



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 09:28 PM UTC

PDB ID : 6HA1 / pdb_00006ha1
EMDB ID : EMD-0176
Title : Cryo-EM structure of a 70S *Bacillus subtilis* ribosome translating the ErmD leader peptide in complex with telithromycin
Authors : Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wilson, D.N.
Deposited on : 2018-08-07
Resolution : 3.10 Å (reported)
Based on initial model : 3J9W

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

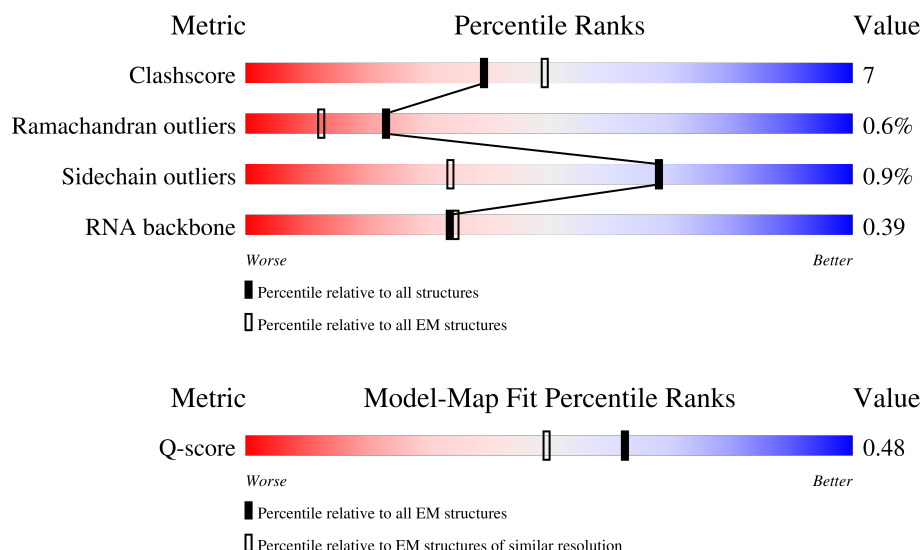
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



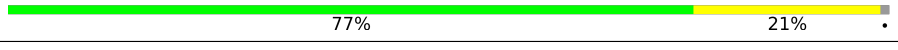
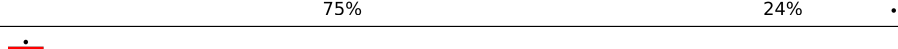
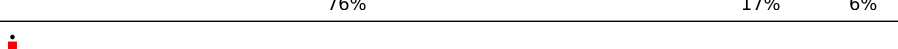
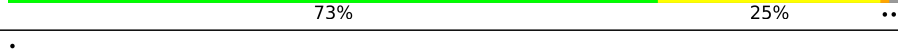
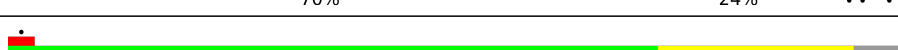
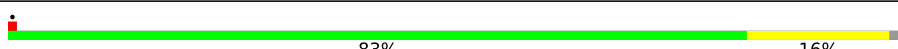
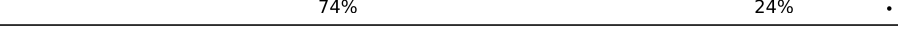
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	2928	
2	B	112	

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Mol	Chain	Length	Quality of chain
3	C	277	
4	D	209	
5	E	207	
6	F	179	
7	G	179	
8	J	145	
9	K	122	
10	L	146	
11	M	144	
12	N	120	
13	O	120	
14	P	115	
15	Q	119	
16	R	102	
17	S	113	
18	T	95	
19	U	103	
20	W	94	
21	X	62	
22	Y	66	
23	Z	59	
24	0	59	
25	1	49	
26	2	44	
27	3	66	

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Mol	Chain	Length	Quality of chain
28	4	37	
29	6	63	
30	7	3	
31	a	1554	
32	b	246	
33	c	218	
34	d	200	
35	e	166	
36	f	95	
37	g	156	
38	h	132	
39	i	130	
40	j	102	
41	k	131	
42	l	138	
43	m	121	
44	n	61	
45	o	89	
46	p	90	
47	q	87	
48	r	79	
49	s	92	
50	t	88	
51	x	87	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
52	TEL	A	3001	X	-	-	-

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 140824 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2887	Total	C	N	O	P	0	0
			61997	27661	11460	19992	2884		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	101	Total	C	N	O		0	0
			786	501	139	146			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	82	Total	C	N	O		0	0
			630	390	123	117			

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 25 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	195	Total	C	N	O	S	0	0
			1568	991	291	284	2		

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	164	Total	C	N	O	S	0	0
			1218	767	225	224	2		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	g	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	k	114	Total	C	N	O	S	0	0
			838	516	164	156	2		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	108	Total	C	N	O	S	0	0
			868	534	176	158			

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	n	60	Total	C	N	O	S	0	0
			497	317	98	77	5		

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	o	85	Total	C	N	O	S	0	0
			710	436	144	129	1		

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	p	88	Total	C	N	O	S	0	0
			695	441	128	124	2		

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	84	Total	C	N	O	S	0	0
			691	435	128	126	2		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	r	64	Total	C	N	O	S	0	0
			518	332	96	88	2		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	s	78	Total	C	N	O	S	0	0
			633	409	112	110	2		

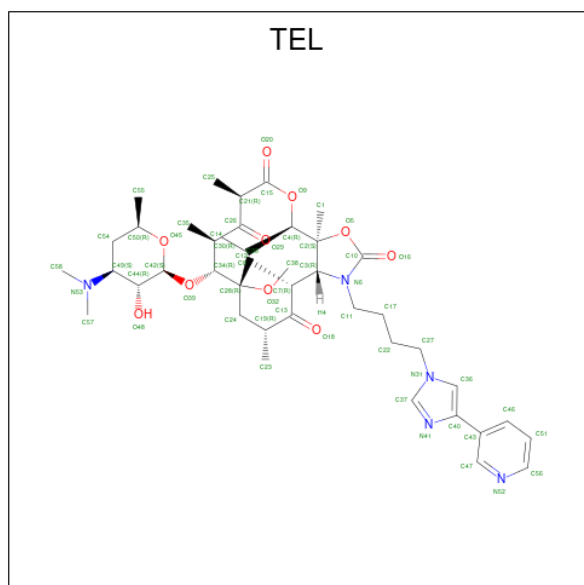
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	t	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 51 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	x	87	Total	C	N	O	P	0	0
			1861	829	333	612	87		

- Molecule 52 is TELITHROMYCIN (CCD ID: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).

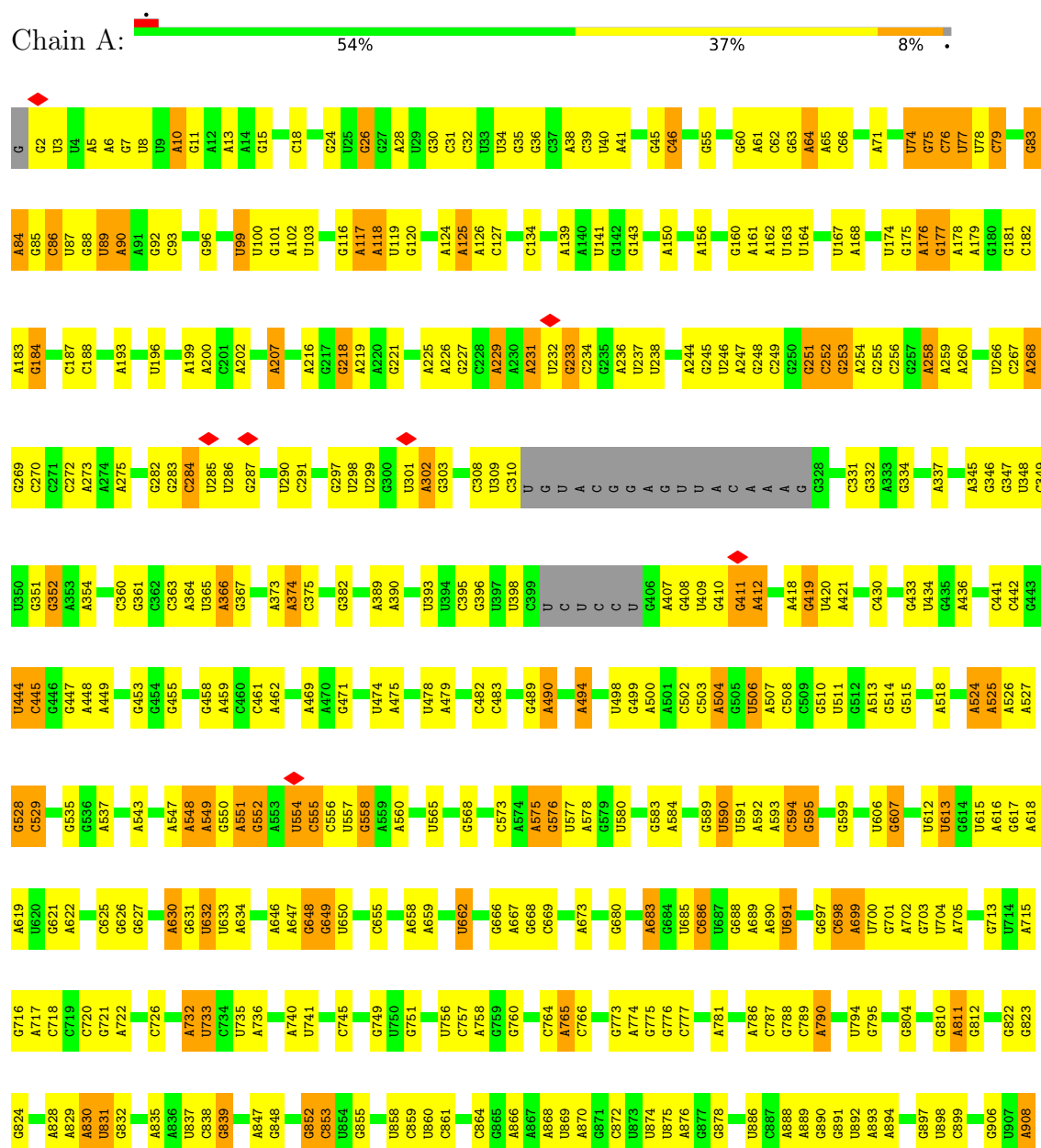


Mol	Chain	Residues	Atoms				AltConf
52	A	1	Total	C	N	O	0
			58	43	5	10	

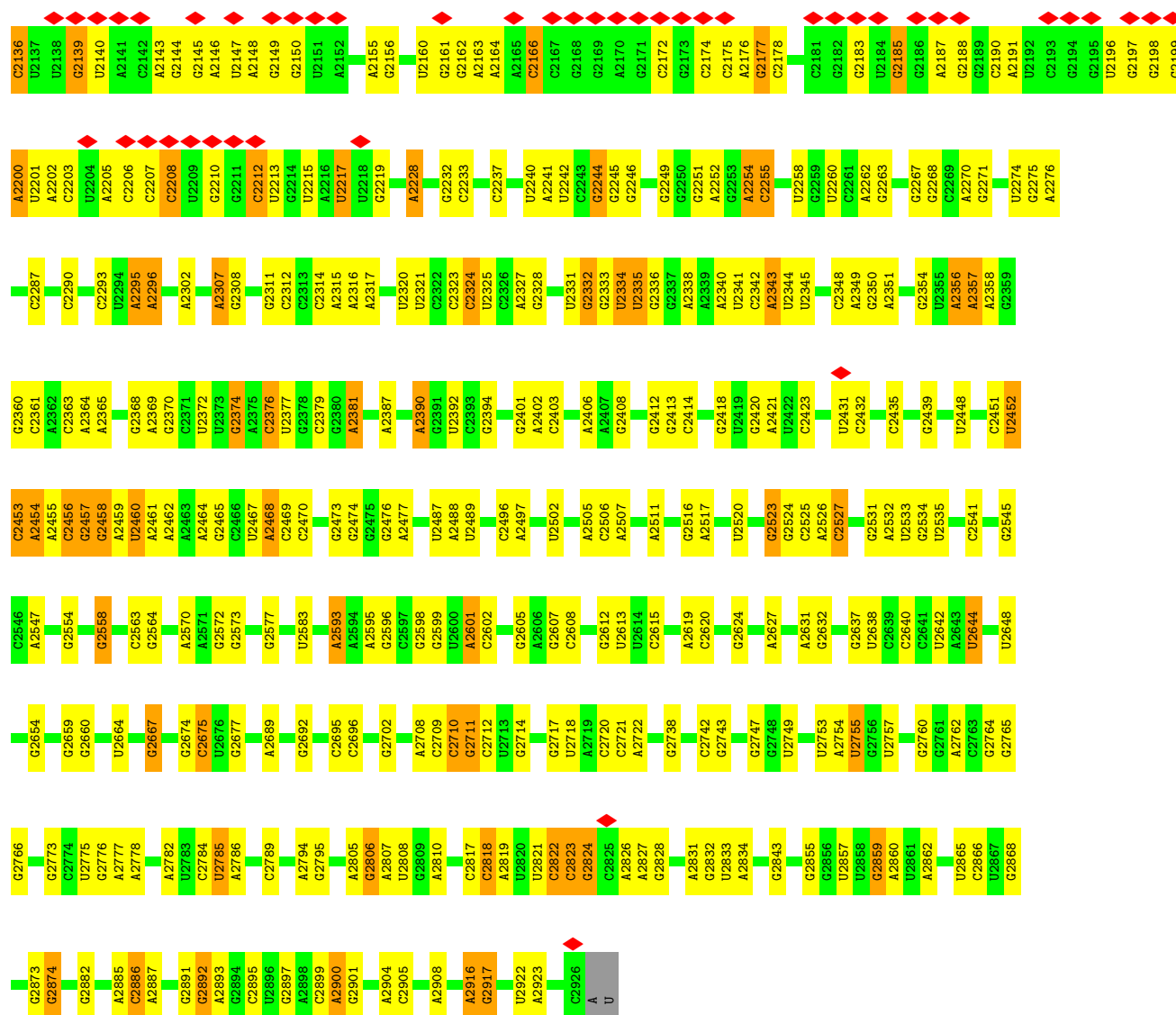
3 Residue-property plots

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

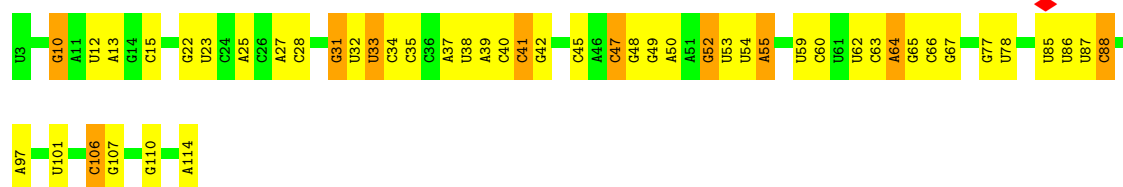
• Molecule 1: 23S ribosomal RNA



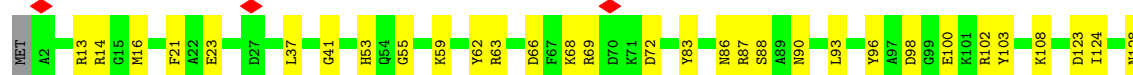


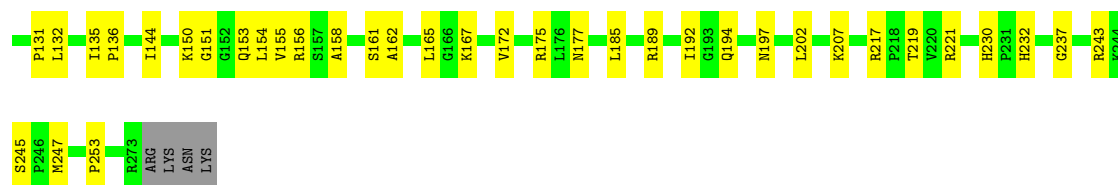


Chain B:



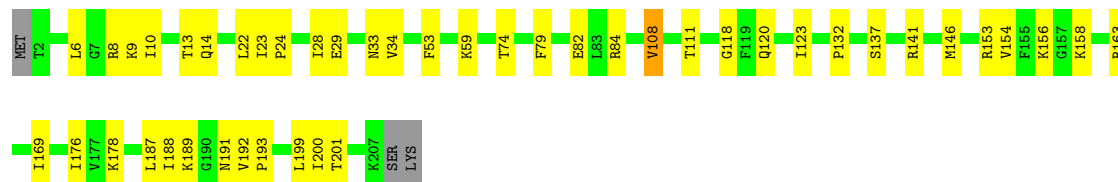
Chain C:





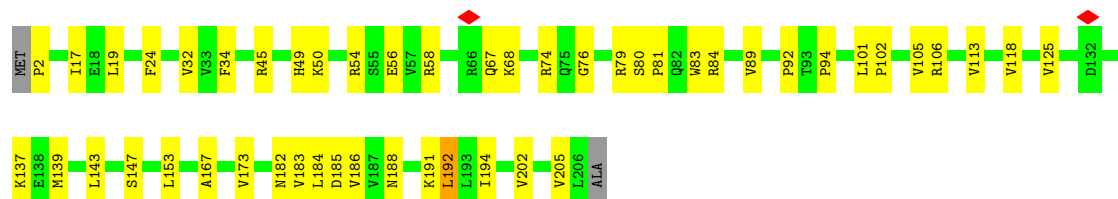
- Molecule 4: 50S ribosomal protein L3

Chain D: 77% 21% .



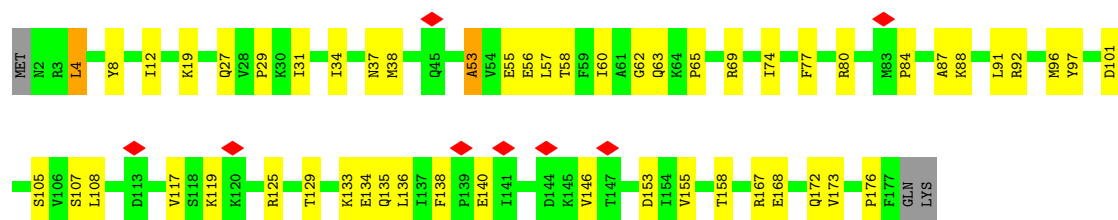
- Molecule 5: 50S ribosomal protein L4

Chain E: 75% 24% .



