LEU:HA	10:F:59:ILE:HG22	1.93	0.50
5:A:807:U:OP2	15:L:41:ARG:NH2	2.44	0.50
23:U:71:ILE:HD11	23:U:82:VAL:HG22	1.93	0.50
5:A:742:A:H2'	5:A:743:A:C8	2.46	0.50
5:A:820:A:H4'	5:A:836:G:H22	1.77	0.50
5:A:1268:A:N6	5:A:2012:G:H21	1.97	0.50
9:E:110:SER:OG	9:E:114:ARG:NH2	2.45	0.50
10:F:157:THR:HG21	10:F:168:LEU:HD21	1.93	0.50
5:A:380:G:N1	5:A:395:U:N3	2.60	0.50
5:A:1464:G:H3'	5:A:1465:G:C8	2.46	0.50
15:L:80:SER:OG	15:L:113:ALA:O	2.27	0.50
5:A:1165:A:H2'	5:A:1166:G:H8	1.76	0.50
5:A:1167:C:H2'	5:A:1168:G:H8	1.75	0.50
5:A:2898:U:H2'	5:A:2899:A:H8	1.74	0.50
8:D:105:LYS:HA	8:D:177:VAL:HG12	1.93	0.50
9:E:170:ARG:HH12	9:E:175:ILE:HA	1.75	0.50
11:G:84:LYS:CD	11:G:140:ILE:HD12	2.22	0.50
11:G:93:TYR:OH	11:G:104:LEU:CD1	2.33	0.50
14:K:42:THR:HB	14:K:57:VAL:HG12	1.92	0.50
16:N:10:LEU:O	16:N:12:ARG:NH1	2.45	0.50
5:A:483:A:OP1	23:U:46:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:1:MET:HG2	8:D:205:PRO:HG2	1.93	0.49
13:J:37:ARG:NH1	13:J:44:TYR:OH	2.45	0.49
15:L:25:SER:O	15:L:25:SER:OG	2.25	0.49
15:L:90:VAL:CB	15:L:122:VAL:HG22	2.42	0.49
22:T:4:GLU:HA	22:T:7:LEU:HB2	1.94	0.49
7:C:36:ASN:HB2	7:C:61:TYR:HB2	1.93	0.49
11:G:71:LEU:HB3	11:G:74:MET:HE3	1.93	0.49
11:G:93:TYR:HD1	11:G:106:LEU:HB3	1.65	0.49
28:Z:44:ARG:NH2	28:Z:58:GLU:OE2	2.45	0.49
5:A:1674:G:N2	5:A:1677:A:N1	2.60	0.49
5:A:2443:C:H2'	5:A:2444:G:H8	1.77	0.49
20:R:49:ILE:CD1	20:R:54:VAL:CA	2.90	0.49
5:A:1464:G:H3'	5:A:1465:G:H8	1.78	0.49
7:C:86:ARG:HG3	7:C:88:ALA:H	1.77	0.49
11:G:84:LYS:HZ2	11:G:141:GLY:HA2	1.77	0.49
13:J:60:ASP:OD1	13:J:60:ASP:N	2.46	0.49
5:A:1694:C:O2	5:A:1695:G:N2	2.46	0.49
5:A:2654:A:N6	5:A:2667:C:H42	2.10	0.49
3:2:22:MET:HE2	3:2:31:LEU:HD13	1.93	0.49
6:B:18:G:H1	6:B:65:U:H3	1.61	0.49
7:C:68:ARG:O	7:C:188:ARG:NH1	2.41	0.49
7:C:141:HIS:ND1	7:C:192:GLY:O	2.42	0.49
10:F:30:VAL:HG23	10:F:95:MET:HE1	1.95	0.49
16:N:97:ILE:CD1	16:N:113:ILE:CD1	2.91	0.49
17:O:35:ILE:HD11	17:O:74:VAL:HG11	1.94	0.49
5:A:290:U:O4	5:A:350:G:O6	2.31	0.48
5:A:1266:G:N2	5:A:2013:A:OP2	2.44	0.48
5:A:1566:A:O4'	7:C:212:TRP:HD1	1.96	0.48
2:1:24:LYS:NZ	2:1:31:GLU:O	2.46	0.48
5:A:1026:G:H2'	5:A:1027:A:H8	1.78	0.48
7:C:97:ASP:OD1	7:C:97:ASP:N	2.41	0.48
7:C:257:ARG:NH2	7:C:266:ILE:CD1	2.76	0.48
24:V:75:GLN:HB2	24:V:92:VAL:HG12	1.94	0.48
27:Y:14:LEU:CD2	27:Y:18:LEU:CD2	2.91	0.48
7:C:51:ARG:HG3	7:C:52:HIS:CD2	2.49	0.48
11:G:52:GLY:HA2	11:G:61:TRP:HZ3	1.78	0.48
11:G:34:ARG:O	11:G:35:THR:C	2.56	0.48
23:U:7:ASP:HA	23:U:24:VAL:HG23	1.96	0.48
5:A:1340:U:OP1	22:T:19:LYS:NZ	2.39	0.48
5:A:1415:U:H3	5:A:1587:G:H1	1.61	0.48
21:S:3:THR:O	21:S:106:VAL:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:411:G:OP2	5:A:2406:A:O2'	2.27	0.48
5:A:1791:A:N6	5:A:1828:G:O2'	2.46	0.48
5:A:2655:G:O2'	5:A:2664:G:O6	2.31	0.48
10:F:37:MET:HG3	10:F:37:MET:O	2.14	0.48
11:G:25:ILE:HD13	11:G:74:MET:HG2	1.95	0.48
5:A:2223:G:C3'	7:C:264:LYS:NZ	2.77	0.48
7:C:209:ALA:HA	7:C:212:TRP:CZ3	2.46	0.48
10:F:94:ARG:C	10:F:98:PHE:CD2	2.83	0.48
10:F:132:ARG:HH22	10:F:148:VAL:HG11	1.78	0.48
5:A:528:A:H5''	13:J:113:PRO:HG3	1.96	0.48
10:F:33:ILE:HG13	10:F:95:MET:HG2	1.96	0.48
14:K:71:ARG:NH1	14:K:105:ARG:NH2	2.56	0.48
23:U:26:ASN:OD1	23:U:27:VAL:N	2.46	0.48
24:V:6:ALA:HB3	24:V:65:VAL:HB	1.95	0.48
5:A:1433:A:H2'	5:A:1434:A:C8	2.48	0.48
5:A:2667:C:H1'	11:G:108:PHE:CE1	2.48	0.48
11:G:26:LYS:HD2	11:G:26:LYS:HA	1.71	0.48
14:K:61:VAL:HG12	14:K:87:LEU:HD11	1.96	0.48
17:O:31:THR:OG1	17:O:34:HIS:O	2.26	0.48
5:A:1016:G:O6	5:A:1147:A:N6	2.47	0.47
5:A:1286:A:N6	5:A:1329:U:O2	2.47	0.47
5:A:2250:G:O2'	5:A:2496:C:OP1	2.32	0.47
7:C:151:GLY:O	7:C:155:ARG:NH1	2.44	0.47
10:F:23:SER:HB3	10:F:26:GLN:HE22	1.79	0.47
20:R:49:ILE:HD11	20:R:54:VAL:CB	2.40	0.47
22:T:25:GLU:OE1	22:T:25:GLU:N	2.47	0.47
1:O:3:GLN:NE2	5:A:2016:U:O2	2.38	0.47
3:2:10:LEU:O	3:2:14:ARG:HB2	2.13	0.47
20:R:95:ASP:OD1	20:R:95:ASP:N	2.43	0.47
23:U:6:ARG:HD2	23:U:6:ARG:HA	1.62	0.47
1:O:32:THR:OG1	1:O:33:SER:N	2.47	0.47
7:C:209:ALA:CA	7:C:212:TRP:CZ3	2.86	0.47
20:R:49:ILE:CG2	20:R:52:PRO:C	2.87	0.47
10:F:15:LEU:HA	10:F:18:GLU:HG2	1.96	0.47
15:L:46:VAL:HG22	15:L:47:ARG:N	2.30	0.47
27:Y:45:GLN:O	27:Y:46:VAL:C	2.56	0.47
7:C:51:ARG:HG3	7:C:52:HIS:ND1	2.29	0.47
5:A:1465:G:N2	5:A:1545:A:H4'	2.30	0.47
5:A:2298:A:H62	5:A:2318:G:H21	1.63	0.47
5:A:2333:A:H2	17:O:9:ARG:HH21	1.57	0.47
10:F:62:GLN:NE2	10:F:89:THR:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1159:U:H2'	5:A:1160:G:H8	1.80	0.47
5:A:1432:G:H2'	5:A:1433:A:C8	2.50	0.47
15:L:67:THR:HG22	15:L:68:SER:O	2.15	0.47
5:A:796:C:H2'	5:A:797:G:C8	2.50	0.47
5:A:1800:C:OP2	7:C:181:ARG:NH2	2.46	0.47
5:A:2377:A:O2'	17:O:117:PHE:O	2.31	0.47
8:D:33:ARG:HE	8:D:73:VAL:HG23	1.80	0.47
17:O:25:ARG:HE	17:O:27:VAL:CG1	2.27	0.47
18:P:91:VAL:CG1	18:P:96:LEU:HD21	2.45	0.47
14:K:62:VAL:HA	14:K:84:CYS:SG	2.55	0.46
17:O:67:ASN:ND2	17:O:69:ASP:OD1	2.48	0.46
8:D:37:VAL:HG22	8:D:48:ILE:HG22	1.96	0.46
16:N:49:GLU:HG2	16:N:94:TYR:HD2	1.80	0.46
4:3:22:LYS:NZ	5:A:630:G:OP2	2.48	0.46
7:C:141:HIS:CD2	7:C:142:ASN:HB2	2.51	0.46
5:A:505:A:HO2'	5:A:509:C:HO2'	1.59	0.46
4:3:22:LYS:HB2	4:3:46:LYS:HD2	1.97	0.46
16:N:55:ALA:HB2	16:N:79:LEU:HD23	1.98	0.46
26:X:57:VAL:HG13	26:X:61:LYS:HE2	1.98	0.46
1:O:12:ARG:HD3	5:A:1263:U:H5''	1.96	0.46
5:A:302:C:H2'	5:A:303:G:H8	1.81	0.46
10:F:43:ILE:HD12	10:F:43:ILE:H	1.81	0.46
13:J:31:GLU:HG3	13:J:142:ILE:HD12	1.98	0.46
24:V:30:ILE:HD13	24:V:91:PHE:CB	2.45	0.46
10:F:73:VAL:HG22	10:F:76:PHE:CG	2.51	0.46
12:H:5:LEU:HD13	12:H:13:GLY:HA2	1.97	0.46
5:A:151:C:H2'	5:A:152:A:H8	1.81	0.46
5:A:2470:G:H2'	5:A:2471:A:H8	1.80	0.46
8:D:170:VAL:HG12	8:D:171:THR:N	2.31	0.46
5:A:1465:G:H21	5:A:1545:A:H4'	1.81	0.46
7:C:171:VAL:O	7:C:182:LYS:HA	2.16	0.46
11:G:19:ASN:HB3	11:G:22:VAL:HG23	1.98	0.46
16:N:24:MET:HE2	16:N:24:MET:HB2	1.89	0.46
17:O:35:ILE:O	17:O:52:SER:OG	2.33	0.46
5:A:1380:G:O2'	5:A:1569:A:N6	2.49	0.45
5:A:2743:U:OP2	5:A:2755:C:N4	2.49	0.45
5:A:2898:U:H2'	5:A:2899:A:C8	2.50	0.45
14:K:13:ASN:HD21	14:K:98:ARG:CG	2.24	0.45
21:S:73:LYS:HB2	21:S:106:VAL:HB	1.99	0.45
24:V:9:ARG:NH2	24:V:28:ALA:O	2.48	0.45
6:B:8:C:O3'	17:O:25:ARG:NH2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:62:LYS:HB2	8:D:62:LYS:HE2	1.70	0.45
2:1:5:ARG:NH1	5:A:2285:C:OP2	2.49	0.45
5:A:2820:A:OP1	16:N:2:ARG:NH1	2.48	0.45
19:Q:47:ARG:HE	19:Q:47:ARG:HB3	1.65	0.45
22:T:33:LYS:HB3	22:T:33:LYS:HE2	1.80	0.45
5:A:626:A:N7	15:L:78:ARG:NH2	2.65	0.45
5:A:1589:U:H2'	5:A:1590:A:C8	2.51	0.45
9:E:41:GLN:HB3	9:E:43:THR:HG23	1.99	0.45
5:A:160:A:N7	5:A:166:U:O4	2.50	0.45
5:A:854:C:H2'	5:A:855:G:H8	1.81	0.45
5:A:2620:C:O2'	8:D:162:ALA:O	2.32	0.45
8:D:179:ARG:HH22	8:D:181:ASP:HB2	1.80	0.45
5:A:864:G:H21	5:A:866:A:H61	1.64	0.45
9:E:130:LYS:HB2	9:E:133:LEU:HD13	1.99	0.45
10:F:23:SER:OG	10:F:24:VAL:N	2.49	0.45
10:F:129:MET:SD	10:F:129:MET:N	2.89	0.45
14:K:25:LEU:HD13	14:K:38:ILE:HG22	1.98	0.45
20:R:38:VAL:HG12	20:R:39:LEU:N	2.32	0.45
4:3:16:THR:OG1	5:A:629:G:OP1	2.35	0.45
5:A:291:G:O6	5:A:349:U:O4	2.34	0.45
5:A:1407:G:H2'	5:A:1408:G:H8	1.81	0.45
5:A:2318:G:H2'	5:A:2319:G:C4	2.52	0.45
5:A:2447:G:N2	5:A:2450:A:OP2	2.39	0.45
22:T:30:ILE:HG22	22:T:85:VAL:HB	1.99	0.45
5:A:796:C:H2'	5:A:797:G:H8	1.81	0.45
5:A:935:C:H2'	5:A:936:A:H8	1.82	0.45
5:A:2471:A:N6	5:A:2476:A:O2'	2.49	0.45
5:A:2506:U:OP2	5:A:2576:G:N1	2.50	0.45
6:B:80:U:O4	24:V:14:LYS:NZ	2.46	0.45
26:X:17:ARG:HA	26:X:17:ARG:HD3	1.71	0.45
26:X:73:ARG:HE	26:X:73:ARG:HB3	1.66	0.45
5:A:1266:G:O2'	5:A:2012:G:O6	2.34	0.44
5:A:2561:U:O3'	14:K:40:LYS:NZ	2.50	0.44
11:G:37:ASN:C	11:G:39:ALA:H	2.24	0.44
5:A:2787:C:H1'	8:D:63:PRO:HG3	1.99	0.44
11:G:34:ARG:NH1	11:G:35:THR:O	2.50	0.44
8:D:124:ARG:HH12	8:D:163:GLY:HA3	1.82	0.44
22:T:58:VAL:HG23	22:T:85:VAL:HG22	1.98	0.44
4:3:33:THR:OG1	5:A:2420:C:OP1	2.32	0.44
5:A:1420:A:O2'	5:A:2211:A:N6	2.49	0.44
7:C:226:PRO:HD3	7:C:233:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:184:ASP:OD1	9:E:184:ASP:N	2.50	0.44
15:L:129:LYS:HA	15:L:129:LYS:HD2	1.77	0.44
5:A:307:G:N1	5:A:310:A:OP2	2.43	0.44
5:A:782:A:C8	7:C:219:VAL:HG11	2.53	0.44
22:T:16:VAL:O	22:T:16:VAL:HG23	2.18	0.44
5:A:559:G:N2	19:Q:51:GLN:HE22	2.16	0.44
18:P:77:SER:HB2	18:P:79:VAL:HG12	2.00	0.44
6:B:115:A:H2'	6:B:116:G:H8	1.83	0.44
8:D:124:ARG:NH1	8:D:163:GLY:HA3	2.33	0.44
11:G:98:LYS:HE2	11:G:103:ASN:HB2	1.99	0.44
24:V:62:THR:HG22	24:V:71:LYS:HD2	2.00	0.44
15:L:89:VAL:HB	15:L:123:ARG:NH2	2.22	0.44
5:A:371:A:HO2'	26:X:60:LYS:NZ	2.03	0.43
9:E:164:LEU:HD23	9:E:164:LEU:HA	1.86	0.43
15:L:73:ILE:O	15:L:73:ILE:CG2	2.64	0.43
23:U:42:LYS:O	23:U:42:LYS:HG3	2.18	0.43
5:A:380:G:C2	5:A:395:U:O2	2.71	0.43
5:A:619:G:OP2	5:A:620:G:N2	2.52	0.43
7:C:269:ARG:NH2	7:C:270:ARG:NH1	2.65	0.43
23:U:3:LYS:HD2	23:U:82:VAL:HB	2.01	0.43
5:A:5:A:H2'	5:A:6:A:H8	1.83	0.43
5:A:959:A:H2'	5:A:960:A:C8	2.54	0.43
