



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 01:32 PM UTC

PDB ID : 5XXB / pdb_00005xxb
EMDB ID : EMD-6778
Title : Large subunit of Toxoplasma gondii ribosome
Authors : Li, Z.; Guo, Q.; Zheng, L.; Ji, Y.; Xie, Y.; Lai, D.; Lun, Z.; Suo, X.; Gao, N.
Deposited on : 2017-07-03
Resolution : 3.17 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

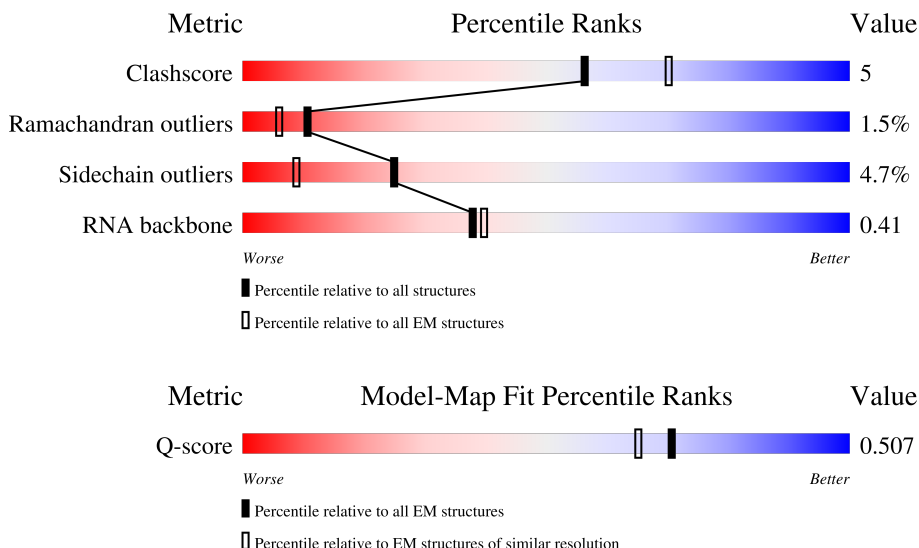
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.17 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.



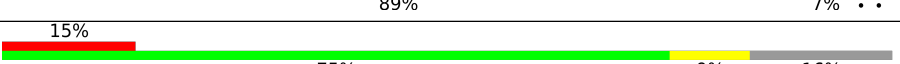
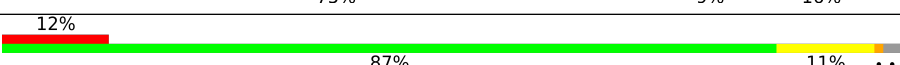
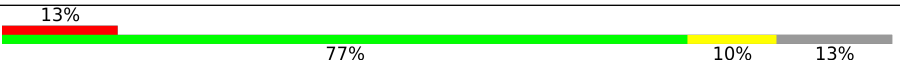
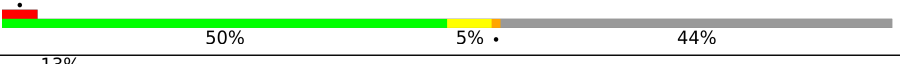
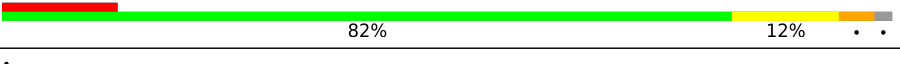
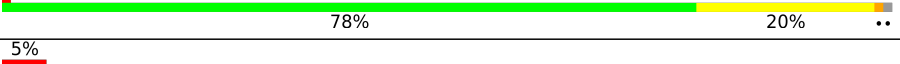
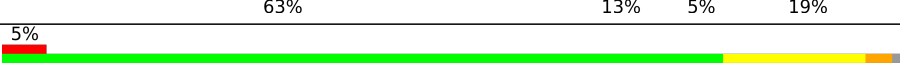
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14465 (2.67 - 3.67)

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	1	3477	
2	3	124	
3	4	158	

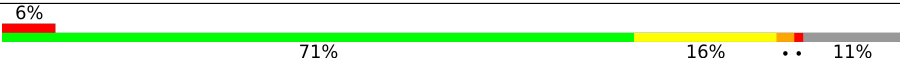
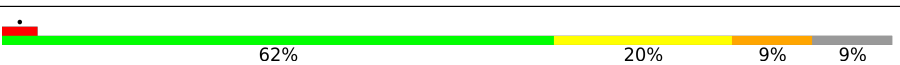
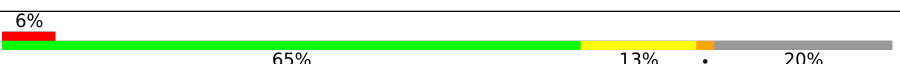
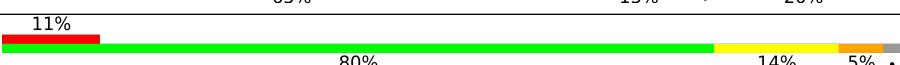
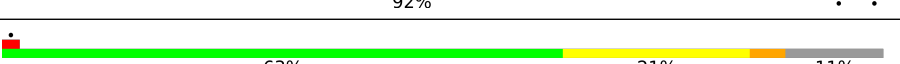
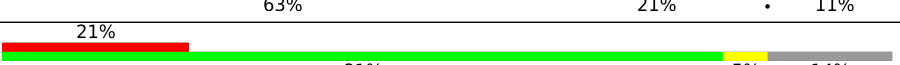
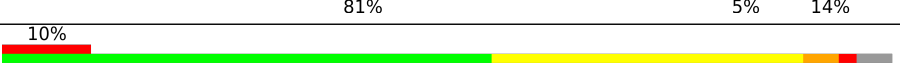
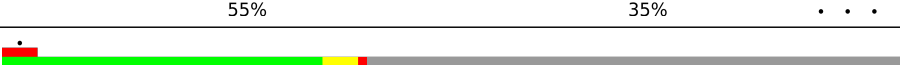
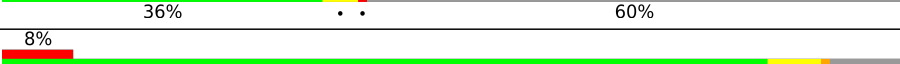
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Mol	Chain	Length	Quality of chain
4	A	260	
5	B	389	
6	C	416	
7	D	310	
8	E	193	
9	F	258	
10	G	276	
11	H	190	
12	I	221	
13	J	175	
14	K	355	
15	L	134	
16	M	205	
17	N	269	
18	O	195	
19	P	187	
20	Q	187	
21	R	183	
22	S	157	
23	T	133	
24	U	139	
25	V	155	
26	W	167	
27	X	141	
28	Y	146	

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Mol	Chain	Length	Quality of chain
29	Z	147	
30	a	54	
31	b	108	
32	c	120	
33	d	134	
34	e	112	
35	f	134	
36	g	123	
37	h	101	
38	i	98	
39	j	84	
40	k	51	
41	l	129	
42	n	105	
43	o	96	
44	p	129	

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 121433 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	3077	Total	C	N	O	P	0	0
			65598	29312	11639	21570	3077		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	118	Total	C	N	O	P	0	0
			2519	1123	452	826	118		

- Molecule 3 is a RNA chain called 5.8S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	157	Total	C	N	O	P	0	0
			3339	1493	586	1103	157		

- Molecule 4 is a protein called Ribosomal protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	246	Total	C	N	O	S	0	0
			1882	1170	379	324	9		

- Molecule 5 is a protein called Ribosomal protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	369	Total	C	N	O	S	0	0
			2942	1867	561	496	18		

- Molecule 6 is a protein called Ribosomal protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	394	Total	C	N	O	S	0	0
			3060	1897	621	528	14		

- Molecule 7 is a protein called Ribosomal protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	261	Total	C	N	O	S	0	0
			2123	1336	406	375	6		

- Molecule 8 is a protein called Ribosomal protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	124	Total	C	N	O	S	0	0
			971	621	177	170	3		

- Molecule 9 is a protein called Ribosomal protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	250	Total	C	N	O	S	0	0
			2059	1324	389	338	8		

- Molecule 10 is a protein called Ribosomal protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	233	Total	C	N	O	S	0	0
			1877	1192	357	319	9		

- Molecule 11 is a protein called Ribosomal protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	187	Total	C	N	O	S	0	0
			1478	938	264	266	10		

- Molecule 12 is a protein called Ribosomal protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	193	Total	C	N	O	S	0	0
			1540	976	296	258	10		

- Molecule 13 is a protein called Ribosomal protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	166	Total	C	N	O	S	0	0
			1343	845	258	236	4		

- Molecule 14 is a protein called Ribosomal protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	199	Total	C	N	O	S	0	0
			1593	1006	321	262	4		

- Molecule 15 is a protein called Ribosomal protein eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	131	Total	C	N	O	S	0	0
			1063	674	203	180	6		

- Molecule 16 is a protein called Ribosomal protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	202	Total	C	N	O	S	0	0
			1683	1060	350	268	5		

- Molecule 17 is a protein called Ribosomal protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	200	Total	C	N	O	S	0	0
			1645	1034	330	272	9		

- Molecule 18 is a protein called Ribosomal protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	158	Total	C	N	O	S	0	0
			1286	805	249	222	10		

- Molecule 19 is a protein called Ribosomal protein eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	186	Total	C	N	O	S	0	0
			1477	918	306	246	7		

- Molecule 20 is a protein called Ribosomal protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	176	Total	C	N	O	S	0	0
			1473	918	309	236	10		

- Molecule 21 is a protein called Ribosomal protein eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	182	Total	C	N	O	S	0	0
			1492	953	282	250	7		

- Molecule 22 is a protein called Ribosomal protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	154	Total	C	N	O	S	0	0
			1231	775	242	208	6		

- Molecule 23 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	99	Total	C	N	O	S	0	0
			827	531	147	145	4		

- Molecule 24 is a protein called Ribosomal protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	129	Total	C	N	O	S	0	0
			968	613	178	168	9		

- Molecule 25 is a protein called Ribosomal protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	63	Total	C	N	O	S	0	0
			533	344	104	82	3		

- Molecule 26 is a protein called Ribosomal protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	127	Total	C	N	O	S	0	0
			1038	655	194	186	3		

- Molecule 27 is a protein called Ribosomal protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	124	Total	C	N	O	S	0	0
			1011	629	207	172	3		

- Molecule 28 is a protein called Ribosomal protein eL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	144	Total	C	N	O	S	0	0
			1163	751	214	191	7		

- Molecule 29 is a protein called Ribosomal protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	145	Total	C	N	O	S	0	0
			1136	724	221	186	5		

- Molecule 30 is a protein called Ribosomal protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	49	Total	C	N	O	S	0	0
			404	243	93	62	6		

- Molecule 31 is a protein called Ribosomal protein eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	96	Total	C	N	O	S	0	0
			725	450	134	134	7		

- Molecule 32 is a protein called Ribosomal protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	107	Total	C	N	O	S	0	0
			908	573	182	151	2		

- Molecule 33 is a protein called Ribosomal protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	122	Total	C	N	O	S	0	0
			1011	639	203	165	4		

- Molecule 34 is a protein called Ribosomal protein eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	105	Total	C	N	O	S	0	0
			854	546	167	140	1		

- Molecule 35 is a protein called Ribosomal protein eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	107	Total	C	N	O	S	0	0
			863	535	191	132	5		

- Molecule 36 is a protein called Ribosomal protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	121	Total	C	N	O	S	0	0
			981	615	199	165	2		

- Molecule 37 is a protein called Ribosomal protein eL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	97	Total	C	N	O	S	0	0
			772	481	165	125	1		

- Molecule 38 is a protein called Ribosomal protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	87	Total	C	N	O	S	0	0
			688	418	152	112	6		

- Molecule 39 is a protein called Ribosomal protein eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	72	Total	C	N	O	S	0	0
			591	376	112	102	1		

- Molecule 40 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	49	Total	C	N	O	S	0	0
			419	264	94	59	2		

- Molecule 41 is a protein called Ribosomal protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	52	Total	C	N	O	S	0	0
			419	263	85	66	5		

- Molecule 42 is a protein called Ribosomal protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	97	Total	C	N	O	S	0	0
			790	503	157	125	5		

- Molecule 43 is a protein called Ribosomal protein eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	90	Total	C	N	O	S	0	0
			684	428	137	113	6		

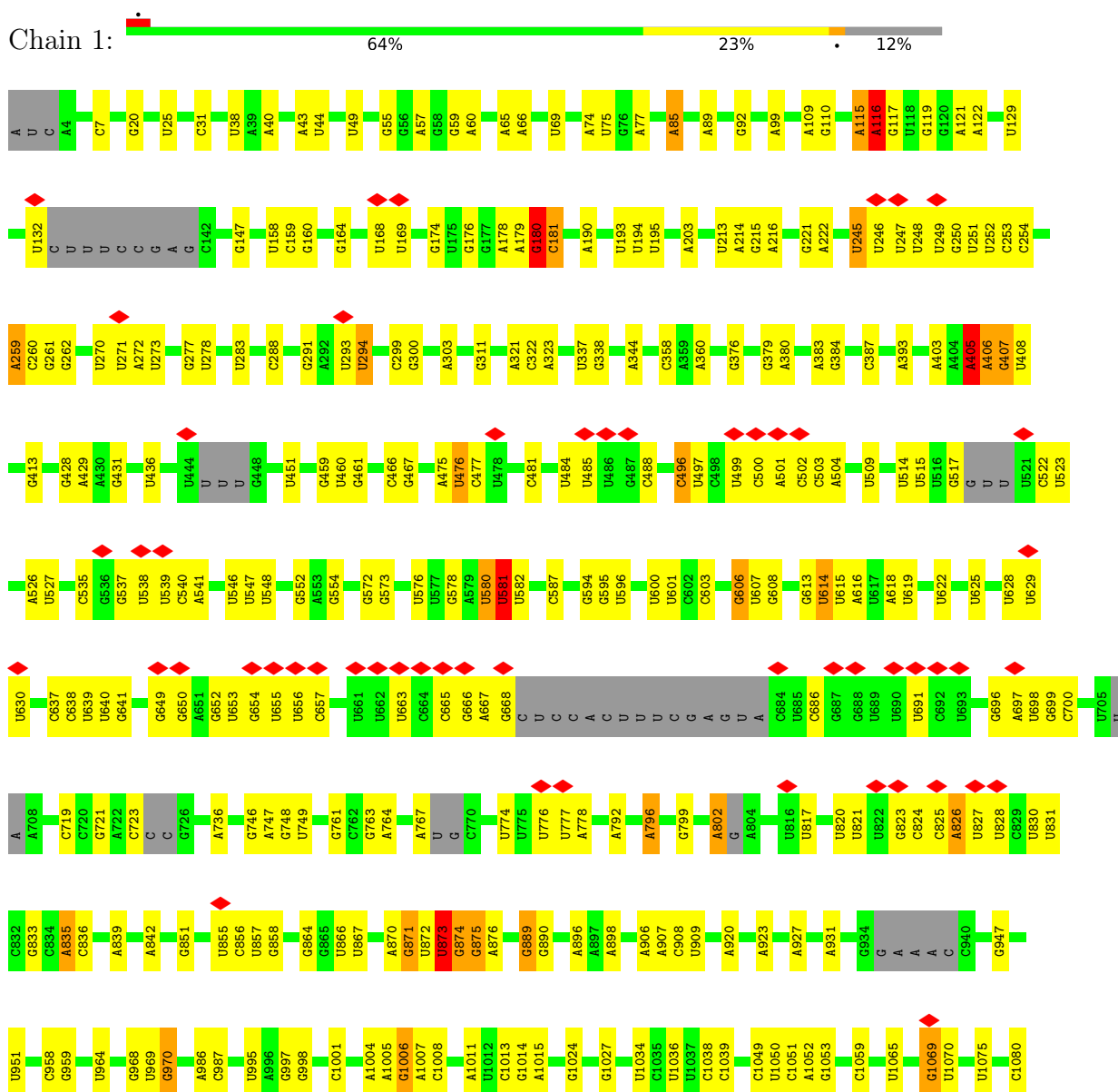
- Molecule 44 is a protein called Ribosomal protein eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	122	Total	C	N	O	S	0	0
			974	607	197	161	9		

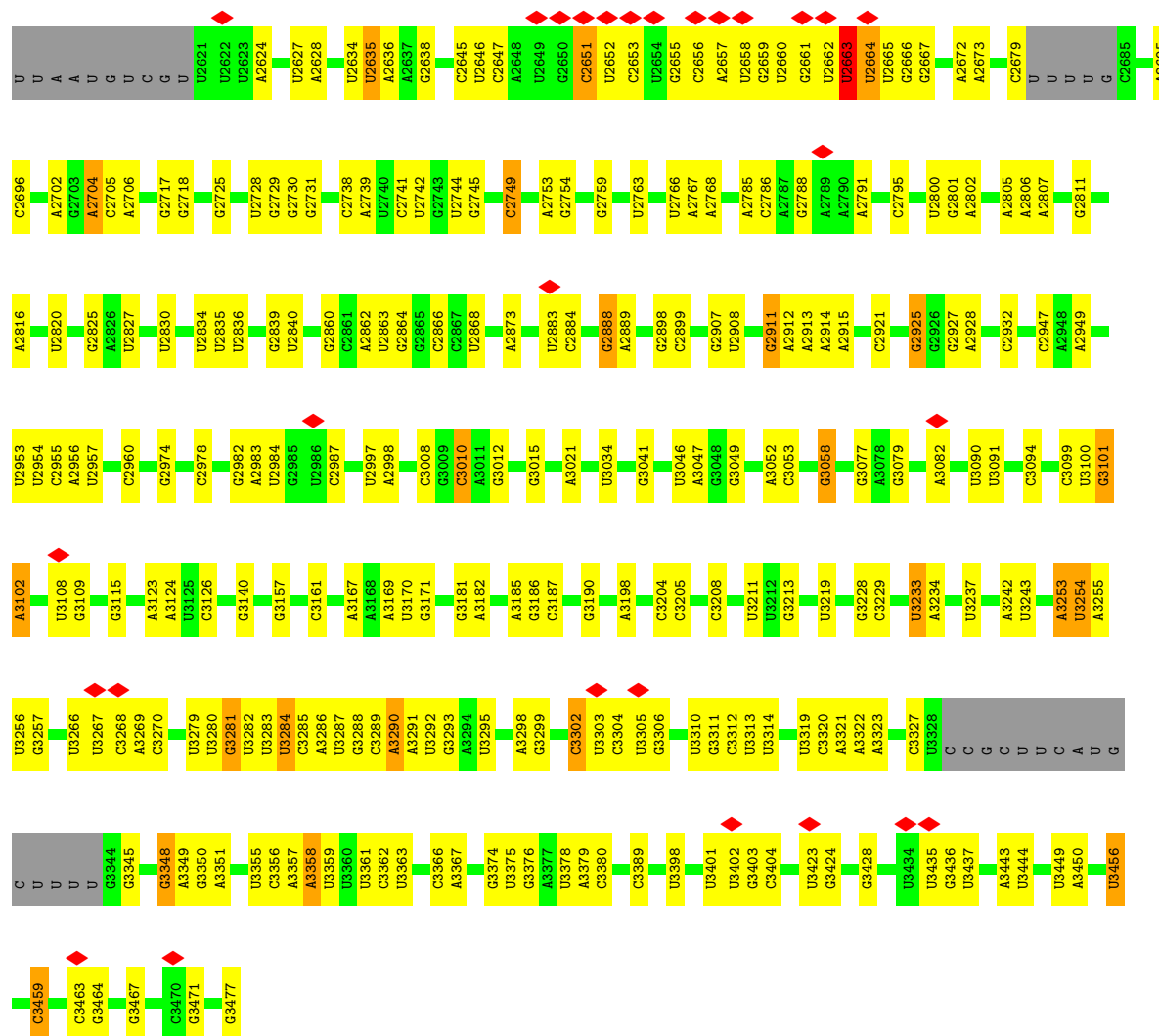
3 Residue-property plots

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: 25S RNA

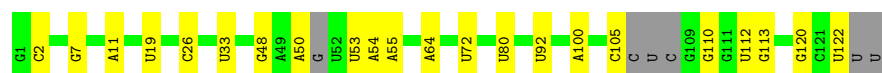






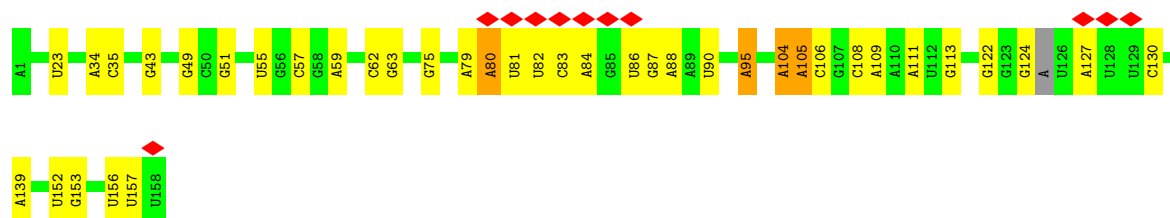
- Molecule 2: 5S RNA

Chain 3: 77% 18% 5%

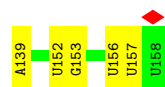


- Molecule 3: 5.8S RNA

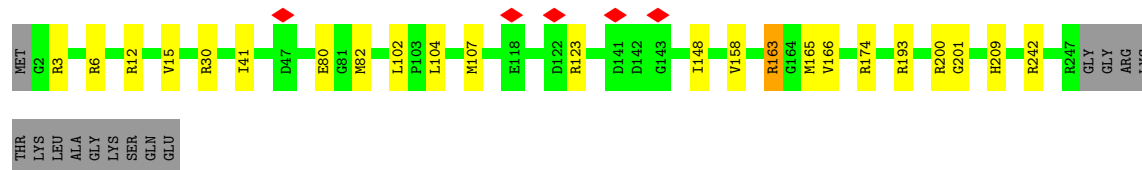
Chain 4: 7% 75% 22%



- Molecule 4: Ribosomal protein uL2

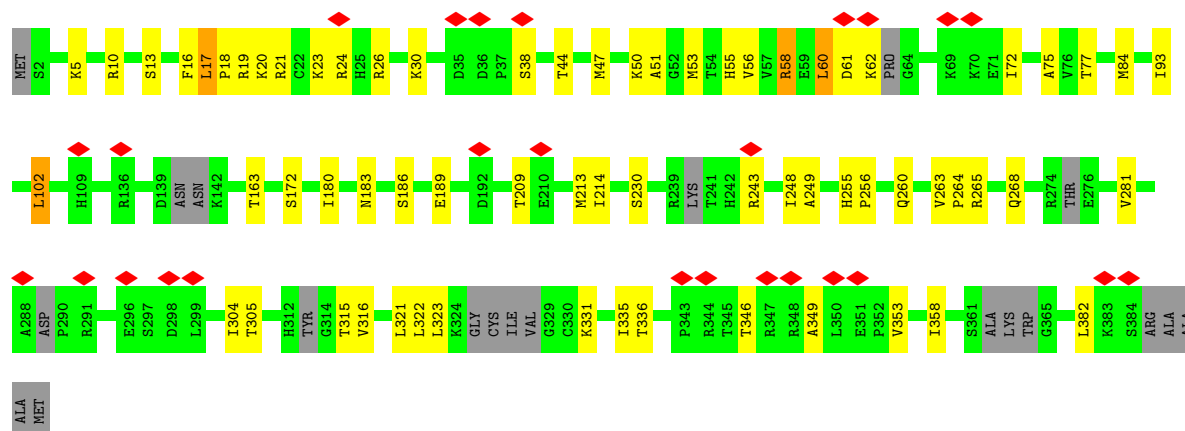


Chain A: 



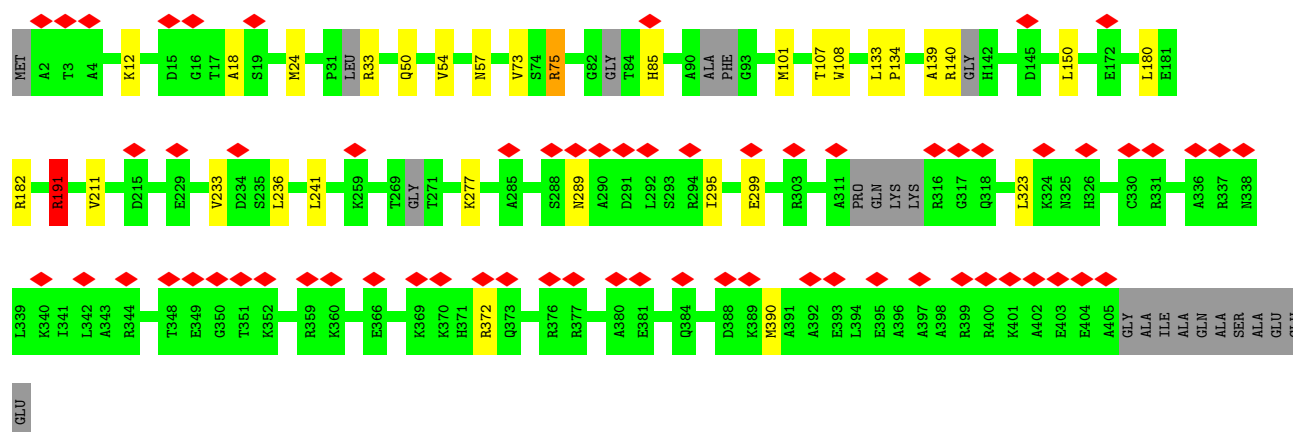
• Molecule 5: Ribosomal protein uL3

Chain B: 



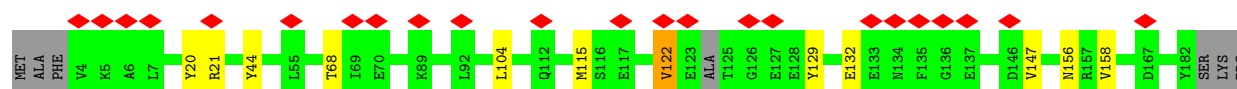
• Molecule 6: Ribosomal protein uL4

Chain C: 

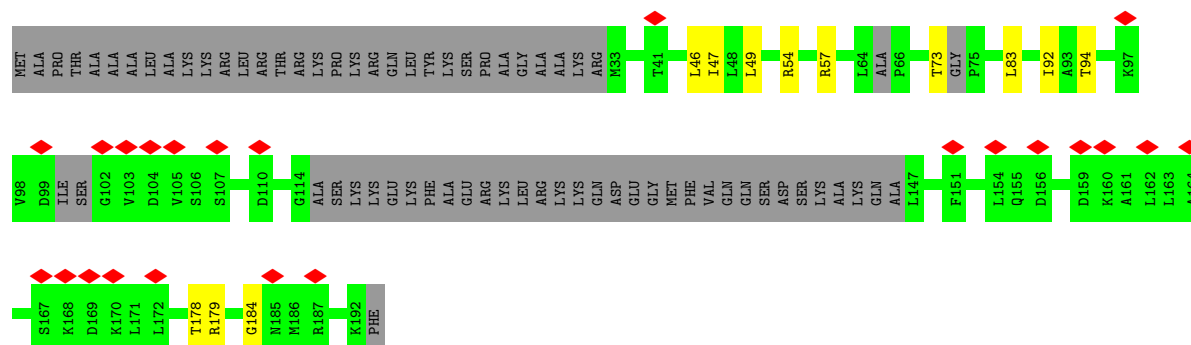


• Molecule 7: Ribosomal protein uL18

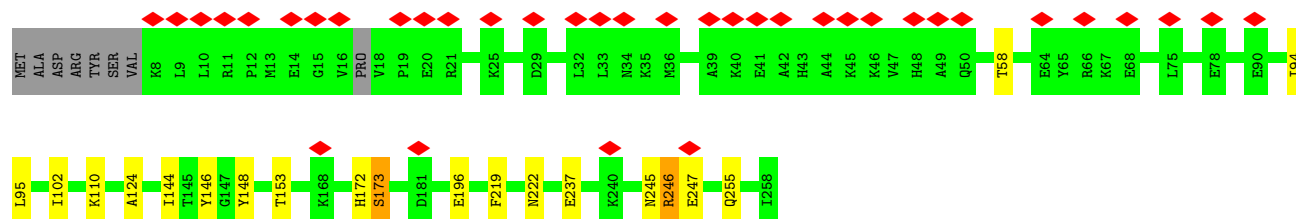
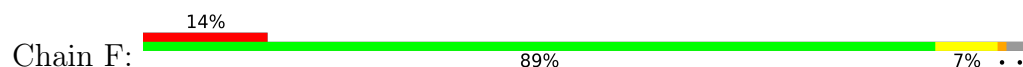
Chain D: 



