



Full wwPDB EM Validation Report ⓘ

Jun 24, 2026 – 02:55 AM EDT

PDB ID : 6PJ6 / pdb_00006pj6
EMDB ID : EMD-20353
Title : High resolution cryo-EM structure of E.coli 50S
Authors : Stojkovic, V.; Myasnikov, A.; Frost, A.; Fujimori, D.G.
Deposited on : 2019-06-27
Resolution : 2.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

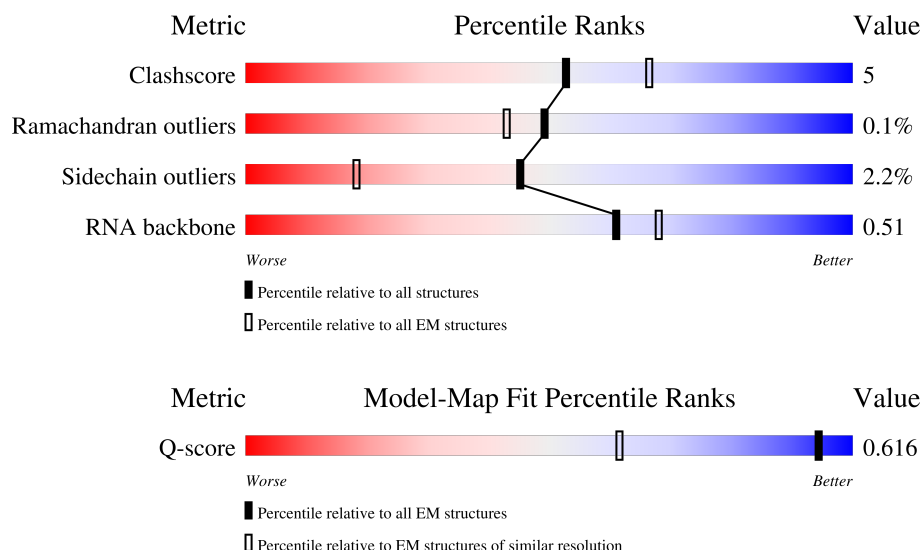
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.20 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	3184 (1.71 - 2.70)

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	I	2904	
2	J	118	
3	K	271	

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Mol	Chain	Length	Quality of chain
4	L	209	
5	M	201	
6	N	177	
7	O	176	
8	P	149	
9	Q	134	
10	R	142	
11	S	122	
12	T	144	
13	U	136	
14	V	120	
15	W	117	
16	X	114	
17	Y	117	
18	Z	103	
19	a	110	
20	b	93	
21	c	102	
22	d	94	
23	e	75	
24	f	77	
25	g	62	
26	h	58	
27	i	56	
28	j	50	

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Mol	Chain	Length	Quality of chain
29	k	46	 78% 20% .
30	l	64	 84% 14% .
31	m	38	 8% 79% 18% .

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 154828 atoms, of which 59910 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 rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	I	2898	Total	C	H	N	O	P	0	0
			93536	27768	31307	11448	20115	2898		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	118	Total	C	H	N	O	P	0	0
			3810	1126	1281	464	821	118		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	271	Total	C	H	N	O	S	1	0
			4261	1294	2167	427	366	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	L	209	Total	C	H	N	O	S	0	0
			3175	979	1610	288	294	4		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	M	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	N	177	Total	C	H	N	O	S	0	0
			2855	899	1444	249	257	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	176	Total	C	H	N	O	S	0	0
			2694	832	1371	243	246	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	149	Total	C	H	N	O	S	0	0
			2258	699	1148	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	134	Total	C	H	N	O	S	0	0
			2007	619	1028	169	185	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	T	144	Total	C	H	N	O	S	0	0
			2169	654	1116	207	190	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	U	136	Total	C	H	N	O	S	0	0
			2229	686	1154	205	178	6		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	120	Total	C	H	N	O	S	
			1960	593	1000	196	166	5	0
									0

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	116	Total	C	H	N	O	S	
			1815	552	923	178	162		0
									0

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	114	Total	C	H	N	O	S	
			1879	574	962	179	163	1	0
									0

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	117	Total	C	H	N	O	S	
			1967	604	1020	192	151		0
									0

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	103	Total	C	H	N	O	S	
			1582	516	766	153	145	2	0
									0

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	110	Total	C	H	N	O	S	
			1779	532	922	166	156	3	0
									0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	93	Total	C	H	N	O	S	
			1546	466	807	139	132	2	0
									0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	102	Total	C	H	N	O	0	0
			1611	492	831	146	142		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	e	75	Total	C	H	N	O	S	0	0
			1156	356	581	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	f	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	g	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	h	58	Total	C	H	N	O	S	0	0
			937	281	488	87	79	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	i	56	Total	C	H	N	O	S	0	0
			902	269	458	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	50	Total	C	H	N	O	0	0
			849	263	440	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	l	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	m	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	I	182	Total	Mg	0
			182	182	
32	J	1	Total	Mg	0
			1	1	
32	K	1	Total	Mg	0
			1	1	
32	L	1	Total	Mg	0
			1	1	

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
33	K	1	Total	Na	0
			1	1	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	m	1	Total 1	Zn 1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	I	3347	Total 3347	O 3347	0
35	J	62	Total 62	O 62	0
35	K	59	Total 59	O 59	0
35	L	41	Total 41	O 41	0
35	M	42	Total 42	O 42	0
35	N	14	Total 14	O 14	0
35	O	13	Total 13	O 13	0
35	P	6	Total 6	O 6	0
35	Q	10	Total 10	O 10	0
35	R	17	Total 17	O 17	0
35	S	7	Total 7	O 7	0
35	T	33	Total 33	O 33	0
35	U	13	Total 13	O 13	0
35	V	23	Total 23	O 23	0
35	W	11	Total 11	O 11	0
35	X	14	Total 14	O 14	0
35	Y	33	Total 33	O 33	0
35	Z	16	Total 16	O 16	0
35	a	18	Total 18	O 18	0

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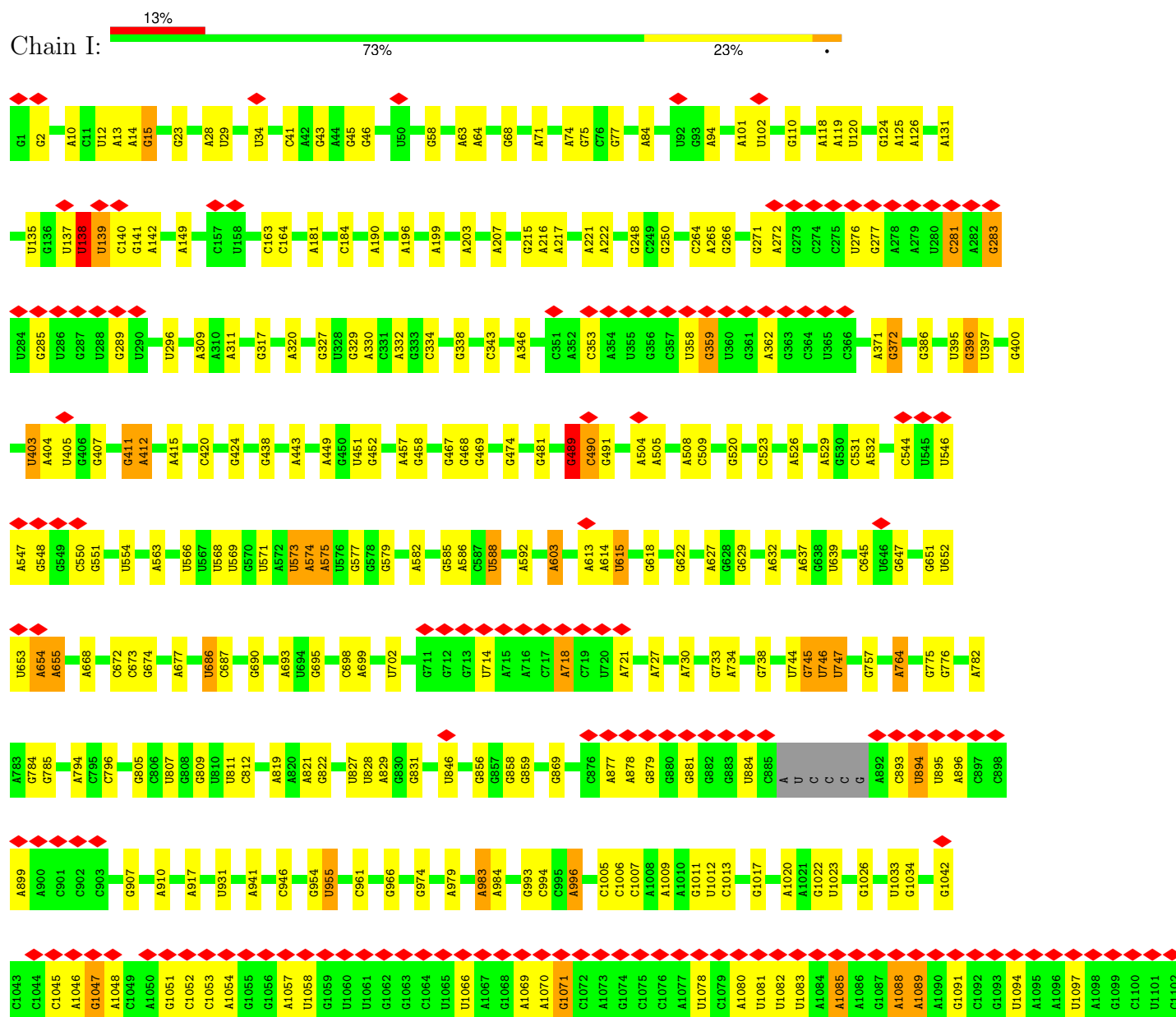
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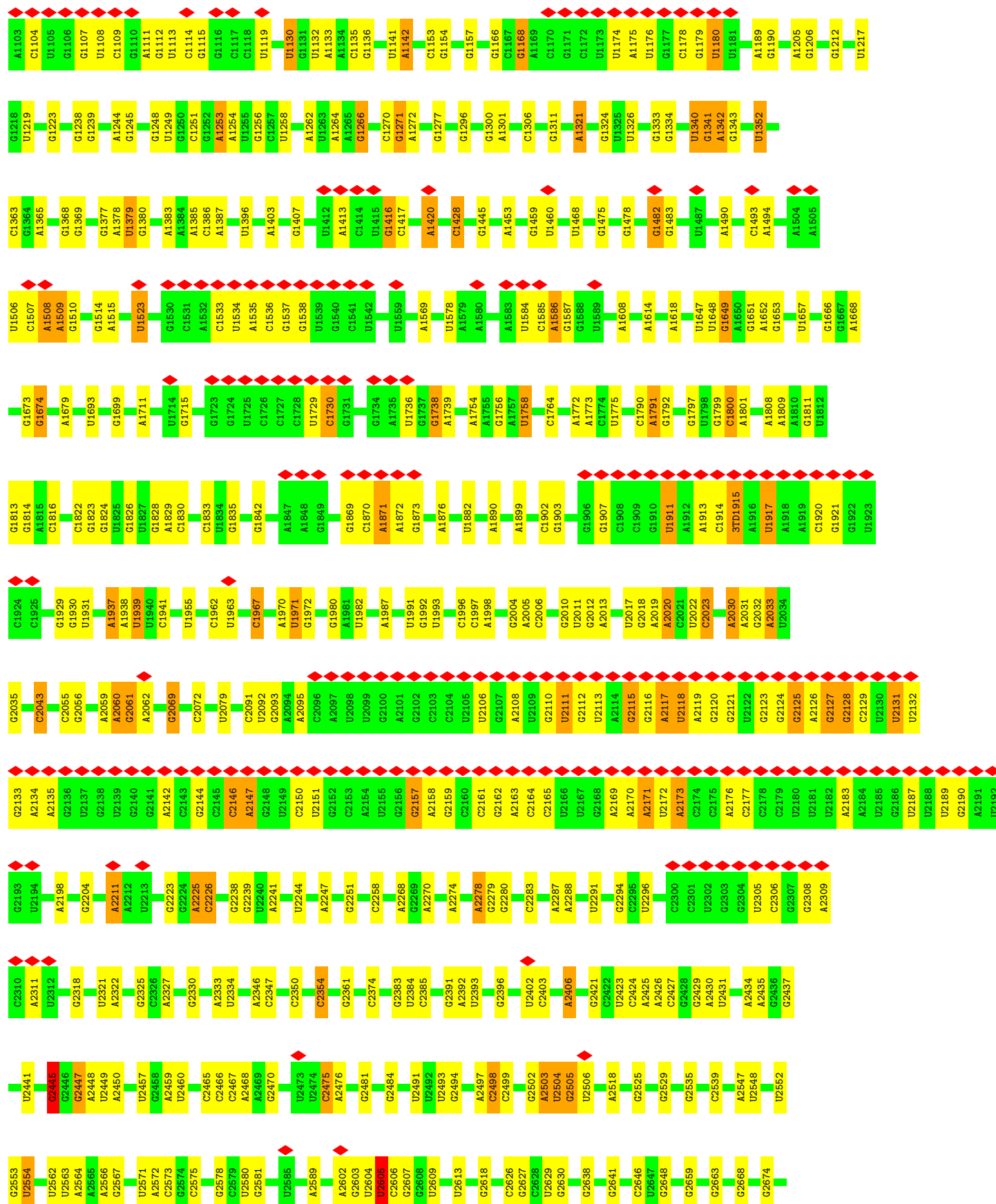
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35	e	13	Total 13	O 13	0
35	f	9	Total 9	O 9	0
35	g	6	Total 6	O 6	0
35	h	4	Total 4	O 4	0
35	i	12	Total 12	O 12	0
35	j	9	Total 9	O 9	0
35	k	11	Total 11	O 11	0
35	l	19	Total 19	O 19	0
35	m	4	Total 4	O 4	0

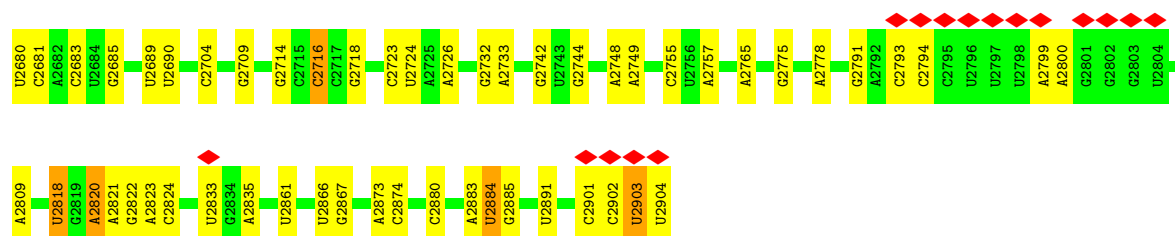
3 Residue-property plots

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.

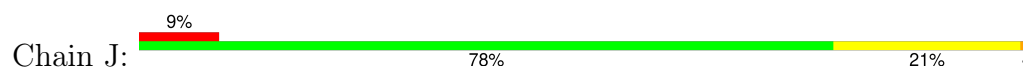
• Molecule 1: 23S rRNA



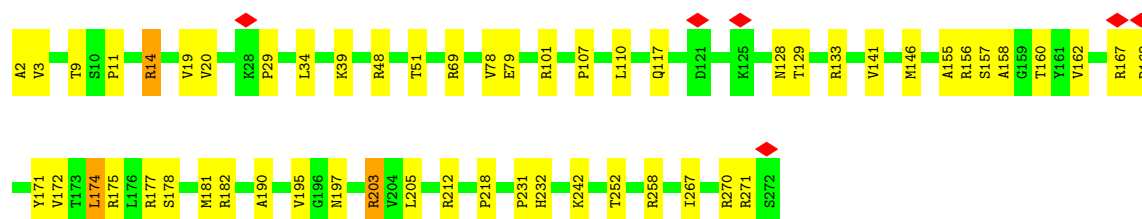
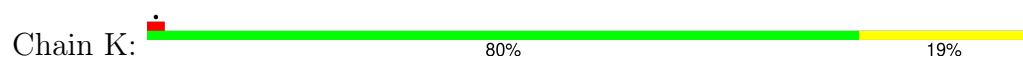




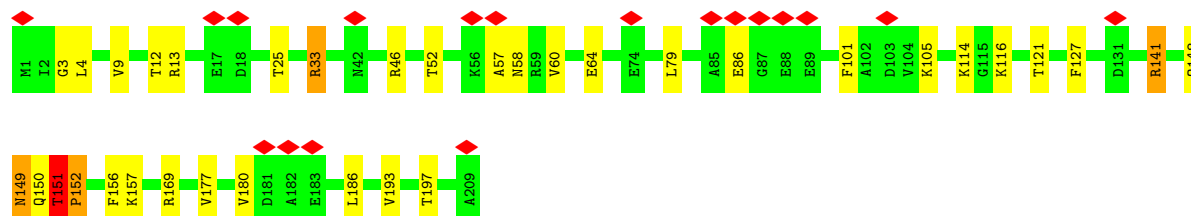
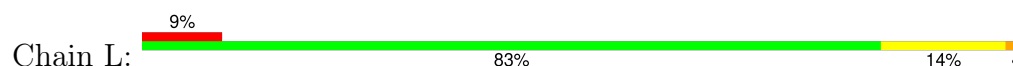
• Molecule 2: 5S rRNA



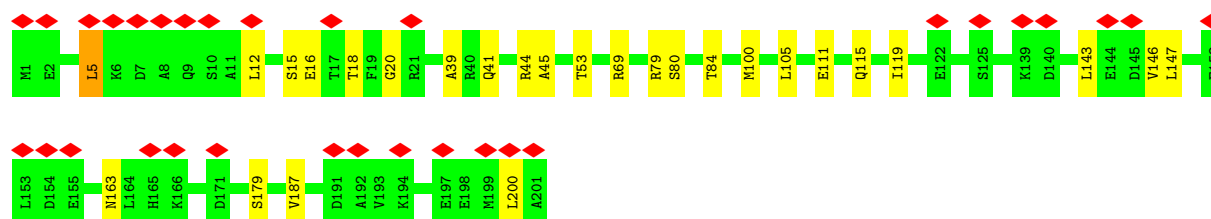
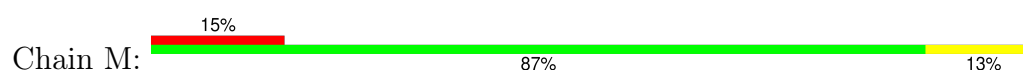
• Molecule 3: 50S ribosomal protein L2