5:A:1280:G:H2'	5:A:1281:G:H8	1.83	0.43
5:A:2223:G:C4'	7:C:264:LYS:HZ1	2.23	0.43
23:U:98:ASN:O	23:U:98:ASN:CG	2.58	0.43
5:A:645:C:H2'	5:A:647:G:C8	2.53	0.43
5:A:1625:C:N4	5:A:1626:A:N1	2.66	0.43
3:2:11:LYS:NZ	5:A:770:G:OP2	2.42	0.43
6:B:114:C:H2'	6:B:115:A:H8	1.84	0.43
9:E:122:GLU:O	9:E:123:LYS:HD2	2.19	0.43
10:F:120:SER:HB2	10:F:127:TYR:CZ	2.53	0.43
1:0:53:VAL:HG22	1:0:54:ILE:H	1.83	0.43
5:A:1796:U:H2'	5:A:1797:G:C8	2.52	0.43
5:A:2245:U:H5''	5:A:2246:G:H5'	2.00	0.43
13:J:1:MET:SD	13:J:1:MET:N	2.82	0.43
5:A:139:U:O2'	5:A:141:G:N2	2.52	0.43
5:A:383:C:H5'	5:A:384:A:H5''	2.01	0.43
5:A:1205:A:N7	9:E:165:HIS:NE2	2.67	0.43
5:A:1386:C:O2'	5:A:1469:A:N3	2.49	0.43
5:A:2699:C:H2'	5:A:2700:A:C8	2.54	0.43
11:G:104:LEU:CD1	11:G:150:TYR:CD2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Q:108:LEU:HD13	20:R:48:LYS:CD	2.49	0.43
22:T:44:LYS:O	22:T:48:GLN:HB2	2.18	0.43
22:T:69:ARG:HB3	22:T:74:ILE:HD13	2.00	0.43
5:A:1465:G:H2'	5:A:1545:A:O3'	2.18	0.43
14:K:1:MET:HE1	14:K:67:LYS:HE3	1.99	0.43
14:K:12:ASP:OD1	14:K:12:ASP:N	2.51	0.43
26:X:2:ARG:HH11	26:X:29:LEU:HD13	1.80	0.43
1:O:37:HIS:ND1	1:O:38:LEU:O	2.42	0.43
5:A:2581:G:N2	5:A:2581:G:OP2	2.51	0.43
11:G:28:LYS:NZ	11:G:79:THR:HA	2.28	0.43
11:G:93:TYR:CG	11:G:151:ARG:HG3	2.53	0.43
13:J:69:ARG:NH1	13:J:90:GLU:HG3	2.33	0.43
22:T:58:VAL:HA	22:T:84:TYR:O	2.18	0.43
5:A:1407:G:H2'	5:A:1408:G:C8	2.54	0.43
5:A:2458:G:H21	5:A:2459:A:H61	1.67	0.43
21:S:24:ILE:HG21	21:S:36:LEU:HD13	2.01	0.43
27:Y:5:GLU:OE1	27:Y:5:GLU:N	2.52	0.43
5:A:291:G:N2	5:A:349:U:O2	2.40	0.42
5:A:2329:U:H2'	5:A:2330:G:C8	2.54	0.42
12:H:8:LYS:HD2	12:H:8:LYS:HA	1.91	0.42
14:K:63:VAL:HG12	14:K:64:ARG:HG3	2.00	0.42
5:A:30:G:OP2	19:Q:4:LYS:NZ	2.40	0.42
5:A:160:A:H62	5:A:166:U:H3	1.67	0.42
5:A:307:G:H21	5:A:330:A:H61	1.67	0.42
7:C:176:ARG:HA	7:C:176:ARG:HD2	1.80	0.42
17:O:24:THR:HG22	17:O:42:PRO:CD	2.41	0.42
18:P:24:THR:HB	18:P:87:ARG:HB3	2.01	0.42
20:R:24:LYS:HA	20:R:94:THR:HG23	2.01	0.42
22:T:34:VAL:HG21	22:T:43:ILE:HD11	2.01	0.42
28:Z:6:ILE:HD11	28:Z:47:ILE:HD11	2.01	0.42
5:A:1114:C:H2'	5:A:1115:G:C8	2.53	0.42
6:B:42:C:C2	10:F:65:LEU:HD21	2.55	0.42
7:C:49:THR:OG1	7:C:50:THR:N	2.51	0.42
18:P:3:ILE:O	18:P:7:LEU:HG	2.18	0.42
25:W:62:LYS:HE3	25:W:62:LYS:HB2	1.75	0.42
5:A:1353:A:N7	5:A:1378:A:N6	2.67	0.42
5:A:2340:A:H2'	5:A:2341:G:H8	1.83	0.42
10:F:37:MET:SD	10:F:56:LEU:CD2	3.08	0.42
22:T:11:LEU:HD22	22:T:32:LEU:HD22	2.01	0.42
9:E:49:ARG:HD2	9:E:76:PRO:HD3	2.01	0.42
10:F:30:VAL:HG12	10:F:157:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:86:CYS:SG	10:F:87:LYS:N	2.93	0.42
24:V:30:ILE:HD13	24:V:91:PHE:HB2	2.00	0.42
10:F:12:VAL:O	10:F:16:MET:CG	2.49	0.42
5:A:774:G:P	7:C:47:ARG:HH12	2.43	0.42
5:A:2505:G:H2'	5:A:2576:G:H1	1.84	0.42
20:R:5:PHE:O	20:R:11:GLN:HA	2.19	0.42
5:A:2822:G:O2'	5:A:2824:C:OP2	2.35	0.42
11:G:151:ARG:HB2	11:G:161:VAL:HG23	2.01	0.42
13:J:11:VAL:HG21	13:J:50:THR:HG22	2.02	0.42
5:A:2720:U:O5'	18:P:52:ARG:NH2	2.53	0.42
23:U:45:GLN:OE1	23:U:46:LYS:N	2.53	0.42
5:A:143:C:H2'	5:A:144:A:H8	1.85	0.42
5:A:300:A:O2'	5:A:318:C:O2	2.38	0.42
5:A:320:A:C2'	9:E:163:ASN:HD22	2.33	0.42
5:A:1141:U:OP2	13:J:65:THR:OG1	2.32	0.42
5:A:2654:A:H4'	5:A:2655:G:H4'	2.02	0.42
10:F:132:ARG:HG3	10:F:133:GLU:HG3	2.01	0.42
15:L:79:LEU:HD23	15:L:79:LEU:HA	1.83	0.42
27:Y:24:GLU:O	27:Y:46:VAL:HG11	2.19	0.42
5:A:5:A:H2'	5:A:6:A:C8	2.55	0.41
5:A:948:C:O2	5:A:984:A:O2'	2.34	0.41
5:A:948:C:H2'	5:A:949:G:C8	2.54	0.41
7:C:209:ALA:CB	7:C:212:TRP:CH2	3.02	0.41
15:L:3:LEU:HD23	15:L:3:LEU:HA	1.86	0.41
15:L:73:ILE:HA	15:L:105:ILE:HD13	2.01	0.41
5:A:1441:G:H2'	5:A:1442:U:C6	2.55	0.41
5:A:2303:G:O6	5:A:2314:A:N6	2.53	0.41
10:F:3:LEU:HA	10:F:6:TYR:HB3	2.01	0.41
11:G:28:LYS:HE3	11:G:78:VAL:O	2.20	0.41
13:J:142:ILE:HD13	13:J:142:ILE:HA	1.92	0.41
5:A:2474:U:H5''	5:A:2475:C:H5	1.85	0.41
5:A:2718:G:O2'	5:A:2847:U:OP1	2.34	0.41
9:E:148:ILE:HD13	9:E:187:VAL:HB	2.03	0.41
17:O:13:ARG:HH12	17:O:16:ARG:HH21	1.68	0.41
24:V:9:ARG:HE	24:V:40:ILE:C	2.28	0.41
28:Z:36:GLU:O	28:Z:37:ARG:NH1	2.47	0.41
4:3:31:ILE:C	4:3:31:ILE:HD12	2.45	0.41
5:A:175:G:H2'	5:A:176:A:H8	1.85	0.41
5:A:2772:C:H5'	8:D:173:GLN:HE22	1.85	0.41
7:C:27:LYS:H	7:C:27:LYS:HG2	1.68	0.41
8:D:11:MET:HE3	8:D:11:MET:HB2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:48:THR:HG22	9:E:86:ALA:HB3	2.02	0.41
14:K:13:ASN:HD22	14:K:98:ARG:CG	2.32	0.41
15:L:74:THR:HA	15:L:107:PHE:HB2	2.02	0.41
19:Q:79:ILE:HA	19:Q:79:ILE:HD13	1.84	0.41
28:Z:18:LYS:HD3	28:Z:18:LYS:HA	1.90	0.41
5:A:1:G:H2'	5:A:2:G:H8	1.85	0.41
5:A:1590:A:H2'	5:A:1591:A:H8	1.84	0.41
9:E:147:LEU:HD21	9:E:170:ARG:HE	1.85	0.41
12:H:9:VAL:O	12:H:10:ALA:C	2.63	0.41
23:U:98:ASN:OD1	23:U:98:ASN:C	2.63	0.41
5:A:2031:A:N3	5:A:2455:G:O2'	2.53	0.41
8:D:169:ARG:C	8:D:170:VAL:HG23	2.46	0.41
13:J:69:ARG:HH22	13:J:90:GLU:HA	1.86	0.41
2:1:24:LYS:HD3	2:1:26:LYS:HE3	2.02	0.41
4:3:30:HIS:NE2	5:A:2392:A:OP2	2.50	0.41
7:C:23:LEU:HD23	7:C:23:LEU:HA	1.85	0.41
7:C:51:ARG:CD	7:C:52:HIS:NE2	2.56	0.41
18:P:23:ASP:OD1	18:P:88:ARG:HA	2.21	0.41
5:A:2411:A:H2'	5:A:2412:A:C8	2.55	0.41
5:A:2855:C:H2'	5:A:2856:A:H8	1.85	0.41
18:P:5:LYS:O	18:P:9:GLN:HG2	2.20	0.41
19:Q:87:VAL:HG11	20:R:48:LYS:HE2	2.01	0.41
20:R:49:ILE:CD1	20:R:54:VAL:HB	2.39	0.41
26:X:58:ILE:CD1	26:X:66:VAL:CG1	2.90	0.41
5:A:974:G:N3	5:A:1186:G:N2	2.68	0.41
5:A:1446:C:H2'	5:A:1447:C:C6	2.56	0.41
5:A:2204:G:H2'	5:A:2205:A:H8	1.86	0.41
5:A:2635:A:O2'	8:D:81:GLU:OE2	2.36	0.41
7:C:198:GLU:OE1	7:C:198:GLU:N	2.53	0.41
7:C:257:ARG:NH2	7:C:266:ILE:HD12	2.36	0.41
14:K:44:LYS:HD3	14:K:44:LYS:HA	1.91	0.41
18:P:36:LYS:HA	18:P:36:LYS:HD3	1.86	0.41
18:P:51:ASN:OD1	18:P:51:ASN:N	2.43	0.41
23:U:97:SER:OG	23:U:97:SER:O	2.39	0.41
5:A:1358:G:H1'	5:A:1374:G:H22	1.85	0.41
9:E:97:ASN:HB2	9:E:100:MET:HB2	2.03	0.41
1:0:11:LYS:HA	1:0:11:LYS:HD3	1.91	0.40
2:1:23:THR:HG22	2:1:24:LYS:N	2.35	0.40
5:A:1342:A:O2'	5:A:1344:U:OP2	2.36	0.40
7:C:200:MET:H	7:C:200:MET:HG2	1.73	0.40
5:A:162:U:C2	5:A:165:A:N6	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:175:G:H2'	5:A:176:A:C8	2.55	0.40
5:A:2093:G:OP1	12:H:24:GLY:N	2.54	0.40
5:A:2749:A:OP1	11:G:1:SER:N	2.54	0.40
6:B:22:U:H2'	6:B:23:G:C8	2.57	0.40
6:B:29:A:H2'	6:B:30:C:C6	2.56	0.40
8:D:106:LYS:HD3	8:D:106:LYS:HA	1.90	0.40
14:K:78:ARG:NH2	18:P:70:GLU:OE1	2.55	0.40
16:N:89:SER:O	16:N:89:SER:OG	2.28	0.40
27:Y:14:LEU:O	27:Y:18:LEU:HD22	2.21	0.40
28:Z:13:ILE:HD13	28:Z:13:ILE:HA	1.88	0.40
3:2:10:LEU:HD12	3:2:10:LEU:HA	1.89	0.40
5:A:505:A:O2'	5:A:509:C:O2'	2.31	0.40
5:A:1592:C:H2'	5:A:1593:A:H8	1.87	0.40
9:E:148:ILE:HB	9:E:169:VAL:HG22	2.03	0.40
15:L:39:LYS:HE2	15:L:39:LYS:HB3	1.68	0.40
5:A:692:C:H2'	5:A:693:A:C8	2.56	0.40
5:A:1155:A:H5''	19:Q:54:ARG:HD3	2.02	0.40
5:A:1340:U:H4'	5:A:1394:U:H1'	2.02	0.40
5:A:1400:U:H2'	5:A:1401:G:C8	2.56	0.40
5:A:2737:G:H2'	5:A:2738:A:C8	2.56	0.40
8:D:33:ARG:CZ	8:D:74:GLU:O	2.70	0.40
10:F:117:SER:OG	10:F:118:ALA:N	2.54	0.40
12:H:5:LEU:HD22	12:H:13:GLY:HA2	2.04	0.40
14:K:99:ILE:HD13	14:K:99:ILE:HA	1.91	0.40
15:L:47:ARG:HG3	15:L:50:PHE:HB2	2.03	0.40
21:S:97:LEU:HA	21:S:97:LEU:HD23	1.88	0.40
5:A:116:C:O2'	5:A:126:A:N3	2.53	0.40
5:A:191:A:H2'	5:A:192:C:C6	2.56	0.40
5:A:1355:G:H2'	5:A:1356:G:H8	1.86	0.40
10:F:27:VAL:O	10:F:29:ARG:NE	2.55	0.40
10:F:103:ILE:CD1	10:F:175:PRO:HD3	2.51	0.40
27:Y:2:LYS:H	27:Y:2:LYS:HG2	1.60	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	47 (87%)	7 (13%)	0	100	100
2	1	46/55 (84%)	44 (96%)	2 (4%)	0	100	100
3	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
4	3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
7	C	269/273 (98%)	245 (91%)	23 (9%)	1 (0%)	30	66
8	D	207/209 (99%)	189 (91%)	17 (8%)	1 (0%)	25	61
9	E	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
10	F	175/179 (98%)	156 (89%)	18 (10%)	1 (1%)	22	58
11	G	171/177 (97%)	154 (90%)	16 (9%)	1 (1%)	22	58
12	H	30/149 (20%)	21 (70%)	9 (30%)	0	100	100
13	J	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	K	120/123 (98%)	107 (89%)	13 (11%)	0	100	100
15	L	141/144 (98%)	118 (84%)	20 (14%)	3 (2%)	5	33
16	N	118/127 (93%)	108 (92%)	10 (8%)	0	100	100
17	O	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
18	P	96/115 (84%)	94 (98%)	2 (2%)	0	100	100
19	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
20	R	101/103 (98%)	92 (91%)	9 (9%)	0	100	100
21	S	108/110 (98%)	102 (94%)	5 (5%)	1 (1%)	14	49
22	T	85/100 (85%)	73 (86%)	12 (14%)	0	100	100
23	U	100/104 (96%)	87 (87%)	13 (13%)	0	100	100
24	V	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
25	W	74/85 (87%)	70 (95%)	4 (5%)	0	100	100
26	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
27	Y	61/63 (97%)	54 (88%)	6 (10%)	1 (2%)	8	38
28	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
All	All	2853/3093 (92%)	2610 (92%)	234 (8%)	9 (0%)	38	71