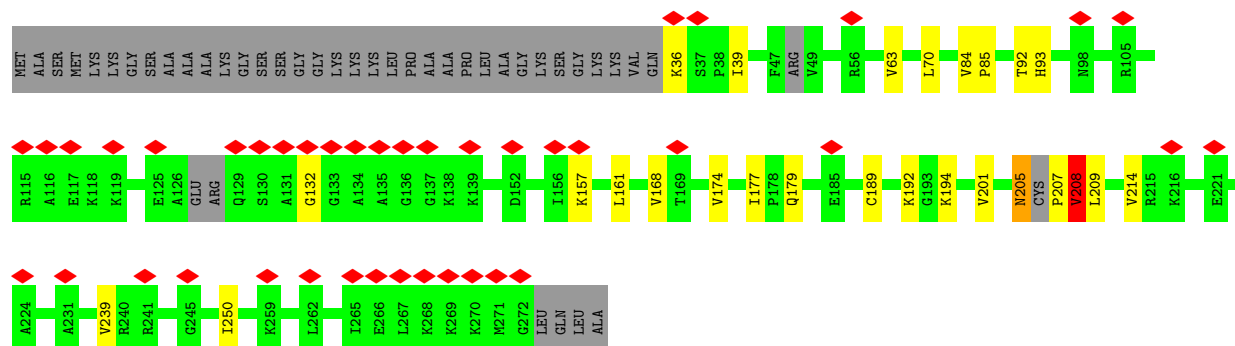
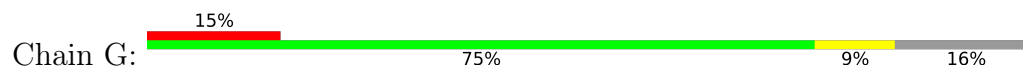
- Molecule 8: Ribosomal protein eL6



- Molecule 9: Ribosomal protein uL30

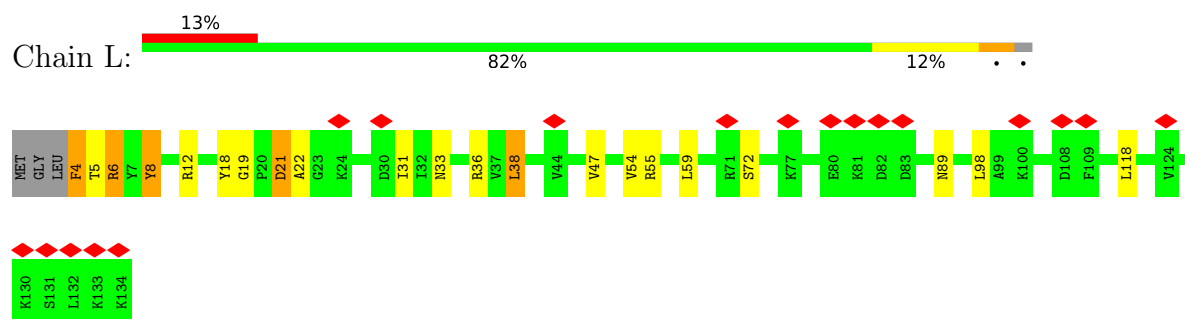


- Molecule 10: Ribosomal protein eL8

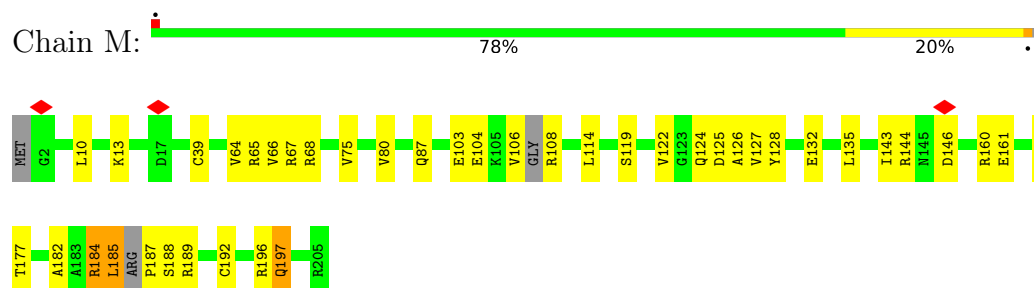


- Molecule 11: Ribosomal protein uL6

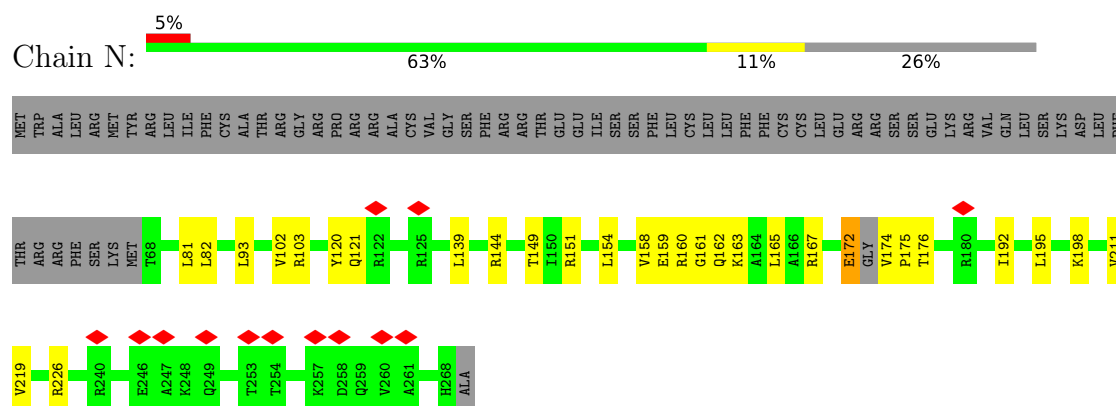
- Molecule 15: Ribosomal protein eL14



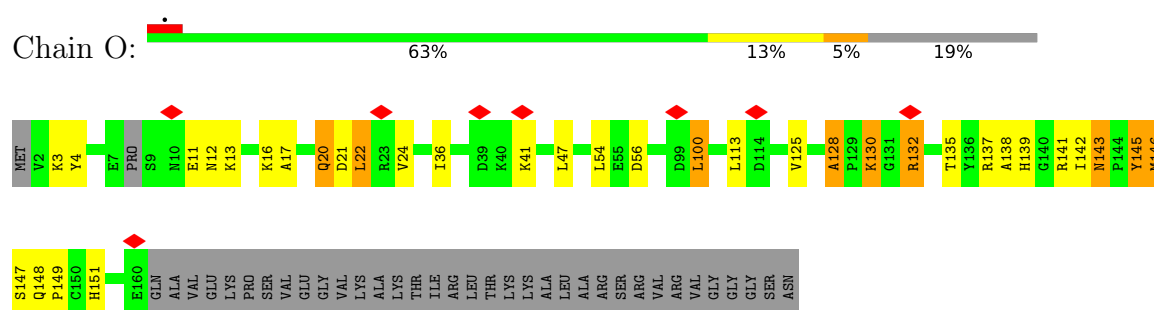
- Molecule 16: Ribosomal protein eL15



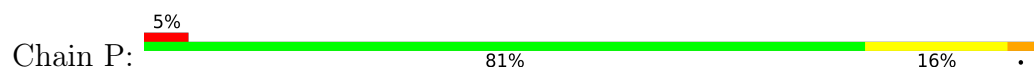
- Molecule 17: Ribosomal protein uL13

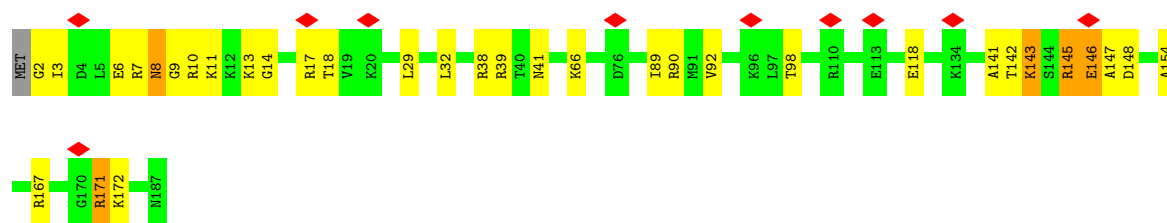


- Molecule 18: Ribosomal protein uL22

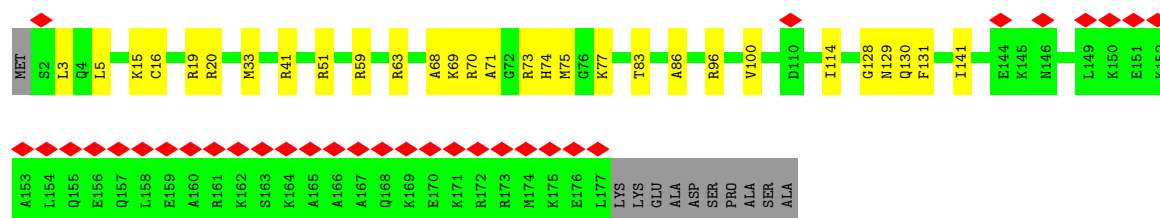
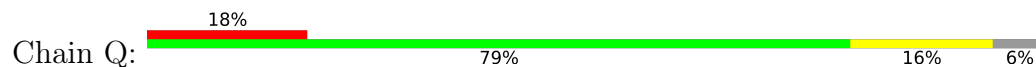


- Molecule 19: Ribosomal protein eL18

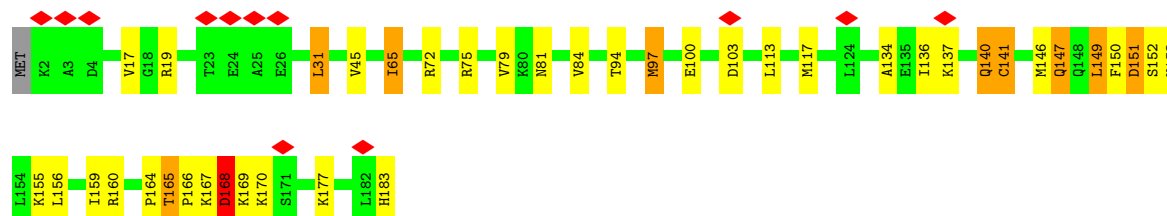
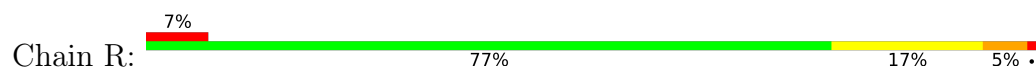




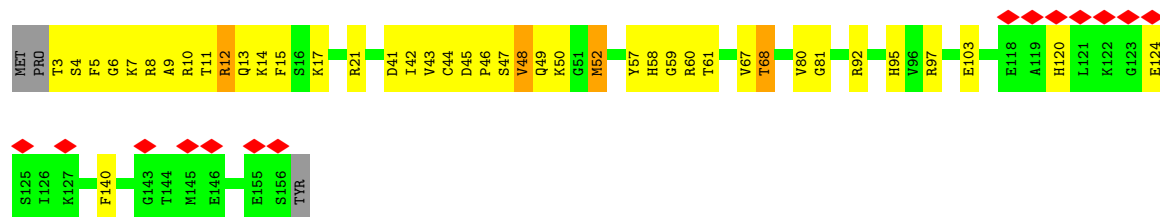
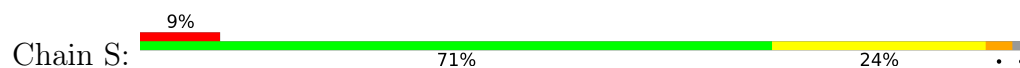
• Molecule 20: Ribosomal protein eL19



• Molecule 21: Ribosomal protein eL20

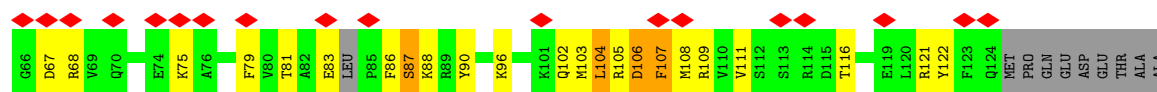


• Molecule 22: Ribosomal protein eL21

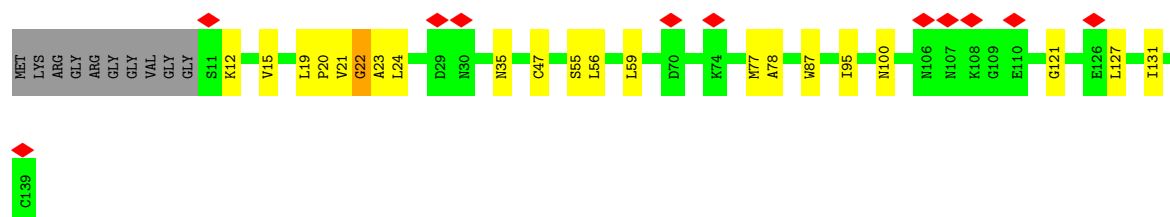
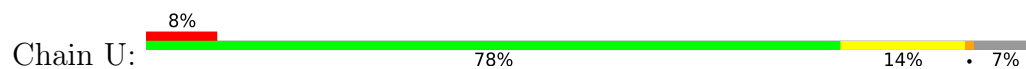


• Molecule 23: Ribosomal protein eL22

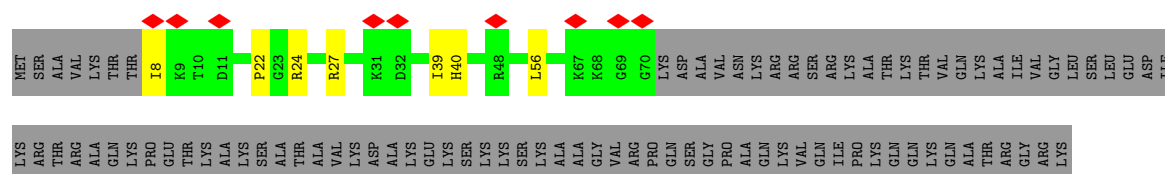
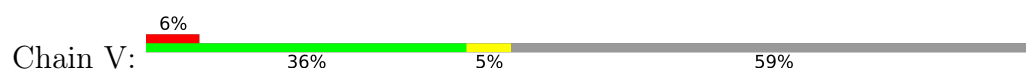




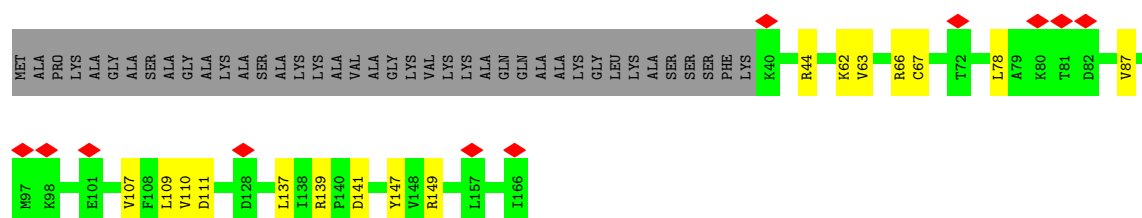
• Molecule 24: Ribosomal protein uL14



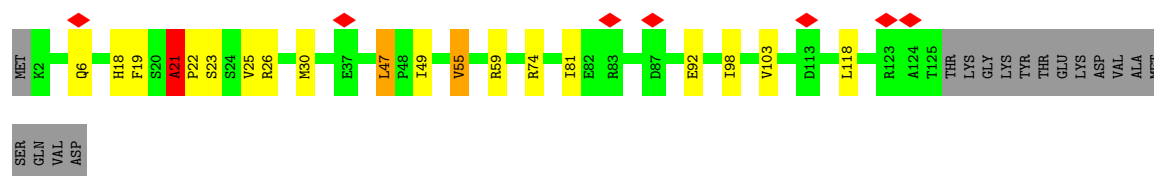
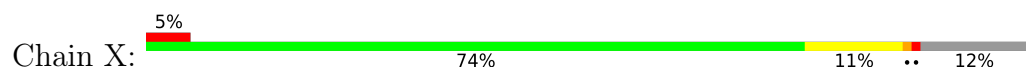
• Molecule 25: Ribosomal protein eL24



• Molecule 26: Ribosomal protein uL23

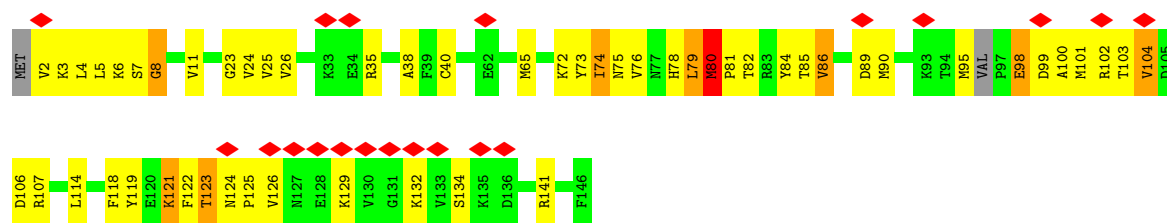


• Molecule 27: Ribosomal protein uL24

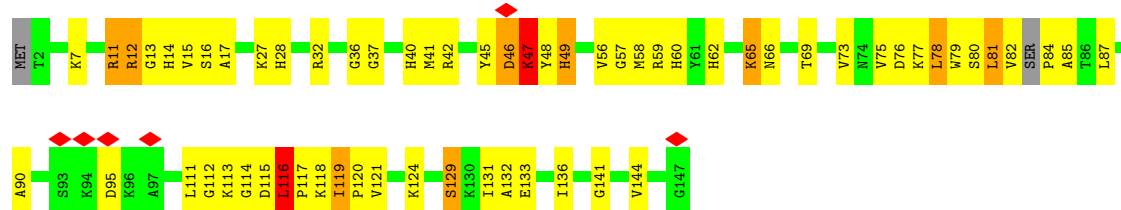


• Molecule 28: Ribosomal protein eL27

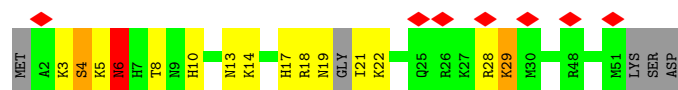




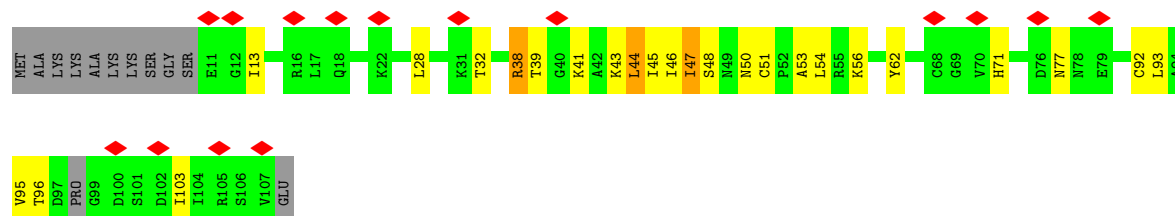
• Molecule 29: Ribosomal protein uL15



• Molecule 30: Ribosomal protein eL29



• Molecule 31: Ribosomal protein eL30

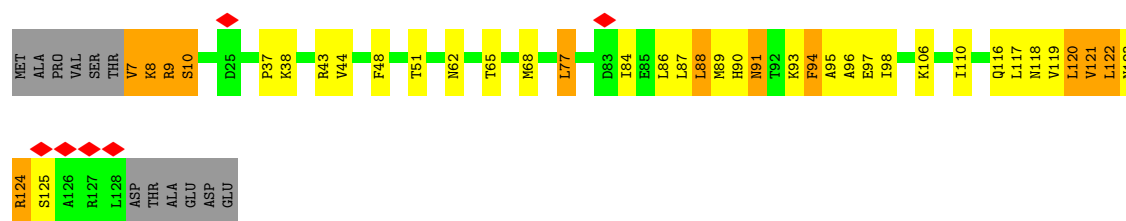


• Molecule 32: Ribosomal protein eL31

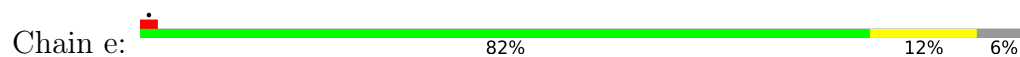


• Molecule 33: Ribosomal protein eL32

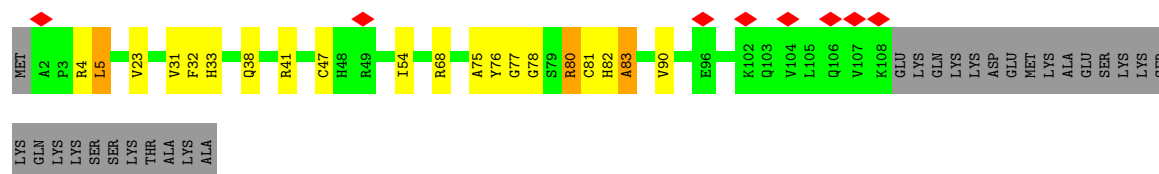




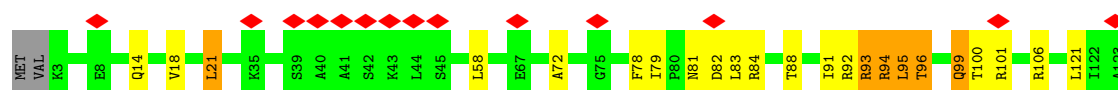
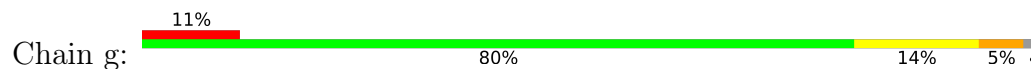
- Molecule 34: Ribosomal protein eL33



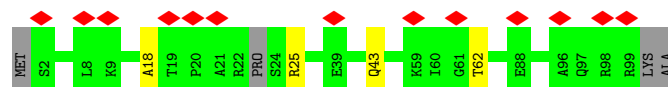
- Molecule 35: Ribosomal protein eL34



- Molecule 36: Ribosomal protein uL29



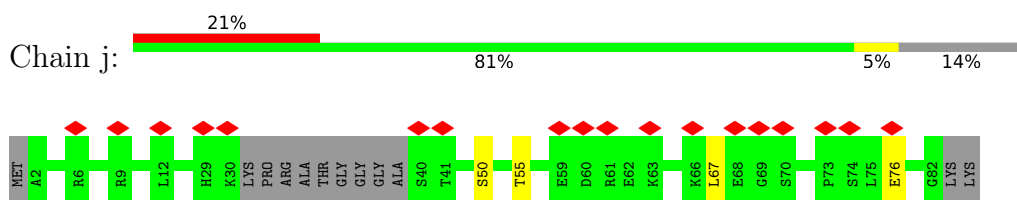
- Molecule 37: Ribosomal protein eL36



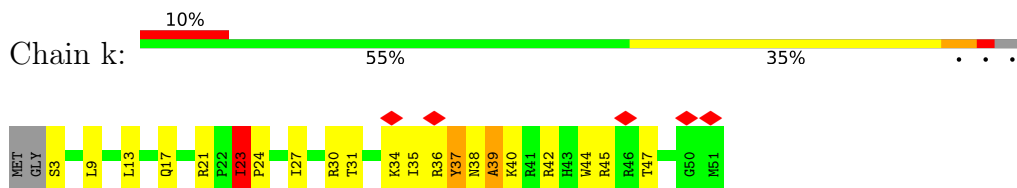
- Molecule 38: Ribosomal protein eL37



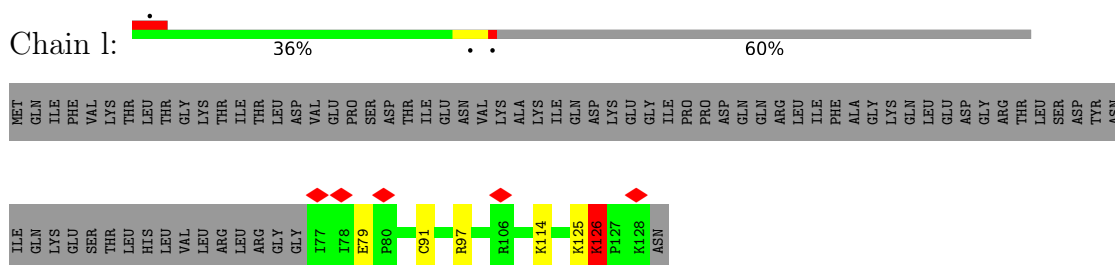
- Molecule 39: Ribosomal protein eL38



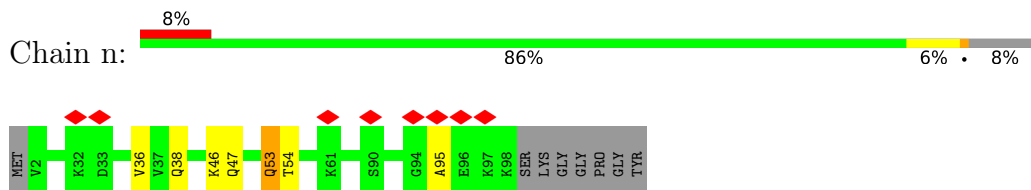
- Molecule 40: Ribosomal protein eL39



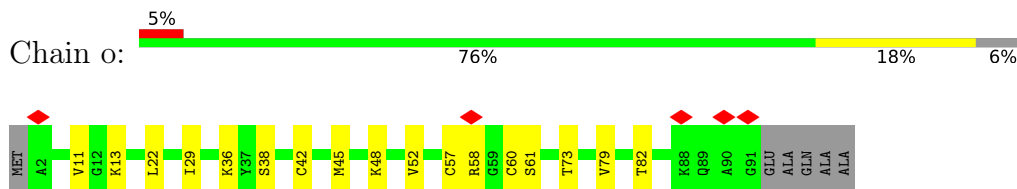
- Molecule 41: Ribosomal protein eL40



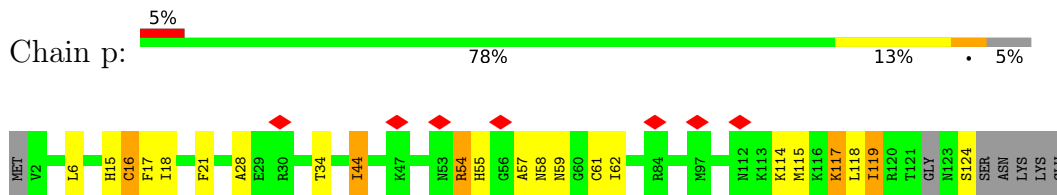
- Molecule 42: Ribosomal protein eL42



- Molecule 43: Ribosomal protein eL43



- Molecule 44: Ribosomal protein eL28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	108162	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.354	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.37	0/73347	0.70	36/114257 (0.0%)
2	3	0.37	0/2813	0.64	0/4379
3	4	0.36	0/3731	0.68	0/5808
4	A	0.48	0/1918	0.72	0/2572
5	B	0.51	0/3006	0.74	1/4023 (0.0%)
6	C	0.53	0/3104	0.76	0/4164
7	D	0.51	0/2158	0.73	0/2891
8	E	0.51	0/981	0.71	0/1311
9	F	0.52	0/2102	0.79	1/2811 (0.0%)
10	G	0.55	0/1905	0.85	1/2546 (0.0%)
11	H	0.50	0/1500	0.71	0/2019
12	I	0.56	0/1570	0.80	4/2099 (0.2%)
13	J	0.53	0/1366	0.75	0/1823
14	K	0.50	0/1621	0.78	0/2172
15	L	0.53	0/1077	0.85	0/1438
16	M	0.51	0/1715	0.82	1/2289 (0.0%)
17	N	0.51	0/1671	0.79	0/2233
18	O	0.58	0/1308	0.98	11/1744 (0.6%)
19	P	0.49	0/1498	0.85	3/1992 (0.2%)
20	Q	0.50	0/1491	0.87	2/1970 (0.1%)
21	R	0.52	0/1523	0.80	3/2043 (0.1%)
22	S	0.56	0/1257	0.86	4/1685 (0.2%)
23	T	0.53	0/840	0.82	2/1120 (0.2%)
24	U	0.51	0/984	0.80	2/1326 (0.2%)
25	V	0.50	0/547	0.74	0/728
26	W	0.53	0/1054	0.77	0/1420
27	X	0.55	0/1026	0.82	3/1367 (0.2%)
28	Y	0.56	1/1182 (0.1%)	0.85	4/1573 (0.3%)
29	Z	0.65	0/1161	1.11	15/1549 (1.0%)
30	a	0.42	0/408	0.91	1/531 (0.2%)
31	b	0.58	0/732	0.93	3/980 (0.3%)
32	c	0.52	0/925	0.79	2/1239 (0.2%)
33	d	0.52	0/1029	1.04	9/1370 (0.7%)
34	e	0.49	0/872	0.69	0/1170