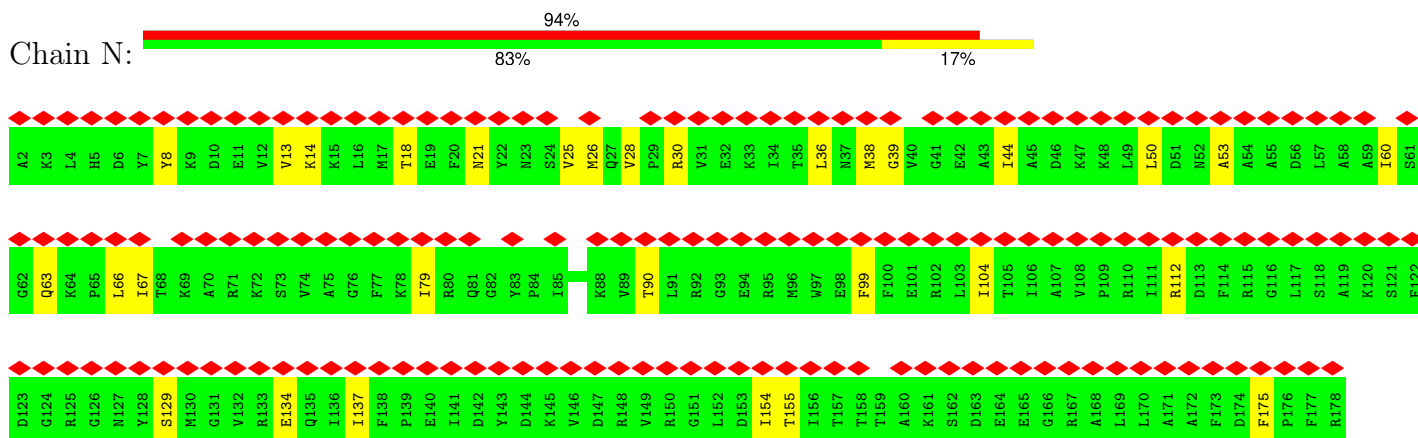
• Molecule 4: 50S ribosomal protein L3



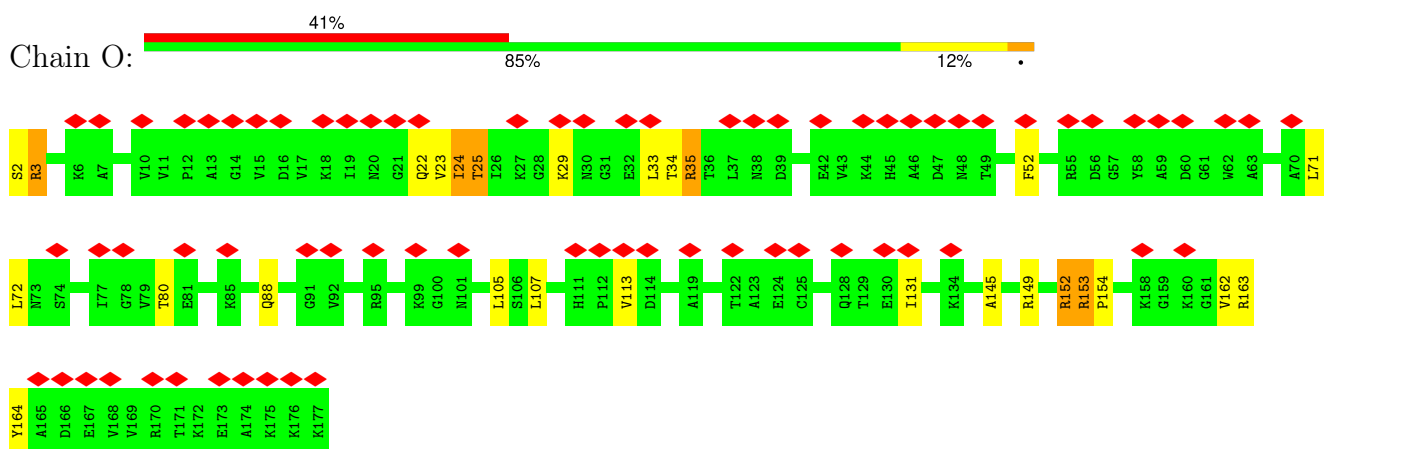
• Molecule 5: 50S ribosomal protein L4



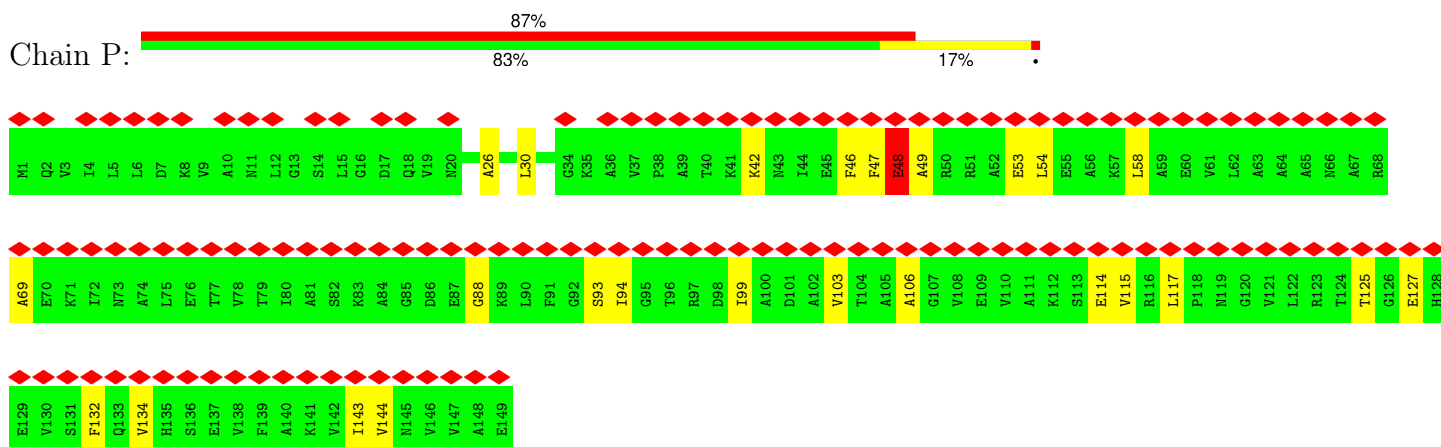
• Molecule 6: 50S ribosomal protein L5



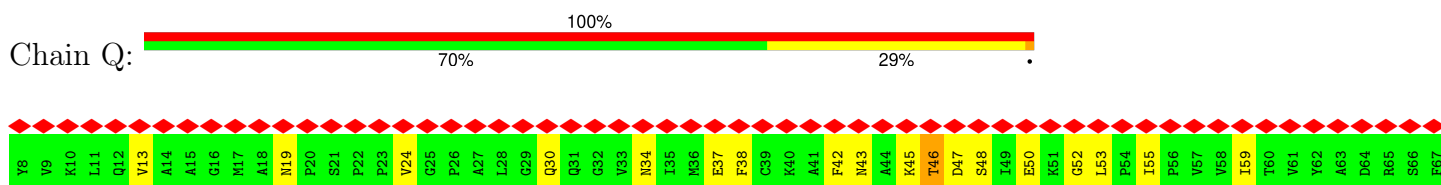
• Molecule 7: 50S ribosomal protein L6

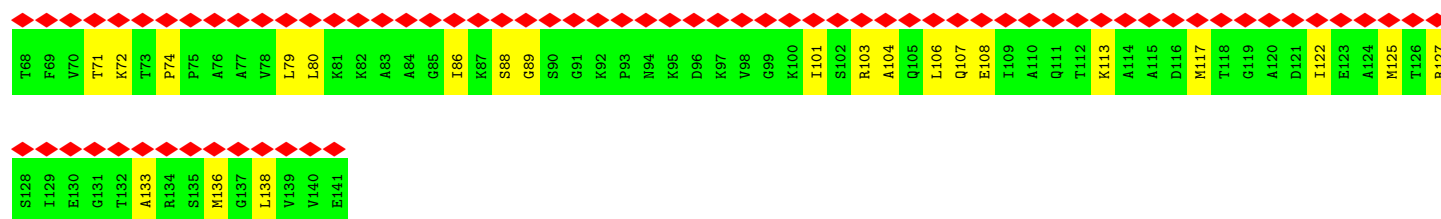


• Molecule 8: 50S ribosomal protein L9

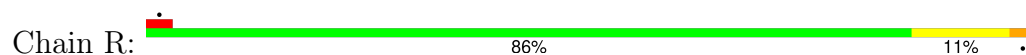


• Molecule 9: 50S ribosomal protein L11

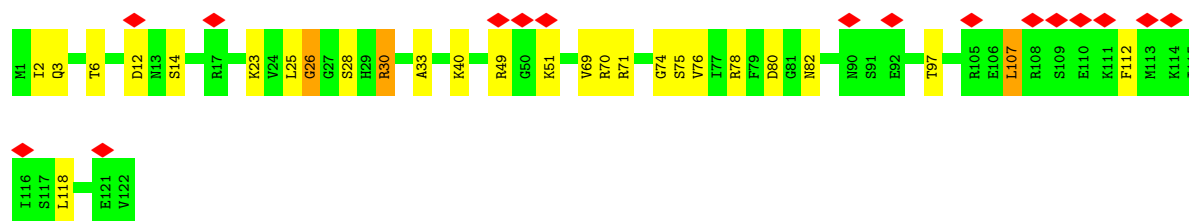
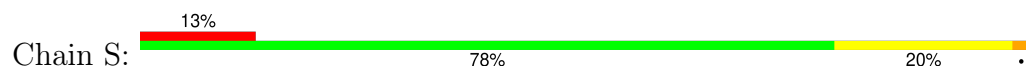




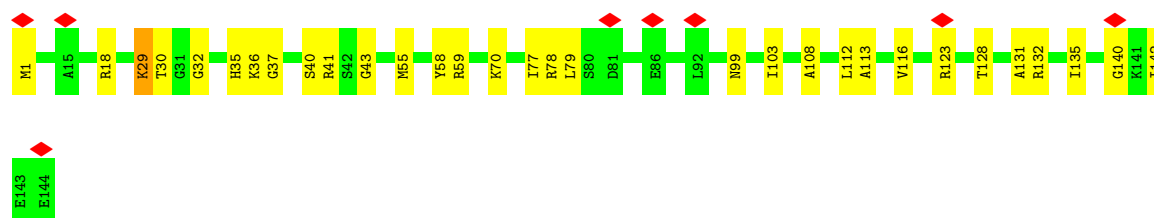
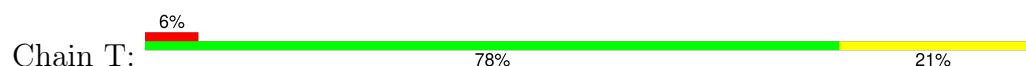
• Molecule 10: 50S ribosomal protein L13



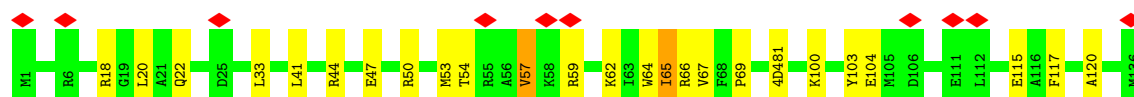
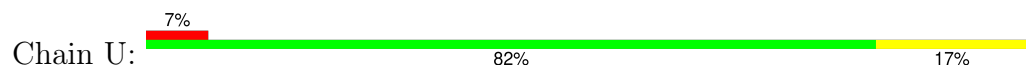
• Molecule 11: 50S ribosomal protein L14



• Molecule 12: 50S ribosomal protein L15

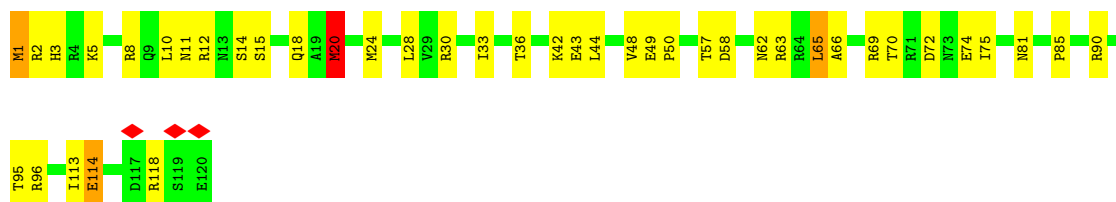


• Molecule 13: 50S ribosomal protein L16

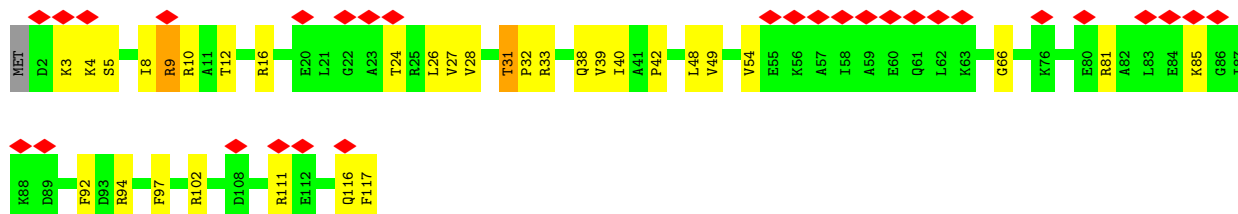


• Molecule 14: 50S ribosomal protein L17

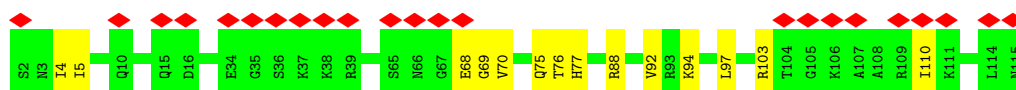
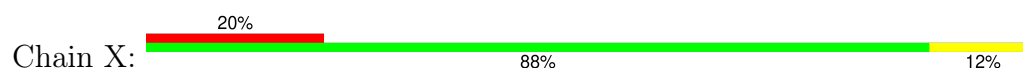




- Molecule 15: 50S ribosomal protein L18



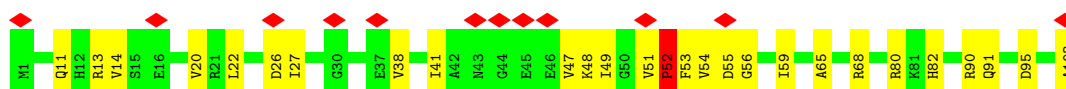
- Molecule 16: 50S ribosomal protein L19



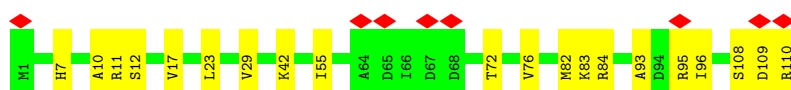
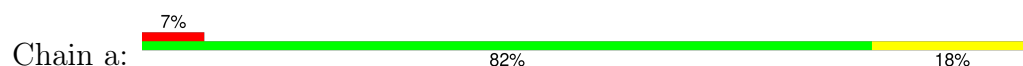
- Molecule 17: 50S ribosomal protein L20



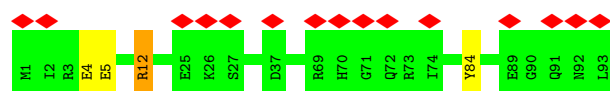
- Molecule 18: 50S ribosomal protein L21



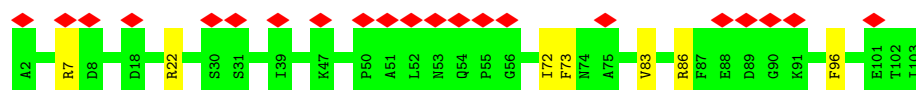
- Molecule 19: 50S ribosomal protein L22



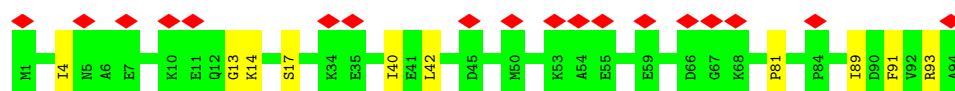
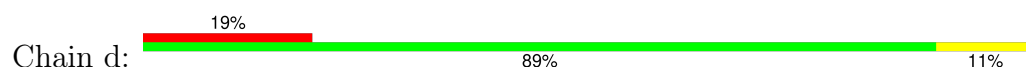
- Molecule 20: 50S ribosomal protein L23



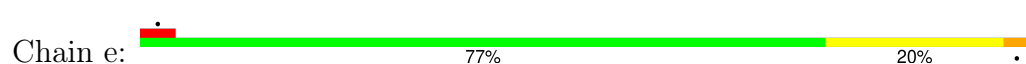
- Molecule 21: 50S ribosomal protein L24



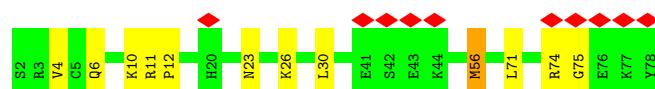
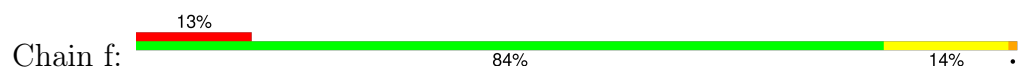
- Molecule 22: 50S ribosomal protein L25



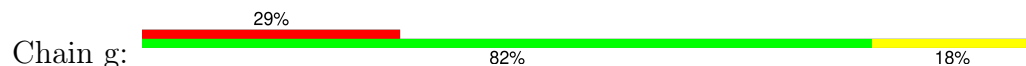
- Molecule 23: 50S ribosomal protein L27



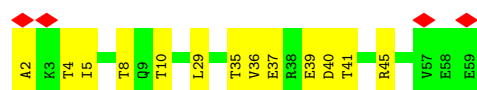
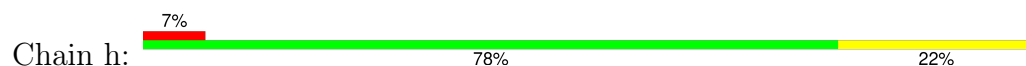
- Molecule 24: 50S ribosomal protein L28



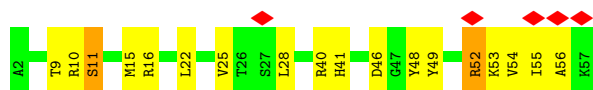
- Molecule 25: 50S ribosomal protein L29



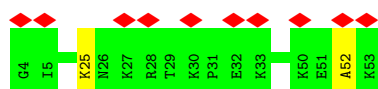
- Molecule 26: 50S ribosomal protein L30



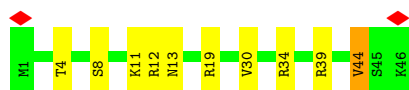
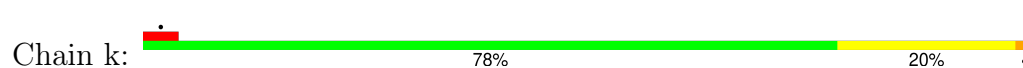
- Molecule 27: 50S ribosomal protein L32



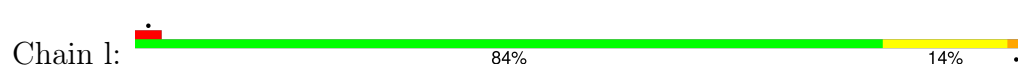
- Molecule 28: 50S ribosomal protein L33



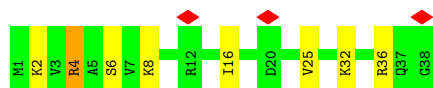
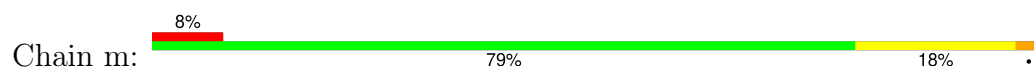
- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	141549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	60827	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	66.611	Depositor
Minimum map value	-32.287	Depositor
Average map value	-0.035	Depositor
Map value standard deviation	2.434	Depositor
Recommended contour level	10	Depositor
Map size ($\text{\AA}$)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, MG, 3TD, H2U, OMG, OMU, 5MU, OMC, 6MZ, NA, ZN, G7M, 2MA, PSU, 1MG, 4D4, 2MG

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	I	0.52	0/69121	0.45	9/107828 (0.0%)
2	J	0.42	0/2828	0.40	0/4410
3	K	0.81	2/2133 (0.1%)	0.92	2/2866 (0.1%)
4	L	0.85	2/1586 (0.1%)	0.93	5/2134 (0.2%)
5	M	0.76	1/1571 (0.1%)	0.90	1/2113 (0.0%)
6	N	0.34	0/1435	0.65	0/1926
7	O	0.53	1/1343 (0.1%)	0.83	2/1816 (0.1%)
8	P	0.43	0/1121	0.77	4/1515 (0.3%)
9	Q	0.34	0/993	0.71	0/1341
10	R	0.77	1/1152 (0.1%)	0.98	3/1551 (0.2%)
11	S	0.77	0/947	0.99	3/1268 (0.2%)
12	T	0.97	2/1062 (0.2%)	1.08	1/1413 (0.1%)
13	U	0.81	1/1081 (0.1%)	1.05	0/1443
14	V	1.06	2/973 (0.2%)	1.35	3/1301 (0.2%)
15	W	0.59	0/902	0.87	1/1209 (0.1%)
16	X	0.63	0/929	0.74	0/1242
17	Y	0.99	3/960 (0.3%)	1.30	9/1278 (0.7%)
18	Z	0.71	0/829	0.90	3/1107 (0.3%)
19	a	0.64	0/864	0.75	0/1156
20	b	0.56	0/745	0.67	0/994
21	c	0.52	0/788	0.75	0/1051
22	d	0.52	0/766	0.58	0/1025
23	e	0.86	1/582 (0.2%)	0.86	0/769
24	f	0.84	0/635	0.93	0/848
25	g	0.53	0/502	0.72	0/667
26	h	0.72	0/453	0.84	0/605
27	i	0.88	1/450 (0.2%)	1.21	2/599 (0.3%)
28	j	0.55	0/416	0.62	0/554
29	k	1.00	0/380	1.44	0/498
30	l	0.86	0/513	1.02	0/676
31	m	0.74	0/303	0.77	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
All	All	0.58	17/98363 (0.0%)	0.59	48/147600 (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
3	K	0	1
8	P	0	1
9	Q	0	2
All	All	0	4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	218	PRO	C-O	-6.85	1.15	1.23
12	T	18	ARG	C-O	-6.52	1.16	1.24
17	Y	92	ARG	C-O	-5.84	1.17	1.24
27	i	11	SER	C-O	-5.81	1.17	1.24
17	Y	56	GLN	C-O	-5.80	1.17	1.24
23	e	40	GLN	C-O	-5.58	1.17	1.23
10	R	97	PRO	C-O	-5.51	1.17	1.24
13	U	69	PRO	C-O	-5.39	1.17	1.24
4	L	169	ARG	C-O	-5.36	1.17	1.23
17	Y	49	ASP	CG-OD1	-5.34	1.15	1.25
14	V	50	PRO	C-O	-5.33	1.17	1.24
3	K	48	ARG	C-O	-5.32	1.17	1.23
4	L	152	PRO	C-O	-5.29	1.17	1.24
5	M	45	ALA	C-O	-5.17	1.17	1.23
7	O	149	ARG	C-O	-5.16	1.17	1.24
14	V	15	SER	C-O	-5.07	1.18	1.24
12	T	43	GLY	C-O	-5.07	1.17	1.24

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2606	C	C4'-C3'-O3'	10.75	129.12	113.00
1	I	2606	C	C1'-C2'-O2'	-9.89	93.56	108.40
1	I	2607	G	C1'-C2'-O2'	-9.00	94.90	108.40
1	I	2607	G	N9-C1'-C2'	-8.14	99.80	112.00
18	Z	52	PRO	CA-N-CD	-7.91	100.93	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2607	G	C4'-C3'-O3'	7.63	124.45	113.00
7	O	153	ARG	CB-CA-C	7.55	121.27	109.42
17	Y	49	ASP	CA-CB-CG	-7.22	105.38	112.60
1	I	2606	C	N1-C1'-C2'	-7.18	101.24	112.00
8	P	47	PHE	N-CA-C	-6.86	104.38	112.89
27	i	10	ARG	CA-C-N	6.82	129.31	120.44
27	i	10	ARG	C-N-CA	6.82	129.31	120.44
3	K	11	PRO	N-CA-C	-6.55	100.92	110.80
17	Y	48	ARG	CA-C-N	6.46	131.50	120.72
17	Y	48	ARG	C-N-CA	6.46	131.50	120.72
10	R	93	ILE	N-CA-C	-6.43	104.06	110.62
3	K	156	ARG	CB-CG-CD	-6.35	96.69	111.30
4	L	151	THR	CB-CA-C	6.13	122.24	110.17
12	T	29	LYS	CB-CA-C	5.96	122.28	110.42
17	Y	49	ASP	CB-CA-C	5.80	122.43	110.31
10	R	14	ASP	CB-CA-C	5.78	119.34	109.80
17	Y	51	ARG	CG-CD-NE	-5.65	99.57	112.00
14	V	3	HIS	CB-CA-C	-5.62	102.25	110.06
4	L	152	PRO	N-CA-C	-5.62	100.90	112.47
4	L	57	ALA	N-CA-C	-5.59	105.19	111.28
10	R	27	ARG	CB-CA-C	5.59	120.35	110.85
18	Z	54	VAL	N-CA-C	-5.55	99.07	107.73
17	Y	6	ARG	CB-CG-CD	-5.55	98.53	111.30
11	S	26	GLY	CA-C-O	-5.47	115.83	120.64
17	Y	6	ARG	NE-CZ-NH1	-5.46	116.04	121.50
4	L	149	ASN	CB-CA-C	-5.42	102.70	110.62
17	Y	50	ARG	CB-CA-C	5.41	120.04	110.85
1	I	138	U	C5'-C4'-O4'	5.38	117.87	109.80
18	Z	52	PRO	N-CA-C	-5.36	101.43	112.47
8	P	48	GLU	N-CA-C	-5.32	107.09	113.21
14	V	90	ARG	CB-CA-C	-5.23	101.48	110.22
7	O	3	ARG	N-CA-C	-5.22	105.66	111.36
17	Y	6	ARG	CB-CA-C	-5.19	101.42	110.09
4	L	148	GLN	CB-CA-C	5.17	120.71	110.42
14	V	20	MET	O-C-N	5.17	127.67	122.09
11	S	30	ARG	CA-C-N	5.15	127.60	120.29
11	S	30	ARG	C-N-CA	5.15	127.60	120.29
1	I	489	G	C2'-C3'-O3'	5.14	117.21	109.50
8	P	48	GLU	CA-C-N	5.14	129.41	120.68
8	P	48	GLU	C-N-CA	5.14	129.41	120.68
15	W	12	THR	CA-C-O	-5.05	115.52	120.82
5	M	79	ARG	CA-C-O	-5.03	115.19	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2225	A	C2'-C3'-O3'	5.02	117.03	109.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	203[B]	ARG	Mainchain
8	P	114	GLU	Peptide
9	Q	19	ASN	Peptide
9	Q	46	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	62229	31307	31319	378	0
2	J	2529	1281	1281	10	0
3	K	2094	2167	2166	46	0
4	L	1565	1610	1616	46	0
5	M	1552	1619	1619	23	0
6	N	1411	1444	1444	18	0
7	O	1323	1371	1371	19	0
8	P	1110	1148	1148	15	0
9	Q	979	1028	1028	27	0
10	R	1129	1162	1162	20	0
11	S	938	1012	1012	24	0
12	T	1053	1116	1129	22	0
13	U	1075	1154	1155	21	0
14	V	960	1000	1000	42	0
15	W	892	923	923	29	0
16	X	917	962	962	13	0
17	Y	947	1020	1019	28	0
18	Z	816	766	839	30	0
19	a	857	922	922	16	0
20	b	739	807	807	4	0
21	c	780	831	831	5	0
22	d	753	780	780	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	e	575	581	592	12	0
24	f	625	652	652	10	0
25	g	501	531	531	8	0
26	h	449	488	488	12	0
27	i	444	458	458	18	0
28	j	409	440	440	1	0
29	k	377	418	418	14	0
30	l	504	572	572	10	0
31	m	302	340	340	7	0
32	I	182	0	0	0	0
32	J	1	0	0	0	0
32	K	1	0	0	0	0
32	L	1	0	0	0	0
33	K	1	0	0	0	0
34	m	1	0	0	0	0
35	I	3347	0	0	151	0
35	J	62	0	0	2	0
35	K	59	0	0	2	0
35	L	41	0	0	0	0
35	M	42	0	0	1	0
35	N	14	0	0	2	0
35	O	13	0	0	0	0
35	P	6	0	0	0	0
35	Q	10	0	0	2	0
35	R	17	0	0	0	0
35	S	7	0	0	0	0
35	T	33	0	0	3	0
35	U	13	0	0	0	0
35	V	23	0	0	0	0
35	W	11	0	0	0	0
35	X	14	0	0	1	0
35	Y	33	0	0	1	0
35	Z	16	0	0	0	0
35	a	18	0	0	0	0
35	b	15	0	0	0	0
35	c	7	0	0	0	0
35	d	9	0	0	0	0
35	e	13	0	0	1	0
35	f	9	0	0	1	0
35	g	6	0	0	0	0
35	h	4	0	0	0	0
35	i	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	j	9	0	0	0	0
35	k	11	0	0	0	0
35	l	19	0	0	2	0
35	m	4	0	0	0	0
All	All	94918	59910	60024	773	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 5.