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	175	PRO
15	L	89	VAL
21	S	66	ILE
27	Y	46	VAL
7	C	194	VAL
8	D	151	THR
15	L	86	GLU
11	G	38	ASP
15	L	30	THR

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	0	47/48 (98%)	47 (100%)	0	100	100
2	1	44/49 (90%)	43 (98%)	1 (2%)	45	64
3	2	38/38 (100%)	37 (97%)	1 (3%)	41	61
4	3	51/52 (98%)	51 (100%)	0	100	100
7	C	216/218 (99%)	214 (99%)	2 (1%)	75	83
8	D	164/164 (100%)	158 (96%)	6 (4%)	29	52
9	E	165/165 (100%)	159 (96%)	6 (4%)	30	52
10	F	148/150 (99%)	141 (95%)	7 (5%)	22	45
11	G	136/138 (99%)	132 (97%)	4 (3%)	37	58
12	H	26/114 (23%)	23 (88%)	3 (12%)	4	20
13	J	116/116 (100%)	113 (97%)	3 (3%)	41	61
14	K	103/104 (99%)	101 (98%)	2 (2%)	52	70
15	L	102/103 (99%)	99 (97%)	3 (3%)	37	58
16	N	100/103 (97%)	98 (98%)	2 (2%)	50	68
17	O	86/87 (99%)	83 (96%)	3 (4%)	31	53
18	P	86/100 (86%)	83 (96%)	3 (4%)	31	53
19	Q	89/90 (99%)	88 (99%)	1 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	84/84 (100%)	83 (99%)	1 (1%)	67	78
21	S	93/93 (100%)	89 (96%)	4 (4%)	25	48
22	T	74/84 (88%)	73 (99%)	1 (1%)	62	75
23	U	83/85 (98%)	79 (95%)	4 (5%)	21	45
24	V	78/78 (100%)	76 (97%)	2 (3%)	41	61
25	W	58/63 (92%)	58 (100%)	0	100	100
26	X	67/68 (98%)	67 (100%)	0	100	100
27	Y	55/55 (100%)	52 (94%)	3 (6%)	18	42
28	Z	48/49 (98%)	47 (98%)	1 (2%)	48	66
All	All	2357/2498 (94%)	2294 (97%)	63 (3%)	41	60