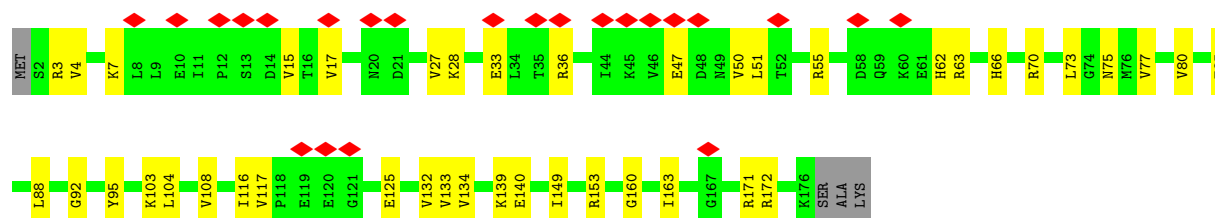
- Molecule 6: 50S ribosomal protein L5

Chain F: 68% 29% ..



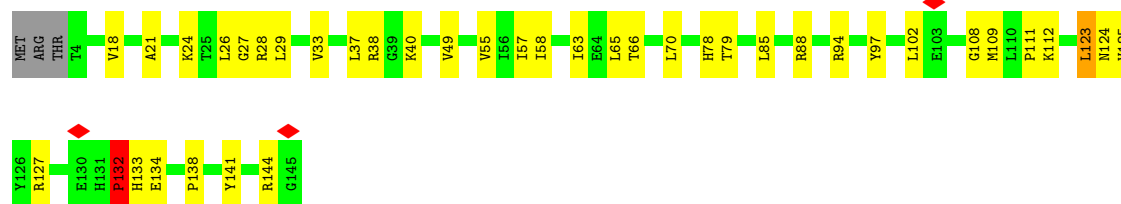
- Molecule 7: 50S ribosomal protein L6

Chain G: 13% 74% 23% .



- Molecule 8: 50S ribosomal protein L13

Chain J:  70% 26% ...



- Molecule 9: 50S ribosomal protein L14

Chain K:  73% 26%



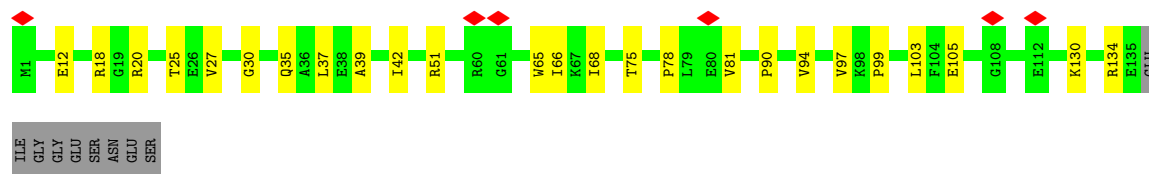
- Molecule 10: 50S ribosomal protein L15

Chain L:  82% 16%



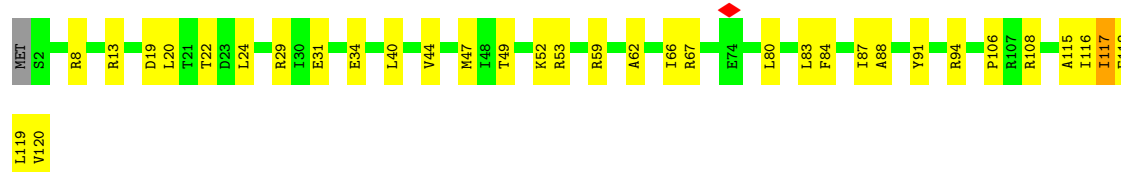
- Molecule 11: 50S ribosomal protein L16

Chain M:  76% 17% 6%



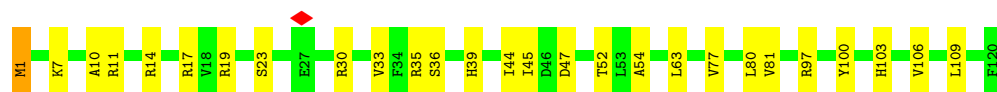
- Molecule 12: 50S ribosomal protein L17

Chain N:  71% 28%



- Molecule 13: 50S ribosomal protein L18

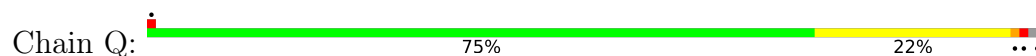
Chain O:  78% 22%



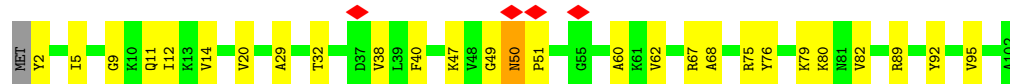
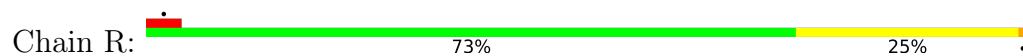
- Molecule 14: 50S ribosomal protein L19



- Molecule 15: 50S ribosomal protein L20



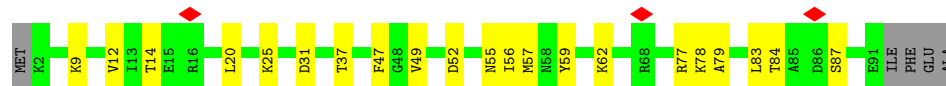
- Molecule 16: 50S ribosomal protein L21



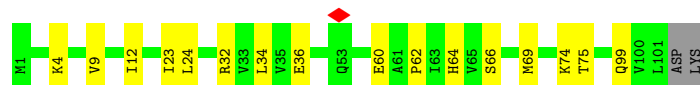
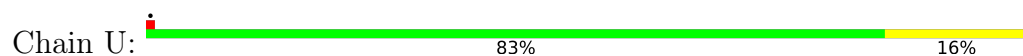
- Molecule 17: 50S ribosomal protein L22



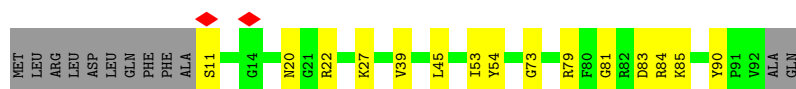
- Molecule 18: 50S ribosomal protein L23



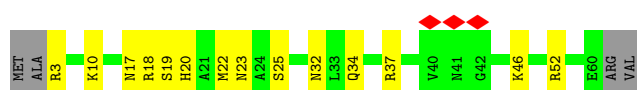
- Molecule 19: 50S ribosomal protein L24



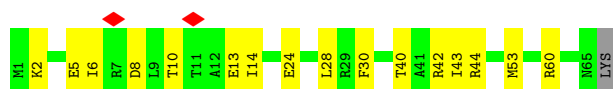
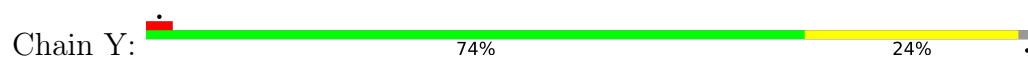
- Molecule 20: 50S ribosomal protein L27



- Molecule 21: 50S ribosomal protein L28



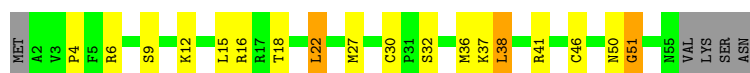
- Molecule 22: 50S ribosomal protein L29



- Molecule 23: 50S ribosomal protein L30



- Molecule 24: 50S ribosomal protein L32



- Molecule 25: 50S ribosomal protein L33 1



- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35

Chain 3:  74% 21% . .



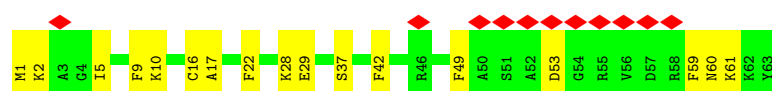
- Molecule 28: 50S ribosomal protein L36

Chain 4:  57% 43%



- Molecule 29: 50S ribosomal protein L31

Chain 6:  17% 73% 27%



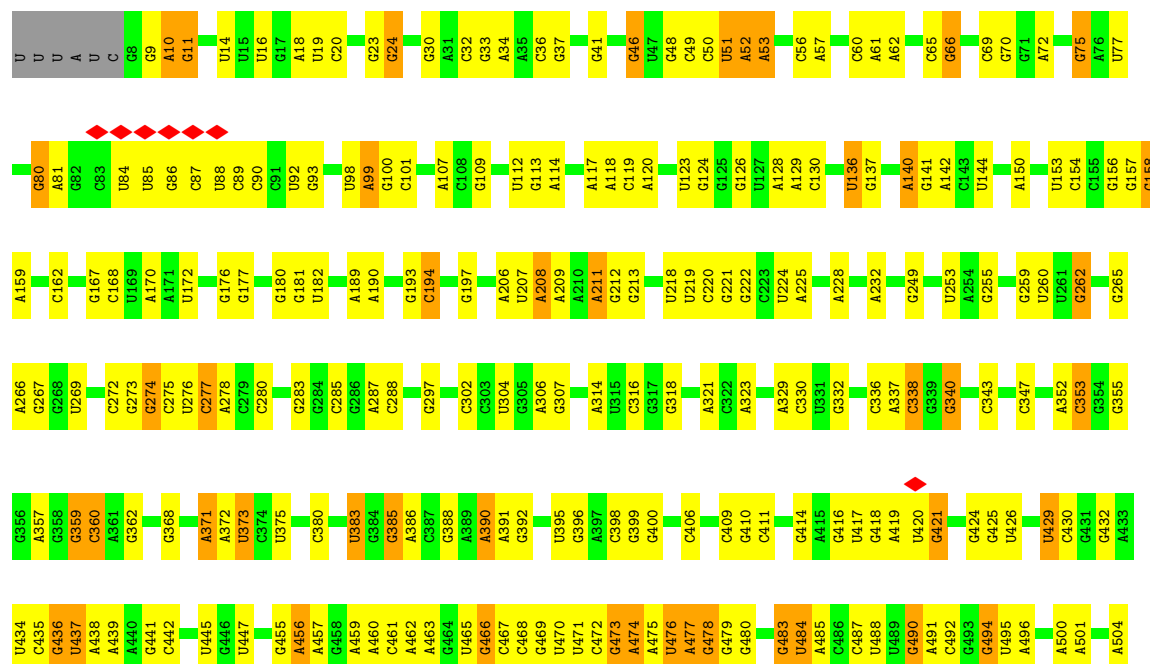
- Molecule 30: mRNA

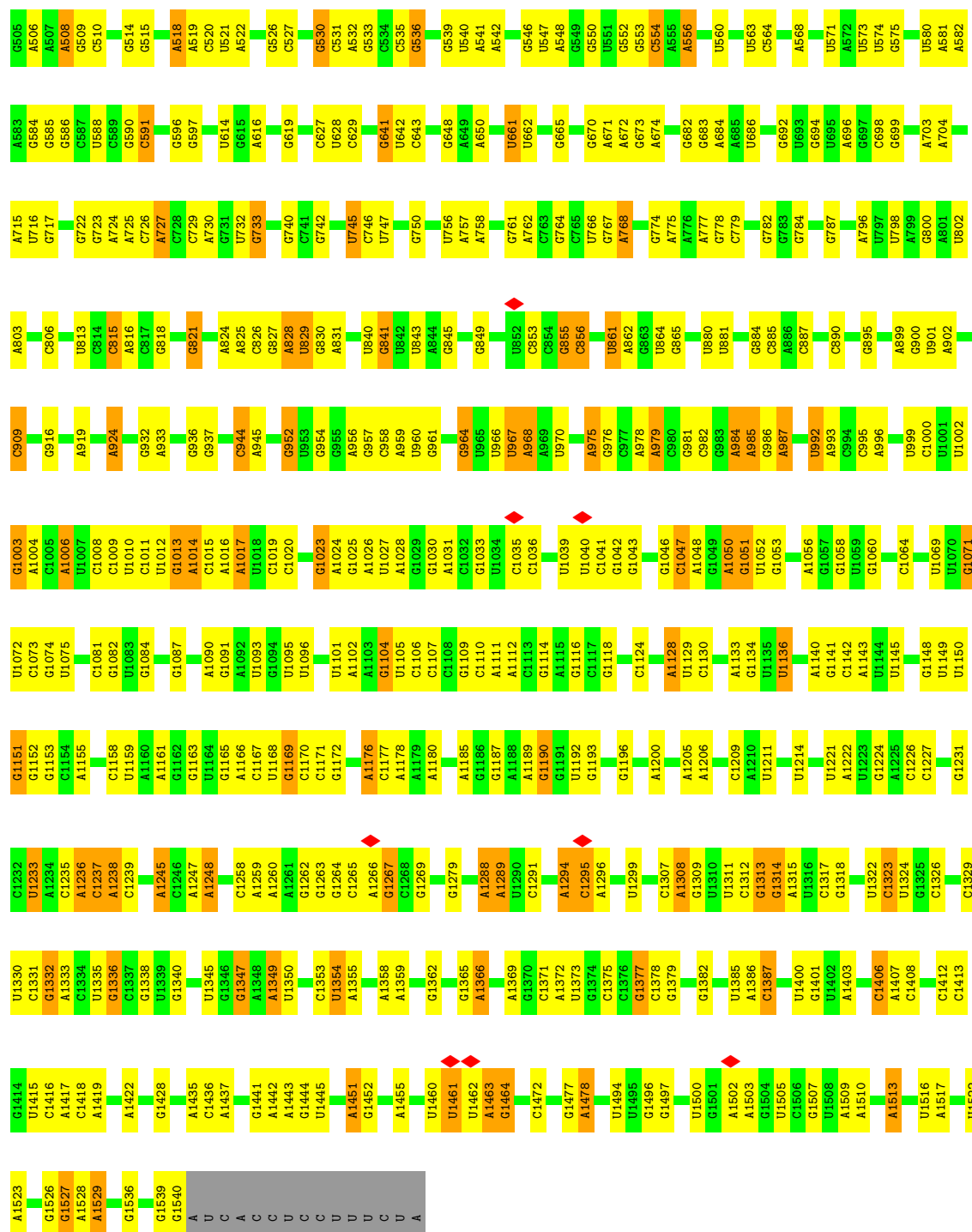
Chain 7:  67% 33%



- Molecule 31: 16S ribosomal RNA

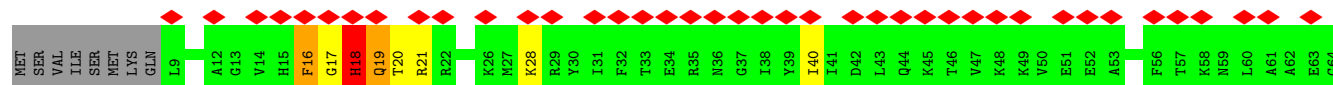
Chain a:  54% 36% 8% .

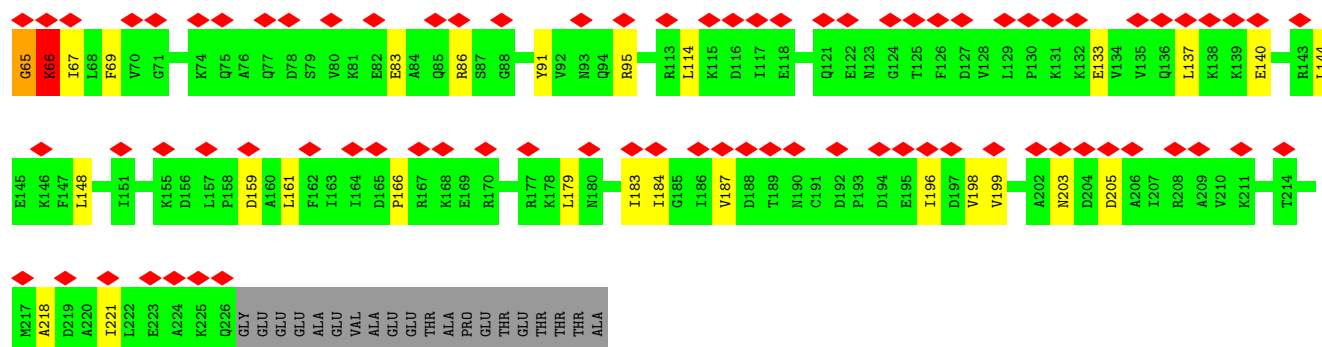




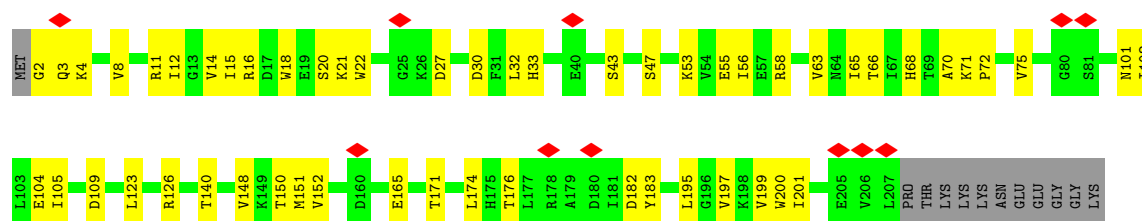
• Molecule 32: 30S ribosomal protein S2

Chain b: 49% 74% 13% 11%

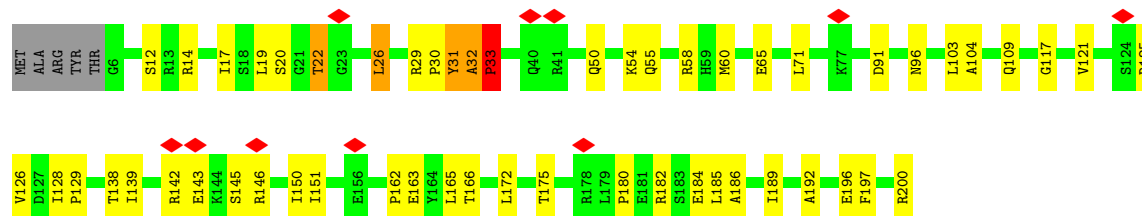




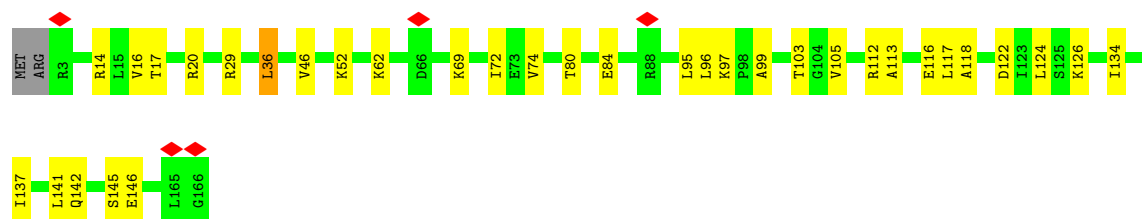
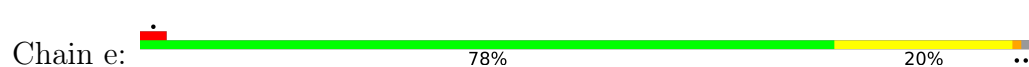
• Molecule 33: 30S ribosomal protein S3