All (773) 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)
7:O:35:ARG:NH1	7:O:71:LEU:HD13	1.45	1.32
11:S:80:ASP:OD2	16:X:69:GLY:HA3	1.16	1.27
1:I:2572:A:OP2	4:L:149:ASN:O	1.59	1.20
26:h:5:ILE:HD12	26:h:45:ARG:NH1	1.62	1.16
1:I:2571:U:O2'	4:L:151:THR:CG2	1.93	1.15
18:Z:51:VAL:HG23	18:Z:52:PRO:HD3	1.16	1.10
1:I:2571:U:O2'	4:L:151:THR:HG23	1.51	1.09
11:S:80:ASP:OD2	16:X:69:GLY:CA	2.01	1.08
18:Z:52:PRO:HD2	18:Z:53:PHE:H	1.07	1.08
13:U:20:LEU:HD13	22:d:81:PRO:HG2	1.31	1.06
7:O:25:THR:HG22	7:O:34:THR:HG23	1.06	1.05
12:T:35:HIS:HE1	35:T:228:HOH:O	1.41	1.03
7:O:25:THR:HG22	7:O:34:THR:CG2	1.92	1.00
18:Z:51:VAL:CG2	18:Z:52:PRO:HD3	1.92	0.99
1:I:1800:C:OP1	3:K:258:ARG:NH2	1.96	0.99
3:K:231:PRO:O	3:K:242:LYS:HE3	1.63	0.99
7:O:35:ARG:HH11	7:O:71:LEU:HD13	1.29	0.98
1:I:1266:G:OP1	27:i:16:ARG:NE	1.96	0.97
3:K:232:HIS:HA	3:K:242:LYS:HE2	1.44	0.96
3:K:242:LYS:NZ	35:K:401:HOH:O	1.98	0.94
7:O:35:ARG:NH1	7:O:71:LEU:CD1	2.33	0.92
1:I:1693:U:O2'	3:K:14:ARG:NH2	2.02	0.91
18:Z:52:PRO:CD	18:Z:53:PHE:H	1.83	0.90
18:Z:52:PRO:HD2	18:Z:53:PHE:N	1.82	0.90
1:I:1652:A:H62	14:V:11:ASN:HD21	1.18	0.87
18:Z:51:VAL:HG23	18:Z:52:PRO:CD	2.05	0.87
14:V:33:ILE:HD13	14:V:114:GLU:HG3	1.53	0.86
14:V:114:GLU:OE2	14:V:118:ARG:NH2	2.08	0.86
1:I:2571:U:O2'	4:L:151:THR:HG21	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2572:A:P	4:L:149:ASN:O	2.34	0.85
1:I:2571:U:O3'	4:L:151:THR:HG21	1.76	0.84
1:I:674:G:O2'	5:M:69:ARG:HD3	1.77	0.84
13:U:20:LEU:HD13	22:d:81:PRO:CG	2.08	0.83
15:W:4:LYS:O	15:W:8:ILE:HD12	1.77	0.83
8:P:48:GLU:OE1	8:P:48:GLU:HA	1.79	0.83
18:Z:14:VAL:CG1	18:Z:20:VAL:HG11	2.09	0.83
5:M:80:SER:O	35:M:301:HOH:O	1.96	0.82
14:V:114:GLU:HG2	14:V:118:ARG:HD2	1.60	0.81
4:L:116:LYS:HD3	14:V:1:MET:HE1	1.61	0.81
15:W:24:THR:HG23	15:W:40:ILE:O	1.80	0.81
18:Z:14:VAL:HG12	18:Z:20:VAL:HG11	1.62	0.80
3:K:231:PRO:O	3:K:242:LYS:CE	2.30	0.80
23:e:25:ARG:NH1	23:e:29:GLU:OE2	2.15	0.80
1:I:2571:U:O3'	4:L:151:THR:CG2	2.28	0.80
13:U:66:ARG:NH1	13:U:104:GLU:OE2	2.13	0.79
10:R:42:ALA:O	17:Y:64:ARG:HD3	1.82	0.79
1:I:250:G:H4'	12:T:59:ARG:HH11	1.47	0.79
13:U:47:GLU:OE2	13:U:50:ARG:NH1	2.16	0.78
7:O:24:ILE:HD11	7:O:72:LEU:HD21	1.66	0.78
1:I:1053:C:N4	35:I:3296:HOH:O	2.16	0.77
4:L:116:LYS:CD	14:V:1:MET:HE1	2.13	0.77
1:I:878:A:N6	1:I:899:A:O2'	2.18	0.77
7:O:24:ILE:CD1	7:O:72:LEU:HD21	2.15	0.77
9:Q:117:MET:O	35:Q:201:HOH:O	2.03	0.76
1:I:822:G:OP2	35:I:3201:HOH:O	2.01	0.76
1:I:1078:U:O2'	1:I:1088:A:OP1	2.03	0.76
1:I:573:U:O2'	1:I:575:A:OP1	2.03	0.75
1:I:1085:A:O2'	1:I:1104:C:O2'	2.04	0.75
1:I:1342:A:OP2	35:I:3202:HOH:O	2.02	0.75
1:I:2306:C:N4	6:N:39:GLY:O	2.18	0.75
24:f:6:GLN:O	24:f:74:ARG:NH1	2.20	0.75
26:h:5:ILE:HD12	26:h:45:ARG:HH11	1.48	0.75
1:I:1980:G:O2'	1:I:1982:U:OP2	2.05	0.74
1:I:1340:U:OP1	20:b:84:TYR:OH	2.05	0.74
31:m:2:LYS:NZ	31:m:32:LYS:O	2.21	0.74
1:I:2571:U:C3'	4:L:151:THR:HG21	2.18	0.74
1:I:1020:A:N1	1:I:1141:U:O2'	2.21	0.73
1:I:438:G:O6	35:I:3204:HOH:O	2.05	0.73
1:I:2144:G:N3	1:I:2147:A:N6	2.36	0.73
4:L:12:THR:CG2	16:X:5:ILE:HG23	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2563:U:H5''	11:S:26:GLY:O	1.89	0.73
1:I:29:U:OP2	35:I:3203:HOH:O	2.05	0.73
1:I:1042:G:O6	35:I:3205:HOH:O	2.06	0.73
15:W:4:LYS:O	15:W:8:ILE:CD1	2.36	0.72
1:I:699:A:OP1	35:I:3209:HOH:O	2.07	0.72
1:I:412:A:OP1	35:I:3206:HOH:O	2.06	0.72
1:I:1453:A:OP1	35:I:3211:HOH:O	2.08	0.72
1:I:2572:A:P	4:L:151:THR:HG22	2.30	0.72
25:g:10:SER:OG	25:g:12:GLU:O	2.08	0.72
26:h:5:ILE:CD1	26:h:45:ARG:NH1	2.48	0.72
1:I:983:A:OP1	35:I:3210:HOH:O	2.07	0.72
1:I:1792:G:N7	35:I:3335:HOH:O	2.23	0.72
12:T:55:MET:HE1	12:T:59:ARG:HH21	1.54	0.72
1:I:881:G:N2	1:I:895:U:O2	2.17	0.71
1:I:1533:C:O2	1:I:1538:G:N2	2.17	0.71
8:P:69:ALA:HB2	8:P:134:VAL:HG11	1.71	0.71
6:N:60:ILE:O	35:N:201:HOH:O	2.08	0.71
1:I:821:A:OP1	35:I:3213:HOH:O	2.08	0.71
1:I:2134:A:N6	1:I:2157:G:O2'	2.23	0.71
15:W:31:THR:HG23	15:W:32:PRO:HD2	1.71	0.71
1:I:1385:A:O2'	1:I:1396:U:O2	2.07	0.71
1:I:1790:C:N3	35:I:3337:HOH:O	2.23	0.71
1:I:2258:C:O2'	1:I:2427:C:OP2	2.09	0.71
1:I:821:A:OP2	35:I:3208:HOH:O	2.07	0.71
16:X:75:GLN:OE1	35:X:201:HOH:O	2.08	0.71
1:I:1711:A:N7	35:I:3348:HOH:O	2.24	0.70
1:I:1797:G:O6	35:I:3222:HOH:O	2.09	0.70
1:I:585:G:N7	17:Y:6:ARG:NH1	2.38	0.70
1:I:1277:G:H5'	14:V:20:MET:CE	2.21	0.70
1:I:811:U:OP1	35:I:3219:HOH:O	2.09	0.70
1:I:1428:C:N3	35:I:3343:HOH:O	2.24	0.70
1:I:2809:A:N7	35:I:3352:HOH:O	2.24	0.70
1:I:474:G:N7	35:I:3347:HOH:O	2.24	0.70
1:I:1179:G:OP2	35:I:3221:HOH:O	2.09	0.70
1:I:2447:G:OP2	35:I:3225:HOH:O	2.10	0.70
1:I:1130:U:O4	4:L:151:THR:O	2.10	0.70
1:I:1352:U:OP2	35:I:3214:HOH:O	2.08	0.70
9:Q:74:PRO:O	9:Q:113:LYS:NZ	2.24	0.70
1:I:1245:G:N7	35:I:3359:HOH:O	2.25	0.70
15:W:31:THR:HG22	15:W:33:ARG:H	1.56	0.70
1:I:141:G:O5'	35:I:3218:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:372:G:O2'	1:I:400:G:O6	2.07	0.70
1:I:1270:C:OP2	35:I:3233:HOH:O	2.10	0.69
9:Q:103:ARG:O	9:Q:107:GLN:N	2.24	0.69
1:I:1007:C:OP2	35:I:3234:HOH:O	2.10	0.69
1:I:1813:G:O6	35:I:3220:HOH:O	2.09	0.69
1:I:1998:A:OP2	4:L:141:ARG:NH2	2.24	0.69
1:I:2685:G:OP1	11:S:78:ARG:NH2	2.25	0.69
9:Q:45:LYS:O	9:Q:48:SER:OG	2.10	0.69
1:I:744:U:OP1	35:I:3216:HOH:O	2.08	0.69
1:I:1523:U:OP2	35:I:3223:HOH:O	2.09	0.69
1:I:1651:G:O6	35:I:3226:HOH:O	2.10	0.69
15:W:5:SER:HA	15:W:8:ILE:HD13	1.73	0.69
1:I:2010:G:N7	35:I:3357:HOH:O	2.25	0.69
1:I:1071:G:N3	1:I:1089:A:O2'	2.25	0.69
1:I:1826:G:O2'	1:I:1971:U:OP2	2.09	0.69
1:I:1869:G:N2	1:I:1871:A:O2'	2.25	0.69
1:I:2668:G:N7	35:I:3355:HOH:O	2.24	0.69
1:I:745:1MG:OP2	35:I:3227:HOH:O	2.10	0.69
1:I:1264:A:OP2	35:I:3230:HOH:O	2.10	0.69
3:K:2:ALA:N	3:K:20:VAL:O	2.25	0.69
1:I:699:A:OP2	35:I:3247:HOH:O	2.11	0.69
1:I:164:C:OP2	35:I:3236:HOH:O	2.11	0.68
1:I:979:A:N7	35:I:3365:HOH:O	2.26	0.68
1:I:1377:G:O6	35:I:3245:HOH:O	2.11	0.68
1:I:2503:2MA:O2'	1:I:2505:G:OP2	2.10	0.68
1:I:317:G:N7	35:I:3362:HOH:O	2.25	0.68
1:I:2618:G:O6	35:I:3241:HOH:O	2.11	0.68
2:J:47:C:OP2	15:W:3:LYS:NZ	2.23	0.68
1:I:1380:G:OP2	35:I:3224:HOH:O	2.10	0.68
1:I:2683:C:O2	11:S:70:ARG:NH2	2.26	0.68
1:I:2646:C:OP2	1:I:2732:G:O2'	2.11	0.68
1:I:894:U:OP1	35:I:3255:HOH:O	2.12	0.68
1:I:2723:C:OP1	4:L:114:LYS:NZ	2.25	0.68
1:I:64:A:OP1	35:I:3242:HOH:O	2.11	0.68
1:I:449:A:OP2	35:I:3256:HOH:O	2.12	0.68
1:I:2641:G:N7	35:I:3373:HOH:O	2.27	0.68
1:I:574:A:OP2	35:I:3252:HOH:O	2.12	0.68
1:I:1822:C:OP2	35:I:3251:HOH:O	2.12	0.68
1:I:2823:A:OP1	35:I:3249:HOH:O	2.12	0.68
1:I:1058:U:N3	1:I:1081:U:O2	2.26	0.67
1:I:1219:U:OP2	17:Y:19:LYS:NZ	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1326:U:OP1	35:I:3238:HOH:O	2.11	0.67
1:I:403:U:OP2	35:I:3240:HOH:O	2.11	0.67
1:I:2330:G:N7	35:I:3380:HOH:O	2.27	0.67
8:P:54:LEU:O	8:P:58:LEU:N	2.26	0.67
24:f:12:PRO:HB3	24:f:30:LEU:HD23	1.76	0.67
1:I:338:G:O6	35:I:3237:HOH:O	2.11	0.67
1:I:2244:U:OP2	35:I:3244:HOH:O	2.11	0.67
27:i:52:ARG:HD3	27:i:54:VAL:CG1	2.25	0.67
1:I:2011:U:OP1	19:a:42:LYS:NZ	2.22	0.67
1:I:2059:A:OP2	35:I:3259:HOH:O	2.13	0.67
1:I:1311:G:OP2	1:I:1311:G:N2	2.22	0.67
1:I:1823:G:N7	35:I:3368:HOH:O	2.26	0.67
8:P:99:ILE:HD12	8:P:117:LEU:HD21	1.77	0.67
1:I:415:A:OP1	35:I:3246:HOH:O	2.11	0.67
1:I:831:G:OP2	35:I:3268:HOH:O	2.13	0.67
1:I:1420:A:O2'	1:I:2211:A:N7	2.27	0.67
1:I:1772:A:OP1	35:I:3258:HOH:O	2.12	0.67
2:J:106:G:N7	35:J:302:HOH:O	2.26	0.67
1:I:2659:G:O6	35:I:3253:HOH:O	2.12	0.66
1:I:1005:C:O2'	10:R:30:THR:HG21	1.95	0.66
1:I:1277:G:H4'	14:V:20:MET:HE2	1.77	0.66
1:I:2498:OMC:OP1	35:I:3254:HOH:O	2.12	0.66
9:Q:38:PHE:O	9:Q:42:PHE:N	2.29	0.66
1:I:207:A:OP2	35:I:3261:HOH:O	2.13	0.66
1:I:1157:G:N7	35:I:3386:HOH:O	2.28	0.66
17:Y:28:ARG:NH1	35:Y:201:HOH:O	2.26	0.66
1:I:2129:C:N4	35:I:3403:HOH:O	2.29	0.66
1:I:2384:U:OP1	35:I:3262:HOH:O	2.13	0.66
1:I:1386:C:OP1	35:I:3269:HOH:O	2.13	0.66
1:I:2017:U:OP2	35:I:3270:HOH:O	2.13	0.66
1:I:1478:G:N7	35:I:3397:HOH:O	2.29	0.66
1:I:1730:C:N3	35:I:3402:HOH:O	2.29	0.66
1:I:285:G:OP2	35:I:3280:HOH:O	2.14	0.66
1:I:1048:A:OP2	1:I:1109:C:N4	2.29	0.66
1:I:1941:C:N3	35:I:3394:HOH:O	2.28	0.66
1:I:2393:U:OP2	35:I:3274:HOH:O	2.14	0.66
1:I:2539:C:H4'	31:m:36:ARG:NH2	2.11	0.66
14:V:49:GLU:OE2	14:V:95:THR:OG1	2.14	0.66
1:I:1258:U:O4	35:I:3231:HOH:O	2.10	0.65
1:I:2023:C:OP1	35:I:3275:HOH:O	2.14	0.65
1:I:2270:A:OP2	35:I:3278:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:184:C:O2'	1:I:217:A:N3	2.29	0.65
1:I:1168:G:O6	35:I:3250:HOH:O	2.12	0.65
1:I:1416:G:O2'	1:I:1417:C:O5'	2.14	0.65
20:b:4:GLU:HG2	25:g:19:LEU:HD22	1.78	0.65
1:I:632:A:OP1	35:I:3272:HOH:O	2.13	0.65
1:I:955:PSU:OP2	35:I:3271:HOH:O	2.13	0.65
1:I:2674:G:H4'	11:S:30:ARG:HD2	1.79	0.65
1:I:1333:G:OP1	35:I:3273:HOH:O	2.13	0.65
1:I:2006:C:OP2	35:I:3266:HOH:O	2.13	0.65
23:e:27:GLY:O	35:e:101:HOH:O	2.13	0.65
12:T:35:HIS:CE1	35:T:228:HOH:O	2.27	0.65
1:I:1006:C:OP2	35:I:3276:HOH:O	2.14	0.65
1:I:1800:C:OP2	3:K:182:ARG:NH1	2.30	0.65
1:I:2135:A:O2'	35:I:3285:HOH:O	2.15	0.65
25:g:9:LYS:O	25:g:60:LYS:NZ	2.30	0.65
1:I:2032:G:N7	35:I:3406:HOH:O	2.29	0.65
1:I:1166:G:O6	35:I:3243:HOH:O	2.11	0.65
1:I:1903:G:OP2	35:I:3283:HOH:O	2.14	0.65
3:K:29:PRO:HG2	3:K:34:LEU:HD11	1.79	0.65
1:I:1379:U:OP2	35:I:3224:HOH:O	2.13	0.64
1:I:2392:A:OP2	30:l:31:HIS:HE1	1.81	0.64
27:i:52:ARG:HD3	27:i:54:VAL:HG13	1.79	0.64
3:K:141:VAL:HG13	3:K:190:ALA:HB1	1.79	0.64
1:I:2061:G:OP2	35:I:3277:HOH:O	2.14	0.64
1:I:309:A:OP2	35:I:3290:HOH:O	2.15	0.64
1:I:1369:G:N7	35:I:3414:HOH:O	2.30	0.64
1:I:1791:A:OP2	35:I:3284:HOH:O	2.15	0.64
1:I:674:G:H1'	5:M:69:ARG:HD2	1.79	0.64
1:I:1047:G:O5'	35:I:3291:HOH:O	2.15	0.64
1:I:2346:A:N1	35:I:3409:HOH:O	2.30	0.63
8:P:26:ALA:HA	8:P:30:LEU:HB2	1.80	0.63
13:U:54:THR:O	13:U:57:VAL:O	2.16	0.63
1:I:2475:C:OP2	35:I:3286:HOH:O	2.15	0.63
1:I:2499:C:OP2	35:I:3288:HOH:O	2.15	0.63
21:c:22:ARG:HD3	21:c:73:PHE:CD1	2.33	0.63
22:d:13:GLY:O	22:d:17:SER:OG	2.07	0.63
3:K:162:VAL:HG11	3:K:174:LEU:HG	1.80	0.63
1:I:1277:G:O3'	14:V:24:MET:HE2	1.99	0.63
1:I:1814:G:H4'	3:K:51:THR:HG21	1.80	0.63
10:R:36:LEU:HD13	10:R:54:ILE:CD1	2.28	0.63
1:I:1130:U:C4	4:L:151:THR:O	2.51	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1508:A:O2'	1:I:1509:A:O4'	2.16	0.63
15:W:8:ILE:HD12	15:W:8:ILE:H	1.63	0.63
1:I:1341:G:O6	35:I:3264:HOH:O	2.13	0.62
9:Q:133:ALA:HA	9:Q:138:LEU:HD12	1.81	0.62
1:I:2468:A:N1	1:I:2481:G:O2'	2.32	0.62
13:U:50:ARG:HD3	13:U:65:ILE:HD11	1.80	0.62
11:S:97:THR:O	11:S:118:LEU:HD13	2.00	0.62
14:V:2:ARG:NH1	14:V:5:LYS:O	2.32	0.62
27:i:52:ARG:CG	27:i:54:VAL:HG13	2.29	0.62
1:I:1475:G:O2'	1:I:1514:G:O6	2.18	0.62
18:Z:68:ARG:HH11	18:Z:90:ARG:HB2	1.64	0.62
10:R:31:GLU:O	10:R:35:ARG:HG3	1.99	0.62
1:I:2755:C:O2	35:I:3279:HOH:O	2.14	0.62
1:I:652:U:OP1	1:I:654:A:N6	2.33	0.61
1:I:1917:PSU:OP1	35:I:3295:HOH:O	2.16	0.61
1:I:2278:A:OP2	23:e:12:ASN:ND2	2.33	0.61
9:Q:59:ILE:O	35:Q:202:HOH:O	2.16	0.61
1:I:1668:A:O2'	1:I:1674:G:N7	2.31	0.61
1:I:1699:G:OP2	35:I:3297:HOH:O	2.16	0.61
1:I:1413:A:N7	35:I:3423:HOH:O	2.31	0.61
3:K:117:GLN:N	3:K:128:ASN:OD1	2.33	0.61
1:I:727:A:C2	3:K:9:THR:HG21	2.35	0.61
35:I:4065:HOH:O	17:Y:13:ARG:HD2	2.01	0.61
12:T:77:ILE:HD11	12:T:108:ALA:HB1	1.83	0.61
1:I:1649:G:N7	35:I:3426:HOH:O	2.31	0.60
1:I:2581:G:O6	35:I:3282:HOH:O	2.14	0.60
6:N:25:VAL:O	6:N:28:VAL:HG12	2.01	0.60
18:Z:65:ALA:HB3	18:Z:95:ASP:HB2	1.83	0.60
1:I:138:U:O2'	1:I:139:U:OP1	2.15	0.60
1:I:673:C:N3	35:I:3427:HOH:O	2.31	0.60
1:I:1180:U:O4'	35:I:3221:HOH:O	2.16	0.60
18:Z:14:VAL:HG11	18:Z:20:VAL:HG11	1.83	0.60
30:l:30:ARG:O	35:l:101:HOH:O	2.17	0.60
1:I:618:G:O6	35:I:3263:HOH:O	2.13	0.60
1:I:2020:A:H5'	27:i:9:THR:CG2	2.31	0.60
1:I:2539:C:H4'	31:m:36:ARG:HH21	1.66	0.60
3:K:79:GLU:OE1	3:K:101:ARG:NE	2.33	0.60
24:f:4:VAL:HG22	24:f:11:ARG:HB3	1.83	0.60
1:I:1081:U:OP1	9:Q:127:ARG:NH1	2.33	0.60
1:I:2571:U:HO2'	4:L:151:THR:HG23	1.65	0.60
9:Q:80:LEU:HD13	9:Q:138:LEU:HD21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:f:4:VAL:HG21	24:f:11:ARG:NH1	2.16	0.59
5:M:147:LEU:HD22	5:M:179:SER:OG	2.02	0.59
9:Q:55:ILE:HD11	9:Q:72:LYS:O	2.02	0.59
1:I:2294:G:P	15:W:94:ARG:HH12	2.25	0.59
1:I:68:G:O6	35:I:3293:HOH:O	2.16	0.59
1:I:2484:G:OP1	13:U:44:ARG:NH2	2.31	0.59