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1	50	GLU
3	2	4	THR
7	C	179	GLU
7	C	186	ASP
8	D	11	MET
8	D	12	THR
8	D	110	THR
8	D	121	THR
8	D	148	GLN
8	D	151	THR
9	E	96	VAL
9	E	105	LEU
9	E	155	GLU
9	E	178	VAL
9	E	186	VAL
9	E	200	LEU
10	F	24	VAL
10	F	73	VAL
10	F	135	ILE
10	F	139	GLU
10	F	168	LEU
10	F	173	ASP
10	F	174	PHE
11	G	8	VAL
11	G	9	VAL

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Mol	Chain	Res	Type
11	G	46	ASP
11	G	126	THR
12	H	9	VAL
12	H	11	ASN
12	H	15	LEU
13	J	45	THR
13	J	80	HIS
13	J	140	LEU
14	K	58	LEU
14	K	69	VAL
15	L	89	VAL
15	L	127	VAL
15	L	142	ILE
16	N	29	VAL
16	N	33	ILE
17	O	47	VAL
17	O	100	HIS
17	O	115	LEU
18	P	63	ILE
18	P	77	SER
18	P	96	LEU
19	Q	33	VAL
20	R	86	GLN
21	S	11	ARG
21	S	35	ILE
21	S	62	ASP
21	S	66	ILE
22	T	89	GLU
23	U	5	ARG
23	U	6	ARG
23	U	85	ARG
23	U	87	GLU
24	V	3	THR
24	V	91	PHE
27	Y	9	LYS
27	Y	44	LYS
27	Y	46	VAL
28	Z	26	LEU

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

Mol	Chain	Res	Type
1	0	5	ASN
3	2	16	HIS
7	C	14	HIS
7	C	36	ASN
7	C	142	ASN
8	D	167	ASN
9	E	163	ASN
10	F	4	HIS
10	F	36	ASN
10	F	51	ASN
11	G	47	ASN
12	H	2	GLN
12	H	11	ASN
13	J	130	HIS
13	J	138	GLN
14	K	13	ASN
14	K	90	ASN
16	N	3	HIS
16	N	107	ASN
18	P	9	GLN
18	P	76	HIS
20	R	82	HIS
22	T	28	ASN
22	T	59	ASN
24	V	5	ASN
27	Y	25	GLN
27	Y	39	GLN
27	Y	45	GLN
27	Y	58	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2374/2904 (81%)	430 (18%)	7 (0%)
6	B	118/120 (98%)	15 (12%)	0
All	All	2492/3024 (82%)	445 (17%)	7 (0%)

All (445) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	A
5	A	14	A

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Mol	Chain	Res	Type
5	A	34	U
5	A	35	G
5	A	45	G
5	A	46	G
5	A	51	G
5	A	63	A
5	A	71	A
5	A	74	A
5	A	75	G
5	A	84	A
5	A	85	G
5	A	91	A
5	A	92	U
5	A	94	A
5	A	100	U
5	A	101	A
5	A	103	A
5	A	110	G
5	A	118	A
5	A	120	U
5	A	134	G
5	A	136	G
5	A	138	U
5	A	139	U
5	A	140	C
5	A	141	G
5	A	142	A
5	A	149	A
5	A	162	U
5	A	178	G
5	A	181	A
5	A	186	G
5	A	196	A
5	A	199	A
5	A	201	C
5	A	204	A
5	A	215	G
5	A	216	A
5	A	222	A
5	A	228	C
5	A	229	C
5	A	230	G

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Mol	Chain	Res	Type
5	A	233	A
5	A	245	G
5	A	247	G
5	A	248	G
5	A	250	G
5	A	255	A
5	A	264	C
5	A	265	A
5	A	266	G
5	A	267	C
5	A	271	G
5	A	302	C
5	A	306	U
5	A	307	G
5	A	311	A
5	A	322	A
5	A	324	A
5	A	329	G
5	A	330	A
5	A	331	C
5	A	371	A
5	A	372	G
5	A	379	G
5	A	382	A
5	A	386	G
5	A	387	U
5	A	388	G
5	A	389	G
5	A	396	G
5	A	404	A
5	A	405	U
5	A	411	G
5	A	412	A
5	A	415	A
5	A	424	G
5	A	425	G
5	A	435	C
5	A	451	U
5	A	452	G
5	A	456	C
5	A	457	A
5	A	464	U

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Mol	Chain	Res	Type
5	A	467	G
5	A	473	G
5	A	480	A
5	A	481	G
5	A	489	G
5	A	490	C
5	A	491	G
5	A	494	G
5	A	500	G
5	A	504	A
5	A	505	A
5	A	508	A
5	A	509	C
5	A	510	C
5	A	512	G
5	A	528	A
5	A	531	C
5	A	532	A
5	A	533	G
5	A	543	G
5	A	544	C
5	A	546	U
5	A	547	A
5	A	548	G
5	A	549	G
5	A	563	A
5	A	569	U
5	A	572	A
5	A	573	U
5	A	574	A
5	A	575	A
5	A	586	A
5	A	603	A
5	A	613	A
5	A	614	A
5	A	615	U
5	A	618	G
5	A	622	G
5	A	627	A
5	A	634	C
5	A	637	A
5	A	645	C

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Mol	Chain	Res	Type
5	A	646	U
5	A	647	G
5	A	654	A
5	A	655	A
5	A	670	A
5	A	686	U
5	A	726	G
5	A	729	G
5	A	730	A
5	A	747	U
5	A	748	G
5	A	764	A
5	A	765	C
5	A	775	G
5	A	776	G
5	A	782	A
5	A	784	G
5	A	785	G
5	A	791	C
5	A	792	A
5	A	805	G
5	A	812	C
5	A	819	A
5	A	827	U
5	A	828	U
5	A	843	G
5	A	845	A
5	A	846	U
5	A	857	G
5	A	859	G
5	A	910	A
5	A	914	G
5	A	938	G
5	A	941	A
5	A	946	C
5	A	959	A
5	A	961	C
5	A	973	A
5	A	974	G
5	A	981	A
5	A	983	A
5	A	989	G

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Mol	Chain	Res	Type
5	A	990	A
5	A	995	C
5	A	996	A
5	A	997	G
5	A	999	U
5	A	1005	C
5	A	1006	C
5	A	1008	A
5	A	1012	U
5	A	1013	C
5	A	1022	G
5	A	1023	U
5	A	1025	G
5	A	1026	G
5	A	1033	U
5	A	1112	G
5	A	1115	G
5	A	1130	U
5	A	1133	A
5	A	1135	C
5	A	1136	G
5	A	1137	G
5	A	1139	G
5	A	1142	A
5	A	1143	A
5	A	1182	G
5	A	1187	G
5	A	1204	A
5	A	1210	G
5	A	1211	C
5	A	1212	G
5	A	1235	G
5	A	1238	G
5	A	1240	U
5	A	1247	A
5	A	1248	G
5	A	1253	A
5	A	1256	G
5	A	1266	G
5	A	1272	A
5	A	1273	U
5	A	1301	A

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Mol	Chain	Res	Type
5	A	1306	C
5	A	1321	A
5	A	1329	U
5	A	1341	G
5	A	1345	C
5	A	1352	U
5	A	1365	A
5	A	1368	G
5	A	1374	G
5	A	1378	A
5	A	1379	U
5	A	1383	A
5	A	1386	C
5	A	1407	G
5	A	1416	G
5	A	1417	C
5	A	1424	G
5	A	1428	C
5	A	1435	G
5	A	1437	C
5	A	1452	G
5	A	1465	G
5	A	1473	G
5	A	1515	A
5	A	1516	G
5	A	1523	U
5	A	1546	G
5	A	1547	C
5	A	1549	A
5	A	1550	C
5	A	1555	G
5	A	1566	A
5	A	1567	G
5	A	1569	A
5	A	1571	A
5	A	1583	A
5	A	1584	U
5	A	1585	C
5	A	1607	C
5	A	1608	A
5	A	1618	A
5	A	1639	C

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Mol	Chain	Res	Type
5	A	1646	C
5	A	1647	U
5	A	1648	U
5	A	1652	A
5	A	1674	G
5	A	1675	C
5	A	1677	A
5	A	1681	G
5	A	1694	C
5	A	1699	G
5	A	1754	A
5	A	1756	G
5	A	1764	C
5	A	1773	A
5	A	1781	U
5	A	1784	A
5	A	1785	A
5	A	1786	A
5	A	1791	A
5	A	1800	C
5	A	1801	A
5	A	1802	A
5	A	1808	A
5	A	1809	A
5	A	1811	G
5	A	1816	C
5	A	1819	A
5	A	1828	G
5	A	1829	A
5	A	1832	C
5	A	1991	U
5	A	1992	G
5	A	1993	U
5	A	1997	C
5	A	2012	G
5	A	2013	A
5	A	2020	A
5	A	2022	U
5	A	2023	C
5	A	2031	A
5	A	2033	A
5	A	2041	U

Continued on next page...