• Molecule 34: 30S ribosomal protein S4

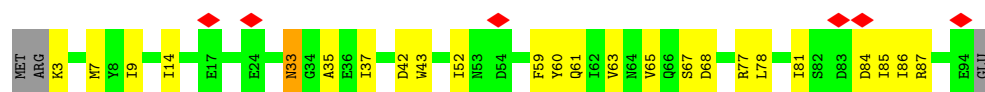


• Molecule 35: 30S ribosomal protein S5

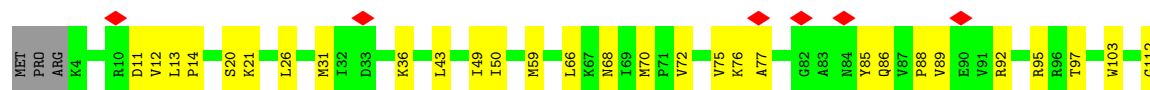


• Molecule 36: 30S ribosomal protein S6





- Molecule 37: 30S ribosomal protein S7



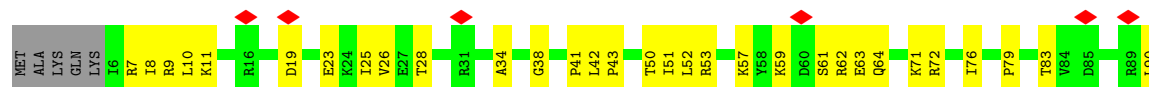
- Molecule 38: 30S ribosomal protein S8



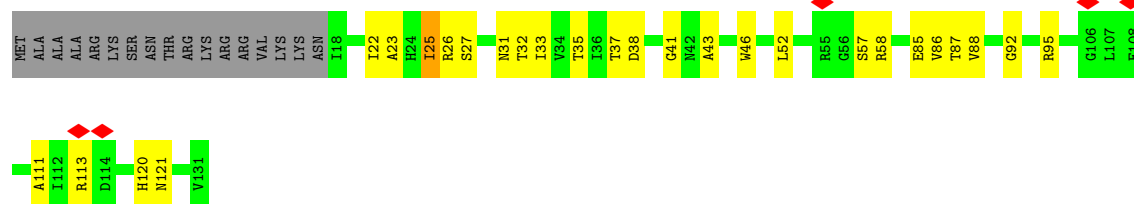
- Molecule 39: 30S ribosomal protein S9



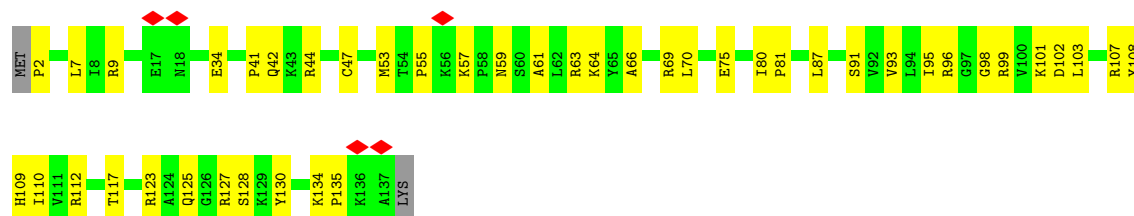
- Molecule 40: 30S ribosomal protein S10



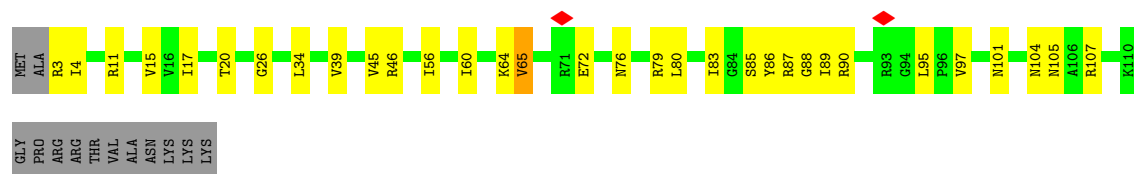
- Molecule 41: 30S ribosomal protein S11



- Molecule 42: 30S ribosomal protein S12



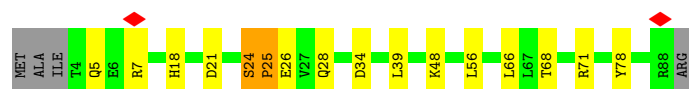
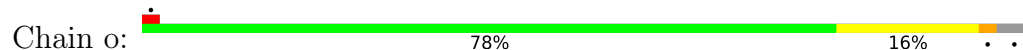
- Molecule 43: 30S ribosomal protein S13



- Molecule 44: 30S ribosomal protein S14

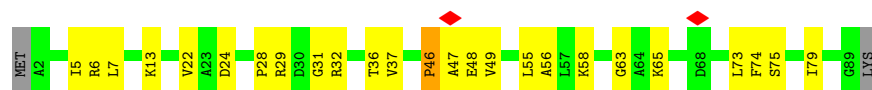


- Molecule 45: 30S ribosomal protein S15



- Molecule 46: 30S ribosomal protein S16

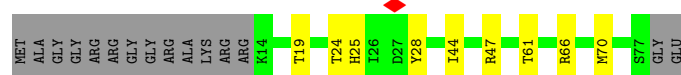




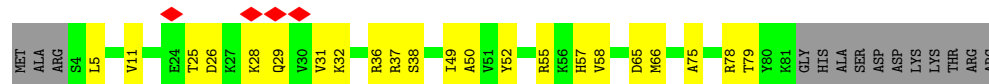
- Molecule 47: 30S ribosomal protein S17



- Molecule 48: 30S ribosomal protein S18



- Molecule 49: 30S ribosomal protein S19



- Molecule 50: 30S ribosomal protein S20



- Molecule 51: P-tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68652	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.425	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.083	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.061, 1.061, 1.061	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/69438	0.49	1/108311 (0.0%)
2	B	0.28	0/2675	0.48	0/4170
3	C	0.42	0/2120	0.76	0/2845
4	D	0.42	0/1591	0.76	0/2132
5	E	0.39	0/1580	0.74	0/2132
6	F	0.35	0/1405	0.80	0/1887
7	G	0.28	0/1360	0.67	0/1832
8	J	0.42	0/1146	0.77	0/1542
9	K	0.40	0/927	0.82	0/1245
10	L	0.40	0/1093	0.76	0/1457
11	M	0.36	0/1099	0.72	0/1468
12	N	0.42	0/960	0.72	0/1284
13	O	0.34	0/921	0.79	0/1236
14	P	0.34	0/957	0.74	0/1279
15	Q	0.46	0/952	0.81	1/1266 (0.1%)
16	R	0.40	0/797	0.83	2/1070 (0.2%)
17	S	0.44	0/851	0.89	4/1146 (0.3%)
18	T	0.33	0/731	0.67	0/974
19	U	0.35	0/772	0.82	0/1032
20	W	0.40	0/638	0.88	0/847
21	X	0.36	0/448	0.81	0/596
22	Y	0.32	0/531	0.73	0/707
23	Z	0.34	0/457	0.73	0/613
24	0	0.40	0/433	0.78	0/574
25	1	0.34	0/406	0.74	0/540
26	2	0.42	0/370	0.70	0/483
27	3	0.38	0/519	0.70	0/680
28	4	0.37	0/299	0.70	0/393
29	6	0.29	0/509	0.75	2/678 (0.3%)
30	7	0.27	0/65	0.44	0/98
31	a	0.40	0/36826	0.49	0/57450
32	b	0.32	0/1782	0.88	7/2392 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	c	0.40	0/1641	0.77	0/2208
34	d	0.41	0/1598	0.86	2/2147 (0.1%)
35	e	0.45	0/1230	0.80	0/1655
36	f	0.37	0/766	0.72	0/1031
37	g	0.40	0/1196	0.82	2/1604 (0.1%)
38	h	0.45	0/1048	0.87	0/1407
39	i	0.39	0/979	0.82	0/1315
40	j	0.46	0/773	0.79	0/1044
41	k	0.38	0/852	0.75	0/1153
42	l	0.44	0/1069	0.83	0/1435
43	m	0.41	0/873	0.93	1/1166 (0.1%)
44	n	0.44	0/507	0.95	2/672 (0.3%)
45	o	0.39	0/718	0.72	0/960
46	p	0.44	0/708	0.92	2/950 (0.2%)
47	q	0.38	0/699	0.79	0/933
48	r	0.38	0/526	0.77	0/705
49	s	0.33	0/649	0.74	0/872
50	t	0.37	0/639	0.79	0/852
51	x	0.33	0/2080	0.47	0/3242
All	All	0.37	0/153209	0.58	26/229710 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	D	0	1
6	F	0	3
8	J	0	1
10	L	0	2
13	O	0	1
15	Q	0	1
16	R	0	2
17	S	0	1
24	0	0	2
29	6	0	1
32	b	0	5
34	d	0	5
35	e	0	1
36	f	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
37	g	0	2
38	h	0	1
42	l	0	2
43	m	0	3
45	o	0	2
48	r	0	2
All	All	0	40

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	b	18	HIS	CA-C-N	8.12	137.06	121.54
32	b	18	HIS	C-N-CA	8.12	137.06	121.54
46	p	46	PRO	CA-C-N	6.99	134.89	121.54
46	p	46	PRO	C-N-CA	6.99	134.89	121.54
32	b	28	LYS	N-CA-C	-6.79	105.28	113.97
17	S	39	THR	N-CA-C	6.61	124.41	109.81
43	m	4	ILE	N-CA-C	6.29	116.78	110.23
32	b	66	LYS	CA-C-N	6.16	133.06	121.97
32	b	66	LYS	C-N-CA	6.16	133.06	121.97
32	b	19	GLN	N-CA-C	6.06	123.70	110.80
17	S	40	PRO	N-CA-C	5.76	124.34	112.47
37	g	114	LYS	CA-C-N	5.71	132.45	121.54
37	g	114	LYS	C-N-CA	5.71	132.45	121.54
17	S	38	LEU	CA-C-N	5.52	135.27	121.80
17	S	38	LEU	C-N-CA	5.52	135.27	121.80
29	6	61	LYS	CA-C-N	5.39	128.91	120.82
29	6	61	LYS	C-N-CA	5.39	128.91	120.82
15	Q	92	ARG	CA-CB-CG	5.32	124.74	114.10
34	d	145	SER	CA-C-N	5.26	128.10	120.79
34	d	145	SER	C-N-CA	5.26	128.10	120.79
1	A	1883	A	C2'-C3'-O3'	5.25	121.57	113.70
44	n	24	CYS	CA-C-N	5.18	131.44	121.54
44	n	24	CYS	C-N-CA	5.18	131.44	121.54
16	R	49	GLY	CA-C-N	5.07	134.18	121.80
16	R	49	GLY	C-N-CA	5.07	134.18	121.80
32	b	17	GLY	N-CA-C	5.06	125.18	113.18

There are no chirality outliers.

