



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:37 AM UTC

PDB ID : 8FN2 / pdb_00008fn2
EMDB ID : EMD-29304
Title : The structure of a 50S ribosomal subunit in the Lyme disease pathogen *Borrelia burgdorferi*
Authors : Sharma, M.R.; Manjari, S.R.; Agrawal, E.K.; Keshavan, P.; Koripella, R.K.; Majumdar, S.; Marcinkiewicz, A.L.; Lin, Y.P.; Agrawal, R.K.; Banavali, N.K.
Deposited on : 2022-12-26
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

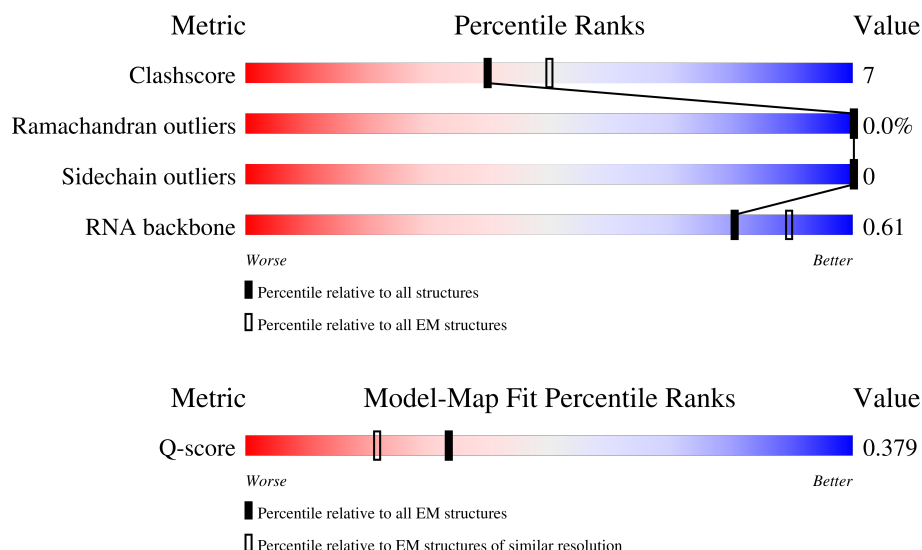
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



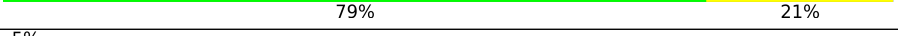
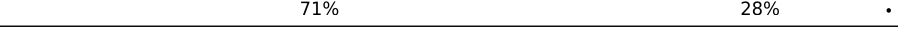
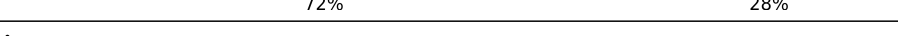
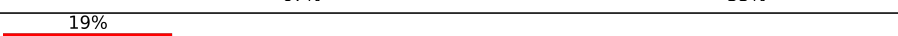
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	2929	
2	B	112	
3	D	277	

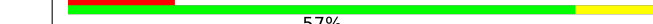
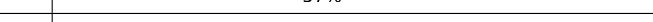
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Mol	Chain	Length	Quality of chain
4	E	206	
5	F	209	
6	G	182	
7	H	180	
8	I	148	
9	J	162	
10	K	139	
11	L	145	
12	M	122	
13	N	145	
14	O	138	
15	P	121	
16	Q	119	
17	R	117	
18	S	114	
19	T	103	
20	U	115	
21	V	98	
22	W	101	
23	X	181	
24	Y	74	
25	Z	91	
26	a	65	
27	b	100	
28	c	81	

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Mol	Chain	Length	Quality of chain
29	d	59	 73% 27% 12%
30	e	51	 57% 43% 12%
31	f	50	 92% 8%
32	g	66	 85% 15% 5%
33	h	37	 78% 22%
34	i	46	 67% 28% 7%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 89742 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2762	Total	C	N	O	P	0	0
			59248	26483	10866	19137	2762		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2398	1071	434	781	112		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	277	Total	C	N	O	S	0	0
			2156	1354	414	383	5		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	206	Total	C	N	O	S	0	0
			1564	995	278	286	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	209	Total	C	N	O	S	0	0
			1658	1056	301	299	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	182	Total	C	N	O	S	0	0
			1439	930	240	265	4		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	180	Total	C	N	O	S	0	0
			1405	895	249	259	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	63	Total	C	N	O	S	0	0
			411	253	76	81	1		

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	132	Total	C	N	O	0	0
			528	264	132	132		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	68	Total	C	N	O	0	0
			272	136	68	68		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	145	Total	C	N	O	S	0	0
			1171	756	211	202	2		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	122	Total	C	N	O	S	0	0
			942	593	174	170	5		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	145	Total	C	N	O	S	0	0
			1129	716	210	201	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	138	Total	C	N	O	S	0	0
			1092	693	204	188	7		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	121	Total	C	N	O	S	0	0
			1004	643	193	164	4		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	119	Total	C	N	O	S	0	0
			968	613	184	170	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	117	Total	C	N	O	S	0	0
			951	613	174	161	3		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	114	Total	C	N	O	S	0	0
			943	597	189	155	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	40	ARG	UNK	conflict	UNP O51206

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	103	Total	C	N	O	S	0	0
			859	552	148	157	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	115	Total	C	N	O	S	0	0
			918	574	180	158	6		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	98	Total	C	N	O	S	0	0
			784	507	134	140	3		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	101	Total	C	N	O	S	0	0
			800	501	155	140	4		

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	181	Total	C	N	O	S	0	0
			1432	912	245	273	2		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	74	Total	C	N	O	0	0
			571	359	112	100		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	91	Total	C	N	O	S	0	0
			705	452	135	115	3		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	65	Total	C	N	O	S	0	0
			553	352	102	95	4		

- Molecule 27 is a protein called 50S ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	100	Total	C	N	O	S	0	0
			814	518	158	133	5		

- Molecule 28 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	58	Total	C	N	O	S	0	0
			466	300	77	87	2		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	59	Total	C	N	O	S	0	0
			484	300	99	80	5		

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	51	Total	C	N	O	S	0	0
			425	266	80	76	3		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			422	260	95	64	3		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	66	Total	C	N	O	S	0	0
			548	346	111	88	3		

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	37	Total	C	N	O	S	0	0
			305	192	63	46	4		

- Molecule 34 is a protein called 50S ribosomal protein bL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	46	Total	C	N	O	S	0	0
			375	236	72	65	2		

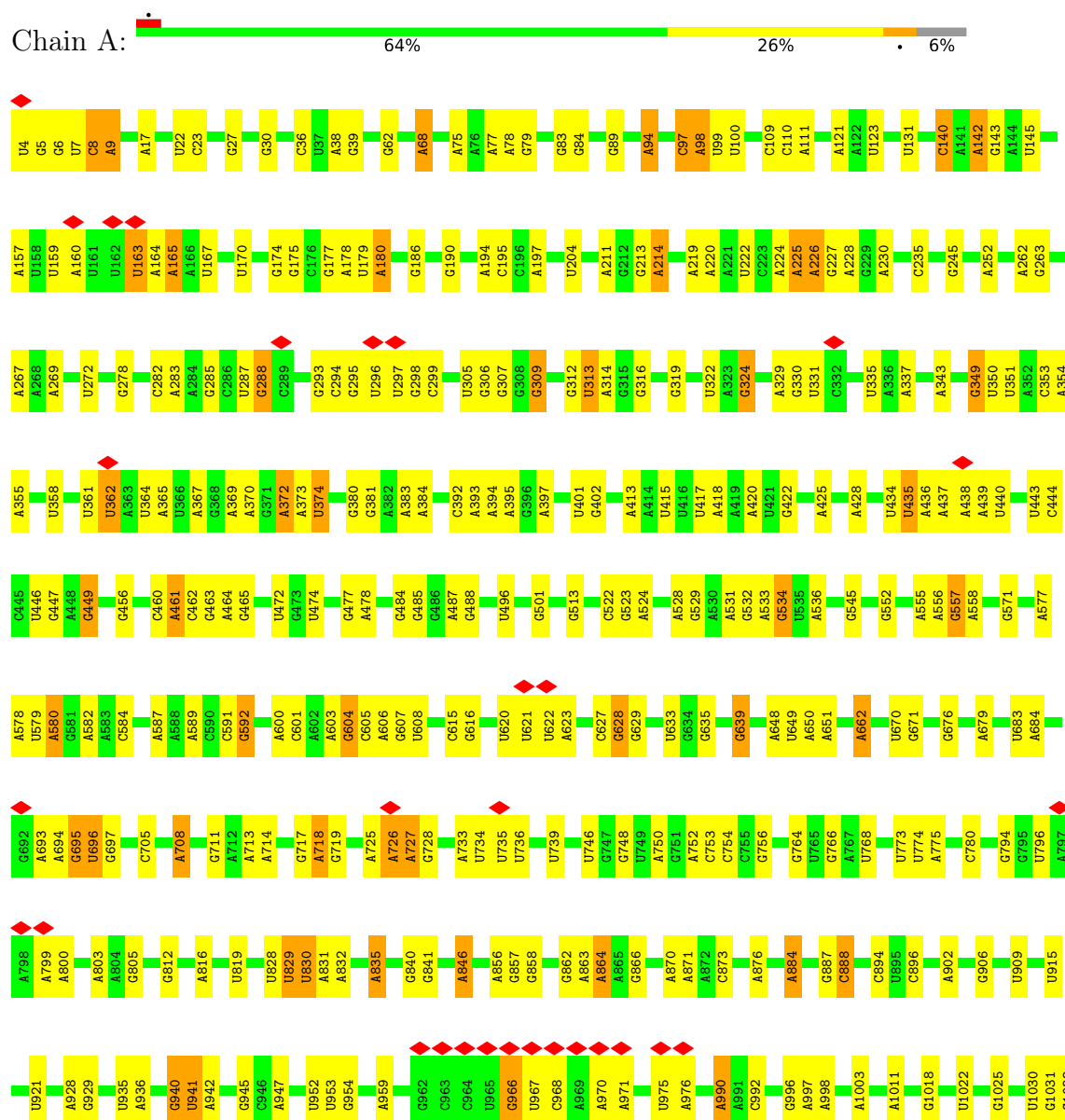
- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
35	d	1	Total	Zn	0
			1	1	
35	h	1	Total	Zn	0
			1	1	

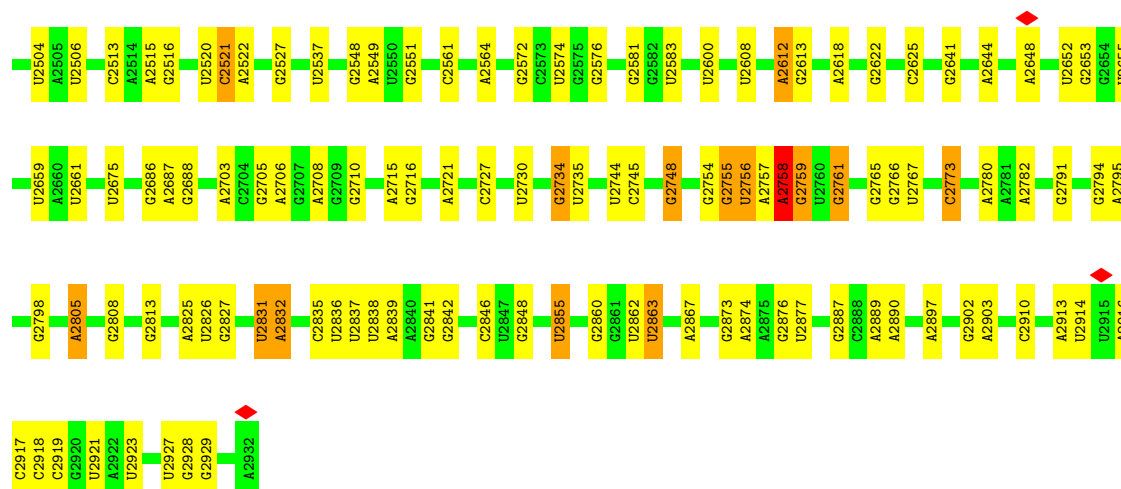
3 Residue-property plots

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

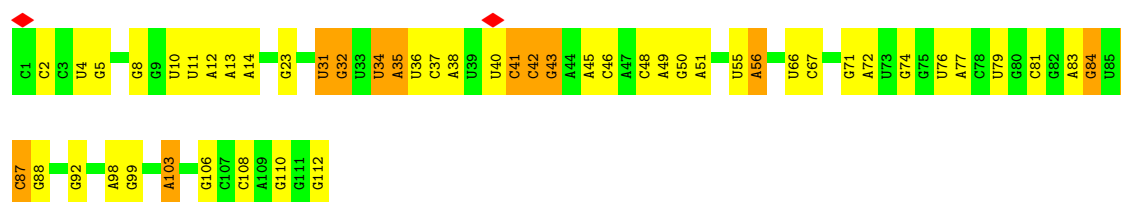
• Molecule 1: 23S ribosomal RNA



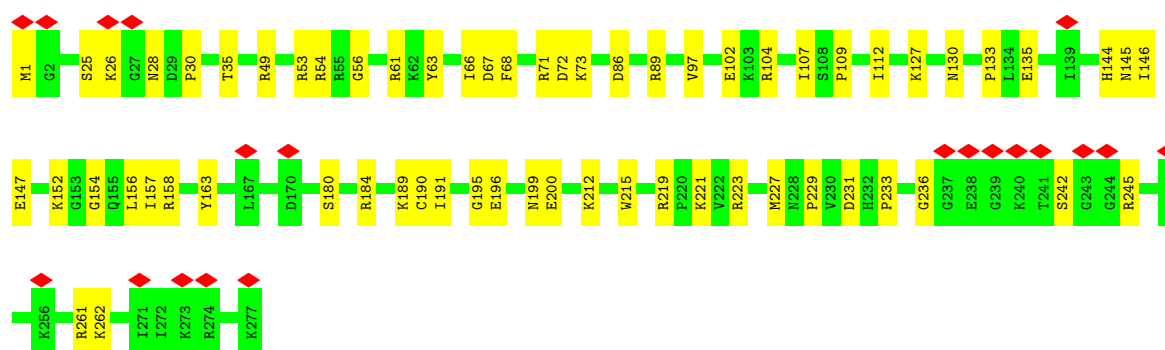
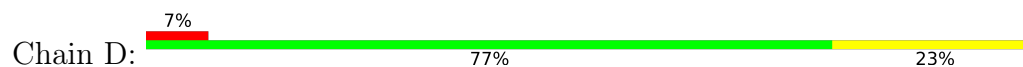




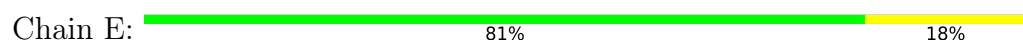
• Molecule 2: 5S ribosomal RNA

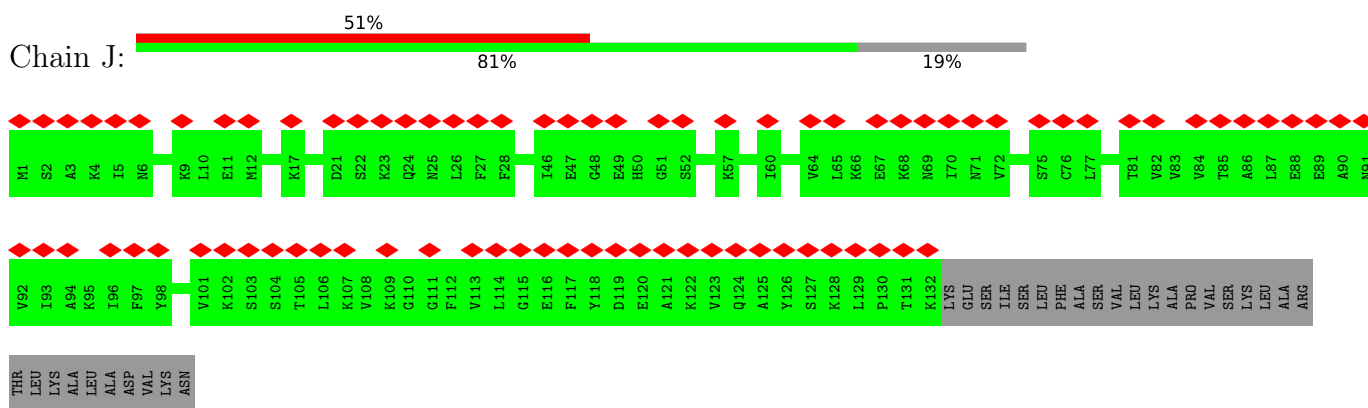


• Molecule 3: 50S ribosomal protein L2

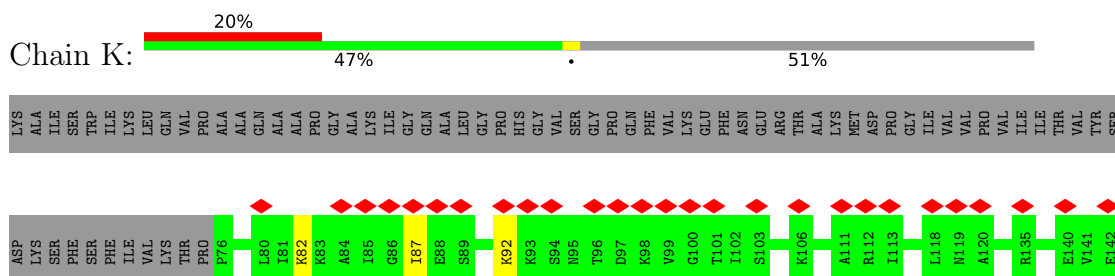


• Molecule 4: 50S ribosomal protein L3

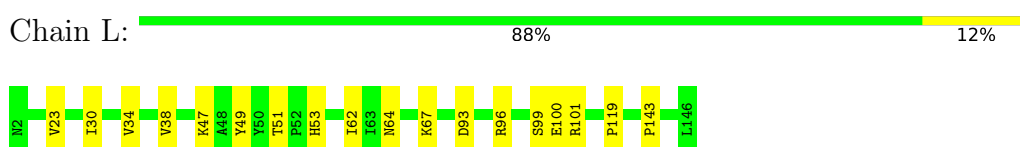




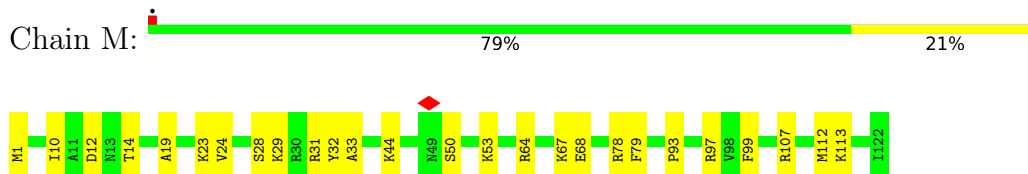
- Molecule 10: 50S ribosomal protein L11



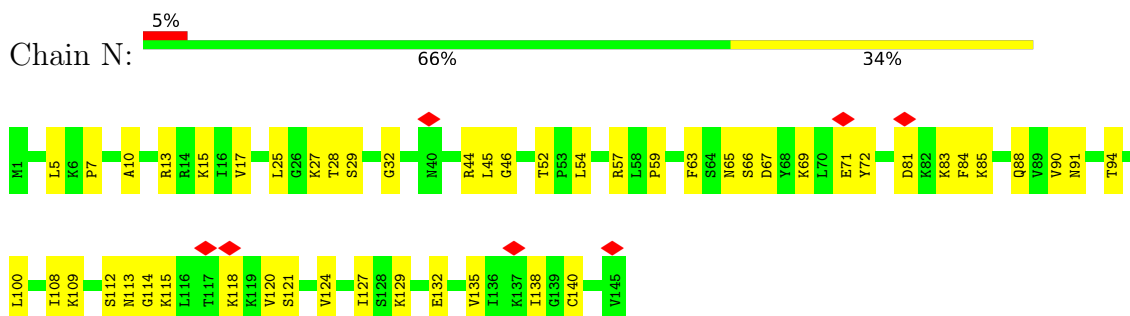
- Molecule 11: 50S ribosomal protein L13



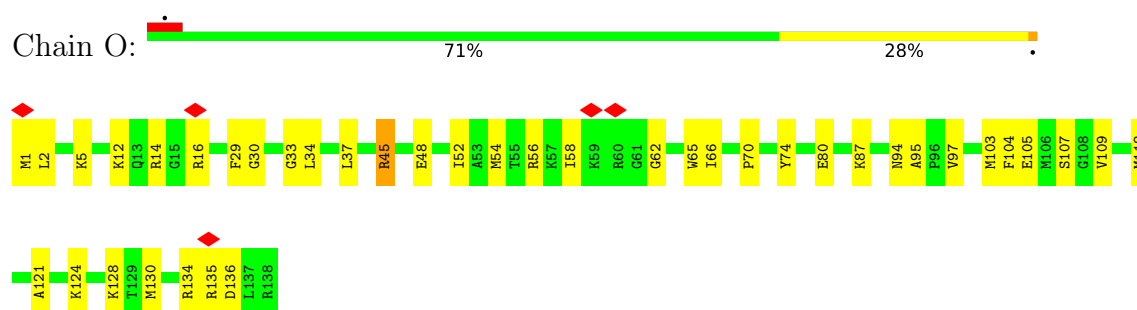
- Molecule 12: 50S ribosomal protein L14



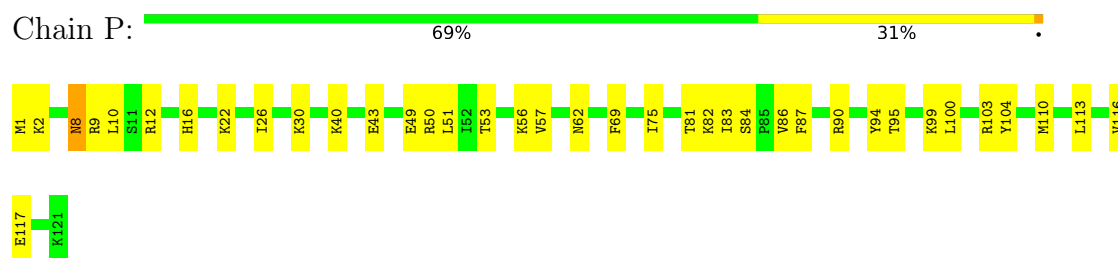
- Molecule 13: 50S ribosomal protein L15