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
35	f	0.54	0/881	0.91	3/1183 (0.3%)
36	g	0.54	0/987	0.92	4/1306 (0.3%)
37	h	0.54	0/779	0.79	0/1033
38	i	0.61	0/700	1.08	2/923 (0.2%)
39	j	0.53	0/599	0.67	0/800
40	k	0.68	1/428 (0.2%)	1.21	7/566 (1.2%)
41	l	0.59	0/426	0.80	2/566 (0.4%)
42	n	0.47	0/802	0.69	0/1057
43	o	0.54	0/693	0.86	0/923
44	p	0.49	0/984	0.89	2/1307 (0.2%)
All	All	0.44	2/130701 (0.0%)	0.74	128/192306 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	k	23	ILE	C-N	6.72	1.39	1.33
28	Y	124	ASN	C-N	6.17	1.39	1.33

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	123	ASN	N-CA-C	10.67	122.91	111.28
10	G	92	THR	N-CA-C	-10.57	100.67	114.31
44	p	17	PHE	N-CA-C	10.24	122.44	111.28
38	i	70	LEU	N-CA-C	9.38	121.58	111.36
18	O	20	GLN	N-CA-C	9.19	121.06	111.14
20	Q	20	ARG	N-CA-C	8.71	120.85	111.36
1	1	1153	A	C4'-C3'-O3'	8.16	121.64	109.40
1	1	1723	U	C4'-C3'-O3'	7.92	121.28	109.40
18	O	146	MET	N-CA-C	7.89	122.09	108.76
1	1	259	A	C4'-C3'-O3'	7.51	120.67	109.40
1	1	2651	C	C2'-C3'-O3'	7.44	120.66	109.50
1	1	1825	G	C2'-C3'-O3'	7.41	120.61	109.50
40	k	23	ILE	CA-C-N	-7.24	114.38	119.66
40	k	23	ILE	C-N-CA	-7.24	114.38	119.66
29	Z	15	VAL	N-CA-C	7.22	117.99	110.62
33	d	122	LEU	N-CA-C	7.06	118.98	111.28
5	B	17	LEU	C-N-CD	6.99	135.99	120.60
38	i	66	ARG	N-CA-C	6.89	118.79	111.28
29	Z	27	LYS	N-CA-C	6.86	118.41	111.07
1	1	1651	A	C2'-C3'-O3'	6.84	119.76	109.50
30	a	6	ASN	N-CA-C	6.81	118.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2704	A	C4'-C3'-O3'	6.80	119.61	109.40
1	1	2664	U	C4'-C3'-O3'	6.74	119.50	109.40
1	1	2635	U	C2'-C3'-O3'	6.69	119.53	109.50
19	P	14	GLY	N-CA-C	6.66	120.72	112.73
1	1	180	G	C2'-C3'-O3'	-6.66	103.71	113.70
23	T	87	SER	N-CA-C	6.63	119.22	108.34
1	1	407	G	C2'-C3'-O3'	6.56	119.35	109.50
44	p	54	ARG	N-CA-C	-6.56	100.72	110.23
1	1	580	U	C2'-C3'-O3'	6.56	119.34	109.50
33	d	94	PHE	N-CA-C	6.48	120.02	109.59
24	U	23	ALA	N-CA-C	6.47	119.62	110.23
35	f	83	ALA	N-CA-C	-6.40	104.31	111.28
1	1	1006	G	C2'-C3'-O3'	-6.36	104.16	113.70
27	X	19	PHE	N-CA-C	6.32	118.25	111.36
29	Z	49	HIS	CA-C-N	-6.32	114.12	120.31
29	Z	49	HIS	C-N-CA	-6.32	114.12	120.31
33	d	125	SER	N-CA-C	-6.30	103.24	111.74
19	P	145	ARG	N-CA-C	6.29	118.99	109.23
1	1	1578	A	C2'-C3'-O3'	6.28	118.92	109.50
1	1	3358	A	C2'-C3'-O3'	6.27	118.91	109.50
1	1	581	U	C4'-C3'-O3'	6.22	118.74	109.40
27	X	21	ALA	CA-C-N	-6.22	113.87	120.03
27	X	21	ALA	C-N-CA	-6.22	113.87	120.03
1	1	3348	G	C4'-C3'-O3'	6.17	118.65	109.40
36	g	72	ALA	N-CA-C	6.10	118.01	111.36
1	1	3233	U	C4'-C3'-O3'	6.01	118.42	109.40
22	S	52	MET	CA-C-N	-6.01	114.57	120.52
22	S	52	MET	C-N-CA	-6.01	114.57	120.52
1	1	405	A	C4'-C3'-O3'	5.98	118.38	109.40
1	1	3254	U	C2'-C3'-O3'	5.98	118.47	109.50
18	O	145	TYR	N-CA-C	-5.97	98.56	108.34
18	O	130	LYS	N-CA-C	5.96	118.40	110.53
29	Z	28	HIS	CA-C-N	-5.94	113.85	119.85
29	Z	28	HIS	C-N-CA	-5.94	113.85	119.85
33	d	124	ARG	N-CA-C	5.93	123.44	110.80
36	g	93	ARG	N-CA-C	-5.91	103.15	110.41
1	1	2226	A	C4'-C3'-O3'	5.88	118.22	109.40
41	l	126	LYS	CA-C-N	-5.82	113.97	119.85
41	l	126	LYS	C-N-CA	-5.82	113.97	119.85
31	b	38	ARG	N-CA-C	-5.78	104.98	111.28
12	I	17	TYR	CA-C-N	-5.77	114.66	120.31
12	I	17	TYR	C-N-CA	-5.77	114.66	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Z	119	ILE	CA-C-N	-5.76	113.61	119.83
29	Z	119	ILE	C-N-CA	-5.76	113.61	119.83
21	R	165	THR	CA-C-N	-5.74	114.02	119.76
21	R	165	THR	C-N-CA	-5.74	114.02	119.76
18	O	148	GLN	CA-C-N	-5.72	114.36	120.03
18	O	148	GLN	C-N-CA	-5.72	114.36	120.03
24	U	22	GLY	N-CA-C	5.71	120.72	113.24
12	I	15	LYS	CA-C-N	-5.67	113.92	119.76
12	I	15	LYS	C-N-CA	-5.67	113.92	119.76
1	1	116	A	C4'-C3'-O3'	5.62	117.84	109.40
23	T	107	PHE	N-CA-C	5.61	117.39	111.28
29	Z	116	LEU	CA-C-N	-5.58	114.51	120.03
29	Z	116	LEU	C-N-CA	-5.58	114.51	120.03
33	d	125	SER	CA-C-N	5.54	127.98	120.44
33	d	125	SER	C-N-CA	5.54	127.98	120.44
1	1	2663	U	C2'-C3'-O3'	5.54	117.81	109.50
1	1	2215	C	C2'-C3'-O3'	5.54	117.81	109.50
28	Y	80	MET	CA-C-N	-5.53	114.56	120.03
28	Y	80	MET	C-N-CA	-5.53	114.56	120.03
18	O	143	ASN	CA-C-N	-5.53	114.27	119.85
18	O	143	ASN	C-N-CA	-5.53	114.27	119.85
16	M	184	ARG	N-CA-C	5.47	117.25	111.28
29	Z	46	ASP	N-CA-C	-5.46	100.21	108.67
20	Q	70	ARG	N-CA-C	-5.45	105.34	111.28
9	F	246	ARG	N-CA-C	-5.39	100.45	109.24
29	Z	81	LEU	N-CA-C	5.38	117.15	111.28
18	O	128	ALA	CA-C-N	-5.38	114.22	119.76
18	O	128	ALA	C-N-CA	-5.38	114.22	119.76
36	g	79	ILE	CA-C-N	-5.37	114.25	119.78
36	g	79	ILE	C-N-CA	-5.37	114.25	119.78
31	b	51	CYS	CA-C-N	-5.32	114.28	119.76
31	b	51	CYS	C-N-CA	-5.32	114.28	119.76
1	1	1439	U	C3'-C2'-O2'	5.32	118.68	110.70
1	1	1675	U	C2'-C3'-O3'	5.31	117.47	109.50
1	1	2215	C	C4'-C3'-O3'	5.31	117.37	109.40
29	Z	47	LYS	N-CA-C	-5.30	99.52	110.80
21	R	147	GLN	N-CA-C	5.26	117.76	111.71
1	1	873	U	C2'-C3'-O3'	-5.26	105.82	113.70
1	1	1941	A	C2'-C3'-O3'	-5.26	105.82	113.70
18	O	132	ARG	N-CA-C	5.23	117.50	109.07
1	1	614	U	C2'-C3'-O3'	5.22	121.53	113.70
33	d	93	LYS	N-CA-C	5.22	117.05	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	S	45	ASP	CA-C-N	-5.21	114.45	119.87
22	S	45	ASP	C-N-CA	-5.21	114.45	119.87
40	k	35	ILE	N-CA-C	5.21	116.40	109.37
1	1	1436	A	C4'-C3'-O3'	5.19	117.19	109.40
1	1	3302	C	C2'-C3'-O3'	5.18	121.47	113.70
35	f	77	GLY	N-CA-C	5.17	118.94	112.73
29	Z	57	GLY	N-CA-C	5.17	121.17	112.85
29	Z	65	LYS	N-CA-C	-5.16	103.58	110.55
1	1	3290	A	C2'-C3'-O3'	5.16	117.23	109.50
40	k	21	ARG	CA-C-N	-5.16	114.47	119.78
40	k	21	ARG	C-N-CA	-5.16	114.47	119.78
40	k	31	THR	N-CA-C	5.16	117.71	110.23
35	f	80	ARG	N-CA-C	5.13	117.61	109.50
1	1	1436	A	C2'-C3'-O3'	5.12	117.19	109.50
33	d	96	ALA	N-CA-C	5.12	117.08	108.73
28	Y	124	ASN	CA-C-N	-5.08	114.74	120.89
28	Y	124	ASN	C-N-CA	-5.08	114.74	120.89
1	1	1440	A	C4'-C3'-O3'	5.08	117.02	109.40
19	P	142	THR	N-CA-C	5.07	116.61	111.14
1	1	1006	G	C4'-C3'-O3'	5.02	120.53	113.00
32	c	75	VAL	CA-C-N	-5.01	114.62	119.78
32	c	75	VAL	C-N-CA	-5.01	114.62	119.78
40	k	39	ALA	N-CA-C	5.01	116.82	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	65598	0	33041	241	0
2	3	2519	0	1277	0	0
3	4	3339	0	1684	7	0
4	A	1882	0	1944	11	0
5	B	2942	0	3034	57	0
6	C	3060	0	3193	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	2123	0	2166	6	0
8	E	971	0	1047	4	0
9	F	2059	0	2185	12	0
10	G	1877	0	2005	10	0
11	H	1478	0	1549	8	0
12	I	1540	0	1584	13	0
13	J	1343	0	1370	25	0
14	K	1593	0	1711	11	0
15	L	1063	0	1142	17	0
16	M	1683	0	1768	56	0
17	N	1645	0	1747	20	0
18	O	1286	0	1325	41	0
19	P	1477	0	1587	45	0
20	Q	1473	0	1600	22	0
21	R	1492	0	1571	47	0
22	S	1231	0	1272	55	0
23	T	827	0	865	54	0
24	U	968	0	1014	14	0
25	V	533	0	555	3	0
26	W	1038	0	1095	9	0
27	X	1011	0	1089	14	0
28	Y	1163	0	1268	78	0
29	Z	1136	0	1194	98	0
30	a	404	0	436	31	0
31	b	725	0	747	37	0
32	c	908	0	942	12	0
33	d	1011	0	1080	48	0
34	e	854	0	897	6	0
35	f	863	0	912	13	0
36	g	981	0	1102	29	0
37	h	772	0	856	2	0
38	i	688	0	703	18	0
39	j	591	0	636	0	0
40	k	419	0	464	17	0
41	l	419	0	464	12	0
42	n	790	0	886	4	0
43	o	684	0	738	12	0
44	p	974	0	1058	43	0
All	All	121433	0	88803	1037	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 (1037) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1436:A:C2	6:C:299:GLU:HG3	1.28	1.67
22:S:49:GLN:HA	22:S:52:MET:CE	1.01	1.47
22:S:49:GLN:CA	22:S:52:MET:CE	1.92	1.44
1:1:2754:G:H5'	30:a:6:ASN:ND2	1.22	1.40
1:1:1436:A:N1	6:C:299:GLU:HG3	1.31	1.39
28:Y:122:PHE:CD2	28:Y:141:ARG:HG2	1.57	1.38
1:1:496:C:C5	29:Z:82:VAL:HG11	1.58	1.36
28:Y:122:PHE:CD2	28:Y:141:ARG:CG	2.11	1.33
3:4:95:A:OP2	38:i:75:ARG:NH2	1.61	1.32
13:J:17:LYS:HE2	13:J:131:GLN:CD	1.52	1.32
30:a:14:LYS:HE2	30:a:18:ARG:NH1	1.42	1.31
1:1:1436:A:C2	6:C:299:GLU:CG	2.15	1.28
29:Z:90:ALA:O	29:Z:119:ILE:HD11	1.32	1.27
21:R:100:GLU:CD	21:R:141:CYS:SG	2.17	1.26
21:R:100:GLU:OE1	21:R:141:CYS:SG	1.94	1.26
17:N:172:GLU:OE1	17:N:219:VAL:HG21	1.29	1.26
16:M:187:PRO:HD2	16:M:192:CYS:SG	1.77	1.23
1:1:2045:U:C5	20:Q:73:ARG:NH1	2.06	1.22
22:S:15:PHE:O	22:S:46:PRO:HG3	1.36	1.21
18:O:20:GLN:O	18:O:151:HIS:HD2	1.24	1.20
18:O:135:THR:OG1	18:O:145:TYR:CD1	1.95	1.20
1:1:496:C:N4	29:Z:82:VAL:HG21	1.59	1.18
1:1:1949:C:N3	18:O:142:ILE:HD11	1.57	1.18
13:J:17:LYS:HE2	13:J:131:GLN:OE1	1.45	1.16
29:Z:90:ALA:O	29:Z:119:ILE:CD1	1.93	1.16
16:M:64:VAL:HG21	16:M:106:VAL:CG2	1.76	1.16
28:Y:122:PHE:HD2	28:Y:141:ARG:CG	1.49	1.15
1:1:1906:G:O2'	35:f:78:GLY:HA3	1.45	1.14
1:1:496:C:C5	29:Z:82:VAL:CG1	2.31	1.13
30:a:3:LYS:HA	30:a:4:SER:HB2	1.16	1.12
41:l:91:CYS:HB3	41:l:126:LYS:CD	1.78	1.12
22:S:49:GLN:CA	22:S:52:MET:HE3	1.67	1.11
22:S:49:GLN:CA	22:S:52:MET:HE1	1.65	1.11
23:T:109:ARG:HH21	23:T:111:VAL:CG2	1.64	1.11
18:O:20:GLN:O	18:O:151:HIS:CD2	2.03	1.10
1:1:3313:U:O4	21:R:169:LYS:HE3	1.51	1.10
22:S:49:GLN:HA	22:S:52:MET:HE3	1.18	1.10
1:1:2045:U:C6	20:Q:73:ARG:NH1	2.16	1.10
1:1:2754:G:C5'	30:a:6:ASN:ND2	2.14	1.10
16:M:64:VAL:CG2	16:M:106:VAL:CG2	2.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1039:C:OP1	19:P:10:ARG:NH2	1.85	1.08
12:I:14:ASN:O	12:I:128:ARG:NH2	1.87	1.08
22:S:49:GLN:C	22:S:52:MET:HE3	1.78	1.08
38:i:25:CYS:SG	38:i:37:CYS:SG	2.52	1.07
41:l:91:CYS:HB3	41:l:126:LYS:CE	1.85	1.07
31:b:39:THR:HG22	31:b:41:LYS:HG3	1.34	1.06
30:a:19:ASN:O	30:a:22:LYS:NZ	1.88	1.06
1:1:1436:A:N1	6:C:299:GLU:CG	2.16	1.05
1:1:180:G:O2'	1:1:181:C:H6	1.39	1.05
16:M:68:ARG:HH22	16:M:124:GLN:NE2	1.54	1.04
28:Y:80:MET:CE	31:b:62:TYR:HE2	1.71	1.04
23:T:109:ARG:HH21	23:T:111:VAL:HG22	1.18	1.04
17:N:172:GLU:OE1	17:N:219:VAL:CG2	2.07	1.02
28:Y:122:PHE:CD2	28:Y:141:ARG:HG3	1.91	1.02
41:l:91:CYS:CB	41:l:126:LYS:HE2	1.89	1.02
1:1:99:A:OP1	16:M:196:ARG:HD3	1.60	1.01
26:W:63:VAL:HG11	36:g:78:PHE:O	1.60	1.01
23:T:57:LYS:HA	23:T:61:LYS:O	1.61	1.01
28:Y:122:PHE:CE2	28:Y:141:ARG:CG	2.43	1.00
29:Z:76:ASP:HB2	29:Z:114:GLY:HA3	1.42	1.00
29:Z:79:TRP:CH2	29:Z:121:VAL:HG11	1.96	1.00
1:1:1039:C:P	19:P:10:ARG:NH2	2.34	1.00
16:M:187:PRO:CD	16:M:192:CYS:SG	2.49	1.00
1:1:300:G:OP2	16:M:68:ARG:NH1	1.93	1.00
9:F:146:TYR:CZ	9:F:245:ASN:HB3	1.97	1.00
5:B:60:LEU:HD21	5:B:62:LYS:CG	1.93	0.98
36:g:95:LEU:H	36:g:95:LEU:HD22	1.29	0.98
1:1:2795:C:OP1	13:J:17:LYS:NZ	1.96	0.98
1:1:2899:C:OP1	29:Z:56:VAL:O	1.82	0.98
28:Y:122:PHE:CE2	28:Y:141:ARG:HG3	1.98	0.98
36:g:96:THR:H	36:g:99:GLN:HE21	0.99	0.98
16:M:68:ARG:NH2	16:M:124:GLN:NE2	2.13	0.97
1:1:299:C:OP1	16:M:68:ARG:HG2	1.66	0.96
28:Y:100:ALA:HB1	28:Y:106:ASP:CG	1.90	0.96
38:i:29:ALA:HB3	38:i:37:CYS:SG	2.05	0.96
1:1:85:A:OP2	29:Z:65:LYS:HE3	1.65	0.96
30:a:14:LYS:CE	30:a:18:ARG:NH1	2.28	0.96
33:d:89:MET:CE	44:p:114:LYS:HB2	1.95	0.95
41:l:91:CYS:HB3	41:l:126:LYS:HD3	1.48	0.95
13:J:14:ARG:HE	13:J:135:PRO:HG3	1.30	0.95
1:1:2754:G:H5'	30:a:6:ASN:HD21	1.28	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:64:VAL:HG21	16:M:106:VAL:HG23	1.49	0.94
33:d:116:GLN:HE22	44:p:124:SER:HA	1.33	0.94
23:T:25:PRO:CB	23:T:83:GLU:OE2	2.15	0.94
6:C:139:ALA:O	44:p:16:CYS:SG	2.26	0.94
16:M:122:VAL:HG11	16:M:132:GLU:HG3	1.47	0.94
18:O:132:ARG:NH1	18:O:132:ARG:HB3	1.83	0.94
22:S:49:GLN:HA	22:S:52:MET:HE2	1.47	0.92
1:1:1039:C:P	19:P:10:ARG:HH21	1.92	0.92
28:Y:80:MET:CE	31:b:62:TYR:CE2	2.52	0.92
1:1:2040:U:O2	20:Q:77:LYS:NZ	2.03	0.91
13:J:17:LYS:HE2	13:J:131:GLN:NE2	1.83	0.91
31:b:50:ASN:HB3	31:b:77:ASN:HB2	1.52	0.91
1:1:1436:A:H2	6:C:299:GLU:CG	1.67	0.91
36:g:95:LEU:HB2	36:g:99:GLN:HG3	1.53	0.90
21:R:155:LYS:O	21:R:156:LEU:HD12	1.71	0.90
28:Y:122:PHE:HD2	28:Y:141:ARG:HG2	0.88	0.90
16:M:68:ARG:HH22	16:M:124:GLN:HE21	1.20	0.89
22:S:15:PHE:O	22:S:46:PRO:CG	2.18	0.89
13:J:17:LYS:CE	13:J:131:GLN:CD	2.44	0.89
20:Q:69:LYS:HG3	20:Q:75:MET:HE3	1.54	0.89
5:B:60:LEU:HD21	5:B:62:LYS:HG3	1.55	0.89
1:1:299:C:OP1	16:M:68:ARG:CG	2.20	0.88
44:p:54:ARG:HD2	44:p:59:ASN:CG	1.98	0.88
1:1:496:C:N4	29:Z:82:VAL:CG2	2.35	0.88
28:Y:118:PHE:O	28:Y:122:PHE:HD1	1.56	0.88
29:Z:124:LYS:HG2	29:Z:144:VAL:HB	1.56	0.88
33:d:8:LYS:O	33:d:8:LYS:NZ	2.06	0.87
41:l:91:CYS:HB3	41:l:126:LYS:HE2	1.49	0.87
1:1:2868:U:H5"	22:S:7:LYS:HE2	1.55	0.87
40:k:27:ILE:O	40:k:30:ARG:HG2	1.74	0.87
1:1:836:C:OP1	19:P:141:ALA:HB1	1.75	0.87
29:Z:12:ARG:HG3	29:Z:12:ARG:HH11	1.38	0.87
1:1:607:U:O2'	21:R:155:LYS:NZ	2.08	0.87
18:O:4:TYR:CE2	18:O:16:LYS:HD3	2.10	0.87
23:T:54:THR:HA	23:T:63:ASN:ND2	1.89	0.87
28:Y:74:ILE:CB	28:Y:79:LEU:HD21	2.04	0.87
1:1:1643:A:O2'	16:M:108:ARG:NH2	2.08	0.86
23:T:25:PRO:HB2	23:T:83:GLU:OE2	1.73	0.86
36:g:101:ARG:O	36:g:101:ARG:NE	2.08	0.86
29:Z:78:LEU:O	29:Z:81:LEU:HB2	1.75	0.85
30:a:14:LYS:HE2	30:a:18:ARG:HH12	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:127:VAL:HG23	16:M:128:TYR:CD2	2.11	0.85
1:1:1436:A:C2	6:C:299:GLU:HA	2.12	0.85
16:M:64:VAL:HG21	16:M:106:VAL:HG21	1.59	0.85
5:B:51:ALA:O	5:B:331:LYS:HG2	1.77	0.85
28:Y:74:ILE:HB	28:Y:79:LEU:HD21	1.59	0.85
22:S:41:ASP:OD1	22:S:61:THR:OG1	1.94	0.84
13:J:17:LYS:CE	13:J:131:GLN:NE2	2.40	0.84
23:T:109:ARG:NH2	23:T:111:VAL:HG22	1.92	0.84
33:d:88:LEU:O	33:d:88:LEU:HD12	1.78	0.84
29:Z:79:TRP:HH2	29:Z:121:VAL:HG11	1.42	0.84
17:N:93:LEU:O	17:N:167:ARG:NH1	2.10	0.84
1:1:1212:U:OP1	12:I:15:LYS:HE3	1.77	0.83
28:Y:80:MET:HE2	31:b:62:TYR:CE2	2.13	0.83
14:K:10:ASN:OD1	19:P:167:ARG:NH1	2.12	0.82
1:1:180:G:O2'	1:1:181:C:C6	2.24	0.82
1:1:872:U:O2'	1:1:873:U:H5'	1.80	0.82
21:R:165:THR:HB	21:R:169:LYS:HD3	1.61	0.82
23:T:102:GLN:O	23:T:104:LEU:CD2	2.27	0.82
1:1:180:G:O6	1:1:245:U:O4	1.97	0.82
44:p:62:ILE:HG12	44:p:118:LEU:CD2	2.08	0.82
28:Y:101:MET:CE	28:Y:107:ARG:HE	1.92	0.82
22:S:48:VAL:O	22:S:52:MET:HE2	1.79	0.81
14:K:10:ASN:CG	19:P:167:ARG:NH1	2.38	0.81
1:1:180:G:O2'	1:1:181:C:O5'	1.97	0.81
16:M:64:VAL:CG2	16:M:106:VAL:HG21	2.10	0.81
16:M:125:ASP:OD1	16:M:126:ALA:N	2.13	0.81
29:Z:79:TRP:HE1	29:Z:117:PRO:HD2	1.45	0.81
1:1:1855:C:OP1	20:Q:15:LYS:NZ	2.11	0.81
30:a:3:LYS:HA	30:a:4:SER:CB	2.05	0.81
23:T:102:GLN:HB2	23:T:104:LEU:HG	1.64	0.80
36:g:96:THR:N	36:g:99:GLN:HE21	1.79	0.80
17:N:102:VAL:CG1	17:N:174:VAL:HG22	2.11	0.80
36:g:96:THR:H	36:g:99:GLN:NE2	1.78	0.80
44:p:54:ARG:HD3	44:p:59:ASN:HB3	1.63	0.80
44:p:62:ILE:HG12	44:p:118:LEU:HD23	1.63	0.80
16:M:189:ARG:HE	16:M:189:ARG:HA	1.46	0.80
23:T:102:GLN:O	23:T:104:LEU:HD21	1.82	0.80
5:B:50:LYS:HB2	5:B:335:ILE:HD11	1.62	0.80
1:1:3313:U:O4	21:R:169:LYS:CE	2.29	0.79
1:1:796:A:N3	29:Z:58:MET:HE3	1.97	0.79
26:W:67:CYS:SG	36:g:82:ASP:OD2	2.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:89:MET:HE1	44:p:114:LYS:HB2	1.63	0.79
29:Z:84:PRO:HD2	29:Z:85:ALA:H	1.47	0.79
31:b:54:LEU:HD23	31:b:54:LEU:O	1.82	0.79
1:1:872:U:H2'	1:1:873:U:C6	2.17	0.79
28:Y:80:MET:HE1	31:b:62:TYR:HE2	1.46	0.79
41:l:126:LYS:NZ	41:l:126:LYS:HB3	1.98	0.79
13:J:18:LEU:HD12	13:J:19:THR:N	1.98	0.79
44:p:54:ARG:CD	44:p:59:ASN:HB3	2.13	0.79
28:Y:74:ILE:CG2	28:Y:79:LEU:HD21	2.12	0.78
33:d:91:ASN:HD21	44:p:117:LYS:HE2	1.46	0.78
1:1:2835:U:OP1	22:S:57:TYR:OH	2.00	0.78
1:1:839:A:O2'	30:a:29:LYS:HE2	1.83	0.78
44:p:62:ILE:CD1	44:p:118:LEU:HD23	2.13	0.78
22:S:49:GLN:HA	22:S:52:MET:HE1	0.78	0.78
28:Y:102:ARG:HH11	28:Y:107:ARG:CZ	1.96	0.78
23:T:25:PRO:HB3	23:T:83:GLU:OE2	1.82	0.78
28:Y:5:LEU:CD1	28:Y:76:VAL:HG23	2.14	0.78
31:b:44:LEU:HD11	31:b:95:VAL:CG2	2.14	0.77
43:o:57:CYS:SG	43:o:60:CYS:HB2	2.24	0.77
1:1:2729:G:OP1	12:I:116:ARG:HD3	1.83	0.77
29:Z:119:ILE:HD12	29:Z:120:PRO:CD	2.14	0.77
1:1:2741:C:OP1	22:S:5:PHE:O	2.02	0.77
1:1:2754:G:H5'	30:a:6:ASN:HD22	0.94	0.77
29:Z:116:LEU:HD12	29:Z:116:LEU:H	1.49	0.77
31:b:39:THR:HG21	31:b:41:LYS:HD2	1.66	0.77
15:L:4:PHE:CZ	21:R:159:ILE:HG12	2.20	0.77
1:1:496:C:H5	29:Z:82:VAL:HG11	1.44	0.77
19:P:6:GLU:O	19:P:7:ARG:HB3	1.85	0.76
29:Z:79:TRP:CZ2	29:Z:119:ILE:CG2	2.68	0.76
36:g:88:THR:OG1	36:g:91:ILE:HG13	1.86	0.76
30:a:3:LYS:CA	30:a:4:SER:HB2	2.04	0.76
33:d:91:ASN:HD21	44:p:117:LYS:CE	1.99	0.76
28:Y:122:PHE:CE2	28:Y:141:ARG:HG2	2.12	0.76
32:c:77:ARG:HG2	32:c:77:ARG:HH11	1.50	0.76
23:T:68:ARG:HG3	23:T:83:GLU:HB2	1.68	0.76
40:k:38:ASN:HD22	40:k:39:ALA:N	1.84	0.75
1:1:179:A:O2'	1:1:180:G:H5'	1.86	0.75
23:T:108:MET:HE2	23:T:122:TYR:CZ	2.21	0.75
1:1:1949:C:C4	18:O:142:ILE:HD11	2.22	0.75
27:X:21:ALA:O	27:X:26:ARG:NH1	2.19	0.75
5:B:21:ARG:NH1	5:B:268:GLN:NE2	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:39:THR:HG22	31:b:41:LYS:CG	2.16	0.75
36:g:95:LEU:HD23	36:g:100:THR:OG1	1.86	0.75
9:F:148:TYR:CD2	9:F:247:GLU:O	2.40	0.75
30:a:19:ASN:HB3	30:a:22:LYS:HZ1	1.51	0.75
1:1:179:A:C2'	1:1:180:G:H5'	2.17	0.75
1:1:180:G:C6	1:1:245:U:O4	2.40	0.75
1:1:496:C:H41	29:Z:82:VAL:HG21	1.48	0.75
16:M:189:ARG:HE	16:M:189:ARG:CA	1.99	0.74
28:Y:122:PHE:HE2	28:Y:141:ARG:HA	1.52	0.74
1:1:2898:G:H1'	29:Z:58:MET:HE2	1.69	0.74
15:L:4:PHE:HZ	21:R:159:ILE:HG12	1.52	0.74
15:L:33:ASN:HA	21:R:149:LEU:HD21	1.67	0.74
1:1:496:C:C6	29:Z:82:VAL:CG1	2.70	0.74
23:T:108:MET:HE3	23:T:122:TYR:CE1	2.23	0.74
29:Z:79:TRP:HH2	29:Z:121:VAL:CG1	2.00	0.74
33:d:84:ILE:HD11	33:d:110:ILE:HG23	1.70	0.74
18:O:22:LEU:N	18:O:22:LEU:HD23	2.03	0.73
38:i:72:ASP:OD1	38:i:75:ARG:NH1	2.21	0.73
23:T:104:LEU:N	23:T:104:LEU:HD23	2.03	0.73
30:a:14:LYS:CE	30:a:18:ARG:HH12	1.97	0.73
44:p:62:ILE:CG1	44:p:118:LEU:HD23	2.18	0.73
5:B:60:LEU:HD23	5:B:61:ASP:N	2.04	0.73
16:M:64:VAL:HG22	16:M:106:VAL:HG22	1.69	0.73
18:O:135:THR:OG1	18:O:145:TYR:HD1	1.66	0.73
33:d:120:LEU:C	33:d:120:LEU:HD13	2.14	0.73
1:1:1436:A:C2	6:C:299:GLU:CA	2.71	0.73
16:M:184:ARG:O	16:M:189:ARG:NH1	2.21	0.73
23:T:109:ARG:HH21	23:T:111:VAL:HG21	1.50	0.73
32:c:66:PHE:CE2	32:c:76:PRO:HG3	2.24	0.73
23:T:103:MET:C	23:T:104:LEU:HD23	2.13	0.73
27:X:22:PRO:HG2	27:X:25:VAL:HG23	1.69	0.73
9:F:146:TYR:CE2	9:F:245:ASN:HB3	2.24	0.73
21:R:100:GLU:OE2	21:R:141:CYS:SG	2.45	0.73
31:b:50:ASN:HB3	31:b:77:ASN:CB	2.19	0.73
1:1:872:U:H2'	1:1:873:U:H6	1.52	0.72
1:1:889:G:OP2	29:Z:32:ARG:NH1	2.22	0.72
23:T:108:MET:CE	23:T:122:TYR:CZ	2.72	0.72
29:Z:14:HIS:HD2	33:d:38:LYS:HE2	1.54	0.72
31:b:48:SER:OG	31:b:77:ASN:HA	1.90	0.72
1:1:2862:A:OP1	22:S:50:LYS:HE2	1.88	0.72
16:M:64:VAL:CG2	16:M:106:VAL:HG22	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:64:VAL:HG22	16:M:106:VAL:CG2	2.19	0.72
1:1:20:G:OP2	36:g:93:ARG:NH1	2.22	0.72
17:N:102:VAL:HG13	17:N:174:VAL:HG22	1.70	0.72
14:K:15:LYS:HD2	16:M:197:GLN:HE22	1.55	0.72
18:O:132:ARG:HB3	18:O:132:ARG:HH11	1.52	0.72
41:l:91:CYS:CB	41:l:126:LYS:CE	2.56	0.72