All (40) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	0	50	ASN	Peptide
24	0	51	GLY	Peptide
29	6	59	PHE	Peptide
3	C	153	GLN	Peptide
4	D	53	PHE	Peptide
6	F	117	VAL	Peptide
6	F	138	PHE	Peptide
6	F	53	ALA	Peptide
8	J	132	PRO	Peptide
10	L	18	ARG	Peptide
10	L	35	HIS	Peptide
13	O	1	MET	Peptide
15	Q	102	ASP	Peptide
16	R	50	ASN	Peptide
16	R	51	PRO	Peptide
17	S	39	THR	Peptide
32	b	148	LEU	Peptide
32	b	16	PHE	Peptide
32	b	18	HIS	Peptide
32	b	65	GLY	Peptide
32	b	66	LYS	Peptide
34	d	117	GLY	Peptide
34	d	192	ALA	Peptide
34	d	31	TYR	Peptide
34	d	32	ALA	Peptide
34	d	33	PRO	Peptide
35	e	20	ARG	Peptide
36	f	33	ASN	Peptide
37	g	114	LYS	Peptide
37	g	129	ASN	Peptide
38	h	98	LEU	Peptide
42	l	34	GLU	Peptide
42	l	57	LYS	Peptide
43	m	104	ASN	Peptide
43	m	3	ARG	Peptide
43	m	65	VAL	Peptide
45	o	24	SER	Peptide
45	o	5	GLN	Peptide
48	r	24	THR	Peptide
48	r	25	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	61997	0	31214	512	0
2	B	2392	0	1213	15	0
3	C	2083	0	2168	49	0
4	D	1569	0	1637	35	0
5	E	1561	0	1647	41	0
6	F	1386	0	1446	41	0
7	G	1342	0	1388	24	0
8	J	1123	0	1162	29	0
9	K	920	0	977	24	0
10	L	1081	0	1132	23	0
11	M	1076	0	1145	15	0
12	N	953	0	983	23	0
13	O	912	0	947	21	0
14	P	944	0	1020	28	0
15	Q	940	0	1005	25	0
16	R	786	0	826	21	0
17	S	842	0	899	19	0
18	T	725	0	770	17	0
19	U	762	0	821	10	0
20	W	630	0	644	12	0
21	X	444	0	487	11	0
22	Y	530	0	568	11	0
23	Z	455	0	491	12	0
24	0	426	0	441	15	0
25	1	401	0	413	18	0
26	2	367	0	410	12	0
27	3	512	0	564	16	0
28	4	296	0	342	13	0
29	6	499	0	491	13	0
30	7	60	0	32	1	0
31	a	32891	0	16559	331	0
32	b	1757	0	1830	17	0
33	c	1619	0	1658	33	0
34	d	1568	0	1604	32	0
35	e	1218	0	1300	22	0
36	f	755	0	746	17	0
37	g	1181	0	1235	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	h	1036	0	1095	17	0
39	i	966	0	1005	25	0
40	j	761	0	795	31	0
41	k	838	0	854	19	0
42	l	1052	0	1112	35	0
43	m	868	0	925	24	0
44	n	497	0	531	23	0
45	o	710	0	735	9	0
46	p	695	0	721	15	0
47	q	691	0	728	18	0
48	r	518	0	555	6	0
49	s	633	0	649	20	0
50	t	637	0	696	17	0
51	x	1861	0	938	18	0
52	A	58	0	65	20	0
All	All	140824	0	93619	1527	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1527) 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:A:334:G:H1	1:A:393:U:H3	1.06	1.03
6:F:80:ARG:NH2	51:x:19:G:O6	1.89	1.03
31:a:455:G:H21	31:a:496:A:H62	1.07	0.96
31:a:964:G:N2	31:a:1236:A:H62	1.64	0.95
1:A:2087:A:H2	52:A:3001:TEL:H351	1.32	0.95
31:a:964:G:H21	31:a:1236:A:N6	1.65	0.93
51:x:1:G:H1	51:x:83:U:H3	0.99	0.92
31:a:964:G:H21	31:a:1236:A:H62	0.93	0.92
1:A:2824:G:H21	1:A:2827:A:H62	1.13	0.90
32:b:133:GLU:O	32:b:137:LEU:HB3	1.72	0.90
1:A:2824:G:N2	1:A:2827:A:N7	2.18	0.90
25:1:5:ILE:HB	25:1:19:SER:O	1.74	0.86
1:A:246:U:OP2	27:3:8:ARG:NH2	2.07	0.86
1:A:1846:G:OP2	3:C:156:ARG:NH2	2.08	0.86
1:A:1088:G:H1	1:A:1159:U:H3	1.24	0.86
31:a:1441:G:HO2'	31:a:1477:G:H1	1.23	0.85
31:a:982:C:OP2	40:j:59:LYS:NZ	2.08	0.85
1:A:2717:G:N1	1:A:2749:U:OP2	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1808:U:OP2	1:A:1813:A:N6	2.12	0.83
1:A:795:G:O6	52:A:3001:TEL:H56	1.80	0.81
1:A:419:G:N2	1:A:448:A:OP2	2.12	0.81
1:A:2307:A:OP2	20:W:20:ASN:ND2	2.13	0.81
31:a:177:G:OP2	50:t:60:LYS:NZ	2.14	0.81
1:A:2087:A:C2	52:A:3001:TEL:H351	2.15	0.81
31:a:535:C:OP2	42:l:101:LYS:NZ	2.13	0.80
31:a:699:G:OP2	41:k:31:ASN:ND2	2.14	0.80
1:A:1856:U:OP2	3:C:221:ARG:NH2	2.16	0.78
1:A:510:G:N2	1:A:513:A:OP2	2.13	0.78
1:A:2824:G:N2	1:A:2827:A:H62	1.82	0.77
20:W:73:GLY:HA3	20:W:90:TYR:O	1.84	0.77
31:a:269:U:OP2	50:t:74:ARG:NH2	2.19	0.76
1:A:2824:G:H21	1:A:2827:A:N6	1.84	0.75
31:a:455:G:H21	31:a:496:A:N6	1.84	0.75
31:a:1369:A:OP2	44:n:35:ARG:NH2	2.19	0.75
31:a:455:G:N2	31:a:496:A:H62	1.84	0.75
52:A:3001:TEL:H112	52:A:3001:TEL:O18	1.87	0.74
31:a:473:G:N1	31:a:476:U:OP2	2.19	0.74
31:a:388:G:N2	31:a:391:A:OP2	2.15	0.74
31:a:1406:C:OP2	35:e:29:ARG:NH2	2.21	0.74
31:a:673:G:H22	31:a:750:G:H1	1.36	0.73
1:A:2390:A:OP2	27:3:24:ARG:NH1	2.21	0.73
31:a:960:U:OP2	43:m:101:ASN:ND2	2.22	0.72
1:A:2640:C:C6	52:A:3001:TEL:H352	2.24	0.72
6:F:96:MET:SD	6:F:96:MET:N	2.62	0.72
1:A:894:A:N6	1:A:980:C:C4	2.57	0.72
1:A:2785:U:OP2	28:4:19:ARG:NE	2.22	0.72
47:q:25:VAL:O	47:q:45:LYS:HA	1.90	0.71
1:A:284:C:O2	1:A:287:G:N2	2.22	0.71
1:A:612:U:N3	1:A:615:U:OP2	2.23	0.71
34:d:12:SER:HB3	34:d:19:LEU:HD22	1.73	0.71
4:D:9:LYS:HB2	4:D:200:ILE:HD12	1.72	0.70
44:n:24:CYS:SG	44:n:25:GLU:N	2.63	0.70
1:A:1820:A:N6	1:A:1857:G:O2'	2.24	0.70
1:A:1257:C:OP2	15:Q:15:LYS:NZ	2.21	0.70
41:k:22:ILE:HG22	41:k:85:GLU:HB3	1.73	0.69
1:A:1043:G:OP2	15:Q:58:ARG:NE	2.24	0.69
1:A:1403:G:N2	1:A:1406:A:OP2	2.22	0.69
47:q:7:ARG:HB2	47:q:64:MET:HE3	1.74	0.69
31:a:665:G:O2'	45:o:28:GLN:NE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1116:G:H5''	33:c:171:THR:HG22	1.74	0.69
31:a:1158:C:OP2	39:i:11:ARG:NH2	2.25	0.69
1:A:721:G:H5''	5:E:76:GLY:H	1.57	0.69
1:A:1381:A:O2'	1:A:1383:U:OP2	2.09	0.69
12:N:20:LEU:HB3	12:N:40:LEU:HD11	1.73	0.69
1:A:607:G:H21	15:Q:37:GLN:HE22	1.37	0.69
31:a:1101:U:N3	31:a:1104:G:OP2	2.19	0.69
1:A:911:G:H21	1:A:913:A:H61	1.40	0.68
1:A:535:G:H4'	17:S:49:LYS:HD2	1.76	0.68
1:A:1380:U:OP2	1:A:1433:U:O2'	2.09	0.68
42:l:44:ARG:HA	42:l:93:VAL:O	1.93	0.68
2:B:13:A:OP2	2:B:67:G:N2	2.26	0.68
6:F:125:ARG:HB3	13:O:1:MET:HG2	1.75	0.68
33:c:66:THR:HA	33:c:101:ASN:O	1.94	0.68
34:d:55:GLN:HA	34:d:58:ARG:HG2	1.76	0.67
14:P:62:ARG:NH1	14:P:100:LEU:O	2.27	0.67
38:h:25:LEU:O	38:h:61:ARG:HA	1.93	0.67
1:A:514:G:OP2	26:2:34:ARG:NH2	2.27	0.67
1:A:999:A:OP2	11:M:18:ARG:NH1	2.26	0.67
1:A:1086:U:H3	1:A:1161:A:H61	1.42	0.67
1:A:1304:G:OP1	24:0:16:ARG:NH2	2.28	0.67
34:d:143:GLU:HA	34:d:146:ARG:HD2	1.75	0.67
11:M:39:ALA:HB2	11:M:99:PRO:HD3	1.76	0.67
15:Q:82:GLY:O	15:Q:86:SER:HB2	1.94	0.67
1:A:2258:U:O2	21:X:34:GLN:NE2	2.28	0.67
34:d:180:PRO:HB2	34:d:185:LEU:HD21	1.76	0.66
9:K:104:ARG:HH22	14:P:34:GLU:HG2	1.60	0.66
36:f:43:TRP:HB2	36:f:60:TYR:HB2	1.77	0.66
3:C:144:ILE:HB	3:C:154:LEU:HB2	1.76	0.66
1:A:688:G:N2	1:A:691:U:OP2	2.21	0.66
1:A:2108:U:O2'	21:X:23:ASN:ND2	2.29	0.66
1:A:1756:U:H5'	1:A:1757:G:H5''	1.77	0.66
31:a:1365:G:H2'	31:a:1366:A:H8	1.60	0.66
1:A:1352:U:OP2	1:A:1353:C:N4	2.25	0.66
31:a:818:G:OP2	45:o:48:LYS:NZ	2.28	0.66
42:l:80:ILE:HG12	42:l:110:ILE:HD12	1.78	0.66
1:A:760:G:H21	1:A:765:A:H2	1.44	0.66
1:A:1292:G:OP2	15:Q:13:ARG:NH2	2.16	0.66
8:J:78:HIS:ND1	8:J:79:THR:O	2.29	0.65
13:O:14:ARG:HG3	13:O:17:ARG:HH12	1.61	0.65
1:A:2624:G:N2	1:A:2627:A:OP2	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:58:PHE:O	27:3:13:ARG:NH1	2.29	0.65
1:A:1377:G:N7	18:T:62:LYS:NZ	2.44	0.65
1:A:580:U:H5'	15:Q:42:SER:HB2	1.77	0.64
1:A:1286:A:H4'	5:E:45:ARG:HH12	1.62	0.64
51:x:9:G:OP1	51:x:22:G:N1	2.28	0.64
1:A:515:G:N7	26:2:39:ARG:NH2	2.46	0.64
31:a:1382:G:H5''	37:g:36:LYS:HD3	1.78	0.64
1:A:1176:U:OP2	1:A:2599:G:N2	2.27	0.64
7:G:85:GLU:HA	7:G:134:VAL:O	1.98	0.64
31:a:52:A:O2'	31:a:368:G:N2	2.30	0.64
34:d:91:ASP:HA	34:d:96:ASN:HD22	1.61	0.64
1:A:911:G:N2	1:A:913:A:H61	1.95	0.64
1:A:254:A:H4'	10:L:47:ARG:HH12	1.63	0.64
1:A:1056:A:OP1	15:Q:66:ASN:ND2	2.31	0.64
1:A:1036:A:O2'	1:A:1038:C:OP2	2.13	0.64
31:a:692:G:N2	41:k:41:GLY:O	2.31	0.64
14:P:39:ARG:HH22	31:a:353:C:H3'	1.63	0.64
23:Z:37:HIS:HB3	23:Z:43:ILE:HD13	1.78	0.64
34:d:196:GLU:OE1	35:e:112:ARG:NH1	2.31	0.64
9:K:7:ARG:HA	9:K:19:VAL:O	1.97	0.64
1:A:650:U:H5''	5:E:102:PRO:HB3	1.79	0.63
1:A:1542:A:O2'	1:A:1544:C:N4	2.31	0.63
9:K:115:VAL:HG13	9:K:121:VAL:HG21	1.80	0.63
1:A:698:C:O2'	1:A:699:A:H5''	1.98	0.63
39:i:65:VAL:HG11	39:i:79:ILE:HG12	1.80	0.63
1:A:253:G:H4'	10:L:59:GLN:HE21	1.63	0.63
29:6:53:ASP:OD2	43:m:64:LYS:HG2	1.98	0.63
11:M:78:PRO:HG2	11:M:81:VAL:HG21	1.81	0.63
31:a:890:C:OP1	42:l:9:ARG:NH2	2.32	0.63
40:j:28:THR:HG21	40:j:90:LEU:HD21	1.81	0.63
1:A:160:G:O2'	1:A:168:A:N6	2.32	0.62
46:p:28:PRO:HG2	46:p:31:GLY:HA3	1.79	0.62
32:b:161:LEU:HB3	32:b:183:ILE:HG22	1.80	0.62
46:p:5:ILE:HG12	46:p:22:VAL:HG22	1.80	0.62
8:J:88:ARG:NH1	8:J:97:TYR:OH	2.32	0.62
17:S:52:LYS:HA	17:S:55:ILE:HD12	1.80	0.62
1:A:363:C:OP2	5:E:137:LYS:NZ	2.29	0.62
31:a:968:A:N7	49:s:55:ARG:NH1	2.48	0.62
19:U:74:LYS:HD3	19:U:75:THR:HG23	1.80	0.62
37:g:76:LYS:HE3	37:g:89:VAL:HG21	1.81	0.62
39:i:11:ARG:HG2	39:i:16:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:A:H61	1:A:2042:A:H5''	1.64	0.62
31:a:1013:G:N2	31:a:1014:A:O2'	2.31	0.62
31:a:1288:A:H5''	40:j:9:ARG:HH22	1.65	0.62
34:d:91:ASP:OD1	34:d:96:ASN:ND2	2.32	0.62
1:A:1397:G:N1	1:A:1411:U:OP2	2.25	0.62
12:N:84:PHE:O	12:N:88:ALA:HB3	2.00	0.62
18:T:9:LYS:HE3	18:T:31:ASP:HB3	1.80	0.62
1:A:1171:G:OP2	1:A:1172:A:O2'	2.16	0.62
31:a:1226:C:OP1	44:n:9:LYS:NZ	2.33	0.62
31:a:560:U:O2'	42:l:96:ARG:NH2	2.33	0.61
38:h:12:THR:HG22	38:h:15:ARG:HH12	1.64	0.61
1:A:1712:G:O2'	1:A:1714:A:N6	2.33	0.61
3:C:72:ASP:OD2	3:C:189:ARG:NH2	2.33	0.61
18:T:20:LEU:HB3	18:T:25:LYS:HG3	1.81	0.61
33:c:16:ARG:NH2	33:c:182:ASP:OD1	2.32	0.61
47:q:81:VAL:HG12	47:q:82:GLU:HG3	1.81	0.61
1:A:1616:G:H4'	3:C:59:LYS:HG3	1.82	0.61
1:A:1991:C:O2'	1:A:1993:G:OP2	2.16	0.61
31:a:421:G:N2	31:a:436:G:O2'	2.33	0.61
9:K:4:GLN:HG2	9:K:5:GLU:HG2	1.82	0.61
1:A:911:G:H21	1:A:913:A:N6	1.98	0.61
1:A:2474:G:OP1	5:E:74:ARG:NH2	2.29	0.61
3:C:66:ASP:OD2	3:C:102:ARG:NH1	2.33	0.61
7:G:4:VAL:O	7:G:70:ARG:NH1	2.33	0.61
23:Z:10:ARG:HB3	23:Z:53:LEU:HA	1.81	0.61
12:N:24:LEU:HD13	12:N:44:VAL:HG21	1.83	0.61
31:a:411:C:H5''	34:d:129:PRO:HD2	1.81	0.61
31:a:733:G:OP2	31:a:864:U:O2'	2.14	0.61
31:a:944:C:O2'	31:a:1353:C:OP2	2.19	0.61
38:h:28:PRO:O	38:h:57:GLN:NE2	2.33	0.61
41:k:92:GLY:H	41:k:95:ARG:HH21	1.48	0.61
48:r:28:TYR:OH	48:r:66:ARG:NH1	2.34	0.61
49:s:50:ALA:HB1	49:s:57:HIS:HB3	1.83	0.61
1:A:1184:G:H21	8:J:109:MET:HE3	1.66	0.61
1:A:2166:C:H42	1:A:2183:G:H1	1.47	0.61
6:F:34:ILE:O	6:F:91:LEU:HB2	2.01	0.61
7:G:47:GLU:HB2	7:G:50:VAL:HB	1.83	0.61
31:a:865:G:OP2	31:a:881:U:N3	2.31	0.60
1:A:2806:G:OP2	1:A:2810:A:O2'	2.15	0.60
12:N:19:ASP:OD1	12:N:67:ARG:NH1	2.34	0.60
3:C:69:ARG:O	3:C:189:ARG:NH1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:G:O2'	1:A:552:G:N2	2.34	0.60
1:A:2640:C:C2	52:A:3001:TEL:H352	2.37	0.60
13:O:44:ILE:HD12	13:O:54:ALA:HB3	1.84	0.60
31:a:445:U:H3	31:a:504:A:H62	1.48	0.60
33:c:27:ASP:HB3	33:c:30:ASP:HB2	1.83	0.60
1:A:894:A:C6	1:A:980:C:N3	2.69	0.60
1:A:2640:C:C5	52:A:3001:TEL:H352	2.36	0.60
37:g:68:ASN:O	37:g:138:ARG:NH2	2.35	0.60
3:C:63:ARG:NH1	3:C:83:TYR:O	2.35	0.60
1:A:1289:U:O2'	10:L:18:ARG:NH2	2.25	0.60
31:a:10:A:N6	34:d:196:GLU:O	2.34	0.60
1:A:445:C:OP1	21:X:32:ASN:ND2	2.35	0.60
31:a:591:C:OP2	31:a:767:G:N2	2.32	0.59
1:A:1831:A:H2	1:A:1844:A:H62	1.50	0.59
1:A:589:G:N2	1:A:590:U:O4	2.32	0.59
1:A:1886:G:OP2	1:A:1886:G:N2	2.32	0.59