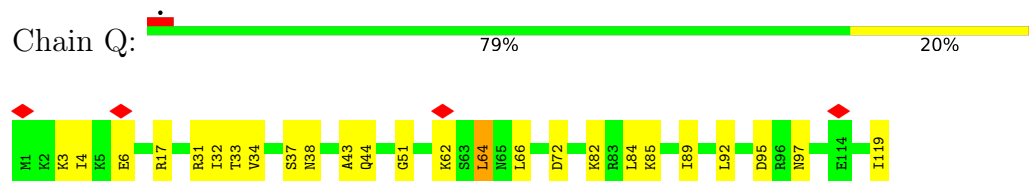
- Molecule 14: 50S ribosomal protein L16



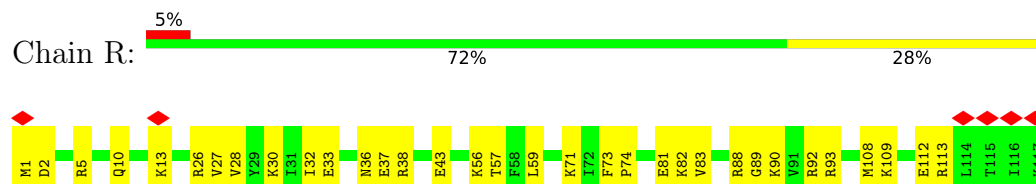
- Molecule 15: 50S ribosomal protein L17



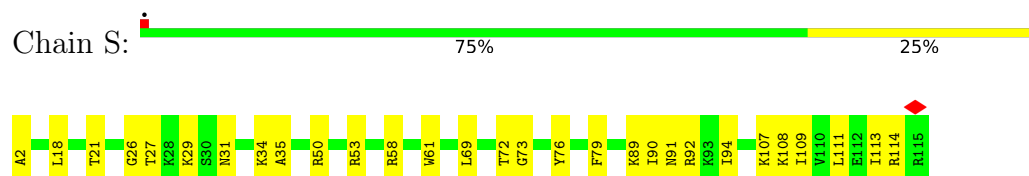
- Molecule 16: 50S ribosomal protein L18



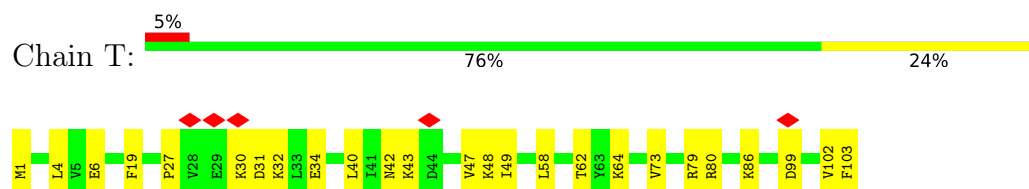
- Molecule 17: 50S ribosomal protein L19



- Molecule 18: 50S ribosomal protein L20

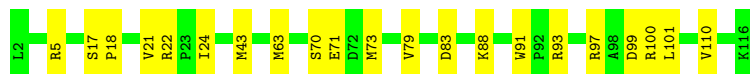


- Molecule 19: 50S ribosomal protein L21



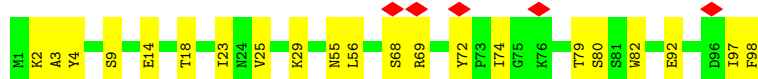
- Molecule 20: 50S ribosomal protein L22

Chain U:  82% 18%



- Molecule 21: 50S ribosomal protein L23

Chain V:  5% 79% 21%



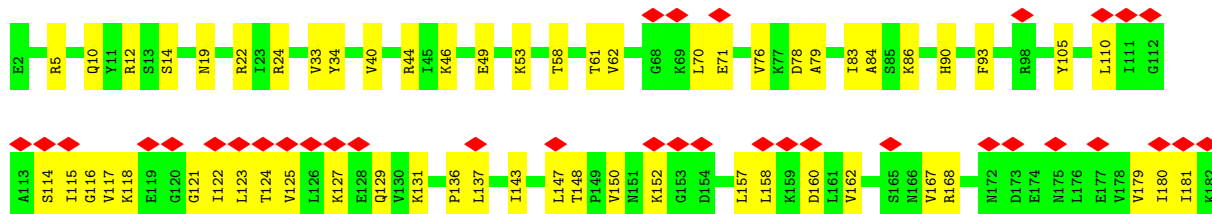
- Molecule 22: 50S ribosomal protein L24

Chain W:  13% 67% 33%



- Molecule 23: 50S ribosomal protein L25

Chain X:  19% 68% 32%



- Molecule 24: 50S ribosomal protein L27

Chain Y:  86% 14%

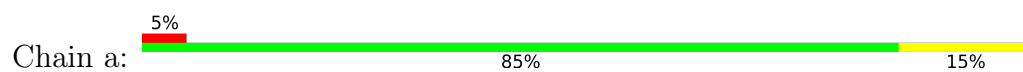


- Molecule 25: 50S ribosomal protein L28

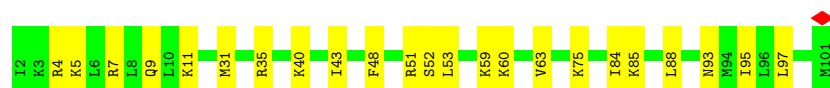
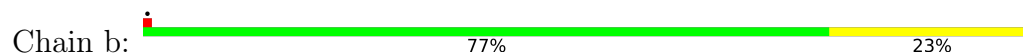
Chain Z:  73% 27%



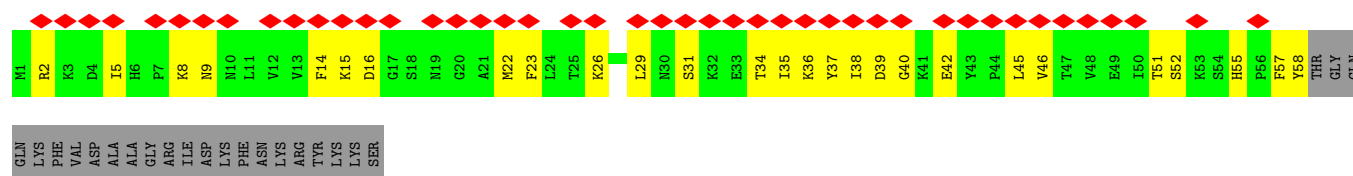
- Molecule 26: 50S ribosomal protein L29



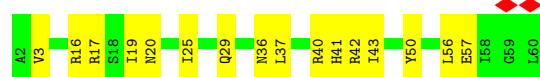
- Molecule 27: 50S ribosomal protein uL30



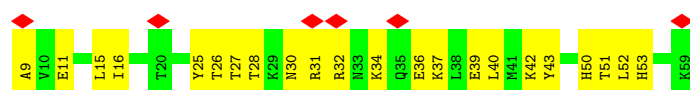
- Molecule 28: 50S ribosomal protein L31 type B



- Molecule 29: 50S ribosomal protein L32



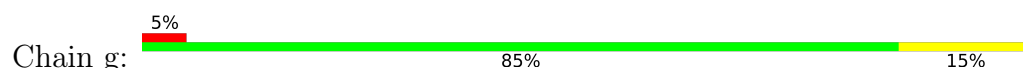
- Molecule 30: 50S ribosomal protein L33

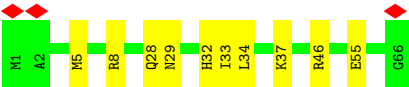


- Molecule 31: 50S ribosomal protein L34

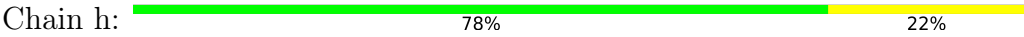


- Molecule 32: 50S ribosomal protein L35

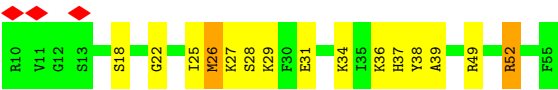




• Molecule 33: 50S ribosomal protein L36



• Molecule 34: 50S ribosomal protein bL38



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12449	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67.527	Depositor
Minimum defocus (nm)	820	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.783	Depositor
Minimum map value	-0.309	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	493.245, 493.245, 493.245	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0961, 1.0961, 1.0961	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.05	0/66391	0.31	93/103525 (0.1%)
2	B	0.05	0/2684	0.12	0/4183
3	D	0.49	0/2196	0.55	0/2935
4	E	0.50	0/1588	0.55	0/2122
5	F	0.48	0/1682	0.52	0/2249
6	G	0.32	0/1460	0.53	1/1955 (0.1%)
7	H	0.33	0/1422	0.44	0/1903
8	I	0.30	0/416	0.44	0/548
9	J	0.11	0/527	0.21	0/657
10	K	0.08	0/271	0.16	0/337
11	L	0.52	0/1197	0.48	0/1612
12	M	0.55	0/951	0.55	0/1276
13	N	0.46	0/1142	0.59	0/1515
14	O	0.53	0/1110	0.74	3/1480 (0.2%)
15	P	0.52	0/1020	0.62	1/1353 (0.1%)
16	Q	0.34	0/979	0.57	1/1299 (0.1%)
17	R	0.53	0/962	0.64	0/1280
18	S	0.62	0/954	0.61	0/1264
19	T	0.51	0/872	0.55	0/1163
20	U	0.54	0/931	0.58	0/1245
21	V	0.42	0/796	0.54	0/1065
22	W	0.41	0/803	0.55	0/1059
23	X	0.30	0/1451	0.45	0/1955
24	Y	0.52	0/577	0.53	0/760
25	Z	0.51	0/713	0.55	0/943
26	a	0.43	0/559	0.64	0/739
27	b	0.52	0/818	0.58	0/1079
28	c	0.25	0/476	0.54	0/640
29	d	0.52	0/492	0.52	0/654
30	e	0.44	0/429	0.69	0/568
31	f	0.54	0/425	0.64	0/551
32	g	0.57	0/554	0.63	1/726 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.54	0/306	0.55	0/400
34	i	0.56	0/381	1.24	5/502 (1.0%)
All	All	0.26	0/97535	0.39	105/145542 (0.1%)

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	E	0	1

There are no bond length outliers.

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1559	G	OP1-P-OP2	-13.54	78.99	119.60
1	A	1558	C	OP2-P-O3'	-12.30	71.09	108.00
34	i	52	ARG	CA-CB-CG	11.34	136.78	114.10
1	A	1559	G	O5'-P-OP1	-9.76	78.71	108.00
1	A	1558	C	OP1-P-O3'	9.66	136.97	108.00
1	A	531	A	OP2-P-O3'	-9.24	80.28	108.00
1	A	1609	U	OP1-P-O3'	-9.23	80.32	108.00
1	A	1286	A	OP1-P-O3'	-9.14	80.59	108.00
1	A	1519	U	OP1-P-O3'	-9.12	80.65	108.00
1	A	1619	G	OP1-P-O3'	-9.09	80.72	108.00
1	A	349	G	OP2-P-O3'	-9.07	80.78	108.00
1	A	177	G	OP1-P-O3'	-9.07	80.79	108.00
1	A	1610	G	OP2-P-O3'	-9.06	80.83	108.00
1	A	1736	G	OP1-P-O3'	-9.04	80.88	108.00
1	A	2836	U	OP2-P-O3'	-9.04	80.88	108.00
1	A	159	U	OP1-P-O3'	-9.01	80.98	108.00
1	A	1560	A	OP2-P-O3'	-8.98	81.06	108.00
1	A	1674	A	OP1-P-O3'	-8.97	81.10	108.00
1	A	1586	G	OP2-P-O3'	-8.95	81.15	108.00
1	A	1500	A	OP1-P-O3'	-8.94	81.19	108.00
1	A	1584	A	OP1-P-O3'	-8.94	81.19	108.00
1	A	1576	A	OP1-P-O3'	-8.93	81.23	108.00
1	A	1520	A	OP1-P-O3'	-8.92	81.23	108.00
1	A	272	U	OP1-P-O3'	-8.92	81.24	108.00
1	A	1585	A	OP1-P-O3'	-8.91	81.27	108.00
1	A	1299	U	OP1-P-O3'	-8.91	81.27	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1633	A	OP1-P-O3'	-8.90	81.29	108.00
1	A	140	C	OP2-P-O3'	-8.90	81.31	108.00
1	A	157	A	OP1-P-O3'	-8.90	81.31	108.00
1	A	1563	A	OP1-P-O3'	-8.89	81.32	108.00
1	A	2447	U	OP1-P-O3'	-8.89	81.32	108.00
1	A	1643	G	OP1-P-O3'	-8.88	81.36	108.00
1	A	1552	U	OP1-P-O3'	-8.88	81.36	108.00
1	A	180	A	OP1-P-O3'	-8.85	81.44	108.00
1	A	1697	A	OP1-P-O3'	-8.85	81.45	108.00
1	A	1559	G	OP1-P-O3'	-8.84	81.47	108.00
1	A	1626	G	OP1-P-O3'	-8.84	81.47	108.00
1	A	2758	A	OP2-P-O3'	-8.83	81.50	108.00
1	A	324	G	OP1-P-O3'	-8.83	81.52	108.00
1	A	1567	U	OP1-P-O3'	-8.82	81.53	108.00
1	A	1287	G	OP2-P-O3'	-8.82	81.55	108.00
1	A	1300	G	OP1-P-O3'	-8.82	81.55	108.00
1	A	1602	U	OP2-P-O3'	-8.80	81.60	108.00
1	A	1490	G	OP1-P-O3'	-8.78	81.65	108.00
1	A	1618	G	OP1-P-O3'	-8.78	81.65	108.00
1	A	1580	C	OP2-P-O3'	-8.75	81.74	108.00
1	A	1587	A	OP2-P-O3'	-8.71	81.87	108.00
1	A	1587	A	OP1-P-O3'	-8.71	81.87	108.00
1	A	1681	A	OP2-P-O3'	-8.69	81.92	108.00
1	A	1681	A	OP1-P-O3'	-8.69	81.93	108.00
1	A	1559	G	OP2-P-O3'	-8.68	81.96	108.00
1	A	2734	G	OP2-P-O3'	-8.67	81.99	108.00
1	A	1580	C	OP1-P-O3'	-8.64	82.09	108.00
1	A	2758	A	OP1-P-O3'	-8.59	82.22	108.00
1	A	1300	G	OP2-P-O3'	-8.46	82.62	108.00
1	A	1618	G	OP2-P-O3'	-8.44	82.68	108.00
1	A	324	G	OP2-P-O3'	-8.43	82.72	108.00
1	A	1490	G	OP2-P-O3'	-8.41	82.77	108.00
1	A	1602	U	OP1-P-O3'	-8.36	82.92	108.00
1	A	1697	A	OP2-P-O3'	-8.34	82.97	108.00
1	A	2447	U	OP2-P-O3'	-8.32	83.03	108.00
1	A	140	C	OP1-P-O3'	-8.30	83.09	108.00
1	A	1287	G	OP1-P-O3'	-8.30	83.09	108.00
1	A	2734	G	OP1-P-O3'	-8.25	83.24	108.00
1	A	1643	G	OP2-P-O3'	-8.19	83.43	108.00
1	A	1552	U	OP2-P-O3'	-8.16	83.53	108.00
1	A	180	A	OP2-P-O3'	-8.14	83.57	108.00
1	A	1563	A	OP2-P-O3'	-8.12	83.63	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	A	OP2-P-O3'	-8.12	83.64	108.00
1	A	272	U	OP2-P-O3'	-8.07	83.78	108.00
1	A	1674	A	OP2-P-O3'	-8.07	83.80	108.00
1	A	1299	U	OP2-P-O3'	-8.05	83.83	108.00
1	A	1520	A	OP2-P-O3'	-8.04	83.89	108.00
1	A	1633	A	OP2-P-O3'	-8.02	83.94	108.00
1	A	1584	A	OP2-P-O3'	-7.98	84.06	108.00
1	A	1586	G	OP1-P-O3'	-7.96	84.12	108.00
1	A	1585	A	OP2-P-O3'	-7.96	84.12	108.00
1	A	1626	G	OP2-P-O3'	-7.93	84.22	108.00
1	A	1576	A	OP2-P-O3'	-7.86	84.41	108.00
1	A	1500	A	OP2-P-O3'	-7.85	84.46	108.00
1	A	1560	A	OP1-P-O3'	-7.79	84.62	108.00
1	A	1567	U	OP2-P-O3'	-7.77	84.70	108.00
1	A	2836	U	OP1-P-O3'	-7.66	85.02	108.00
1	A	1610	G	OP1-P-O3'	-7.63	85.10	108.00
1	A	1736	G	OP2-P-O3'	-7.59	85.22	108.00
1	A	177	G	OP2-P-O3'	-7.57	85.28	108.00
1	A	1286	A	OP2-P-O3'	-7.55	85.35	108.00
1	A	159	U	OP2-P-O3'	-7.55	85.35	108.00
1	A	349	G	OP1-P-O3'	-7.47	85.59	108.00
34	i	26	MET	CA-CB-CG	7.43	128.96	114.10
1	A	1609	U	OP2-P-O3'	-7.37	85.90	108.00
1	A	1519	U	OP2-P-O3'	-7.31	86.06	108.00
1	A	1619	G	OP2-P-O3'	-7.29	86.13	108.00
1	A	531	A	OP1-P-O3'	-7.26	86.22	108.00
6	G	29	MET	CB-CG-SD	7.23	134.39	112.70
1	A	1559	G	O5'-P-OP2	7.15	129.44	108.00
34	i	52	ARG	CG-CD-NE	7.00	127.39	112.00
32	g	55	GLU	CB-CG-CD	6.05	122.89	112.60
14	O	80	GLU	CA-CB-CG	5.99	126.07	114.10
14	O	45	ARG	CA-CB-CG	-5.86	102.38	114.10
16	Q	64	LEU	CD1-CG-CD2	-5.41	98.91	110.80
15	P	8	ASN	N-CA-C	-5.25	106.78	114.39
34	i	25	ILE	CA-C-N	-5.21	114.50	122.62
34	i	25	ILE	C-N-CA	-5.21	114.50	122.62
14	O	16	ARG	CA-CB-CG	5.10	124.30	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	163	MET	Mainchain

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	59248	0	29718	393	0
2	B	2398	0	1205	24	0
3	D	2156	0	2261	49	0
4	E	1564	0	1651	27	0
5	F	1658	0	1752	29	0
6	G	1439	0	1512	43	0
7	H	1405	0	1494	33	0
8	I	411	0	348	8	0
9	J	528	0	146	0	0
10	K	272	0	77	2	0
11	L	1171	0	1235	13	0
12	M	942	0	1008	19	0
13	N	1129	0	1232	40	0
14	O	1092	0	1163	31	0
15	P	1004	0	1090	26	0
16	Q	968	0	1039	20	0
17	R	951	0	1037	22	0
18	S	943	0	1033	30	0
19	T	859	0	902	23	0
20	U	918	0	975	13	0
21	V	784	0	847	16	0
22	W	800	0	895	26	0
23	X	1432	0	1486	39	0
24	Y	571	0	611	6	0
25	Z	705	0	784	20	0
26	a	553	0	595	11	0
27	b	814	0	922	15	0
28	c	466	0	478	26	0
29	d	484	0	500	13	0
30	e	425	0	456	16	0
31	f	422	0	480	4	0
32	g	548	0	619	10	0
33	h	305	0	357	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	i	375	0	393	10	0
35	d	1	0	0	0	0
35	h	1	0	0	0	0
All	All	89742	0	60301	919	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 7.