1:1:2811:G:H5''	22:S:17:LYS:HG2	1.69	0.72
5:B:21:ARG:HH12	5:B:268:GLN:HE22	1.36	0.72
10:G:207:PRO:O	10:G:208:VAL:HG22	1.90	0.71
21:R:166:PRO:HD2	21:R:169:LYS:CD	2.20	0.71
40:k:42:ARG:HG3	40:k:47:THR:HG23	1.71	0.71
29:Z:36:GLY:HA3	29:Z:40:HIS:CE1	2.26	0.71
1:1:2754:G:C5'	30:a:6:ASN:HD21	1.92	0.71
1:1:802:A:OP1	29:Z:131:ILE:HB	1.90	0.71
14:K:10:ASN:CG	19:P:167:ARG:HH11	1.98	0.71
1:1:836:C:P	19:P:141:ALA:HB1	2.31	0.71
28:Y:122:PHE:HE2	28:Y:141:ARG:CA	2.04	0.71
21:R:167:LYS:O	21:R:168:ASP:HB3	1.90	0.71
23:T:54:THR:HA	23:T:63:ASN:HD21	1.55	0.70
28:Y:102:ARG:NH1	28:Y:107:ARG:HG3	2.06	0.70
1:1:3157:G:OP1	5:B:19:ARG:NH2	2.24	0.70
30:a:19:ASN:HB3	30:a:22:LYS:NZ	2.04	0.70
1:1:839:A:HO2'	30:a:29:LYS:HE2	1.54	0.70
22:S:49:GLN:O	22:S:52:MET:HE3	1.90	0.70
27:X:21:ALA:HB3	27:X:26:ARG:NH1	2.05	0.70
1:1:496:C:C4	29:Z:82:VAL:CG2	2.75	0.70
1:1:496:C:C4	29:Z:82:VAL:HG21	2.26	0.70
19:P:13:LYS:CE	19:P:17:ARG:HH12	2.04	0.70
21:R:97:MET:HE2	21:R:117:MET:HE1	1.73	0.70
20:Q:69:LYS:CG	20:Q:75:MET:HE3	2.21	0.70
21:R:136:ILE:CG2	21:R:140:GLN:HB3	2.21	0.70
28:Y:74:ILE:HG21	28:Y:79:LEU:CD2	2.22	0.70
29:Z:119:ILE:HD12	29:Z:120:PRO:HD2	1.73	0.70
1:1:2469:A:N3	18:O:137:ARG:NH2	2.39	0.69
5:B:60:LEU:HD23	5:B:61:ASP:H	1.57	0.69
23:T:26:VAL:HG12	23:T:27:LYS:N	2.07	0.69
29:Z:90:ALA:O	29:Z:119:ILE:HD13	1.87	0.69
28:Y:2:VAL:HG13	28:Y:6:LYS:NZ	2.07	0.69
28:Y:74:ILE:HG21	28:Y:79:LEU:HD21	1.72	0.69
5:B:50:LYS:HB2	5:B:335:ILE:CD1	2.22	0.69
36:g:95:LEU:HD22	36:g:95:LEU:N	2.01	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1646:U:OP1	38:i:44:ASN:ND2	2.25	0.69
1:1:2754:G:C5'	30:a:6:ASN:HD22	1.88	0.69
18:O:128:ALA:HB3	18:O:149:PRO:O	1.92	0.69
5:B:21:ARG:HH12	5:B:268:GLN:NE2	1.89	0.69
6:C:54:VAL:HG21	6:C:101:MET:HE1	1.73	0.69
21:R:166:PRO:HD2	21:R:169:LYS:HD3	1.75	0.69
38:i:22:CYS:SG	38:i:25:CYS:N	2.64	0.69
28:Y:5:LEU:HD12	28:Y:76:VAL:HG23	1.75	0.69
33:d:89:MET:CE	44:p:114:LYS:CB	2.71	0.69
1:1:835:A:O3'	19:P:141:ALA:HA	1.93	0.69
1:1:1949:C:C2	18:O:142:ILE:HD11	2.27	0.69
33:d:86:LEU:HD21	44:p:28:ALA:HA	1.73	0.69
1:1:1781:U:O4	23:T:60:GLY:N	2.23	0.68
1:1:3284:U:H2'	17:N:163:LYS:HD3	1.73	0.68
19:P:92:VAL:CG1	29:Z:87:LEU:HD21	2.24	0.68
13:J:17:LYS:CE	13:J:131:GLN:OE1	2.35	0.68
21:R:166:PRO:O	21:R:169:LYS:HB3	1.94	0.68
31:b:39:THR:CG2	31:b:41:LYS:HG3	2.19	0.68
17:N:154:LEU:HD12	17:N:165:LEU:HD21	1.75	0.68
40:k:23:ILE:HD12	40:k:24:PRO:O	1.92	0.68
27:X:47:LEU:HD11	27:X:118:LEU:HD21	1.74	0.68
1:1:1906:G:O2'	35:f:78:GLY:CA	2.36	0.68
1:1:1978:G:O6	20:Q:19:ARG:NH1	2.26	0.68
19:P:13:LYS:HE3	19:P:17:ARG:HH12	1.57	0.68
24:U:12:LYS:HG3	24:U:127:LEU:HD21	1.76	0.68
41:l:91:CYS:SG	41:l:126:LYS:HE2	2.34	0.68
33:d:43:ARG:HD3	33:d:51:THR:HG21	1.76	0.68
29:Z:12:ARG:HH11	29:Z:12:ARG:CG	2.04	0.68
40:k:36:ARG:O	40:k:37:TYR:O	2.12	0.68
33:d:43:ARG:HB2	33:d:48:PHE:HD2	1.58	0.67
28:Y:101:MET:HG3	28:Y:102:ARG:H	1.57	0.67
29:Z:76:ASP:CB	29:Z:114:GLY:HA3	2.21	0.67
22:S:21:ARG:HG3	22:S:21:ARG:HH11	1.58	0.67
23:T:108:MET:CE	23:T:122:TYR:OH	2.42	0.67
36:g:101:ARG:HE	36:g:101:ARG:C	2.00	0.67
1:1:802:A:H5'	29:Z:131:ILE:HD12	1.76	0.67
28:Y:101:MET:HE1	28:Y:107:ARG:HE	1.59	0.67
36:g:95:LEU:N	36:g:95:LEU:HD13	2.10	0.67
15:L:21:ASP:OD1	15:L:21:ASP:N	2.27	0.67
31:b:46:ILE:HD12	31:b:93:LEU:HD12	1.76	0.67
21:R:167:LYS:HD2	34:e:42:ASP:OD1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:50:LYS:HG2	22:S:92:ARG:HH21	1.60	0.66
1:1:2868:U:C5'	22:S:7:LYS:HE2	2.24	0.66
33:d:9:ARG:HG2	33:d:10:SER:N	2.10	0.66
1:1:178:A:N6	1:1:179:A:C6	2.63	0.66
1:1:1578:A:O2'	1:1:1961:A:H1'	1.94	0.66
1:1:180:G:HO2'	1:1:181:C:H6	1.10	0.66
44:p:15:HIS:CE1	44:p:18:ILE:HG13	2.30	0.66
33:d:91:ASN:HD21	44:p:117:LYS:NZ	1.93	0.66
22:S:44:CYS:H	22:S:58:HIS:CD2	2.13	0.66
32:c:77:ARG:HG2	32:c:77:ARG:NH1	2.09	0.66
1:1:1039:C:P	19:P:10:ARG:HH22	2.19	0.66
18:O:21:ASP:OD2	18:O:149:PRO:HB2	1.96	0.65
28:Y:2:VAL:HG13	28:Y:6:LYS:CE	2.27	0.65
43:o:60:CYS:O	43:o:61:SER:OG	2.12	0.65
27:X:22:PRO:HG2	27:X:25:VAL:CG2	2.27	0.65
1:1:299:C:OP1	16:M:68:ARG:HG3	1.97	0.65
1:1:496:C:C5	29:Z:82:VAL:HG13	2.30	0.65
1:1:3161:C:O2'	5:B:55:HIS:HD2	1.79	0.65
16:M:196:ARG:O	16:M:196:ARG:HG3	1.95	0.65
9:F:146:TYR:CZ	9:F:245:ASN:CB	2.78	0.65
21:R:141:CYS:O	21:R:147:GLN:NE2	2.29	0.65
41:l:126:LYS:HB3	41:l:126:LYS:HZ3	1.60	0.65
28:Y:7:SER:OG	28:Y:26:VAL:O	2.07	0.65
29:Z:79:TRP:NE1	29:Z:117:PRO:HD2	2.11	0.65
30:a:14:LYS:HE2	30:a:18:ARG:CZ	2.24	0.65
1:1:719:C:OP1	17:N:159:GLU:HB2	1.97	0.65
1:1:1135:A:H5''	12:I:16:PRO:HG3	1.78	0.65
28:Y:75:ASN:HB3	28:Y:78:HIS:CD2	2.32	0.65
44:p:57:ALA:O	44:p:58:ASN:HB2	1.97	0.65
13:J:14:ARG:HD2	13:J:135:PRO:HD3	1.79	0.65
23:T:102:GLN:O	23:T:104:LEU:HD23	1.95	0.65
26:W:63:VAL:HG21	36:g:78:PHE:HB3	1.79	0.65
28:Y:121:LYS:O	28:Y:125:PRO:HB3	1.97	0.65
30:a:28:ARG:HD2	30:a:29:LYS:H	1.62	0.64
1:1:180:G:O2'	1:1:181:C:P	2.54	0.64
1:1:1436:A:H2	6:C:299:GLU:CD	2.04	0.64
23:T:68:ARG:HG3	23:T:83:GLU:CB	2.27	0.64
1:1:1038:C:O3'	19:P:10:ARG:NH2	2.30	0.64
26:W:66:ARG:HA	36:g:82:ASP:HB2	1.80	0.64
28:Y:100:ALA:HB1	28:Y:106:ASP:OD2	1.97	0.64
28:Y:119:TYR:O	28:Y:123:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:95:MET:HE3	28:Y:114:LEU:HD22	1.80	0.64
29:Z:14:HIS:CD2	33:d:38:LYS:HE2	2.33	0.64
28:Y:40:CYS:SG	28:Y:79:LEU:CD1	2.87	0.63
28:Y:118:PHE:O	28:Y:122:PHE:CD1	2.46	0.63
38:i:36:THR:HG23	38:i:43:PRO:HD2	1.80	0.63
29:Z:84:PRO:CD	29:Z:85:ALA:H	2.12	0.63
30:a:8:THR:HG22	30:a:10:HIS:H	1.62	0.63
20:Q:68:ALA:O	20:Q:71:ALA:HB3	1.98	0.63
28:Y:2:VAL:HG13	28:Y:6:LYS:HE3	1.81	0.63
5:B:213:MET:HE3	5:B:349:ALA:HB2	1.80	0.63
1:l:874:G:O2'	19:P:90:ARG:NH1	2.31	0.62
40:k:24:PRO:HD2	40:k:27:ILE:HD12	1.81	0.62
42:n:46:LYS:HD3	42:n:54:THR:HG21	1.81	0.62
28:Y:75:ASN:OD1	28:Y:76:VAL:N	2.32	0.62
35:f:81:CYS:O	35:f:82:HIS:ND1	2.32	0.62
33:d:88:LEU:HD12	33:d:88:LEU:C	2.22	0.62
18:O:4:TYR:CZ	18:O:16:LYS:HD3	2.34	0.62
33:d:91:ASN:ND2	44:p:117:LYS:HE2	2.14	0.62
5:B:53:MET:CE	5:B:75:ALA:HB1	2.30	0.62
29:Z:79:TRP:CZ2	29:Z:119:ILE:HG21	2.35	0.62
43:o:36:LYS:O	43:o:45:MET:HE2	1.99	0.62
1:l:1436:A:C2	6:C:299:GLU:CD	2.78	0.62
6:C:236:LEU:HD22	6:C:241:LEU:HD11	1.82	0.62
14:K:10:ASN:ND2	19:P:167:ARG:HH11	1.97	0.62
44:p:115:MET:O	44:p:119:ILE:CD1	2.48	0.62
23:T:109:ARG:NH2	23:T:111:VAL:CG2	2.49	0.61
1:l:2745:G:O6	22:S:3:THR:HG21	2.00	0.61
5:B:60:LEU:CD2	5:B:62:LYS:CG	2.74	0.61
5:B:84:MET:HE1	5:B:180:ILE:HD11	1.82	0.61
35:f:75:ALA:O	35:f:76:TYR:HB2	1.99	0.61
1:l:802:A:OP2	29:Z:111:LEU:HB3	2.01	0.61
19:P:13:LYS:HE3	19:P:17:ARG:NH1	2.14	0.61
1:l:2835:U:P	22:S:57:TYR:OH	2.58	0.61
18:O:138:ALA:O	18:O:139:HIS:HB2	2.01	0.61
44:p:15:HIS:NE2	44:p:18:ILE:HG13	2.16	0.61
22:S:4:SER:O	22:S:10:ARG:NH1	2.34	0.61
12:I:115:MET:O	12:I:116:ARG:HB2	2.00	0.60
18:O:130:LYS:HD3	18:O:146:MET:HE3	1.82	0.60
1:l:3313:U:C4	21:R:169:LYS:HE3	2.33	0.60
1:l:2749:C:O2	22:S:60:ARG:NH2	2.35	0.60
21:R:165:THR:OG1	21:R:170:LYS:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:53:ALA:HA	31:b:56:LYS:HE2	1.82	0.60
29:Z:82:VAL:HG12	29:Z:82:VAL:O	2.01	0.60
1:l:2468:G:H4'	18:O:145:TYR:CE2	2.37	0.60
32:c:71:GLY:O	32:c:72:ILE:HG22	2.02	0.60
44:p:62:ILE:HD13	44:p:118:LEU:HD23	1.82	0.60
14:K:10:ASN:ND2	19:P:167:ARG:NH1	2.50	0.60
44:p:55:HIS:N	44:p:61:CYS:O	2.30	0.60
28:Y:5:LEU:HD11	28:Y:76:VAL:HG23	1.84	0.59
33:d:116:GLN:NE2	44:p:124:SER:HA	2.13	0.59
43:o:42:CYS:SG	43:o:60:CYS:HB2	2.42	0.59
1:l:496:C:C4	29:Z:82:VAL:CG1	2.83	0.59
13:J:161:ILE:HG23	13:J:172:VAL:HG11	1.84	0.59
16:M:103:GLU:OE2	16:M:119:SER:OG	2.13	0.59
35:f:5:LEU:HD23	35:f:32:PHE:CZ	2.38	0.59
5:B:16:PHE:O	5:B:17:LEU:HG	2.02	0.59
44:p:62:ILE:HG12	44:p:118:LEU:HD21	1.84	0.59
29:Z:116:LEU:HD12	29:Z:116:LEU:N	2.18	0.59
19:P:143:LYS:NZ	19:P:143:LYS:HB3	2.18	0.59
21:R:136:ILE:HG23	21:R:140:GLN:HB3	1.84	0.59
33:d:90:HIS:NE2	44:p:34:THR:O	2.30	0.59
43:o:42:CYS:SG	43:o:57:CYS:SG	3.01	0.59
1:l:294:U:O2	16:M:184:ARG:NH1	2.36	0.59
13:J:18:LEU:HD12	13:J:19:THR:H	1.64	0.59
44:p:54:ARG:HD2	44:p:59:ASN:CB	2.32	0.59
1:l:3058:G:N3	5:B:249:ALA:HB1	2.17	0.59
22:S:44:CYS:H	22:S:58:HIS:HD2	1.51	0.59
23:T:57:LYS:CA	23:T:61:LYS:O	2.44	0.59
29:Z:111:LEU:HD23	29:Z:129:SER:HB3	1.85	0.59
23:T:96:LYS:HG2	23:T:105:ARG:NH1	2.18	0.59
28:Y:40:CYS:SG	28:Y:79:LEU:HD12	2.43	0.59
28:Y:5:LEU:O	28:Y:6:LYS:HG2	2.02	0.58
1:l:178:A:C5	1:l:179:A:C5	2.91	0.58
16:M:144:ARG:NH1	36:g:94:ARG:O	2.36	0.58
23:T:26:VAL:HG12	23:T:27:LYS:H	1.68	0.58
28:Y:73:TYR:OH	28:Y:101:MET:HG2	2.03	0.58
1:l:3253:A:OP1	5:B:23:LYS:NZ	2.37	0.58
18:O:142:ILE:C	18:O:143:ASN:HD22	2.12	0.58
1:l:970:G:C8	18:O:138:ALA:CB	2.87	0.58
5:B:93:ILE:HD11	5:B:102:LEU:HG	1.86	0.58
5:B:60:LEU:HD12	5:B:72:ILE:HD11	1.85	0.58
15:L:38:LEU:HD12	21:R:79:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:289:ASN:HB2	6:C:295:ILE:HD11	1.86	0.58
16:M:196:ARG:O	16:M:197:GLN:HG2	2.03	0.58
1:1:3456:U:O2'	1:1:3459:C:OP2	2.22	0.58
18:O:132:ARG:HB3	18:O:132:ARG:CZ	2.33	0.58
28:Y:104:VAL:HG12	28:Y:104:VAL:O	2.03	0.58
22:S:9:ALA:O	22:S:10:ARG:HB2	2.04	0.58
23:T:83:GLU:OE1	23:T:83:GLU:HA	2.03	0.58
28:Y:122:PHE:CE2	28:Y:141:ARG:HA	2.36	0.58
36:g:95:LEU:HB2	36:g:99:GLN:CG	2.31	0.58
5:B:60:LEU:HD21	5:B:62:LYS:CB	2.33	0.57
23:T:29:LYS:HE3	23:T:79:PHE:HB3	1.85	0.57
33:d:77:LEU:HD12	44:p:21:PHE:CD1	2.39	0.57
20:Q:59:ARG:O	20:Q:63:ARG:HG3	2.05	0.57
1:1:3187:C:OP1	32:c:74:ASN:ND2	2.36	0.57
13:J:13:ILE:HD11	13:J:159:ASP:OD2	2.04	0.57
31:b:48:SER:OG	31:b:77:ASN:CA	2.52	0.57
30:a:14:LYS:NZ	30:a:18:ARG:HH12	2.01	0.57
29:Z:47:LYS:O	29:Z:48:TYR:HB2	2.05	0.57
1:1:1949:C:N3	18:O:142:ILE:CD1	2.50	0.57
29:Z:11:ARG:HA	29:Z:11:ARG:NE	2.19	0.57
30:a:6:ASN:OD1	30:a:6:ASN:N	2.37	0.57
40:k:38:ASN:HD22	40:k:38:ASN:C	2.11	0.57
4:A:107:MET:HE2	4:A:166:VAL:HG22	1.87	0.56
9:F:102:ILE:HD11	19:P:2:GLY:C	2.30	0.56
29:Z:79:TRP:HZ2	29:Z:119:ILE:CG2	2.18	0.56
1:1:1436:A:N1	6:C:299:GLU:HA	2.19	0.56
6:C:12:LYS:HG2	6:C:18:ALA:HB2	1.86	0.56
28:Y:40:CYS:SG	28:Y:79:LEU:HD11	2.45	0.56
13:J:14:ARG:HE	13:J:135:PRO:CG	2.12	0.56
23:T:62:CYS:O	23:T:63:ASN:HB2	2.05	0.56
27:X:22:PRO:CG	27:X:25:VAL:HG23	2.35	0.56
28:Y:38:ALA:O	28:Y:76:VAL:HB	2.05	0.56
33:d:7:VAL:O	33:d:8:LYS:HB3	2.05	0.56
1:1:2045:U:H6	20:Q:73:ARG:HH11	1.39	0.56
29:Z:14:HIS:HD2	33:d:38:LYS:CE	2.16	0.56
19:P:143:LYS:HB3	19:P:143:LYS:HZ3	1.71	0.56
31:b:44:LEU:O	31:b:44:LEU:HD12	2.06	0.56
1:1:178:A:C6	1:1:179:A:C5	2.93	0.56
1:1:496:C:C6	29:Z:82:VAL:HG13	2.39	0.56
28:Y:126:VAL:HG22	28:Y:132:LYS:O	2.05	0.56
31:b:13:ILE:HG13	31:b:103:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:38:U:H4'	29:Z:32:ARG:HD2	1.86	0.56
33:d:89:MET:HE3	44:p:114:LYS:CG	2.36	0.56
40:k:42:ARG:HG3	40:k:47:THR:CG2	2.35	0.56
1:1:1578:A:O2'	1:1:1961:A:N3	2.33	0.56
18:O:36:ILE:HD11	18:O:54:LEU:HD21	1.87	0.56
38:i:37:CYS:SG	38:i:40:CYS:SG	3.01	0.56
1:1:2745:G:O6	22:S:3:THR:CG2	2.54	0.56
16:M:68:ARG:NH1	16:M:124:GLN:HE22	2.04	0.56
16:M:68:ARG:CZ	16:M:124:GLN:NE2	2.69	0.56
16:M:68:ARG:HH12	16:M:124:GLN:HE22	1.52	0.56
31:b:44:LEU:CD1	31:b:95:VAL:HB	2.36	0.56
1:1:1642:U:OP1	16:M:67:ARG:HD3	2.06	0.55
11:H:88:GLN:HA	11:H:146:THR:HG22	1.88	0.55
32:c:41:LEU:HD22	32:c:59:ILE:HD12	1.86	0.55
21:R:166:PRO:HD2	21:R:169:LYS:HD2	1.86	0.55
22:S:43:VAL:O	22:S:95:HIS:O	2.24	0.55
29:Z:16:SER:O	29:Z:17:ALA:HB3	2.06	0.55
29:Z:79:TRP:CH2	29:Z:121:VAL:CG1	2.76	0.55
1:1:1436:A:C2	6:C:299:GLU:CB	2.87	0.55
1:1:923:A:OP1	20:Q:83:THR:HG21	2.06	0.55
1:1:2261:A:OP2	4:A:200:ARG:NH1	2.39	0.55
28:Y:79:LEU:N	28:Y:79:LEU:HD23	2.20	0.55
1:1:44:U:H1'	42:n:54:THR:HG23	1.88	0.55
1:1:178:A:N7	1:1:179:A:N7	2.54	0.55
1:1:875:G:OP1	19:P:66:LYS:HD3	2.06	0.55
1:1:3161:C:H5'	5:B:53:MET:O	2.07	0.55
22:S:11:THR:O	22:S:14:LYS:N	2.40	0.55
40:k:38:ASN:ND2	40:k:40:LYS:H	2.04	0.55
1:1:3008:C:H5''	41:l:125:LYS:HD2	1.89	0.55
11:H:127:MET:HE1	11:H:160:ILE:HD11	1.88	0.55
31:b:54:LEU:HD23	31:b:54:LEU:C	2.32	0.55
31:b:44:LEU:HD11	31:b:95:VAL:HG21	1.87	0.55
16:M:122:VAL:HG11	16:M:132:GLU:CG	2.29	0.55
29:Z:115:ASP:OD2	29:Z:116:LEU:N	2.40	0.55
1:1:796:A:C2	29:Z:58:MET:CE	2.90	0.54
7:D:214:LEU:HD21	7:D:221:LYS:HB3	1.90	0.54
21:R:165:THR:HB	21:R:169:LYS:CD	2.36	0.54
22:S:17:LYS:HD3	22:S:47:SER:HB2	1.88	0.54
27:X:22:PRO:CG	27:X:25:VAL:CG2	2.85	0.54
19:P:145:ARG:O	19:P:146:GLU:C	2.48	0.54
29:Z:75:VAL:CG2	29:Z:112:GLY:HA2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:58:ARG:HH21	5:B:353:VAL:HA	1.72	0.54
18:O:132:ARG:HG2	18:O:146:MET:SD	2.47	0.54
1:1:606:G:N3	1:1:606:G:H2'	2.22	0.54
22:S:49:GLN:C	22:S:52:MET:CE	2.53	0.54
28:Y:101:MET:HG3	28:Y:102:ARG:N	2.23	0.54
33:d:86:LEU:HD21	44:p:28:ALA:CA	2.37	0.54
44:p:54:ARG:HD2	44:p:59:ASN:HB3	1.89	0.54
1:1:836:C:H5''	19:P:143:LYS:HG2	1.89	0.54
28:Y:119:TYR:O	28:Y:123:THR:CG2	2.56	0.54
34:e:57:VAL:HG12	34:e:71:VAL:HG12	1.90	0.54
36:g:88:THR:O	36:g:92:ARG:HG3	2.08	0.54
23:T:108:MET:HE2	23:T:122:TYR:OH	2.06	0.54
36:g:93:ARG:O	36:g:94:ARG:HG3	2.08	0.54
13:J:16:GLU:OE2	13:J:137:ASN:ND2	2.41	0.54
21:R:155:LYS:C	21:R:156:LEU:HD12	2.33	0.54
24:U:12:LYS:HG3	24:U:127:LEU:HD11	1.89	0.54
29:Z:46:ASP:O	29:Z:47:LYS:HG2	2.08	0.54
1:1:2497:A:H61	17:N:162:GLN:NE2	2.05	0.54
20:Q:69:LYS:HZ3	20:Q:69:LYS:HB2	1.72	0.53
31:b:39:THR:CG2	31:b:41:LYS:CD	2.87	0.53
31:b:44:LEU:HD12	31:b:95:VAL:HB	1.90	0.53
43:o:57:CYS:SG	43:o:60:CYS:CB	2.94	0.53
1:1:1651:A:O2'	1:1:1652:U:O4'	2.26	0.53
17:N:160:ARG:HG3	17:N:161:GLY:N	2.22	0.53
23:T:107:PHE:C	23:T:108:MET:HG3	2.34	0.53
44:p:55:HIS:O	44:p:59:ASN:HA	2.08	0.53
1:1:2834:U:O3'	22:S:57:TYR:OH	2.27	0.53
1:1:719:C:H5''	17:N:160:ARG:HB3	1.89	0.53
31:b:45:ILE:O	31:b:71:HIS:HA	2.09	0.53
44:p:115:MET:O	44:p:119:ILE:HD11	2.07	0.53
9:F:146:TYR:CE1	9:F:245:ASN:CB	2.92	0.53
22:S:43:VAL:O	22:S:43:VAL:HG13	2.08	0.53
22:S:49:GLN:CB	22:S:52:MET:HE1	2.35	0.53
28:Y:2:VAL:CG1	28:Y:6:LYS:HE3	2.37	0.53
28:Y:101:MET:HE1	28:Y:107:ARG:NE	2.23	0.53
33:d:62:ASN:HB3	33:d:65:THR:HG22	1.89	0.53
44:p:15:HIS:CE1	44:p:18:ILE:HD11	2.43	0.53
1:1:1730:U:O2'	28:Y:78:HIS:CD2	2.62	0.53
5:B:44:THR:HG21	5:B:183:ASN:HD22	1.74	0.53
5:B:248:ILE:HD11	5:B:264:PRO:HG2	1.89	0.53
17:N:82:LEU:HD21	17:N:149:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:3099:C:O2	5:B:265:ARG:NH1	2.41	0.52
5:B:304:ILE:HD11	5:B:322:LEU:HD21	1.90	0.52
12:I:9:TYR:CG	12:I:97:LEU:HD21	2.43	0.52
6:C:134:PRO:HG3	6:C:150:LEU:HD12	1.91	0.52
19:P:9:GLY:HA2	19:P:10:ARG:C	2.34	0.52
28:Y:90:MET:HB3	28:Y:121:LYS:HD2	1.91	0.52
23:T:86:PHE:CE1	23:T:90:TYR:HD2	2.27	0.52
5:B:53:MET:HB3	5:B:77:THR:HA	1.90	0.52
22:S:48:VAL:O	22:S:52:MET:CE	2.52	0.52
32:c:36:ARG:HB2	32:c:72:ILE:O	2.08	0.52
1:1:178:A:C5	1:1:179:A:N7	2.78	0.52
1:1:2663:U:C2'	1:1:2663:U:O2	2.57	0.52
1:1:2888:G:C5	29:Z:60:HIS:CE1	2.97	0.52
21:R:141:CYS:SG	21:R:146:MET:HG3	2.50	0.52
29:Z:79:TRP:HE1	29:Z:117:PRO:CD	2.21	0.52
33:d:9:ARG:CG	33:d:10:SER:N	2.72	0.52
1:1:2001:G:O2'	24:U:20:PRO:HD2	2.10	0.52
15:L:8:TYR:CD1	15:L:59:LEU:HD21	2.44	0.52
19:P:13:LYS:CE	19:P:17:ARG:NH1	2.73	0.52
1:1:970:G:C8	18:O:138:ALA:HB1	2.45	0.52
12:I:60:ILE:HD12	12:I:129:VAL:HG21	1.91	0.52
14:K:15:LYS:HD2	16:M:197:GLN:NE2	2.23	0.52
15:L:21:ASP:OD2	15:L:47:VAL:HG13	2.10	0.52
1:1:1924:A:N3	1:1:1924:A:H2'	2.25	0.52
5:B:60:LEU:CD2	5:B:61:ASP:N	2.73	0.52
13:J:60:ILE:HD13	13:J:66:ILE:HD12	1.91	0.52
18:O:137:ARG:HB2	18:O:141:ARG:HB2	1.92	0.52
27:X:30:MET:HE1	27:X:74:ARG:HA	1.92	0.52
20:Q:114:ILE:HD11	20:Q:141:ILE:HD13	1.92	0.51
23:T:25:PRO:O	23:T:26:VAL:HB	2.10	0.51
23:T:108:MET:HE3	23:T:122:TYR:CZ	2.42	0.51
24:U:95:ILE:HD13	25:V:27:ARG:HB2	1.92	0.51
1:1:995:U:O2'	4:A:12:ARG:NH2	2.43	0.51
5:B:23:LYS:O	5:B:23:LYS:HG3	2.10	0.51
16:M:187:PRO:HD3	16:M:192:CYS:SG	2.45	0.51
23:T:106:ASP:OD1	23:T:106:ASP:N	2.42	0.51
44:p:15:HIS:CE1	44:p:18:ILE:CG1	2.94	0.51
16:M:189:ARG:CA	16:M:189:ARG:NE	2.73	0.51
19:P:9:GLY:HA3	19:P:11:LYS:HG3	1.91	0.51
29:Z:14:HIS:CD2	33:d:38:LYS:CE	2.93	0.51
5:B:305:THR:HG22	5:B:315:THR:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:124:ALA:HB3	9:F:219:PHE:HB2	1.93	0.51
27:X:21:ALA:CB	27:X:26:ARG:NH1	2.73	0.51
43:o:48:LYS:HD2	43:o:58:ARG:NH2	2.25	0.51
23:T:26:VAL:CG1	23:T:27:LYS:N	2.73	0.51
33:d:87:LEU:HD22	33:d:94:PHE:HB2	1.93	0.51
1:1:871:G:C2'	1:1:872:U:H5'	2.41	0.51
1:1:2754:G:C4'	30:a:6:ASN:HD21	2.23	0.51
1:1:2947:C:O4'	1:1:2947:C:O2	2.28	0.51
31:b:39:THR:CG2	31:b:41:LYS:HD2	2.40	0.51
1:1:836:C:P	19:P:141:ALA:CB	2.99	0.51
18:O:145:TYR:O	18:O:146:MET:HG2	2.11	0.51
1:1:85:A:P	29:Z:65:LYS:HE3	2.51	0.51
1:1:802:A:C8	29:Z:113:LYS:HD2	2.45	0.51
15:L:33:ASN:HA	21:R:149:LEU:CD2	2.37	0.51
13:J:17:LYS:HE3	13:J:131:GLN:NE2	2.23	0.50
14:K:63:ARG:CB	29:Z:69:THR:HG21	2.41	0.50
29:Z:119:ILE:O	29:Z:121:VAL:HG13	2.11	0.50
31:b:39:THR:HG21	31:b:41:LYS:CD	2.38	0.50
34:e:14:VAL:HG21	34:e:49:TYR:HE1	1.75	0.50
35:f:76:TYR:O	35:f:80:ARG:HB2	2.10	0.50
1:1:970:G:C8	18:O:138:ALA:HB2	2.46	0.50
1:1:1769:G:OP1	23:T:87:SER:OG	2.29	0.50
5:B:53:MET:HB3	5:B:77:THR:HG22	1.92	0.50
20:Q:83:THR:HG23	20:Q:86:ALA:H	1.75	0.50
31:b:54:LEU:HD21	35:f:90:VAL:HG12	1.92	0.50
1:1:288:C:H4'	16:M:184:ARG:HH21	1.77	0.50
1:1:2729:G:OP1	12:I:116:ARG:CD	2.57	0.50
21:R:165:THR:CB	21:R:169:LYS:HD3	2.37	0.50
1:1:796:A:N3	29:Z:58:MET:CE	2.71	0.50
27:X:55:VAL:HG22	27:X:103:VAL:HG22	1.92	0.50
1:1:1059:C:OP1	30:a:19:ASN:ND2	2.43	0.50
21:R:81:ASN:ND2	21:R:150:PHE:CZ	2.80	0.50
29:Z:132:ALA:O	29:Z:136:ILE:HG13	2.11	0.50
1:1:1468:G:OP1	29:Z:16:SER:HB3	2.10	0.50
35:f:82:HIS:CG	35:f:83:ALA:N	2.79	0.50
9:F:95:LEU:HD11	9:F:124:ALA:HB1	1.93	0.50
16:M:177:THR:HG23	16:M:182:ALA:HB2	1.94	0.50
28:Y:126:VAL:HG13	28:Y:132:LYS:O	2.11	0.50
29:Z:41:MET:O	29:Z:45:TYR:HD2	1.94	0.50
29:Z:84:PRO:CD	29:Z:85:ALA:N	2.73	0.50
3:4:43:G:O6	38:i:68:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:60:LEU:CD2	5:B:62:LYS:HB2	2.41	0.50
1:1:1279:C:N4	1:1:1389:A:OP2	2.45	0.49
28:Y:102:ARG:NH1	28:Y:107:ARG:NH1	2.60	0.49
1:1:1436:A:N1	6:C:299:GLU:CB	2.74	0.49
31:b:39:THR:CG2	31:b:41:LYS:CG	2.86	0.49
31:b:44:LEU:CD1	31:b:44:LEU:C	2.85	0.49
22:S:42:ILE:O	22:S:59:GLY:N	2.41	0.49
1:1:55:G:O2'	16:M:108:ARG:NH1	2.45	0.49
16:M:185:LEU:C	16:M:185:LEU:CD2	2.86	0.49
19:P:92:VAL:HG13	29:Z:87:LEU:HD21	1.92	0.49
21:R:97:MET:CE	21:R:117:MET:HE1	2.43	0.49
30:a:17:HIS:CE1	30:a:21:ILE:HD11	2.47	0.49
1:1:405:A:H4'	1:1:406:A:OP1	2.12	0.49
23:T:30:PHE:O	23:T:31:THR:CG2	2.60	0.49