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Mol	Chain	Res	Type
5	A	2043	C
5	A	2051	A
5	A	2052	A
5	A	2053	G
5	A	2055	C
5	A	2056	G
5	A	2060	A
5	A	2061	G
5	A	2062	A
5	A	2069	G
5	A	2093	G
5	A	2095	A
5	A	2198	A
5	A	2203	U
5	A	2204	G
5	A	2211	A
5	A	2212	A
5	A	2225	A
5	A	2226	C
5	A	2238	G
5	A	2239	G
5	A	2250	G
5	A	2259	U
5	A	2271	G
5	A	2283	C
5	A	2286	G
5	A	2287	A
5	A	2288	A
5	A	2297	A
5	A	2305	U
5	A	2306	C
5	A	2308	G
5	A	2311	A
5	A	2312	U
5	A	2319	G
5	A	2322	A
5	A	2325	G
5	A	2326	C
5	A	2327	A
5	A	2333	A
5	A	2334	U
5	A	2335	A

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Mol	Chain	Res	Type
5	A	2347	C
5	A	2350	C
5	A	2361	G
5	A	2365	G
5	A	2376	A
5	A	2383	G
5	A	2385	C
5	A	2390	U
5	A	2402	U
5	A	2406	A
5	A	2422	C
5	A	2425	A
5	A	2426	A
5	A	2429	G
5	A	2430	A
5	A	2434	A
5	A	2435	A
5	A	2441	U
5	A	2445	G
5	A	2448	A
5	A	2475	C
5	A	2476	A
5	A	2481	G
5	A	2491	U
5	A	2494	G
5	A	2498	C
5	A	2502	G
5	A	2503	A
5	A	2504	U
5	A	2505	G
5	A	2507	C
5	A	2518	A
5	A	2519	U
5	A	2520	C
5	A	2529	G
5	A	2531	A
5	A	2532	G
5	A	2535	G
5	A	2566	A
5	A	2567	G
5	A	2570	G
5	A	2572	A

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Mol	Chain	Res	Type
5	A	2573	C
5	A	2576	G
5	A	2582	G
5	A	2585	U
5	A	2586	U
5	A	2587	A
5	A	2602	A
5	A	2603	G
5	A	2604	U
5	A	2609	U
5	A	2610	C
5	A	2613	U
5	A	2629	U
5	A	2639	A
5	A	2646	C
5	A	2663	G
5	A	2689	U
5	A	2690	U
5	A	2714	G
5	A	2718	G
5	A	2720	U
5	A	2726	A
5	A	2729	G
5	A	2733	A
5	A	2744	G
5	A	2748	A
5	A	2756	U
5	A	2759	G
5	A	2764	A
5	A	2765	A
5	A	2766	A
5	A	2776	A
5	A	2778	A
5	A	2780	G
5	A	2811	G
5	A	2818	U
5	A	2820	A
5	A	2825	G
5	A	2835	A
5	A	2849	U
5	A	2861	U
5	A	2867	G

Continued on next page...

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Mol	Chain	Res	Type
5	A	2872	A
5	A	2879	A
5	A	2880	C
5	A	2883	A
5	A	2884	U
5	A	2885	G
5	A	2886	A
5	A	2887	A
6	B	2	G
6	B	9	G
6	B	13	G
6	B	15	A
6	B	31	C
6	B	35	C
6	B	37	C
6	B	41	G
6	B	56	G
6	B	66	A
6	B	89	U
6	B	90	C
6	B	99	A
6	B	105	G
6	B	109	A

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	404	A
5	A	479	A
5	A	1378	A
5	A	2211	A
5	A	2304	G
5	A	2326	C
5	A	2425	A

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

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

5.5 Carbohydrates [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.

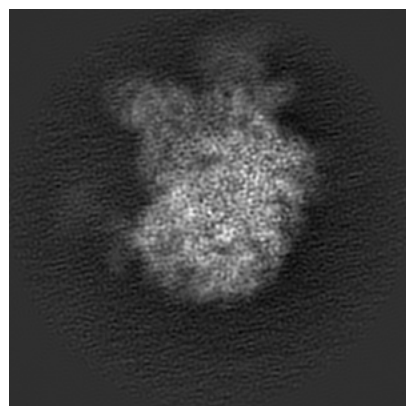
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61605. These allow visual inspection of the internal detail of the map and identification of artifacts.

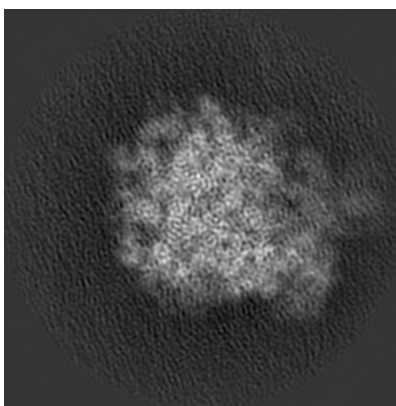
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

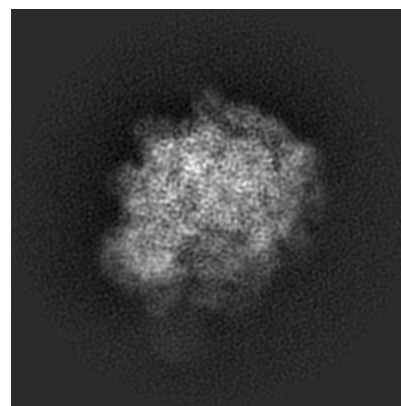
6.1.1 Primary map



X

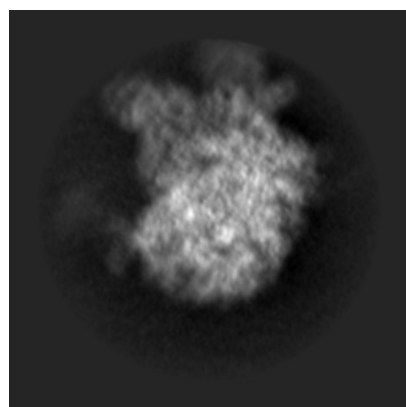


Y

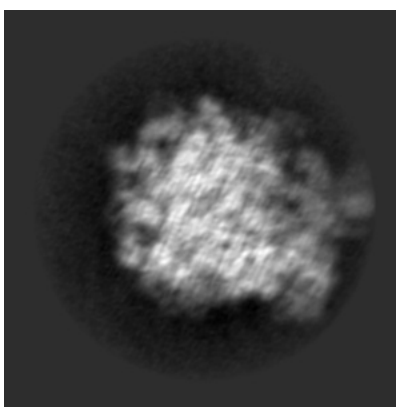


Z

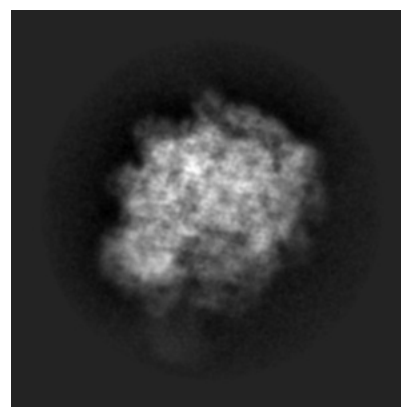
6.1.2 Raw map



X



Y

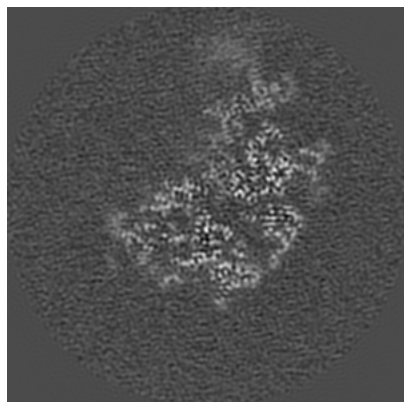


Z

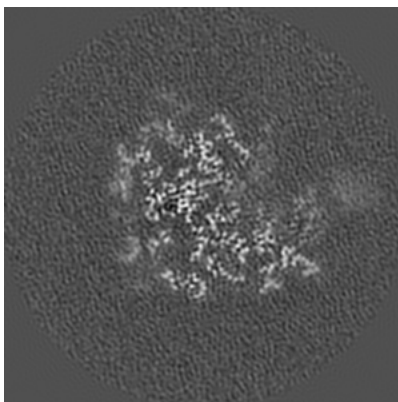
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

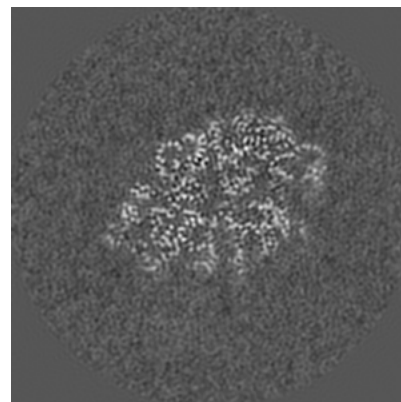
6.2.1 Primary map



X Index: 240

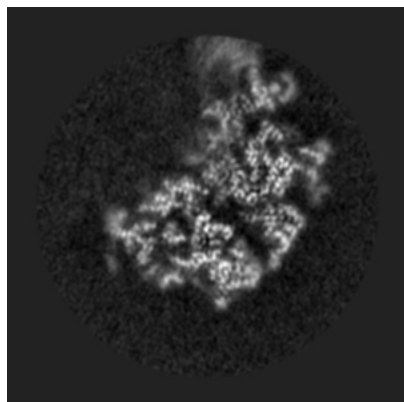


Y Index: 240

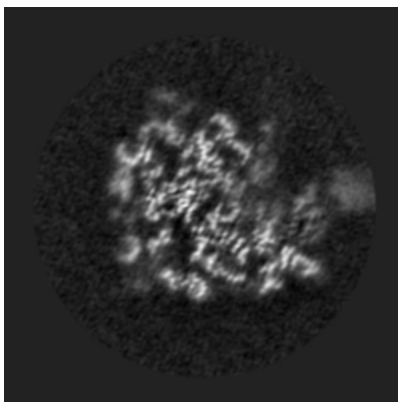


Z Index: 240

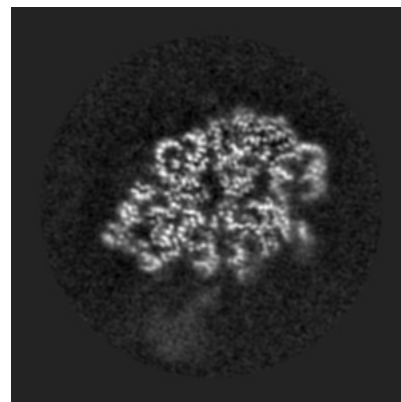
6.2.2 Raw map



X Index: 240



Y Index: 240

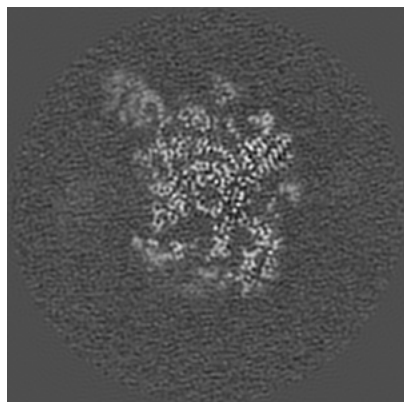


Z Index: 240

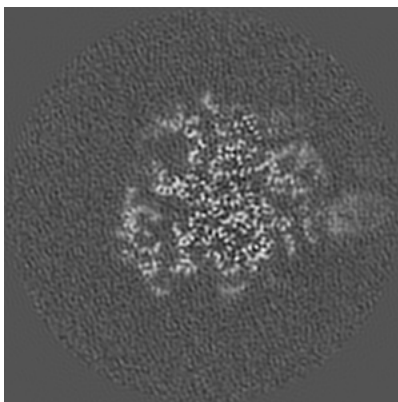
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