All (919) 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)
14:O:34:LEU:HB2	14:O:118:MET:HE3	1.53	0.90
6:G:66:GLN:NE2	6:G:93:THR:O	2.06	0.88
17:R:90:LYS:HB2	17:R:113:ARG:HG3	1.55	0.88
13:N:81:ASP:OD1	13:N:118:LYS:NZ	2.10	0.85
7:H:121:ILE:HD11	7:H:140:LYS:HB3	1.59	0.82
13:N:44:ARG:NH1	13:N:44:ARG:O	2.13	0.82
17:R:26:ARG:HD3	17:R:43:GLU:HG2	1.60	0.81
3:D:30:PRO:HB2	3:D:35:THR:HG21	1.62	0.80
27:b:31:MET:HE1	27:b:93:ASN:HA	1.62	0.80
3:D:86:ASP:OD2	3:D:89:ARG:NH1	2.15	0.79
13:N:72:TYR:HE2	13:N:109:LYS:HB2	1.47	0.79
17:R:33:GLU:OE2	17:R:38:ARG:NH1	2.16	0.78
23:X:110:LEU:HD11	23:X:147:LEU:HG	1.66	0.78
3:D:144:HIS:ND1	3:D:195:GLY:O	2.17	0.78
32:g:32:HIS:O	32:g:34:LEU:HG	1.85	0.77
13:N:17:VAL:HG23	13:N:25:LEU:HB3	1.67	0.76
28:c:52:SER:O	28:c:55:HIS:ND1	2.18	0.76
3:D:25:SER:O	3:D:28:ASN:ND2	2.20	0.75
14:O:62:GLY:HA3	14:O:107:SER:O	1.86	0.74
15:P:56:LYS:NZ	15:P:87:PHE:O	2.20	0.74
4:E:113:LYS:O	4:E:164:ALA:HB1	1.87	0.74
3:D:26:LYS:O	3:D:28:ASN:ND2	2.20	0.74
11:L:93:ASP:OD2	11:L:101:ARG:NH2	2.22	0.73
18:S:50:ARG:NH2	19:T:73:VAL:O	2.22	0.73
22:W:21:ARG:NH1	22:W:40:CYS:SG	2.62	0.72
17:R:89:GLY:HA2	17:R:112:GLU:HA	1.71	0.71
23:X:114:SER:HB2	23:X:147:LEU:HB3	1.72	0.71
12:M:93:PRO:HD2	12:M:113:LYS:HD2	1.73	0.71
14:O:30:GLY:N	14:O:105:GLU:OE2	2.23	0.71
7:H:9:ILE:HB	7:H:50:VAL:HB	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:30:LYS:NZ	17:R:81:GLU:OE2	2.19	0.71
23:X:83:ILE:O	23:X:86:LYS:NZ	2.23	0.71
23:X:14:SER:HB3	23:X:19:ASN:HB3	1.73	0.70
1:A:1075:A:H4'	18:S:91:ASN:HD21	1.56	0.70
7:H:43:VAL:HG22	7:H:52:VAL:HG12	1.74	0.70
16:Q:66:LEU:HD12	16:Q:72:ASP:HA	1.71	0.70
14:O:70:PRO:HA	14:O:95:ALA:HB2	1.74	0.70
20:U:91:TRP:HB2	20:U:101:LEU:HD22	1.74	0.70
13:N:45:LEU:HA	32:g:8:ARG:HH22	1.56	0.69
1:A:2389:U:HO2'	1:A:2419:A:HO2'	1.40	0.69
32:g:29:ASN:O	32:g:37:LYS:NZ	2.25	0.69
5:F:10:GLY:HA2	5:F:146:PHE:HE1	1.59	0.68
15:P:90:ARG:NH2	15:P:117:GLU:OE1	2.25	0.68
1:A:1517:A:H62	1:A:1635:G:H21	1.42	0.68
22:W:97:ASN:HB2	22:W:99:GLN:HE22	1.59	0.68
28:c:16:ASP:OD2	28:c:51:THR:OG1	2.09	0.68
1:A:2256:U:H3	1:A:2267:G:H1	1.41	0.68
13:N:44:ARG:O	13:N:46:GLY:N	2.27	0.68
1:A:1346:A:H61	1:A:2065:U:H3	1.40	0.68
25:Z:18:VAL:HG22	25:Z:37:LYS:HG2	1.76	0.68
7:H:126:ASP:HB2	7:H:130:LYS:HB2	1.75	0.67
20:U:63:MET:HE1	20:U:71:GLU:HG2	1.77	0.67
14:O:58:ILE:HD12	14:O:109:VAL:HG11	1.75	0.67
1:A:313:U:H3	1:A:446:U:H3	1.42	0.67
1:A:316:G:H1	1:A:443:U:H3	1.42	0.67
13:N:85:LYS:HA	13:N:118:LYS:HD2	1.75	0.67
3:D:227:MET:HE3	3:D:231:ASP:HB3	1.76	0.67
1:A:829:U:O2'	20:U:97:ARG:NH2	2.27	0.67
25:Z:24:ALA:HB2	25:Z:32:GLN:HE21	1.60	0.67
11:L:23:VAL:HG23	11:L:143:PRO:HB2	1.76	0.66
24:Y:31:VAL:HB	24:Y:35:GLU:HG3	1.77	0.66
22:W:46:VAL:HG12	22:W:58:ILE:HG12	1.77	0.65
7:H:1:MET:SD	7:H:6:ARG:NH1	2.70	0.65
1:A:1690:C:N4	1:A:1705:A:OP2	2.29	0.65
6:G:77:ILE:HG22	6:G:82:ILE:HB	1.78	0.65
15:P:10:LEU:HD21	15:P:43:GLU:HG3	1.77	0.65
3:D:135:GLU:OE2	3:D:189:LYS:NZ	2.18	0.65
23:X:114:SER:OG	23:X:150:VAL:O	2.13	0.65
6:G:147:ASP:OD1	6:G:148:LYS:N	2.30	0.65
1:A:474:U:OP2	25:Z:10:LYS:NZ	2.30	0.65
1:A:449:G:H5''	25:Z:74:LYS:HZ3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:A:H61	1:A:1805:U:H3	1.41	0.65
1:A:990:A:H62	14:O:12:LYS:HA	1.62	0.65
13:N:91:ASN:H	13:N:94:THR:HG22	1.62	0.65
30:e:9:ALA:O	30:e:30:ASN:ND2	2.30	0.65
1:A:1072:A:OP1	18:S:50:ARG:NH1	2.29	0.64
1:A:1172:G:H21	1:A:1177:A:H62	1.46	0.64
1:A:2046:G:N2	1:A:2050:C:O2'	2.29	0.64
2:B:71:G:H21	2:B:98:A:H62	1.46	0.64
1:A:639:G:OP2	19:T:79:ARG:NH1	2.30	0.64
1:A:990:A:N3	1:A:2310:C:O2'	2.30	0.64
18:S:26:GLY:O	18:S:29:LYS:NZ	2.30	0.64
1:A:1149:G:H1'	1:A:1168:G:H2'	1.77	0.64
18:S:18:LEU:HA	18:S:21:THR:HG22	1.80	0.64
1:A:343:A:N6	1:A:435:U:O2'	2.30	0.64
5:F:126:ILE:HB	5:F:146:PHE:HE2	1.63	0.64
23:X:33:VAL:HG22	23:X:93:PHE:HB2	1.80	0.64
2:B:41:C:O3'	28:c:2:ARG:NH2	2.31	0.64
1:A:1147:A:H4'	1:A:1148:A:H5''	1.80	0.63
1:A:616:G:H1	1:A:627:C:H42	1.45	0.63
18:S:27:THR:OG1	18:S:31:ASN:OD1	2.16	0.63
15:P:30:LYS:HB2	15:P:75:ILE:HD11	1.81	0.63
1:A:460:C:H2'	1:A:462:C:H41	1.63	0.63
1:A:2794:G:OP1	7:H:74:ASN:ND2	2.31	0.63
1:A:2114:A:N7	5:F:73:ARG:NH2	2.47	0.63
1:A:1142:C:N4	1:A:1147:A:O2'	2.31	0.63
7:H:44:LYS:NZ	7:H:53:ASP:OD1	2.32	0.63
19:T:43:LYS:NZ	19:T:103:PHE:OXT	2.31	0.63
5:F:155:ILE:HB	5:F:176:ILE:HD13	1.81	0.62
1:A:2464:G:OP1	32:g:46:ARG:NH1	2.32	0.62
1:A:2052:A:OP2	4:E:139:ARG:NH2	2.32	0.62
1:A:717:G:OP1	13:N:129:LYS:NZ	2.33	0.62
1:A:1749:G:H1	1:A:2048:C:H42	1.46	0.62
2:B:55:U:H4'	2:B:56:A:H5'	1.81	0.62
1:A:1103:G:H1	1:A:1218:G:H1	1.47	0.62
1:A:627:C:H3'	1:A:628:G:H5''	1.80	0.62
14:O:65:TRP:HZ3	14:O:107:SER:HB3	1.64	0.62
14:O:135:ARG:HG3	23:X:86:LYS:HE3	1.82	0.62
23:X:19:ASN:OD1	23:X:22:ARG:NH1	2.29	0.62
23:X:124:THR:HB	23:X:180:ILE:HG22	1.81	0.62
1:A:1813:A:HO2'	1:A:2761:G:HO2'	1.48	0.62
6:G:136:THR:OG1	6:G:137:GLU:OE1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2073:A:H61	1:A:2089:G:H1	1.48	0.61
4:E:132:SER:OG	4:E:133:HIS:N	2.31	0.61
12:M:50:SER:O	12:M:53:LYS:NZ	2.30	0.61
16:Q:34:VAL:O	16:Q:97:ASN:ND2	2.28	0.61
22:W:91:ILE:HB	22:W:100:ARG:HH12	1.65	0.61
1:A:648:A:OP2	19:T:80:ARG:NH2	2.29	0.61
5:F:139:LEU:O	5:F:143:ILE:HD12	2.01	0.61
6:G:179:PRO:HB3	28:c:58:TYR:HE1	1.65	0.61
26:a:57:GLU:OE1	26:a:63:ARG:NH2	2.32	0.61
1:A:2842:G:H1	1:A:2918:C:H42	1.48	0.61
3:D:73:LYS:NZ	3:D:102:GLU:OE2	2.30	0.61
6:G:179:PRO:HB3	28:c:58:TYR:CE1	2.36	0.61
24:Y:37:ILE:HG22	24:Y:38:VAL:HG23	1.82	0.61
1:A:393:A:N3	5:F:170:ASN:ND2	2.48	0.60
13:N:72:TYR:CE2	13:N:109:LYS:HB2	2.31	0.60
20:U:93:ARG:NH1	20:U:99:ASP:OD1	2.30	0.60
1:A:1843:A:OP2	3:D:223:ARG:NH1	2.33	0.60
1:A:392:C:OP2	5:F:137:LYS:NZ	2.29	0.60
17:R:27:VAL:HG12	17:R:83:VAL:HG22	1.84	0.60
1:A:555:A:H4'	1:A:556:A:H5'	1.82	0.60
23:X:78:ASP:OD1	23:X:79:ALA:N	2.34	0.60
1:A:1043:U:O2'	1:A:2319:A:N3	2.33	0.60
1:A:394:A:O2'	1:A:413:A:N3	2.34	0.60
1:A:477:G:N7	25:Z:70:ARG:NH2	2.46	0.60
1:A:1747:A:H61	1:A:2050:C:H42	1.50	0.60
1:A:1387:G:OP2	31:f:9:ARG:NH2	2.35	0.59
1:A:2513:C:O2	14:O:124:LYS:NZ	2.35	0.59
1:A:1471:U:H4'	1:A:1686:A:H4'	1.83	0.59
23:X:167:VAL:C	23:X:168:ARG:HD3	2.27	0.59
33:h:1:MET:HG2	33:h:2:LYS:HG3	1.84	0.59
4:E:3:GLY:HA2	4:E:201:VAL:O	2.02	0.59
22:W:66:ASP:OD1	22:W:67:ILE:N	2.35	0.59
1:A:921:U:H3	1:A:1018:G:H1	1.49	0.58
28:c:15:LYS:HD3	28:c:22:MET:HG2	1.83	0.58
1:A:2276:G:H1'	25:Z:45:ASN:HB3	1.85	0.58
11:L:38:VAL:HG21	11:L:62:ILE:HD11	1.85	0.58
1:A:2285:G:OP1	3:D:245:ARG:NH2	2.35	0.58
1:A:1437:A:H62	1:A:1448:G:H21	1.51	0.58
1:A:2118:C:O2'	1:A:2297:G:N2	2.37	0.58
3:D:1:MET:SD	3:D:199:ASN:HA	2.43	0.58
14:O:29:PHE:N	14:O:105:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:115:ILE:HA	23:X:118:LYS:HD2	1.86	0.58
30:e:27:THR:HG22	30:e:28:THR:H	1.69	0.58
1:A:2576:G:N7	7:H:172:LYS:NZ	2.52	0.57
19:T:40:LEU:HD12	19:T:49:ILE:HG22	1.86	0.57
1:A:1233:G:OP2	18:S:58:ARG:NH2	2.31	0.57
2:B:110:G:O3'	16:Q:62:LYS:NZ	2.37	0.57
11:L:64:ASN:OD1	11:L:67:LYS:NZ	2.37	0.57
16:Q:66:LEU:HB3	16:Q:72:ASP:HB3	1.86	0.57
1:A:2515:A:O2'	14:O:56:ARG:NH1	2.38	0.57
1:A:2548:G:H5''	1:A:2549:A:H5''	1.85	0.57
4:E:115:LYS:HD2	15:P:1:MET:HE2	1.85	0.57
10:K:82:LYS:O	10:K:87:ILE:N	2.35	0.57
1:A:832:A:OP1	1:A:1698:C:N4	2.37	0.57
1:A:1853:G:N7	3:D:180:SER:OG	2.36	0.57
4:E:179:ASP:OD2	4:E:182:LYS:HB2	2.05	0.57
2:B:34:U:O2'	2:B:35:A:O5'	2.21	0.57
18:S:109:ILE:O	18:S:113:ILE:HG12	2.05	0.57
1:A:819:U:H3	1:A:841:G:H1	1.52	0.57
1:A:713:A:O3'	13:N:65:ASN:ND2	2.38	0.57
1:A:2705:G:N2	1:A:2708:A:OP2	2.38	0.57
3:D:146:ILE:HB	3:D:156:LEU:HB2	1.85	0.57
14:O:1:MET:HE1	14:O:45:ARG:HG3	1.86	0.57
34:i:37:HIS:HB2	34:i:49:ARG:HH12	1.70	0.57
1:A:2612:A:N1	12:M:28:SER:OG	2.38	0.56
1:A:2703:A:H62	1:A:2710:G:H21	1.53	0.56
5:F:126:ILE:HD12	5:F:146:PHE:CE2	2.39	0.56
1:A:381:G:H21	1:A:402:G:H21	1.53	0.56
1:A:2686:G:OP1	11:L:101:ARG:NH1	2.39	0.56
5:F:7:SER:N	5:F:11:LYS:O	2.23	0.56
23:X:105:TYR:HB3	23:X:129:GLN:HG3	1.87	0.56
1:A:952:U:OP2	14:O:5:LYS:NZ	2.38	0.56
1:A:1192:U:O2'	1:A:1193:A:OP1	2.21	0.56
1:A:1373:G:OP1	1:A:2755:G:O2'	2.20	0.56
2:B:84:G:O6	27:b:35:ARG:NH2	2.39	0.56
14:O:130:MET:HE1	23:X:84:ALA:O	2.06	0.56
18:S:76:TYR:HA	18:S:79:PHE:HB3	1.88	0.56
23:X:117:VAL:HG21	23:X:123:LEU:HD22	1.87	0.56
6:G:104:TYR:HH	28:c:23:PHE:HD1	1.53	0.56
18:S:72:THR:OG1	18:S:114:ARG:NH2	2.38	0.56
1:A:109:C:O2	1:A:367:A:O2'	2.23	0.56
1:A:1163:A:O2'	1:A:1184:U:O2'	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:2:ASP:HB2	17:R:5:ARG:HD3	1.87	0.56
21:V:68:SER:OG	21:V:69:ARG:N	2.39	0.56
4:E:54:ASP:OD2	4:E:77:LYS:NZ	2.25	0.56
7:H:35:GLN:OE1	7:H:36:ASP:N	2.39	0.56
1:A:1003:A:H4'	24:Y:29:GLN:HG3	1.88	0.56
1:A:1792:C:O2'	1:A:2889:A:N3	2.35	0.56
8:I:9:PHE:HB2	8:I:12:LEU:HB2	1.87	0.56
29:d:16:ARG:O	29:d:20:ASN:ND2	2.35	0.56
7:H:28:GLY:HA3	7:H:79:VAL:HB	1.88	0.56
19:T:43:LYS:HE2	19:T:103:PHE:HB2	1.87	0.56
1:A:190:G:N2	1:A:190:G:OP2	2.37	0.55
1:A:1467:U:H3	1:A:1472:A:H62	1.54	0.55
1:A:1559:G:N2	1:A:1589:A:O2'	2.39	0.55
1:A:2073:A:H1'	18:S:34:LYS:HE2	1.86	0.55
13:N:28:THR:OG1	13:N:32:GLY:O	2.25	0.55
13:N:66:SER:O	13:N:67:ASP:HB2	2.06	0.55
1:A:2715:A:OP1	34:i:49:ARG:NH1	2.40	0.55
1:A:2721:A:H4'	12:M:29:LYS:HB2	1.86	0.55
15:P:12:ARG:HD3	15:P:16:HIS:CD2	2.42	0.55
1:A:2520:U:OP2	1:A:2521:C:N4	2.27	0.55
30:e:39:GLU:HB3	30:e:52:LEU:HD11	1.88	0.55
1:A:1303:A:OP1	19:T:86:LYS:NZ	2.36	0.55
1:A:2734:G:N1	1:A:2767:U:OP2	2.40	0.55
1:A:2773:C:O2	12:M:67:LYS:NZ	2.39	0.55
19:T:58:LEU:H	19:T:102:VAL:HB	1.71	0.55
33:h:25:ILE:HB	33:h:34:GLN:HB2	1.88	0.55
6:G:114:VAL:HB	6:G:117:PHE:HB2	1.88	0.55
1:A:1033:G:H1	1:A:1042:U:H3	1.53	0.55
1:A:1808:C:OP1	17:R:93:ARG:NH1	2.39	0.55
1:A:2755:G:O2'	1:A:2756:U:OP1	2.24	0.55
14:O:97:VAL:HG11	14:O:103:MET:HE2	1.89	0.55
5:F:153:VAL:HG22	5:F:192:ASN:HB2	1.89	0.55
7:H:103:LEU:HD11	7:H:123:VAL:HG11	1.88	0.55
29:d:29:GLN:OE1	29:d:40:ARG:NH1	2.40	0.55
1:A:22:U:OP1	18:S:29:LYS:NZ	2.39	0.54
1:A:1085:U:H3	1:A:1216:G:H1	1.54	0.54
6:G:59:GLU:O	6:G:63:ILE:HG12	2.07	0.54
18:S:108:LYS:NZ	19:T:47:VAL:O	2.38	0.54
28:c:52:SER:HA	28:c:55:HIS:CE1	2.42	0.54
1:A:2835:C:O2'	1:A:2839:A:N3	2.33	0.54
1:A:1566:U:H3	1:A:1586:G:H22	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2860:G:OP1	4:E:56:LYS:NZ	2.40	0.54
3:D:56:GLY:HA3	3:D:219:ARG:HG3	1.89	0.54
6:G:101:GLU:HG3	28:c:26:LYS:HB2	1.88	0.54
13:N:90:VAL:HG23	13:N:120:VAL:HG11	1.88	0.54
16:Q:92:LEU:HB2	16:Q:119:ILE:HG22	1.90	0.54
1:A:522:C:OP1	18:S:2:ALA:N	2.41	0.54
11:L:96:ARG:O	11:L:100:GLU:HG3	2.07	0.54
23:X:147:LEU:HD13	23:X:181:ILE:HD11	1.88	0.54
28:c:38:ILE:HD12	28:c:38:ILE:H	1.71	0.54
5:F:4:LYS:HE3	5:F:12:GLU:HG3	1.88	0.54
19:T:4:LEU:HB2	19:T:40:LEU:HB3	1.89	0.54
1:A:775:A:O2'	1:A:1430:A:N3	2.37	0.54
1:A:1529:C:O2'	1:A:1530:G:N2	2.40	0.54
22:W:48:LYS:O	22:W:50:ARG:NH1	2.41	0.54
1:A:362:U:N3	1:A:417:U:OP1	2.35	0.54
1:A:633:U:O2'	11:L:53:HIS:O	2.23	0.54
1:A:1854:C:OP2	3:D:184:ARG:NH2	2.40	0.54
7:H:59:LYS:N	7:H:59:LYS:HD2	2.23	0.54
1:A:1141:G:N2	10:K:92:LYS:O	2.37	0.54
7:H:59:LYS:HD2	7:H:59:LYS:H	1.71	0.54
1:A:1066:C:OP1	27:b:51:ARG:NH2	2.36	0.54
1:A:1455:A:O2'	1:A:1457:G:OP2	2.26	0.54
1:A:2468:C:H5	32:g:32:HIS:HE1	1.56	0.54
3:D:144:HIS:HA	3:D:157:ILE:HD11	1.89	0.54
6:G:80:PHE:HB2	6:G:82:ILE:HG12	1.90	0.54
1:A:2105:U:O2	1:A:2106:A:N6	2.41	0.53
3:D:233:PRO:HB3	3:D:245:ARG:NH1	2.24	0.53
19:T:32:LYS:HE2	19:T:62:THR:HG22	1.90	0.53
30:e:43:TYR:HB2	30:e:50:HIS:CE1	2.42	0.53
6:G:51:LYS:HD3	6:G:150:GLU:HG2	1.90	0.53
1:A:369:A:O3'	22:W:90:LYS:NZ	2.41	0.53
1:A:1134:G:H4'	1:A:1165:A:H8	1.73	0.53
1:A:1753:C:O2	1:A:2047:U:O2'	2.24	0.53
7:H:72:ILE:HA	7:H:75:MET:HE2	1.90	0.53
8:I:51:ARG:O	8:I:56:LYS:N	2.27	0.53
15:P:8:ASN:C	15:P:10:LEU:H	2.14	0.53
1:A:718:A:OP1	13:N:112:SER:OG	2.24	0.53
1:A:858:G:H1	1:A:2126:C:H5''	1.73	0.53
8:I:29:TYR:HD2	8:I:30:LEU:HD23	1.73	0.53
15:P:100:LEU:HD13	29:d:43:ILE:HD12	1.90	0.53
16:Q:82:LYS:HA	16:Q:85:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:89:LYS:NZ	19:T:6:GLU:OE1	2.42	0.53
19:T:34:GLU:HG2	19:T:58:LEU:HD12	1.91	0.53
22:W:91:ILE:HB	22:W:100:ARG:NH1	2.24	0.53
23:X:34:TYR:HB3	23:X:40:VAL:HG12	1.90	0.53
27:b:4:ARG:HA	27:b:7:ARG:HG2	1.90	0.53
1:A:863:A:OP1	3:D:219:ARG:NH2	2.41	0.53
17:R:1:MET:HE3	17:R:1:MET:HA	1.89	0.53
1:A:2393:C:OP1	30:e:42:LYS:NZ	2.38	0.53
6:G:77:ILE:O	6:G:82:ILE:N	2.33	0.53
31:f:49:LYS:O	31:f:50:LYS:HB2	2.09	0.53
34:i:31:GLU:O	34:i:34:LYS:HB2	2.08	0.53
1:A:750:A:N6	1:A:752:A:O2'	2.42	0.53
1:A:902:A:N3	1:A:1022:U:O2'	2.40	0.53
12:M:107:ARG:HD2	12:M:112:MET:SD	2.49	0.53
22:W:19:ARG:O	22:W:21:ARG:N	2.42	0.53
13:N:27:LYS:HG3	13:N:28:THR:N	2.22	0.53
1:A:252:A:O2'	1:A:461:A:OP1	2.26	0.53
1:A:288:G:H22	1:A:335:U:H3	1.57	0.53
1:A:1872:U:O2'	3:D:156:LEU:O	2.24	0.53
1:A:2887:G:N2	1:A:2890:A:OP2	2.34	0.53
13:N:85:LYS:HG3	13:N:88:GLN:HE22	1.74	0.53
1:A:608:U:H3	1:A:635:G:H1	1.57	0.52
3:D:145:ASN:OD1	3:D:154:GLY:HA3	2.09	0.52
18:S:91:ASN:OD1	18:S:92:ARG:N	2.42	0.52
1:A:23:C:O2'	1:A:629:G:O2'	2.28	0.52
1:A:794:G:O6	1:A:800:A:N6	2.42	0.52
5:F:154:VAL:HG22	5:F:175:LYS:HB2	1.90	0.52
1:A:870:A:OP1	1:A:873:C:N4	2.37	0.52
1:A:2765:G:O2'	1:A:2877:U:OP1	2.27	0.52
23:X:125:VAL:HA	23:X:179:VAL:HG12	1.91	0.52
1:A:374:U:OP2	22:W:80:ARG:NH2	2.26	0.52
15:P:100:LEU:HD11	29:d:56:LEU:HD11	1.92	0.52
22:W:93:TYR:HD2	22:W:98:GLY:HA2	1.73	0.52
23:X:10:GLN:OE1	23:X:46:LYS:NZ	2.42	0.52
5:F:138:ASP:O	5:F:142:ILE:HG12	2.09	0.52
1:A:434:U:H2'	1:A:435:U:H4'	1.92	0.52
30:e:27:THR:HG22	30:e:28:THR:N	2.24	0.52
28:c:55:HIS:HB3	28:c:57:PHE:H	1.75	0.52
1:A:190:G:O2'	1:A:884:A:N3	2.42	0.52
1:A:552:G:O2'	1:A:577:A:N6	2.42	0.52
17:R:88:ARG:O	17:R:112:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1856:A:OP1	1:A:1869:A:N6	2.28	0.52
1:A:2438:A:OP2	32:g:32:HIS:ND1	2.32	0.52
4:E:163:MET:O	4:E:164:ALA:HB3	2.09	0.52
1:A:370:A:H5''	22:W:83:ILE:HD11	1.92	0.51
1:A:1351:A:OP1	1:A:1729:C:N4	2.43	0.51
13:N:54:LEU:HD13	13:N:57:ARG:HH21	1.75	0.51
1:A:571:G:OP2	20:U:5:ARG:NH1	2.43	0.51
1:A:1579:C:H2'	1:A:1580:C:H4'	1.91	0.51
2:B:77:A:H62	2:B:92:G:H21	1.58	0.51
20:U:88:LYS:HD2	20:U:100:ARG:NH2	2.24	0.51
23:X:116:GLY:O	23:X:121:GLY:N	2.43	0.51
1:A:1436:A:OP2	1:A:1448:G:N2	2.36	0.51
7:H:42:ASN:C	7:H:44:LYS:HZ3	2.18	0.51
15:P:49:GLU:OE1	15:P:94:TYR:N	2.41	0.51
1:A:418:A:N3	1:A:420:A:N6	2.59	0.51
1:A:1089:A:H5''	18:S:76:TYR:HE2	1.74	0.51
1:A:269:A:O2'	1:A:444:C:O2	2.27	0.51
14:O:74:TYR:HB2	14:O:94:ASN:OD1	2.10	0.51
1:A:1852:U:H5''	3:D:261:ARG:HB2	1.93	0.51
2:B:38:A:H2	2:B:45:A:H61	1.58	0.51
19:T:19:PHE:HE1	19:T:64:LYS:HG3	1.74	0.51
28:c:15:LYS:HB2	28:c:45:LEU:HD11	1.93	0.51
1:A:224:A:N6	1:A:487:A:O4'	2.44	0.51
6:G:178:MET:SD	6:G:179:PRO:HD2	2.51	0.51
24:Y:12:ASN:HA	24:Y:14:ARG:NH2	2.25	0.51
1:A:726:A:H5''	1:A:727:A:H2'	1.92	0.51
1:A:1736:G:H21	15:P:2:LYS:HE3	1.75	0.51
1:A:62:G:O2'	1:A:77:A:N1	2.38	0.51
1:A:592:G:OP1	29:d:17:ARG:NH1	2.44	0.51
1:A:828:U:H5'	1:A:830:U:H1'	1.92	0.51
1:A:1880:C:O2'	1:A:2025:U:OP2	2.23	0.51
26:a:10:GLU:CD	26:a:10:GLU:H	2.18	0.51
1:A:780:C:O2'	1:A:816:A:N6	2.44	0.50
1:A:140:C:N4	1:A:142:A:O2'	2.43	0.50
4:E:121:MET:HG3	4:E:126:PHE:O	2.11	0.50
5:F:8:LYS:HA	5:F:126:ILE:HD11	1.93	0.50
13:N:7:PRO:HG2	13:N:10:ALA:HB2	1.93	0.50
14:O:37:LEU:HD21	14:O:130:MET:HB2	1.92	0.50
18:S:90:ILE:HG22	18:S:91:ASN:H	1.75	0.50
1:A:235:C:O2'	1:A:684:A:N3	2.40	0.50
1:A:764:G:O6	1:A:876:A:N6	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:A:H5''	3:D:49:ARG:HH12	1.76	0.50
1:A:997:A:H5''	1:A:2314:A:H61	1.77	0.50
1:A:2370:U:H3	1:A:2377:G:H1	1.59	0.50
1:A:746:U:OP1	13:N:15:LYS:NZ	2.36	0.50
1:A:1872:U:H2'	3:D:158:ARG:HB2	1.93	0.50
17:R:32:ILE:HG22	17:R:37:GLU:HG3	1.93	0.50
3:D:53:ARG:HB2	3:D:54:ARG:HG3	1.94	0.50
18:S:69:LEU:HD12	18:S:76:TYR:HB3	1.93	0.50
1:A:1488:U:O4	1:A:1489:A:N6	2.45	0.50
1:A:1651:G:H5'	3:D:61:ARG:HA	1.93	0.50
3:D:163:TYR:HB3	3:D:196:GLU:HG2	1.93	0.50
7:H:54:ARG:HH11	7:H:65:HIS:CD2	2.29	0.50
14:O:52:ILE:HG22	14:O:56:ARG:HH21	1.76	0.50
15:P:83:ILE:O	15:P:86:VAL:HG22	2.11	0.50
28:c:37:TYR:HD1	28:c:39:ASP:H	1.59	0.50
6:G:80:PHE:O	6:G:81:LYS:HG3	2.11	0.50
8:I:9:PHE:HZ	8:I:35:PHE:CD2	2.29	0.50
17:R:28:VAL:HB	17:R:82:LYS:HG2	1.93	0.50
1:A:225:A:H4'	1:A:226:A:O5'	2.11	0.50
23:X:14:SER:HB3	23:X:19:ASN:CB	2.40	0.50
1:A:472:U:O2'	25:Z:13:MET:SD	2.69	0.50
1:A:662:A:O2'	1:A:753:C:O2'	2.29	0.50
1:A:1089:A:O2'	1:A:1231:C:O2	2.30	0.50
6:G:151:ARG:NH1	6:G:152:ILE:O	2.45	0.50
17:R:88:ARG:CZ	17:R:113:ARG:HH12	2.25	0.50
21:V:2:LYS:HD2	21:V:3:ALA:H	1.77	0.50
1:A:1845:A:N6	1:A:1882:G:O2'	2.43	0.49
1:A:2756:U:H2'	1:A:2757:A:C8	2.47	0.49
23:X:122:ILE:O	23:X:181:ILE:HA	2.12	0.49
1:A:36:C:N4	1:A:524:A:OP2	2.45	0.49
1:A:397:A:OP2	1:A:1282:A:N6	2.45	0.49
2:B:41:C:O2'	6:G:67:LYS:O	2.24	0.49
17:R:10:GLN:O	17:R:13:LYS:NZ	2.45	0.49
29:d:36:ASN:OD1	29:d:37:LEU:N	2.45	0.49
31:f:8:SER:OG	31:f:9:ARG:N	2.46	0.49
1:A:534:G:O2'	1:A:545:G:O6	2.31	0.49
1:A:846:A:N1	1:A:1843:A:O2'	2.45	0.49
3:D:109:PRO:HD2	3:D:112:ILE:HD13	1.93	0.49
7:H:36:ASP:OD2	7:H:37:ILE:N	2.45	0.49
21:V:79:THR:HG22	21:V:80:SER:H	1.76	0.49
34:i:28:SER:HA	34:i:36:LYS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:U:O2'	1:A:1783:A:N7	2.43	0.49
1:A:2025:U:H1'	3:D:242:SER:HB3	1.93	0.49
3:D:54:ARG:HD2	3:D:221:LYS:HA	1.93	0.49
11:L:51:THR:HG22	11:L:53:HIS:H	1.78	0.49
1:A:683:U:H2'	1:A:684:A:H8	1.77	0.49
1:A:888:C:O2	1:A:2490:G:O2'	2.27	0.49
4:E:37:LYS:HG3	4:E:48:LEU:HD23	1.95	0.49
21:V:4:TYR:HD1	26:a:20:LYS:HB3	1.78	0.49
27:b:40:LYS:HB3	27:b:43:ILE:HD13	1.94	0.49
30:e:43:TYR:HA	30:e:50:HIS:HA	1.93	0.49
27:b:31:MET:CE	27:b:93:ASN:HA	2.40	0.49
1:A:1061:C:N3	27:b:11:LYS:NZ	2.60	0.49
1:A:2831:U:H2'	1:A:2832:A:C8	2.48	0.49
21:V:4:TYR:CD1	26:a:20:LYS:HB3	2.47	0.49
1:A:222:U:O4	1:A:496:U:O2'	2.29	0.48
1:A:896:C:O2'	1:A:1301:G:N2	2.45	0.48
1:A:1806:A:H2'	1:A:1807:G:C8	2.48	0.48
13:N:84:PHE:O	13:N:118:LYS:HE3	2.13	0.48
1:A:30:G:H1'	1:A:589:A:H61	1.78	0.48
1:A:1500:A:H2'	1:A:1501:G:C8	2.48	0.48
14:O:135:ARG:HA	14:O:135:ARG:NE	2.28	0.48
1:A:437:A:H2'	1:A:438:A:C8	2.47	0.48
29:d:57:GLU:OE1	29:d:57:GLU:N	2.47	0.48
1:A:7:U:H3	1:A:2929:G:H1	1.60	0.48
1:A:354:A:H2'	1:A:355:A:C8	2.48	0.48
1:A:896:C:HO2'	1:A:1301:G:N2	2.11	0.48
19:T:27:PRO:HA	19:T:30:LYS:HG3	1.96	0.48
14:O:66:ILE:HG12	14:O:104:PHE:HE1	1.79	0.48
22:W:41:ASN:HB2	22:W:65:ILE:HD11	1.95	0.48
33:h:33:LYS:O	33:h:34:GLN:HG3	2.13	0.48
1:A:717:G:O2'	1:A:719:G:O2'	2.26	0.48
1:A:941:U:H2'	1:A:942:A:H8	1.78	0.48
4:E:25:THR:OG1	4:E:189:GLY:O	2.27	0.48
15:P:99:LYS:O	29:d:43:ILE:HG13	2.13	0.48
20:U:63:MET:HE1	20:U:71:GLU:CG	2.43	0.48
27:b:59:LYS:O	27:b:63:VAL:HG23	2.14	0.48
1:A:465:G:H5'	25:Z:25:LYS:HB2	1.96	0.48
1:A:2758:A:H2'	1:A:2759:G:C8	2.48	0.48
6:G:103:LEU:O	6:G:107:ILE:HG22	2.14	0.48
6:G:114:VAL:HG22	6:G:140:ILE:HG21	1.94	0.48
21:V:79:THR:HG22	21:V:80:SER:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:G:OP2	1:A:2452:A:O2'	2.31	0.48
1:A:2420:C:N4	1:A:2421:G:O6	2.46	0.48
21:V:23:ILE:HG13	21:V:25:VAL:HG23	1.95	0.48
1:A:906:G:H1	1:A:915:U:H3	1.61	0.48
1:A:1636:U:O4	1:A:1637:A:N6	2.46	0.48
28:c:8:LYS:NZ	28:c:9:ASN:O	2.43	0.48
1:A:591:C:O2'	20:U:22:ARG:NH2	2.47	0.48
1:A:1287:G:OP1	1:A:1288:A:O2'	2.29	0.48
1:A:2766:G:H4'	1:A:2876:G:H4'	1.96	0.48
1:A:1668:U:O2'	1:A:1669:A:O5'	2.32	0.47
7:H:163:LYS:NZ	7:H:164:TYR:O	2.45	0.47
19:T:31:ASP:OD1	19:T:31:ASP:N	2.45	0.47
6:G:67:LYS:HD3	28:c:5:ILE:HD12	1.96	0.47
6:G:143:GLU:OE2	28:c:29:LEU:N	2.47	0.47
16:Q:64:LEU:HB3	16:Q:66:LEU:HD23	1.96	0.47
1:A:633:U:H5''	11:L:119:PRO:HB2	1.96	0.47
1:A:1055:G:O2'	1:A:1234:A:O2'	2.31	0.47
1:A:2249:U:H2'	1:A:2250:C:C6	2.49	0.47
2:B:87:C:N4	2:B:88:G:O6	2.48	0.47
23:X:116:GLY:HA2	23:X:152:LYS:HG3	1.95	0.47
1:A:364:U:H2'	1:A:365:A:H8	1.79	0.47
1:A:766:G:O2'	1:A:870:A:N7	2.41	0.47
1:A:2572:G:H1	1:A:2583:U:H3	1.61	0.47
8:I:5:LEU:HD23	8:I:9:PHE:HD2	1.78	0.47
26:a:21:LYS:HA	26:a:21:LYS:HE2	1.97	0.47
1:A:556:A:OP2	22:W:45:LYS:NZ	2.47	0.47
1:A:1500:A:H2'	1:A:1501:G:H8	1.79	0.47
1:A:1986:A:H62	1:A:2022:G:H21	1.61	0.47
1:A:2622:G:O2'	1:A:2625:C:OP2	2.32	0.47
6:G:163:ALA:HB1	6:G:168:GLU:HB2	1.96	0.47
18:S:76:TYR:CD1	18:S:76:TYR:N	2.80	0.47
1:A:446:U:H5''	1:A:447:G:H5'	1.96	0.47
1:A:1066:C:O2'	1:A:1079:A:N3	2.44	0.47
1:A:1617:A:H4'	1:A:1618:G:O5'	2.13	0.47
7:H:148:ILE:O	7:H:151:LEU:HB2	2.14	0.47
1:A:23:C:HO2'	1:A:629:G:HO2'	1.62	0.47
1:A:756:G:H5''	5:F:75:GLY:N	2.29	0.47
1:A:1107:A:H5''	14:O:128:LYS:HE2	1.96	0.47
28:c:14:PHE:CD1	28:c:46:VAL:HB	2.50	0.47
32:g:28:GLN:HG3	32:g:29:ASN:OD1	2.15	0.47