29:Z:7:LYS:O	29:Z:11:ARG:HB2	2.13	0.49
16:M:122:VAL:CG1	16:M:132:GLU:HG3	2.32	0.49
16:M:185:LEU:HD13	16:M:185:LEU:H	1.77	0.49
26:W:87:VAL:HA	26:W:110:VAL:HG12	1.94	0.49
40:k:37:TYR:O	40:k:37:TYR:HD1	1.95	0.49
18:O:4:TYR:CD2	18:O:16:LYS:HD3	2.47	0.49
9:F:58:THR:HG23	9:F:196:GLU:HG2	1.95	0.49
20:Q:73:ARG:O	20:Q:74:HIS:HB2	2.13	0.49
29:Z:79:TRP:CZ2	29:Z:119:ILE:HG23	2.46	0.49
30:a:17:HIS:CE1	30:a:21:ILE:CD1	2.95	0.49
31:b:48:SER:OG	31:b:77:ASN:N	2.46	0.49
32:c:80:ARG:HG3	32:c:106:VAL:HG21	1.93	0.49
1:1:2505:C:O2'	5:B:265:ARG:NH2	2.46	0.49
11:H:45:ILE:HG23	11:H:54:LEU:HD21	1.95	0.49
28:Y:5:LEU:HD11	28:Y:76:VAL:CG2	2.43	0.49
33:d:120:LEU:C	33:d:120:LEU:CD1	2.85	0.49
41:l:126:LYS:HB3	41:l:126:LYS:HZ2	1.77	0.48
1:1:2911:G:O6	29:Z:42:ARG:NH2	2.46	0.48
5:B:214:ILE:HD12	5:B:281:VAL:CG2	2.43	0.48
36:g:101:ARG:NE	36:g:101:ARG:HA	2.26	0.48
16:M:185:LEU:C	16:M:185:LEU:HD22	2.38	0.48
17:N:139:LEU:HD13	17:N:144:ARG:HG3	1.95	0.48
5:B:60:LEU:HD22	5:B:62:LYS:N	2.28	0.48
10:G:179:GLN:HE22	37:h:43:GLN:HG2	1.78	0.48
14:K:6:ASN:O	29:Z:49:HIS:HE1	1.97	0.48
5:B:214:ILE:HD12	5:B:281:VAL:HG21	1.95	0.48
17:N:81:LEU:HD11	17:N:195:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:11:GLU:C	18:O:13:LYS:N	2.72	0.48
21:R:167:LYS:CG	34:e:42:ASP:OD1	2.61	0.48
23:T:54:THR:HA	23:T:63:ASN:HD22	1.77	0.48
1:1:180:G:C2'	1:1:181:C:C6	2.96	0.48
1:1:1592:U:H5	1:1:1938:A:N1	2.11	0.48
5:B:60:LEU:CD2	5:B:62:LYS:CB	2.91	0.48
11:H:34:ILE:HD11	11:H:148:THR:HB	1.96	0.48
15:L:8:TYR:CE1	15:L:59:LEU:HD21	2.49	0.48
18:O:4:TYR:CE2	18:O:16:LYS:CD	2.91	0.48
31:b:43:LYS:HE3	31:b:43:LYS:HA	1.94	0.48
24:U:15:VAL:HG13	24:U:87:TRP:CD1	2.49	0.48
28:Y:74:ILE:CG2	28:Y:79:LEU:CD2	2.85	0.48
44:p:54:ARG:CD	44:p:59:ASN:CB	2.85	0.48
28:Y:5:LEU:CD1	28:Y:76:VAL:CG2	2.90	0.48
1:1:2663:U:O2	1:1:2663:U:H2'	2.12	0.48
5:B:60:LEU:HD21	5:B:62:LYS:HG2	1.90	0.48
16:M:169:GLY:HA2	16:M:172:TYR:CE2	2.49	0.48
27:X:18:HIS:O	27:X:21:ALA:HB2	2.14	0.48
44:p:115:MET:O	44:p:119:ILE:HG12	2.14	0.48
1:1:2264:G:H4'	43:o:22:LEU:HD21	1.96	0.48
15:L:5:THR:HG22	15:L:6:ARG:N	2.29	0.47
24:U:56:LEU:HD21	24:U:121:GLY:HA3	1.96	0.47
1:1:2957:U:O2	1:1:2957:U:O4'	2.30	0.47
28:Y:101:MET:CG	28:Y:102:ARG:H	2.24	0.47
36:g:101:ARG:NE	36:g:101:ARG:CA	2.76	0.47
40:k:38:ASN:C	40:k:38:ASN:ND2	2.72	0.47
1:1:158:U:OP2	36:g:106:ARG:NH2	2.48	0.47
1:1:1710:A:OP2	1:1:1924:A:N6	2.47	0.47
22:S:21:ARG:HG3	22:S:21:ARG:NH1	2.26	0.47
23:T:26:VAL:CG1	23:T:27:LYS:H	2.27	0.47
28:Y:4:LEU:HD12	28:Y:81:PRO:HG2	1.96	0.47
32:c:41:LEU:HD21	32:c:67:ILE:HD12	1.96	0.47
33:d:119:VAL:O	33:d:119:VAL:HG13	2.14	0.47
1:1:2925:G:P	6:C:75:ARG:HH22	2.37	0.47
13:J:17:LYS:CE	13:J:131:GLN:HE22	2.21	0.47
18:O:132:ARG:HH11	18:O:132:ARG:CB	2.24	0.47
31:b:47:ILE:HG22	31:b:92:CYS:SG	2.54	0.47
21:R:136:ILE:HG22	21:R:137:LYS:O	2.14	0.47
23:T:108:MET:CE	23:T:122:TYR:CE1	2.90	0.47
28:Y:95:MET:HE3	28:Y:114:LEU:CD2	2.44	0.47
1:1:89:A:N7	19:P:172:LYS:NZ	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2045:U:C5	20:Q:73:ARG:CZ	2.92	0.47
5:B:26:ARG:HD2	5:B:47:MET:HE1	1.97	0.47
11:H:93:PHE:CE1	11:H:178:ILE:HD12	2.49	0.47
24:U:21:VAL:HG13	24:U:22:GLY:N	2.29	0.47
24:U:24:LEU:HD11	24:U:35:ASN:HB3	1.96	0.47
28:Y:24:VAL:HG12	28:Y:25:VAL:O	2.15	0.47
33:d:89:MET:HE3	44:p:114:LYS:HG3	1.97	0.47
44:p:15:HIS:CE1	44:p:18:ILE:CD1	2.98	0.47
1:1:889:G:P	29:Z:32:ARG:NH1	2.88	0.47
8:E:73:THR:OG1	8:E:83:LEU:HD23	2.13	0.47
17:N:154:LEU:CD1	17:N:165:LEU:HD21	2.44	0.47
23:T:30:PHE:C	23:T:31:THR:HG23	2.39	0.47
27:X:21:ALA:HB3	27:X:26:ARG:CZ	2.44	0.47
28:Y:100:ALA:HB1	28:Y:106:ASP:OD1	2.12	0.47
10:G:174:VAL:HG13	10:G:177:ILE:HD12	1.96	0.47
21:R:152:SER:O	21:R:153:LYS:HB2	2.14	0.47
22:S:11:THR:OG1	22:S:15:PHE:CG	2.67	0.47
1:1:180:G:C6	1:1:245:U:C4	3.03	0.47
1:1:1462:U:O2'	19:P:10:ARG:HD3	2.14	0.47
15:L:12:ARG:HD2	15:L:59:LEU:HD22	1.97	0.47
18:O:11:GLU:C	18:O:13:LYS:H	2.22	0.47
21:R:167:LYS:CD	34:e:42:ASP:OD1	2.62	0.47
25:V:39:ILE:HD12	25:V:40:HIS:CD2	2.50	0.47
28:Y:98:GLU:OE1	28:Y:99:ASP:N	2.48	0.47
28:Y:103:THR:O	28:Y:104:VAL:HB	2.14	0.47
33:d:86:LEU:CD2	44:p:28:ALA:HA	2.42	0.47
1:1:3010:C:O2'	1:1:3012:G:OP2	2.33	0.46
7:D:104:LEU:HD23	7:D:250:ILE:HG23	1.97	0.46
19:P:7:ARG:C	19:P:8:ASN:ND2	2.73	0.46
20:Q:16:CYS:HB3	20:Q:51:ARG:HD3	1.96	0.46
38:i:29:ALA:HB1	38:i:38:GLY:H	1.80	0.46
1:1:874:G:H5'	1:1:875:G:OP1	2.15	0.46
1:1:2745:G:O3'	12:I:15:LYS:NZ	2.48	0.46
1:1:3281:G:C2	1:1:3367:A:C2	3.02	0.46
17:N:120:TYR:CE2	17:N:211:VAL:HG11	2.50	0.46
22:S:9:ALA:CB	22:S:10:ARG:HH11	2.28	0.46
1:1:1168:C:O2	7:D:115:MET:HE1	2.15	0.46
4:A:30:ARG:O	4:A:163:ARG:NH2	2.49	0.46
42:n:47:GLN:HE21	42:n:53:GLN:HB2	1.80	0.46
1:1:796:A:H2	29:Z:58:MET:HE1	1.80	0.46
1:1:1858:C:H5''	23:T:109:ARG:HH22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:82:MET:HE1	4:A:165:MET:HE1	1.97	0.46
29:Z:78:LEU:O	29:Z:81:LEU:CB	2.58	0.46
1:1:376:G:O2'	40:k:34:LYS:NZ	2.44	0.46
1:1:796:A:C2	29:Z:58:MET:HE3	2.51	0.46
1:1:970:G:N7	18:O:138:ALA:HB1	2.29	0.46
1:1:1069:G:N3	1:1:1069:G:H2'	2.31	0.46
28:Y:82:THR:HG22	28:Y:84:TYR:H	1.81	0.46
28:Y:101:MET:CG	28:Y:102:ARG:N	2.78	0.46
21:R:84:VAL:HG11	21:R:113:LEU:CD2	2.46	0.46
1:1:836:C:H5''	19:P:143:LYS:CG	2.45	0.46
4:A:201:GLY:HA3	4:A:209:HIS:CD2	2.51	0.46
18:O:11:GLU:O	18:O:13:LYS:N	2.36	0.46
29:Z:121:VAL:O	29:Z:141:GLY:HA2	2.16	0.46
1:1:25:U:OP1	38:i:61:THR:HG21	2.15	0.46
15:L:5:THR:O	15:L:6:ARG:HB2	2.16	0.46
7:D:147:VAL:HG12	7:D:158:VAL:HG11	1.96	0.46
16:M:189:ARG:NE	16:M:189:ARG:O	2.48	0.46
1:1:115:A:H3'	1:1:116:A:C5'	2.46	0.45
3:4:57:C:OP1	38:i:71:LYS:HE2	2.16	0.45
5:B:60:LEU:HD21	5:B:62:LYS:HB2	1.97	0.45
10:G:36:LYS:HA	10:G:39:ILE:HD12	1.98	0.45
16:M:80:VAL:HG21	16:M:87:GLN:HA	1.98	0.45
20:Q:129:ASN:O	20:Q:131:PHE:N	2.49	0.45
10:G:84:VAL:HA	10:G:85:PRO:HD3	1.80	0.45
18:O:135:THR:OG1	18:O:145:TYR:CE1	2.46	0.45
24:U:15:VAL:HG13	24:U:87:TRP:CG	2.51	0.45
3:4:57:C:P	38:i:71:LYS:HE2	2.57	0.45
13:J:14:ARG:CD	13:J:135:PRO:HD3	2.47	0.45
32:c:41:LEU:HD22	32:c:59:ILE:CD1	2.47	0.45
28:Y:8:GLY:O	28:Y:85:THR:OG1	2.31	0.45
33:d:91:ASN:H	33:d:91:ASN:HD22	1.63	0.45
43:o:11:VAL:HG12	43:o:11:VAL:O	2.16	0.45
1:1:1919:U:H2'	1:1:1919:U:O2	2.17	0.45
1:1:3161:C:C4'	5:B:53:MET:O	2.65	0.45
21:R:81:ASN:HD21	21:R:150:PHE:HE1	1.65	0.45
7:D:214:LEU:HD21	7:D:221:LYS:CB	2.47	0.45
21:R:45:VAL:HG13	21:R:65:ILE:CD1	2.47	0.45
28:Y:122:PHE:HD2	28:Y:141:ARG:CD	2.21	0.45
11:H:127:MET:HE3	11:H:145:LEU:HD11	1.97	0.45
31:b:44:LEU:HD11	31:b:95:VAL:HG23	1.94	0.45
32:c:100:LEU:HD12	32:c:100:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:95:ALA:HB1	33:d:120:LEU:HD12	1.98	0.45
40:k:44:TRP:CZ3	40:k:45:ARG:HG2	2.52	0.45
1:1:3101:G:P	5:B:18:PRO:HB2	2.57	0.45
5:B:60:LEU:CD2	5:B:62:LYS:HG2	2.47	0.45
6:C:211:VAL:HG12	6:C:233:VAL:HG22	1.99	0.45
16:M:189:ARG:HE	16:M:189:ARG:C	2.25	0.45
22:S:11:THR:HG23	22:S:12:ARG:N	2.32	0.45
28:Y:86:VAL:CG1	28:Y:90:MET:HE3	2.47	0.45
29:Z:84:PRO:HD2	29:Z:85:ALA:N	2.23	0.45
33:d:43:ARG:CD	33:d:51:THR:HG21	2.45	0.45
1:1:496:C:C4	29:Z:82:VAL:HG22	2.51	0.45
1:1:3161:C:O2'	5:B:55:HIS:CD2	2.65	0.45
1:1:1480:G:OP2	6:C:191:ARG:NH2	2.49	0.45
1:1:2742:U:OP1	22:S:6:GLY:HA3	2.16	0.45
33:d:91:ASN:HD22	33:d:91:ASN:N	2.15	0.45
35:f:81:CYS:O	35:f:82:HIS:CG	2.70	0.45
1:1:180:G:O2'	1:1:181:C:O4'	2.35	0.44
19:P:89:ILE:HG12	29:Z:80:SER:HB2	1.99	0.44
20:Q:3:LEU:O	20:Q:5:LEU:N	2.50	0.44
26:W:107:VAL:HG22	26:W:147:TYR:CD1	2.53	0.44
38:i:57:LYS:O	38:i:61:THR:HG23	2.17	0.44
1:1:2728:U:OP1	30:a:3:LYS:HB3	2.17	0.44
3:4:75:G:O4'	40:k:30:ARG:HA	2.17	0.44
22:S:9:ALA:HB1	22:S:10:ARG:HH11	1.82	0.44
23:T:107:PHE:H	23:T:107:PHE:HD2	1.65	0.44
29:Z:59:ARG:H	29:Z:59:ARG:HG2	1.56	0.44
10:G:201:VAL:HG21	10:G:209:LEU:HD21	1.98	0.44
1:1:842:A:H61	1:1:872:U:H3	1.66	0.44
1:1:1136:A:N3	1:1:2744:U:O2'	2.50	0.44
5:B:55:HIS:CD2	5:B:55:HIS:H	2.35	0.44
28:Y:3:LYS:HA	31:b:38:ARG:O	2.17	0.44
29:Z:79:TRP:CH2	29:Z:119:ILE:HG21	2.53	0.44
30:a:13:ASN:O	30:a:17:HIS:HD2	2.00	0.44
38:i:38:GLY:O	38:i:48:ARG:NE	2.50	0.44
1:1:2786:C:N4	13:J:23:CYS:SG	2.91	0.44
29:Z:79:TRP:CH2	29:Z:119:ILE:CG2	3.01	0.44
36:g:94:ARG:C	36:g:95:LEU:HD13	2.42	0.44
38:i:72:ASP:CG	38:i:75:ARG:NH1	2.75	0.44
5:B:44:THR:HG21	5:B:183:ASN:ND2	2.33	0.44
12:I:9:TYR:CD2	12:I:97:LEU:HD21	2.53	0.44
23:T:96:LYS:HG2	23:T:105:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:107:PHE:CD2	23:T:107:PHE:N	2.84	0.44
35:f:81:CYS:SG	35:f:83:ALA:HB3	2.57	0.44
1:1:1221:G:O2'	1:1:2753:A:N3	2.43	0.44
16:M:114:LEU:HB2	16:M:135:LEU:HD23	1.99	0.44
16:M:114:LEU:CB	16:M:135:LEU:HD23	2.48	0.44
20:Q:96:ARG:O	20:Q:100:VAL:HG23	2.18	0.44
40:k:23:ILE:CG2	40:k:38:ASN:HB2	2.48	0.44
5:B:256:PRO:HG2	5:B:260:GLN:HE21	1.83	0.44
23:T:108:MET:HG2	23:T:121:ARG:O	2.18	0.44
40:k:37:TYR:O	40:k:37:TYR:CD1	2.70	0.44
10:G:93:HIS:CD2	10:G:239:VAL:HG11	2.52	0.44
18:O:145:TYR:C	18:O:146:MET:HG2	2.43	0.44
33:d:120:LEU:HD13	33:d:121:VAL:N	2.32	0.44
36:g:21:LEU:HD22	36:g:21:LEU:O	2.18	0.44
4:A:102:LEU:HB2	4:A:107:MET:HE3	2.00	0.43
11:H:93:PHE:CZ	11:H:143:ILE:HG13	2.53	0.43
33:d:97:GLU:OE1	33:d:122:LEU:HD23	2.17	0.43
3:4:104:A:C8	3:4:105:A:C8	3.06	0.43
28:Y:102:ARG:NH1	28:Y:107:ARG:CZ	2.73	0.43
33:d:8:LYS:HA	33:d:8:LYS:HD2	1.81	0.43
1:1:1906:G:HO2'	35:f:78:GLY:HA3	1.72	0.43
7:D:122:VAL:HG21	7:D:129:TYR:CG	2.53	0.43
11:H:89:TYR:CZ	11:H:183:THR:HG22	2.53	0.43
23:T:27:LYS:HE3	23:T:81:THR:CG2	2.48	0.43
34:e:37:LEU:CD2	34:e:105:VAL:HG21	2.48	0.43
1:1:1651:A:O2'	1:1:1652:U:O5'	2.33	0.43
1:1:3100:U:H2'	1:1:3101:G:O4'	2.18	0.43
22:S:52:MET:HB3	22:S:95:HIS:NE2	2.32	0.43
22:S:80:VAL:HG23	22:S:80:VAL:O	2.18	0.43
26:W:109:LEU:HD23	26:W:109:LEU:HA	1.92	0.43
33:d:91:ASN:ND2	44:p:117:LYS:NZ	2.65	0.43
12:I:89:ILE:HD13	12:I:136:MET:HG2	1.99	0.43
15:L:89:ASN:HD21	15:L:98:LEU:HD11	1.83	0.43
9:F:94:ILE:HD12	9:F:146:TYR:CD1	2.54	0.43
22:S:5:PHE:CD2	22:S:5:PHE:N	2.86	0.43
1:1:871:G:H2'	1:1:872:U:H5'	1.99	0.43
1:1:2634:U:OP1	4:A:123:ARG:NH1	2.52	0.43
1:1:1825:G:C2'	1:1:1825:G:N3	2.81	0.43
20:Q:69:LYS:HB2	20:Q:69:LYS:NZ	2.32	0.43
1:1:178:A:C4	1:1:179:A:C8	3.07	0.43
1:1:1695:U:OP2	20:Q:41:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:146:TYR:CE1	9:F:245:ASN:HB2	2.53	0.43
18:O:11:GLU:O	18:O:12:ASN:HB2	2.19	0.43
29:Z:37:GLY:HA2	29:Z:45:TYR:CE2	2.54	0.43
1:1:796:A:C2	29:Z:58:MET:HE1	2.54	0.43
1:1:3319:U:O3'	8:E:178:THR:HG22	2.19	0.43
10:G:63:VAL:HG21	26:W:44:ARG:HD2	2.01	0.43
21:R:150:PHE:O	21:R:151:ASP:HB3	2.19	0.43
24:U:12:LYS:HG3	24:U:127:LEU:CD2	2.45	0.43
4:A:104:LEU:CD1	4:A:148:ILE:HD11	2.49	0.42
5:B:53:MET:HB3	5:B:77:THR:CG2	2.48	0.42
5:B:56:VAL:HG23	5:B:358:ILE:HA	2.00	0.42
16:M:187:PRO:O	16:M:188:SER:OG	2.36	0.42
19:P:17:ARG:C	19:P:18:THR:HG23	2.44	0.42
24:U:19:LEU:HD21	24:U:100:ASN:OD1	2.17	0.42
32:c:75:VAL:CG1	32:c:76:PRO:HD2	2.49	0.42
6:C:390:MET:HE2	21:R:134:ALA:CB	2.49	0.42
16:M:103:GLU:OE2	16:M:119:SER:CB	2.66	0.42
22:S:49:GLN:CB	22:S:52:MET:CE	2.89	0.42
29:Z:75:VAL:HB	29:Z:112:GLY:HA2	2.01	0.42
6:C:54:VAL:HG21	6:C:101:MET:CE	2.47	0.42
19:P:145:ARG:NH1	19:P:147:ALA:HB3	2.34	0.42
15:L:8:TYR:O	15:L:31:ILE:HD11	2.18	0.42
19:P:9:GLY:HA2	19:P:10:ARG:CB	2.49	0.42
19:P:98:THR:HG23	19:P:118:GLU:HB3	2.01	0.42
22:S:17:LYS:HG2	22:S:46:PRO:HG2	2.02	0.42
29:Z:62:HIS:CG	29:Z:62:HIS:O	2.70	0.42
38:i:39:ALA:O	38:i:48:ARG:HB3	2.18	0.42
16:M:65:ARG:HD2	16:M:128:TYR:CD1	2.55	0.42
36:g:81:ASN:OD1	36:g:81:ASN:N	2.53	0.42
1:1:322:C:OP2	37:h:25:ARG:NH2	2.50	0.42
10:G:194:LYS:HE3	10:G:205:ASN:ND2	2.35	0.42
22:S:57:TYR:HA	22:S:60:ARG:HG3	2.01	0.42
30:a:5:LYS:HB3	30:a:5:LYS:HE2	1.65	0.42
33:d:37:PRO:HG2	33:d:44:VAL:HB	2.01	0.42
1:1:85:A:OP2	29:Z:65:LYS:CE	2.51	0.42
1:1:1005:A:N3	1:1:1005:A:H2'	2.35	0.42
18:O:22:LEU:N	18:O:22:LEU:CD2	2.73	0.42
26:W:63:VAL:HG21	36:g:78:PHE:CB	2.49	0.42
1:1:1268:U:H3'	21:R:170:LYS:NZ	2.34	0.42
19:P:89:ILE:HG12	29:Z:80:SER:CB	2.50	0.42
29:Z:118:LYS:HE3	29:Z:118:LYS:HB3	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:54:LEU:C	31:b:54:LEU:CD2	2.93	0.42
1:1:475:A:H3'	1:1:476:U:H5''	2.02	0.42
1:1:2496:C:OP2	17:N:151:ARG:NH2	2.53	0.42
1:1:2741:C:P	22:S:5:PHE:O	2.77	0.42
13:J:8:ASN:N	13:J:9:PRO:HD2	2.34	0.42
24:U:15:VAL:HB	24:U:55:SER:HB2	2.00	0.42
36:g:14:GLN:O	36:g:18:VAL:HG23	2.20	0.42
1:1:1265:A:N3	1:1:1415:C:O2'	2.53	0.42
4:A:148:ILE:HD12	4:A:158:VAL:HG21	2.02	0.42
10:G:208:VAL:O	10:G:208:VAL:HG23	2.20	0.42
19:P:145:ARG:O	19:P:147:ALA:N	2.53	0.42
22:S:43:VAL:HG11	22:S:97:ARG:HH11	1.84	0.42
33:d:98:ILE:HG12	33:d:110:ILE:HG21	2.00	0.42
33:d:120:LEU:HD22	33:d:121:VAL:N	2.34	0.42
36:g:93:ARG:O	36:g:94:ARG:CB	2.68	0.42
1:1:3102:A:OP1	5:B:20:LYS:HB2	2.20	0.41
13:J:60:ILE:HD13	13:J:66:ILE:CD1	2.50	0.41
17:N:192:ILE:O	21:R:160:ARG:NH2	2.53	0.41
22:S:11:THR:CG2	22:S:12:ARG:N	2.83	0.41
1:1:872:U:C2'	1:1:873:U:C6	2.97	0.41
1:1:872:U:C2'	1:1:873:U:H6	2.27	0.41
3:4:79:A:H3'	3:4:80:A:H4'	2.02	0.41
5:B:13:SER:OG	5:B:16:PHE:HD2	2.03	0.41
15:L:55:ARG:NH1	21:R:164:PRO:HB3	2.35	0.41
18:O:17:ALA:HB3	18:O:100:LEU:HD23	2.01	0.41
43:o:38:SER:HA	43:o:45:MET:HA	2.02	0.41
44:p:119:ILE:N	44:p:119:ILE:HD13	2.35	0.41
1:1:872:U:H2'	1:1:873:U:C5	2.52	0.41
8:E:47:ILE:HG22	8:E:57:ARG:HG2	2.02	0.41
13:J:18:LEU:HD12	13:J:129:TYR:O	2.21	0.41
19:P:171:ARG:O	19:P:172:LYS:CB	2.68	0.41
23:T:29:LYS:HG3	23:T:81:THR:OG1	2.20	0.41
1:1:825:C:O2'	1:1:826:A:O5'	2.38	0.41
15:L:18:TYR:CG	15:L:19:GLY:N	2.87	0.41
18:O:21:ASP:OD2	18:O:149:PRO:CB	2.66	0.41
21:R:150:PHE:O	21:R:151:ASP:CB	2.69	0.41
29:Z:12:ARG:CG	29:Z:12:ARG:NH1	2.72	0.41
31:b:43:LYS:HG2	31:b:96:THR:O	2.19	0.41
1:1:3058:G:C2	5:B:249:ALA:HB1	2.56	0.41
5:B:55:HIS:HE1	25:V:22:PRO:O	2.02	0.41
8:E:49:LEU:HD11	8:E:92:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:81:ILE:HD11	27:X:98:ILE:HD11	2.03	0.41
28:Y:11:VAL:HG22	28:Y:23:GLY:O	2.21	0.41
29:Z:13:GLY:O	33:d:38:LYS:HD2	2.20	0.41
29:Z:59:ARG:HH21	42:n:38:GLN:HG2	1.84	0.41
1:1:1730:U:O2'	28:Y:78:HIS:HD2	2.02	0.41
21:R:19:ARG:HB3	21:R:31:LEU:HD23	2.02	0.41
43:o:48:LYS:HD2	43:o:58:ARG:CZ	2.51	0.41
1:1:180:G:O2'	1:1:181:C:C5'	2.69	0.41
1:1:581:U:O2	1:1:581:U:O4'	2.37	0.41
1:1:761:G:OP1	6:C:33:ARG:NH2	2.53	0.41
1:1:1825:G:N3	1:1:1825:G:H2'	2.35	0.41
16:M:127:VAL:HG23	16:M:128:TYR:CE2	2.51	0.41
19:P:13:LYS:HD3	19:P:17:ARG:NH2	2.36	0.41
1:1:178:A:H2'	1:1:179:A:O4'	2.20	0.41
5:B:260:GLN:O	5:B:263:VAL:HG12	2.21	0.41
1:1:311:G:C2	1:1:321:A:C2	3.09	0.41
1:1:1435:U:OP1	19:P:38:ARG:NH1	2.53	0.41
12:I:76:MET:HE3	12:I:138:ILE:HD13	2.03	0.41
13:J:18:LEU:HD12	13:J:18:LEU:C	2.41	0.41
14:K:63:ARG:HB3	29:Z:69:THR:HG21	2.02	0.41
21:R:81:ASN:ND2	21:R:150:PHE:CE1	2.88	0.41
1:1:344:A:O2'	6:C:50:GLN:NE2	2.54	0.41
5:B:255:HIS:HA	5:B:256:PRO:C	2.45	0.41
23:T:87:SER:O	23:T:88:LYS:C	2.62	0.41
35:f:80:ARG:HD3	35:f:80:ARG:HA	1.60	0.41
43:o:79:VAL:HA	43:o:82:THR:HG22	2.02	0.41
13:J:111:ILE:HD13	13:J:123:ILE:HD12	2.03	0.40
23:T:102:GLN:C	23:T:104:LEU:CD2	2.94	0.40
33:d:117:LEU:O	33:d:118:ASN:HB2	2.21	0.40
1:1:873:U:O2'	1:1:874:G:P	2.79	0.40
1:1:1641:U:O2'	1:1:2281:A:N3	2.49	0.40
1:1:3219:U:OP1	41:l:114:LYS:NZ	2.47	0.40
4:A:104:LEU:HD13	4:A:148:ILE:HD11	2.02	0.40
15:L:6:ARG:NH2	21:R:183:HIS:C	2.79	0.40
17:N:103:ARG:HG3	17:N:174:VAL:CG2	2.52	0.40
17:N:158:VAL:CG1	17:N:159:GLU:N	2.84	0.40
22:S:11:THR:OG1	22:S:15:PHE:HB2	2.22	0.40
24:U:59:LEU:HD12	24:U:78:ALA:O	2.21	0.40
31:b:44:LEU:CD1	31:b:95:VAL:CG2	2.91	0.40
33:d:89:MET:HE3	44:p:114:LYS:CB	2.49	0.40
35:f:23:VAL:HG21	35:f:33:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:i:37:CYS:HB3	38:i:41:GLY:H	1.86	0.40
19:P:9:GLY:CA	19:P:10:ARG:C	2.94	0.40
40:k:37:TYR:CD1	40:k:37:TYR:C	3.00	0.40
1:l:1216:A:H5''	12:I:13:LYS:HZ2	1.87	0.40
14:K:50:SER:OG	14:K:51:GLY:N	2.55	0.40
1:l:1460:A:O2'	9:F:173:SER:O	2.31	0.40
1:l:1924:A:N3	1:l:1924:A:C2'	2.85	0.40
1:l:2753:A:O2'	30:a:6:ASN:ND2	2.55	0.40
1:l:2868:U:C5'	22:S:7:LYS:CE	2.97	0.40
23:T:30:PHE:C	23:T:31:THR:CG2	2.95	0.40
24:U:12:LYS:CG	24:U:127:LEU:HD21	2.47	0.40
27:X:21:ALA:HB1	27:X:26:ARG:HG3	2.03	0.40
28:Y:102:ARG:HD3	28:Y:107:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	244/260 (94%)	228 (93%)	15 (6%)	1 (0%)	30	60
5	B	351/389 (90%)	312 (89%)	33 (9%)	6 (2%)	7	32
6	C	380/416 (91%)	345 (91%)	30 (8%)	5 (1%)	9	38
7	D	253/310 (82%)	225 (89%)	24 (10%)	4 (2%)	7	34
8	E	114/193 (59%)	101 (89%)	12 (10%)	1 (1%)	14	45
9	F	246/258 (95%)	226 (92%)	19 (8%)	1 (0%)	30	60
10	G	225/276 (82%)	209 (93%)	12 (5%)	4 (2%)	6	31
11	H	185/190 (97%)	169 (91%)	16 (9%)	0	100	100
12	I	185/221 (84%)	168 (91%)	15 (8%)	2 (1%)	11	41
13	J	164/175 (94%)	145 (88%)	16 (10%)	3 (2%)	6	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	K	193/355 (54%)	167 (86%)	20 (10%)	6 (3%)	3	19
15	L	129/134 (96%)	118 (92%)	8 (6%)	3 (2%)	5	26
16	M	196/205 (96%)	180 (92%)	15 (8%)	1 (0%)	24	57
17	N	196/269 (73%)	187 (95%)	6 (3%)	3 (2%)	8	35
18	O	154/195 (79%)	140 (91%)	13 (8%)	1 (1%)	21	53
19	P	184/187 (98%)	172 (94%)	10 (5%)	2 (1%)	11	41
20	Q	174/187 (93%)	165 (95%)	7 (4%)	2 (1%)	11	41
21	R	180/183 (98%)	159 (88%)	16 (9%)	5 (3%)	4	22
22	S	152/157 (97%)	141 (93%)	6 (4%)	5 (3%)	3	18
23	T	95/133 (71%)	85 (90%)	7 (7%)	3 (3%)	3	19
24	U	127/139 (91%)	117 (92%)	10 (8%)	0	100	100
25	V	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
26	W	125/167 (75%)	107 (86%)	16 (13%)	2 (2%)	7	34
27	X	122/141 (86%)	111 (91%)	10 (8%)	1 (1%)	16	47
28	Y	140/146 (96%)	123 (88%)	11 (8%)	6 (4%)	2	14
29	Z	141/147 (96%)	126 (89%)	11 (8%)	4 (3%)	4	22
30	a	45/54 (83%)	42 (93%)	1 (2%)	2 (4%)	2	13
31	b	92/108 (85%)	83 (90%)	9 (10%)	0	100	100
32	c	103/120 (86%)	93 (90%)	7 (7%)	3 (3%)	3	21
33	d	120/134 (90%)	111 (92%)	6 (5%)	3 (2%)	4	24
34	e	101/112 (90%)	94 (93%)	6 (6%)	1 (1%)	12	43
35	f	105/134 (78%)	98 (93%)	6 (6%)	1 (1%)	12	43
36	g	119/123 (97%)	113 (95%)	4 (3%)	2 (2%)	7	32
37	h	93/101 (92%)	89 (96%)	2 (2%)	2 (2%)	5	26
38	i	81/98 (83%)	77 (95%)	3 (4%)	1 (1%)	10	39
39	j	68/84 (81%)	63 (93%)	4 (6%)	1 (2%)	8	35
40	k	47/51 (92%)	45 (96%)	1 (2%)	1 (2%)	5	27
41	l	50/129 (39%)	48 (96%)	1 (2%)	1 (2%)	6	28
42	n	95/105 (90%)	86 (90%)	7 (7%)	2 (2%)	5	27
43	o	88/96 (92%)	82 (93%)	5 (6%)	1 (1%)	11	41
44	p	118/129 (92%)	107 (91%)	10 (8%)	1 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6041/7166 (84%)	5517 (91%)	431 (7%)	93 (2%)	11	35