12:T:1:MET:O	12:T:1:MET:HG2	2.02	0.59
1:I:2146:C:O2'	1:I:2147:A:O5'	2.15	0.59
1:I:2605:PSU:H6	1:I:2605:PSU:H5'	1.66	0.59
6:N:63:GLN:NE2	6:N:90:THR:O	2.35	0.59
1:I:1459:G:N7	35:I:3430:HOH:O	2.31	0.59
1:I:320:A:N3	5:M:163:ASN:ND2	2.51	0.59
35:I:4403:HOH:O	5:M:100:MET:SD	2.57	0.58
10:R:4:PHE:O	17:Y:64:ARG:NH2	2.36	0.58
1:I:568:U:H1'	1:I:2030:6MZ:H9C1	1.85	0.58
6:N:38:MET:HE3	6:N:53:ALA:HB1	1.85	0.58
1:I:1153:C:OP1	17:Y:92:ARG:NH2	2.35	0.58
1:I:1244:A:N7	35:I:3436:HOH:O	2.32	0.58
5:M:111:GLU:HG3	5:M:115:GLN:NE2	2.19	0.58
1:I:332:A:O2'	1:I:334:C:OP2	2.13	0.58
1:I:1907:G:N3	35:I:3435:HOH:O	2.31	0.58
1:I:2018:G:OP2	35:I:3298:HOH:O	2.17	0.58
1:I:2902:C:OP2	1:I:2903:U:O2'	2.14	0.58
4:L:12:THR:HG21	16:X:5:ILE:HG23	1.85	0.58
2:J:5:U:O2'	2:J:27:C:O2	2.21	0.58
26:h:39:GLU:HG3	26:h:41:THR:HG23	1.86	0.58
1:I:690:G:N7	35:I:3438:HOH:O	2.32	0.58
23:e:25:ARG:HD2	23:e:31:VAL:HG12	1.86	0.58
1:I:1249:U:OP1	35:I:3299:HOH:O	2.17	0.58
1:I:1277:G:C5'	14:V:20:MET:CE	2.82	0.58
12:T:99:ASN:OD1	35:T:201:HOH:O	2.16	0.58
19:a:83:LYS:HD2	19:a:95:ARG:CZ	2.33	0.57
29:k:12:ARG:NH1	29:k:44:VAL:CG2	2.66	0.57
1:I:1277:G:C4'	14:V:20:MET:HE2	2.34	0.57
1:I:2421:G:N7	30:l:31:HIS:HD2	2.00	0.57
26:h:4:THR:HG22	26:h:37:GLU:CG	2.33	0.57
1:I:1094:U:N3	1:I:1097:U:OP2	2.38	0.57
1:I:1824:G:O2'	3:K:252:THR:HG21	2.04	0.57
2:J:80:U:O4	22:d:14:LYS:NZ	2.37	0.57
23:e:21:LEU:HA	23:e:39:ARG:HB2	1.85	0.57
1:I:1141:U:H5''	10:R:27:ARG:HH21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:U:53:MET:HE1	13:U:103:TYR:CD1	2.40	0.57
16:X:88:ARG:NH2	16:X:110:ILE:O	2.33	0.57
1:I:1277:G:C5'	14:V:20:MET:HE2	2.34	0.57
1:I:1445:G:O6	35:I:3265:HOH:O	2.13	0.57
13:U:53:MET:HE1	13:U:103:TYR:CG	2.38	0.57
15:W:66:GLY:HA2	15:W:102:ARG:NH2	2.20	0.57
1:I:526:A:O2'	1:I:2043:C:O2	2.20	0.57
5:M:111:GLU:HG3	5:M:115:GLN:HE21	1.69	0.57
12:T:79:LEU:HD11	12:T:112:LEU:HD12	1.86	0.57
26:h:4:THR:HG22	26:h:37:GLU:HG3	1.86	0.57
1:I:124:G:O6	35:I:3294:HOH:O	2.16	0.57
4:L:33:ARG:HH22	4:L:52:THR:HA	1.70	0.57
23:e:38:VAL:O	23:e:58:THR:OG1	2.17	0.57
26:h:2:ALA:CB	26:h:39:GLU:HB2	2.34	0.57
12:T:135:ILE:HG22	12:T:140:GLY:HA3	1.87	0.56
1:I:622:G:OP1	12:T:103:ILE:HD12	2.05	0.56
4:L:116:LYS:HD2	14:V:1:MET:HE1	1.87	0.56
9:Q:122:ILE:HG23	9:Q:125:MET:HE1	1.86	0.56
13:U:53:MET:HE2	13:U:117:PHE:HD1	1.70	0.56
13:U:115:GLU:HA	13:U:115:GLU:OE1	2.05	0.56
23:e:75:LYS:HB2	23:e:77:ARG:HG3	1.88	0.56
1:I:2575:C:H5'	4:L:149:ASN:HB2	1.86	0.56
1:I:1113:U:O4	35:I:3205:HOH:O	2.17	0.56
1:I:1869:G:N2	1:I:1871:A:HO2'	2.04	0.56
6:N:36:LEU:HD21	6:N:99:PHE:CE1	2.41	0.56
7:O:52:PHE:HZ	7:O:72:LEU:HD22	1.70	0.56
1:I:2092:U:N3	1:I:2226:C:OP2	2.39	0.56
4:L:156:PHE:CG	10:R:81:ILE:HG12	2.41	0.56
9:Q:42:PHE:O	9:Q:46:THR:N	2.39	0.56
1:I:395:U:O2'	1:I:396:G:N7	2.26	0.55
1:I:993:G:N3	18:Z:91:GLN:NE2	2.54	0.55
1:I:1800:C:H5'	3:K:146:MET:HE1	1.88	0.55
3:K:158:ALA:HB1	3:K:197:ASN:O	2.06	0.55
5:M:105:LEU:HB3	5:M:200:LEU:HD21	1.89	0.55
1:I:698:C:O2'	1:I:734:A:N6	2.38	0.55
7:O:105:LEU:HD21	7:O:131:ILE:HD11	1.87	0.55
1:I:994:C:O2'	1:I:996:A:OP1	2.24	0.55
1:I:1992:G:N2	1:I:1996:C:O2'	2.39	0.55
17:Y:94:ILE:HD12	18:Z:13:ARG:HB2	1.88	0.55
1:I:520:G:N7	35:I:3449:HOH:O	2.33	0.55
18:Z:38:VAL:HG12	18:Z:59:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:603:A:O5'	1:I:655:A:N6	2.37	0.55
6:N:38:MET:CE	6:N:53:ALA:HB1	2.37	0.55
1:I:467:G:OP2	29:k:34:ARG:HD2	2.06	0.55
1:I:1271:G:O6	35:I:3260:HOH:O	2.13	0.55
1:I:125:A:OP2	29:k:19:ARG:NH2	2.36	0.55
1:I:489:G:O2'	1:I:490:C:OP1	2.20	0.55
3:K:78:VAL:HG21	3:K:110:LEU:HD21	1.88	0.55
1:I:1223:G:OP2	18:Z:90:ARG:NH1	2.30	0.55
1:I:2571:U:C2'	4:L:151:THR:HG21	2.36	0.54
8:P:127:GLU:OE1	8:P:143:ILE:HG21	2.07	0.54
12:T:78:ARG:CZ	12:T:113:ALA:HB1	2.37	0.54
14:V:57:THR:O	14:V:62:ASN:ND2	2.30	0.54
27:i:52:ARG:CD	27:i:54:VAL:HG13	2.37	0.54
1:I:1673:G:OP1	35:I:3300:HOH:O	2.18	0.54
19:a:82:MET:SD	19:a:84:ARG:NH1	2.80	0.54
1:I:1006:C:O4'	10:R:30:THR:HG23	2.07	0.54
4:L:12:THR:HG22	16:X:5:ILE:HG23	1.89	0.54
11:S:2:ILE:HG23	11:S:6:THR:HG21	1.88	0.54
13:U:53:MET:HE2	13:U:117:PHE:CD1	2.42	0.54
14:V:66:ALA:O	14:V:70:THR:HB	2.07	0.54
29:k:12:ARG:NH1	29:k:44:VAL:HG22	2.23	0.54
1:I:468:G:N7	29:k:39:ARG:NH2	2.50	0.54
9:Q:34:ASN:OD1	9:Q:37:GLU:N	2.40	0.54
19:a:83:LYS:HD2	19:a:95:ARG:NE	2.23	0.54
1:I:250:G:C4'	12:T:59:ARG:HH11	2.20	0.54
1:I:1277:G:O3'	14:V:24:MET:CE	2.56	0.54
7:O:22:GLN:O	7:O:24:ILE:HG22	2.08	0.54
11:S:12:ASP:OD1	11:S:14:SER:OG	2.24	0.54
7:O:105:LEU:N	7:O:113:VAL:O	2.40	0.54
1:I:1296:G:OP1	1:I:2709:G:O2'	2.23	0.54
3:K:141:VAL:CG1	3:K:190:ALA:HB1	2.37	0.54
15:W:26:LEU:HD13	15:W:39:VAL:CG2	2.37	0.54
27:i:48:TYR:CZ	27:i:53:LYS:HD3	2.43	0.53
14:V:70:THR:HG22	14:V:72:ASP:H	1.73	0.53
1:I:190:A:OP2	24:f:26:LYS:HE2	2.09	0.53
1:I:1586:A:OP2	35:I:3304:HOH:O	2.19	0.53
1:I:1679:A:N7	35:I:3464:HOH:O	2.34	0.53
1:I:2170:A:O2'	1:I:2171:A:OP2	2.25	0.53
11:S:70:ARG:HH12	11:S:74:GLY:HA2	1.72	0.53
1:I:2571:U:O3'	4:L:151:THR:HG22	2.04	0.53
1:I:693:A:OP1	3:K:39:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:137:ILE:N	35:N:202:HOH:O	2.41	0.53
23:e:25:ARG:HH11	23:e:29:GLU:CD	2.17	0.53
1:I:1334:G:OP2	35:I:3273:HOH:O	2.18	0.53
9:Q:80:LEU:HD22	9:Q:138:LEU:HD11	1.91	0.53
13:U:22:GLN:O	13:U:100:LYS:NZ	2.29	0.53
13:U:47:GLU:CD	13:U:50:ARG:HH11	2.13	0.53
1:I:1754:A:O2'	16:X:103:ARG:NH2	2.42	0.52
13:U:20:LEU:CD1	22:d:81:PRO:HG2	2.22	0.52
14:V:81:ASN:O	14:V:85:PRO:HG2	2.09	0.52
26:h:8:THR:HG1	26:h:35:THR:HG1	1.51	0.52
15:W:116:GLN:N	15:W:116:GLN:OE1	2.41	0.52
1:I:452:G:C8	5:M:53:THR:HG21	2.44	0.52
14:V:114:GLU:HG2	14:V:118:ARG:CD	2.33	0.52
15:W:111:ARG:NH1	15:W:117:PHE:O	2.42	0.52
4:L:157:LYS:HD2	10:R:79:GLY:O	2.09	0.52
9:Q:104:ALA:O	9:Q:108:GLU:N	2.42	0.52
17:Y:91:ASP:O	17:Y:95:LEU:HD23	2.09	0.52
27:i:46:ASP:O	27:i:53:LYS:HE2	2.10	0.52
3:K:107:PRO:HD2	3:K:110:LEU:HD22	1.91	0.52
4:L:156:PHE:HB3	10:R:81:ILE:CG1	2.39	0.52
18:Z:52:PRO:CD	18:Z:53:PHE:N	2.47	0.52
5:M:5:LEU:HD12	5:M:5:LEU:N	2.24	0.52
1:I:674:G:HO2'	5:M:69:ARG:HD3	1.75	0.52
1:I:733:G:OP2	35:I:3306:HOH:O	2.19	0.52
6:N:129:SER:OG	6:N:154:ILE:O	2.09	0.52
9:Q:42:PHE:O	9:Q:46:THR:HG23	2.09	0.52
15:W:27:VAL:HG21	15:W:40:ILE:HD12	1.92	0.52
5:M:5:LEU:N	5:M:5:LEU:CD1	2.73	0.51
9:Q:80:LEU:HD11	9:Q:136:MET:SD	2.50	0.51
14:V:24:MET:HB3	14:V:44:LEU:HD13	1.91	0.51
1:I:568:U:OP1	12:T:36:LYS:HD2	2.11	0.51
1:I:2079:U:O2'	24:f:23:ASN:OD1	2.23	0.51
1:I:2638:G:O2'	1:I:2775:G:N2	2.39	0.51
17:Y:109:LEU:HD23	18:Z:49:ILE:HD13	1.92	0.51
18:Z:48:LYS:HE3	18:Z:103:ALA:HB1	1.91	0.51
1:I:1324:G:O2'	1:I:1326:U:OP2	2.23	0.51
6:N:129:SER:HB2	6:N:155:THR:HG23	1.91	0.51
11:S:71:ARG:HB2	11:S:75:SER:OG	2.10	0.51
15:W:54:VAL:HG13	15:W:54:VAL:O	2.09	0.51
1:I:1034:G:N7	35:I:3472:HOH:O	2.34	0.51
4:L:177:VAL:HG13	4:L:177:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:A:N3	35:I:3453:HOH:O	2.34	0.51
1:I:687:C:H1'	29:k:4:THR:HG22	1.93	0.51
11:S:2:ILE:HG23	11:S:6:THR:CG2	2.41	0.51
17:Y:87:SER:O	18:Z:51:VAL:O	2.29	0.51
27:i:11:SER:O	27:i:15:MET:HG3	2.11	0.51
1:I:571:U:OP1	18:Z:80:ARG:NH1	2.44	0.51
1:I:1385:A:OP1	35:I:3269:HOH:O	2.19	0.51
1:I:1799:G:OP2	3:K:270:ARG:NH2	2.37	0.51
3:K:168:ASP:OD1	3:K:171:TYR:HB2	2.11	0.51
18:Z:38:VAL:CG1	18:Z:59:ILE:HD12	2.41	0.51
29:k:12:ARG:CZ	29:k:44:VAL:HG22	2.41	0.51
1:I:2006:C:O2'	1:I:2823:A:N3	2.41	0.50
6:N:44:ILE:HG21	6:N:79:ILE:HG22	1.94	0.50
13:U:33:LEU:HD13	13:U:117:PHE:HB3	1.92	0.50
17:Y:91:ASP:O	17:Y:95:LEU:CD2	2.59	0.50
8:P:49:ALA:O	8:P:53:GLU:N	2.43	0.50
1:I:1052:C:N4	1:I:1107:G:O6	2.45	0.50
27:i:52:ARG:HB2	27:i:52:ARG:CZ	2.41	0.50
1:I:1657:U:OP2	4:L:141:ARG:HG3	2.12	0.50
4:L:46:ARG:HH12	4:L:86:GLU:H	1.57	0.50
11:S:70:ARG:HG3	11:S:70:ARG:HH11	1.76	0.50
19:a:29:VAL:CG1	19:a:55:ILE:HD11	2.42	0.50
1:I:1251:C:OP2	17:Y:6:ARG:HD2	2.12	0.50
1:I:2742:G:OP1	31:m:36:ARG:HD3	2.10	0.50
1:I:695:G:OP1	1:I:1380:G:O2'	2.30	0.50
1:I:1791:A:N6	1:I:1828:G:O2'	2.40	0.50
1:I:2091:C:H4'	24:f:56:MET:HE3	1.92	0.50
18:Z:14:VAL:HG12	18:Z:20:VAL:CG1	2.39	0.50
1:I:1189:A:OP1	18:Z:82:HIS:ND1	2.40	0.50
4:L:156:PHE:HB3	10:R:81:ILE:HG13	1.94	0.50
17:Y:66:ASN:O	17:Y:70:ARG:HB2	2.11	0.50
1:I:588:U:OP2	35:I:3305:HOH:O	2.19	0.49
1:I:1937:A:H1'	1:I:1939:5MU:H72	1.94	0.49
2:J:58:A:OP2	35:J:301:HOH:O	2.20	0.49
12:T:77:ILE:CD1	12:T:108:ALA:HB1	2.41	0.49
17:Y:87:SER:C	18:Z:51:VAL:O	2.55	0.49
1:I:281:C:H42	1:I:359:G:H22	1.60	0.49
24:f:23:ASN:ND2	35:f:102:HOH:O	2.45	0.49
1:I:2004:G:OP1	35:I:3308:HOH:O	2.19	0.49
9:Q:71:THR:HG22	9:Q:72:LYS:H	1.77	0.49
1:I:2291:U:O2'	1:I:2374:C:O2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:42:C:C5	6:N:66:LEU:HD22	2.48	0.49
14:V:8:ARG:HB2	14:V:43:GLU:CD	2.38	0.49
27:i:41:HIS:HA	27:i:49:TYR:OH	2.13	0.49
7:O:24:ILE:HG12	7:O:24:ILE:O	2.13	0.49
10:R:36:LEU:HD13	10:R:54:ILE:HD12	1.94	0.49
14:V:30:ARG:NH1	14:V:74:GLU:OE1	2.45	0.49
1:I:2605:PSU:H5'	1:I:2605:PSU:C6	2.48	0.49
1:I:727:A:H2	3:K:9:THR:HG21	1.78	0.49
1:I:2445:2MG:OP1	5:M:69:ARG:NH2	2.46	0.49
1:I:203:A:N7	35:I:3478:HOH:O	2.35	0.48
6:N:8:TYR:O	6:N:13:VAL:HG23	2.12	0.48
3:K:157:SER:HB3	3:K:160:THR:HG21	1.95	0.48
1:I:443:A:OP1	5:M:41:GLN:N	2.46	0.48
1:I:579:G:O2'	1:I:2019:A:OP1	2.30	0.48
1:I:2241:A:N7	35:I:3476:HOH:O	2.35	0.48
1:I:2294:G:OP1	15:W:10:ARG:HD3	2.13	0.48
15:W:24:THR:HG23	15:W:40:ILE:C	2.39	0.48
1:I:28:A:N3	17:Y:11:ARG:NH2	2.61	0.48
1:I:2131:U:OP2	35:I:3310:HOH:O	2.20	0.48
2:J:40:U:O2'	2:J:43:C:OP2	2.26	0.48
18:Z:48:LYS:HE3	18:Z:103:ALA:CB	2.43	0.48
29:k:12:ARG:NE	29:k:44:VAL:HG22	2.28	0.48
1:I:1652:A:N6	14:V:11:ASN:HD21	1.99	0.48
27:i:52:ARG:NH2	27:i:52:ARG:CB	2.77	0.48
1:I:397:U:OP2	24:f:10:LYS:NZ	2.41	0.48
1:I:2005:A:N7	35:I:3479:HOH:O	2.35	0.48
1:I:2589:A:OP2	35:I:3309:HOH:O	2.20	0.48
26:h:4:THR:CG2	26:h:37:GLU:CG	2.92	0.48
26:h:40:ASP:OD1	26:h:45:ARG:NE	2.45	0.48
30:l:32:ILE:O	30:l:32:ILE:HG22	2.13	0.48
3:K:203[A]:ARG:NH2	3:K:205:LEU:HD11	2.29	0.48
9:Q:43:ASN:O	9:Q:47:ASP:N	2.44	0.48
19:a:17:VAL:HG12	19:a:76:VAL:HG21	1.96	0.48
10:R:36:LEU:HD21	10:R:122:LEU:HB2	1.96	0.47
13:U:53:MET:HE3	13:U:120:ALA:CB	2.44	0.47
19:a:109:ASP:OD1	19:a:110:ARG:N	2.45	0.47
24:f:71:LEU:O	24:f:75:GLY:O	2.32	0.47
1:I:1266:G:O2'	1:I:2012:G:O6	2.27	0.47
1:I:2306:C:N3	35:I:3473:HOH:O	2.35	0.47
5:M:119:ILE:HB	5:M:187:VAL:HG22	1.96	0.47
1:I:2334:U:O4	15:W:16:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2818:U:OP2	14:V:42:LYS:NZ	2.41	0.47
15:W:26:LEU:HD12	15:W:38:GLN:O	2.15	0.47
5:M:16:GLU:O	5:M:20:GLY:CA	2.62	0.47
17:Y:32:TYR:CD1	17:Y:32:TYR:C	2.92	0.47
4:L:121:THR:HB	4:L:127:PHE:CD2	2.49	0.47
4:L:151:THR:HG23	4:L:152:PRO:HD3	1.97	0.47
1:I:411:G:OP2	1:I:2406:A:O2'	2.30	0.47
1:I:686:U:O4	29:k:12:ARG:HB2	2.13	0.47
1:I:2296:U:OP2	15:W:9:ARG:NH2	2.42	0.47
1:I:2437:G:N7	35:I:3485:HOH:O	2.35	0.47
1:I:2450:A:OP1	1:I:2497:A:O2'	2.25	0.47
3:K:232:HIS:CA	3:K:242:LYS:HE2	2.32	0.47
9:Q:86:ILE:HG22	9:Q:88:SER:H	1.80	0.47
14:V:70:THR:HG21	14:V:75:ILE:HB	1.97	0.47
22:d:4:ILE:CG2	22:d:42:LEU:HD22	2.44	0.47
29:k:12:ARG:CZ	29:k:44:VAL:CG2	2.92	0.47
1:I:2704:C:OP2	35:I:3315:HOH:O	2.21	0.47
10:R:32:LEU:O	10:R:36:LEU:HB2	2.14	0.47
11:S:2:ILE:HB	11:S:33:ALA:HB3	1.96	0.47
1:I:2318:G:O2'	1:I:2321:U:O4	2.26	0.47
5:M:16:GLU:O	5:M:20:GLY:N	2.48	0.47
12:T:128:THR:OG1	12:T:131:ALA:HB3	2.15	0.47
25:g:44:LYS:O	25:g:48:ARG:HG3	2.13	0.47
1:I:1114:C:N4	1:I:1115:G:O6	2.48	0.46
1:I:1190:G:H5''	12:T:32:GLY:O	2.15	0.46
1:I:1792:G:O2'	1:I:1830:C:OP1	2.30	0.46
23:e:59:LEU:HD12	23:e:80:ILE:HD12	1.97	0.46
1:I:1009:A:O4'	17:Y:59:GLN:HG3	2.15	0.46
1:I:1799:G:N7	3:K:178:SER:OG	2.47	0.46
1:I:1902:C:H4'	3:K:242:LYS:O	2.14	0.46
3:K:178:SER:O	3:K:271:ARG:HB2	2.16	0.46
10:R:36:LEU:HD13	10:R:54:ILE:HD13	1.96	0.46
26:h:39:GLU:O	26:h:39:GLU:HG2	2.15	0.46
1:I:125:A:H1'	29:k:13:ASN:HD22	1.80	0.46
21:c:22:ARG:HD3	21:c:73:PHE:CE1	2.50	0.46
1:I:1011:G:OP1	17:Y:77:SER:OG	2.26	0.46
1:I:2274:A:OP2	35:I:3314:HOH:O	2.20	0.46
15:W:24:THR:OG1	15:W:42:PRO:HD3	2.15	0.46
8:P:42:LYS:O	8:P:46:PHE:N	2.49	0.46
16:X:92:VAL:HG21	16:X:97:LEU:HD21	1.97	0.46