1:A:195:C:O2'	1:A:2290:U:OP1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1623:C:H2'	1:A:1624:A:C8	2.50	0.47
12:M:68:GLU:HB3	12:M:78:ARG:HB2	1.96	0.47
13:N:17:VAL:HG22	13:N:29:SER:HB3	1.97	0.47
13:N:135:VAL:CG1	13:N:140:CYS:HB2	2.44	0.47
16:Q:3:LYS:O	16:Q:6:GLU:HG3	2.15	0.47
18:S:94:ILE:HG21	19:T:4:LEU:HD13	1.95	0.47
25:Z:71:SER:O	25:Z:75:ILE:HG22	2.15	0.47
26:a:58:TYR:CE1	26:a:63:ARG:HD2	2.50	0.47
1:A:219:A:N1	1:A:262:A:O2'	2.48	0.47
1:A:558:A:H5''	22:W:46:VAL:HG21	1.96	0.47
1:A:670:U:H2'	1:A:671:G:C8	2.50	0.47
23:X:105:TYR:HE1	23:X:131:LYS:HB2	1.80	0.47
1:A:372:A:N1	1:A:395:A:O2'	2.39	0.47
1:A:620:U:H3	1:A:623:A:H2	1.63	0.47
1:A:1504:A:N6	1:A:1654:A:OP2	2.34	0.47
2:B:74:G:H21	23:X:90:HIS:CE1	2.33	0.47
4:E:12:THR:OG1	4:E:13:GLN:N	2.47	0.47
7:H:44:LYS:HB3	7:H:46:GLU:OE1	2.14	0.47
20:U:17:SER:O	20:U:21:VAL:HG23	2.15	0.47
29:d:25:ILE:HD12	29:d:25:ILE:H	1.80	0.47
1:A:1232:C:OP1	18:S:92:ARG:NH2	2.35	0.46
1:A:1752:A:H61	1:A:2047:U:H3	1.62	0.46
34:i:18:SER:N	34:i:22:GLY:O	2.41	0.46
4:E:113:LYS:O	4:E:164:ALA:CB	2.60	0.46
17:R:57:THR:HG22	17:R:74:PRO:HA	1.97	0.46
22:W:97:ASN:CB	22:W:99:GLN:HE22	2.27	0.46
1:A:945:G:H21	1:A:947:A:H61	1.64	0.46
2:B:10:U:H3	2:B:103:A:H61	1.63	0.46
1:A:213:G:H4'	1:A:214:A:H4'	1.95	0.46
1:A:1121:C:H2'	1:A:1122:G:C8	2.50	0.46
1:A:1500:A:O2'	1:A:1579:C:O2'	2.20	0.46
1:A:1805:U:H2'	1:A:1806:A:H8	1.81	0.46
13:N:69:LYS:HB3	13:N:71:GLU:HG2	1.98	0.46
13:N:114:GLY:O	13:N:115:LYS:HE2	2.15	0.46
1:A:1365:U:H5	1:A:1403:U:H3	1.64	0.46
1:A:2350:G:H1	1:A:2358:U:H3	1.62	0.46
6:G:51:LYS:NZ	6:G:150:GLU:HB3	2.30	0.46
16:Q:33:THR:HG22	16:Q:95:ASP:HB3	1.96	0.46
20:U:79:VAL:HG22	20:U:110:VAL:HG22	1.97	0.46
21:V:97:ILE:HG23	21:V:98:PHE:HD2	1.80	0.46
28:c:14:PHE:CE1	28:c:46:VAL:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2641:G:N2	1:A:2644:A:OP2	2.41	0.46
18:S:111:LEU:HD13	18:S:114:ARG:HH12	1.80	0.46
1:A:1143:U:O2	1:A:1151:A:N6	2.49	0.46
1:A:2056:G:P	15:P:9:ARG:HH21	2.39	0.46
1:A:2846:C:O2	1:A:2913:A:O2'	2.34	0.46
3:D:68:PHE:HE1	3:D:107:ILE:HD11	1.81	0.46
23:X:62:VAL:HG11	23:X:136:PRO:O	2.16	0.46
1:A:998:A:N3	2:B:79:U:O2'	2.41	0.46
1:A:1855:A:OP2	3:D:152:LYS:NZ	2.45	0.46
1:A:2754:G:H2'	1:A:2755:G:H8	1.81	0.46
2:B:76:U:OP1	23:X:24:ARG:NH2	2.46	0.46
7:H:1:MET:SD	7:H:2:SER:N	2.89	0.46
16:Q:84:LEU:HD11	16:Q:89:ILE:HB	1.98	0.46
20:U:24:ILE:HD12	20:U:43:MET:SD	2.56	0.46
20:U:70:SER:H	20:U:73:MET:HE2	1.81	0.46
22:W:42:MET:HE3	22:W:60:ASP:HB3	1.97	0.46
23:X:127:LYS:HZ2	23:X:158:LEU:HD11	1.81	0.46
1:A:484:G:H2'	1:A:485:G:H8	1.80	0.46
1:A:725:A:H61	1:A:2395:G:H21	1.63	0.46
1:A:2841:G:H1	1:A:2919:C:H42	1.64	0.46
5:F:10:GLY:HA2	5:F:146:PHE:CE1	2.44	0.46
14:O:33:GLY:C	14:O:118:MET:HE1	2.41	0.46
30:e:15:LEU:HB2	30:e:25:TYR:HB2	1.97	0.46
1:A:1563:A:O2'	1:A:1564:U:O4'	2.34	0.46
1:A:1683:C:H2'	1:A:1684:G:H8	1.80	0.46
1:A:2574:U:H5''	7:H:172:LYS:HZ3	1.80	0.46
23:X:105:TYR:CE1	23:X:131:LYS:HB2	2.51	0.46
34:i:29:LYS:HG2	34:i:38:TYR:CE1	2.51	0.46
1:A:587:A:O2'	1:A:1294:U:OP1	2.26	0.45
1:A:1134:G:O2'	1:A:1182:A:N6	2.50	0.45
1:A:1637:A:O2'	1:A:1638:G:O5'	2.33	0.45
2:B:31:U:H2'	2:B:32:G:C8	2.51	0.45
12:M:12:ASP:OD2	12:M:14:THR:HG23	2.16	0.45
14:O:134:ARG:C	14:O:136:ASP:H	2.23	0.45
26:a:6:ASN:OD1	26:a:6:ASN:N	2.49	0.45
27:b:5:LYS:O	27:b:9:GLN:HG3	2.16	0.45
1:A:676:G:H1	1:A:739:U:H3	1.63	0.45
1:A:862:G:N1	3:D:231:ASP:OD1	2.42	0.45
1:A:1035:G:OP2	14:O:14:ARG:NH1	2.48	0.45
6:G:132:SER:HA	6:G:157:ILE:O	2.16	0.45
17:R:36:ASN:OD1	17:R:37:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:34:LYS:HD2	18:S:34:LYS:HA	1.70	0.45
1:A:1505:C:N4	1:A:1653:A:OP2	2.39	0.45
1:A:1586:G:H1'	1:A:1587:A:C8	2.52	0.45
14:O:54:MET:HE1	14:O:104:PHE:CG	2.52	0.45
16:Q:64:LEU:O	16:Q:66:LEU:HD22	2.15	0.45
1:A:628:G:H2'	1:A:629:G:C8	2.52	0.45
1:A:748:G:H1'	32:g:5:MET:HG3	1.97	0.45
1:A:2050:C:N4	12:M:32:TYR:OH	2.39	0.45
6:G:76:ALA:HB2	6:G:84:GLN:H	1.81	0.45
26:a:12:MET:SD	26:a:54:MET:HE2	2.56	0.45
1:A:485:G:H1	1:A:496:U:H3	1.64	0.45
15:P:51:LEU:HD11	15:P:69:PHE:CD2	2.51	0.45
26:a:12:MET:HE1	26:a:54:MET:HB3	1.97	0.45
30:e:16:ILE:O	30:e:53:HIS:HA	2.17	0.45
33:h:1:MET:HE1	33:h:31:LYS:HA	1.99	0.45
1:A:380:G:N2	1:A:383:A:OP2	2.48	0.45
1:A:383:A:P	22:W:19:ARG:HH12	2.40	0.45
1:A:1184:U:H2'	1:A:1185:G:H8	1.82	0.45
1:A:1287:G:N2	1:A:1313:G:O2'	2.49	0.45
3:D:147:GLU:HB3	3:D:190:CYS:HB3	1.99	0.45
4:E:69:LYS:HG3	4:E:70:SER:N	2.32	0.45
4:E:75:GLU:O	4:E:77:LYS:HD3	2.17	0.45
4:E:163:MET:O	4:E:164:ALA:CB	2.64	0.45
15:P:95:THR:HB	15:P:113:LEU:HD11	1.99	0.45
1:A:711:G:N2	1:A:714:A:OP2	2.37	0.45
1:A:718:A:H8	13:N:113:ASN:HD21	1.64	0.45
1:A:1538:U:H4'	1:A:1539:C:O5'	2.15	0.45
1:A:1741:C:H2'	1:A:1742:A:C8	2.52	0.45
2:B:106:G:N2	16:Q:51:GLY:O	2.50	0.45
25:Z:23:LEU:HB3	25:Z:29:GLY:HA3	1.97	0.45
1:A:1074:C:OP1	18:S:53:ARG:NH1	2.50	0.45
1:A:1498:G:N3	1:A:1574:A:N6	2.64	0.45
13:N:118:LYS:O	13:N:120:VAL:HG23	2.17	0.45
13:N:120:VAL:HG12	13:N:121:SER:N	2.32	0.45
1:A:2798:G:OP1	1:A:2798:G:N2	2.38	0.45
2:B:86:U:H4'	2:B:87:C:O5'	2.15	0.45
6:G:59:GLU:OE1	6:G:138:GLN:NE2	2.50	0.45
15:P:22:LYS:O	15:P:26:ILE:HG12	2.17	0.45
22:W:51:THR:N	22:W:52:PRO:HD2	2.32	0.45
31:f:50:LYS:HE2	31:f:50:LYS:HB3	1.75	0.45
23:X:12:ARG:HB3	23:X:44:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:U:H2'	1:A:306:G:C8	2.52	0.44
2:B:42:C:O2	6:G:95:ARG:NH1	2.50	0.44
3:D:35:THR:HA	3:D:63:TYR:O	2.17	0.44
5:F:2:GLU:OE2	5:F:15:THR:HB	2.16	0.44
13:N:45:LEU:H	13:N:45:LEU:HD23	1.82	0.44
13:N:120:VAL:O	13:N:140:CYS:HB3	2.16	0.44
18:S:72:THR:OG1	18:S:73:GLY:N	2.50	0.44
1:A:1540:C:HO2'	1:A:2748:G:HO2'	1.63	0.44
1:A:2727:C:OP2	4:E:113:LYS:NZ	2.44	0.44
3:D:71:ARG:NH2	3:D:147:GLU:OE1	2.49	0.44
1:A:774:U:H2'	1:A:775:A:C8	2.53	0.44
1:A:1625:U:H2'	1:A:1626:G:C8	2.52	0.44
4:E:180:GLU:OE1	4:E:180:GLU:N	2.44	0.44
16:Q:32:ILE:HD12	16:Q:44:GLN:O	2.17	0.44
17:R:71:LYS:HG2	17:R:73:PHE:CE2	2.52	0.44
21:V:29:LYS:HG2	21:V:82:TRP:CZ3	2.52	0.44
29:d:41:HIS:O	29:d:42:ARG:HD3	2.18	0.44
4:E:41:ASP:OD1	4:E:41:ASP:N	2.45	0.44
13:N:135:VAL:O	13:N:138:ILE:HG22	2.17	0.44
14:O:2:LEU:HD12	14:O:2:LEU:HA	1.88	0.44
16:Q:37:SER:OG	16:Q:38:ASN:N	2.51	0.44
1:A:464:A:P	25:Z:20:ARG:HH22	2.40	0.44
1:A:725:A:H2'	1:A:727:A:C8	2.53	0.44
1:A:2913:A:OP1	29:d:50:TYR:OH	2.35	0.44
22:W:72:ILE:HG21	22:W:81:LEU:HD21	1.98	0.44
1:A:1208:A:O2'	1:A:2561:C:O2'	2.35	0.44
2:B:8:G:OP1	16:Q:31:ARG:NH1	2.47	0.44
12:M:1:MET:HE3	12:M:1:MET:HB2	1.90	0.44
15:P:81:THR:HG22	15:P:82:LYS:HD2	1.99	0.44
19:T:43:LYS:HZ3	19:T:103:PHE:HD2	1.66	0.44
27:b:48:PHE:CE2	27:b:75:LYS:HD3	2.53	0.44
17:R:109:LYS:HB2	17:R:109:LYS:HE2	1.79	0.44
25:Z:58:ARG:HD2	25:Z:59:SER:O	2.18	0.44
30:e:15:LEU:HD11	30:e:40:LEU:HD12	1.99	0.44
1:A:4:U:H2'	1:A:5:G:C8	2.53	0.44
1:A:2439:U:H5''	13:N:59:PRO:HB3	1.99	0.44
1:A:2465:U:H4'	30:e:26:THR:HG21	1.99	0.44
5:F:62:LYS:NZ	5:F:74:VAL:O	2.41	0.44
6:G:107:ILE:HG23	6:G:108:HIS:ND1	2.33	0.44
6:G:109:LEU:C	6:G:112:PRO:HD2	2.42	0.44
22:W:22:ILE:HD13	22:W:73:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:G:H2'	1:A:696:U:C2	2.52	0.44
1:A:1514:U:O2'	1:A:1595:G:O2'	2.27	0.44
1:A:2143:U:H2'	1:A:2144:A:C8	2.53	0.44
5:F:6:PHE:HA	5:F:12:GLU:HA	1.99	0.44
12:M:78:ARG:NH2	17:R:59:LEU:HD11	2.33	0.44
21:V:4:TYR:HD1	26:a:20:LYS:HD3	1.83	0.44
1:A:840:G:H2'	1:A:841:G:H8	1.83	0.43
1:A:1683:C:H2'	1:A:1684:G:C8	2.53	0.43
15:P:87:PHE:CE2	15:P:94:TYR:HB3	2.53	0.43
1:A:945:G:H21	1:A:947:A:N6	2.16	0.43
7:H:44:LYS:HB2	7:H:44:LYS:HE2	1.75	0.43
23:X:143:ILE:HD11	23:X:162:VAL:O	2.18	0.43
30:e:51:THR:OG1	30:e:52:LEU:N	2.45	0.43
1:A:2848:G:H4'	1:A:2867:A:H4'	2.00	0.43
3:D:66:ILE:HG22	3:D:67:ASP:N	2.33	0.43
5:F:35:ALA:O	5:F:39:GLU:HG3	2.19	0.43
19:T:43:LYS:HZ2	19:T:48:LYS:HE2	1.83	0.43
22:W:1:MET:N	22:W:33:ASN:OD1	2.51	0.43
25:Z:2:ALA:O	25:Z:4:LYS:N	2.50	0.43
27:b:84:ILE:O	27:b:88:LEU:HG	2.18	0.43
1:A:306:G:H2'	1:A:307:G:C8	2.53	0.43
28:c:2:ARG:NH2	28:c:5:ILE:HD11	2.32	0.43
1:A:2134:A:OP1	25:Z:21:LYS:HD3	2.18	0.43
2:B:48:C:H2'	2:B:49:A:C8	2.54	0.43
30:e:11:GLU:OE2	30:e:31:ARG:NE	2.52	0.43
1:A:1525:U:H2'	1:A:1526:A:C8	2.54	0.43
1:A:2313:A:H5''	1:A:2314:A:H5'	2.01	0.43
7:H:42:ASN:HB3	7:H:44:LYS:NZ	2.33	0.43
29:d:19:ILE:HD13	29:d:19:ILE:HA	1.87	0.43
1:A:773:U:OP1	3:D:219:ARG:NH1	2.50	0.43
1:A:2056:G:H2'	1:A:2057:G:H8	1.84	0.43
1:A:68:A:H61	1:A:94:A:H61	1.67	0.43
1:A:578:A:H4'	1:A:580:A:H5''	2.01	0.43
12:M:24:VAL:HG13	12:M:33:ALA:HB2	2.00	0.43
1:A:461:A:N6	1:A:488:G:O6	2.51	0.43
1:A:648:A:H61	1:A:2083:G:H21	1.67	0.43
6:G:34:LEU:HD23	6:G:161:THR:HG22	2.01	0.43
6:G:105:LYS:HA	6:G:109:LEU:HD12	1.99	0.43
17:R:56:LYS:HE3	17:R:56:LYS:HB2	1.61	0.43
23:X:117:VAL:HG21	23:X:123:LEU:CD2	2.48	0.43
1:A:1402:G:OP1	1:A:1730:G:O2'	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1594:A:HO2'	1:A:1639:U:HO2'	1.65	0.43
3:D:67:ASP:OD1	3:D:104:ARG:NH1	2.48	0.43
3:D:133:PRO:HA	3:D:191:ILE:HA	2.01	0.43
14:O:1:MET:HE1	14:O:45:ARG:HE	1.84	0.43
15:P:10:LEU:HD12	15:P:40:LYS:HG2	2.01	0.43
21:V:14:GLU:O	21:V:18:THR:HG23	2.19	0.43
23:X:5:ARG:NH2	23:X:137:LEU:O	2.50	0.43
23:X:70:LEU:HD12	23:X:71:GLU:H	1.84	0.43
1:A:267:A:OP2	1:A:309:G:N1	2.46	0.42
1:A:285:G:O6	1:A:331:U:N3	2.51	0.42
1:A:354:A:H2'	1:A:355:A:H8	1.84	0.42
1:A:364:U:H3	1:A:422:G:H1	1.65	0.42
2:B:37:C:H2'	2:B:38:A:C8	2.54	0.42
4:E:4:LEU:HD12	4:E:100:PHE:HE2	1.83	0.42
5:F:4:LYS:HA	5:F:4:LYS:HD2	1.87	0.42
5:F:5:VAL:HA	5:F:125:VAL:HG13	2.01	0.42
7:H:155:GLU:OE1	7:H:157:TYR:N	2.52	0.42
12:M:44:LYS:HA	12:M:44:LYS:HD2	1.89	0.42
14:O:1:MET:HE1	14:O:45:ARG:NE	2.34	0.42
1:A:278:G:H1	1:A:299:C:H42	1.67	0.42
1:A:522:C:N4	1:A:523:G:O6	2.51	0.42
1:A:1582:U:H4'	3:D:97:VAL:HG11	2.00	0.42
4:E:118:GLN:OE1	4:E:122:LYS:HD3	2.19	0.42
6:G:63:ILE:O	6:G:105:LYS:NZ	2.44	0.42
13:N:83:LYS:HG2	13:N:100:LEU:HD21	2.00	0.42
24:Y:53:LEU:HD21	24:Y:57:TYR:HD1	1.84	0.42
28:c:31:SER:OG	28:c:45:LEU:O	2.31	0.42
1:A:945:G:H1	1:A:992:C:H42	1.68	0.42
1:A:1522:U:H2'	1:A:1523:G:C8	2.54	0.42
1:A:1850:U:H3	1:A:1877:G:H1	1.66	0.42
1:A:2069:A:C2	29:d:3:VAL:HG12	2.54	0.42
1:A:2146:U:N3	1:A:2272:G:OP2	2.48	0.42
1:A:2855:U:O4	4:E:162:ARG:NH2	2.36	0.42
4:E:150:PRO:HG3	4:E:154:PHE:CZ	2.54	0.42
7:H:13:ASP:OD1	7:H:14:ALA:N	2.50	0.42
12:M:31:ARG:HH11	12:M:31:ARG:HD2	1.73	0.42
16:Q:4:ILE:HD12	16:Q:4:ILE:H	1.85	0.42
17:R:108:MET:HG3	17:R:108:MET:O	2.19	0.42
19:T:1:MET:HA	19:T:42:ASN:O	2.19	0.42
1:A:1622:G:O2'	1:A:1623:C:OP1	2.33	0.42
1:A:2442:G:H5''	25:Z:25:LYS:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:42:ASN:O	7:H:44:LYS:NZ	2.52	0.42
28:c:55:HIS:HB3	28:c:58:TYR:H	1.84	0.42
1:A:670:U:H2'	1:A:671:G:H8	1.83	0.42
1:A:2082:U:H3	1:A:2087:A:H62	1.67	0.42
1:A:2351:U:H5''	6:G:134:GLY:HA3	2.01	0.42
3:D:67:ASP:OD1	3:D:104:ARG:HD3	2.19	0.42
3:D:72:ASP:OD1	3:D:73:LYS:HG2	2.20	0.42
6:G:75:LYS:HE3	6:G:75:LYS:HB2	1.92	0.42
6:G:135:ILE:HD13	6:G:140:ILE:HD11	2.00	0.42
21:V:72:TYR:O	21:V:74:ILE:HG23	2.19	0.42
30:e:31:ARG:HG3	30:e:32:ARG:HG2	2.00	0.42
1:A:1192:U:H2'	1:A:1193:A:H8	1.84	0.42
1:A:1743:C:H2'	1:A:1744:G:H8	1.85	0.42
1:A:1850:U:H2'	1:A:1851:C:C6	2.55	0.42
1:A:2442:G:H5''	25:Z:25:LYS:NZ	2.35	0.42
11:L:47:LYS:HD3	11:L:49:TYR:CZ	2.54	0.42
13:N:127:ILE:HG12	13:N:132:GLU:HB3	2.01	0.42
15:P:84:SER:O	15:P:87:PHE:N	2.50	0.42
16:Q:62:LYS:HD3	16:Q:62:LYS:N	2.34	0.42
28:c:34:THR:HB	28:c:42:GLU:CD	2.45	0.42
32:g:33:ILE:HG13	32:g:33:ILE:O	2.18	0.42
1:A:83:G:H2'	1:A:84:G:C8	2.55	0.42
1:A:456:G:O2'	1:A:2278:C:OP1	2.32	0.42
1:A:2862:U:H5''	1:A:2863:U:H2'	2.02	0.42
6:G:43:VAL:HG13	6:G:43:VAL:O	2.19	0.42
18:S:58:ARG:HA	18:S:61:TRP:CE3	2.55	0.42
20:U:18:PRO:HG3	20:U:83:ASP:HB3	2.02	0.42
1:A:8:C:H2'	1:A:9:A:C8	2.54	0.42
1:A:97:C:O2'	1:A:98:A:O4'	2.37	0.42
1:A:1427:C:O2	1:A:1656:A:O2'	2.38	0.42
1:A:2687:A:H2'	1:A:2688:G:C8	2.55	0.42
15:P:94:TYR:O	15:P:116:VAL:HG22	2.19	0.42
23:X:58:THR:O	23:X:61:THR:HG22	2.19	0.42
32:g:32:HIS:CG	32:g:33:ILE:H	2.38	0.42
1:A:705:C:O2'	1:A:739:U:OP1	2.37	0.42
1:A:718:A:C6	1:A:733:A:H4'	2.55	0.42
1:A:2248:U:H2'	1:A:2249:U:C6	2.55	0.42
1:A:2264:U:OP1	25:Z:59:SER:OG	2.32	0.42
3:D:229:PRO:HD3	3:D:236:GLY:N	2.35	0.42
5:F:123:PHE:CE2	5:F:193:LEU:HD22	2.55	0.42
11:L:96:ARG:O	11:L:99:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:108:ILE:HD11	13:N:124:VAL:HG12	2.02	0.42
18:S:107:LYS:O	18:S:111:LEU:HD23	2.20	0.42
25:Z:7:ILE:HG21	25:Z:80:PHE:CE1	2.54	0.42
1:A:110:C:H2'	1:A:111:A:C8	2.55	0.42
1:A:708:A:O2'	1:A:717:G:N2	2.45	0.42
1:A:1587:A:N6	1:A:1588:G:N7	2.68	0.42
1:A:2706:A:N7	7:H:175:LYS:NZ	2.63	0.42
12:M:64:ARG:HD2	12:M:79:PHE:CD1	2.55	0.42
13:N:5:LEU:HD23	13:N:5:LEU:O	2.20	0.42
15:P:103:ARG:HB2	15:P:110:MET:HG2	2.02	0.42
28:c:35:ILE:HG21	28:c:45:LEU:HD13	2.02	0.42
1:A:2504:U:O2'	1:A:2506:U:O4	2.34	0.41
1:A:2716:G:OP2	34:i:52:ARG:NH2	2.53	0.41
2:B:43:G:H1'	2:B:46:C:H42	1.85	0.41
3:D:127:LYS:HB3	3:D:130:ASN:ND2	2.35	0.41
4:E:38:LYS:O	4:E:46:SER:HA	2.20	0.41
11:L:30:ILE:O	11:L:34:VAL:HG23	2.20	0.41
1:A:942:A:H62	1:A:996:G:H21	1.67	0.41
1:A:1272:G:N7	13:N:13:ARG:NH1	2.64	0.41
3:D:66:ILE:HG22	3:D:67:ASP:H	1.86	0.41
5:F:52:THR:O	5:F:56:VAL:HG23	2.20	0.41
21:V:55:ASN:O	21:V:56:LEU:HD23	2.21	0.41
27:b:52:SER:OG	27:b:53:LEU:N	2.53	0.41
33:h:4:ARG:O	33:h:37:LYS:N	2.52	0.41
1:A:529:G:N2	1:A:534:G:O4'	2.52	0.41
1:A:831:A:H61	1:A:835:A:H2	1.68	0.41
1:A:1278:U:H2'	1:A:1279:G:C8	2.56	0.41
1:A:1294:U:H2'	1:A:1295:A:C8	2.55	0.41
1:A:1463:C:H2'	1:A:1464:G:C8	2.55	0.41
1:A:1572:G:H21	1:A:1575:A:H2'	1.86	0.41
1:A:1871:G:OP1	3:D:89:ARG:NH2	2.53	0.41
1:A:2340:C:H5	16:Q:17:ARG:HH12	1.68	0.41
1:A:2754:G:H2'	1:A:2755:G:C8	2.55	0.41
1:A:2805:A:C4	7:H:67:LEU:HD21	2.55	0.41
6:G:46:ALA:HA	6:G:49:ASN:O	2.20	0.41
8:I:3:VAL:O	8:I:18:THR:HA	2.20	0.41
19:T:32:LYS:HB2	19:T:32:LYS:HE3	1.83	0.41
21:V:9:SER:HB2	26:a:31:VAL:HG21	2.02	0.41
23:X:49:GLU:HG3	23:X:53:LYS:HE2	2.02	0.41
1:A:2730:U:O2'	12:M:68:GLU:OE2	2.36	0.41
1:A:2744:U:H2'	1:A:2745:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:209:LYS:HB2	5:F:209:LYS:HE3	1.87	0.41
6:G:49:ASN:ND2	6:G:52:LEU:HG	2.35	0.41
14:O:45:ARG:O	14:O:48:GLU:HG3	2.21	0.41
30:e:37:LYS:HD3	30:e:37:LYS:HA	1.73	0.41
1:A:536:A:H62	1:A:545:G:H21	1.68	0.41
1:A:2051:A:H2'	1:A:2052:A:C8	2.55	0.41
3:D:212:LYS:HA	3:D:215:TRP:CD2	2.55	0.41
6:G:16:ILE:O	6:G:20:VAL:HG23	2.20	0.41
23:X:157:LEU:HB2	23:X:160:ASP:CG	2.46	0.41
1:A:5:G:H2'	1:A:6:G:C8	2.56	0.41
1:A:110:C:H2'	1:A:111:A:H8	1.85	0.41
1:A:935:U:H2'	1:A:936:A:C8	2.56	0.41
1:A:1572:G:H21	1:A:1575:A:H8	1.68	0.41
1:A:2056:G:H2'	1:A:2057:G:C8	2.55	0.41
4:E:181:GLU:HG2	4:E:182:LYS:N	2.34	0.41
5:F:197:GLU:OE1	5:F:197:GLU:N	2.40	0.41
8:I:8:ASP:OD1	8:I:9:PHE:N	2.54	0.41
12:M:10:ILE:HD11	12:M:19:ALA:HB2	2.02	0.41
18:S:94:ILE:CG2	19:T:4:LEU:HD13	2.51	0.41
1:A:600:A:O2'	1:A:2098:U:O4'	2.32	0.41
1:A:1448:G:N2	1:A:1449:U:O4	2.54	0.41
2:B:4:U:H2'	2:B:5:G:C8	2.56	0.41
5:F:92:LYS:HD3	5:F:92:LYS:HA	1.91	0.41
14:O:87:LYS:HD2	14:O:87:LYS:HA	1.95	0.41
21:V:92:GLU:OE1	21:V:92:GLU:N	2.47	0.41
28:c:36:LYS:HD2	28:c:40:GLY:HA2	2.02	0.41
1:A:753:C:H2'	1:A:754:C:C6	2.56	0.41
1:A:966:G:H1	1:A:971:A:H61	1.68	0.41
1:A:1526:A:O2'	1:A:1608:G:O2'	2.32	0.41
1:A:1861:G:N2	1:A:1864:A:OP2	2.43	0.41
1:A:2394:U:H2'	1:A:2395:G:C8	2.56	0.41
15:P:50:ARG:O	15:P:53:THR:HG22	2.20	0.41
16:Q:32:ILE:HD11	16:Q:43:ALA:HB1	2.03	0.41
16:Q:62:LYS:HD3	16:Q:62:LYS:H	1.86	0.41
21:V:29:LYS:HG2	21:V:82:TRP:CE3	2.56	0.41
24:Y:24:LYS:HA	24:Y:24:LYS:HD3	1.93	0.41
1:A:97:C:O2'	1:A:98:A:O5'	2.39	0.41
1:A:163:U:OP2	1:A:165:A:N6	2.54	0.41
1:A:186:G:H5''	25:Z:14:PHE:CD2	2.56	0.41
1:A:863:A:H5''	1:A:864:A:C8	2.55	0.41
1:A:1521:C:H2'	1:A:1522:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1807:G:H5''	17:R:92:ARG:HD3	2.02	0.41
1:A:2249:U:O2'	1:A:2250:C:OP1	2.36	0.41
1:A:2927:U:H2'	1:A:2928:G:C8	2.55	0.41
4:E:5:ILE:HD11	4:E:81:ILE:HG12	2.02	0.41
6:G:7:LEU:HD23	6:G:7:LEU:HA	1.90	0.41
6:G:119:GLY:O	6:G:120:ILE:HD13	2.21	0.41
8:I:2:LYS:HG3	8:I:39:SER:HB3	2.02	0.41
12:M:23:LYS:HA	12:M:23:LYS:HD3	1.89	0.41
12:M:97:ARG:NH1	12:M:99:PHE:CE2	2.88	0.41
13:N:52:THR:O	13:N:57:ARG:NH1	2.54	0.41
19:T:62:THR:HG23	19:T:99:ASP:OD2	2.21	0.41
28:c:55:HIS:CB	28:c:58:TYR:H	2.33	0.41
1:A:1030:U:H2'	1:A:1031:G:H8	1.86	0.41
1:A:1825:C:H2'	1:A:1826:G:C8	2.56	0.41
1:A:2345:G:H2'	1:A:2346:A:H8	1.86	0.41
1:A:2489:C:H2'	1:A:2490:G:H8	1.86	0.41
2:B:81:C:O3'	27:b:60:LYS:NZ	2.48	0.41
5:F:50:THR:O	5:F:92:LYS:NZ	2.41	0.41
6:G:64:THR:OG1	6:G:65:GLY:N	2.54	0.41
7:H:44:LYS:HB3	7:H:46:GLU:OE2	2.21	0.41
13:N:90:VAL:HA	13:N:94:THR:HG21	2.02	0.41
22:W:83:ILE:HD12	22:W:90:LYS:HE2	2.03	0.41
23:X:76:VAL:HG22	23:X:93:PHE:HE1	1.86	0.41
23:X:114:SER:HA	23:X:148:THR:HA	2.03	0.41
1:A:401:U:H4'	22:W:66:ASP:OD2	2.21	0.40
1:A:1432:G:H2'	1:A:1433:G:C8	2.56	0.40
1:A:2374:A:H2'	1:A:2375:A:C8	2.56	0.40
15:P:103:ARG:HG2	15:P:104:TYR:O	2.21	0.40
22:W:74:VAL:HG13	22:W:75:LYS:HG2	2.02	0.40
1:A:601:C:N4	1:A:2826:U:OP2	2.35	0.40
1:A:603:A:H4'	1:A:604:G:H21	1.87	0.40
1:A:953:U:H2'	1:A:954:G:C8	2.56	0.40
1:A:1050:C:O2'	1:A:1062:A:N3	2.53	0.40
1:A:2489:C:H2'	1:A:2490:G:C8	2.56	0.40
3:D:200:GLU:OE1	3:D:200:GLU:N	2.41	0.40
5:F:77:LYS:HB2	5:F:77:LYS:HE2	1.91	0.40
6:G:112:PRO:HG3	28:c:55:HIS:NE2	2.36	0.40
13:N:63:PHE:HD1	13:N:63:PHE:HA	1.78	0.40
14:O:54:MET:HG3	14:O:121:ALA:HB2	2.03	0.40
27:b:85:LYS:HE3	27:b:85:LYS:HB2	1.90	0.40
1:A:174:G:H3'	1:A:175:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:A:OP2	1:A:1213:A:O2'	2.31	0.40
1:A:1193:A:H2'	1:A:1194:C:C6	2.57	0.40
1:A:1462:A:O2'	1:A:1473:U:O2	2.30	0.40
1:A:1526:A:H2'	1:A:1527:G:C8	2.56	0.40
7:H:37:ILE:HD11	7:H:41:ILE:HB	2.03	0.40
7:H:84:SER:HB2	7:H:134:GLU:HG3	2.03	0.40
30:e:34:LYS:O	30:e:36:GLU:HG3	2.22	0.40
34:i:26:MET:HB3	34:i:39:ALA:HA	2.01	0.40
34:i:27:LYS:HB2	34:i:38:TYR:CE1	2.56	0.40
1:A:557:G:OP2	22:W:46:VAL:HG22	2.21	0.40
1:A:615:C:H2'	1:A:616:G:H8	1.87	0.40
1:A:940:G:HO2'	1:A:941:U:P	2.44	0.40
1:A:1597:U:H2'	1:A:1598:G:C8	2.56	0.40
1:A:1875:A:H2'	1:A:1876:G:C8	2.56	0.40
1:A:2008:G:O2'	1:A:2010:U:O4	2.33	0.40
1:A:2652:U:H2'	1:A:2653:G:C8	2.56	0.40
1:A:2782:A:OP1	34:i:49:ARG:NE	2.54	0.40
7:H:130:LYS:HE2	7:H:130:LYS:HB3	1.93	0.40
25:Z:53:ILE:HG13	25:Z:88:ILE:HD11	2.02	0.40
1:A:1287:G:H5'	1:A:1288:A:H2'	2.03	0.40
1:A:1524:C:H2'	1:A:1525:U:C6	2.56	0.40
1:A:1542:A:H2'	1:A:1543:G:C8	2.55	0.40
1:A:2873:G:H2'	1:A:2874:A:C8	2.56	0.40
3:D:262:LYS:HE2	3:D:262:LYS:HB3	1.86	0.40
11:L:34:VAL:O	11:L:38:VAL:HG23	2.22	0.40
15:P:57:VAL:HG13	15:P:62:ASN:ND2	2.37	0.40
18:S:21:THR:HG21	18:S:35:ALA:HB1	2.03	0.40
27:b:95:ILE:HD12	27:b:97:LEU:HD21	2.03	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	
3	D	275/277 (99%)	259 (94%)	16 (6%)	0	100	100
4	E	204/206 (99%)	194 (95%)	9 (4%)	1 (0%)	24	54
5	F	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
6	G	180/182 (99%)	167 (93%)	13 (7%)	0	100	100
7	H	178/180 (99%)	170 (96%)	8 (4%)	0	100	100
8	I	61/148 (41%)	52 (85%)	9 (15%)	0	100	100
9	J	130/162 (80%)	123 (95%)	7 (5%)	0	100	100
10	K	66/139 (48%)	65 (98%)	1 (2%)	0	100	100
11	L	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
12	M	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
13	N	143/145 (99%)	116 (81%)	27 (19%)	0	100	100
14	O	136/138 (99%)	119 (88%)	17 (12%)	0	100	100
15	P	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
16	Q	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
17	R	115/117 (98%)	105 (91%)	10 (9%)	0	100	100
18	S	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
19	T	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
20	U	113/115 (98%)	108 (96%)	5 (4%)	0	100	100
21	V	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	W	99/101 (98%)	91 (92%)	8 (8%)	0	100	100
23	X	179/181 (99%)	169 (94%)	10 (6%)	0	100	100
24	Y	72/74 (97%)	69 (96%)	3 (4%)	0	100	100
25	Z	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
26	a	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
27	b	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
28	c	56/81 (69%)	49 (88%)	7 (12%)	0	100	100
29	d	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
30	e	49/51 (96%)	42 (86%)	7 (14%)	0	100	100
31	f	48/50 (96%)	42 (88%)	6 (12%)	0	100	100
32	g	64/66 (97%)	56 (88%)	8 (12%)	0	100	100
33	h	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
34	i	44/46 (96%)	38 (86%)	6 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3569/3842 (93%)	3318 (93%)	250 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	164	ALA