8:J:63:ILE:O	8:J:94:ARG:NH1	2.34	0.59
31:a:1375:C:O2'	40:j:62:ARG:NH2	2.35	0.59
1:A:1699:A:N1	1:A:2077:G:O2'	2.35	0.59
3:C:167:LYS:HG2	3:C:172:VAL:HG22	1.85	0.59
16:R:67:ARG:HH21	16:R:89:ARG:HB2	1.67	0.59
47:q:15:VAL:HB	47:q:24:THR:HG23	1.84	0.59
11:M:51:ARG:HG3	11:M:66:ILE:HD11	1.84	0.59
17:S:6:VAL:HG13	17:S:104:THR:HG22	1.83	0.59
31:a:1264:G:O2'	31:a:1267:G:N3	2.31	0.59
37:g:20:SER:HB2	37:g:59:MET:HE1	1.83	0.59
42:l:70:LEU:HD21	42:l:95:ILE:HD12	1.84	0.59
1:A:2857:U:H5'	1:A:2859:G:H5'	1.85	0.59
9:K:80:ASP:OD2	14:P:62:ARG:NH2	2.33	0.59
31:a:150:A:OP2	31:a:168:C:N4	2.34	0.59
1:A:75:G:O2'	1:A:76:C:OP2	2.17	0.59
1:A:2648:U:H5'	4:D:156:LYS:HG2	1.85	0.59
13:O:97:ARG:NH2	13:O:100:TYR:O	2.35	0.59
2:B:31:G:N2	2:B:33:U:O4	2.36	0.59
41:k:38:ASP:O	41:k:41:GLY:N	2.34	0.59
2:B:10:G:OP2	20:W:79:ARG:NH2	2.35	0.58
5:E:182:ASN:ND2	5:E:185:ASP:OD2	2.35	0.58
50:t:10:ARG:O	50:t:14:ASN:HB2	2.02	0.58
1:A:2394:G:O6	27:3:43:LYS:NZ	2.37	0.58
31:a:530:G:N7	42:l:63:ARG:NH1	2.51	0.58
37:g:148:ASN:OD1	41:k:58:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:G:O6	21:X:52:ARG:NH1	2.36	0.58
1:A:1036:A:N3	16:R:75:ARG:NH1	2.51	0.58
18:T:56:ILE:HG21	18:T:77:ARG:HH21	1.67	0.58
40:j:34:ALA:HB2	40:j:83:THR:HG21	1.83	0.58
1:A:1289:U:HO2'	10:L:18:ARG:HH22	1.51	0.58
1:A:2776:G:OP1	7:G:75:ASN:ND2	2.36	0.58
15:Q:92:ARG:NH1	16:R:9:GLY:O	2.36	0.58
31:a:1081:C:H2'	31:a:1082:G:H8	1.69	0.58
44:n:3:LYS:NZ	44:n:28:GLY:O	2.28	0.58
1:A:713:G:H1'	27:3:4:MET:HE2	1.85	0.58
1:A:920:G:H2'	1:A:921:G:H8	1.69	0.58
16:R:76:TYR:HA	16:R:82:VAL:O	2.04	0.58
17:S:24:ILE:HD11	17:S:36:LEU:HD21	1.84	0.58
1:A:828:A:OP1	3:C:217:ARG:NH1	2.36	0.58
1:A:2121:U:H4'	1:A:2122:G:H5'	1.84	0.58
1:A:2135:G:N2	1:A:2212:C:C2	2.71	0.58
1:A:2710:C:O2	1:A:2712:C:N4	2.36	0.58
22:Y:14:ILE:HG23	22:Y:53:MET:HE2	1.86	0.58
30:7:27:U:OP1	31:a:1412:C:N4	2.37	0.58
31:a:383:U:O2	46:p:29:ARG:NH2	2.36	0.58
35:e:97:LYS:HB2	35:e:124:LEU:HB2	1.84	0.58
1:A:2290:C:OP1	20:W:27:LYS:NZ	2.33	0.58
34:d:104:ALA:HB1	34:d:109:GLN:HB3	1.85	0.58
47:q:30:TYR:HB2	47:q:41:LYS:HA	1.84	0.58
8:J:24:LYS:HD2	8:J:29:LEU:HD12	1.86	0.58
10:L:61:LEU:O	27:3:13:ARG:NH1	2.37	0.58
31:a:232:A:OP1	50:t:69:LYS:NZ	2.37	0.58
40:j:41:PRO:HA	40:j:72:ARG:HG2	1.86	0.58
1:A:1033:C:OP1	23:Z:10:ARG:NH2	2.36	0.58
1:A:1649:C:O2'	1:A:1655:A:N6	2.37	0.58
10:L:19:VAL:HG12	10:L:31:ALA:HB1	1.86	0.58
20:W:79:ARG:HD2	20:W:81:GLY:H	1.69	0.58
29:6:49:PHE:HZ	43:m:64:LYS:HA	1.67	0.58
29:6:53:ASP:OD2	43:m:64:LYS:HE2	2.04	0.58
31:a:267:G:OP1	50:t:78:ARG:NH2	2.37	0.58
32:b:65:GLY:HA3	32:b:159:ASP:HB2	1.86	0.58
33:c:11:ARG:NH2	33:c:176:THR:O	2.37	0.58
36:f:33:ASN:HD21	36:f:68:ASP:H	1.52	0.58
13:O:45:ILE:HG12	13:O:52:THR:HG22	1.85	0.58
31:a:1159:U:H4'	40:j:43:PRO:HG3	1.86	0.58
1:A:2523:G:OP1	20:W:11:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:A:N3	2:B:78:U:O2'	2.37	0.57
1:A:2712:C:OP1	14:P:51:ARG:NH1	2.36	0.57
24:0:32:SER:OG	24:0:46:CYS:SG	2.62	0.57
25:1:9:CYS:SG	25:1:10:THR:N	2.76	0.57
34:d:60:MET:HG3	34:d:189:ILE:HD11	1.85	0.57
1:A:2274:U:H5''	1:A:2275:G:H5'	1.87	0.57
1:A:2709:C:H5'	4:D:193:PRO:HA	1.86	0.57
3:C:124:ILE:HG13	3:C:192:ILE:HD13	1.87	0.57
25:1:29:ARG:HG3	25:1:47:GLU:HB3	1.87	0.57
1:A:2361:C:OP1	20:W:84:ARG:NH1	2.37	0.57
13:O:45:ILE:HA	13:O:52:THR:HA	1.87	0.57
31:a:1231:G:H5''	49:s:78:ARG:HH11	1.69	0.57
36:f:52:ILE:HG21	36:f:86:ILE:HG23	1.85	0.57
1:A:2054:C:OP1	4:D:153:ARG:NE	2.31	0.57
6:F:8:TYR:O	6:F:12:ILE:HB	2.04	0.57
13:O:63:LEU:HD22	13:O:80:LEU:HD21	1.86	0.57
32:b:184:ILE:HA	32:b:198:VAL:HB	1.86	0.57
1:A:1830:G:OP2	3:C:150:LYS:NZ	2.37	0.57
44:n:26:ARG:NH2	44:n:46:GLU:OE1	2.37	0.57
1:A:125:A:H5'	26:2:18:PHE:HB3	1.86	0.57
11:M:68:ILE:HD13	11:M:103:LEU:HD22	1.86	0.57
31:a:14:U:O2'	31:a:924:A:OP2	2.20	0.57
31:a:855:G:OP2	48:r:19:THR:OG1	2.19	0.57
1:A:99:U:O4	19:U:4:LYS:NZ	2.35	0.57
1:A:852:G:N2	1:A:876:A:OP1	2.38	0.57
1:A:2640:C:C4	52:A:3001:TEL:C35	2.87	0.57
1:A:2873:G:O2'	1:A:2893:A:N6	2.38	0.57
3:C:123:ASP:O	3:C:128:ASN:ND2	2.38	0.57
6:F:107:SER:OG	6:F:108:LEU:N	2.38	0.57
12:N:8:ARG:O	12:N:13:ARG:NH2	2.37	0.57
18:T:20:LEU:HD22	18:T:25:LYS:HD2	1.86	0.57
36:f:42:ASP:OD1	36:f:61:GLN:NE2	2.37	0.57
37:g:31:MET:HE2	37:g:36:LYS:HG3	1.87	0.57
31:a:285:C:OP1	47:q:47:LYS:NZ	2.34	0.57
31:a:1324:U:O2'	31:a:1369:A:N3	2.35	0.57
51:x:5:A:O2'	51:x:6:G:H5'	2.05	0.57
5:E:2:PRO:HG2	5:E:19:LEU:HB2	1.86	0.57
12:N:83:LEU:HA	12:N:87:ILE:HD12	1.87	0.57
33:c:8:VAL:HG23	33:c:183:TYR:HB3	1.85	0.57
33:c:14:VAL:HG12	33:c:15:ILE:HG13	1.87	0.57
6:F:4:LEU:HB3	6:F:97:TYR:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:77:VAL:HB	10:L:111:ILE:HG12	1.87	0.56
4:D:178:LYS:NZ	14:P:11:GLU:OE2	2.35	0.56
1:A:2577:G:O2'	9:K:4:GLN:OE1	2.22	0.56
2:B:55:A:O2'	6:F:27:GLN:NE2	2.37	0.56
31:a:66:G:OP1	31:a:390:A:N6	2.38	0.56
31:a:1109:G:H3'	32:b:95:ARG:HH22	1.70	0.56
44:n:21:TYR:OH	44:n:23:ARG:NH2	2.38	0.56
38:h:30:SER:H	38:h:33:LYS:HD2	1.69	0.56
44:n:40:CYS:SG	44:n:41:ARG:N	2.79	0.56
1:A:2376:C:O2'	25:1:17:TYR:OH	2.23	0.56
11:M:20:ARG:HD3	11:M:99:PRO:HG2	1.87	0.56
31:a:1025:G:O2'	44:n:15:LYS:NZ	2.39	0.56
1:A:1042:A:H4'	15:Q:92:ARG:HD3	1.86	0.56
35:e:16:VAL:HG12	35:e:17:THR:HG23	1.88	0.56
1:A:2376:C:OP1	25:1:34:LYS:NZ	2.34	0.56
52:A:3001:TEL:H122	52:A:3001:TEL:C11	2.36	0.56
35:e:80:THR:HG22	35:e:122:ASP:HB2	1.87	0.56
1:A:1847:U:O2'	3:C:154:LEU:O	2.24	0.56
17:S:73:GLN:HB2	17:S:106:VAL:HB	1.88	0.56
49:s:31:VAL:HB	49:s:49:ILE:HG22	1.87	0.56
1:A:193:A:H5''	1:A:207:A:H61	1.71	0.56
1:A:2874:G:O6	1:A:2892:G:N3	2.39	0.56
11:M:75:THR:HA	11:M:90:PRO:HA	1.88	0.56
31:a:1096:U:H3	31:a:1109:G:H22	1.52	0.56
38:h:52:VAL:HB	38:h:59:ILE:HB	1.87	0.56
31:a:1069:U:O2'	44:n:45:ARG:NH2	2.39	0.56
31:a:37:G:O2'	42:l:128:SER:O	2.22	0.55
43:m:17:ILE:O	43:m:20:THR:OG1	2.23	0.55
11:M:25:THR:O	11:M:35:GLN:NE2	2.40	0.55
26:2:34:ARG:HG3	26:2:42:LEU:HD12	1.89	0.55
31:a:490:G:O2'	31:a:492:C:N4	2.39	0.55
46:p:6:ARG:NH1	46:p:24:ASP:O	2.39	0.55
1:A:774:A:OP1	1:A:1477:A:O2'	2.18	0.55
1:A:2148:A:H61	1:A:2197:G:H21	1.54	0.55
52:A:3001:TEL:H122	52:A:3001:TEL:H111	1.89	0.55
16:R:5:ILE:O	16:R:11:GLN:HA	2.07	0.55
31:a:48:G:O2'	31:a:373:U:O2	2.24	0.55
31:a:277:C:H2'	31:a:278:A:H8	1.72	0.55
31:a:1165:G:O2'	31:a:1189:A:N1	2.33	0.55
6:F:105:SER:HA	29:6:37:SER:HB3	1.88	0.55
12:N:94:ARG:NH1	12:N:120:VAL:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:g:72:VAL:HB	37:g:142:HIS:HE1	1.72	0.55
39:i:115:LYS:HB2	39:i:118:LEU:HD12	1.88	0.55
47:q:8:LYS:HB3	47:q:65:GLU:HG2	1.88	0.55
1:A:2372:U:HO2'	1:A:2402:A:HO2'	1.52	0.55
1:A:795:G:O6	52:A:3001:TEL:C56	2.53	0.55
28:4:1:MET:HE2	28:4:35:LYS:HE3	1.88	0.55
31:a:1004:A:O2'	44:n:12:ARG:NH2	2.39	0.55
40:j:19:ASP:OD1	40:j:72:ARG:NH1	2.40	0.55
41:k:27:SER:HA	41:k:32:THR:HA	1.88	0.55
1:A:1263:G:OP2	16:R:89:ARG:NH2	2.40	0.55
1:A:1668:G:H2'	1:A:1669:G:H8	1.72	0.55
24:0:12:LYS:HD3	24:0:15:LEU:HD12	1.89	0.55
34:d:50:GLN:HB3	34:d:197:PHE:HB2	1.88	0.55
44:n:29:ARG:NE	44:n:40:CYS:SG	2.77	0.55
1:A:1055:A:OP2	8:J:40:LYS:NZ	2.25	0.55
3:C:37:LEU:HG	3:C:62:TYR:HB2	1.87	0.55
4:D:22:LEU:HD12	9:K:74:GLY:HA3	1.89	0.55
6:F:31:ILE:HA	6:F:158:THR:HA	1.87	0.55
16:R:67:ARG:HB3	16:R:89:ARG:HB3	1.89	0.55
1:A:2526:A:H1'	1:A:2527:C:H5	1.71	0.55
3:C:23:GLU:OE1	3:C:90:ASN:ND2	2.40	0.55
4:D:178:LYS:HB3	4:D:187:LEU:HD12	1.88	0.55
34:d:121:VAL:HG22	34:d:139:ILE:HG12	1.89	0.55
1:A:268:A:O2'	1:A:475:A:N6	2.40	0.54
3:C:100:GLU:OE1	3:C:102:ARG:NH2	2.40	0.54
14:P:27:ARG:NH1	14:P:44:GLU:OE2	2.40	0.54
37:g:13:LEU:HD22	37:g:21:LYS:HE3	1.88	0.54
8:J:18:VAL:HG23	8:J:138:PRO:HB2	1.89	0.54
21:X:18:ARG:HH21	21:X:22:MET:HB3	1.73	0.54
31:a:661:U:O4	31:a:761:G:O2'	2.24	0.54
31:a:703:A:N1	31:a:796:A:O2'	2.40	0.54
31:a:985:A:N6	40:j:50:THR:OG1	2.40	0.54
35:e:105:VAL:O	35:e:112:ARG:NH2	2.40	0.54
40:j:34:ALA:HB1	40:j:76:ILE:HG23	1.89	0.54
14:P:114:ARG:NH2	31:a:1451:A:O2'	2.41	0.54
31:a:1314:G:HO2'	31:a:1315:A:H8	1.56	0.54
43:m:39:VAL:HG11	43:m:56:ILE:HD11	1.89	0.54
7:G:36:ARG:NH2	7:G:140:GLU:OE1	2.41	0.54
31:a:1082:G:OP1	35:e:62:LYS:NZ	2.36	0.54
34:d:166:THR:OG1	34:d:175:THR:OG1	2.24	0.54
25:1:2:ARG:HD2	25:1:20:LYS:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1387:C:O2'	37:g:92:ARG:NH1	2.41	0.54
37:g:13:LEU:HA	37:g:21:LYS:HD2	1.90	0.54
47:q:78:VAL:HG12	47:q:79:GLU:HG2	1.90	0.54
3:C:132:LEU:HD23	3:C:135:ILE:HD12	1.89	0.54
13:O:19:ARG:HH12	13:O:23:SER:HA	1.71	0.54
31:a:726:C:O3'	41:k:121:ASN:ND2	2.41	0.54
1:A:751:G:O2'	1:A:774:A:N6	2.41	0.54
1:A:839:G:N3	1:A:2101:G:O2'	2.35	0.54
1:A:2024:U:O2	9:K:3:GLN:NE2	2.37	0.54
1:A:2708:A:H5'	4:D:169:ILE:HD13	1.90	0.54
6:F:91:LEU:HB3	6:F:96:MET:HG3	1.90	0.54
12:N:29:ARG:NH2	12:N:118:GLU:OE2	2.40	0.54
1:A:1742:G:OP2	1:A:1743:A:O2'	2.21	0.54
1:A:2775:U:H5''	7:G:139:LYS:HB3	1.89	0.54
4:D:34:VAL:HG21	4:D:74:THR:HG21	1.90	0.54
6:F:37:ASN:HB3	6:F:153:ASP:HB2	1.90	0.54
1:A:2190:C:H2'	1:A:2191:A:H8	1.73	0.54
6:F:4:LEU:HD12	6:F:97:TYR:HD1	1.73	0.54
34:d:14:ARG:HB2	34:d:33:PRO:HD3	1.90	0.54
1:A:183:A:OP2	1:A:184:G:H5''	2.07	0.54
1:A:548:A:OP2	1:A:548:A:H8	1.91	0.54
1:A:1135:G:N2	1:A:1136:U:O4	2.41	0.54
1:A:1188:A:H4'	8:J:28:ARG:HH22	1.73	0.54
1:A:1243:A:O2'	1:A:1244:A:OP1	2.26	0.54
1:A:1893:U:OP1	1:A:2439:G:O2'	2.26	0.54
31:a:1169:G:H1	31:a:1185:A:H61	1.55	0.54
39:i:30:VAL:N	39:i:33:ARG:O	2.38	0.54
1:A:1067:A:H61	1:A:1188:A:H61	1.55	0.53
9:K:24:VAL:HG11	9:K:30:ARG:HD2	1.89	0.53
42:l:69:ARG:HB2	42:l:75:GLU:HG2	1.89	0.53
3:C:230:HIS:HD2	3:C:232:HIS:H	1.56	0.53
31:a:318:G:H5''	46:p:32:ARG:HB3	1.91	0.53
31:a:546:G:H5''	42:l:123:ARG:HH22	1.70	0.53
31:a:954:G:N1	31:a:1347:G:OP2	2.34	0.53
42:l:66:ALA:HB2	42:l:80:ILE:HD11	1.88	0.53
46:p:74:PHE:HD1	46:p:79:ILE:HD13	1.74	0.53
1:A:351:G:H21	1:A:374:A:H62	1.54	0.53
4:D:132:PRO:O	4:D:137:SER:OG	2.27	0.53
31:a:211:A:N1	31:a:228:A:O2'	2.38	0.53
31:a:1023:G:N2	31:a:1026:A:OP2	2.32	0.53
31:a:1136:U:OP1	40:j:7:ARG:NH2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1387:C:O4'	37:g:95:ARG:NH2	2.41	0.53
50:t:67:VAL:O	50:t:71:THR:OG1	2.26	0.53
6:F:12:ILE:HD12	6:F:172:GLN:HB3	1.90	0.53
10:L:18:ARG:HH21	10:L:21:ARG:HG2	1.72	0.53
12:N:59:ARG:HD2	12:N:80:LEU:HD21	1.90	0.53
31:a:1365:G:H2'	31:a:1366:A:C8	2.43	0.53
39:i:44:LEU:O	39:i:48:ILE:HB	2.09	0.53
41:k:25:ILE:HG23	41:k:88:VAL:HA	1.91	0.53
1:A:835:A:OP1	1:A:838:C:N4	2.35	0.53
1:A:1106:U:H1'	1:A:1108:G:H5'	1.90	0.53
13:O:7:LYS:O	13:O:11:ARG:HB2	2.07	0.53
13:O:30:ARG:NH2	13:O:47:ASP:OD1	2.41	0.53
31:a:224:U:H4'	31:a:473:G:H4'	1.91	0.53
51:x:69:A:H1'	51:x:71:U:OP2	2.09	0.53
1:A:1292:G:H1	15:Q:37:GLN:HE21	1.56	0.53
3:C:88:SER:O	3:C:197:ASN:ND2	2.41	0.53
31:a:1248:A:H62	31:a:1308:A:H61	1.55	0.53
1:A:89:U:H3'	1:A:90:A:H2'	1.91	0.53