3:K:162:VAL:CG1	3:K:174:LEU:HG	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:175:ARG:HE	3:K:181:MET:HE1	1.81	0.46
14:V:8:ARG:HB2	14:V:43:GLU:OE2	2.16	0.46
1:I:1420:A:N3	35:I:3492:HOH:O	2.36	0.46
9:Q:53:LEU:HD22	9:Q:79:LEU:HD21	1.97	0.46
20:b:4:GLU:HG2	25:g:19:LEU:CD2	2.44	0.46
3:K:167:ARG:HG2	3:K:167:ARG:NH2	2.31	0.46
8:P:103:VAL:HG22	8:P:106:ALA:HB3	1.98	0.46
9:Q:13:VAL:CG2	9:Q:24:VAL:HG13	2.46	0.46
31:m:4:ARG:HG3	31:m:6:SER:O	2.16	0.45
1:I:2723:C:H4'	14:V:1:MET:HG3	1.99	0.45
3:K:177:ARG:HG3	3:K:177:ARG:HH21	1.81	0.45
7:O:88:GLN:N	7:O:163:ARG:O	2.48	0.45
26:h:29:LEU:HD21	26:h:36:VAL:HG22	1.98	0.45
1:I:764:A:N3	3:K:212:ARG:NH2	2.60	0.45
1:I:2013:A:H4'	19:a:96:ILE:HG22	1.98	0.45
3:K:133:ARG:HD3	35:K:433:HOH:O	2.15	0.45
1:I:2467:C:OP1	31:m:8:LYS:NZ	2.44	0.45
11:S:14:SER:O	11:S:51:LYS:HG3	2.16	0.45
21:c:72:ILE:HD12	21:c:96:PHE:CE1	2.52	0.45
30:l:42:ARG:NH1	35:l:102:HOH:O	2.43	0.45
1:I:2571:U:C2'	4:L:151:THR:CG2	2.90	0.45
4:L:101:PHE:O	4:L:180:VAL:HG21	2.17	0.45
15:W:26:LEU:HD13	15:W:39:VAL:HG23	1.96	0.45
15:W:48:LEU:O	15:W:85:LYS:NZ	2.48	0.45
19:a:72:THR:HG21	19:a:108:SER:CB	2.47	0.45
1:I:2280:G:O6	23:e:14:ARG:HD2	2.17	0.45
9:Q:42:PHE:HZ	9:Q:55:ILE:HG23	1.82	0.45
13:U:44:ARG:HG2	13:U:44:ARG:HH21	1.82	0.45
16:X:76:THR:HG23	16:X:77:HIS:CD2	2.52	0.45
1:I:807:U:O2'	1:I:2060:A:N1	2.43	0.45
1:I:2548:U:O2	11:S:23:LYS:NZ	2.50	0.45
1:I:77:G:O2'	25:g:7:ARG:NH2	2.49	0.45
1:I:1253:A:OP1	35:I:3318:HOH:O	2.21	0.45
1:I:2125:G:C2'	1:I:2173:A:H61	2.30	0.45
1:I:2393:U:O2'	30:l:13:ARG:NH1	2.49	0.45
3:K:3:VAL:HG12	3:K:19:VAL:HG22	1.99	0.45
15:W:28:VAL:HG21	15:W:92:PHE:CZ	2.52	0.45
17:Y:49:ASP:OD1	17:Y:52:GLN:NE2	2.49	0.45
22:d:40:ILE:HD12	22:d:42:LEU:HD21	1.99	0.45
1:I:2884:U:O2'	27:i:40:ARG:NH2	2.50	0.44
6:N:104:ILE:HD11	6:N:175:PHE:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:29:LYS:HE3	7:O:80:THR:HA	1.99	0.44
14:V:65:LEU:HD12	14:V:65:LEU:HA	1.83	0.44
1:I:2294:G:P	15:W:94:ARG:NH1	2.89	0.44
4:L:186:LEU:HD11	16:X:4:ILE:HG23	1.99	0.44
18:Z:55:ASP:OD1	18:Z:56:GLY:N	2.45	0.44
3:K:167:ARG:HG2	3:K:167:ARG:HH21	1.82	0.44
3:K:177:ARG:HG3	3:K:177:ARG:NH2	2.31	0.44
13:U:62:LYS:HD3	13:U:64:TRP:CZ2	2.53	0.44
14:V:12:ARG:NH1	14:V:20:MET:HE1	2.32	0.44
1:I:714:U:O4'	1:I:718:A:N6	2.51	0.44
9:Q:30:GLN:NE2	9:Q:30:GLN:O	2.50	0.44
19:a:12:SER:OG	19:a:17:VAL:HG23	2.17	0.44
4:L:3:GLY:O	4:L:4:LEU:HD12	2.18	0.44
5:M:5:LEU:CD1	5:M:5:LEU:H	2.31	0.44
8:P:103:VAL:HG22	8:P:106:ALA:CB	2.48	0.44
9:Q:50:GLU:O	9:Q:52:GLY:N	2.49	0.44
29:k:8:SER:HB3	29:k:11:LYS:HB2	1.98	0.44
1:I:250:G:H4'	12:T:59:ARG:HD2	2.00	0.44
1:I:126:A:O5'	29:k:19:ARG:HG3	2.17	0.44
3:K:19:VAL:HG23	3:K:203[A]:ARG:HB3	1.98	0.44
28:j:25:LYS:NZ	28:j:52:ALA:HB1	2.32	0.44
1:I:2033:A:O2'	1:I:2035:G:OP2	2.34	0.44
1:I:2460:U:O2	1:I:2493:U:N3	2.51	0.44
12:T:128:THR:OG1	12:T:131:ALA:CB	2.66	0.44
17:Y:89:GLU:O	18:Z:11:GLN:NE2	2.45	0.44
18:Z:68:ARG:HE	18:Z:90:ARG:HB2	1.83	0.44
1:I:1758:U:OP1	35:I:3317:HOH:O	2.21	0.44
13:U:41:LEU:HD23	13:U:41:LEU:HA	1.90	0.44
18:Z:26:ASP:O	18:Z:27:ILE:HD13	2.18	0.44
29:k:30:VAL:O	29:k:34:ARG:HG3	2.18	0.44
1:I:2820:A:P	14:V:2:ARG:NH2	2.91	0.43
1:I:592:A:O2'	30:l:64:TYR:OH	2.28	0.43
1:I:2822:G:O2'	1:I:2824:C:OP2	2.34	0.43
7:O:107:LEU:HD13	7:O:152:ARG:HB2	2.00	0.43
14:V:10:LEU:HD11	14:V:43:GLU:OE1	2.18	0.43
14:V:28:LEU:HD23	14:V:48:VAL:HG21	2.00	0.43
21:c:72:ILE:HD11	21:c:83:VAL:HG22	2.00	0.43
1:I:1071:G:O2'	1:I:1089:A:OP2	2.25	0.43
1:I:2749:A:OP1	7:O:2:SER:N	2.51	0.43
8:P:115:VAL:HG23	8:P:132:PHE:CD1	2.53	0.43
15:W:24:THR:CG2	15:W:40:ILE:O	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:338:G:N7	35:I:3500:HOH:O	2.36	0.43
1:I:523:C:O2	1:I:554:U:O2'	2.34	0.43
7:O:154:PRO:HD3	7:O:162:VAL:O	2.18	0.43
11:S:69:VAL:O	11:S:76:VAL:HG23	2.19	0.43
15:W:94:ARG:HD2	15:W:97:PHE:O	2.18	0.43
1:I:954:G:O2'	1:I:2274:A:N1	2.37	0.43
1:I:2117:A:O2'	1:I:2118:U:OP2	2.23	0.43
4:L:151:THR:HG23	4:L:152:PRO:CD	2.49	0.43
5:M:143:LEU:HD13	5:M:146:VAL:HG21	2.00	0.43
14:V:44:LEU:HD23	14:V:113:ILE:HD13	2.01	0.43
1:I:283:G:N2	1:I:358:U:O2	2.51	0.43
1:I:1754:A:N1	1:I:2716:C:O2'	2.46	0.43
1:I:277:G:N7	35:I:3506:HOH:O	2.37	0.43
1:I:629:G:N3	1:I:639:U:O2'	2.51	0.43
1:I:672:C:H4'	5:M:84:THR:HG23	2.01	0.43
1:I:2279:G:O2'	1:I:2327:A:O2'	2.35	0.43
8:P:46:PHE:O	8:P:49:ALA:HB3	2.18	0.43
31:m:16:ILE:HD13	31:m:25:VAL:HG22	2.01	0.43
1:I:13:A:O2'	1:I:15:G:N7	2.40	0.43
1:I:467:G:O2'	1:I:796:C:O2'	2.30	0.43
1:I:1869:G:N2	1:I:1872:A:OP2	2.48	0.43
2:J:54:G:H21	6:N:26:MET:CE	2.32	0.43
4:L:9:VAL:O	4:L:197:THR:HG23	2.18	0.43
6:N:14:LYS:O	6:N:18:THR:HG22	2.19	0.43
4:L:25:THR:HG21	4:L:193:VAL:HG22	2.01	0.43
9:Q:101:ILE:HD11	9:Q:106:LEU:HD21	2.00	0.43
11:S:70:ARG:HG3	11:S:70:ARG:NH1	2.33	0.43
1:I:615:U:O4	5:M:39:ALA:HB2	2.19	0.42
7:O:33:LEU:HD23	7:O:33:LEU:HA	1.88	0.42
21:c:22:ARG:HD3	21:c:73:PHE:CG	2.54	0.42
1:I:1920:C:N4	1:I:1921:G:O6	2.52	0.42
3:K:69:ARG:HB2	3:K:129:THR:HG21	2.00	0.42
10:R:89:PHE:CE1	10:R:100:VAL:HG11	2.54	0.42
12:T:58:TYR:O	30:l:13:ARG:NE	2.52	0.42
14:V:70:THR:HG22	14:V:72:ASP:N	2.33	0.42
1:I:966:G:OP2	35:I:3312:HOH:O	2.20	0.42
1:I:2115:G:N2	1:I:2119:A:OP1	2.49	0.42
16:X:68:GLU:O	16:X:70:VAL:HG23	2.19	0.42
17:Y:28:ARG:NH2	17:Y:38:ALA:HB1	2.34	0.42
5:M:15:SER:HB3	5:M:18:THR:HG22	2.00	0.42
1:I:458:G:O2'	1:I:469:G:O6	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1154:G:OP1	35:I:3325:HOH:O	2.22	0.42
1:I:2820:A:OP2	14:V:2:ARG:NH2	2.51	0.42
11:S:70:ARG:NH1	11:S:74:GLY:O	2.52	0.42
15:W:26:LEU:HD13	15:W:39:VAL:HG22	2.01	0.42
1:I:569:U:O2'	1:I:983:A:N1	2.52	0.42
3:K:167:ARG:HG3	3:K:172:VAL:HG12	2.02	0.42
17:Y:58:ARG:HA	17:Y:61:TRP:CE3	2.55	0.42
22:d:89:ILE:HG21	22:d:91:PHE:CZ	2.55	0.42
30:l:26:HIS:NE2	30:l:48:ALA:HB2	2.34	0.42
1:I:577:G:O2'	1:I:1254:A:OP1	2.36	0.42
1:I:1217:U:OP2	17:Y:15:LYS:NZ	2.50	0.42
4:L:60:VAL:HG22	4:L:64:GLU:HB2	2.02	0.42
27:i:52:ARG:HG2	27:i:54:VAL:HG13	2.00	0.42
1:I:727:A:N1	3:K:9:THR:HG21	2.34	0.42
3:K:155:ALA:HB2	3:K:162:VAL:HG23	2.01	0.42
1:I:1141:U:H4'	1:I:1142:A:O4'	2.20	0.42
1:I:41:C:OP1	35:I:3320:HOH:O	2.21	0.42
1:I:2127:G:N1	1:I:2128:G:O6	2.53	0.42
7:O:145:ALA:HB1	7:O:164:TYR:HE1	1.85	0.42
10:R:99:ARG:HD2	10:R:99:ARG:HA	1.76	0.42
1:I:1363:C:O2'	1:I:1809:A:N3	2.49	0.41
1:I:1666:G:OP1	11:S:82:ASN:ND2	2.47	0.41
1:I:2354:C:O2	23:e:36:ILE:HD12	2.20	0.41
4:L:150:GLN:O	4:L:150:GLN:CG	2.67	0.41
8:P:88:GLY:O	8:P:125:THR:N	2.49	0.41
14:V:58:ASP:OD2	14:V:63:ARG:NH2	2.52	0.41
27:i:55:ILE:HG22	27:i:56:ALA:N	2.34	0.41
1:I:2111:U:O5'	35:I:3323:HOH:O	2.21	0.41
2:J:90:C:H5'	13:U:18:ARG:HG2	2.02	0.41
6:N:50:LEU:HD21	6:N:67:ILE:HG23	2.02	0.41
9:Q:88:SER:OG	9:Q:89:GLY:N	2.52	0.41
11:S:3:GLN:O	11:S:6:THR:HG22	2.19	0.41
2:J:66:A:O4'	2:J:108:A:N6	2.53	0.41
17:Y:90:ILE:HG22	17:Y:95:LEU:HD22	2.02	0.41
1:I:566:U:O2'	1:I:809:G:OP2	2.33	0.41
11:S:107:LEU:HD23	11:S:112:PHE:HB3	2.02	0.41
15:W:49:VAL:HG13	15:W:81:ARG:HB2	2.02	0.41
1:I:582:A:OP1	17:Y:14:HIS:ND1	2.52	0.41
1:I:2553:G:N1	1:I:2554:U:O2	2.53	0.41
1:I:2564:A:OP1	1:I:2648:G:O2'	2.25	0.41
3:K:107:PRO:HA	3:K:195:VAL:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:46:ARG:NH1	4:L:86:GLU:H	2.16	0.41
4:L:156:PHE:CD2	10:R:81:ILE:HG12	2.55	0.41
11:S:70:ARG:HH12	11:S:74:GLY:CA	2.33	0.41
12:T:29:LYS:HG2	12:T:30:THR:HG23	2.02	0.41
1:I:94:A:OP2	35:I:3321:HOH:O	2.21	0.41
1:I:2571:U:C4'	4:L:151:THR:HG21	2.51	0.41
1:I:2820:A:OP1	14:V:2:ARG:NH2	2.51	0.41
14:V:24:MET:SD	14:V:36:THR:HG21	2.60	0.41
27:i:25:VAL:HG11	27:i:28:LEU:HD21	2.01	0.41
1:I:1738:G:O2'	1:I:1739:A:O4'	2.39	0.41
1:I:2146:C:HO2'	1:I:2147:A:P	2.40	0.41
18:Z:41:ILE:O	18:Z:47:VAL:HA	2.21	0.41
19:a:7:HIS:CD2	19:a:10:ALA:HB2	2.55	0.41
19:a:23:LEU:HD21	27:i:22:LEU:O	2.21	0.41
23:e:19:LYS:HA	23:e:19:LYS:HD3	1.80	0.41
1:I:1614:A:C2	19:a:93:ALA:HB2	2.55	0.41
1:I:2121:G:H22	1:I:2176:A:H2	1.69	0.41
4:L:105:LYS:O	4:L:177:VAL:HG12	2.21	0.41
10:R:28:LEU:C	10:R:28:LEU:HD12	2.45	0.41
10:R:93:ILE:HD13	10:R:93:ILE:HA	1.97	0.41
11:S:25:LEU:HD21	11:S:40:LYS:HB2	2.03	0.41
22:d:93:ARG:HH11	22:d:93:ARG:HD2	1.75	0.41
27:i:48:TYR:CE1	27:i:53:LYS:HD3	2.56	0.41
1:I:1653:G:H3'	14:V:2:ARG:HB2	2.03	0.41
1:I:1754:A:C8	16:X:94:LYS:HE2	2.55	0.41
1:I:1967:C:OP2	35:I:3328:HOH:O	2.22	0.41
1:I:2626:C:H2'	1:I:2627:G:O4'	2.20	0.41
1:I:829:A:N7	1:I:2247:A:O2'	2.51	0.40
1:I:1066:U:N3	1:I:1069:A:OP2	2.48	0.40
1:I:1321:A:O2'	19:a:11:ARG:NH2	2.54	0.40
1:I:1482:G:H1	1:I:1507:C:H42	1.68	0.40
19:a:17:VAL:HG12	19:a:17:VAL:O	2.21	0.40
1:I:1239:G:N7	35:I:3518:HOH:O	2.37	0.40
30:l:33:LEU:O	30:l:41:LYS:NZ	2.50	0.40
1:I:1775:U:OP2	35:I:3326:HOH:O	2.22	0.40
1:I:2553:G:N2	35:I:3959:HOH:O	2.53	0.40
1:I:2709:G:OP1	14:V:18:GLN:NE2	2.42	0.40
17:Y:52:GLN:HE21	17:Y:52:GLN:HB2	1.66	0.40
25:g:11:VAL:HG12	25:g:15:ASN:ND2	2.36	0.40
6:N:112:ARG:NH2	6:N:134:GLU:OE2	2.55	0.40
8:P:93:SER:OG	8:P:94:ILE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:99:ILE:HG23	8:P:144:VAL:HG11	2.03	0.40
12:T:37:GLY:O	12:T:41:ARG:HG2	2.21	0.40
20:b:12:ARG:HA	25:g:29:ARG:HE	1.85	0.40
1:I:994:C:P	17:Y:50:ARG:HD2	2.61	0.40
12:T:132:ARG:HG3	12:T:142:ILE:CD1	2.51	0.40
19:a:72:THR:HG21	19:a:108:SER:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	270/271 (100%)	254 (94%)	16 (6%)	0	100	100
4	L	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	24	27
5	M	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
6	N	175/177 (99%)	152 (87%)	23 (13%)	0	100	100
7	O	174/176 (99%)	162 (93%)	12 (7%)	0	100	100
8	P	147/149 (99%)	126 (86%)	21 (14%)	0	100	100
9	Q	132/134 (98%)	110 (83%)	22 (17%)	0	100	100
10	R	140/142 (99%)	140 (100%)	0	0	100	100
11	S	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
12	T	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
13	U	133/136 (98%)	129 (97%)	4 (3%)	0	100	100
14	V	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
15	W	114/117 (97%)	105 (92%)	9 (8%)	0	100	100
16	X	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
17	Y	115/117 (98%)	115 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Z	101/103 (98%)	96 (95%)	4 (4%)	1 (1%)	12	11
19	a	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
20	b	91/93 (98%)	87 (96%)	4 (4%)	0	100	100
21	c	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
22	d	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
23	e	73/75 (97%)	73 (100%)	0	0	100	100
24	f	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
25	g	60/62 (97%)	55 (92%)	5 (8%)	0	100	100
26	h	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
27	i	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
28	j	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
All	All	3298/3357 (98%)	3112 (94%)	184 (6%)	2 (0%)	49	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	Z	52	PRO
4	L	151	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	
3	K	217/216 (100%)	214 (99%)	3 (1%)	59	75
4	L	164/164 (100%)	158 (96%)	6 (4%)	30	41
5	M	165/165 (100%)	162 (98%)	3 (2%)	51	68
6	N	148/148 (100%)	146 (99%)	2 (1%)	59	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	O	137/137 (100%)	130 (95%)	7 (5%)	21	27
8	P	114/114 (100%)	113 (99%)	1 (1%)	70	84
9	Q	104/104 (100%)	104 (100%)	0	100	100
10	R	116/116 (100%)	113 (97%)	3 (3%)	40	55
11	S	103/103 (100%)	100 (97%)	3 (3%)	37	51
12	T	103/103 (100%)	99 (96%)	4 (4%)	28	39
13	U	108/108 (100%)	104 (96%)	4 (4%)	30	41
14	V	100/100 (100%)	93 (93%)	7 (7%)	14	16
15	W	86/87 (99%)	84 (98%)	2 (2%)	44	59
16	X	99/99 (100%)	99 (100%)	0	100	100
17	Y	89/89 (100%)	87 (98%)	2 (2%)	45	61
18	Z	84/84 (100%)	83 (99%)	1 (1%)	63	78
19	a	93/93 (100%)	93 (100%)	0	100	100
20	b	80/80 (100%)	78 (98%)	2 (2%)	42	56
21	c	83/83 (100%)	81 (98%)	2 (2%)	43	58
22	d	78/78 (100%)	78 (100%)	0	100	100
23	e	57/57 (100%)	55 (96%)	2 (4%)	32	43
24	f	67/67 (100%)	66 (98%)	1 (2%)	57	73
25	g	54/54 (100%)	54 (100%)	0	100	100
26	h	48/48 (100%)	47 (98%)	1 (2%)	47	63
27	i	47/47 (100%)	46 (98%)	1 (2%)	47	63
28	j	45/45 (100%)	45 (100%)	0	100	100
29	k	38/38 (100%)	37 (97%)	1 (3%)	40	55
30	l	51/51 (100%)	50 (98%)	1 (2%)	48	64
31	m	34/34 (100%)	33 (97%)	1 (3%)	37	51
All	All	2712/2712 (100%)	2652 (98%)	60 (2%)	45	61