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	
3	D	229/229 (100%)	229 (100%)	0	100	100
4	E	168/168 (100%)	168 (100%)	0	100	100
5	F	181/181 (100%)	181 (100%)	0	100	100
6	G	155/155 (100%)	155 (100%)	0	100	100
7	H	156/156 (100%)	156 (100%)	0	100	100
8	I	34/134 (25%)	34 (100%)	0	100	100
11	L	127/127 (100%)	127 (100%)	0	100	100
12	M	103/103 (100%)	103 (100%)	0	100	100
13	N	124/124 (100%)	124 (100%)	0	100	100
14	O	115/115 (100%)	115 (100%)	0	100	100
15	P	110/110 (100%)	110 (100%)	0	100	100
16	Q	104/104 (100%)	104 (100%)	0	100	100
17	R	103/103 (100%)	103 (100%)	0	100	100
18	S	99/99 (100%)	99 (100%)	0	100	100
19	T	96/96 (100%)	96 (100%)	0	100	100
20	U	100/100 (100%)	100 (100%)	0	100	100
21	V	88/88 (100%)	88 (100%)	0	100	100
22	W	89/89 (100%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	X	163/163 (100%)	163 (100%)	0	100	100
24	Y	60/60 (100%)	60 (100%)	0	100	100
25	Z	76/76 (100%)	76 (100%)	0	100	100
26	a	61/61 (100%)	61 (100%)	0	100	100
27	b	93/93 (100%)	93 (100%)	0	100	100
28	c	54/73 (74%)	54 (100%)	0	100	100
29	d	54/54 (100%)	54 (100%)	0	100	100
30	e	48/48 (100%)	48 (100%)	0	100	100
31	f	44/44 (100%)	44 (100%)	0	100	100
32	g	61/61 (100%)	61 (100%)	0	100	100
33	h	36/36 (100%)	36 (100%)	0	100	100
34	i	40/40 (100%)	40 (100%)	0	100	100
All	All	2971/3090 (96%)	2971 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	124	HIS
4	E	125	ASN
5	F	128	ASN
6	G	156	ASN
7	H	42	ASN
13	N	51	GLN
13	N	113	ASN
15	P	8	ASN
15	P	61	HIS
16	Q	52	HIS
17	R	51	ASN
17	R	101	ASN
22	W	88	ASN
23	X	90	HIS
23	X	99	ASN
25	Z	55	ASN
27	b	42	ASN
29	d	54	GLN
32	g	50	ASN