12:N:34:GLU:HG2	12:N:115:ALA:HB2	1.91	0.53
31:a:424:G:H2'	31:a:425:G:H8	1.74	0.53
31:a:724:A:H2'	31:a:725:A:C8	2.44	0.53
35:e:14:ARG:HH21	35:e:113:ALA:HA	1.73	0.53
47:q:24:THR:HA	47:q:46:PHE:O	2.09	0.53
1:A:929:G:H1	1:A:941:U:H3	1.56	0.53
1:A:2357:A:H2'	1:A:2358:A:C8	2.44	0.53
1:A:2874:G:O6	1:A:2892:G:C2	2.61	0.53
7:G:125:GLU:HB2	7:G:133:VAL:HB	1.90	0.53
1:A:2640:C:O4'	52:A:3001:TEL:H81	2.09	0.53
1:A:926:G:H2'	1:A:927:G:H8	1.73	0.53
31:a:779:C:O2'	31:a:909:C:N3	2.35	0.53
31:a:1129:U:OP1	39:i:85:ARG:NH1	2.42	0.53
1:A:490:A:OP1	5:E:45:ARG:HG3	2.08	0.52
1:A:1362:G:OP1	17:S:98:LYS:NZ	2.42	0.52
20:W:39:VAL:HG11	20:W:45:LEU:HD21	1.92	0.52
31:a:531:C:H41	42:l:63:ARG:HH22	1.57	0.52
37:g:113:GLU:H	37:g:119:ARG:HD2	1.73	0.52
1:A:499:G:C8	5:E:58:ARG:HG2	2.44	0.52
19:U:74:LYS:HB2	19:U:99:GLN:HG3	1.90	0.52
23:Z:6:ILE:HG23	23:Z:54:VAL:HG13	1.90	0.52
23:Z:11:SER:OG	23:Z:12:VAL:N	2.40	0.52
1:A:1570:U:H4'	1:A:1571:G:OP2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2374:G:OP2	25:1:34:LYS:HD3	2.10	0.52
1:A:2717:G:OP1	1:A:2742:C:N4	2.42	0.52
7:G:7:LYS:HB2	7:G:70:ARG:HH22	1.74	0.52
31:a:967:U:H5'	31:a:968:A:OP2	2.09	0.52
1:A:253:G:OP1	27:3:13:ARG:NH2	2.42	0.52
31:a:1262:G:H2'	31:a:1263:G:H8	1.74	0.52
37:g:85:TYR:HH	41:k:57:SER:HG	1.57	0.52
47:q:66:THR:OG1	47:q:67:ARG:N	2.43	0.52
1:A:84:A:H5''	19:U:4:LYS:HG3	1.92	0.52
1:A:786:A:H8	1:A:786:A:OP2	1.92	0.52
1:A:2572:G:H2'	1:A:2573:G:C8	2.45	0.52
1:A:2640:C:C4	52:A:3001:TEL:H352	2.45	0.52
6:F:63:GLN:HG2	29:6:1:MET:HE1	1.91	0.52
31:a:1322:U:H3'	49:s:5:LEU:HD13	1.92	0.52
31:a:1335:U:H2'	31:a:1336:G:H8	1.75	0.52
1:A:2314:C:OP2	25:1:2:ARG:NH2	2.41	0.52
3:C:13:ARG:NH1	3:C:16:MET:SD	2.83	0.52
31:a:126:G:O2'	47:q:7:ARG:NH1	2.43	0.52
31:a:682:G:H5'	36:f:87:ARG:HH12	1.74	0.52
39:i:15:SER:HB3	39:i:70:GLY:HA3	1.92	0.52
1:A:2049:A:H5'	24:0:9:SER:HB3	1.92	0.52
1:A:2196:U:H3	1:A:2200:A:H62	1.57	0.52
4:D:8:ARG:HH21	4:D:79:PHE:HE2	1.58	0.52
23:Z:23:VAL:HG21	23:Z:53:LEU:HD22	1.92	0.52
42:l:61:ALA:HB3	42:l:63:ARG:HH11	1.74	0.52
1:A:86:C:H4'	1:A:103:U:H1'	1.92	0.52
1:A:589:G:C2	1:A:595:G:C2	2.98	0.52
4:D:22:LEU:HD11	14:P:75:PRO:HG3	1.91	0.52
6:F:19:LYS:NZ	6:F:168:GLU:OE1	2.40	0.52
31:a:548:A:OP2	42:l:125:GLN:NE2	2.43	0.52
31:a:722:G:H2'	31:a:723:G:C8	2.45	0.52
40:j:10:LEU:HD22	40:j:96:VAL:HB	1.92	0.52
1:A:1053:C:H5''	1:A:1054:A:H2'	1.91	0.52
1:A:2526:A:OP2	1:A:2526:A:H8	1.92	0.52
2:B:52:G:OP2	2:B:52:G:H8	1.92	0.52
17:S:19:LEU:HB3	24:0:22:LEU:HD23	1.91	0.52
19:U:32:ARG:HB3	19:U:62:PRO:HB2	1.91	0.52
25:1:8:ALA:HA	25:1:15:ARG:HA	1.92	0.52
34:d:54:LYS:NZ	34:d:65:GLU:OE2	2.43	0.52
45:o:18:HIS:N	45:o:21:ASP:OD2	2.37	0.52
1:A:2102:C:HO2'	1:A:2627:A:HO2'	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:1187:G:N2	31:a:1190:G:OP2	2.43	0.51
31:a:1375:C:OP1	39:i:119:LYS:NZ	2.39	0.51
43:m:79:ARG:NH1	49:s:65:ASP:O	2.43	0.51
1:A:334:G:N2	1:A:393:U:O2	2.35	0.51
1:A:732:A:O2'	1:A:735:U:O4	2.22	0.51
1:A:2619:A:OP2	3:C:237:GLY:HA2	2.09	0.51
31:a:968:A:N3	31:a:995:C:O2'	2.41	0.51
39:i:88:LEU:HD11	39:i:104:LEU:HD11	1.92	0.51
1:A:1365:U:O2'	1:A:1366:C:O4'	2.28	0.51
2:B:41:C:O2	6:F:92:ARG:NE	2.44	0.51
3:C:41:GLY:HA2	3:C:55:GLY:HA3	1.92	0.51
3:C:158:ALA:HB1	3:C:197:ASN:HB2	1.92	0.51
31:a:1245:A:H4'	31:a:1313:G:H4'	1.91	0.51
1:A:32:C:N4	1:A:494:A:OP2	2.43	0.51
1:A:721:G:H5''	5:E:76:GLY:N	2.25	0.51
1:A:1941:A:N6	31:a:1416:C:O2'	2.43	0.51
1:A:2048:U:OP2	24:O:6:ARG:NH2	2.42	0.51
25:1:5:ILE:HG13	25:1:21:LYS:HG2	1.91	0.51
31:a:483:G:OP2	46:p:75:SER:HB2	2.10	0.51
1:A:721:G:H1'	5:E:74:ARG:HH11	1.76	0.51
1:A:1185:G:O2'	1:A:1189:A:N1	2.40	0.51
1:A:2593:A:OP1	1:A:2677:G:O2'	2.28	0.51
4:D:10:ILE:HD11	4:D:29:GLU:HB2	1.92	0.51
6:F:4:LEU:HD11	6:F:173:VAL:HG13	1.93	0.51
7:G:62:HIS:O	7:G:66:HIS:HB2	2.11	0.51
16:R:40:PHE:HD1	16:R:47:LYS:HB3	1.76	0.51
31:a:536:G:O6	42:l:59:ASN:ND2	2.43	0.51
31:a:596:G:OP1	38:h:86:ARG:NH2	2.44	0.51
31:a:683:G:H2'	31:a:684:A:H8	1.75	0.51
31:a:766:U:OP1	31:a:831:A:O2'	2.27	0.51
31:a:778:G:H4'	31:a:1523:A:H4'	1.93	0.51
31:a:1318:G:OP1	43:m:87:ARG:NH1	2.44	0.51
1:A:221:G:H22	1:A:238:U:H4'	1.75	0.51
28:4:17:ILE:HD12	28:4:26:ILE:HD12	1.93	0.51
1:A:957:A:N3	1:A:2293:C:O2'	2.38	0.51
8:J:21:ALA:HB1	8:J:63:ILE:HD12	1.93	0.51
28:4:2:LYS:HB2	28:4:34:GLN:HG2	1.92	0.51
31:a:277:C:H2'	31:a:278:A:C8	2.46	0.51
31:a:919:A:N3	31:a:1422:A:O2'	2.39	0.51
31:a:1047:C:H2'	31:a:1048:A:C8	2.46	0.51
31:a:1441:G:N2	31:a:1478:A:OP2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:61:SER:O	40:j:61:SER:OG	2.25	0.51
45:o:24:SER:O	45:o:26:GLU:N	2.44	0.51
1:A:273:A:OP2	1:A:297:G:N2	2.28	0.51
1:A:2315:A:H2'	25:1:26:ASN:HD21	1.75	0.51
31:a:260:U:O2	31:a:283:G:N2	2.44	0.51
31:a:715:A:H5''	41:k:26:ARG:HH21	1.76	0.51
34:d:126:VAL:HG12	34:d:128:ILE:H	1.76	0.51
14:P:37:ARG:NH2	31:a:353:C:OP2	2.44	0.50
31:a:62:A:OP1	31:a:109:G:N2	2.44	0.50
31:a:1359:A:OP1	39:i:123:ARG:NH1	2.44	0.50
1:A:245:G:N1	1:A:258:A:OP2	2.37	0.50
1:A:830:A:O2'	1:A:1808:U:O2	2.28	0.50
1:A:2757:U:O2	4:D:191:ASN:ND2	2.44	0.50
31:a:956:A:H2'	31:a:957:G:H8	1.76	0.50
37:g:116:MET:HA	37:g:119:ARG:HE	1.75	0.50
40:j:10:LEU:O	40:j:71:LYS:HA	2.11	0.50
44:n:24:CYS:SG	44:n:28:GLY:HA2	2.50	0.50
49:s:55:ARG:HH22	49:s:79:THR:HG21	1.75	0.50
1:A:256:C:OP2	27:3:5:LYS:NZ	2.44	0.50
1:A:448:A:H2'	1:A:449:A:C8	2.46	0.50
1:A:537:A:H8	1:A:537:A:OP2	1.94	0.50
1:A:698:C:HO2'	1:A:699:A:H8	1.55	0.50
9:K:97:ARG:NE	31:a:347:C:OP2	2.45	0.50
9:K:107:ARG:HE	9:K:115:VAL:HG11	1.76	0.50
12:N:22:THR:HG22	12:N:66:ILE:HG23	1.93	0.50
12:N:31:GLU:HG2	12:N:116:ILE:HG12	1.94	0.50
1:A:697:G:OP1	27:3:19:SER:OG	2.29	0.50
4:D:6:LEU:H	4:D:33:ASN:HD21	1.59	0.50
12:N:106:PRO:HG3	17:S:40:PRO:HG3	1.92	0.50
41:k:87:THR:HG22	41:k:113:ARG:HD2	1.92	0.50
51:x:1:G:N2	51:x:83:U:O2	2.35	0.50
1:A:1089:C:O2'	1:A:1094:A:O2'	2.30	0.50
1:A:2572:G:H21	1:A:2675:C:H5''	1.77	0.50
31:a:584:G:O2'	31:a:830:G:OP2	2.30	0.50
31:a:784:G:N2	31:a:813:U:O4	2.44	0.50
31:a:1238:A:O2'	51:x:31:C:OP1	2.29	0.50
41:k:37:THR:HA	41:k:43:ALA:HA	1.93	0.50
1:A:1403:G:OP1	21:X:3:ARG:NH1	2.34	0.50
15:Q:70:ARG:HE	15:Q:75:SER:HA	1.76	0.50
31:a:107:A:H61	31:a:332:G:H1'	1.76	0.50
31:a:775:A:OP2	31:a:821:G:N2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:151:MET:HA	33:c:165:GLU:O	2.12	0.50
35:e:142:GLN:NE2	35:e:146:GLU:OE2	2.39	0.50
1:A:2640:C:N1	52:A:3001:TEL:H352	2.27	0.50
5:E:153:LEU:HD12	5:E:192:LEU:HD12	1.93	0.50
31:a:417:U:C2	31:a:441:G:O6	2.64	0.50
31:a:462:A:H5'	31:a:463:A:OP2	2.11	0.50
31:a:468:C:H2'	31:a:469:G:H8	1.77	0.50
1:A:1088:G:N2	1:A:1159:U:O2	2.37	0.50
1:A:2605:G:O2'	1:A:2608:C:OP2	2.21	0.50
18:T:49:VAL:HG11	18:T:83:LEU:HD13	1.93	0.50
32:b:140:GLU:HG2	32:b:144:LEU:HD13	1.93	0.50
40:j:51:ILE:HG23	44:n:41:ARG:HG2	1.93	0.50
43:m:87:ARG:HG3	43:m:97:VAL:HG13	1.94	0.50
1:A:64:A:H61	1:A:90:A:H61	1.60	0.50
1:A:200:A:H8	1:A:200:A:OP2	1.95	0.50
1:A:364:A:O2'	1:A:366:A:OP2	2.20	0.50
38:h:13:ARG:HD2	38:h:27:ILE:HG12	1.93	0.50
1:A:633:U:H2'	1:A:634:A:H8	1.76	0.49
5:E:101:LEU:O	5:E:106:ARG:NH2	2.36	0.49
31:a:590:G:H8	31:a:590:G:OP2	1.95	0.49
1:A:630:A:H5'	5:E:89:VAL:HG21	1.93	0.49
1:A:1075:A:N6	1:A:1171:G:O2'	2.45	0.49
9:K:38:VAL:HG22	9:K:61:VAL:HG22	1.93	0.49
31:a:18:A:N3	31:a:1090:A:O2'	2.43	0.49
31:a:1237:C:OP2	43:m:107:ARG:NH2	2.43	0.49
31:a:1526:G:H2'	31:a:1528:A:OP2	2.12	0.49
49:s:36:ARG:NH2	49:s:75:ALA:O	2.45	0.49
1:A:1077:G:O2'	28:4:7:VAL:O	2.30	0.49
2:B:35:C:O2	13:O:103:HIS:NE2	2.36	0.49
15:Q:97:ASP:HA	15:Q:100:VAL:HB	1.94	0.49
31:a:815:C:H2'	31:a:816:A:H8	1.78	0.49
1:A:252:C:OP2	1:A:2423:C:O2'	2.28	0.49
1:A:894:A:N6	1:A:980:C:N4	2.60	0.49
6:F:176:PRO:HB2	29:6:42:PHE:HE2	1.77	0.49
8:J:33:VAL:HG13	8:J:55:VAL:HG11	1.94	0.49
8:J:78:HIS:HA	8:J:85:LEU:HA	1.94	0.49
14:P:6:GLU:O	14:P:10:LYS:HB2	2.12	0.49
18:T:59:TYR:HE2	18:T:78:LYS:HD3	1.77	0.49
31:a:1025:G:N3	31:a:1227:C:O2'	2.40	0.49
33:c:20:SER:HB2	33:c:22:TRP:CZ3	2.47	0.49
36:f:9:ILE:HA	36:f:59:PHE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:A:H5''	26:2:19:ARG:HG2	1.95	0.49
1:A:411:G:H4'	1:A:412:A:OP2	2.12	0.49
1:A:621:G:O2'	1:A:1294:A:OP1	2.29	0.49
1:A:775:G:H4'	3:C:13:ARG:HE	1.77	0.49
5:E:147:SER:O	5:E:191:LYS:NZ	2.46	0.49
6:F:101:ASP:O	6:F:105:SER:OG	2.28	0.49
12:N:29:ARG:HA	12:N:117:ILE:O	2.12	0.49
31:a:1087:G:N2	31:a:1090:A:OP2	2.39	0.49
1:A:1615:A:OP2	3:C:83:TYR:OH	2.21	0.49
3:C:161:SER:H	3:C:177:ASN:HD21	1.60	0.49
8:J:124:ASN:N	8:J:124:ASN:OD1	2.46	0.49
9:K:20:LEU:HD13	9:K:44:LYS:HE3	1.95	0.49
14:P:21:ARG:HD3	14:P:22:PRO:HD2	1.93	0.49
14:P:60:THR:HA	14:P:73:THR:HA	1.93	0.49
18:T:84:THR:OG1	18:T:87:SER:OG	2.30	0.49
21:X:19:SER:OG	21:X:20:HIS:N	2.45	0.49
31:a:532:A:H61	42:l:102:ASP:HB2	1.78	0.49
31:a:827:G:O2'	31:a:829:U:OP2	2.30	0.49
33:c:72:PRO:HD3	33:c:104:GLU:HG3	1.95	0.49
45:o:68:THR:HG22	45:o:71:ARG:HH12	1.76	0.49
1:A:2882:G:N2	1:A:2885:A:OP2	2.33	0.49
16:R:68:ALA:O	16:R:89:ARG:NE	2.45	0.49
1:A:1010:C:O2'	1:A:2302:A:N3	2.42	0.49
1:A:1105:G:OP2	1:A:1106:U:H3'	2.13	0.49
1:A:1184:G:N2	8:J:109:MET:HE3	2.28	0.49
1:A:1366:C:O2'	12:N:108:ARG:NH2	2.46	0.49
1:A:1379:U:OP2	18:T:57:MET:HE1	2.13	0.49
1:A:2315:A:N6	25:1:19:SER:OG	2.45	0.49
7:G:171:ARG:NH2	28:4:28:GLU:O	2.46	0.49
9:K:63:VAL:HG13	9:K:102:VAL:HG13	1.95	0.49
17:S:76:VAL:HG22	17:S:103:ILE:HG13	1.94	0.49
31:a:682:G:H4'	36:f:87:ARG:HH22	1.78	0.49
31:a:900:G:O2'	31:a:916:G:O6	2.25	0.49
1:A:1325:A:H2'	1:A:1327:U:OP2	2.12	0.49
1:A:1709:A:H61	1:A:2025:C:H5	1.61	0.49
1:A:2356:A:H2'	1:A:2357:A:C8	2.47	0.49
7:G:103:LYS:HG2	7:G:117:VAL:HG22	1.94	0.49
12:N:91:TYR:OH	12:N:119:LEU:O	2.30	0.49
31:a:861:U:H5'	31:a:862:A:OP2	2.12	0.49
31:a:1084:G:O6	31:a:1093:U:O2	2.30	0.49
33:c:58:ARG:HD3	33:c:63:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:h:40:LEU:HD21	38:h:131:VAL:HG21	1.94	0.49
41:k:23:ALA:HB3	41:k:86:VAL:HG22	1.93	0.49
1:A:869:U:H2'	1:A:870:A:H8	1.78	0.49
1:A:1036:A:O2'	1:A:1037:C:OP1	2.27	0.49
1:A:1945:A:H61	31:a:1417:A:HO2'	1.61	0.49
2:B:88:C:H5'	11:M:18:ARG:HB3	1.95	0.49
3:C:53:HIS:HA	3:C:217:ARG:HB2	1.95	0.49
10:L:23:ILE:HA	10:L:28:GLY:HA3	1.93	0.49
19:U:24:LEU:HB2	19:U:34:LEU:HD12	1.95	0.49
31:a:956:A:H2'	31:a:957:G:C8	2.47	0.48
42:l:98:GLY:H	42:l:108:TYR:HA	1.78	0.48
44:n:7:ILE:HD11	44:n:28:GLY:HA3	1.95	0.48
1:A:26:G:OP2	1:A:26:G:H8	1.97	0.48
1:A:853:C:OP2	10:L:41:ARG:NH2	2.41	0.48
1:A:1033:C:O2'	1:A:1046:A:N3	2.38	0.48
1:A:2895:C:OP1	12:N:53:ARG:NH1	2.46	0.48
31:a:1260:A:N3	31:a:1378:C:O2'	2.41	0.48
33:c:70:ALA:HB2	33:c:105:ILE:HB	1.95	0.48
37:g:11:ASP:N	37:g:11:ASP:OD1	2.44	0.48
47:q:22:THR:HG21	47:q:73:LYS:HE2	1.94	0.48
1:A:733:U:O2'	26:2:4:THR:O	2.28	0.48
1:A:1941:A:H8	31:a:1505:U:H1'	1.78	0.48
8:J:141:TYR:OH	8:J:144:ARG:NH2	2.46	0.48