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	14	ARG
3	K	174	LEU
3	K	267	ILE

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Mol	Chain	Res	Type
4	L	13	ARG
4	L	33	ARG
4	L	58	ASN
4	L	79	LEU
4	L	141	ARG
4	L	151	THR
5	M	5	LEU
5	M	12	LEU
5	M	44	ARG
6	N	21	ASN
6	N	30	ARG
7	O	3	ARG
7	O	23	VAL
7	O	24	ILE
7	O	25	THR
7	O	35	ARG
7	O	152	ARG
7	O	153	ARG
8	P	48	GLU
10	R	11	VAL
10	R	36	LEU
10	R	81	ILE
11	S	28	SER
11	S	49	ARG
11	S	107	LEU
12	T	40	SER
12	T	70	LYS
12	T	116	VAL
12	T	123	ARG
13	U	57	VAL
13	U	59	ARG
13	U	65	ILE
13	U	67	VAL
14	V	1	MET
14	V	14	SER
14	V	20	MET
14	V	65	LEU
14	V	69	ARG
14	V	96	ARG
14	V	114	GLU
15	W	9	ARG
15	W	31	THR

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Mol	Chain	Res	Type
17	Y	9	ILE
17	Y	52	GLN
18	Z	22	LEU
20	b	5	GLU
20	b	12	ARG
21	c	7	ARG
21	c	86	ARG
23	e	19	LYS
23	e	38	VAL
24	f	56	MET
26	h	10	THR
27	i	52	ARG
29	k	44	VAL
30	l	31	HIS
31	m	4	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	134	ASN
3	K	153	GLN
3	K	200	HIS
4	L	173	GLN
5	M	115	GLN
5	M	165	HIS
7	O	30	ASN
7	O	115	HIS
8	P	11	ASN
9	Q	30	GLN
10	R	80	HIS
12	T	35	HIS
12	T	104	GLN
13	U	13	HIS
14	V	11	ASN
14	V	23	ASN
14	V	31	HIS
15	W	104	GLN
17	Y	52	GLN
18	Z	91	GLN
19	a	7	HIS
19	a	9	HIS
24	f	16	ASN

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Mol	Chain	Res	Type
27	i	5	GLN
28	j	19	HIS
30	l	31	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	454 (15%)	23 (0%)
2	J	117/118 (99%)	14 (11%)	0
All	All	3013/3022 (99%)	468 (15%)	23 (0%)

All (468) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	12	U
1	I	14	A
1	I	15	G
1	I	23	G
1	I	34	U
1	I	43	G
1	I	45	G
1	I	46	G
1	I	58	G
1	I	63	A
1	I	71	A
1	I	74	A
1	I	75	G
1	I	84	A
1	I	101	A
1	I	102	U
1	I	110	G
1	I	118	A
1	I	119	A
1	I	120	U
1	I	131	A
1	I	135	U
1	I	137	U
1	I	138	U
1	I	139	U

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Mol	Chain	Res	Type
1	I	140	C
1	I	142	A
1	I	163	C
1	I	181	A
1	I	196	A
1	I	215	G
1	I	216	A
1	I	221	A
1	I	222	A
1	I	248	G
1	I	264	C
1	I	265	A
1	I	266	G
1	I	272	A
1	I	276	U
1	I	281	C
1	I	283	G
1	I	289	G
1	I	296	U
1	I	311	A
1	I	327	G
1	I	329	G
1	I	330	A
1	I	343	C
1	I	346	A
1	I	353	C
1	I	359	G
1	I	362	A
1	I	371	A
1	I	372	G
1	I	386	G
1	I	396	G
1	I	403	U
1	I	405	U
1	I	407	G
1	I	411	G
1	I	412	A
1	I	420	C
1	I	424	G
1	I	451	U
1	I	457	A
1	I	481	G

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Mol	Chain	Res	Type
1	I	490	C
1	I	491	G
1	I	504	A
1	I	505	A
1	I	508	A
1	I	509	C
1	I	529	A
1	I	531	C
1	I	532	A
1	I	544	C
1	I	546	U
1	I	547	A
1	I	548	G
1	I	550	C
1	I	551	G
1	I	563	A
1	I	573	U
1	I	574	A
1	I	575	A
1	I	586	A
1	I	588	U
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	627	A
1	I	637	A
1	I	645	C
1	I	647	G
1	I	651	G
1	I	653	U
1	I	654	A
1	I	655	A
1	I	668	A
1	I	677	A
1	I	686	U
1	I	702	U
1	I	718	A
1	I	721	A
1	I	730	A
1	I	738	G
1	I	746	PSU

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Mol	Chain	Res	Type
1	I	747	5MU
1	I	757	G
1	I	764	A
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	794	A
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	846	U
1	I	856	G
1	I	858	G
1	I	859	G
1	I	869	G
1	I	877	A
1	I	879	G
1	I	884	U
1	I	893	C
1	I	894	U
1	I	896	A
1	I	907	G
1	I	910	A
1	I	917	A
1	I	931	U
1	I	941	A
1	I	946	C
1	I	961	C
1	I	974	G
1	I	983	A
1	I	996	A
1	I	1012	U
1	I	1013	C
1	I	1017	G
1	I	1022	G
1	I	1023	U
1	I	1026	G
1	I	1033	U

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Mol	Chain	Res	Type
1	I	1045	C
1	I	1046	A
1	I	1047	G
1	I	1051	G
1	I	1054	A
1	I	1057	A
1	I	1070	A
1	I	1071	G
1	I	1080	A
1	I	1082	U
1	I	1083	U
1	I	1085	A
1	I	1088	A
1	I	1089	A
1	I	1091	G
1	I	1108	U
1	I	1111	A
1	I	1112	G
1	I	1119	U
1	I	1130	U
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1168	G
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1178	C
1	I	1180	U
1	I	1206	G
1	I	1212	G
1	I	1238	G
1	I	1248	G
1	I	1253	A
1	I	1256	G
1	I	1262	A
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1300	G

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Mol	Chain	Res	Type
1	I	1301	A
1	I	1306	C
1	I	1321	A
1	I	1340	U
1	I	1341	G
1	I	1343	G
1	I	1352	U
1	I	1365	A
1	I	1368	G
1	I	1378	A
1	I	1379	U
1	I	1383	A
1	I	1387	A
1	I	1403	A
1	I	1407	G
1	I	1416	G
1	I	1420	A
1	I	1428	C
1	I	1460	U
1	I	1468	U
1	I	1482	G
1	I	1483	G
1	I	1490	A
1	I	1493	C
1	I	1494	A
1	I	1506	U
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1523	U
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1537	G
1	I	1569	A
1	I	1578	U
1	I	1584	U
1	I	1585	C
1	I	1586	A
1	I	1587	G
1	I	1608	A

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Mol	Chain	Res	Type
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1674	G
1	I	1715	G
1	I	1729	U
1	I	1730	C
1	I	1736	U
1	I	1738	G
1	I	1756	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1791	A
1	I	1800	C
1	I	1801	A
1	I	1808	A
1	I	1811	G
1	I	1816	C
1	I	1829	A
1	I	1833	C
1	I	1842	G
1	I	1870	C
1	I	1871	A
1	I	1873	G
1	I	1876	A
1	I	1882	U
1	I	1890	A
1	I	1899	A
1	I	1911	PSU
1	I	1913	A
1	I	1914	C
1	I	1915	3TD
1	I	1929	G
1	I	1930	G
1	I	1931	U
1	I	1937	A
1	I	1938	A
1	I	1955	U
1	I	1963	U
1	I	1967	C
1	I	1970	A

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Mol	Chain	Res	Type
1	I	1971	U
1	I	1972	G
1	I	1987	A
1	I	1991	U
1	I	1993	U
1	I	1997	C
1	I	2020	A
1	I	2022	U
1	I	2023	C
1	I	2031	A
1	I	2033	A
1	I	2043	C
1	I	2055	C
1	I	2056	G
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2069	G7M
1	I	2072	C
1	I	2093	G
1	I	2095	A
1	I	2106	U
1	I	2108	A
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2113	U
1	I	2115	G
1	I	2116	G
1	I	2117	A
1	I	2118	U
1	I	2120	G
1	I	2123	G
1	I	2124	G
1	I	2125	G
1	I	2126	A
1	I	2127	G
1	I	2128	G
1	I	2131	U
1	I	2132	U
1	I	2133	G
1	I	2142	A

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Mol	Chain	Res	Type
1	I	2146	C
1	I	2147	A
1	I	2150	C
1	I	2151	U
1	I	2157	G
1	I	2158	A
1	I	2159	G
1	I	2161	C
1	I	2162	G
1	I	2163	A
1	I	2164	C
1	I	2165	C
1	I	2169	A
1	I	2171	A
1	I	2172	U
1	I	2173	A
1	I	2177	C
1	I	2183	A
1	I	2187	U
1	I	2189	U
1	I	2190	G
1	I	2198	A
1	I	2204	G
1	I	2211	A
1	I	2223	G
1	I	2225	A
1	I	2226	C
1	I	2238	G
1	I	2239	G
1	I	2268	A
1	I	2278	A
1	I	2283	C
1	I	2287	A
1	I	2288	A
1	I	2305	U
1	I	2308	G
1	I	2309	A
1	I	2311	A
1	I	2322	A
1	I	2325	G
1	I	2333	A
1	I	2347	C

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Mol	Chain	Res	Type
1	I	2350	C
1	I	2354	C
1	I	2361	G
1	I	2383	G
1	I	2385	C
1	I	2391	G
1	I	2396	G
1	I	2402	U
1	I	2403	C
1	I	2406	A
1	I	2423	U
1	I	2424	C
1	I	2425	A
1	I	2426	A
1	I	2429	G
1	I	2430	A
1	I	2431	U
1	I	2434	A
1	I	2435	A
1	I	2441	U
1	I	2445	2MG
1	I	2447	G
1	I	2448	A
1	I	2459	A
1	I	2465	C
1	I	2466	C
1	I	2470	G
1	I	2475	C
1	I	2476	A
1	I	2491	U
1	I	2494	G
1	I	2502	G
1	I	2504	PSU
1	I	2505	G
1	I	2506	U
1	I	2518	A
1	I	2525	G
1	I	2529	G
1	I	2535	G
1	I	2547	A
1	I	2554	U
1	I	2562	U

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Mol	Chain	Res	Type
1	I	2566	A
1	I	2567	G
1	I	2573	C
1	I	2578	G
1	I	2602	A
1	I	2603	G
1	I	2605	PSU
1	I	2609	U
1	I	2613	U
1	I	2629	U
1	I	2630	G
1	I	2663	G
1	I	2681	C
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2716	C
1	I	2718	G
1	I	2724	U
1	I	2726	A
1	I	2733	A
1	I	2744	G
1	I	2748	A
1	I	2757	A
1	I	2765	A
1	I	2778	A
1	I	2791	G
1	I	2793	C
1	I	2794	C
1	I	2799	A
1	I	2800	A
1	I	2818	U
1	I	2820	A
1	I	2821	A
1	I	2833	U
1	I	2835	A
1	I	2861	U
1	I	2866	U
1	I	2867	G
1	I	2873	A
1	I	2874	C
1	I	2880	C

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Mol	Chain	Res	Type
1	I	2883	A
1	I	2884	U
1	I	2885	G
1	I	2891	U
1	I	2901	C
1	I	2903	U
1	I	2904	U
2	J	3	C
2	J	9	G
2	J	17	C
2	J	32	U
2	J	35	C
2	J	45	A
2	J	56	G
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	99	A
2	J	109	A
2	J	119	A

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	138	U
1	I	199	A
1	I	271	G
1	I	404	A
1	I	489	G
1	I	504	A
1	I	784	G
1	I	984	A
1	I	1205	A
1	I	1340	U
1	I	1342	A
1	I	1608	A
1	I	1930	G
1	I	2146	C
1	I	2162	G
1	I	2225	A
1	I	2425	A

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Mol	Chain	Res	Type
1	I	2430	A
1	I	2447	G
1	I	2680	U
1	I	2866	U
1	I	2873	A
1	I	2903	U

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	4D4	U	81	13	9,11,12	2.70	3 (33%)	7,13,15	1.23	0
1	G7M	I	2069	1	23,26,27	2.56	7 (30%)	34,39,42	1.93	10 (29%)
1	2MA	I	2503	1	22,25,26	3.65	11 (50%)	32,37,40	2.19	8 (25%)
1	3TD	I	1915	1	19,22,23	4.28	7 (36%)	23,32,35	1.65	2 (8%)
1	OMG	I	2251	1	23,26,27	2.24	8 (34%)	32,38,41	1.70	7 (21%)
1	PSU	I	1917	1	18,21,22	1.46	3 (16%)	21,30,33	2.02	4 (19%)
1	1MG	I	745	1	23,26,27	2.95	8 (34%)	33,39,42	2.20	9 (27%)
1	H2U	I	2449	1	18,21,22	1.58	3 (16%)	19,30,33	0.63	0
1	5MU	I	1939	1	19,22,23	4.77	7 (36%)	27,32,35	3.59	9 (33%)
1	5MC	I	1962	1	19,22,23	3.30	8 (42%)	26,32,35	1.17	2 (7%)
1	5MU	I	747	1	19,22,23	4.61	7 (36%)	27,32,35	3.59	9 (33%)
1	OMU	I	2552	1	19,22,23	2.89	8 (42%)	25,31,34	1.78	5 (20%)
1	PSU	I	2605	1	18,21,22	3.01	10 (55%)	21,30,33	2.70	7 (33%)
1	6MZ	I	2030	1	22,25,26	2.61	6 (27%)	29,36,39	3.12	11 (37%)
1	PSU	I	955	1	18,21,22	1.66	5 (27%)	21,30,33	1.90	4 (19%)
1	PSU	I	2504	1,32	18,21,22	1.71	5 (27%)	21,30,33	1.78	4 (19%)
1	PSU	I	746	1	18,21,22	1.66	6 (33%)	21,30,33	1.84	4 (19%)
1	OMC	I	2498	1,32	19,22,23	2.71	7 (36%)	25,31,34	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	I	1835	1	23,26,27	2.69	8 (34%)	33,38,41	2.00	7 (21%)
1	PSU	I	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.35	3 (14%)
1	2MG	I	2445	1	23,26,27	2.67	8 (34%)	33,38,41	1.93	8 (24%)
1	PSU	I	2604	1	18,21,22	2.66	9 (50%)	21,30,33	2.84	6 (28%)
1	PSU	I	2580	1	18,21,22	1.87	6 (33%)	21,30,33	1.81	5 (23%)
1	6MZ	I	1618	1	22,25,26	2.44	6 (27%)	29,36,39	3.18	12 (41%)
1	PSU	I	2457	1	18,21,22	1.67	4 (22%)	21,30,33	2.05	3 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	4D4	U	81	13	-	2/11/12/14	-
1	G7M	I	2069	1	-	1/7/25/26	0/3/3/3
1	2MA	I	2503	1	-	1/7/25/26	0/3/3/3
1	3TD	I	1915	1	-	3/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	0/9/27/28	0/3/3/3
1	PSU	I	1917	1	-	2/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	H2U	I	2449	1	-	0/7/38/39	0/2/2/2
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	PSU	I	2605	1	-	2/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	2/9/27/28	0/3/3/3
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2504	1,32	-	2/7/25/26	0/2/2/2
1	PSU	I	746	1	-	1/7/25/26	0/2/2/2
1	OMC	I	2498	1,32	-	0/9/27/28	0/2/2/2
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	I	1911	1	-	2/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	I	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	1618	1	-	1/9/27/28	0/3/3/3
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1915	3TD	C6-C5	12.97	1.49	1.35
1	I	1939	5MU	C2-N1	10.81	1.55	1.38
1	I	2503	2MA	C4-N3	10.51	1.47	1.34
1	I	747	5MU	C2-N1	10.38	1.54	1.38
1	I	1939	5MU	C6-N1	10.17	1.55	1.38
1	I	747	5MU	C6-N1	9.96	1.55	1.38
1	I	1939	5MU	C4-C5	9.96	1.61	1.44
1	I	1915	3TD	C2-N1	9.53	1.48	1.37
1	I	747	5MU	C4-C5	9.25	1.59	1.44
1	I	2030	6MZ	C6-N6	9.16	1.44	1.34
1	I	1618	6MZ	C6-N6	9.15	1.44	1.34
1	I	745	1MG	C2-N2	8.14	1.48	1.34
1	I	1962	5MC	C6-C5	7.60	1.47	1.34
1	I	1939	5MU	C4-N3	-7.46	1.24	1.38
1	I	747	5MU	C4-N3	-7.44	1.24	1.38
1	I	1835	2MG	C2-N3	7.09	1.45	1.32
1	I	2445	2MG	C2-N3	6.65	1.44	1.32
1	I	2552	OMU	C2-N1	6.62	1.48	1.38
1	I	2503	2MA	C2-N3	6.61	1.45	1.34
1	I	2503	2MA	C6-N1	6.59	1.43	1.35
1	I	2552	OMU	C2-N3	6.37	1.49	1.38
13	U	81	4D4	CZ-NE	6.27	1.45	1.33
1	I	2069	G7M	C5-N7	-6.26	1.32	1.39
1	I	1962	5MC	C4-N3	6.24	1.44	1.34
1	I	1835	2MG	C4-N3	6.11	1.48	1.34
1	I	2605	PSU	C2-N1	-6.02	1.28	1.36
1	I	1939	5MU	C6-C5	5.88	1.44	1.34
1	I	2445	2MG	C4-N3	5.81	1.47	1.34
1	I	2498	OMC	C2-N3	5.79	1.47	1.36
1	I	2251	OMG	C4-N3	5.79	1.47	1.34
1	I	1915	3TD	C6-N1	5.78	1.45	1.36
1	I	745	1MG	C4-N3	5.73	1.47	1.34
1	I	747	5MU	C6-C5	5.66	1.43	1.34
1	I	1962	5MC	C2-N3	5.65	1.47	1.36
1	I	2069	G7M	C4-N3	5.61	1.47	1.34
1	I	745	1MG	C2-N3	5.45	1.42	1.33
1	I	2498	OMC	C6-C5	5.35	1.47	1.35
1	I	2605	PSU	C4-N3	-5.30	1.28	1.38
1	I	1915	3TD	C2-N3	5.25	1.49	1.38
1	I	2604	PSU	C4-N3	-5.24	1.29	1.38
1	I	2605	PSU	C2-N3	-5.24	1.28	1.37
1	I	2503	2MA	C2-N1	5.18	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2445	2MG	C2-N2	5.12	1.44	1.33
1	I	1962	5MC	C5-C4	5.05	1.47	1.44
1	I	2251	OMG	C2-N3	5.04	1.45	1.33
1	I	1835	2MG	C2-N2	5.02	1.43	1.33
1	I	2552	OMU	C6-C5	4.91	1.46	1.35
1	I	2604	PSU	C2-N3	-4.74	1.29	1.37
1	I	2498	OMC	C4-N3	4.63	1.43	1.34
1	I	745	1MG	C2-N1	4.49	1.45	1.37
1	I	2069	G7M	C2-N3	4.37	1.43	1.33
1	I	2030	6MZ	C5-N7	-4.27	1.31	1.39
1	I	2552	OMU	C4-N3	4.22	1.45	1.38
1	I	2605	PSU	C6-N1	-4.18	1.29	1.36
1	I	2604	PSU	C6-N1	-4.16	1.29	1.36
1	I	2604	PSU	C2-N1	-4.15	1.31	1.36
1	I	1835	2MG	C2-N1	4.06	1.43	1.36
1	I	2445	2MG	C2-N1	4.06	1.43	1.36
1	I	2498	OMC	C4-N4	4.05	1.43	1.33
1	I	745	1MG	C5-N7	-4.02	1.31	1.39
1	I	1917	PSU	C6-C5	4.01	1.39	1.35
1	I	1962	5MC	C2-N1	3.92	1.48	1.40
1	I	1618	6MZ	C5-N7	-3.91	1.31	1.39
1	I	2580	PSU	C4-N3	-3.89	1.31	1.38
1	I	2030	6MZ	C8-N9	-3.88	1.31	1.37
1	I	2069	G7M	C2-N2	3.87	1.43	1.34
1	I	745	1MG	O6-C6	-3.84	1.15	1.23
1	I	2449	H2U	C2-N3	-3.83	1.31	1.38
1	I	2504	PSU	C4-N3	-3.80	1.31	1.38
1	I	2503	2MA	C5-C6	3.77	1.51	1.41
1	I	2498	OMC	C2-N1	3.76	1.47	1.40
13	U	81	4D4	CZ-NH2	3.73	1.45	1.32
1	I	746	PSU	C4-N3	-3.68	1.32	1.38
1	I	2449	H2U	C4-N3	-3.68	1.31	1.37
1	I	1835	2MG	C5-N7	-3.64	1.31	1.39
1	I	2580	PSU	C6-C5	3.63	1.39	1.35
1	I	1962	5MC	C4-N4	3.62	1.43	1.34
1	I	1962	5MC	C6-N1	3.62	1.44	1.38
1	I	2445	2MG	C5-N7	-3.60	1.31	1.39
1	I	2251	OMG	C2-N2	3.60	1.42	1.34
1	I	1911	PSU	C6-C5	3.53	1.39	1.35
1	I	2580	PSU	C2-N1	-3.51	1.32	1.36
1	I	955	PSU	C2-N1	-3.43	1.32	1.36
1	I	2503	2MA	C5-N7	-3.43	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2457	PSU	C4-N3	-3.41	1.32	1.38
1	I	2069	G7M	C5-C6	3.35	1.52	1.43
1	I	2030	6MZ	C5-C4	-3.31	1.33	1.39
1	I	747	5MU	O2-C2	-3.31	1.17	1.23
1	I	955	PSU	C4-N3	-3.29	1.32	1.38
1	I	2069	G7M	C4-N9	-3.29	1.29	1.38
1	I	2449	H2U	C2-N1	-3.28	1.31	1.35
1	I	1618	6MZ	C5-C4	-3.28	1.33	1.39
1	I	2251	OMG	C5-N7	-3.28	1.32	1.39
1	I	747	5MU	O4-C4	-3.27	1.17	1.23
1	I	2604	PSU	C1'-C5	-3.22	1.43	1.50
1	I	2503	2MA	C4-N9	-3.21	1.31	1.37
1	I	2504	PSU	C6-C5	3.17	1.38	1.35
1	I	2457	PSU	C2-N3	-3.15	1.32	1.37
1	I	2552	OMU	O4-C4	-3.14	1.18	1.24
1	I	1939	5MU	O4-C4	-3.14	1.17	1.23
1	I	1915	3TD	C4-N3	3.14	1.46	1.40
1	I	2498	OMC	O2-C2	-3.13	1.17	1.23
1	I	2605	PSU	C2'-C1'	-3.08	1.49	1.53
1	I	2503	2MA	C6-N6	-3.08	1.26	1.34
1	I	2457	PSU	C2-N1	-3.07	1.32	1.36
1	I	746	PSU	C2-N3	-3.07	1.32	1.37
1	I	2445	2MG	O6-C6	-3.07	1.17	1.23
1	I	1962	5MC	O2-C2	-3.06	1.18	1.23
1	I	2580	PSU	C2-N3	-3.05	1.32	1.37
1	I	1939	5MU	O2-C2	-3.02	1.17	1.23
1	I	745	1MG	C5-C6	2.99	1.53	1.45
1	I	2251	OMG	O6-C6	-2.98	1.17	1.23
1	I	2069	G7M	O6-C6	-2.92	1.18	1.23
1	I	2030	6MZ	C6-N1	-2.92	1.30	1.35
1	I	2498	OMC	C6-N1	2.88	1.44	1.38
1	I	2604	PSU	C2'-C1'	-2.84	1.49	1.53
1	I	955	PSU	C2-N3	-2.81	1.32	1.37
1	I	1835	2MG	O6-C6	-2.81	1.18	1.23
1	I	2605	PSU	O5'-C5'	-2.79	1.36	1.44
1	I	2552	OMU	O2-C2	-2.78	1.18	1.23
1	I	2504	PSU	C2-N1	-2.75	1.33	1.36
1	I	2503	2MA	C8-N9	-2.71	1.32	1.37
1	I	746	PSU	O4'-C1'	-2.70	1.40	1.43
1	I	2504	PSU	C2-N3	-2.69	1.33	1.37
1	I	2457	PSU	C6-C5	2.69	1.38	1.35
1	I	1917	PSU	C4-N3	-2.68	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C5-C4	-2.67	1.34	1.39
1	I	2445	2MG	C4-N9	-2.63	1.31	1.38
1	I	2030	6MZ	C5-C6	-2.57	1.35	1.41
1	I	2604	PSU	O4-C4	-2.56	1.18	1.23
1	I	1618	6MZ	C8-N9	-2.52	1.33	1.37
1	I	1915	3TD	O2-C2	-2.51	1.18	1.23
1	I	2552	OMU	C6-N1	2.49	1.44	1.38
1	I	746	PSU	C6-C5	2.47	1.38	1.35
1	I	2251	OMG	C4-N9	-2.46	1.31	1.38
1	I	2504	PSU	C6-N1	-2.45	1.32	1.36
1	I	955	PSU	C6-N1	-2.45	1.32	1.36
1	I	2605	PSU	O4'-C4'	-2.44	1.39	1.45
1	I	2604	PSU	O2-C2	-2.44	1.18	1.23
1	I	1911	PSU	C4-N3	-2.43	1.34	1.38
13	U	81	4D4	CZ-NH1	-2.42	1.25	1.34
1	I	2604	PSU	O4'-C1'	-2.33	1.40	1.43
1	I	745	1MG	C4-N9	-2.33	1.32	1.38
1	I	1618	6MZ	C5-C6	-2.31	1.36	1.41
1	I	2251	OMG	C2-N1	2.26	1.43	1.37
1	I	955	PSU	C6-C5	2.25	1.37	1.35
1	I	2580	PSU	O4'-C1'	-2.23	1.40	1.43
1	I	2580	PSU	C6-N1	-2.23	1.32	1.36
1	I	2605	PSU	O4-C4	-2.22	1.19	1.23
1	I	2251	OMG	C5-C6	2.20	1.52	1.44
1	I	746	PSU	C6-N1	-2.17	1.32	1.36
1	I	2605	PSU	C3'-C2'	-2.16	1.47	1.53
1	I	2552	OMU	C5-C4	2.16	1.48	1.43
1	I	2445	2MG	C5-C6	2.14	1.52	1.44
1	I	1618	6MZ	C6-N1	-2.14	1.31	1.35
1	I	1835	2MG	C5-C6	2.13	1.52	1.44
1	I	1835	2MG	C4-N9	-2.12	1.32	1.38
1	I	2605	PSU	C3'-C4'	-2.08	1.47	1.53
1	I	746	PSU	C2-N1	-2.07	1.34	1.36
1	I	2503	2MA	C8-N7	2.06	1.35	1.31
1	I	1911	PSU	C2-N1	-2.04	1.34	1.36
1	I	1917	PSU	C2-N3	-2.02	1.34	1.37
1	I	1915	3TD	O4-C4	-2.02	1.18	1.23