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	5	LYS
6	C	191	ARG
7	D	156	ASN
14	K	60	PRO
20	Q	130	GLN
21	R	151	ASP
22	S	12	ARG
23	T	26	VAL
28	Y	104	VAL
32	c	72	ILE
33	d	124	ARG
36	g	94	ARG
40	k	37	TYR
44	p	44	ILE
5	B	30	LYS
5	B	38	SER
12	I	144	ASN
13	J	115	ILE
14	K	74	PHE
14	K	154	LYS
14	K	155	ILE
15	L	22	ALA
16	M	197	GLN
17	N	176	THR
19	P	146	GLU
21	R	168	ASP
22	S	120	HIS
22	S	124	GLU
23	T	75	LYS
28	Y	8	GLY
29	Z	77	LYS
29	Z	78	LEU
30	a	4	SER
32	c	111	ASN
38	i	28	ARG
43	o	13	LYS
6	C	85	HIS

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Mol	Chain	Res	Type
7	D	20	TYR
7	D	21	ARG
7	D	44	TYR
13	J	119	PRO
15	L	8	TYR
17	N	198	LYS
20	Q	128	GLY
21	R	31	LEU
27	X	21	ALA
29	Z	47	LYS
29	Z	66	ASN
30	a	29	LYS
32	c	94	LYS
36	g	84	ARG
42	n	95	ALA
4	A	3	ARG
6	C	57	ASN
6	C	133	LEU
10	G	157	LYS
10	G	168	VAL
10	G	208	VAL
13	J	56	ARG
15	L	36	ARG
18	O	3	LYS
19	P	154	ALA
21	R	140	GLN
26	W	62	LYS
28	Y	35	ARG
28	Y	129	LYS
28	Y	134	SER
33	d	9	ARG
35	f	68	ARG
37	h	62	THR
41	l	79	GLU
5	B	24	ARG
5	B	186	SER
5	B	316	VAL
6	C	323	LEU
14	K	145	SER
21	R	177	LYS
22	S	68	THR
23	T	41	ASN

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Mol	Chain	Res	Type
26	W	141	ASP
28	Y	89	ASP
33	d	10	SER
39	j	76	GLU
34	e	10	VAL
37	h	18	ALA
22	S	81	GLY
10	G	132	GLY
14	K	51	GLY
17	N	175	PRO
42	n	36	VAL
9	F	237	GLU
12	I	196	GLY
8	E	184	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	190/200 (95%)	182 (96%)	8 (4%)	26	56
5	B	315/330 (96%)	300 (95%)	15 (5%)	23	53
6	C	313/326 (96%)	302 (96%)	11 (4%)	32	61
7	D	218/253 (86%)	213 (98%)	5 (2%)	44	68
8	E	110/163 (68%)	106 (96%)	4 (4%)	31	60
9	F	216/223 (97%)	208 (96%)	8 (4%)	30	59
10	G	204/233 (88%)	196 (96%)	8 (4%)	28	58
11	H	167/169 (99%)	159 (95%)	8 (5%)	23	53
12	I	159/180 (88%)	154 (97%)	5 (3%)	35	62
13	J	141/151 (93%)	137 (97%)	4 (3%)	38	64
14	K	170/303 (56%)	160 (94%)	10 (6%)	18	47
15	L	116/118 (98%)	109 (94%)	7 (6%)	17	46
16	M	171/176 (97%)	159 (93%)	12 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	178/240 (74%)	175 (98%)	3 (2%)	53	72
18	O	139/168 (83%)	130 (94%)	9 (6%)	15	44
19	P	154/155 (99%)	145 (94%)	9 (6%)	18	47
20	Q	154/162 (95%)	153 (99%)	1 (1%)	78	82
21	R	162/163 (99%)	152 (94%)	10 (6%)	16	45
22	S	134/137 (98%)	127 (95%)	7 (5%)	21	51
23	T	93/111 (84%)	87 (94%)	6 (6%)	15	44
24	U	100/105 (95%)	97 (97%)	3 (3%)	36	63
25	V	56/131 (43%)	53 (95%)	3 (5%)	20	50
26	W	116/139 (84%)	111 (96%)	5 (4%)	26	56
27	X	113/128 (88%)	106 (94%)	7 (6%)	16	45
28	Y	128/130 (98%)	119 (93%)	9 (7%)	14	41
29	Z	116/118 (98%)	109 (94%)	7 (6%)	17	46
30	a	44/48 (92%)	43 (98%)	1 (2%)	44	68
31	b	80/89 (90%)	76 (95%)	4 (5%)	22	52
32	c	99/110 (90%)	91 (92%)	8 (8%)	11	36
33	d	112/122 (92%)	103 (92%)	9 (8%)	11	37
34	e	91/97 (94%)	86 (94%)	5 (6%)	19	49
35	f	91/115 (79%)	84 (92%)	7 (8%)	12	38
36	g	103/105 (98%)	96 (93%)	7 (7%)	14	42
37	h	79/82 (96%)	79 (100%)	0	100	100
38	i	69/79 (87%)	61 (88%)	8 (12%)	5	22
39	j	66/73 (90%)	63 (96%)	3 (4%)	24	55
40	k	44/45 (98%)	39 (89%)	5 (11%)	5	22
41	l	47/116 (40%)	45 (96%)	2 (4%)	26	56
42	n	88/93 (95%)	87 (99%)	1 (1%)	65	77
43	o	68/71 (96%)	65 (96%)	3 (4%)	25	55
44	p	108/114 (95%)	103 (95%)	5 (5%)	24	54
All	All	5322/6071 (88%)	5070 (95%)	252 (5%)	25	54

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	6	ARG
4	A	15	VAL
4	A	41	ILE
4	A	80	GLU
4	A	163	ARG
4	A	174	ARG
4	A	193	ARG
4	A	242	ARG
5	B	10	ARG
5	B	58	ARG
5	B	60	LEU
5	B	102	LEU
5	B	163	THR
5	B	172	SER
5	B	189	GLU
5	B	209	THR
5	B	230	SER
5	B	243	ARG
5	B	321	LEU
5	B	323	LEU
5	B	336	THR
5	B	346	THR
5	B	382	LEU
6	C	24	MET
6	C	73	VAL
6	C	75	ARG
6	C	107	THR
6	C	108	TRP
6	C	140	ARG
6	C	180	LEU
6	C	182	ARG
6	C	191	ARG
6	C	277	LYS
6	C	372	ARG
7	D	68	THR
7	D	122	VAL
7	D	132	GLU
7	D	196	GLU
7	D	240	GLU
8	E	46	LEU
8	E	54	ARG
8	E	94	THR
8	E	179	ARG

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Mol	Chain	Res	Type
9	F	110	LYS
9	F	144	ILE
9	F	153	THR
9	F	172	HIS
9	F	173	SER
9	F	222	ASN
9	F	246	ARG
9	F	255	GLN
10	G	70	LEU
10	G	161	LEU
10	G	189	CYS
10	G	192	LYS
10	G	205	ASN
10	G	208	VAL
10	G	214	VAL
10	G	250	ILE
11	H	23	ARG
11	H	25	VAL
11	H	40	HIS
11	H	57	GLU
11	H	138	ASN
11	H	141	ASP
11	H	145	LEU
11	H	170	ASP
12	I	52	LEU
12	I	63	GLU
12	I	99	ILE
12	I	130	ASP
12	I	133	GLN
13	J	14	ARG
13	J	23	CYS
13	J	113	LEU
13	J	115	ILE
14	K	52	LEU
14	K	54	ARG
14	K	57	VAL
14	K	68	VAL
14	K	115	LEU
14	K	155	ILE
14	K	167	ARG
14	K	168	CYS
14	K	177	GLU

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Mol	Chain	Res	Type
14	K	180	PHE
15	L	4	PHE
15	L	6	ARG
15	L	21	ASP
15	L	38	LEU
15	L	54	VAL
15	L	72	SER
15	L	118	LEU
16	M	10	LEU
16	M	13	LYS
16	M	39	CYS
16	M	66	VAL
16	M	75	VAL
16	M	104	GLU
16	M	143	ILE
16	M	146	ASP
16	M	160	ARG
16	M	161	GLU
16	M	175	LEU
16	M	185	LEU
17	N	121	GLN
17	N	172	GLU
17	N	226	ARG
18	O	22	LEU
18	O	24	VAL
18	O	41	LYS
18	O	47	LEU
18	O	56	ASP
18	O	100	LEU
18	O	113	LEU
18	O	125	VAL
18	O	147	SER
19	P	3	ILE
19	P	8	ASN
19	P	29	LEU
19	P	32	LEU
19	P	39	ARG
19	P	41	ASN
19	P	143	LYS
19	P	148	ASP
19	P	171	ARG
20	Q	33	MET

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Mol	Chain	Res	Type
21	R	17	VAL
21	R	65	ILE
21	R	72	ARG
21	R	75	ARG
21	R	94	THR
21	R	97	MET
21	R	103	ASP
21	R	141	CYS
21	R	149	LEU
21	R	168	ASP
22	S	8	ARG
22	S	13	GLN
22	S	48	VAL
22	S	67	VAL
22	S	68	THR
22	S	103	GLU
22	S	140	PHE
23	T	62	CYS
23	T	63	ASN
23	T	67	ASP
23	T	104	LEU
23	T	106	ASP
23	T	116	THR
24	U	47	CYS
24	U	77	MET
24	U	131	ILE
25	V	8	ILE
25	V	24	ARG
25	V	56	LEU
26	W	78	LEU
26	W	111	ASP
26	W	137	LEU
26	W	139	ARG
26	W	149	ARG
27	X	6	GLN
27	X	23	SER
27	X	47	LEU
27	X	49	ILE
27	X	55	VAL
27	X	59	ARG
27	X	92	GLU
28	Y	65	MET

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Mol	Chain	Res	Type
28	Y	72	LYS
28	Y	74	ILE
28	Y	79	LEU
28	Y	80	MET
28	Y	86	VAL
28	Y	98	GLU
28	Y	121	LYS
28	Y	123	THR
29	Z	11	ARG
29	Z	12	ARG
29	Z	73	VAL
29	Z	95	ASP
29	Z	116	LEU
29	Z	129	SER
29	Z	133	GLU
30	a	6	ASN
31	b	28	LEU
31	b	32	THR
31	b	44	LEU
31	b	47	ILE
32	c	21	THR
32	c	43	GLU
32	c	52	MET
32	c	72	ILE
32	c	79	VAL
32	c	81	VAL
32	c	100	LEU
32	c	104	VAL
33	d	7	VAL
33	d	8	LYS
33	d	68	MET
33	d	77	LEU
33	d	88	LEU
33	d	91	ASN
33	d	106	LYS
33	d	120	LEU
33	d	121	VAL
34	e	28	GLN
34	e	35	LEU
34	e	53	ARG
34	e	103	VAL
34	e	107	LEU

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Mol	Chain	Res	Type
35	f	4	ARG
35	f	5	LEU
35	f	31	VAL
35	f	38	GLN
35	f	41	ARG
35	f	47	CYS
35	f	54	ILE
36	g	21	LEU
36	g	58	LEU
36	g	83	LEU
36	g	95	LEU
36	g	96	THR
36	g	99	GLN
36	g	121	LEU
38	i	8	THR
38	i	18	THR
38	i	21	LEU
38	i	22	CYS
38	i	25	CYS
38	i	40	CYS
38	i	67	CYS
38	i	70	LEU
39	j	50	SER
39	j	55	THR
39	j	67	LEU
40	k	3	SER
40	k	9	LEU
40	k	13	LEU
40	k	17	GLN
40	k	23	ILE
41	l	97	ARG
41	l	126	LYS
42	n	53	GLN
43	o	29	ILE
43	o	52	VAL
43	o	73	THR
44	p	6	LEU
44	p	16	CYS
44	p	44	ILE
44	p	117	LYS
44	p	119	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102)

such sidechains are listed below:

Mol	Chain	Res	Type
5	B	55	HIS
5	B	152	ASN
5	B	162	HIS
5	B	164	GLN
5	B	181	GLN
5	B	260	GLN
5	B	268	GLN
5	B	286	ASN
5	B	312	HIS
6	C	50	GLN
6	C	105	ASN
6	C	216	ASN
6	C	289	ASN
6	C	302	GLN
6	C	373	GLN
6	C	384	GLN
7	D	112	GLN
7	D	225	GLN
7	D	284	HIS
7	D	291	GLN
8	E	112	GLN
8	E	174	GLN
9	F	178	GLN
9	F	236	ASN
9	F	251	ASN
10	G	89	ASN
10	G	93	HIS
10	G	248	ASN
11	H	138	ASN
12	I	73	ASN
13	J	40	GLN
13	J	63	ASN
13	J	131	GLN
13	J	141	HIS
14	K	102	ASN
15	L	34	GLN
15	L	102	GLN
15	L	126	GLN
16	M	41	GLN
16	M	124	GLN
17	N	80	HIS
17	N	108	ASN

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Mol	Chain	Res	Type
17	N	121	GLN
17	N	162	GLN
17	N	169	GLN
17	N	215	HIS
18	O	20	GLN
18	O	143	ASN
18	O	151	HIS
19	P	8	ASN
19	P	41	ASN
19	P	45	ASN
20	Q	98	GLN
20	Q	129	ASN
20	Q	130	GLN
21	R	21	GLN
21	R	81	ASN
21	R	127	ASN
21	R	145	HIS
21	R	147	GLN
22	S	13	GLN
22	S	58	HIS
22	S	69	GLN
22	S	90	HIS
22	S	102	ASN
22	S	117	HIS
23	T	63	ASN
26	W	118	GLN
27	X	18	HIS
28	Y	15	ASN
28	Y	78	HIS
28	Y	127	ASN
29	Z	14	HIS
29	Z	25	HIS
29	Z	49	HIS
29	Z	60	HIS
29	Z	92	GLN
30	a	6	ASN
30	a	13	ASN
30	a	17	HIS
31	b	14	ASN
31	b	77	ASN
31	b	78	ASN
32	c	23	HIS

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Mol	Chain	Res	Type
32	c	64	ASN
33	d	56	ASN
33	d	91	ASN
33	d	101	ASN
33	d	116	GLN
34	e	36	GLN
34	e	80	HIS
34	e	93	ASN
35	f	103	GLN
36	g	99	GLN
36	g	112	GLN
37	h	92	ASN
40	k	38	ASN
40	k	43	HIS
41	l	120	GLN
42	n	47	GLN
44	p	55	HIS
44	p	59	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3053/3477 (87%)	745 (24%)	91 (2%)
2	3	115/124 (92%)	21 (18%)	1 (0%)
3	4	155/158 (98%)	35 (22%)	2 (1%)
All	All	3323/3759 (88%)	801 (24%)	94 (2%)

All (801) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	7	C
1	1	31	C
1	1	40	A
1	1	43	A
1	1	49	U
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	69	U

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Mol	Chain	Res	Type
1	1	74	A
1	1	75	U
1	1	77	A
1	1	85	A
1	1	92	G
1	1	109	A
1	1	110	G
1	1	115	A
1	1	116	A
1	1	117	G
1	1	119	G
1	1	121	A
1	1	122	A
1	1	129	U
1	1	132	U
1	1	147	G
1	1	159	C
1	1	160	G
1	1	164	G
1	1	168	U
1	1	169	U
1	1	174	G
1	1	176	G
1	1	180	G
1	1	181	C
1	1	190	A
1	1	193	U
1	1	194	U
1	1	195	U
1	1	203	A
1	1	213	U
1	1	214	A
1	1	215	G
1	1	216	A
1	1	221	G
1	1	222	A
1	1	245	U
1	1	246	U
1	1	247	U
1	1	248	U
1	1	249	U
1	1	250	G

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Mol	Chain	Res	Type
1	1	251	U
1	1	252	U
1	1	253	C
1	1	254	C
1	1	259	A
1	1	260	C
1	1	261	G
1	1	262	G
1	1	270	U
1	1	271	U
1	1	272	A
1	1	273	U
1	1	277	G
1	1	278	U
1	1	283	U
1	1	291	G
1	1	293	U
1	1	294	U
1	1	303	A
1	1	323	A
1	1	337	U
1	1	338	G
1	1	358	C
1	1	360	A
1	1	379	G
1	1	380	A
1	1	383	A
1	1	384	G
1	1	387	C
1	1	393	A
1	1	403	A
1	1	405	A
1	1	406	A
1	1	408	U
1	1	428	G
1	1	429	A
1	1	431	G
1	1	436	U
1	1	451	U
1	1	459	G
1	1	461	G
1	1	466	C

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Mol	Chain	Res	Type
1	1	467	G
1	1	476	U
1	1	477	C
1	1	481	C
1	1	484	U
1	1	485	U
1	1	488	C
1	1	496	C
1	1	497	U
1	1	499	U
1	1	500	C
1	1	501	A
1	1	502	C
1	1	503	C
1	1	504	A
1	1	509	U
1	1	514	U
1	1	515	U
1	1	517	G
1	1	522	C
1	1	523	U
1	1	526	A
1	1	527	U
1	1	535	C
1	1	537	G
1	1	538	U
1	1	539	U
1	1	540	C
1	1	541	A
1	1	546	U
1	1	547	U
1	1	548	U
1	1	552	G
1	1	554	G
1	1	572	G
1	1	573	G
1	1	576	U
1	1	580	U
1	1	581	U
1	1	582	U
1	1	587	C
1	1	594	G

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Mol	Chain	Res	Type
1	1	595	G
1	1	596	U
1	1	600	U
1	1	601	U
1	1	603	C
1	1	606	G
1	1	608	G
1	1	613	G
1	1	615	U
1	1	616	A
1	1	618	A
1	1	619	U
1	1	622	U
1	1	625	U
1	1	628	U
1	1	629	U
1	1	630	U
1	1	637	C
1	1	638	C
1	1	639	U
1	1	640	U
1	1	641	G
1	1	649	G
1	1	650	G
1	1	652	G
1	1	653	U
1	1	654	G
1	1	655	U
1	1	656	U
1	1	657	C
1	1	663	U
1	1	665	C
1	1	666	G
1	1	667	A
1	1	668	G
1	1	686	C
1	1	691	U
1	1	696	G
1	1	697	A
1	1	698	U
1	1	699	G
1	1	700	C

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Mol	Chain	Res	Type
1	1	721	G
1	1	723	C
1	1	736	A
1	1	746	G
1	1	747	A
1	1	748	G
1	1	749	U
1	1	763	G
1	1	764	A
1	1	767	A
1	1	774	U
1	1	776	U
1	1	777	U
1	1	778	A
1	1	792	A
1	1	796	A
1	1	799	G
1	1	802	A
1	1	817	U
1	1	820	U
1	1	821	U
1	1	824	C
1	1	826	A
1	1	827	U
1	1	828	U
1	1	830	U
1	1	831	U
1	1	833	G
1	1	835	A
1	1	851	G
1	1	855	U
1	1	856	C
1	1	857	U
1	1	858	G
1	1	864	G
1	1	866	U
1	1	867	U
1	1	870	A
1	1	871	G
1	1	873	U
1	1	874	G
1	1	875	G

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Mol	Chain	Res	Type
1	1	876	A
1	1	889	G
1	1	896	A
1	1	898	A
1	1	907	A
1	1	908	C
1	1	909	U
1	1	920	A
1	1	927	A
1	1	931	A
1	1	947	G
1	1	951	U
1	1	958	C
1	1	959	G
1	1	964	U
1	1	968	G
1	1	969	U
1	1	970	G
1	1	986	A
1	1	987	C
1	1	997	G
1	1	998	G
1	1	1001	C
1	1	1004	A
1	1	1006	G
1	1	1007	A
1	1	1008	C
1	1	1011	A
1	1	1013	C
1	1	1014	G
1	1	1015	A
1	1	1024	G
1	1	1027	G
1	1	1034	U
1	1	1036	U
1	1	1049	C
1	1	1050	U
1	1	1051	C
1	1	1052	A
1	1	1053	G
1	1	1065	U
1	1	1069	G

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Mol	Chain	Res	Type
1	1	1070	U
1	1	1075	U
1	1	1080	C
1	1	1082	G
1	1	1083	G
1	1	1089	C
1	1	1090	G
1	1	1091	A
1	1	1099	G
1	1	1102	G
1	1	1121	C
1	1	1123	C
1	1	1124	G
1	1	1125	A
1	1	1126	C
1	1	1134	C
1	1	1136	A
1	1	1138	C
1	1	1153	A
1	1	1154	U
1	1	1157	A
1	1	1160	G
1	1	1164	A
1	1	1165	C
1	1	1168	C
1	1	1170	U
1	1	1171	U
1	1	1183	A
1	1	1184	U
1	1	1185	U
1	1	1186	A
1	1	1191	G
1	1	1202	G
1	1	1204	G
1	1	1209	U
1	1	1218	G
1	1	1231	U
1	1	1239	G
1	1	1240	C
1	1	1246	A
1	1	1249	C
1	1	1250	U

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Mol	Chain	Res	Type
1	1	1268	U
1	1	1269	G
1	1	1277	A
1	1	1278	U
1	1	1279	C
1	1	1283	U
1	1	1284	A
1	1	1288	U
1	1	1289	A
1	1	1293	G
1	1	1296	G
1	1	1299	G
1	1	1304	A
1	1	1305	U
1	1	1382	G
1	1	1388	A
1	1	1392	U
1	1	1394	G
1	1	1396	U
1	1	1400	G
1	1	1403	G
1	1	1404	A
1	1	1409	G
1	1	1417	A
1	1	1427	A
1	1	1431	C
1	1	1432	U
1	1	1435	U
1	1	1436	A
1	1	1437	A
1	1	1438	U
1	1	1439	U
1	1	1440	A
1	1	1441	U
1	1	1442	C
1	1	1443	A
1	1	1449	C
1	1	1451	U
1	1	1452	U
1	1	1453	U
1	1	1454	U
1	1	1455	G

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Mol	Chain	Res	Type
1	1	1456	U
1	1	1489	G
1	1	1496	U
1	1	1498	G
1	1	1514	G
1	1	1516	A
1	1	1517	C
1	1	1531	G
1	1	1533	U
1	1	1534	C
1	1	1543	A
1	1	1547	G
1	1	1549	A
1	1	1552	U
1	1	1570	G
1	1	1572	A
1	1	1578	A
1	1	1579	A
1	1	1580	G
1	1	1599	G
1	1	1605	C
1	1	1620	U
1	1	1624	C
1	1	1628	C
1	1	1630	U
1	1	1633	G
1	1	1636	A
1	1	1637	C
1	1	1639	G
1	1	1644	A
1	1	1650	U
1	1	1651	A
1	1	1652	U
1	1	1653	A
1	1	1654	C
1	1	1672	C
1	1	1674	U
1	1	1675	U
1	1	1676	U
1	1	1678	G
1	1	1681	A
1	1	1683	A

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Mol	Chain	Res	Type
1	1	1687	A
1	1	1691	G
1	1	1714	C
1	1	1717	G
1	1	1718	G
1	1	1722	C
1	1	1723	U
1	1	1724	G
1	1	1726	A
1	1	1731	A
1	1	1733	C
1	1	1736	A
1	1	1737	A
1	1	1738	G
1	1	1751	C
1	1	1777	G
1	1	1794	G
1	1	1818	C
1	1	1826	C
1	1	1829	G
1	1	1831	G
1	1	1841	G
1	1	1842	C
1	1	1843	U
1	1	1851	A
1	1	1852	G
1	1	1859	U
1	1	1861	G
1	1	1872	U
1	1	1877	G
1	1	1878	G
1	1	1882	G
1	1	1884	U
1	1	1899	A
1	1	1911	A
1	1	1916	U
1	1	1917	G
1	1	1918	U
1	1	1919	U
1	1	1920	A
1	1	1921	U
1	1	1922	U

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Mol	Chain	Res	Type
1	1	1932	G
1	1	1942	A
1	1	1944	A
1	1	1945	A
1	1	1949	C
1	1	1950	A
1	1	1953	A
1	1	1961	A
1	1	1962	A
1	1	1969	U
1	1	1974	U
1	1	1981	G
1	1	1982	A
1	1	1983	U
1	1	1987	A
1	1	1989	A
1	1	1996	A
1	1	2009	G
1	1	2011	A
1	1	2013	A
1	1	2029	C
1	1	2033	A
1	1	2042	G
1	1	2055	G
1	1	2213	A
1	1	2215	C
1	1	2216	U
1	1	2217	C
1	1	2224	G
1	1	2225	G
1	1	2226	A
1	1	2227	G
1	1	2228	C
1	1	2232	C
1	1	2235	G
1	1	2236	G
1	1	2245	A
1	1	2258	A
1	1	2259	A
1	1	2263	A
1	1	2264	G
1	1	2272	A

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Mol	Chain	Res	Type
1	1	2274	G
1	1	2278	A
1	1	2283	U
1	1	2299	U
1	1	2307	G
1	1	2314	G
1	1	2318	U
1	1	2338	U
1	1	2357	A
1	1	2359	G
1	1	2362	G
1	1	2365	A
1	1	2373	U
1	1	2385	G
1	1	2386	G
1	1	2387	U
1	1	2398	C
1	1	2401	G
1	1	2419	C
1	1	2420	G
1	1	2423	U
1	1	2426	A
1	1	2427	U
1	1	2428	G
1	1	2431	U
1	1	2448	G
1	1	2449	U
1	1	2476	A
1	1	2485	A
1	1	2486	A
1	1	2487	C
1	1	2488	G
1	1	2504	G
1	1	2506	G
1	1	2510	A
1	1	2514	A
1	1	2515	A
1	1	2516	G
1	1	2517	A
1	1	2518	C
1	1	2519	C
1	1	2524	U

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Mol	Chain	Res	Type
1	1	2525	G
1	1	2535	C
1	1	2537	A
1	1	2548	G
1	1	2550	G
1	1	2624	A
1	1	2627	U
1	1	2628	A
1	1	2636	A
1	1	2638	G
1	1	2645	C
1	1	2646	U
1	1	2647	C
1	1	2651	C
1	1	2652	U
1	1	2653	C
1	1	2655	G
1	1	2656	C
1	1	2657	A
1	1	2658	U
1	1	2659	G
1	1	2660	U
1	1	2661	G
1	1	2662	U
1	1	2663	U
1	1	2664	U
1	1	2665	U
1	1	2666	G
1	1	2667	G
1	1	2672	A
1	1	2673	A
1	1	2679	C
1	1	2695	A
1	1	2696	C
1	1	2702	A
1	1	2704	A
1	1	2705	C
1	1	2706	A
1	1	2717	G
1	1	2718	G
1	1	2725	G
1	1	2730	G

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Mol	Chain	Res	Type
1	1	2731	G
1	1	2739	A
1	1	2749	C
1	1	2759	G
1	1	2763	U
1	1	2766	U
1	1	2767	A
1	1	2768	A
1	1	2785	A
1	1	2788	G
1	1	2791	A
1	1	2800	U
1	1	2801	G
1	1	2802	A
1	1	2805	A
1	1	2806	A
1	1	2807	A
1	1	2816	A
1	1	2820	U
1	1	2825	G
1	1	2827	U
1	1	2830	U
1	1	2836	U
1	1	2839	G
1	1	2840	U
1	1	2860	G
1	1	2863	U
1	1	2864	G
1	1	2866	C
1	1	2873	A
1	1	2883	U
1	1	2884	C
1	1	2888	G
1	1	2889	A
1	1	2907	G
1	1	2908	U
1	1	2911	G
1	1	2912	A
1	1	2913	A
1	1	2914	A
1	1	2915	A
1	1	2921	C

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Mol	Chain	Res	Type
1	1	2925	G
1	1	2927	G
1	1	2928	A
1	1	2932	C
1	1	2949	A
1	1	2953	U
1	1	2954	U
1	1	2955	C
1	1	2956	A
1	1	2960	C
1	1	2974	G
1	1	2978	C
1	1	2982	G
1	1	2983	A
1	1	2984	U
1	1	2987	C
1	1	2998	A
1	1	3010	C
1	1	3015	G
1	1	3021	A
1	1	3034	U
1	1	3041	G
1	1	3046	U
1	1	3047	A
1	1	3049	G
1	1	3052	A
1	1	3053	C
1	1	3058	G
1	1	3077	G
1	1	3079	G
1	1	3082	A
1	1	3090	U
1	1	3091	U
1	1	3094	C
1	1	3101	G
1	1	3102	A
1	1	3108	U
1	1	3109	G
1	1	3115	G
1	1	3123	A
1	1	3124	A
1	1	3126	C

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Mol	Chain	Res	Type
1	1	3140	G
1	1	3169	A
1	1	3170	U
1	1	3171	G
1	1	3181	G
1	1	3182	A
1	1	3185	A
1	1	3186	G
1	1	3190	G
1	1	3198	A
1	1	3204	C
1	1	3205	C
1	1	3208	C
1	1	3211	U
1	1	3213	G
1	1	3228	G
1	1	3229	C
1	1	3234	A
1	1	3237	U
1	1	3242	A
1	1	3243	U
1	1	3253	A
1	1	3254	U
1	1	3255	A
1	1	3256	U
1	1	3257	G
1	1	3266	U
1	1	3267	U
1	1	3268	C
1	1	3269	A
1	1	3270	C
1	1	3279	U
1	1	3280	U
1	1	3282	U
1	1	3283	U
1	1	3284	U
1	1	3285	C
1	1	3286	A
1	1	3287	U
1	1	3288	G
1	1	3289	C
1	1	3290	A

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Mol	Chain	Res	Type
1	1	3291	A
1	1	3292	U
1	1	3293	G
1	1	3295	U
1	1	3298	A
1	1	3299	G
1	1	3302	C
1	1	3303	U
1	1	3304	C
1	1	3305	U
1	1	3306	G
1	1	3310	U
1	1	3311	G
1	1	3312	C
1	1	3314	U
1	1	3320	C
1	1	3321	A
1	1	3322	A
1	1	3323	A
1	1	3327	C
1	1	3345	G
1	1	3349	A
1	1	3350	G
1	1	3351	A
1	1	3355	U
1	1	3356	C
1	1	3357	A
1	1	3358	A
1	1	3359	U
1	1	3361	U
1	1	3362	C
1	1	3363	U
1	1	3366	C
1	1	3374	G
1	1	3375	U
1	1	3376	G
1	1	3378	U
1	1	3379	A
1	1	3380	C
1	1	3389	C
1	1	3398	U
1	1	3401	U

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Mol	Chain	Res	Type
1	1	3402	U
1	1	3403	G
1	1	3404	C
1	1	3423	U
1	1	3424	G
1	1	3428	G
1	1	3435	U
1	1	3436	G
1	1	3437	U
1	1	3443	A
1	1	3444	U
1	1	3449	U
1	1	3450	A
1	1	3456	U
1	1	3459	C
1	1	3463	C
1	1	3464	G
1	1	3467	G
1	1	3471	G
1	1	3477	G
2	3	2	C
2	3	7	G
2	3	11	A
2	3	19	U
2	3	26	C
2	3	33	U
2	3	48	G
2	3	50	A
2	3	53	U
2	3	54	A
2	3	55	A
2	3	64	A
2	3	72	U
2	3	80	U
2	3	92	U
2	3	100	A
2	3	105	C
2	3	110	G
2	3	113	G
2	3	120	G
2	3	122	U
3	4	23	U

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Mol	Chain	Res	Type
3	4	34	A
3	4	35	C
3	4	49	G
3	4	51	G
3	4	55	U
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	A
3	4	86	U
3	4	87	G
3	4	88	A
3	4	90	U
3	4	95	A
3	4	104	A
3	4	105	A
3	4	106	C
3	4	108	C
3	4	109	A
3	4	111	A
3	4	113	G
3	4	122	G
3	4	124	G
3	4	127	A
3	4	130	C
3	4	139	A
3	4	152	U
3	4	153	G
3	4	156	U
3	4	157	U

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	116	A
1	1	180	G
1	1	193	U
1	1	259	A

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Mol	Chain	Res	Type
1	1	405	A
1	1	407	G
1	1	413	G
1	1	460	U
1	1	537	G
1	1	547	U
1	1	578	G
1	1	580	U
1	1	581	U
1	1	614	U
1	1	649	G
1	1	654	G
1	1	748	G
1	1	823	G
1	1	826	A
1	1	873	U
1	1	874	G
1	1	875	G
1	1	890	G
1	1	906	A
1	1	986	A
1	1	1006	G
1	1	1027	G
1	1	1049	C
1	1	1051	C
1	1	1082	G
1	1	1089	C
1	1	1153	A
1	1	1239	G
1	1	1241	U
1	1	1277	A
1	1	1283	U
1	1	1403	G
1	1	1436	A
1	1	1439	U
1	1	1440	A
1	1	1651	A
1	1	1675	U
1	1	1699	A
1	1	1723	U
1	1	1724	G
1	1	1737	A

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Mol	Chain	Res	Type
1	1	1751	C
1	1	1825	G
1	1	1841	G
1	1	1897	U
1	1	1915	U
1	1	1937	U
1	1	1944	A
1	1	1961	A
1	1	1982	A
1	1	2212	U
1	1	2215	C
1	1	2224	G
1	1	2226	A
1	1	2258	A
1	1	2427	U
1	1	2485	A
1	1	2487	C
1	1	2635	U
1	1	2651	C
1	1	2663	U
1	1	2664	U
1	1	2704	A
1	1	2738	C
1	1	2791	A
1	1	2800	U
1	1	2806	A
1	1	2839	G
1	1	2997	U
1	1	3090	U
1	1	3167	A
1	1	3204	C
1	1	3205	C
1	1	3233	U
1	1	3254	U
1	1	3255	A
1	1	3269	A
1	1	3281	G
1	1	3288	G
1	1	3290	A
1	1	3302	C
1	1	3348	G
1	1	3356	C

Continued on next page...

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Mol	Chain	Res	Type
1	1	3358	A
1	1	3362	C
1	1	3456	U
2	3	112	U
3	4	83	C
3	4	87	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

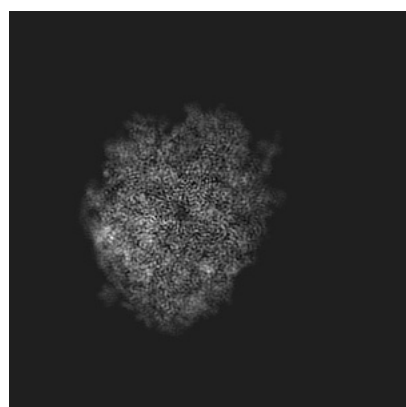
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6778. These allow visual inspection of the internal detail of the map and identification of artifacts.

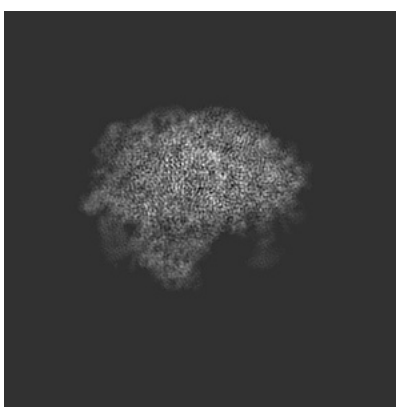
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

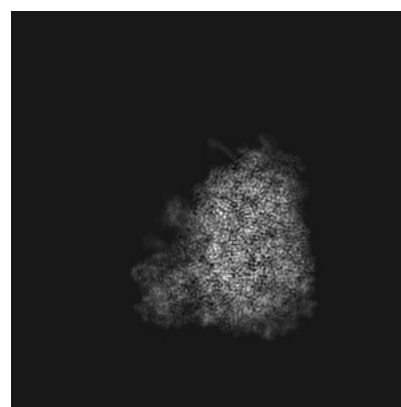
6.1.1 Primary map



X



Y

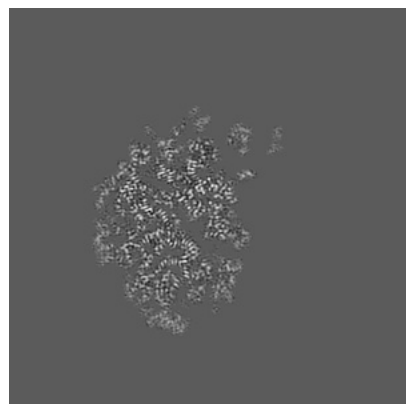


Z

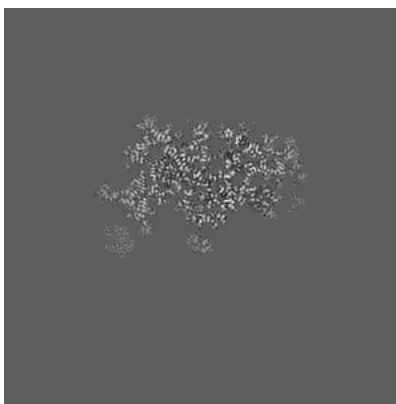
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 160



Y Index: 160

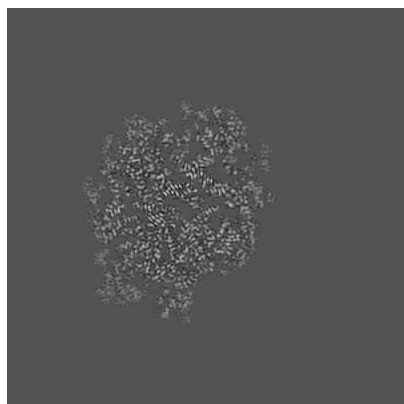


Z Index: 160

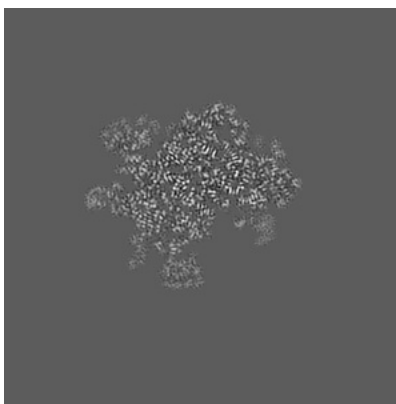
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

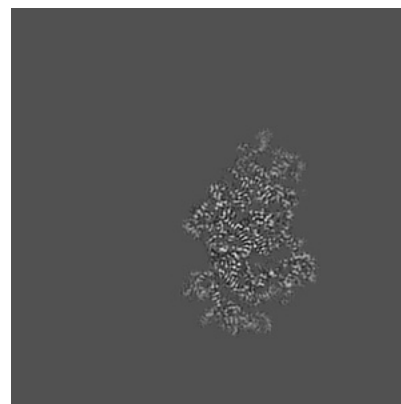
6.3.1 Primary map



X Index: 187



Y Index: 111

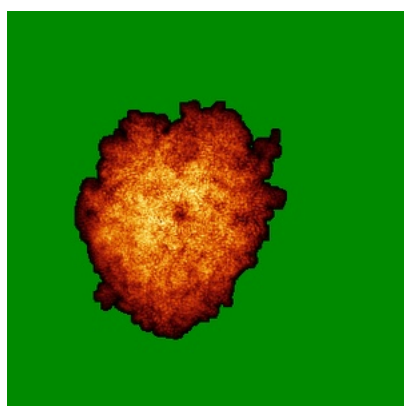


Z Index: 171

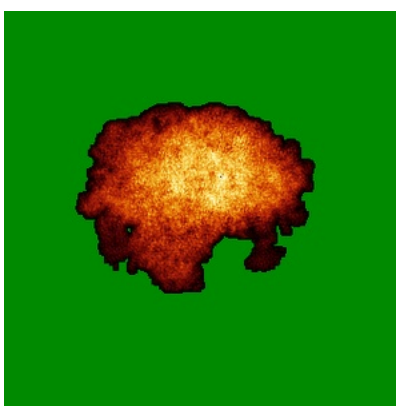
The images above show the largest variance slices of the map in three orthogonal directions.