10:L:33:LYS:HE3	10:L:40:ALA:HA	1.95	0.48
12:N:24:LEU:HD22	12:N:44:VAL:HG11	1.95	0.48
33:c:148:VAL:HG22	33:c:201:ILE:HG23	1.96	0.48
45:o:71:ARG:NH2	45:o:78:TYR:OH	2.46	0.48
1:A:117:A:OP2	1:A:118:A:H2'	2.14	0.48
1:A:1379:U:H2'	18:T:57:MET:HE3	1.95	0.48
11:M:37:LEU:HD21	11:M:130:LYS:HD3	1.96	0.48
25:1:36:CYS:O	25:1:40:LYS:N	2.47	0.48
31:a:434:U:OP1	34:d:31:TYR:OH	2.29	0.48
31:a:495:U:H2'	31:a:496:A:H8	1.77	0.48
31:a:1091:G:OP2	35:e:52:LYS:NZ	2.42	0.48
47:q:7:ARG:HB3	47:q:65:GLU:HG3	1.95	0.48
1:A:740:A:O2'	1:A:1392:A:N3	2.42	0.48
1:A:897:G:H21	23:Z:46:MET:HE3	1.78	0.48
1:A:1478:G:H2'	1:A:1479:G:C8	2.48	0.48
1:A:2520:U:H5'	1:A:2599:G:H5''	1.94	0.48
31:a:840:U:H5'	32:b:21:ARG:HD2	1.94	0.48
40:j:50:THR:HG22	40:j:64:GLN:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:U:OP2	8:J:66:THR:OG1	2.27	0.48
1:A:1619:A:H2'	1:A:1620:A:C8	2.48	0.48
1:A:2360:G:O2'	1:A:2365:A:N1	2.43	0.48
6:F:57:LEU:HB2	6:F:65:PRO:HG3	1.96	0.48
31:a:56:C:OP1	31:a:359:G:N2	2.45	0.48
31:a:1133:A:H4'	40:j:38:GLY:HA3	1.94	0.48
33:c:32:LEU:HD21	44:n:53:ILE:HA	1.95	0.48
37:g:70:MET:HE2	37:g:97:THR:HG22	1.96	0.48
1:A:5:A:H2'	1:A:6:A:C8	2.49	0.48
1:A:15:G:H4'	24:0:18:THR:HG22	1.96	0.48
1:A:2121:U:O2	1:A:2254:A:O2'	2.31	0.48
8:J:97:TYR:HA	8:J:127:ARG:HH21	1.78	0.48
17:S:18:ARG:HD2	17:S:76:VAL:HB	1.96	0.48
32:b:86:ARG:HH21	32:b:218:ALA:HB3	1.78	0.48
37:g:66:LEU:HB3	37:g:70:MET:HE3	1.95	0.48
46:p:36:THR:OG1	46:p:37:VAL:O	2.30	0.48
1:A:549:A:N3	1:A:551:A:O2'	2.43	0.48
12:N:84:PHE:O	12:N:88:ALA:CB	2.62	0.48
14:P:35:GLY:C	14:P:37:ARG:H	2.20	0.48
27:3:32:LEU:O	27:3:36:LYS:NZ	2.34	0.48
31:a:100:G:H2'	31:a:101:C:H6	1.78	0.48
31:a:194:C:N4	47:q:5:ASN:O	2.42	0.48
31:a:937:G:O2'	31:a:1513:A:N7	2.38	0.48
34:d:103:LEU:HD22	34:d:151:ILE:HG23	1.94	0.48
1:A:444:U:OP2	21:X:10:LYS:HD3	2.14	0.48
1:A:594:C:OP2	16:R:92:TYR:OH	2.29	0.48
1:A:1186:C:H5'	8:J:27:GLY:HA3	1.95	0.48
1:A:1883:A:H3'	1:A:1884:G:H8	1.79	0.48
1:A:2130:G:H22	1:A:2217:U:H3	1.62	0.48
5:E:186:VAL:HG13	5:E:192:LEU:HD13	1.95	0.48
31:a:330:C:O2	31:a:340:G:N2	2.46	0.48
31:a:477:A:H3'	31:a:478:G:C8	2.49	0.48
48:r:44:ILE:HG21	48:r:61:THR:HG22	1.96	0.48
1:A:77:U:H3'	22:Y:2:LYS:HD2	1.95	0.48
1:A:2640:C:O4'	52:A:3001:TEL:H252	2.14	0.48
5:E:32:VAL:HG13	5:E:105:VAL:HG13	1.96	0.48
22:Y:8:ASP:HB3	22:Y:13:GLU:HB2	1.96	0.48
31:a:477:A:H3'	31:a:478:G:H8	1.79	0.48
31:a:1050:A:H2'	31:a:1051:G:C8	2.49	0.48
35:e:72:ILE:HD11	35:e:145:SER:HB3	1.95	0.48
38:h:41:LYS:HD3	38:h:48:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:m:80:LEU:HA	43:m:83:ILE:HG12	1.94	0.48
1:A:648:G:O2'	1:A:649:G:OP2	2.29	0.47
1:A:1322:G:N2	1:A:1325:A:OP2	2.46	0.47
1:A:2778:A:H4'	7:G:63:ARG:HB3	1.94	0.47
6:F:119:LYS:HA	6:F:167:ARG:HH12	1.79	0.47
11:M:30:GLY:O	11:M:134:ARG:NH2	2.46	0.47
39:i:20:ARG:HG3	39:i:64:LEU:HB2	1.94	0.47
51:x:9:G:O2'	51:x:10:G:N7	2.45	0.47
1:A:143:G:O2'	18:T:37:THR:OG1	2.24	0.47
1:A:1847:U:OP2	3:C:87:ARG:NH1	2.46	0.47
5:E:80:SER:HG	5:E:83:TRP:CD1	2.31	0.47
7:G:3:ARG:HH22	7:G:55:ARG:HH22	1.61	0.47
16:R:2:TYR:HA	16:R:14:VAL:O	2.14	0.47
31:a:1128:A:H8	31:a:1128:A:OP2	1.96	0.47
1:A:529:C:O2'	1:A:543:A:N1	2.47	0.47
1:A:576:G:OP1	1:A:2050:G:O2'	2.23	0.47
1:A:1177:G:H5'	8:J:85:LEU:HD22	1.96	0.47
4:D:111:THR:HG1	4:D:201:THR:HG1	1.61	0.47
5:E:113:VAL:HG21	5:E:183:VAL:HG13	1.95	0.47
11:M:42:ILE:HD12	11:M:97:VAL:HG21	1.95	0.47
31:a:825:A:OP1	31:a:1536:G:O2'	2.28	0.47
42:l:81:PRO:HB2	42:l:130:TYR:HE1	1.79	0.47
1:A:268:A:N1	1:A:474:U:O2'	2.45	0.47
1:A:626:G:H2'	1:A:627:G:C8	2.49	0.47
6:F:57:LEU:HD23	6:F:60:ILE:HD12	1.94	0.47
31:a:468:C:H2'	31:a:469:G:C8	2.49	0.47
51:x:29:U:H2'	51:x:30:A:C8	2.50	0.47
1:A:499:G:H5'	5:E:79:ARG:HH12	1.79	0.47
1:A:1542:A:H2'	1:A:1542:A:OP2	2.14	0.47
6:F:38:MET:HB3	6:F:87:ALA:H	1.79	0.47
31:a:158:G:H5'	31:a:159:A:OP2	2.15	0.47
34:d:20:SER:OG	34:d:22:THR:OG1	2.27	0.47
36:f:7:MET:HE3	48:r:70:MET:HG3	1.95	0.47
48:r:44:ILE:HD13	48:r:61:THR:HG22	1.96	0.47
1:A:28:A:N6	1:A:558:G:O2'	2.48	0.47
1:A:1165:U:H2'	1:A:1166:G:H8	1.79	0.47
1:A:2817:C:O2'	1:A:2834:A:N3	2.43	0.47
31:a:273:G:H4'	47:q:70:SER:HA	1.97	0.47
31:a:445:U:O4	31:a:504:A:N7	2.47	0.47
40:j:42:LEU:HD22	40:j:71:LYS:HD2	1.96	0.47
1:A:776:G:H8	1:A:811:A:OP2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:G:H4'	1:A:1837:U:H3	1.79	0.47
1:A:2496:C:OP1	28:4:8:LYS:NZ	2.44	0.47
52:A:3001:TEL:H333	52:A:3001:TEL:O45	2.15	0.47
17:S:41:ARG:O	17:S:44:SER:OG	2.27	0.47
31:a:51:U:N3	31:a:372:A:C6	2.83	0.47
31:a:435:C:O2'	31:a:550:G:OP1	2.29	0.47
31:a:686:U:H3	31:a:722:G:H22	1.63	0.47
31:a:992:U:H5''	44:n:6:MET:HE2	1.97	0.47
31:a:1129:U:H2'	31:a:1130:C:H6	1.80	0.47
33:c:152:VAL:HG22	33:c:197:VAL:HG22	1.97	0.47
35:e:36:LEU:HD13	35:e:134:ILE:HG12	1.97	0.47
37:g:12:VAL:HG12	37:g:14:PRO:HD2	1.97	0.47
49:s:32:LYS:HA	49:s:50:ALA:HB3	1.96	0.47
1:A:365:U:H5''	5:E:136:THR:HG23	1.97	0.47
1:A:2782:A:O2'	28:4:15:LYS:NZ	2.48	0.47
6:F:8:TYR:OH	6:F:29:PRO:O	2.33	0.47
31:a:684:A:H1'	41:k:120:HIS:CD2	2.49	0.47
31:a:1003:G:O2'	31:a:1004:A:N7	2.48	0.47
33:c:56:ILE:HG12	33:c:65:ILE:HG12	1.96	0.47
40:j:53:ARG:O	44:n:45:ARG:NH2	2.47	0.47
47:q:22:THR:HG22	47:q:49:HIS:HA	1.95	0.47
1:A:1700:A:H4'	4:D:120:GLN:HA	1.96	0.47
1:A:2377:U:OP2	27:3:38:GLN:HG2	2.13	0.47
1:A:2392:U:OP1	27:3:40:GLN:NE2	2.48	0.47
2:B:47:C:OP1	13:O:35:ARG:NH2	2.43	0.47
13:O:44:ILE:HD11	13:O:81:VAL:HG13	1.96	0.47
15:Q:28:LYS:HG2	15:Q:34:VAL:HG12	1.96	0.47
31:a:417:U:O2	31:a:441:G:C6	2.68	0.47
31:a:1151:G:H5''	31:a:1152:G:OP2	2.15	0.47
31:a:1354:U:OP1	39:i:122:ARG:NH2	2.42	0.47
31:a:1415:U:O2	31:a:1527:G:N2	2.45	0.47
1:A:83:G:N2	1:A:102:A:OP2	2.35	0.47
1:A:631:G:H22	10:L:33:LYS:HE2	1.80	0.47
1:A:2320:U:O2'	1:A:2403:C:O2	2.32	0.47
1:A:2640:C:C5	52:A:3001:TEL:C35	2.98	0.47
14:P:51:ARG:O	14:P:57:GLU:HA	2.15	0.47
26:2:33:ARG:HA	26:2:36:ARG:HG2	1.97	0.47
32:b:203:ASN:ND2	32:b:205:ASP:OD1	2.48	0.47
33:c:18:TRP:HB2	33:c:21:LYS:HG2	1.97	0.47
40:j:59:LYS:HE2	40:j:62:ARG:NH2	2.30	0.47
42:l:53:MET:HE3	42:l:103:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:o:7:ARG:HH11	45:o:34:ASP:HB3	1.80	0.47
1:A:662:U:H5''	5:E:106:ARG:HD3	1.96	0.46
1:A:910:A:H2'	1:A:911:G:C8	2.50	0.46
3:C:68:LYS:HA	3:C:151:GLY:HA2	1.97	0.46
22:Y:28:LEU:HB3	22:Y:43:ILE:HG12	1.96	0.46
31:a:716:U:H2'	31:a:717:G:C8	2.50	0.46
31:a:968:A:C5	49:s:55:ARG:HD3	2.50	0.46
33:c:33:HIS:HE2	44:n:38:LYS:HB3	1.79	0.46
49:s:25:THR:OG1	49:s:26:ASP:N	2.48	0.46
1:A:259:A:H2'	1:A:260:A:C8	2.50	0.46
1:A:560:A:N3	1:A:625:C:O2'	2.43	0.46
1:A:704:U:H2'	1:A:705:A:C8	2.50	0.46
16:R:79:LYS:HB2	16:R:80:LYS:HD2	1.96	0.46
31:a:208:A:OP1	50:t:56:LYS:HG3	2.15	0.46
31:a:798:U:H2'	31:a:800:G:OP2	2.15	0.46
31:a:1377:G:OP1	40:j:64:GLN:NE2	2.47	0.46
34:d:182:ARG:NH1	34:d:186:ALA:O	2.32	0.46
51:x:5:A:C2'	51:x:6:G:H5'	2.46	0.46
1:A:120:G:H4'	1:A:150:A:H5'	1.97	0.46
1:A:683:A:OP2	10:L:113:GLY:N	2.48	0.46
1:A:864:C:O2'	1:A:886:U:OP1	2.28	0.46
1:A:2664:U:O2'	4:D:82:GLU:OE1	2.33	0.46
15:Q:105:ALA:HB1	16:R:40:PHE:HZ	1.80	0.46
31:a:124:G:OP1	31:a:614:U:O2'	2.23	0.46
31:a:1400:U:H2'	31:a:1401:G:C8	2.50	0.46
38:h:17:ALA:HB2	38:h:25:LEU:HD21	1.97	0.46
43:m:11:ARG:HB3	43:m:46:ARG:HB3	1.97	0.46
1:A:184:G:H8	26:2:36:ARG:HD2	1.81	0.46
10:L:49:GLY:H	27:3:61:MET:HE3	1.80	0.46
16:R:60:ALA:HB1	16:R:95:VAL:HG13	1.97	0.46
25:1:21:LYS:NZ	25:1:26:ASN:O	2.47	0.46
31:a:46:G:OP2	46:p:13:LYS:HB2	2.15	0.46
31:a:417:U:O2	31:a:441:G:O6	2.33	0.46
50:t:78:ARG:HE	50:t:82:LYS:HG3	1.81	0.46
1:A:789:C:H2'	1:A:790:A:C8	2.50	0.46
1:A:1571:G:OP2	1:A:1571:G:H8	1.98	0.46
1:A:2172:C:H42	1:A:2177:G:H1	1.63	0.46
3:C:155:VAL:HG21	3:C:162:ALA:HB2	1.97	0.46
6:F:53:ALA:HA	6:F:56:GLU:HB3	1.97	0.46
8:J:63:ILE:HD13	8:J:102:LEU:HD21	1.97	0.46
25:1:34:LYS:O	25:1:42:SER:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:436:G:O2'	34:d:29:ARG:NH1	2.49	0.46
31:a:671:A:H2'	31:a:672:A:C8	2.50	0.46
31:a:815:C:H2'	31:a:816:A:C8	2.51	0.46
34:d:163:GLU:N	34:d:184:GLU:OE2	2.48	0.46
35:e:16:VAL:HG21	35:e:137:ILE:HD11	1.97	0.46
35:e:74:VAL:HG11	35:e:118:ALA:HB1	1.98	0.46
50:t:32:ILE:HG12	50:t:79:LEU:HD11	1.97	0.46
1:A:1377:G:H5''	18:T:14:THR:HG22	1.98	0.46
1:A:1472:G:H8	1:A:1472:G:OP2	1.98	0.46
1:A:2711:G:C2	4:D:24:PRO:HB3	2.51	0.46
4:D:123:ILE:HD12	4:D:141:ARG:HA	1.96	0.46
6:F:101:ASP:HB3	29:6:22:PHE:HE2	1.81	0.46
31:a:416:G:H5'	34:d:109:GLN:HB2	1.98	0.46
31:a:777:A:N3	31:a:1522:U:O2'	2.48	0.46
42:l:47:CYS:HB2	42:l:91:SER:H	1.80	0.46
46:p:37:VAL:HG11	46:p:56:ALA:HB2	1.97	0.46
1:A:1338:G:H22	1:A:1685:A:H5''	1.81	0.46
1:A:2343:A:H1'	6:F:155:VAL:HG11	1.97	0.46
1:A:2900:A:OP2	1:A:2900:A:H8	1.98	0.46
31:a:590:G:N2	31:a:768:A:OP2	2.42	0.46
31:a:1084:G:OP1	35:e:69:LYS:NZ	2.43	0.46
31:a:1200:A:H5''	33:c:4:LYS:HE2	1.97	0.46
32:b:16:PHE:HB2	32:b:40:ILE:HG12	1.97	0.46
1:A:1002:G:N2	1:A:1006:A:OP2	2.47	0.46
1:A:1657:C:H5'	26:2:7:PRO:HG3	1.98	0.46
1:A:2541:C:O2'	4:D:158:LYS:NZ	2.48	0.46
20:W:22:ARG:H	20:W:22:ARG:HD3	1.80	0.46
26:2:35:ARG:HG3	26:2:42:LEU:HD11	1.98	0.46
31:a:23:G:H2'	31:a:24:G:C8	2.51	0.46
31:a:466:G:O6	31:a:484:U:O4	2.33	0.46
31:a:716:U:H2'	31:a:717:G:H8	1.79	0.46
31:a:727:A:OP2	31:a:729:C:N4	2.48	0.46
31:a:774:G:N1	31:a:821:G:O2'	2.42	0.46
37:g:112:GLY:HA2	37:g:119:ARG:HH21	1.81	0.46
51:x:1:G:O6	51:x:83:U:O4	2.33	0.46
1:A:633:U:H2'	1:A:634:A:C8	2.51	0.46
1:A:722:A:O2'	5:E:67:GLN:OE1	2.22	0.46
1:A:1886:G:O2'	1:A:1887:G:O4'	2.31	0.46
1:A:2619:A:H2'	1:A:2620:C:H6	1.81	0.46
4:D:146:MET:HE3	4:D:154:VAL:HG11	1.98	0.46
5:E:50:LYS:NZ	5:E:56:GLU:OE1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:22:ILE:HD12	9:K:40:VAL:HG12	1.97	0.46
31:a:996:A:N3	49:s:52:TYR:OH	2.45	0.46
32:b:83:GLU:OE1	32:b:86:ARG:NH2	2.49	0.46
33:c:53:LYS:NZ	33:c:55:GLU:OE2	2.49	0.46
33:c:75:VAL:HG12	33:c:102:ILE:HD13	1.98	0.46
42:l:63:ARG:HB2	42:l:103:LEU:HD12	1.98	0.46
1:A:669:C:OP2	10:L:104:LYS:NZ	2.42	0.46
29:6:10:LYS:HD2	29:6:29:GLU:HG2	1.98	0.46
31:a:958:C:H2'	31:a:959:A:H8	1.81	0.46
32:b:114:LEU:HB2	32:b:144:LEU:HD23	1.97	0.46
35:e:14:ARG:NH2	35:e:116:GLU:OE1	2.35	0.46
37:g:103:TRP:HB3	37:g:134:ALA:HB1	1.98	0.46
1:A:632:U:H2'	1:A:633:U:C6	2.51	0.45
1:A:2287:C:O2'	1:A:2456:C:OP2	2.30	0.45
6:F:62:GLY:H	29:6:9:PHE:HZ	1.63	0.45
21:X:17:ASN:HB3	21:X:25:SER:HB2	1.98	0.45
31:a:265:G:H2'	31:a:266:A:H8	1.80	0.45
31:a:1262:G:H2'	31:a:1263:G:C8	2.51	0.45
32:b:69:PHE:O	32:b:91:TYR:HA	2.16	0.45
35:e:72:ILE:HG21	35:e:141:LEU:HD22	1.97	0.45
1:A:1613:C:H5''	3:C:21:PHE:HE2	1.81	0.45
1:A:2075:G:H5'	24:0:16:ARG:HG2	1.99	0.45
1:A:2818:C:H1'	1:A:2916:A:H2	1.81	0.45
14:P:93:ARG:O	14:P:94:ARG:NH1	2.50	0.45
31:a:385:G:H5'	31:a:386:A:OP2	2.15	0.45
31:a:470:U:H2'	31:a:471:U:C6	2.52	0.45