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1939	5MU	C5-C4-N3	11.97	125.73	115.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	747	5MU	C5-C4-N3	11.37	125.20	115.32
1	I	747	5MU	C5-C6-N1	-8.82	113.73	123.31
1	I	2604	PSU	N1-C2-N3	8.61	124.25	115.17
1	I	1939	5MU	C5-C6-N1	-8.56	114.02	123.31
1	I	2605	PSU	N1-C2-N3	7.70	123.29	115.17
1	I	1618	6MZ	C5-C4-N3	-7.36	116.58	126.72
1	I	1911	PSU	N1-C2-N3	7.34	122.91	115.17
1	I	2030	6MZ	C4-N9-C1'	-6.86	110.59	126.63
1	I	1618	6MZ	C1'-N9-C8	6.77	142.13	127.09
1	I	2030	6MZ	C1'-N9-C8	6.75	142.07	127.09
1	I	2030	6MZ	C5-C4-N3	-6.70	117.49	126.72
1	I	2457	PSU	N1-C2-N3	6.62	122.15	115.17
1	I	1618	6MZ	C4-N9-C1'	-6.39	111.69	126.63
1	I	1917	PSU	N1-C2-N3	6.32	121.84	115.17
1	I	2604	PSU	C4-N3-C2	-5.99	118.12	126.37
1	I	1835	2MG	C2-N3-C4	5.95	119.44	112.00
1	I	747	5MU	O4-C4-C5	-5.89	118.18	124.92
1	I	1618	6MZ	C4-C5-C6	5.86	121.65	116.78
1	I	2503	2MA	N9-C8-N7	-5.76	105.76	113.94
1	I	955	PSU	N1-C2-N3	5.72	121.20	115.17
1	I	745	1MG	C5-C4-N3	-5.70	119.32	128.39
1	I	745	1MG	C1'-N9-C8	5.68	142.88	126.73
1	I	746	PSU	N1-C2-N3	5.67	121.14	115.17
1	I	2445	2MG	C2-N3-C4	5.66	119.08	112.00
1	I	2504	PSU	N1-C2-N3	5.60	121.08	115.17
1	I	2030	6MZ	C4-C5-C6	5.56	121.40	116.78
1	I	745	1MG	C1'-N9-C4	-5.55	110.09	126.49
1	I	2552	OMU	C4-N3-C2	-5.52	119.76	126.61
1	I	1835	2MG	C5-C4-N3	-5.50	119.63	128.39
1	I	2580	PSU	N1-C2-N3	5.39	120.85	115.17
1	I	2069	G7M	CN7-N7-C5	5.36	133.49	126.80
1	I	1618	6MZ	N3-C4-N9	5.18	135.97	127.17
1	I	2503	2MA	C4-N9-C8	5.16	111.16	105.74
1	I	1915	3TD	N1-C2-N3	5.12	119.85	116.13
1	I	747	5MU	C4-N3-C2	-5.06	120.70	127.34
1	I	1939	5MU	O4-C4-C5	-5.06	119.13	124.92
1	I	1618	6MZ	N1-C2-N3	-5.02	120.99	128.58
1	I	2030	6MZ	N3-C4-N9	5.01	135.69	127.17
1	I	747	5MU	N3-C2-N1	5.01	121.42	114.89
1	I	1939	5MU	C4-N3-C2	-4.83	121.01	127.34
1	I	2251	OMG	C5-C4-N3	-4.82	120.71	128.39
1	I	2445	2MG	C5-C4-N3	-4.75	120.83	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2605	PSU	C4-N3-C2	-4.75	119.83	126.37
1	I	2503	2MA	C5-C4-N3	-4.75	122.18	127.18
1	I	2030	6MZ	N1-C2-N3	-4.71	121.45	128.58
1	I	1911	PSU	C4-N3-C2	-4.67	119.94	126.37
1	I	1939	5MU	C5M-C5-C4	4.60	123.69	118.78
1	I	1911	PSU	O2-C2-N1	-4.52	118.12	122.79
1	I	1939	5MU	N3-C2-N1	4.47	120.70	114.89
1	I	2030	6MZ	C9-N6-C6	4.44	126.97	122.85
1	I	747	5MU	O2-C2-N1	-4.42	117.05	122.80
1	I	1915	3TD	C4-N3-C2	-4.28	120.08	124.61
1	I	2069	G7M	CN7-N7-C8	-4.21	118.41	124.79
1	I	1618	6MZ	C2-N3-C4	4.14	121.94	111.83
1	I	1835	2MG	C2-N1-C6	-4.09	119.61	124.55
1	I	955	PSU	O2-C2-N1	-4.08	118.59	122.79
1	I	2605	PSU	C5'-C4'-C3'	-4.02	100.75	115.21
1	I	2604	PSU	O2-C2-N3	-3.97	114.81	121.86
1	I	1939	5MU	C5M-C5-C6	-3.92	117.54	122.85
1	I	2251	OMG	C2-N3-C4	3.92	119.05	112.30
1	I	1917	PSU	C4-N3-C2	-3.90	121.00	126.37
1	I	2605	PSU	C6-C5-C4	-3.88	115.56	118.17
1	I	2503	2MA	N3-C2-N1	-3.76	119.14	125.77
1	I	2552	OMU	N3-C2-N1	3.75	119.77	114.89
1	I	745	1MG	C2-N3-C4	3.74	120.38	111.98
1	I	2457	PSU	C4-N3-C2	-3.67	121.32	126.37
1	I	2445	2MG	C2-N1-C6	-3.60	120.20	124.55
1	I	2030	6MZ	C2-N3-C4	3.59	120.59	111.83
1	I	2457	PSU	O2-C2-N1	-3.57	119.11	122.79
1	I	2580	PSU	O2-C2-N1	-3.54	119.14	122.79
1	I	2069	G7M	C2-N3-C4	3.54	118.39	112.30
1	I	746	PSU	C4-N3-C2	-3.53	121.51	126.37
1	I	747	5MU	C5M-C5-C6	-3.48	118.14	122.85
1	I	2503	2MA	N3-C4-N9	3.48	131.40	126.99
1	I	2503	2MA	CM2-C2-N1	3.46	122.30	117.13
1	I	1962	5MC	CM5-C5-C6	-3.45	118.18	122.85
1	I	745	1MG	N9-C4-N3	3.43	132.82	125.95
1	I	1939	5MU	O2-C2-N1	-3.37	118.41	122.80
1	I	2552	OMU	C5-C4-N3	3.37	119.52	114.80
1	I	1835	2MG	N9-C4-N3	3.32	132.59	125.95
1	I	1917	PSU	O2-C2-N1	-3.26	119.42	122.79
1	I	747	5MU	C5M-C5-C4	3.23	122.23	118.78
1	I	1618	6MZ	C6-C5-N7	-3.22	128.91	132.43
1	I	2069	G7M	C5-C6-N1	3.19	118.43	111.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2605	PSU	O2-C2-N3	-3.17	116.23	121.86
1	I	2069	G7M	O6-C6-C5	-3.10	121.08	128.01
1	I	1618	6MZ	C5-C6-N1	3.09	121.47	118.15
1	I	746	PSU	C6-C5-C4	-3.08	116.09	118.17
1	I	2504	PSU	O2-C2-N1	-3.08	119.61	122.79
1	I	2580	PSU	C6-C5-C4	-3.05	116.11	118.17
1	I	955	PSU	C4-N3-C2	-3.00	122.24	126.37
1	I	2030	6MZ	N9-C8-N7	-2.94	109.77	113.94
1	I	2069	G7M	C5-C4-N3	-2.92	122.64	128.15
1	I	2552	OMU	O4-C4-C5	-2.88	120.20	125.16
1	I	2251	OMG	C2-N1-C6	-2.84	119.96	125.11
1	I	2503	2MA	C5-N7-C8	2.81	107.87	103.45
1	I	1618	6MZ	C9-N6-C6	2.78	125.43	122.85
1	I	745	1MG	CM1-N1-C6	2.76	121.92	117.64
1	I	2503	2MA	N6-C6-N1	2.76	120.75	117.03
1	I	2445	2MG	N9-C8-N7	-2.75	108.30	113.40
1	I	2504	PSU	C4-N3-C2	-2.67	122.69	126.37
1	I	2445	2MG	N9-C4-N3	2.67	131.29	125.95
1	I	1939	5MU	O4-C4-N3	-2.65	115.14	120.11
1	I	1618	6MZ	N9-C8-N7	-2.57	110.28	113.94
1	I	1835	2MG	N1-C2-N2	2.56	119.18	116.56
1	I	2251	OMG	N9-C4-N3	2.56	131.08	125.95
1	I	2030	6MZ	C6-C5-N7	-2.54	129.66	132.43
1	I	2604	PSU	O4'-C4'-C3'	-2.54	100.12	105.15
1	I	2504	PSU	C6-C5-C4	-2.50	116.48	118.17
1	I	1962	5MC	C5-C6-N1	-2.48	120.62	123.31
1	I	1835	2MG	O6-C6-C5	-2.46	120.04	126.53
1	I	2069	G7M	N2-C2-N1	2.45	121.93	116.76
1	I	2251	OMG	N9-C8-N7	-2.45	108.86	113.40
1	I	955	PSU	C6-C5-C4	-2.44	116.53	118.17
1	I	1835	2MG	C5-C6-N1	2.42	119.42	113.25
1	I	2030	6MZ	C5-N7-C8	2.41	107.23	103.45
1	I	2580	PSU	C4-N3-C2	-2.40	123.06	126.37
1	I	1917	PSU	C6-C5-C4	-2.38	116.57	118.17
1	I	2069	G7M	C2-N1-C6	-2.35	120.85	125.11
1	I	2251	OMG	C5-C6-N1	2.33	119.18	113.25
1	I	2445	2MG	N1-C2-N2	2.32	118.93	116.56
1	I	2445	2MG	C5-C6-N1	2.28	119.05	113.25
1	I	745	1MG	CM1-N1-C2	-2.26	118.36	120.70
1	I	2552	OMU	O2-C2-N1	-2.26	119.86	122.80
1	I	2445	2MG	C1'-N9-C4	-2.25	119.83	126.49
1	I	2069	G7M	C1'-N9-C8	-2.25	119.14	126.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2069	G7M	N9-C8-N7	-2.24	107.03	112.48
1	I	2605	PSU	O2-C2-N1	-2.24	120.48	122.79
1	I	2604	PSU	O4-C4-C5	-2.23	118.46	124.01
1	I	745	1MG	C5-C6-N1	2.18	119.04	115.02
1	I	746	PSU	O2-C2-N1	-2.18	120.54	122.79
1	I	745	1MG	N9-C8-N7	-2.16	109.40	113.40
1	I	2604	PSU	C5-C6-N1	-2.13	119.18	122.14
1	I	1618	6MZ	C5-N7-C8	2.10	106.75	103.45
1	I	2580	PSU	O4'-C1'-C2'	2.09	108.05	105.15
1	I	2251	OMG	O6-C6-C5	-2.06	121.09	126.53
1	I	2605	PSU	C6-N1-C2	-2.06	120.78	122.69
1	I	747	5MU	C6-N1-C2	-2.01	119.31	121.30

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1911	PSU	O4'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	1917	PSU	O4'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2605	PSU	C3'-C4'-C5'-O5'
1	I	2605	PSU	O4'-C4'-C5'-O5'
1	I	1911	PSU	C3'-C4'-C5'-O5'
1	I	2030	6MZ	O4'-C4'-C5'-O5'
1	I	2030	6MZ	C3'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
1	I	1917	PSU	C3'-C4'-C5'-O5'
1	I	2445	2MG	O4'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C1'-C5-C4
13	U	81	4D4	CG-CD-NE-CZ
1	I	2069	G7M	C4'-C5'-O5'-P
1	I	746	PSU	O4'-C4'-C5'-O5'
13	U	81	4D4	O-C-CA-CB
1	I	1618	6MZ	N1-C6-N6-C9
1	I	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	2503	2MA	1	0
1	I	1917	PSU	1	0
1	I	745	1MG	1	0
1	I	1939	5MU	1	0
1	I	2605	PSU	2	0
1	I	2030	6MZ	1	0
1	I	955	PSU	1	0
1	I	2498	OMC	1	0
1	I	2445	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 187 ligands modelled in this entry, 187 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.

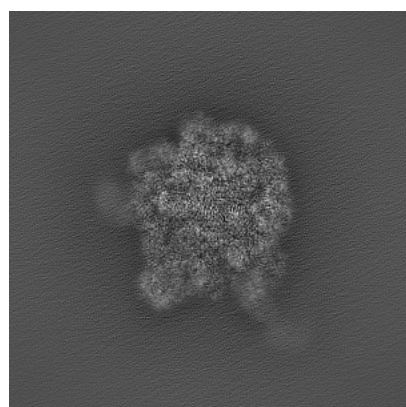
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20353. These allow visual inspection of the internal detail of the map and identification of artifacts.

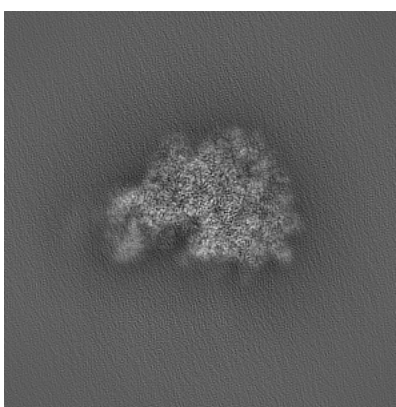
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

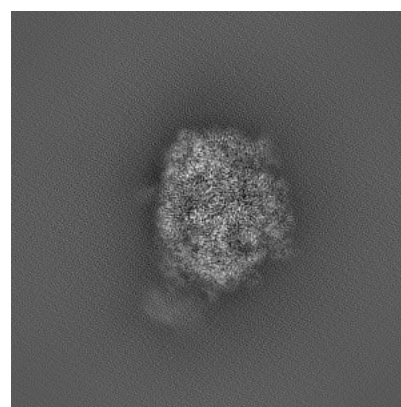
6.1.1 Primary map



X



Y

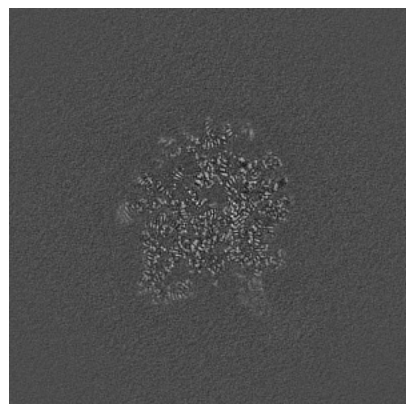


Z

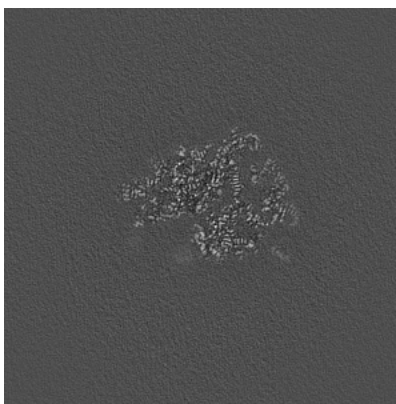
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

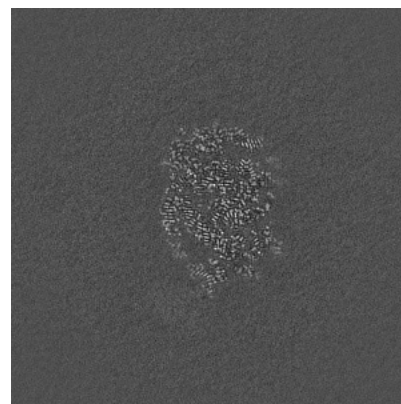
6.2.1 Primary map



X Index: 256



Y Index: 256

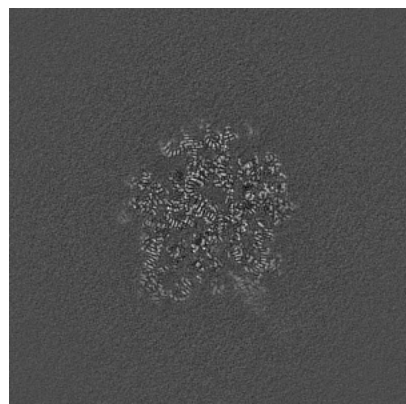


Z Index: 256

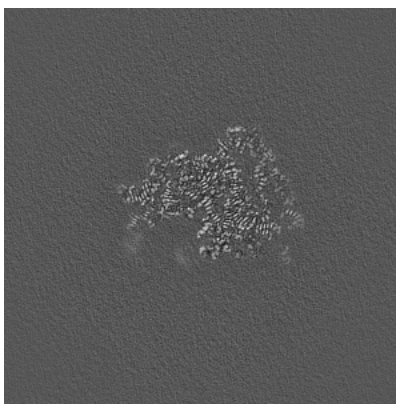
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

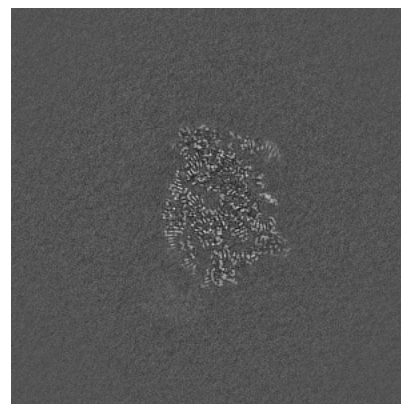
6.3.1 Primary map



X Index: 261



Y Index: 247

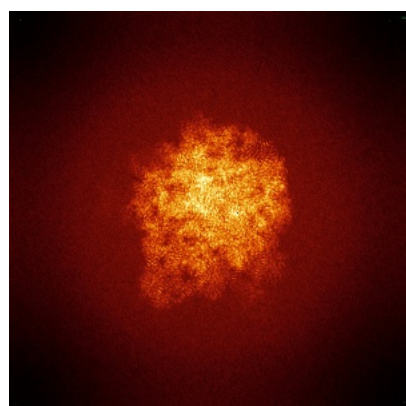


Z Index: 266

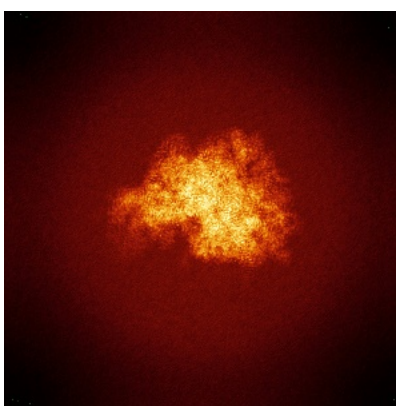
The images above show the largest variance slices of the map in three orthogonal directions.