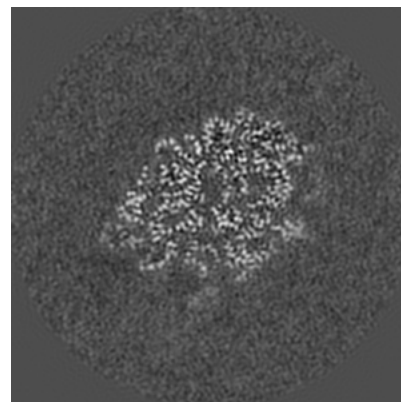
6.3.1 Primary map



X Index: 188

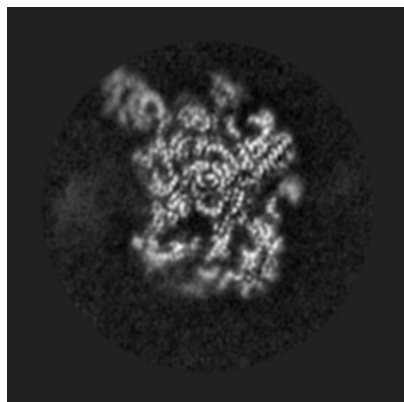


Y Index: 292

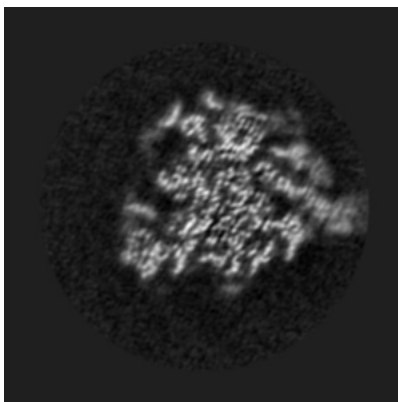


Z Index: 233

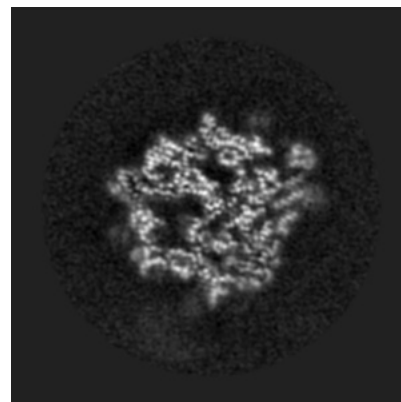
6.3.2 Raw map



X Index: 188



Y Index: 298

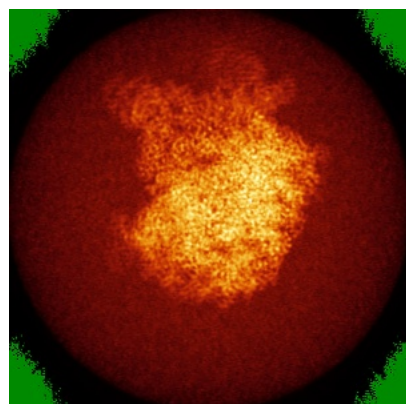


Z Index: 211

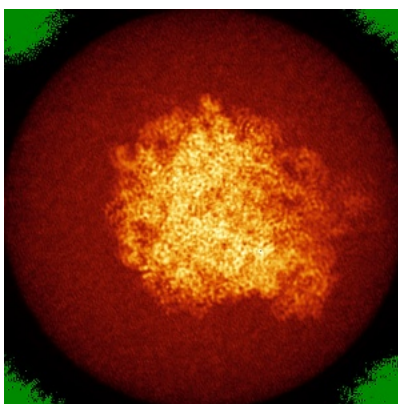
The images above show the largest variance slices of the map in three orthogonal directions.

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

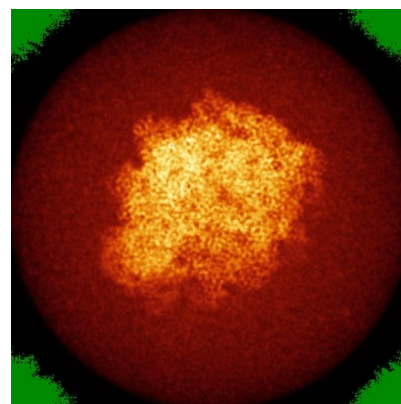
6.4.1 Primary map



X

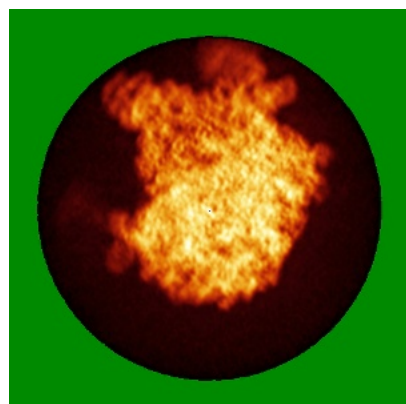


Y

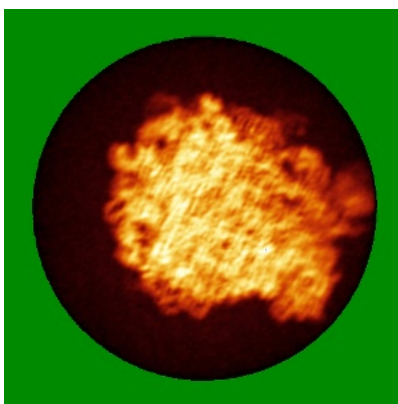


Z

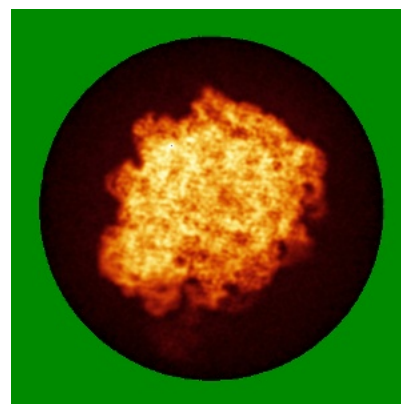
6.4.2 Raw map



X



Y

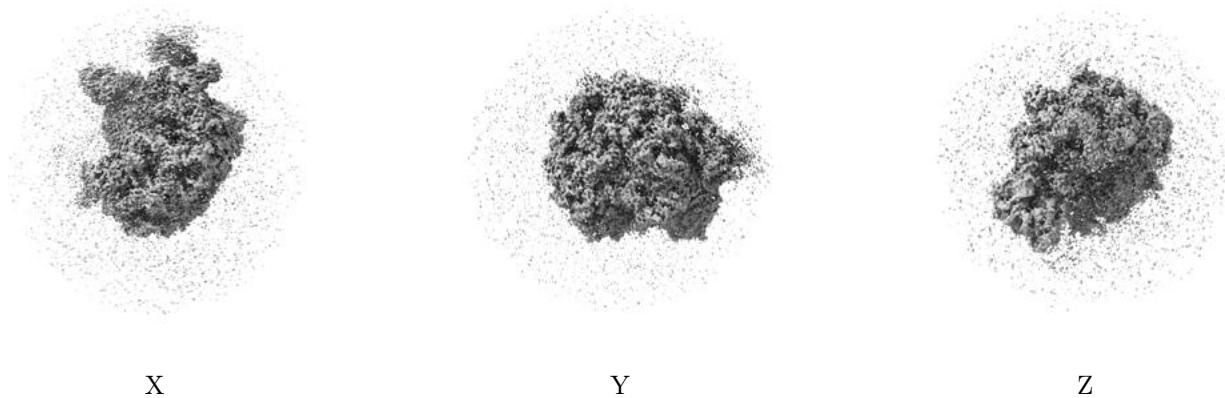


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

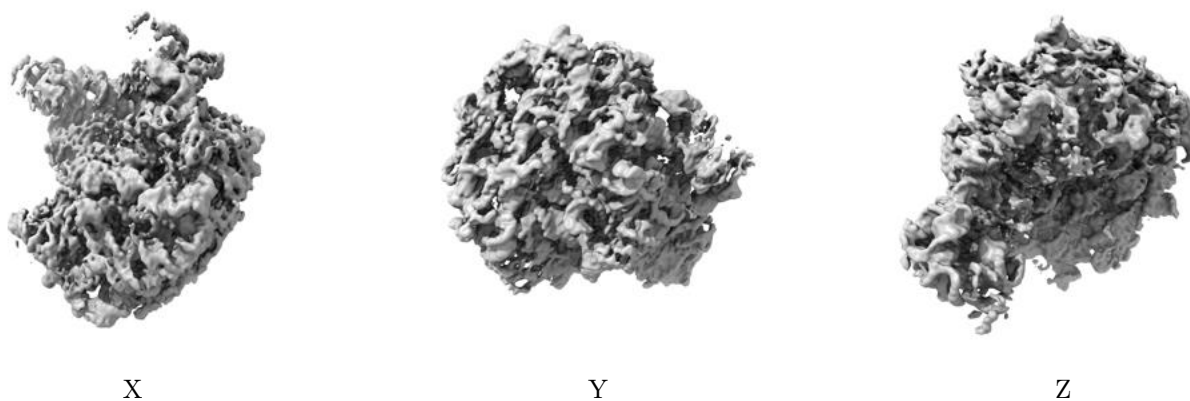
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

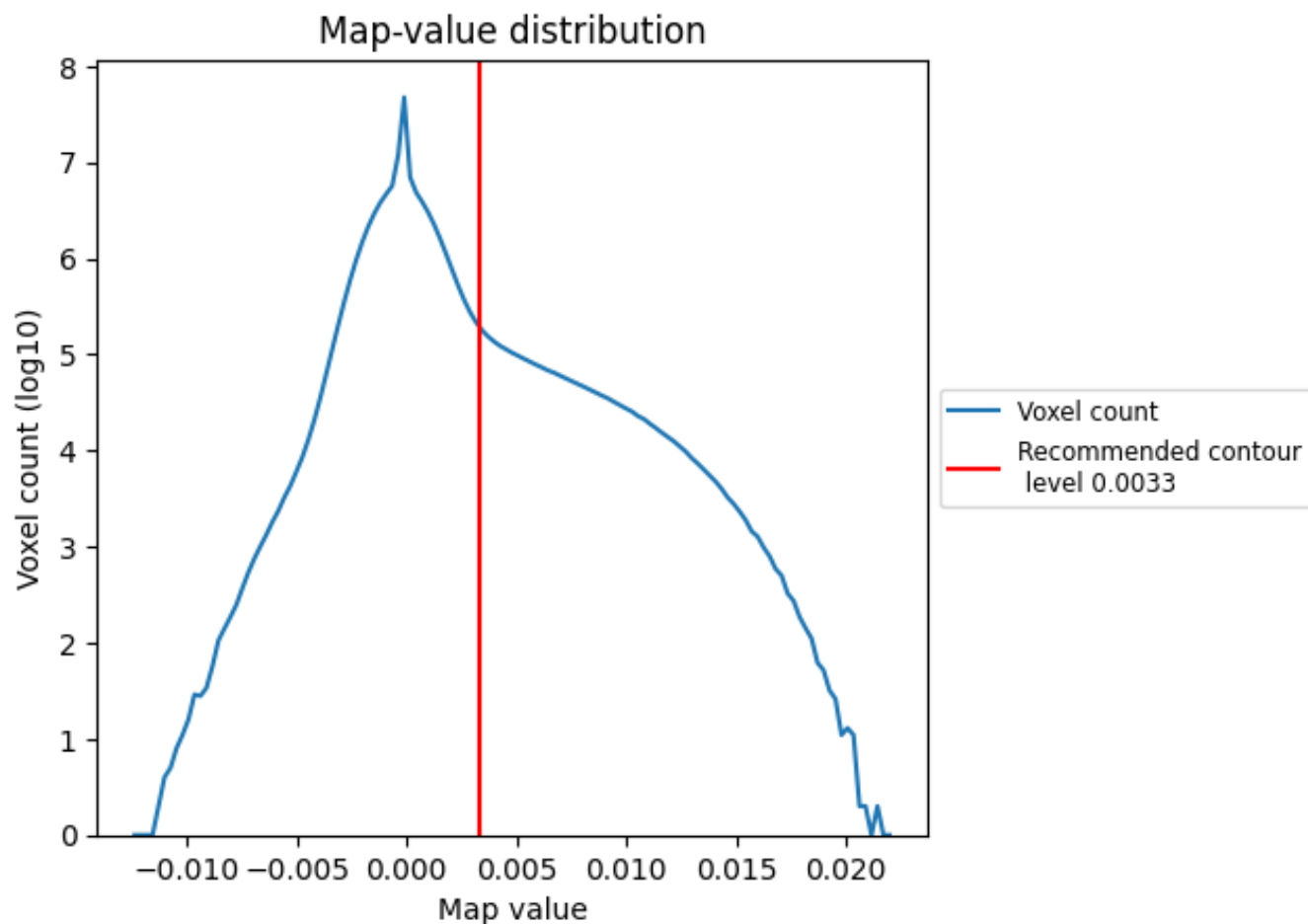
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