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Mol	Chain	Res	Type
34	i	32	ASN
34	i	46	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2756/2929 (94%)	400 (14%)	29 (1%)
2	B	111/112 (99%)	28 (25%)	4 (3%)
All	All	2867/3041 (94%)	428 (14%)	33 (1%)

All (428) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	A
1	A	17	A
1	A	27	G
1	A	38	A
1	A	39	G
1	A	68	A
1	A	75	A
1	A	78	A
1	A	79	G
1	A	89	G
1	A	94	A
1	A	97	C
1	A	98	A
1	A	99	U
1	A	100	U
1	A	121	A
1	A	123	U
1	A	131	U
1	A	143	G
1	A	145	U
1	A	160	A
1	A	163	U
1	A	164	A
1	A	165	A
1	A	167	U
1	A	170	U
1	A	178	A
1	A	179	U

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Mol	Chain	Res	Type
1	A	180	A
1	A	194	A
1	A	197	A
1	A	204	U
1	A	211	A
1	A	214	A
1	A	220	A
1	A	226	A
1	A	227	G
1	A	228	A
1	A	230	A
1	A	245	G
1	A	263	G
1	A	282	C
1	A	283	A
1	A	287	U
1	A	288	G
1	A	293	G
1	A	294	C
1	A	295	G
1	A	296	U
1	A	297	U
1	A	298	G
1	A	309	G
1	A	312	G
1	A	313	U
1	A	314	A
1	A	319	G
1	A	322	U
1	A	324	G
1	A	330	G
1	A	337	A
1	A	349	G
1	A	350	U
1	A	351	U
1	A	353	C
1	A	358	U
1	A	361	U
1	A	362	U
1	A	373	A
1	A	374	U
1	A	384	A

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Mol	Chain	Res	Type
1	A	415	U
1	A	425	A
1	A	428	A
1	A	435	U
1	A	436	A
1	A	439	A
1	A	440	U
1	A	449	G
1	A	461	A
1	A	463	G
1	A	478	A
1	A	501	G
1	A	513	G
1	A	528	A
1	A	532	G
1	A	533	A
1	A	534	G
1	A	557	G
1	A	579	U
1	A	580	A
1	A	582	A
1	A	584	C
1	A	592	G
1	A	604	G
1	A	605	C
1	A	606	A
1	A	607	G
1	A	621	U
1	A	622	U
1	A	628	G
1	A	639	G
1	A	649	U
1	A	650	A
1	A	651	A
1	A	662	A
1	A	679	A
1	A	693	A
1	A	694	A
1	A	695	G
1	A	696	U
1	A	697	G
1	A	708	A

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Mol	Chain	Res	Type
1	A	718	A
1	A	726	A
1	A	727	A
1	A	728	G
1	A	734	U
1	A	735	U
1	A	736	U
1	A	768	U
1	A	796	U
1	A	799	A
1	A	803	A
1	A	805	G
1	A	812	G
1	A	829	U
1	A	830	U
1	A	835	A
1	A	846	A
1	A	857	G
1	A	864	A
1	A	866	G
1	A	871	A
1	A	884	A
1	A	887	G
1	A	888	C
1	A	894	C
1	A	909	U
1	A	929	G
1	A	940	G
1	A	941	U
1	A	959	A
1	A	966	G
1	A	967	U
1	A	968	C
1	A	970	A
1	A	975	U
1	A	976	A
1	A	990	A
1	A	1011	A
1	A	1025	G
1	A	1032	G
1	A	1038	A
1	A	1040	G

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Mol	Chain	Res	Type
1	A	1053	G
1	A	1062	A
1	A	1075	A
1	A	1090	A
1	A	1092	U
1	A	1100	G
1	A	1104	A
1	A	1111	G
1	A	1124	A
1	A	1125	A
1	A	1139	U
1	A	1140	G
1	A	1142	C
1	A	1147	A
1	A	1148	A
1	A	1149	G
1	A	1151	A
1	A	1152	G
1	A	1156	U
1	A	1157	A
1	A	1158	C
1	A	1159	C
1	A	1162	U
1	A	1163	A
1	A	1164	A
1	A	1166	G
1	A	1168	G
1	A	1169	U
1	A	1174	A
1	A	1175	A
1	A	1186	G
1	A	1191	G
1	A	1193	A
1	A	1201	G
1	A	1211	U
1	A	1212	A
1	A	1214	C
1	A	1221	A
1	A	1230	A
1	A	1261	A
1	A	1286	A
1	A	1288	A

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Mol	Chain	Res	Type
1	A	1294	U
1	A	1304	A
1	A	1307	U
1	A	1315	G
1	A	1333	G
1	A	1348	G
1	A	1349	A
1	A	1350	A
1	A	1377	A
1	A	1378	A
1	A	1379	A
1	A	1398	A
1	A	1402	G
1	A	1410	C
1	A	1418	U
1	A	1427	C
1	A	1429	U
1	A	1442	A
1	A	1455	A
1	A	1456	U
1	A	1457	G
1	A	1460	A
1	A	1473	U
1	A	1484	C
1	A	1485	U
1	A	1490	G
1	A	1493	U
1	A	1494	C
1	A	1498	G
1	A	1505	C
1	A	1520	A
1	A	1524	C
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1538	U
1	A	1539	C
1	A	1554	A
1	A	1559	G
1	A	1560	A
1	A	1561	U
1	A	1563	A

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Mol	Chain	Res	Type
1	A	1564	U
1	A	1565	C
1	A	1568	A
1	A	1571	A
1	A	1577	A
1	A	1578	U
1	A	1580	C
1	A	1581	G
1	A	1588	G
1	A	1594	A
1	A	1603	G
1	A	1610	G
1	A	1611	C
1	A	1616	U
1	A	1618	G
1	A	1620	U
1	A	1621	A
1	A	1623	C
1	A	1627	A
1	A	1630	U
1	A	1631	G
1	A	1636	U
1	A	1637	A
1	A	1638	G
1	A	1649	A
1	A	1652	A
1	A	1655	U
1	A	1662	U
1	A	1668	U
1	A	1669	A
1	A	1670	G
1	A	1671	G
1	A	1679	G
1	A	1680	G
1	A	1681	A
1	A	1682	C
1	A	1691	A
1	A	1704	U
1	A	1709	G
1	A	1729	C
1	A	1730	G
1	A	1731	C

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Mol	Chain	Res	Type
1	A	1736	G
1	A	1737	A
1	A	1757	G
1	A	1810	U
1	A	1811	A
1	A	1812	A
1	A	1818	G
1	A	1827	A
1	A	1841	A
1	A	1854	C
1	A	1870	A
1	A	1883	A
1	A	1984	G
1	A	2009	U
1	A	2024	A
1	A	2026	G
1	A	2045	U
1	A	2047	U
1	A	2051	A
1	A	2073	A
1	A	2074	A
1	A	2075	G
1	A	2076	U
1	A	2077	A
1	A	2084	A
1	A	2085	A
1	A	2086	G
1	A	2087	A
1	A	2097	C
1	A	2106	A
1	A	2109	C
1	A	2110	G
1	A	2114	A
1	A	2115	G
1	A	2116	A
1	A	2122	U
1	A	2123	G
1	A	2130	U
1	A	2149	G
1	A	2153	U
1	A	2154	G
1	A	2158	A

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Mol	Chain	Res	Type
1	A	2244	A
1	A	2245	G
1	A	2249	U
1	A	2250	C
1	A	2252	A
1	A	2253	A
1	A	2256	U
1	A	2271	A
1	A	2284	G
1	A	2285	G
1	A	2329	C
1	A	2333	A
1	A	2334	A
1	A	2351	U
1	A	2354	G
1	A	2355	A
1	A	2379	A
1	A	2393	C
1	A	2396	U
1	A	2418	U
1	A	2429	G
1	A	2431	C
1	A	2452	A
1	A	2469	U
1	A	2471	A
1	A	2474	G
1	A	2475	A
1	A	2476	A
1	A	2477	U
1	A	2487	U
1	A	2494	A
1	A	2516	G
1	A	2521	C
1	A	2522	A
1	A	2527	G
1	A	2537	U
1	A	2551	G
1	A	2564	A
1	A	2581	G
1	A	2600	U
1	A	2608	U
1	A	2612	A

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Mol	Chain	Res	Type
1	A	2613	G
1	A	2618	A
1	A	2648	A
1	A	2655	U
1	A	2659	U
1	A	2661	U
1	A	2675	U
1	A	2735	U
1	A	2748	G
1	A	2756	U
1	A	2758	A
1	A	2759	G
1	A	2761	G
1	A	2773	C
1	A	2780	A
1	A	2791	G
1	A	2795	A
1	A	2805	A
1	A	2808	G
1	A	2813	G
1	A	2825	A
1	A	2827	G
1	A	2832	A
1	A	2837	U
1	A	2838	U
1	A	2855	U
1	A	2863	U
1	A	2897	A
1	A	2902	G
1	A	2903	A
1	A	2910	C
1	A	2914	U
1	A	2916	A
1	A	2917	C
1	A	2921	U
1	A	2923	U
2	B	2	C
2	B	11	U
2	B	12	A
2	B	13	A
2	B	14	A
2	B	23	G

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Mol	Chain	Res	Type
2	B	31	U
2	B	32	G
2	B	35	A
2	B	36	U
2	B	40	U
2	B	41	C
2	B	42	C
2	B	43	G
2	B	50	G
2	B	51	A
2	B	56	A
2	B	66	U
2	B	67	C
2	B	72	A
2	B	83	A
2	B	84	G
2	B	86	U
2	B	87	C
2	B	99	G
2	B	103	A
2	B	108	C
2	B	112	G

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	C
1	A	142	A
1	A	179	U
1	A	225	A
1	A	329	A
1	A	350	U
1	A	372	A
1	A	532	G
1	A	928	A
1	A	940	G
1	A	1091	A
1	A	1146	G
1	A	1155	A
1	A	1192	U
1	A	1426	C
1	A	1484	C

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Mol	Chain	Res	Type
1	A	1523	G
1	A	1538	U
1	A	1577	A
1	A	1617	A
1	A	1622	G
1	A	1635	G
1	A	1636	U
1	A	1668	U
1	A	2152	U
1	A	2249	U
1	A	2755	G
1	A	2831	U
1	A	2837	U
2	B	31	U
2	B	34	U
2	B	35	A
2	B	86	U

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

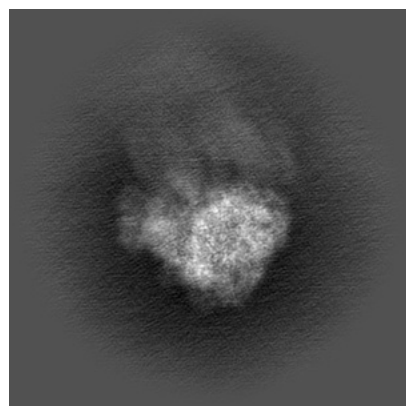
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29304. These allow visual inspection of the internal detail of the map and identification of artifacts.