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

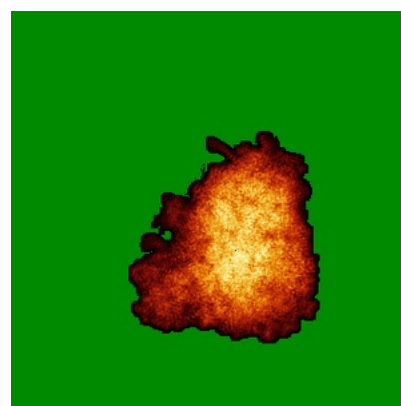
6.4.1 Primary map



X



Y

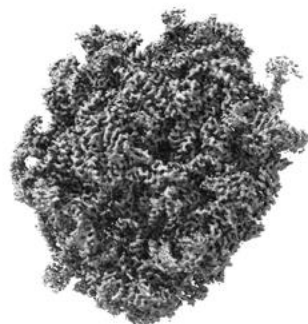


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

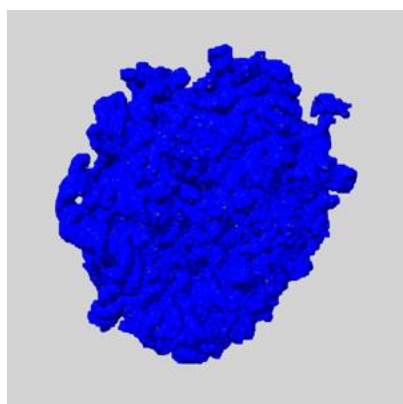
6.6 Mask visualisation [i](#)

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

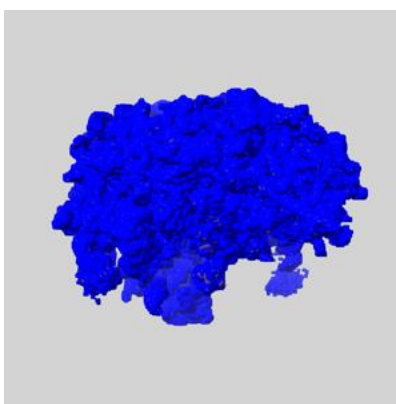
A mask typically either:

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

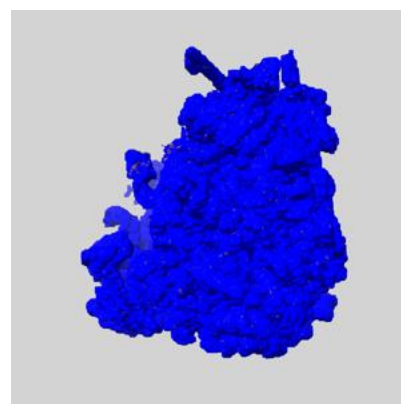
6.6.1 emd_6778_msk_1.map [i](#)



X



Y

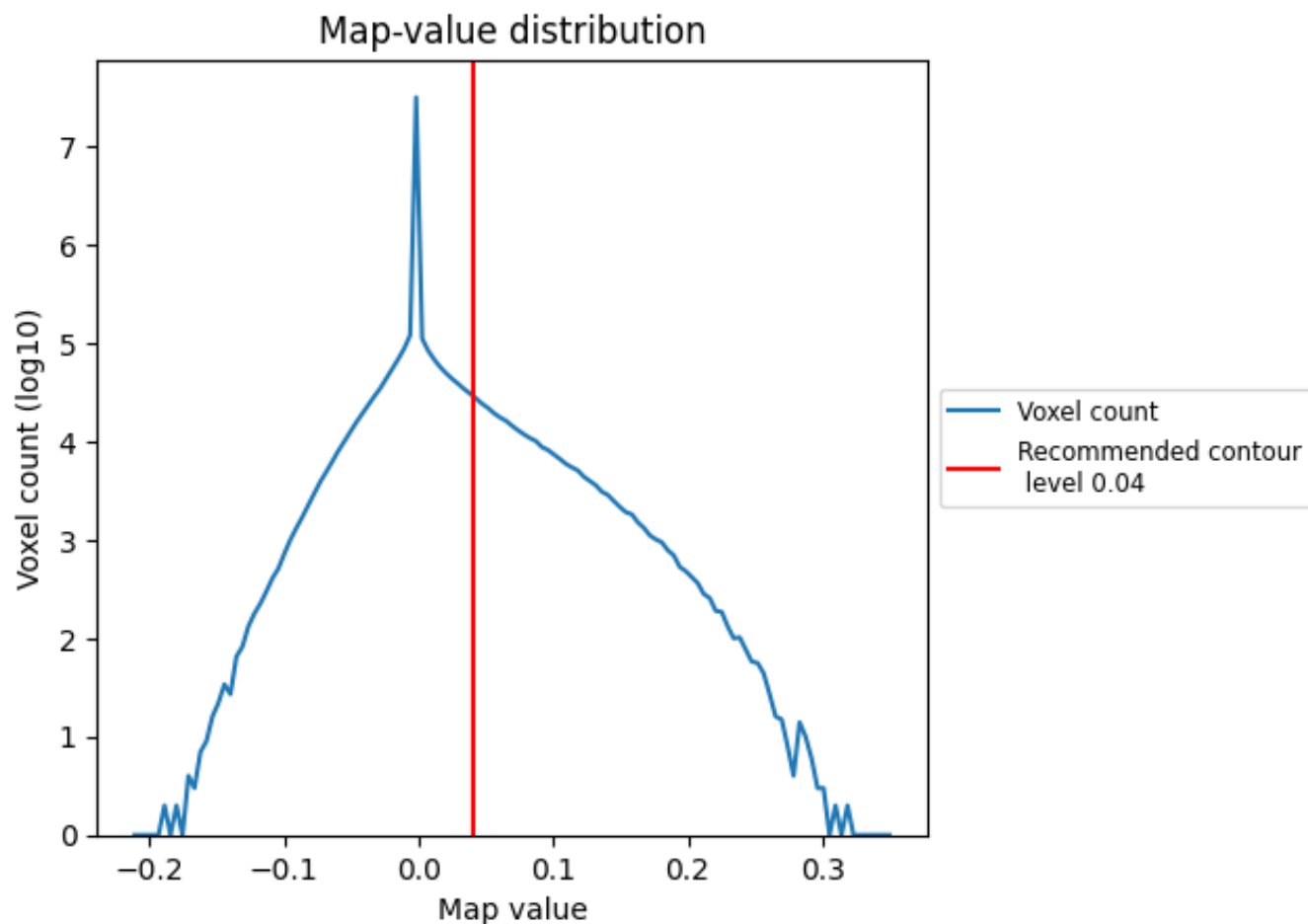


Z

7 Map analysis [i](#)

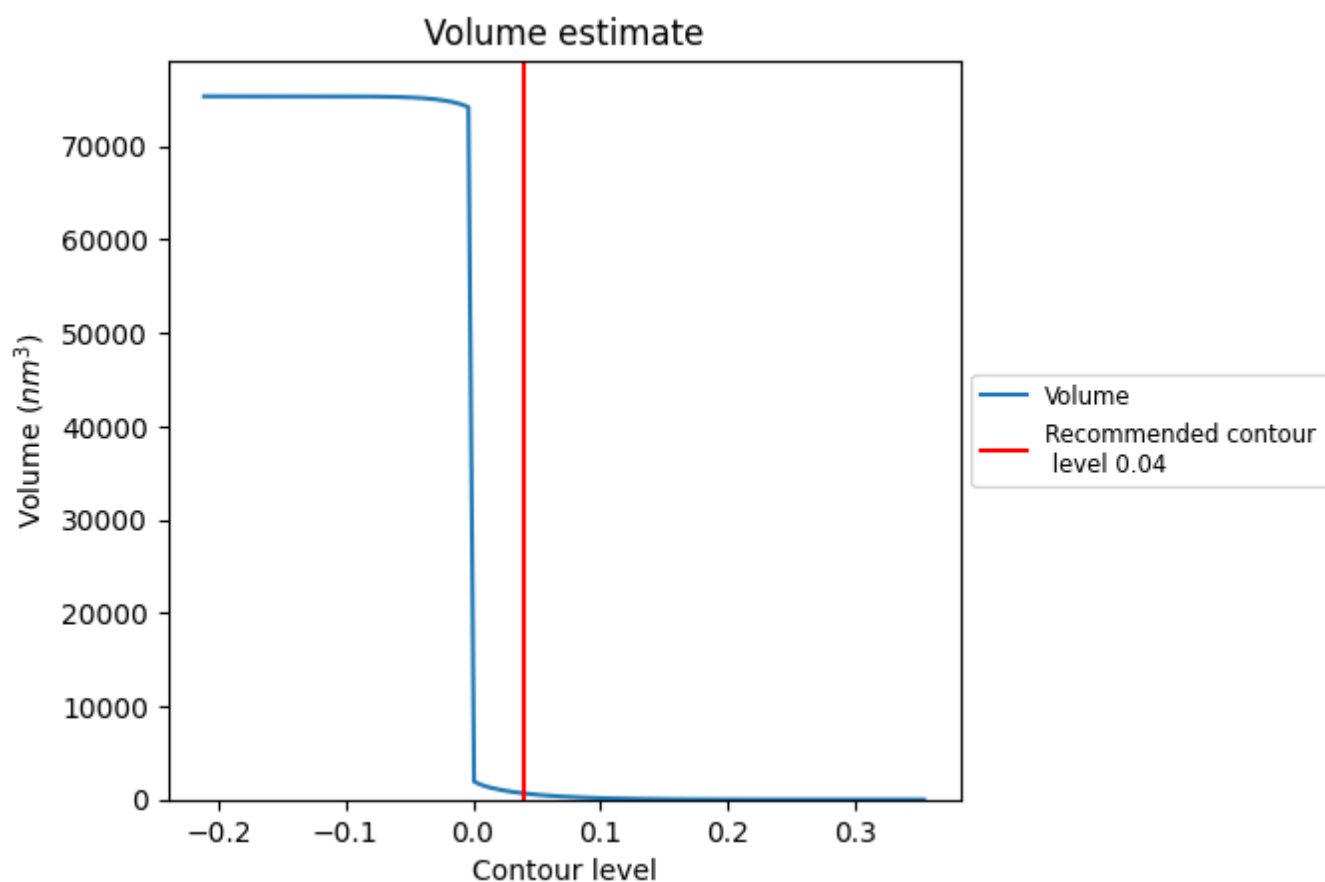
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

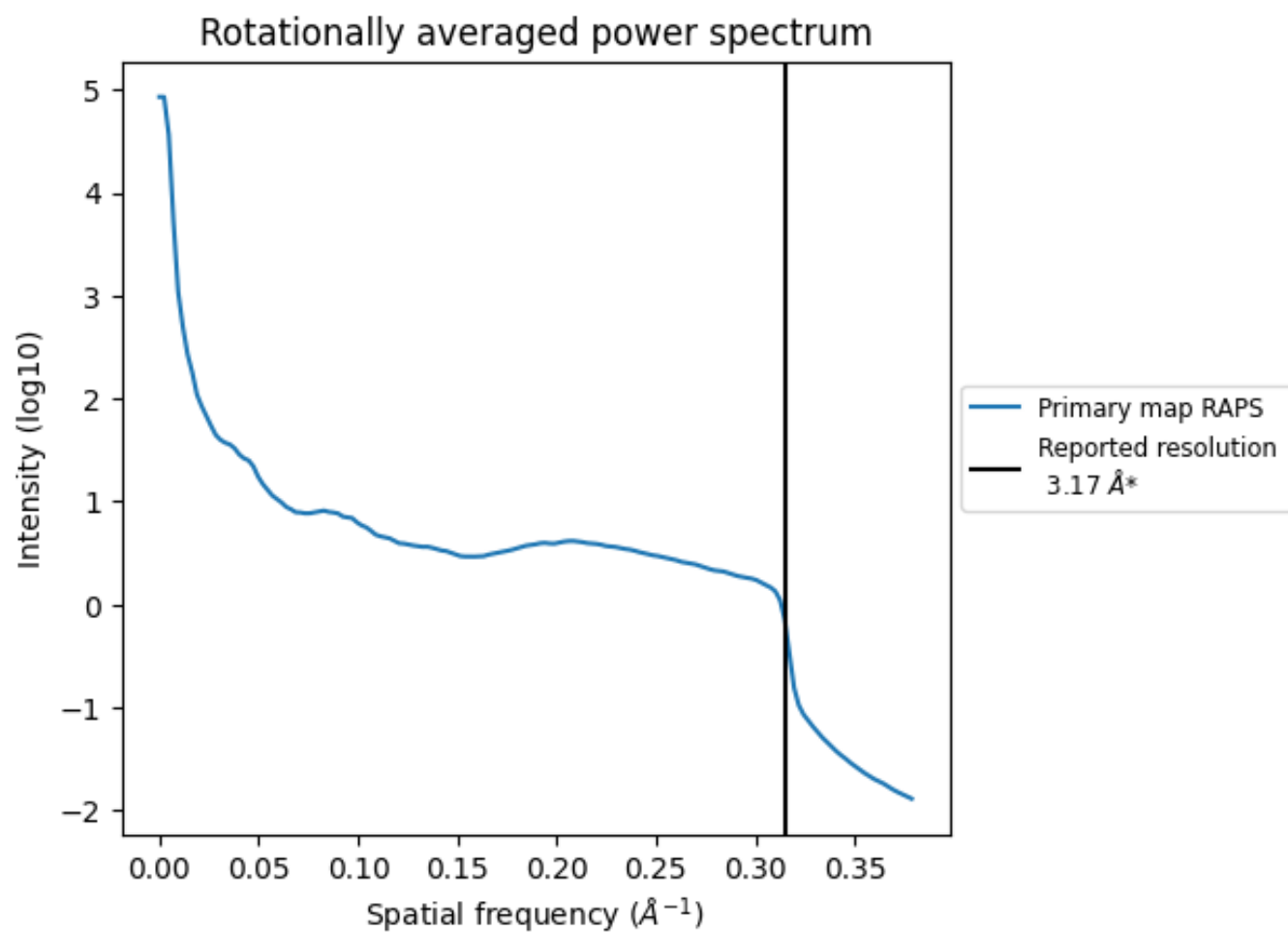
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 664 nm^3 ; this corresponds to an approximate mass of 600 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 ⓘ

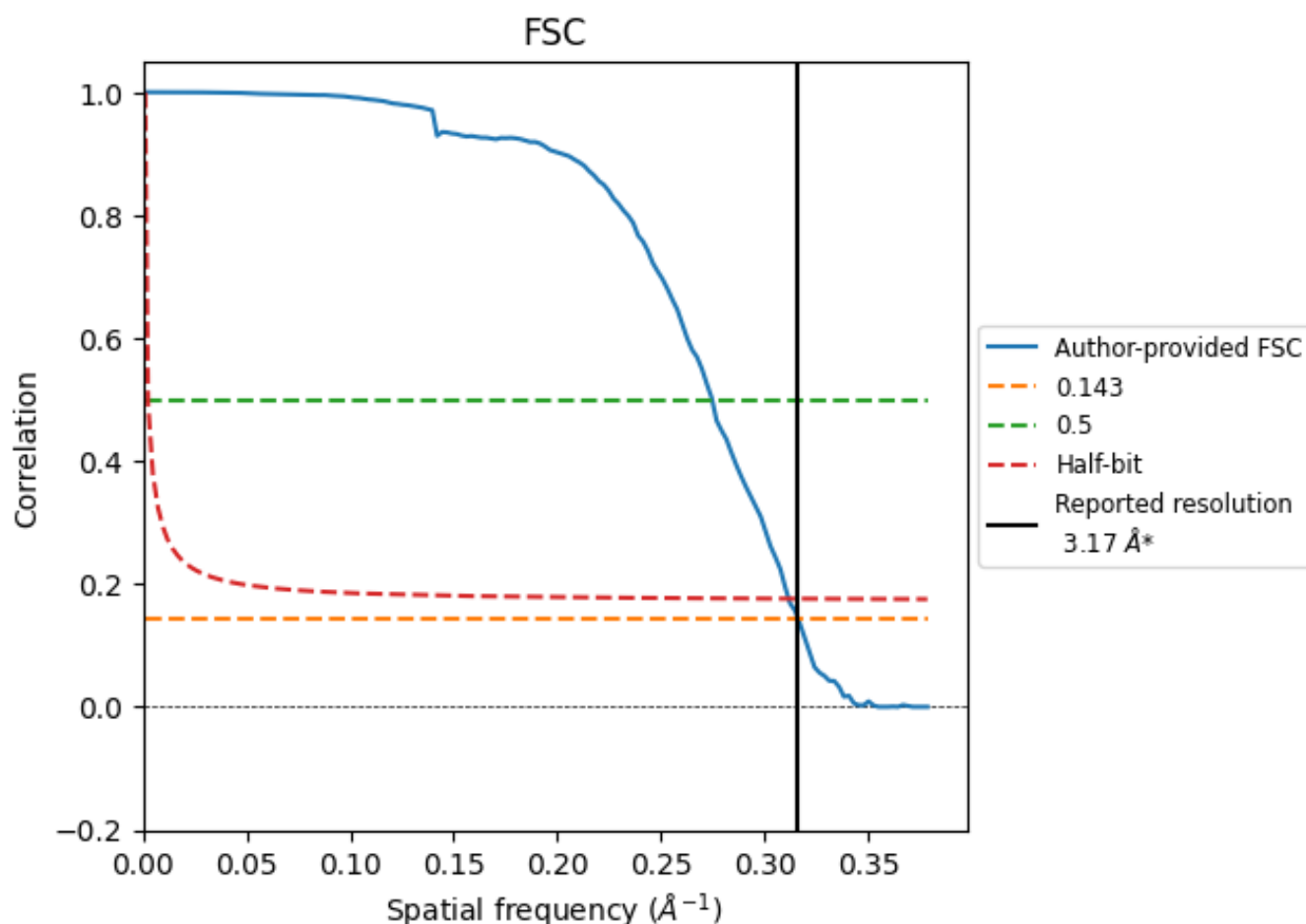


*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.315 Å⁻¹

8.2 Resolution estimates [i](#)

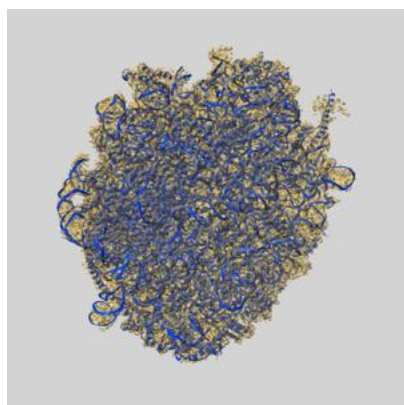
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.16	3.64	3.21
Unmasked-calculated*	-	-	-

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

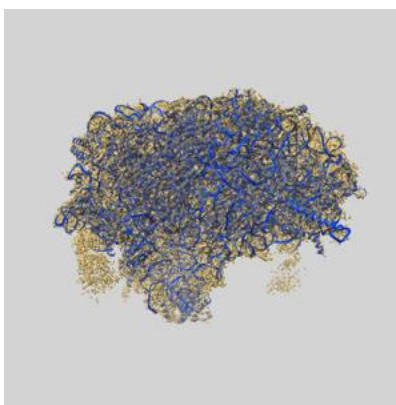
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6778 and PDB model 5XXB. Per-residue inclusion information can be found in section [3](#) on page [12](#).

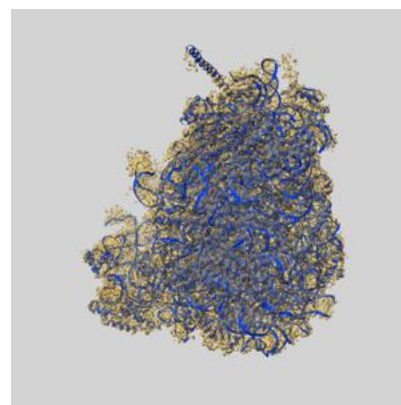
9.1 Map-model overlay [i](#)



X



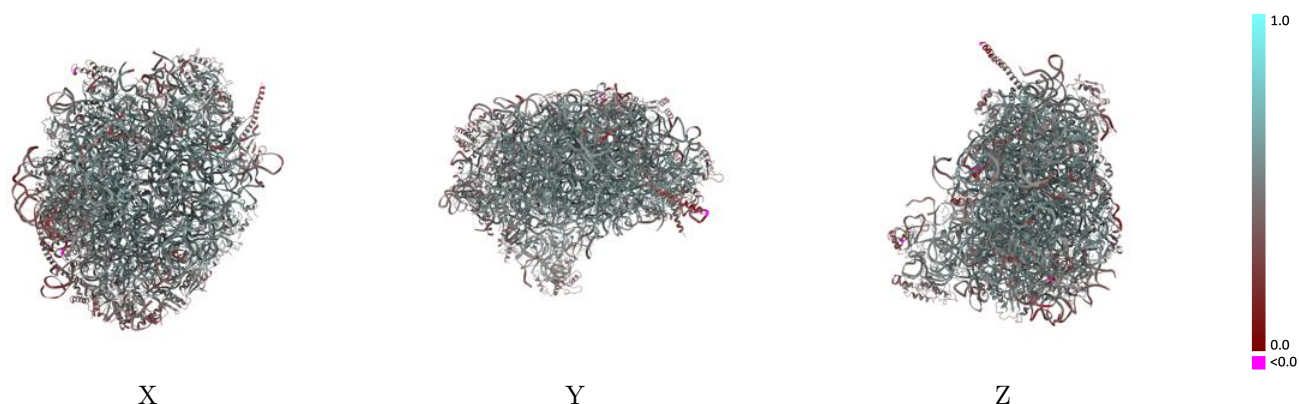
Y



Z

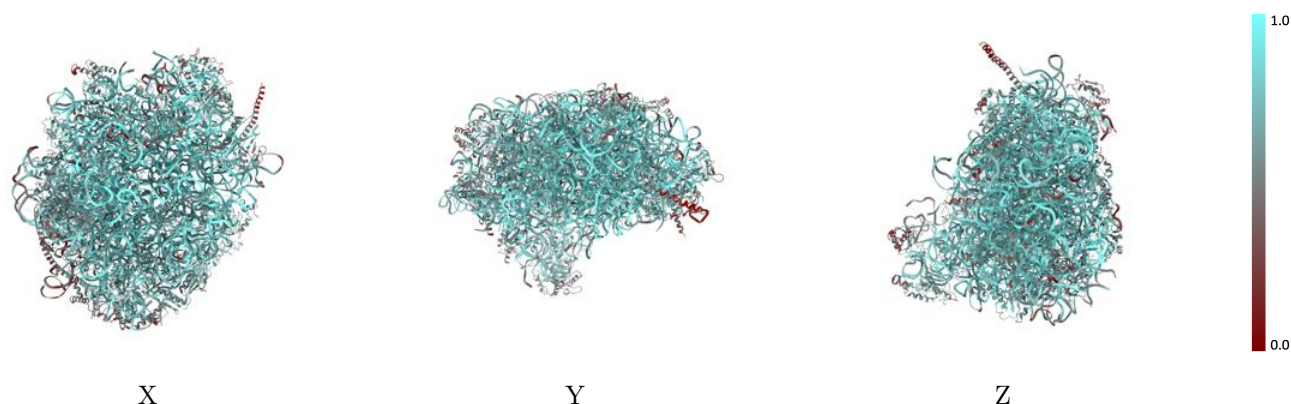
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



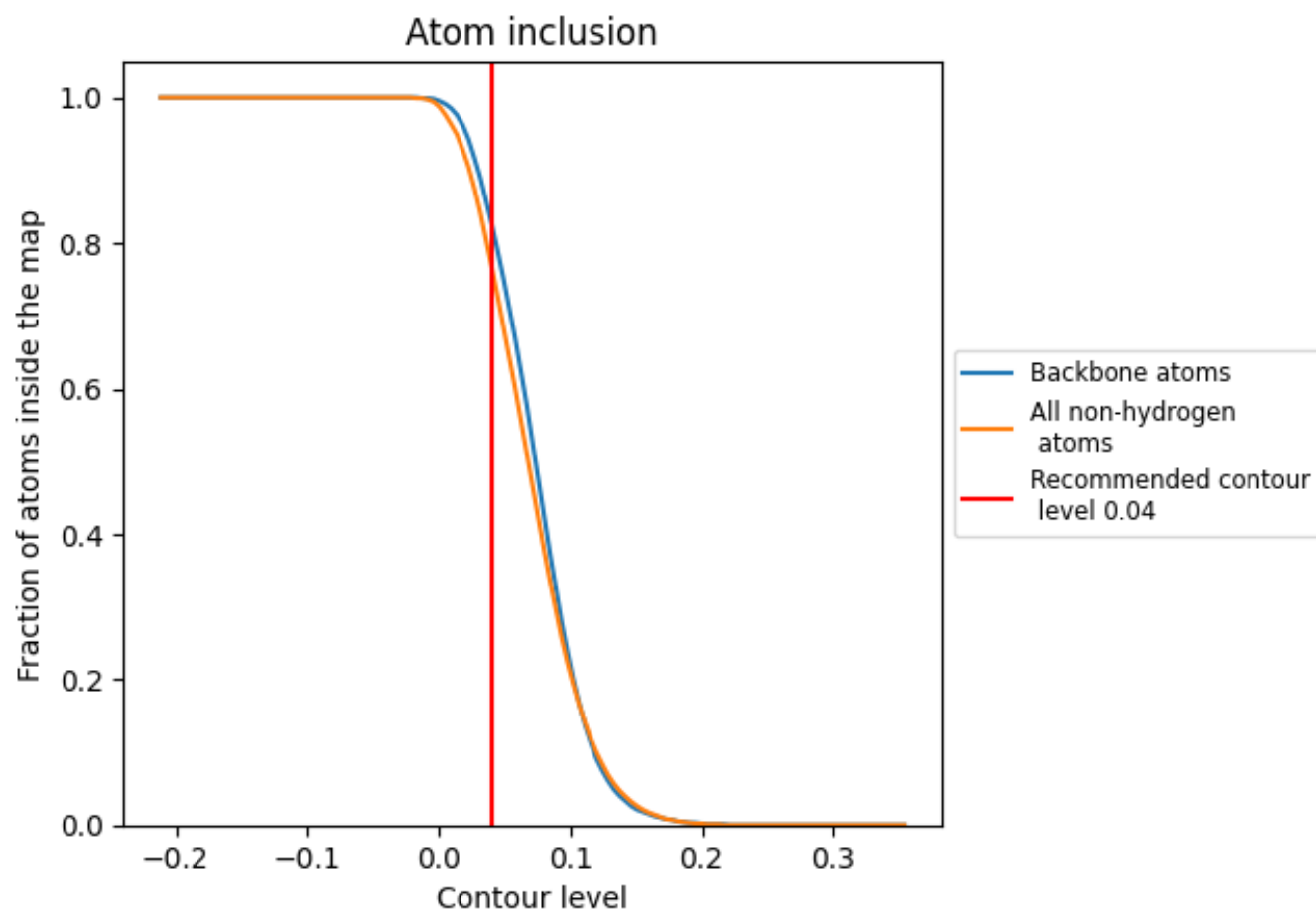
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.5070
1	 0.8450	 0.5240
3	 0.8350	 0.4940
4	 0.8480	 0.5300
A	 0.7680	 0.5420
B	 0.7140	 0.5060
C	 0.6490	 0.4720
D	 0.5930	 0.4270
E	 0.5770	 0.4330
F	 0.6460	 0.4740
G	 0.6260	 0.4550
H	 0.6130	 0.4500
I	 0.6260	 0.4630
J	 0.4530	 0.3490
K	 0.7050	 0.4850
L	 0.6380	 0.4410
M	 0.7980	 0.5520
N	 0.6840	 0.5000
O	 0.7190	 0.5180
P	 0.7030	 0.5080
Q	 0.6200	 0.4670
R	 0.6760	 0.4990
S	 0.6710	 0.4930
T	 0.4880	 0.4010
U	 0.6650	 0.5060
V	 0.6580	 0.4900
W	 0.6940	 0.4930
X	 0.6930	 0.4980
Y	 0.6560	 0.4730
Z	 0.7840	 0.5380
a	 0.6990	 0.5310
b	 0.6050	 0.4520
c	 0.6990	 0.4980
d	 0.7250	 0.5210
e	 0.7640	 0.5270



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Chain	Atom inclusion	Q-score
f	 0.7420	 0.5120
g	 0.6680	 0.4930
h	 0.6370	 0.4530
i	 0.8110	 0.5500
j	 0.5380	 0.4240
k	 0.7690	 0.5400
l	 0.6730	 0.4910
n	 0.6530	 0.4910
o	 0.7120	 0.5210
p	 0.6550	 0.4710