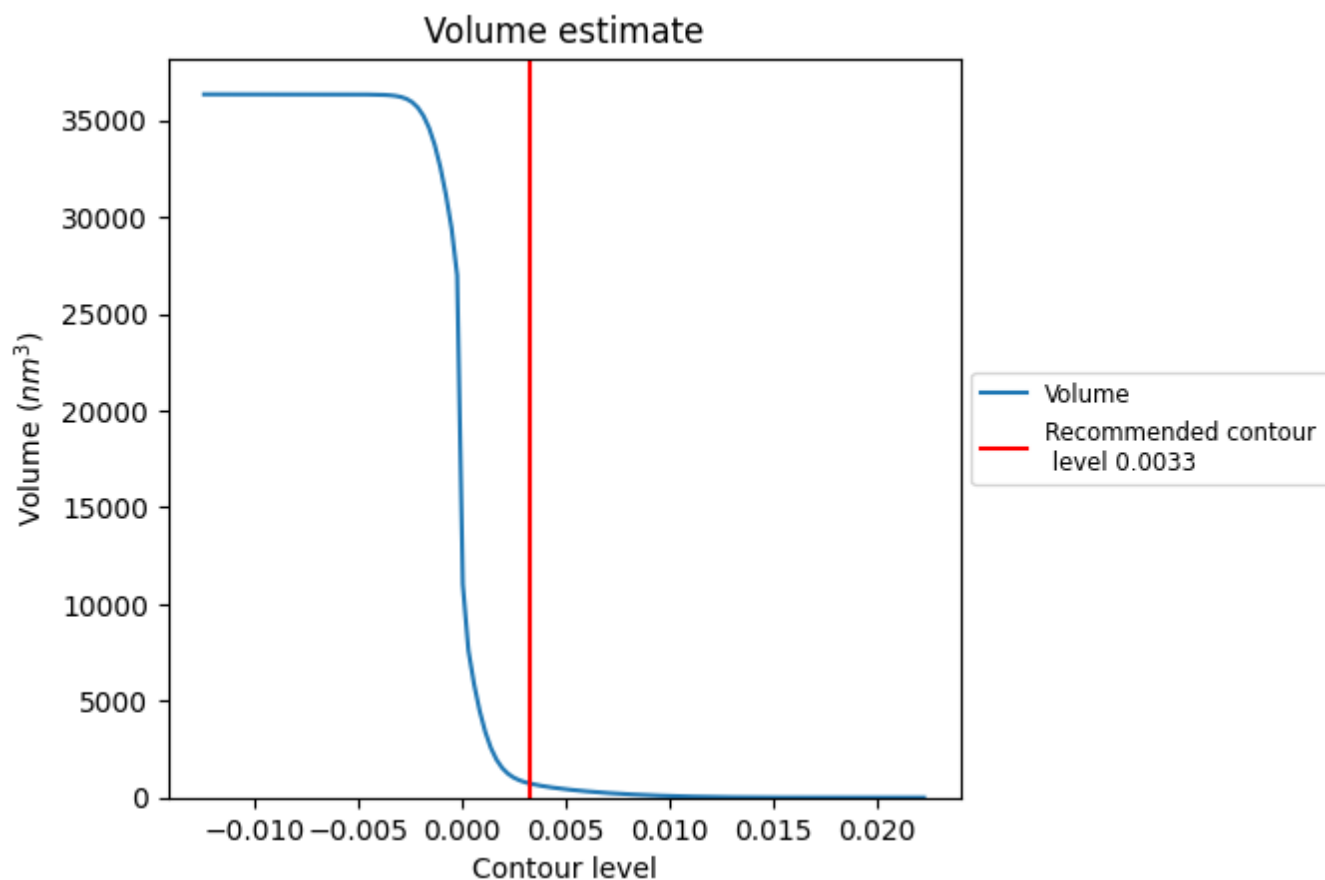
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

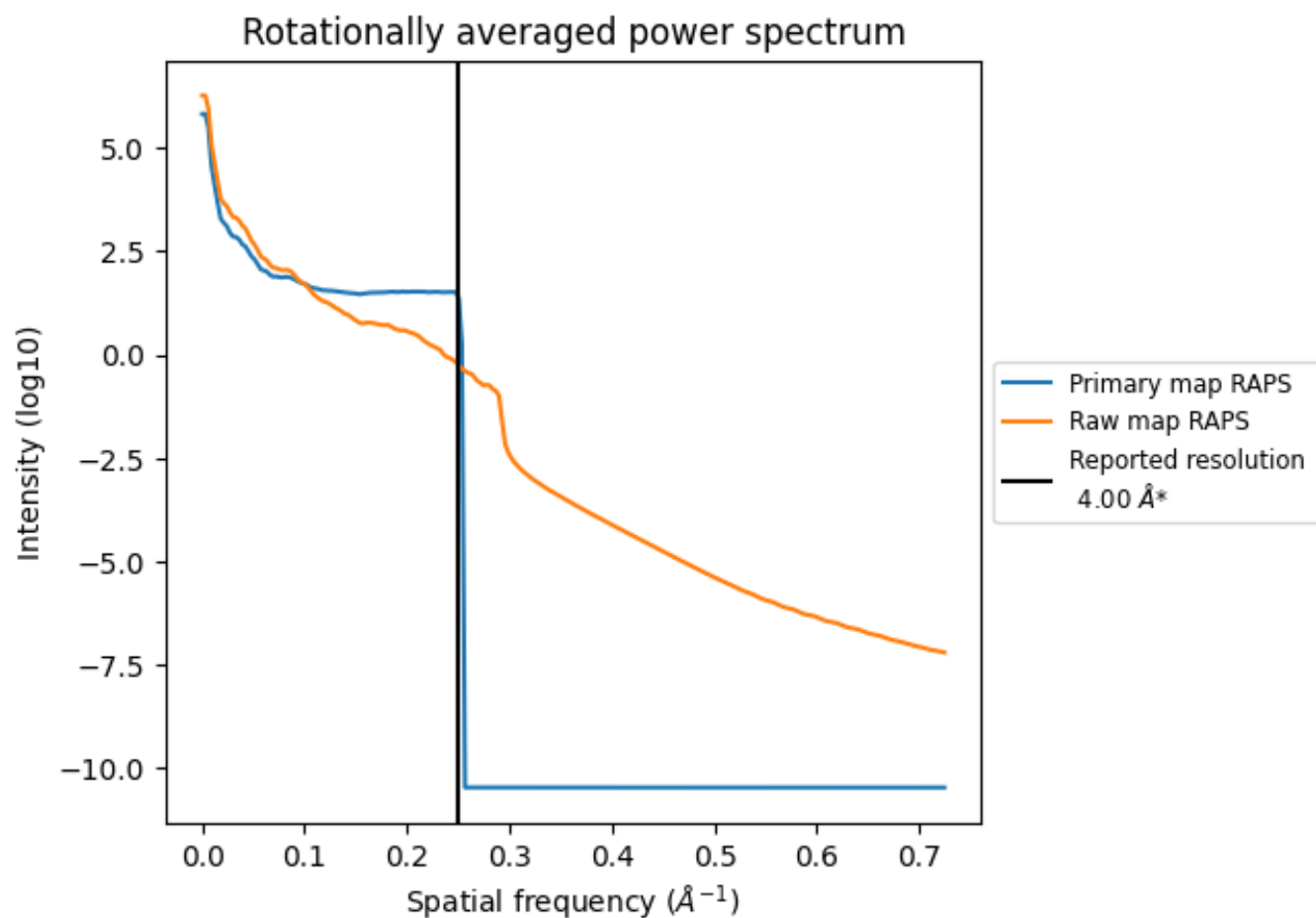
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 723 nm³; this corresponds to an approximate mass of 653 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 ⓘ

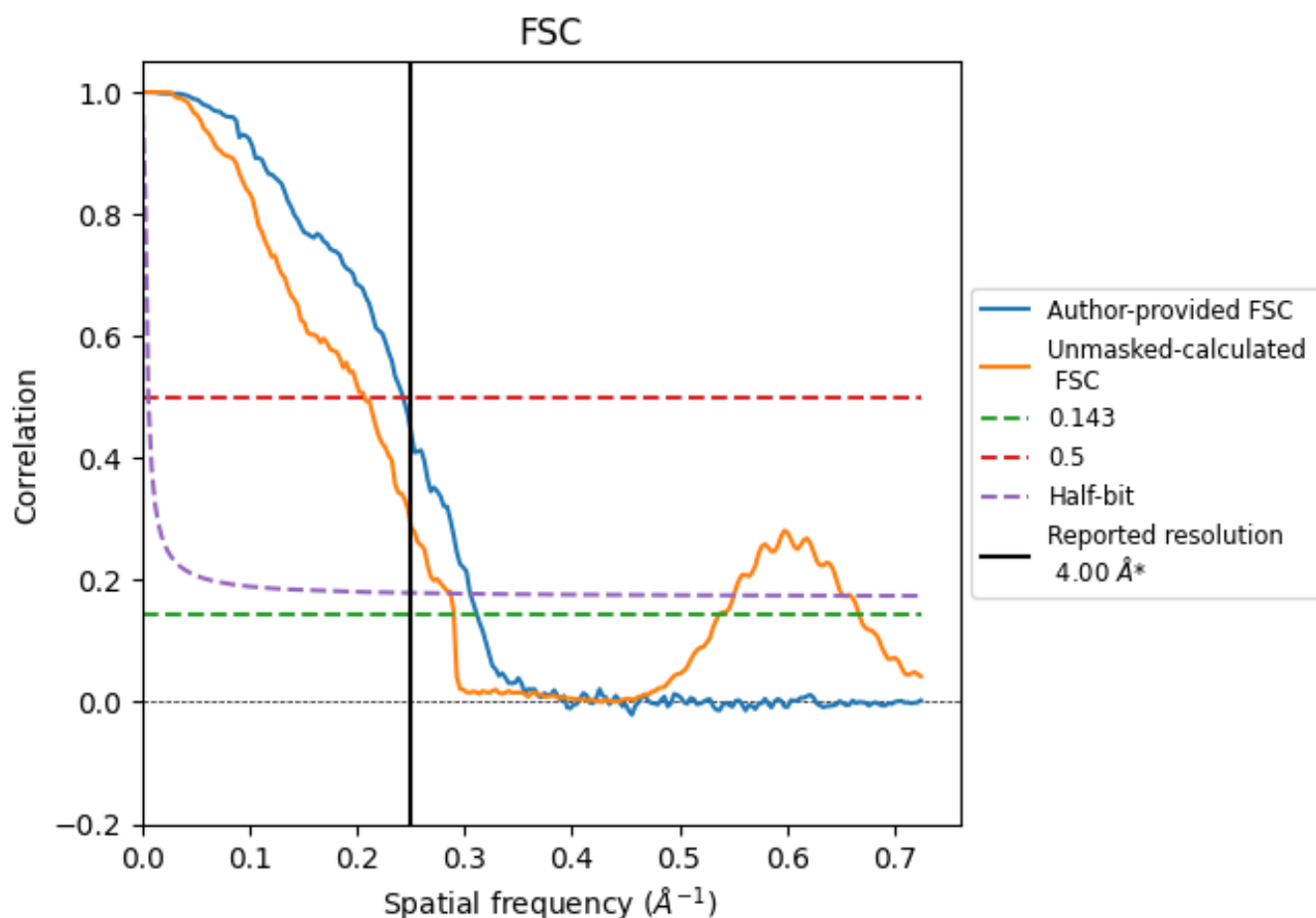


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

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 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.21	4.12	3.27
Unmasked-calculated*	3.45	4.83	3.48