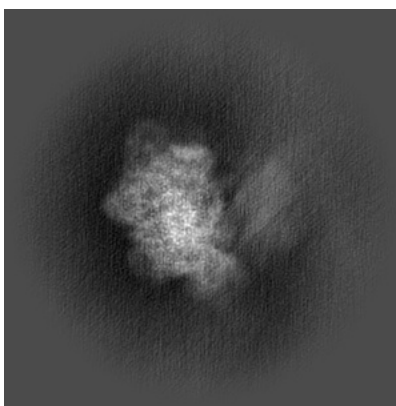
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

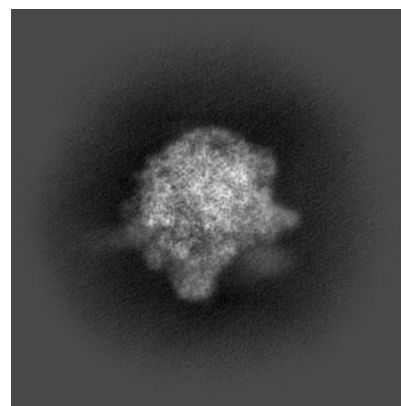
6.1.1 Primary map



X

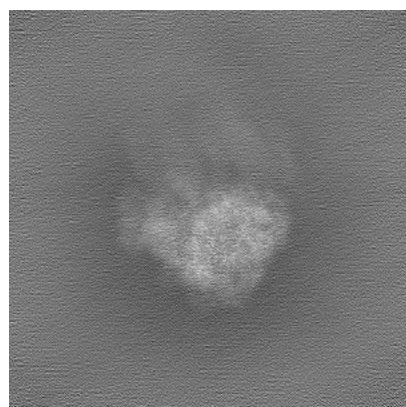


Y

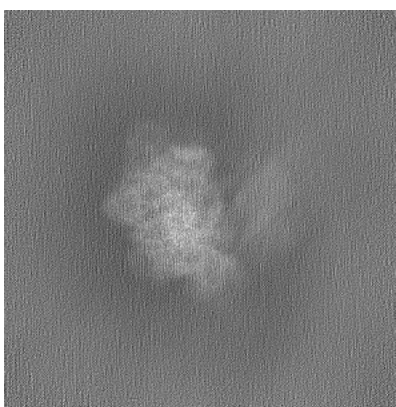


Z

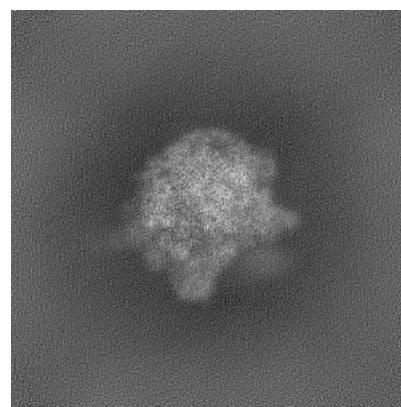
6.1.2 Raw map



X



Y

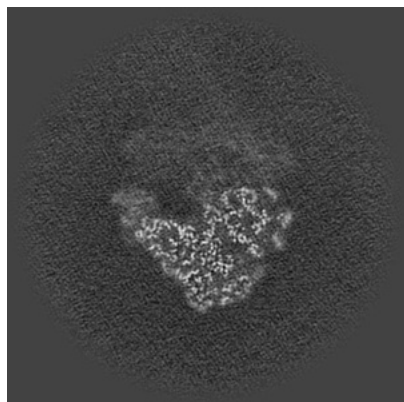


Z

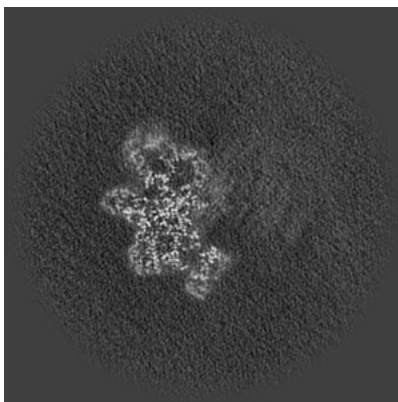
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

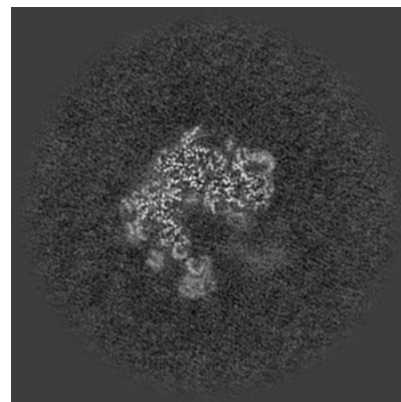
6.2.1 Primary map



X Index: 225

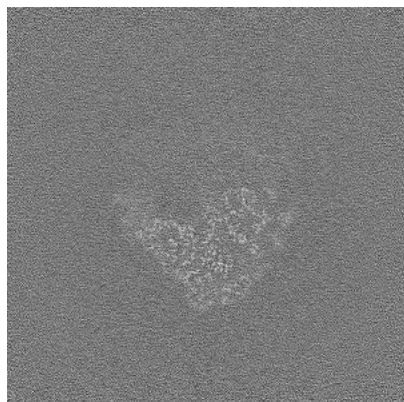


Y Index: 225

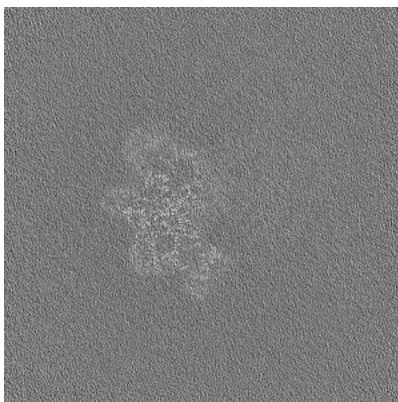


Z Index: 225

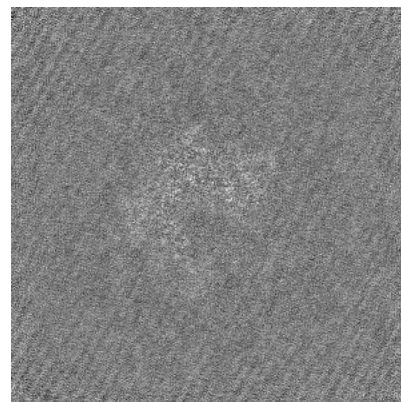
6.2.2 Raw map



X Index: 225



Y Index: 225

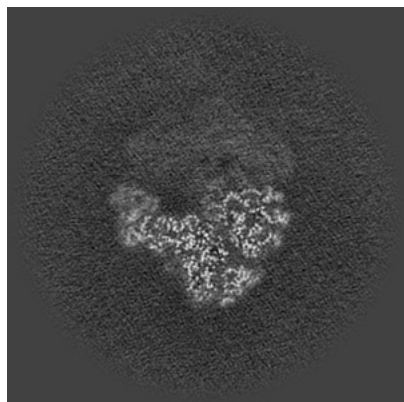


Z Index: 225

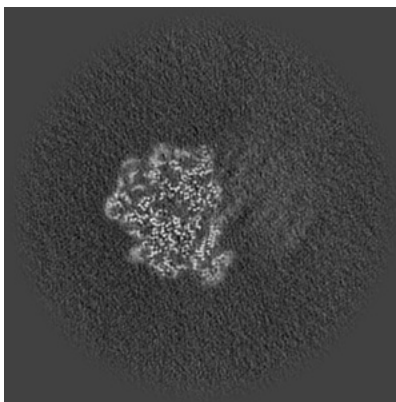
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

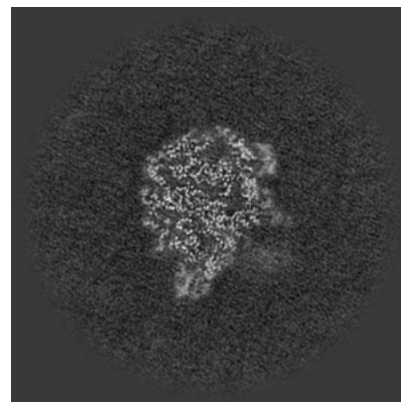
6.3.1 Primary map



X Index: 220

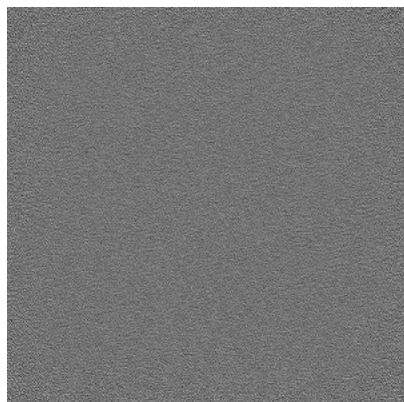


Y Index: 242

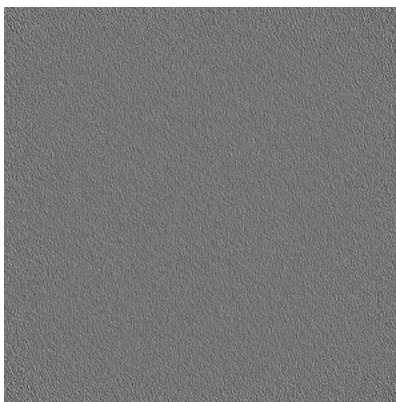


Z Index: 192

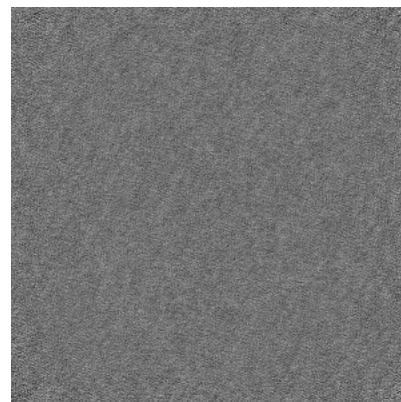
6.3.2 Raw map



X Index: 0



Y Index: 0

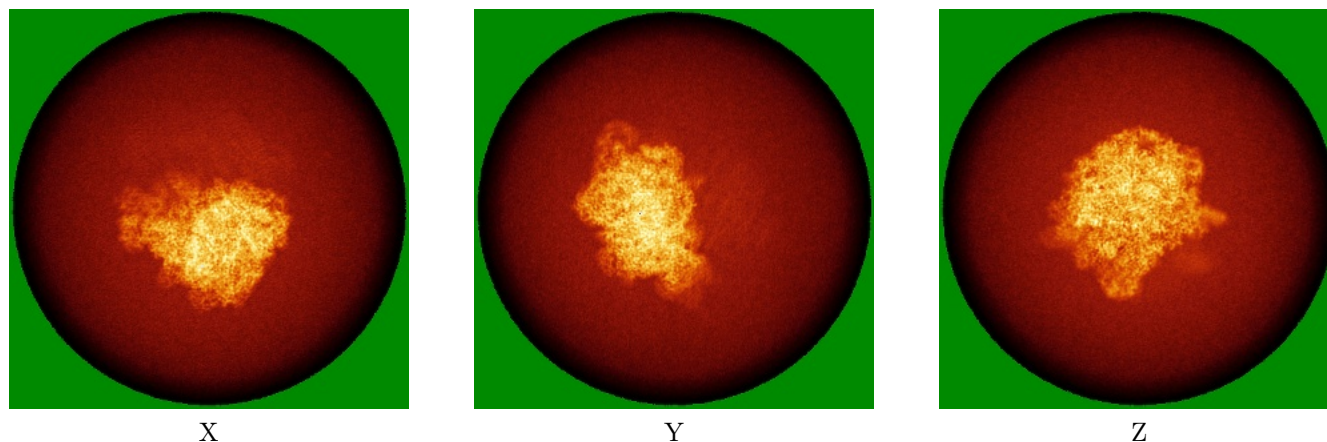


Z Index: 0

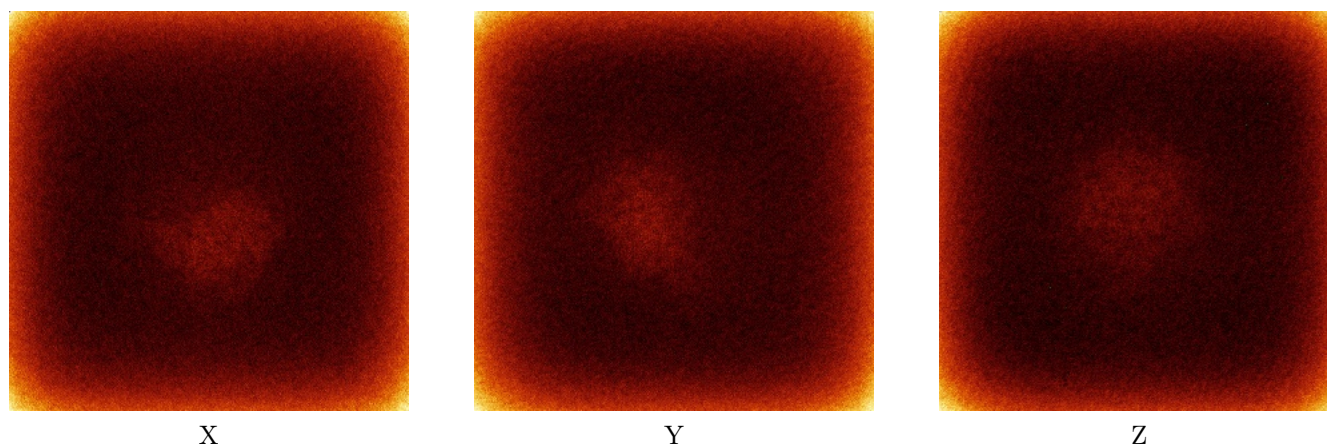
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



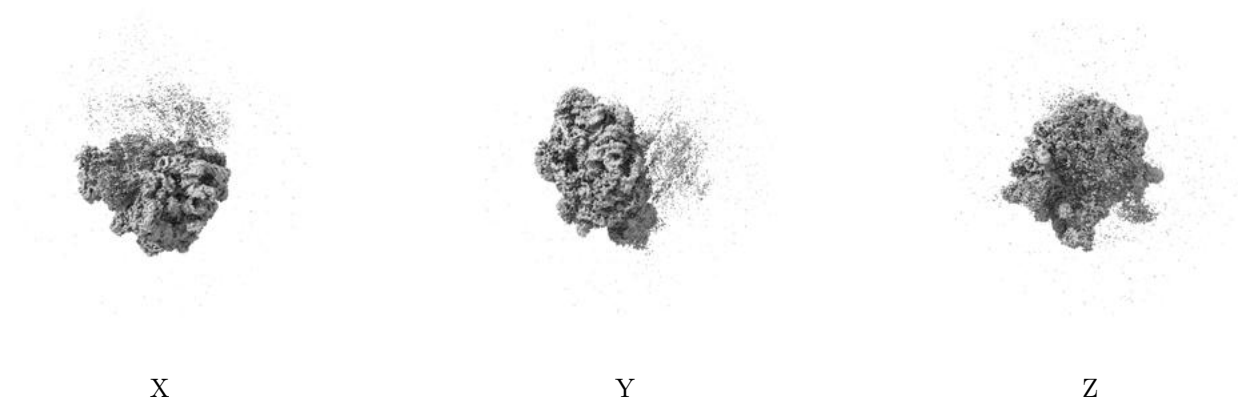
6.4.2 Raw map



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.

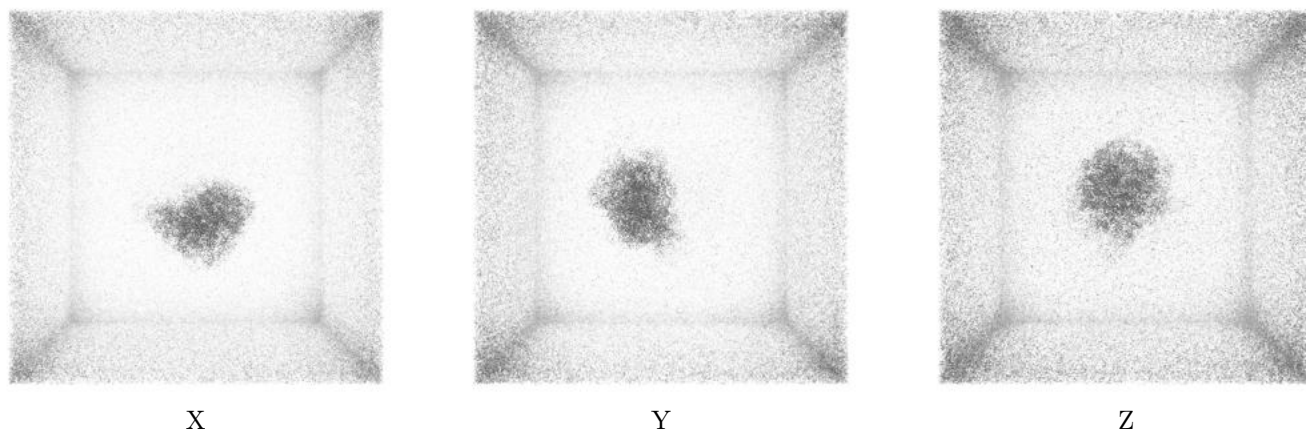
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

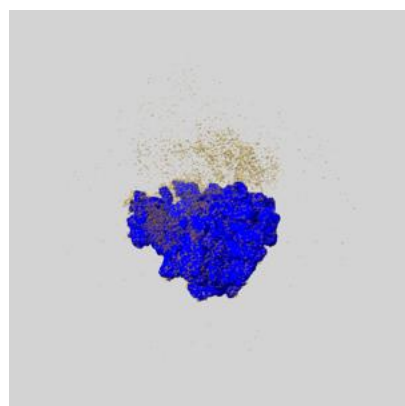
6.6 Mask visualisation [i](#)

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

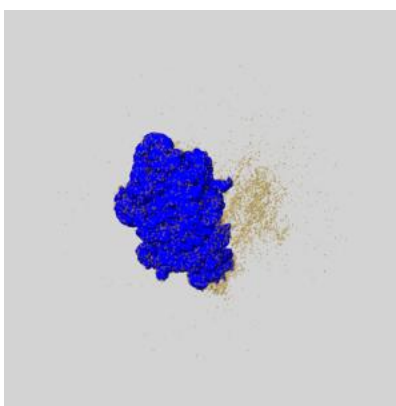
A mask typically either:

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

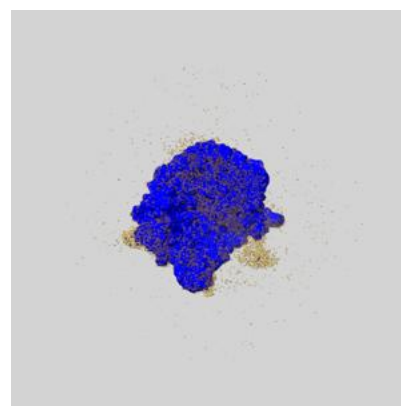
6.6.1 emd_29304_msk_1.map [i](#)