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

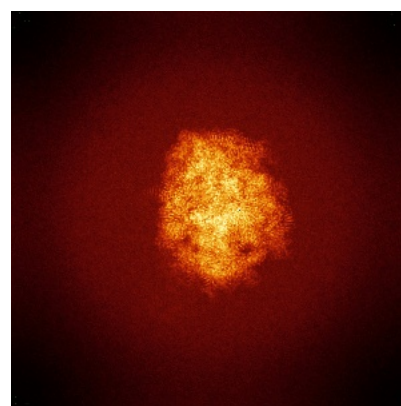
6.4.1 Primary map



X



Y

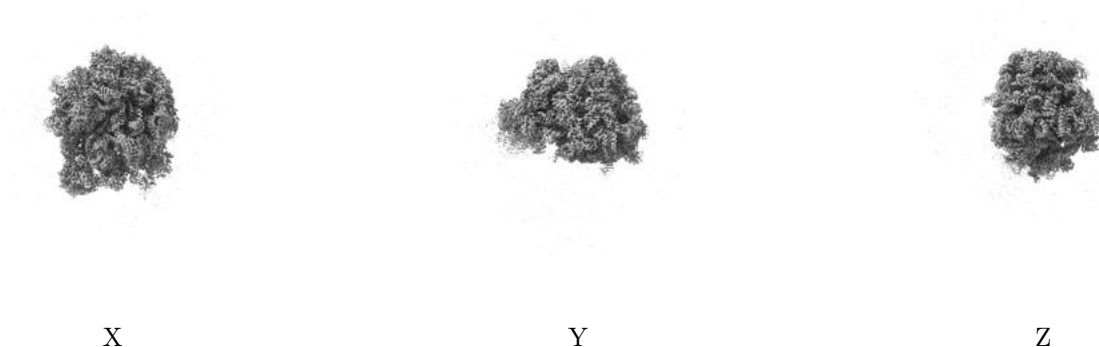


Z

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 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

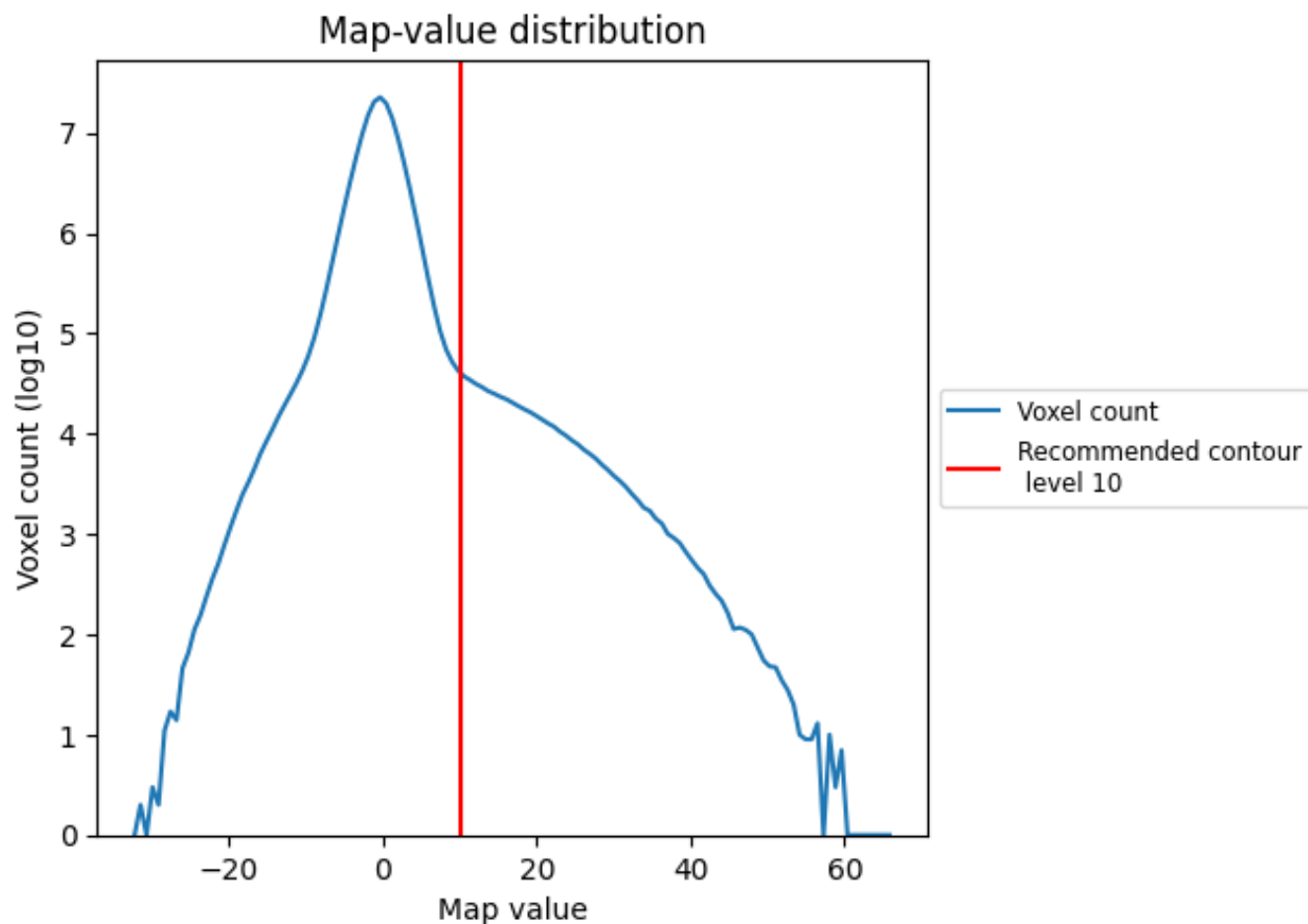
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

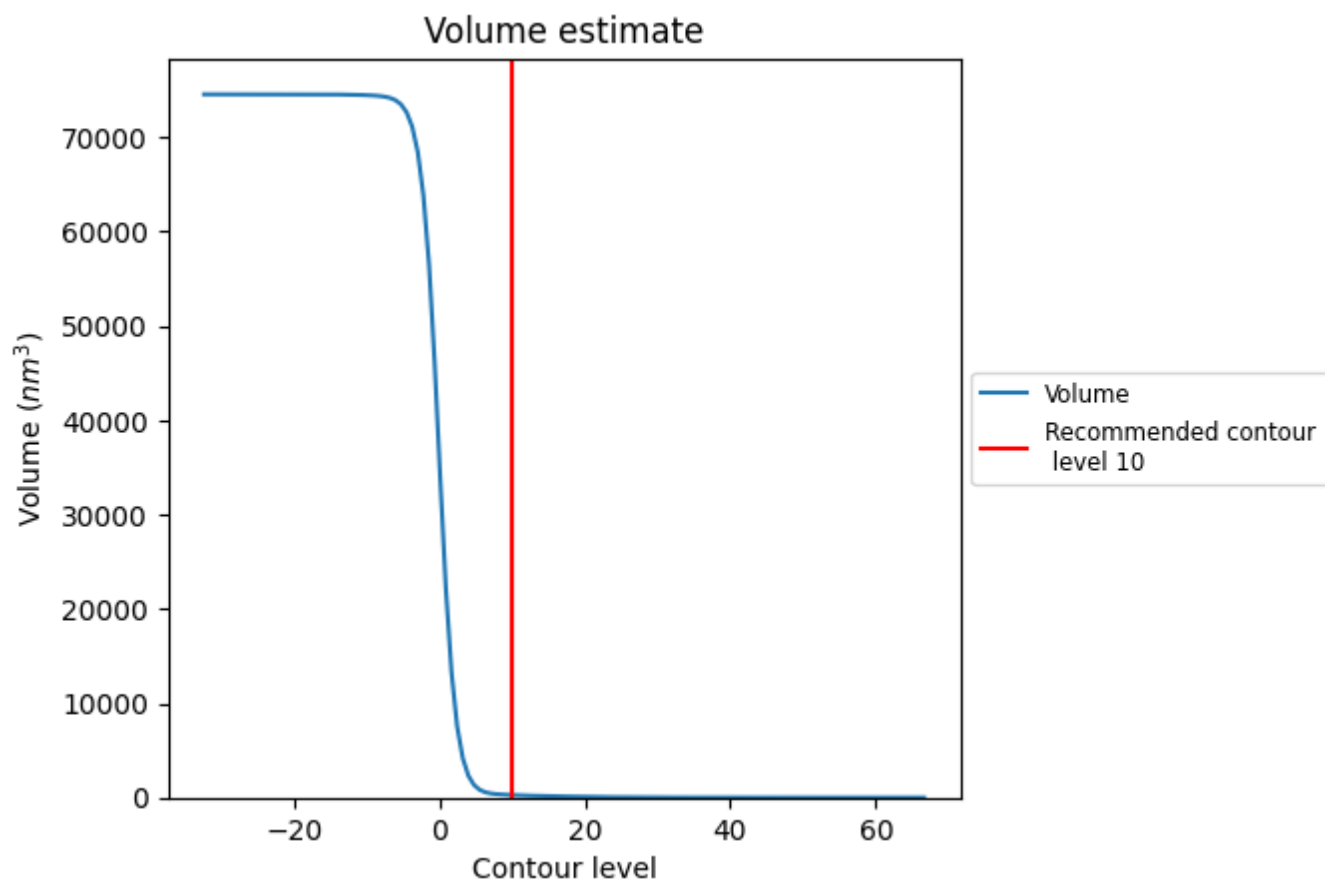
This section contains the results of statistical analysis of the map.

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.

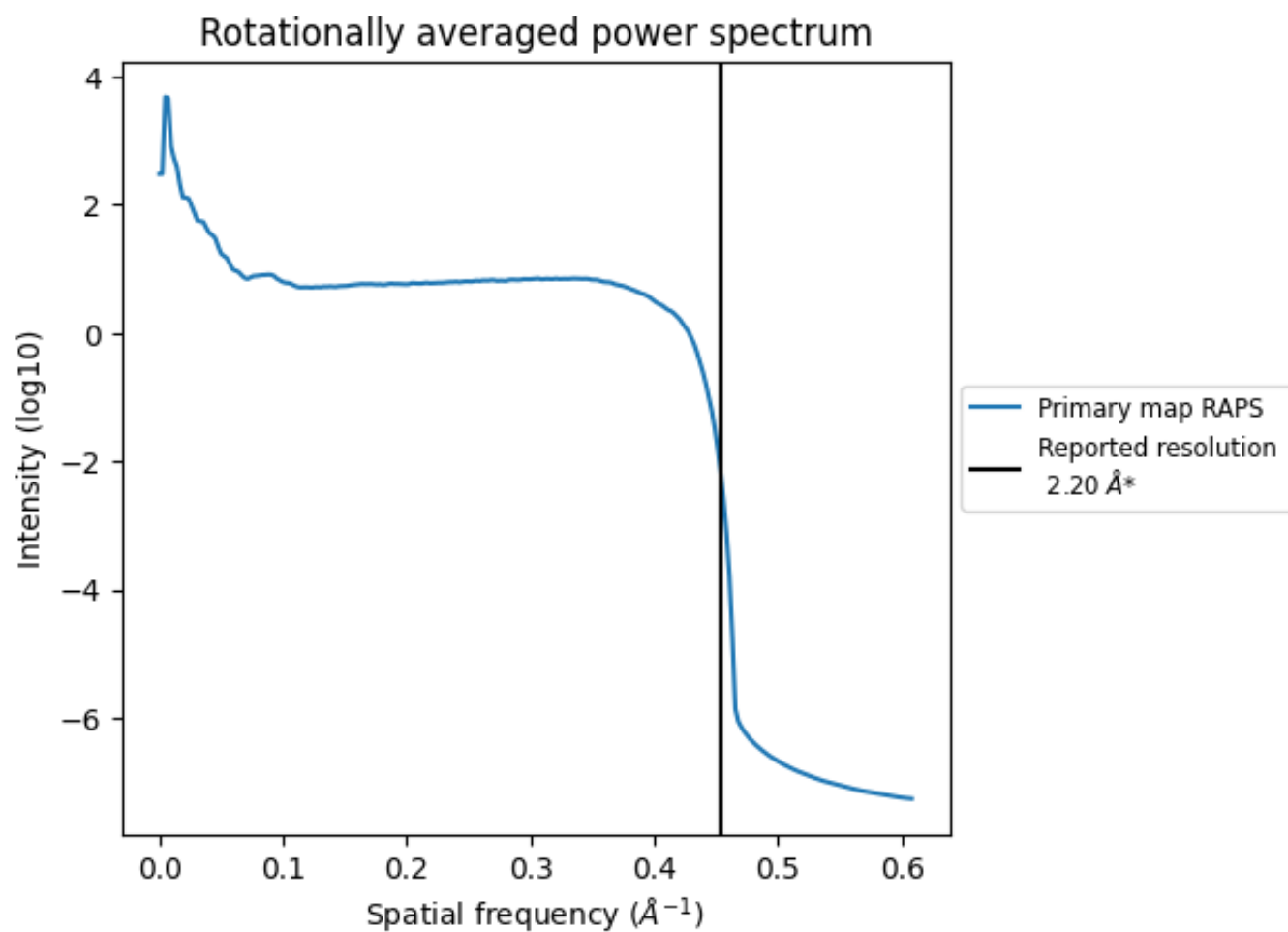
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266 nm^3 ; this corresponds to an approximate mass of 240 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 0.455 Å⁻¹

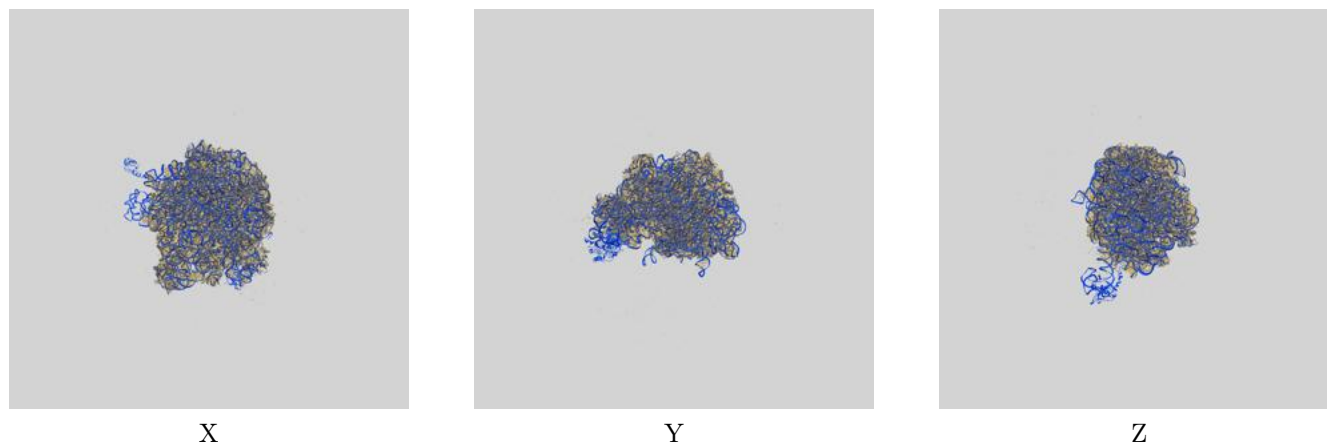
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

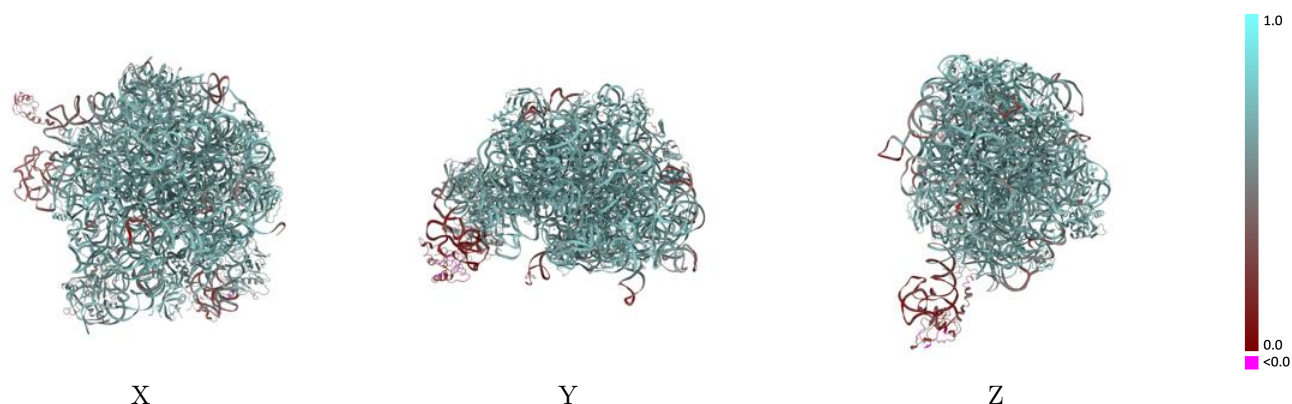
This section contains information regarding the fit between EMDB map EMD-20353 and PDB model 6PJ6. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

9.1 Map-model overlay [i](#)



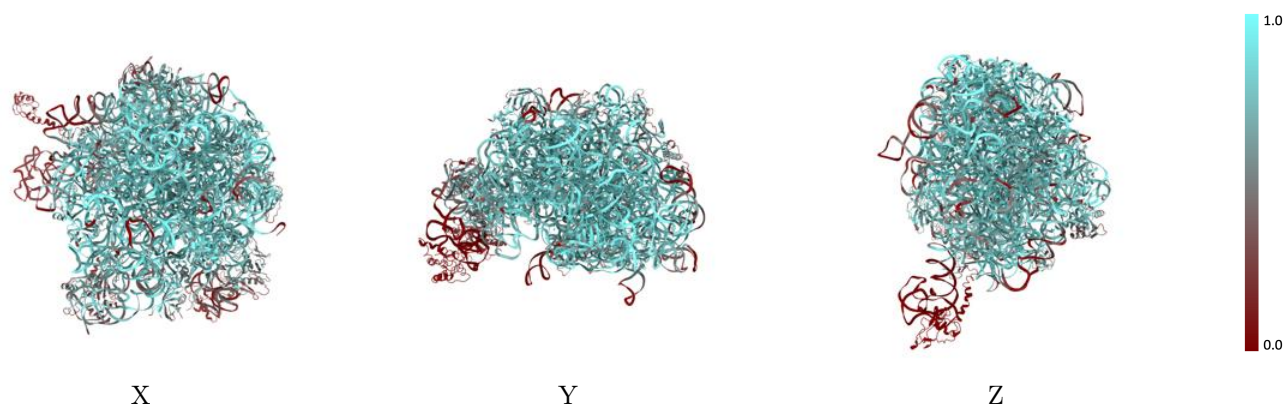
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



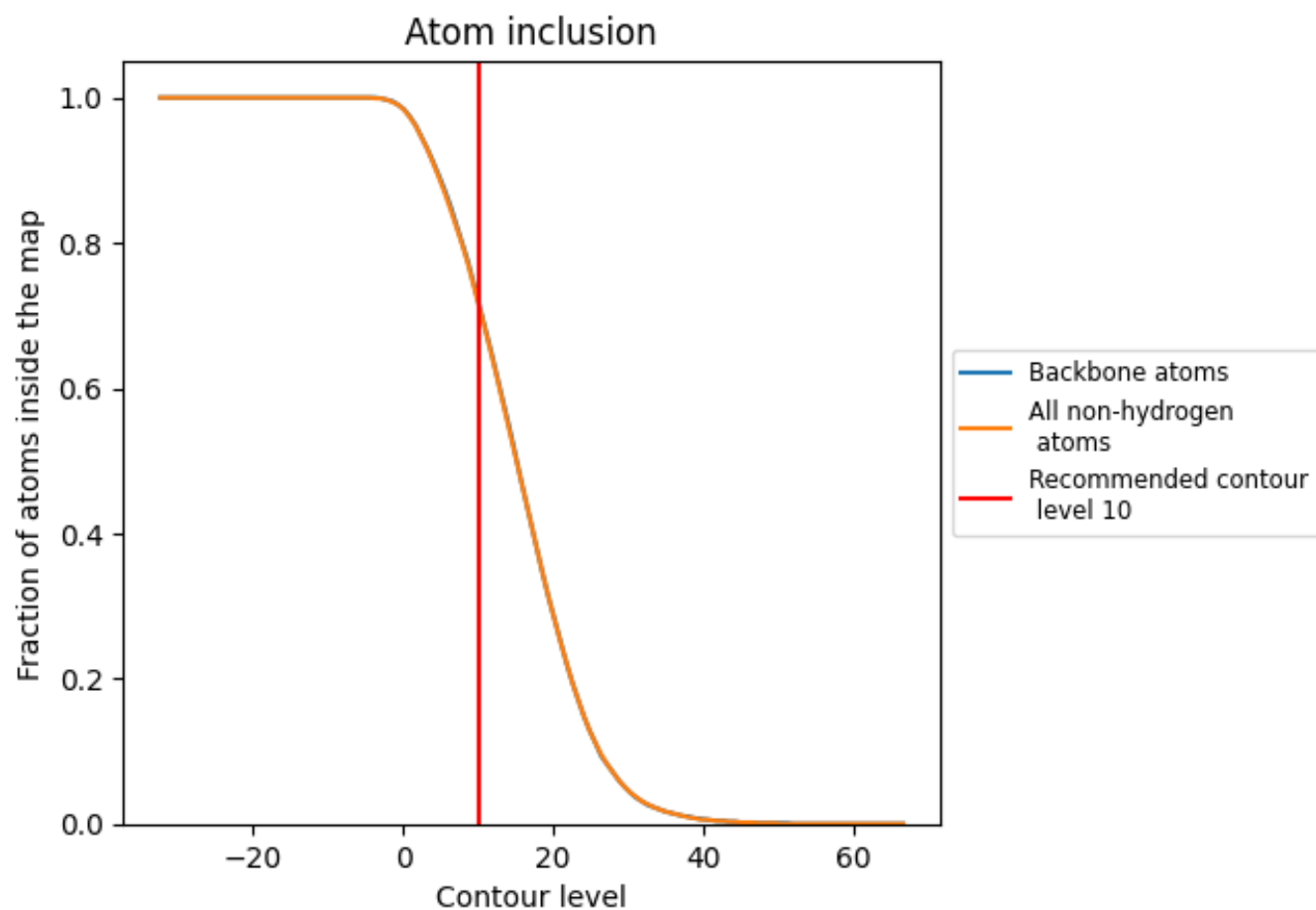
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (10).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% 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 (10) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.6160
I	 0.7610	 0.6180
J	 0.6860	 0.6150
K	 0.7910	 0.6730
L	 0.7800	 0.6700
M	 0.6780	 0.6470
N	 0.1220	 0.4500
O	 0.4460	 0.5820
P	 0.1270	 0.3310
Q	 0.0000	 0.2260
R	 0.7690	 0.6740
S	 0.6980	 0.6520
T	 0.7520	 0.6650
U	 0.7400	 0.6650
V	 0.8400	 0.6810
W	 0.5700	 0.6060
X	 0.6670	 0.6330
Y	 0.8390	 0.6930
Z	 0.7290	 0.6440
a	 0.7490	 0.6570
b	 0.6390	 0.6360
c	 0.5990	 0.6150
d	 0.6350	 0.6360
e	 0.7910	 0.6630
f	 0.7140	 0.6620
g	 0.5400	 0.6070
h	 0.7480	 0.6580
i	 0.7520	 0.6600
j	 0.5960	 0.6200
k	 0.8370	 0.6900
l	 0.8370	 0.6870
m	 0.7070	 0.6500