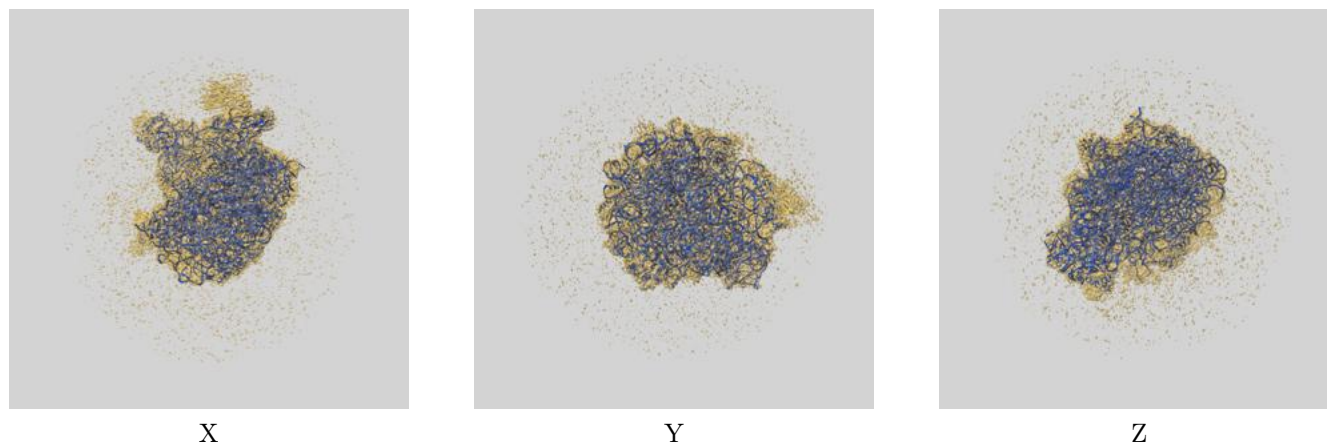
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.21 differs from the reported value 4.0 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 4.0 by more than 10 %

9 Map-model fit [i](#)

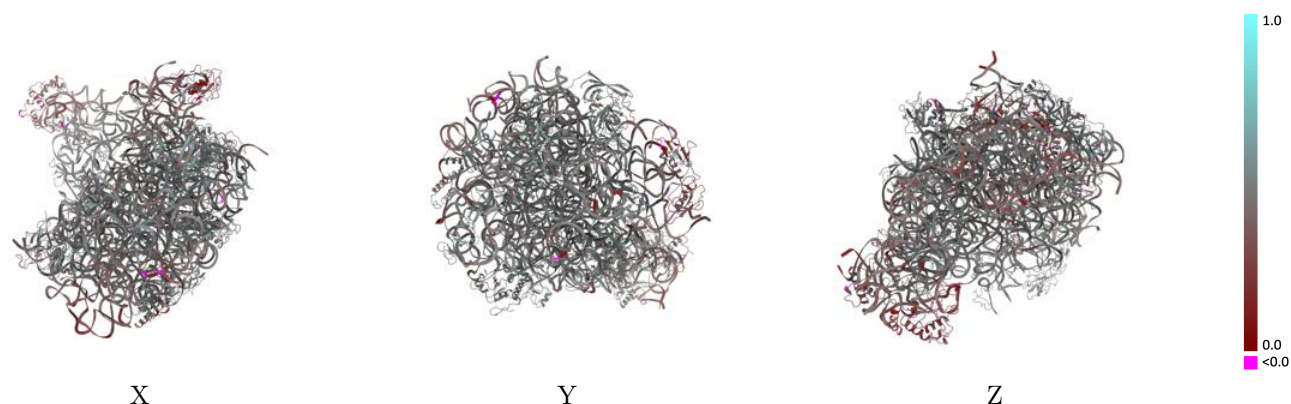
This section contains information regarding the fit between EMDB map EMD-61605 and PDB model 9JMK. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



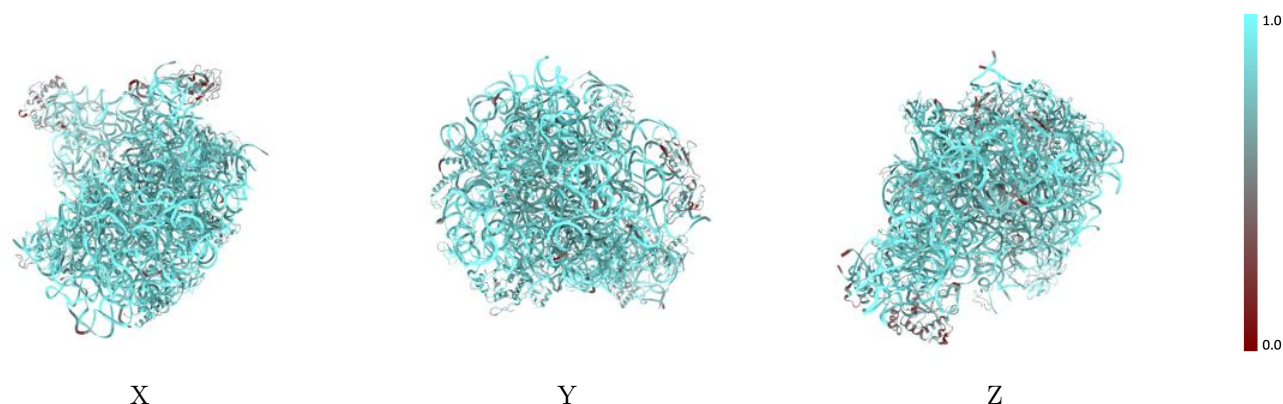
The images above show the 3D surface view of the map at the recommended contour level 0.0033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



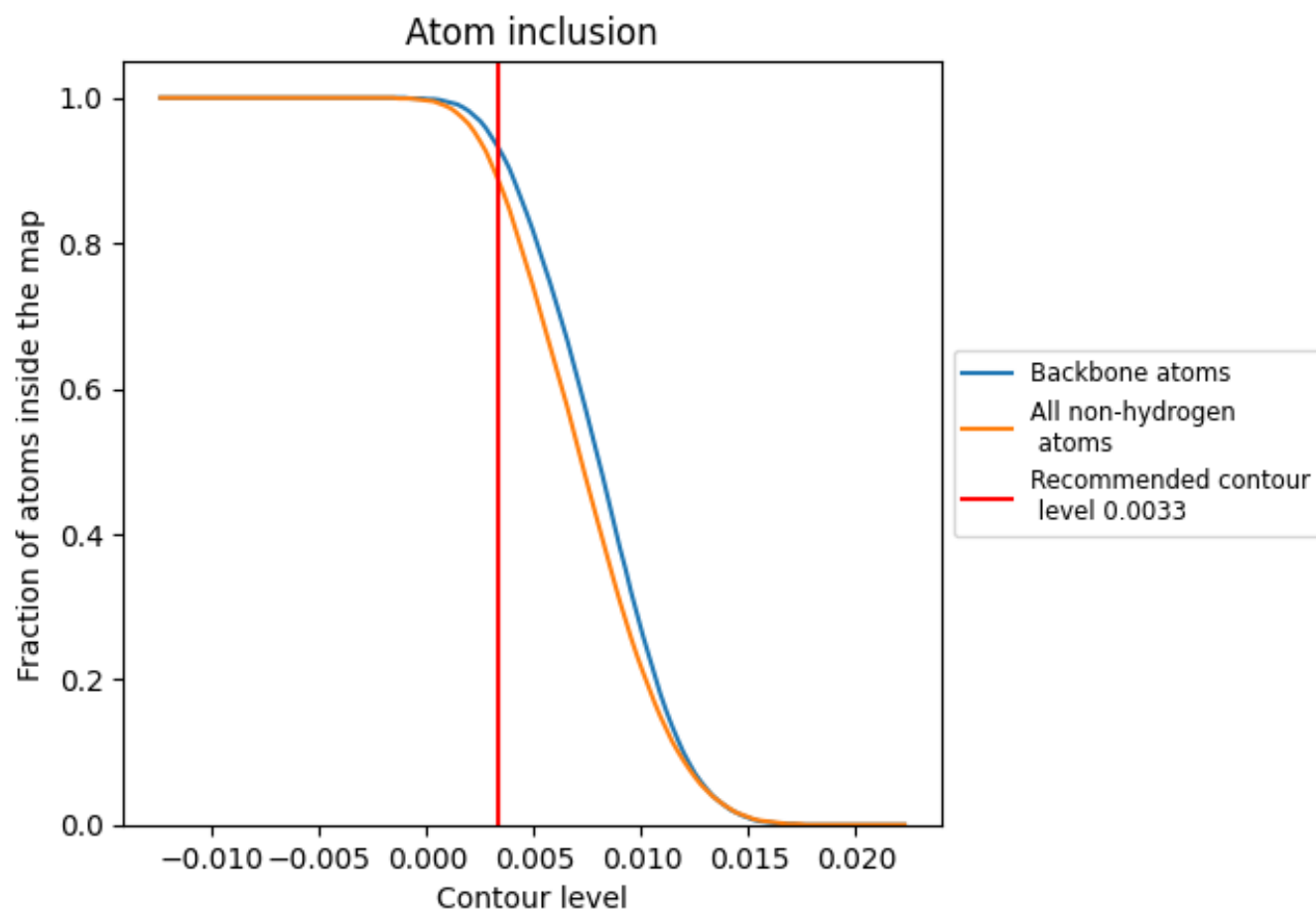
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0033).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.0033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.4510
0	 0.8600	 0.4830
1	 0.8760	 0.4920
2	 0.8420	 0.5050
3	 0.8660	 0.5120
A	 0.9310	 0.4520
B	 0.8850	 0.3900
C	 0.7960	 0.4690
D	 0.8510	 0.4900
E	 0.8290	 0.4870
F	 0.5200	 0.2800
G	 0.5240	 0.2900
H	 0.5670	 0.3460
J	 0.8640	 0.5080
K	 0.8000	 0.4580
L	 0.8420	 0.4690
N	 0.8860	 0.5010
O	 0.7550	 0.4030
P	 0.8410	 0.4760
Q	 0.8930	 0.5010
R	 0.8850	 0.5070
S	 0.8290	 0.4970
T	 0.8170	 0.4570
U	 0.8920	 0.4810
V	 0.7260	 0.4220
W	 0.8370	 0.5060
X	 0.8450	 0.4930
Y	 0.8210	 0.4450
Z	 0.8540	 0.4960