X



Y

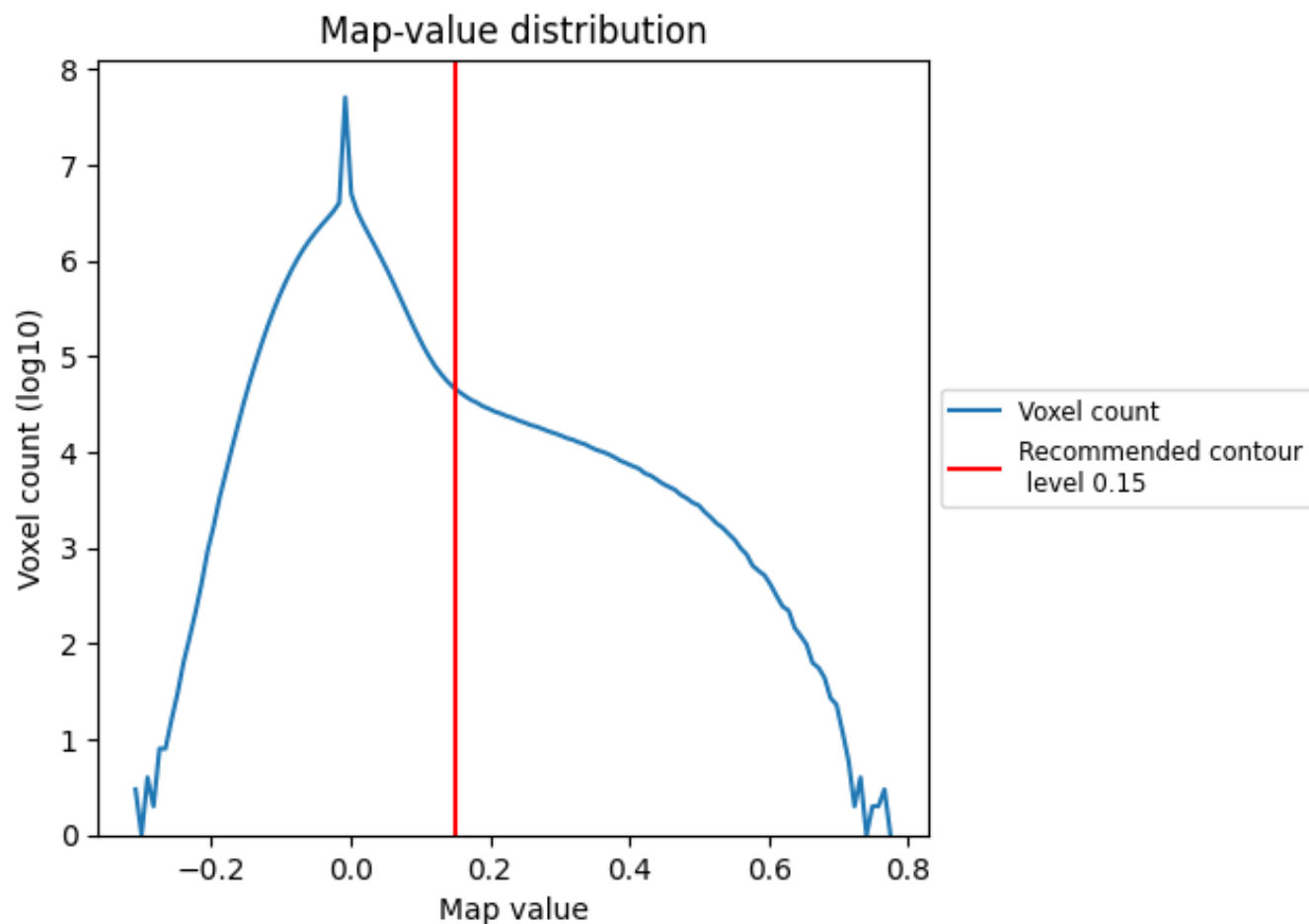


Z

7 Map analysis [i](#)

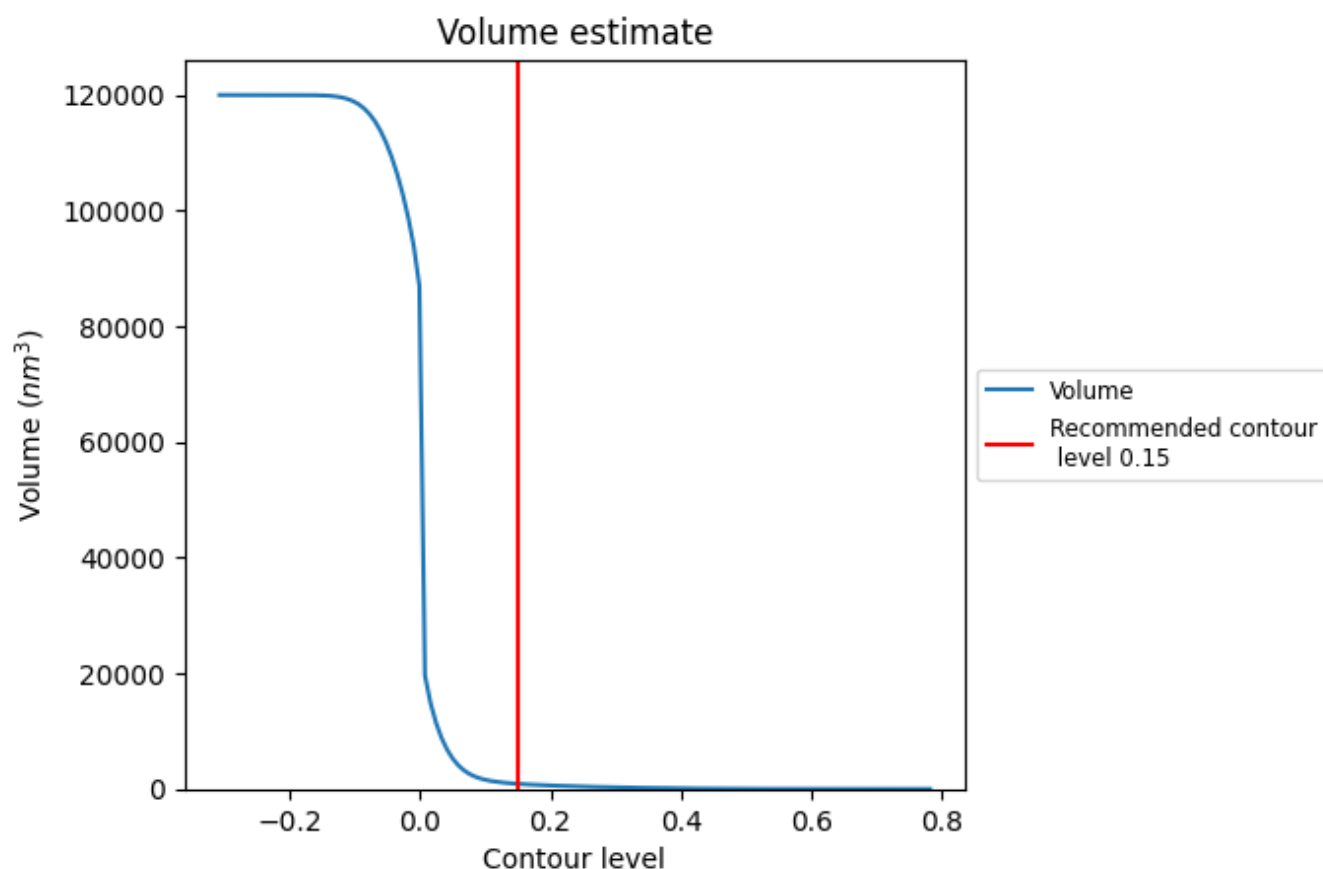
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

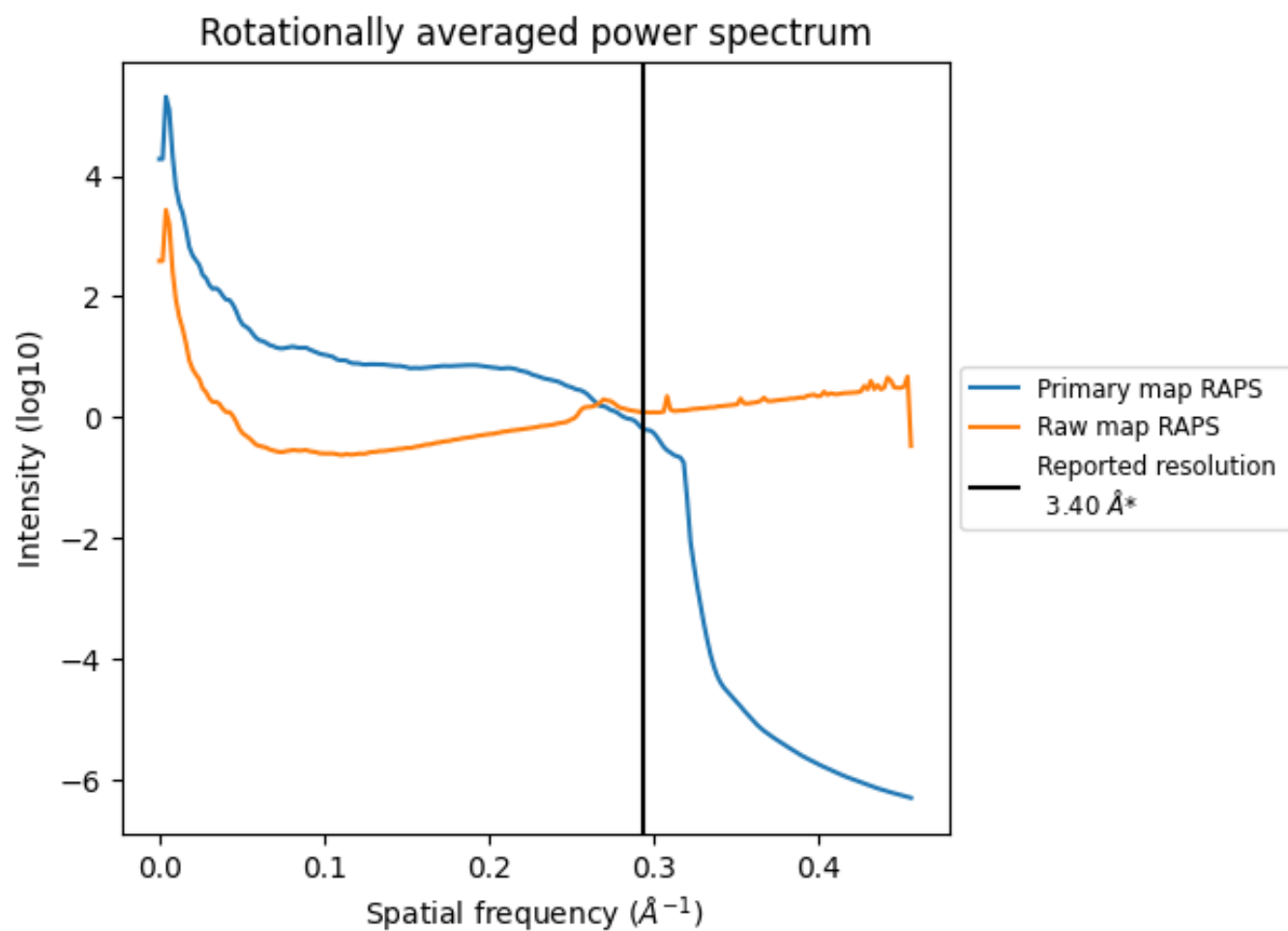
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 888 nm^3 ; this corresponds to an approximate mass of 802 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](#)

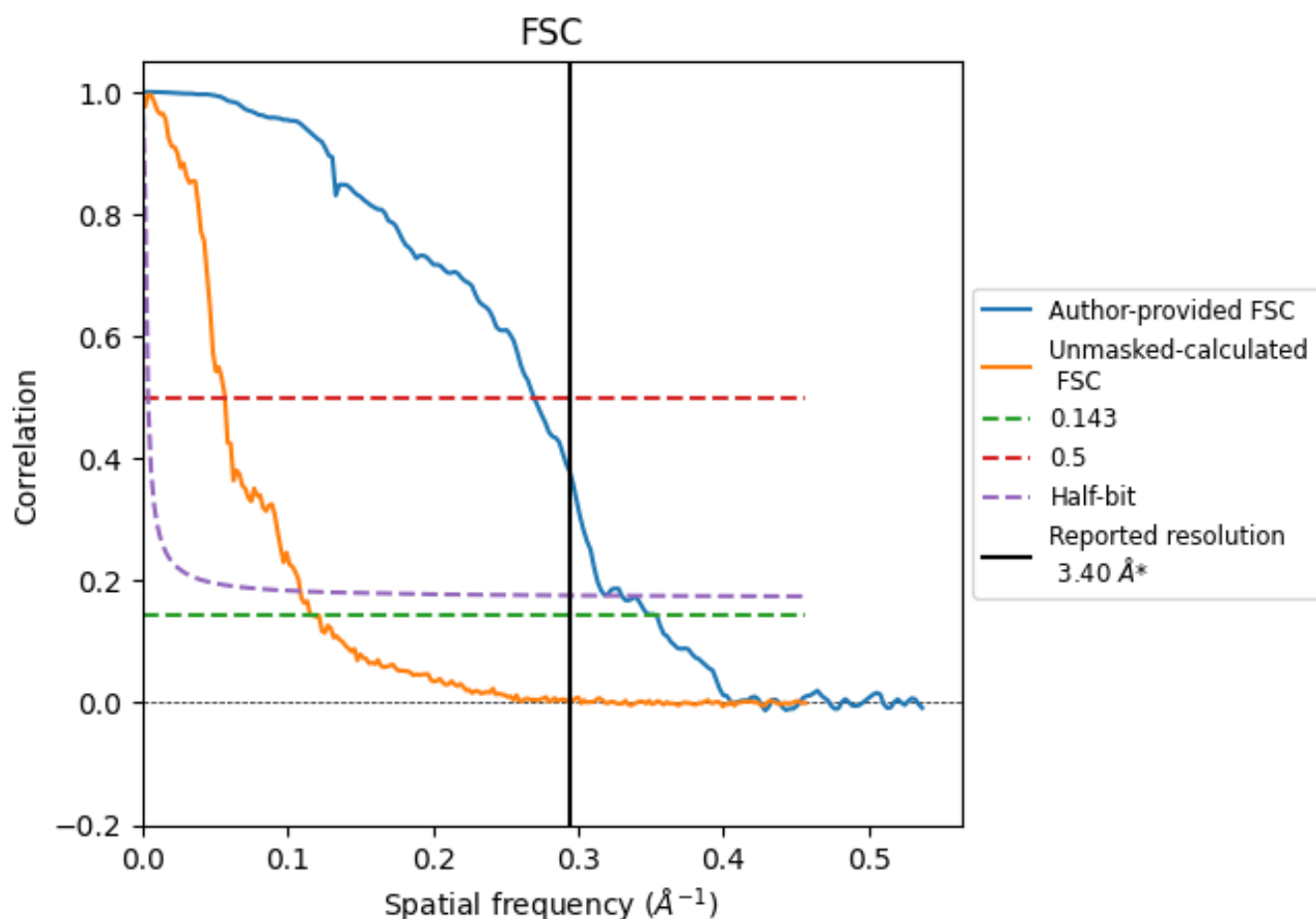


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	2.83	3.71	3.03
Unmasked-calculated*	8.56	17.61	9.20

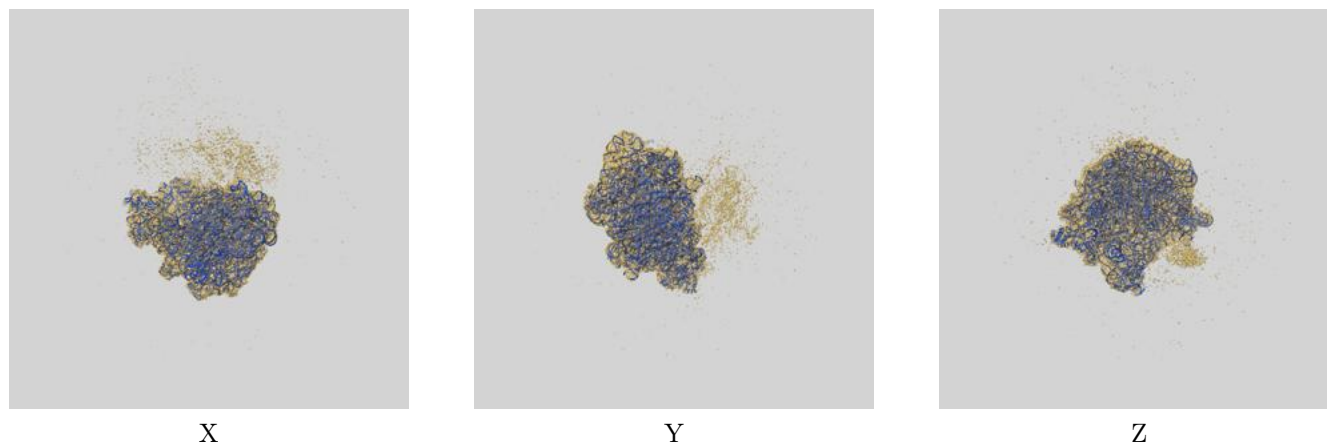
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.83 differs from the reported value 3.4 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.56 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

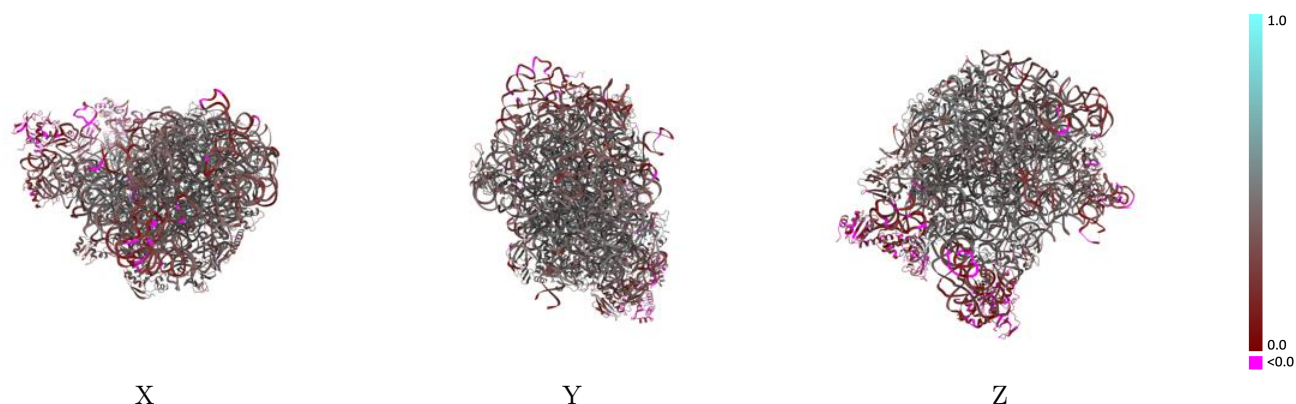
This section contains information regarding the fit between EMDB map EMD-29304 and PDB model 8FN2. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



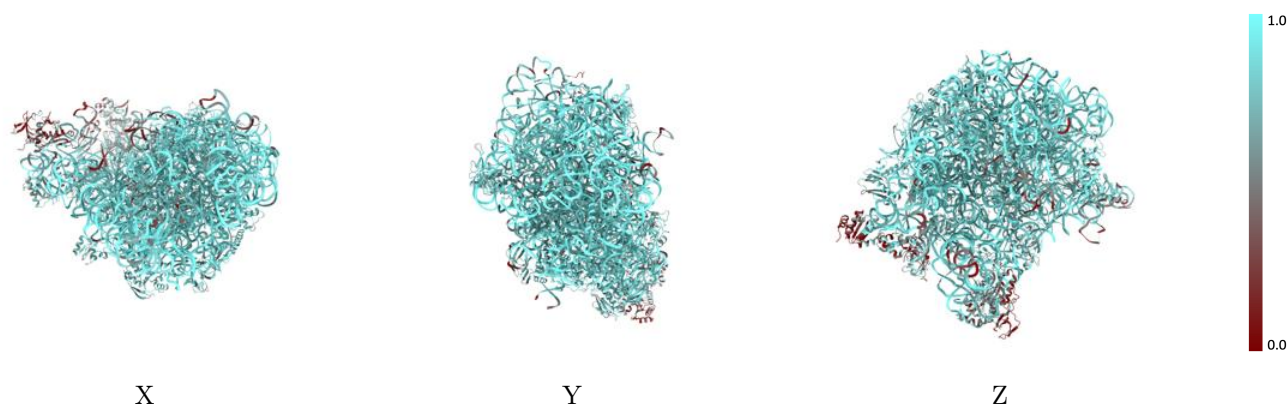
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



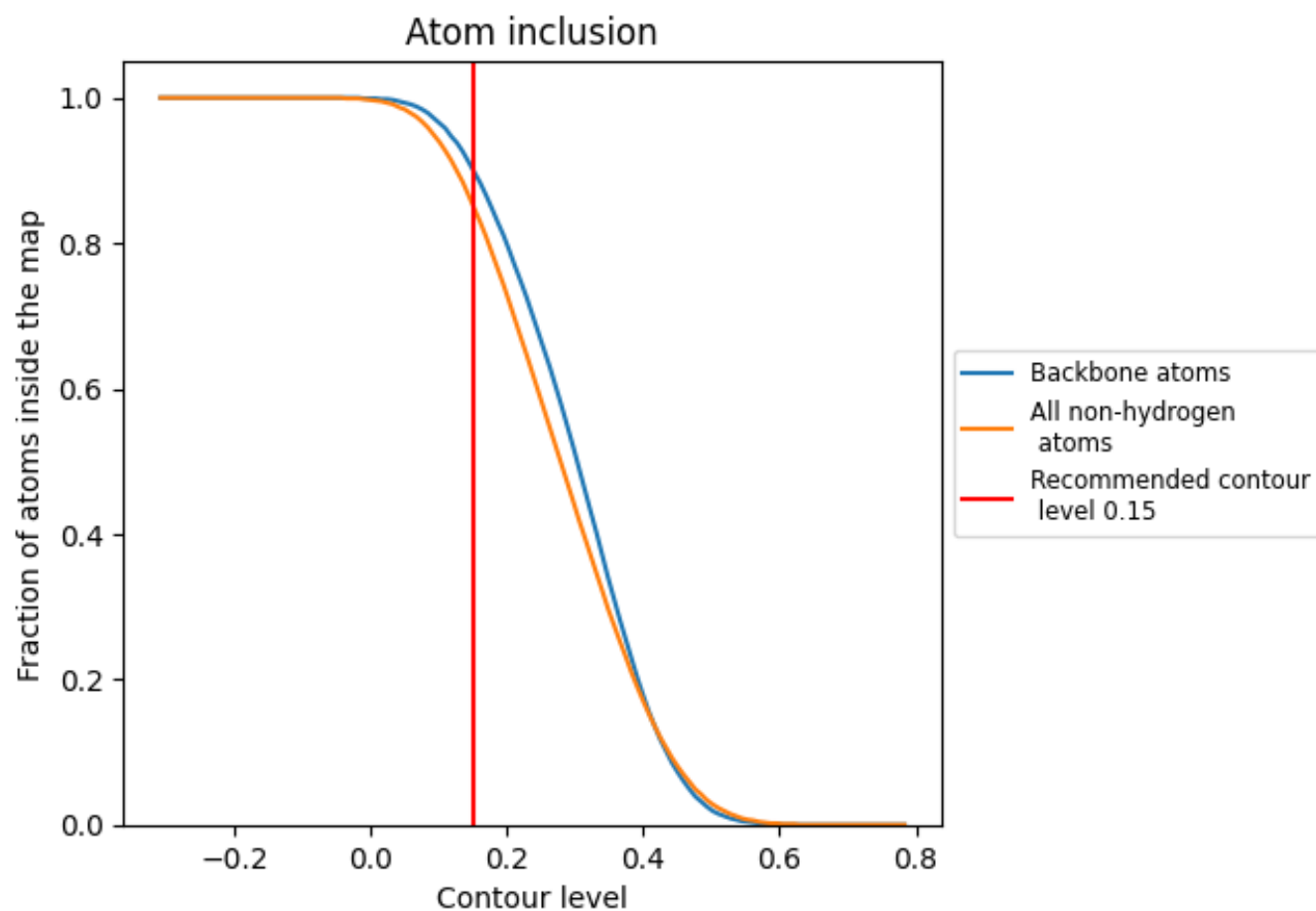
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 85% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.3790
A	 0.9040	 0.3840
B	 0.8670	 0.2810
D	 0.7870	 0.4120
E	 0.8290	 0.4580
F	 0.8020	 0.4350
G	 0.4380	 0.1240
H	 0.7640	 0.3160
I	 0.4700	 0.2440
J	 0.3300	 0.0820
K	 0.4410	 0.1380
L	 0.8560	 0.4610
M	 0.8280	 0.4500
N	 0.7710	 0.4030
O	 0.7700	 0.4310
P	 0.8480	 0.4660
Q	 0.6920	 0.2590
R	 0.7530	 0.4080
S	 0.8400	 0.4570
T	 0.7800	 0.4350
U	 0.8250	 0.4700
V	 0.7850	 0.4070
W	 0.6800	 0.3480
X	 0.6480	 0.2740
Y	 0.8410	 0.4760
Z	 0.7840	 0.4240
a	 0.7800	 0.3520
b	 0.8110	 0.4600
c	 0.2300	 0.0510
d	 0.8460	 0.4530
e	 0.6840	 0.3570
f	 0.8450	 0.4940
g	 0.8150	 0.4720
h	 0.8020	 0.4450
i	 0.8000	 0.3120