36:f:14:ILE:HD11	36:f:84:ASP:HB2	1.99	0.45
39:i:12:ARG:O	39:i:15:SER:OG	2.29	0.45
1:A:1475:G:H8	1:A:1475:G:OP2	1.99	0.45
12:N:52:LYS:NZ	12:N:94:ARG:O	2.49	0.45
31:a:272:C:O2'	47:q:68:PRO:O	2.32	0.45
31:a:456:A:H2	31:a:495:U:H3	1.63	0.45
31:a:508:A:O4'	31:a:556:A:N6	2.50	0.45
31:a:843:U:OP1	48:r:47:ARG:NH2	2.39	0.45
33:c:174:LEU:HD21	33:c:200:TRP:CD1	2.52	0.45
39:i:119:LYS:HE2	39:i:125:PRO:HB3	1.97	0.45
1:A:10:A:H3'	1:A:11:G:H8	1.81	0.45
1:A:331:C:H2'	1:A:332:G:C8	2.52	0.45
1:A:1042:A:O2'	15:Q:92:ARG:NH1	2.49	0.45
1:A:1366:C:N4	1:A:1692:U:O2	2.49	0.45
5:E:50:LYS:HB2	5:E:94:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:VAL:HG11	7:G:51:LEU:HD21	1.97	0.45
12:N:22:THR:HG21	12:N:67:ARG:H	1.80	0.45
22:Y:40:THR:O	22:Y:43:ILE:HB	2.16	0.45
31:a:51:U:C4	31:a:372:A:C6	3.05	0.45
1:A:1371:G:N7	1:A:1654:A:O2'	2.43	0.45
1:A:1825:U:H2'	1:A:1826:C:H6	1.81	0.45
1:A:2334:U:O2'	1:A:2335:U:O4'	2.35	0.45
1:A:2886:C:H2'	1:A:2887:A:H8	1.81	0.45
16:R:12:ILE:HG21	16:R:20:VAL:HG11	1.97	0.45
23:Z:5:GLU:HB2	23:Z:57:LYS:HB3	1.97	0.45
31:a:11:G:OP2	35:e:126:LYS:HD2	2.16	0.45
31:a:855:G:H2'	31:a:856:C:C6	2.51	0.45
41:k:85:GLU:HG3	41:k:111:ALA:HB3	1.98	0.45
42:l:99:ARG:HH12	42:l:107:ARG:HE	1.64	0.45
3:C:131:PRO:HA	3:C:189:ARG:HA	1.98	0.45
14:P:88:ARG:NH2	31:a:1472:C:OP1	2.48	0.45
15:Q:80:MET:HE2	15:Q:93:LYS:HE3	1.98	0.45
31:a:36:C:H1'	42:l:42:GLN:HE22	1.82	0.45
31:a:723:G:H2'	31:a:724:A:C8	2.51	0.45
1:A:2332:G:H21	6:F:129:THR:HG21	1.81	0.45
1:A:2922:U:H2'	1:A:2923:A:C8	2.52	0.45
22:Y:6:ILE:HA	22:Y:60:ARG:HH21	1.82	0.45
23:Z:12:VAL:HG12	23:Z:20:ARG:HE	1.81	0.45
25:1:5:ILE:O	25:1:18:ILE:HA	2.16	0.45
31:a:136:U:OP1	46:p:65:LYS:NZ	2.43	0.45
31:a:474:A:H2'	31:a:475:A:C8	2.52	0.45
31:a:952:G:H21	39:i:126:GLN:NE2	2.15	0.45
40:j:42:LEU:HB3	40:j:71:LYS:HG3	1.98	0.45
1:A:735:U:H2'	1:A:736:A:H8	1.81	0.45
1:A:2314:C:H5	25:1:2:ARG:HH12	1.64	0.45
4:D:146:MET:HA	4:D:158:LYS:HE2	1.99	0.45
8:J:78:HIS:HD2	8:J:85:LEU:HB3	1.82	0.45
9:K:120:GLU:OE2	14:P:63:LYS:NZ	2.45	0.45
14:P:17:LEU:HD22	14:P:84:ILE:HB	1.99	0.45
27:3:24:ARG:HD3	27:3:50:VAL:HG22	1.97	0.45
28:4:27:CYS:SG	28:4:28:GLU:N	2.90	0.45
31:a:984:A:OP2	44:n:41:ARG:NH2	2.50	0.45
32:b:166:PRO:HB3	32:b:196:ILE:HD11	1.98	0.45
1:A:698:C:OP2	1:A:698:C:H6	1.99	0.45
1:A:1339:A:H4'	1:A:1340:A:H5'	1.97	0.45
1:A:1529:G:H2'	1:A:1530:G:H8	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:6:LEU:HA	4:D:201:THR:HA	1.99	0.45
15:Q:93:LYS:H	15:Q:93:LYS:HD2	1.82	0.45
23:Z:7:THR:HG22	23:Z:34:THR:HG22	1.99	0.45
31:a:473:G:H21	31:a:477:A:H2	1.65	0.45
31:a:1322:U:OP2	49:s:5:LEU:HB2	2.16	0.45
49:s:50:ALA:HA	49:s:58:VAL:O	2.16	0.45
51:x:74:C:H2'	51:x:75:G:H8	1.82	0.45
1:A:720:C:H5''	5:E:80:SER:HB2	1.98	0.45
1:A:1859:C:H2'	1:A:1860:G:H8	1.82	0.45
6:F:55:GLU:O	6:F:58:THR:OG1	2.35	0.45
31:a:206:A:H4'	50:t:52:THR:HG22	1.98	0.45
37:g:50:ILE:HD11	37:g:121:ALA:HA	1.99	0.45
41:k:85:GLU:OE2	41:k:113:ARG:NH2	2.50	0.45
1:A:606:U:H2'	1:A:616:A:H1'	1.99	0.44
1:A:2502:U:OP1	1:A:2558:G:N2	2.47	0.44
5:E:184:LEU:O	5:E:188:ASN:HB2	2.17	0.44
14:P:23:GLY:HA3	14:P:92:VAL:HG21	1.99	0.44
15:Q:61:TRP:HB3	15:Q:93:LYS:HB3	1.99	0.44
20:W:53:ILE:HG12	20:W:85:LYS:HB2	1.98	0.44
24:0:38:LEU:HD12	24:0:41:ARG:HD2	1.98	0.44
31:a:455:G:O6	31:a:494:G:O2'	2.29	0.44
41:k:35:THR:HG22	41:k:46:TRP:HB2	1.99	0.44
42:l:117:THR:O	42:l:117:THR:OG1	2.35	0.44
43:m:60:ILE:HG23	43:m:65:VAL:HG21	1.99	0.44
1:A:79:C:O2'	1:A:390:A:N3	2.43	0.44
1:A:1245:G:OP1	10:L:4:HIS:HE1	1.99	0.44
1:A:2066:A:H2'	1:A:2067:G:C8	2.52	0.44
1:A:2100:A:H2'	1:A:2101:G:C8	2.52	0.44
1:A:2104:U:OP1	3:C:243:ARG:NH2	2.50	0.44
1:A:2865:U:H5''	12:N:49:THR:HG21	1.99	0.44
18:T:47:PHE:HZ	22:Y:30:PHE:HE2	1.65	0.44
31:a:1158:C:O2'	31:a:1289:A:N1	2.45	0.44
37:g:26:LEU:HD22	37:g:43:LEU:HD12	1.99	0.44
50:t:69:LYS:HA	50:t:72:ALA:HB3	1.99	0.44
1:A:89:U:H5''	1:A:90:A:OP2	2.17	0.44
1:A:331:C:H2'	1:A:332:G:H8	1.82	0.44
1:A:1709:A:H2	9:K:1:MET:HE2	1.82	0.44
1:A:2135:G:H5'	1:A:2136:C:OP2	2.17	0.44
1:A:2452:U:H1'	1:A:2454:A:C5	2.52	0.44
3:C:202:LEU:HD21	31:a:782:G:H5'	1.98	0.44
4:D:13:THR:HG22	14:P:5:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:34:PHE:HB2	10:L:1:MET:HE2	1.99	0.44
8:J:132:PRO:O	8:J:134:GLU:N	2.50	0.44
11:M:30:GLY:N	11:M:105:GLU:OE1	2.48	0.44
11:M:65:TRP:HB2	11:M:105:GLU:HB2	2.00	0.44
14:P:49:LYS:HD3	14:P:51:ARG:HG2	1.99	0.44
28:4:25:VAL:HB	28:4:34:GLN:HB2	1.98	0.44
31:a:30:G:O2'	31:a:304:U:OP1	2.27	0.44
31:a:57:A:OP2	31:a:360:C:N4	2.49	0.44
31:a:958:C:OP1	43:m:107:ARG:N	2.48	0.44
1:A:554:U:H4'	1:A:555:C:OP2	2.17	0.44
3:C:14:ARG:HA	3:C:14:ARG:HD3	1.79	0.44
1:A:1095:C:H2'	1:A:1096:A:H8	1.83	0.44
12:N:47:MET:HE1	12:N:62:ALA:HA	1.98	0.44
16:R:32:THR:HA	16:R:60:ALA:O	2.17	0.44
17:S:18:ARG:NE	17:S:76:VAL:O	2.49	0.44
31:a:302:C:OP1	31:a:619:G:O2'	2.30	0.44
31:a:323:A:O2'	31:a:338:C:O2'	2.33	0.44
39:i:20:ARG:HH11	39:i:22:VAL:HG11	1.82	0.44
43:m:15:VAL:HG22	43:m:45:VAL:HG12	1.98	0.44
1:A:461:C:H2'	1:A:462:A:C8	2.52	0.44
1:A:1027:A:N1	1:A:2056:G:O2'	2.49	0.44
1:A:2460:U:O2'	1:A:2462:A:N7	2.49	0.44
22:Y:10:THR:HG22	22:Y:60:ARG:HH11	1.82	0.44
31:a:729:C:H2'	31:a:730:A:C8	2.53	0.44
31:a:1071:G:N7	33:c:2:GLY:N	2.66	0.44
38:h:107:SER:HA	38:h:112:VAL:HA	2.00	0.44
40:j:63:GLU:OE2	44:n:49:TYR:OH	2.29	0.44
1:A:229:A:O2'	1:A:231:A:N1	2.46	0.44
1:A:631:G:OP2	10:L:21:ARG:NH2	2.51	0.44
1:A:869:U:H2'	1:A:870:A:C8	2.52	0.44
1:A:1289:U:HO2'	10:L:18:ARG:NH2	2.12	0.44
1:A:2115:U:H2'	1:A:2116:G:C8	2.52	0.44
2:B:27:A:OP2	13:O:36:SER:OG	2.35	0.44
3:C:136:PRO:HG3	36:f:81:ILE:HG23	2.00	0.44
7:G:104:LEU:HD23	7:G:116:ILE:HD12	1.99	0.44
8:J:65:LEU:HD12	8:J:70:LEU:HD23	2.00	0.44
19:U:12:ILE:HD11	19:U:69:MET:HG3	2.00	0.44
24:0:27:MET:HB3	24:0:36:MET:HE3	2.00	0.44
31:a:933:A:O2'	31:a:1408:C:OP2	2.31	0.44
42:l:2:PRO:HG2	42:l:7:LEU:HG	1.99	0.44
1:A:1072:A:OP2	1:A:1180:C:O2'	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2045:U:O2'	24:0:4:PRO:O	2.26	0.44
1:A:2244:G:OP2	1:A:2244:G:H8	2.01	0.44
1:A:2667:G:OP2	4:D:84:ARG:NH1	2.44	0.44
9:K:90:ASP:OD1	9:K:91:LYS:N	2.50	0.44
31:a:745:U:H2'	31:a:746:C:C6	2.53	0.44
31:a:1335:U:H2'	31:a:1336:G:C8	2.52	0.44
31:a:1526:G:N1	31:a:1529:A:OP2	2.47	0.44
36:f:33:ASN:ND2	36:f:68:ASP:H	2.15	0.44
36:f:77:ARG:HD3	36:f:78:LEU:HG	2.00	0.44
1:A:1465:A:H2'	1:A:1467:G:N7	2.33	0.44
1:A:2150:G:OP1	1:A:2199:G:N2	2.51	0.44
1:A:2516:G:H2'	1:A:2517:A:C8	2.52	0.44
2:B:45:C:OP2	13:O:7:LYS:HE3	2.18	0.44
3:C:245:SER:HB2	3:C:253:PRO:HB3	1.99	0.44
28:4:3:VAL:HA	28:4:35:LYS:O	2.17	0.44
29:6:2:LYS:HB3	29:6:5:ILE:HD12	2.00	0.44
31:a:987:A:N6	31:a:1233:U:O4'	2.51	0.44
31:a:1091:G:OP2	31:a:1091:G:H8	2.00	0.44
1:A:888:A:H2'	1:A:889:A:C8	2.52	0.43
1:A:1240:U:H1'	15:Q:4:VAL:HG22	1.98	0.43
1:A:1340:A:H1'	1:A:1341:U:H5''	2.00	0.43
1:A:1965:A:OP2	1:A:1990:C:N4	2.51	0.43
1:A:2121:U:N3	1:A:2255:C:OP2	2.45	0.43
6:F:38:MET:HB2	6:F:57:LEU:HD11	2.00	0.43
10:L:81:LYS:HD3	10:L:101:VAL:HG13	2.00	0.43
31:a:14:U:H4'	31:a:535:C:H4'	1.99	0.43
31:a:1016:A:H3'	31:a:1017:A:H8	1.83	0.43
31:a:1071:G:OP2	33:c:2:GLY:HA3	2.17	0.43
31:a:1176:A:H2'	31:a:1176:A:OP1	2.18	0.43
35:e:99:ALA:HB1	35:e:103:THR:HG21	1.99	0.43
1:A:524:A:H2'	1:A:525:A:C8	2.53	0.43
1:A:1317:G:H2'	1:A:1318:G:H8	1.83	0.43
40:j:11:LYS:HB3	40:j:71:LYS:HB3	1.99	0.43
42:l:96:ARG:HE	42:l:109:HIS:CD2	2.35	0.43
46:p:55:LEU:HG	46:p:58:LYS:HE3	1.99	0.43
1:A:24:G:O2'	17:S:78:GLU:O	2.36	0.43
1:A:515:G:OP2	26:2:37:LYS:HE3	2.19	0.43
16:R:5:ILE:HG22	16:R:38:VAL:HG22	2.00	0.43
22:Y:24:GLU:OE2	22:Y:42:ARG:NH2	2.51	0.43
31:a:61:A:H5''	31:a:395:U:H5''	1.99	0.43
34:d:71:LEU:HD23	34:d:71:LEU:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:A:H8	1:A:831:U:H5''	1.83	0.43
1:A:1220:G:O6	1:A:1221:A:N6	2.51	0.43
1:A:2270:A:H2'	1:A:2271:G:C8	2.53	0.43
1:A:2473:G:OP2	5:E:68:LYS:HD2	2.19	0.43
1:A:2754:A:H1'	1:A:2755:U:H2'	1.99	0.43
52:A:3001:TEL:H572	52:A:3001:TEL:H541	1.68	0.43
14:P:35:GLY:C	14:P:37:ARG:N	2.76	0.43
14:P:49:LYS:O	14:P:59:PHE:HA	2.19	0.43
31:a:462:A:H3'	31:a:463:A:H8	1.83	0.43
31:a:1509:A:OP2	31:a:1510:A:OP2	2.37	0.43
34:d:125:ARG:HB3	34:d:142:ARG:HH21	1.83	0.43
1:A:490:A:H2'	5:E:45:ARG:HD3	2.00	0.43
1:A:908:A:N3	2:B:77:G:O2'	2.45	0.43
1:A:1681:U:H2'	1:A:1682:C:C6	2.54	0.43
1:A:1839:A:OP2	1:A:1839:A:H8	2.00	0.43
1:A:2037:C:H2'	1:A:2038:G:H8	1.84	0.43
1:A:2251:G:H4'	3:C:185:LEU:HD11	2.00	0.43
1:A:2573:G:H1'	1:A:2675:C:H5'	2.01	0.43
5:E:143:LEU:HD13	5:E:173:VAL:HG21	2.00	0.43
7:G:51:LEU:HD13	7:G:73:LEU:HD13	2.00	0.43
8:J:37:LEU:HD11	8:J:123:LEU:HD13	2.00	0.43
31:a:212:G:H2'	31:a:213:G:H8	1.84	0.43
31:a:1161:A:O5'	40:j:72:ARG:NH2	2.52	0.43
35:e:84:GLU:HA	35:e:96:LEU:O	2.18	0.43
39:i:31:ASN:O	39:i:33:ARG:NH1	2.52	0.43
44:n:24:CYS:HB3	44:n:29:ARG:H	1.84	0.43
51:x:53:A:H5''	51:x:54:G:OP2	2.18	0.43
1:A:249:C:N4	27:3:8:ARG:HG2	2.33	0.43
1:A:565:U:H5''	17:S:25:ARG:HH12	1.84	0.43
1:A:1713:A:O2'	1:A:1719:G:N7	2.41	0.43
1:A:2262:A:H2'	1:A:2263:G:C8	2.54	0.43
4:D:28:ILE:HD12	4:D:188:ILE:HD12	2.01	0.43
5:E:50:LYS:HD3	5:E:94:PRO:HD3	2.00	0.43
5:E:139:MET:HG3	5:E:167:ALA:HB2	2.01	0.43
7:G:15:VAL:HG11	7:G:77:VAL:HG13	2.01	0.43
7:G:92:GLY:HA3	7:G:95:TYR:CG	2.53	0.43
16:R:29:ALA:HA	16:R:62:VAL:HG12	2.00	0.43
21:X:37:ARG:HA	21:X:46:LYS:HA	2.01	0.43
31:a:16:U:H2'	31:a:18:A:OP2	2.18	0.43
31:a:383:U:H5'	46:p:7:LEU:HD12	2.01	0.43
40:j:52:LEU:HD22	40:j:59:LYS:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:l:87:LEU:HD21	42:l:117:THR:HG22	1.99	0.43
45:o:39:LEU:HB3	45:o:56:LEU:HD12	1.99	0.43
1:A:176:A:OP2	1:A:177:G:OP2	2.37	0.43
1:A:231:A:H1'	1:A:233:G:H5'	2.00	0.43
1:A:957:A:H62	11:M:12:GLU:HA	1.83	0.43
1:A:1356:G:H2'	1:A:1357:A:H8	1.84	0.43
1:A:1673:G:H2'	1:A:1674:G:H8	1.83	0.43
6:F:133:LYS:HG2	6:F:134:GLU:HG3	2.01	0.43
7:G:88:LEU:HB2	7:G:132:VAL:O	2.19	0.43
13:O:30:ARG:HE	13:O:45:ILE:HB	1.83	0.43
14:P:49:LYS:HB3	14:P:60:THR:HG22	2.01	0.43
23:Z:8:LEU:HD21	23:Z:28:LEU:HB3	2.01	0.43
26:2:25:LYS:HA	26:2:28:ARG:HE	1.83	0.43
31:a:1349:A:O2'	51:x:32:C:O2'	2.26	0.43
31:a:1385:U:H2'	31:a:1386:A:C8	2.54	0.43
31:a:1436:C:H2'	31:a:1437:A:H8	1.83	0.43
38:h:38:GLU:HG2	38:h:42:ARG:HH21	1.84	0.43
1:A:139:A:H2	1:A:1448:U:H1'	1.84	0.43
1:A:251:G:O2'	1:A:2461:A:OP1	2.30	0.43
1:A:1102:G:N2	1:A:1147:U:OP2	2.51	0.43
1:A:1174:A:O4'	1:A:2545:G:O2'	2.36	0.43
1:A:2054:C:P	4:D:153:ARG:HE	2.40	0.43
1:A:2874:G:OP1	14:P:93:ARG:NE	2.43	0.43
1:A:2900:A:OP2	1:A:2900:A:H2'	2.19	0.43
52:A:3001:TEL:H7	52:A:3001:TEL:H13	1.49	0.43
5:E:80:SER:HG	5:E:83:TRP:HD1	1.66	0.43
22:Y:5:GLU:HG2	22:Y:53:MET:HE3	2.01	0.43
25:1:34:LYS:HB2	25:1:45:HIS:CE1	2.53	0.43
31:a:123:U:O3'	31:a:641:G:N2	2.52	0.43
31:a:265:G:H2'	31:a:266:A:C8	2.54	0.43
31:a:409:C:H2'	31:a:410:G:C8	2.54	0.43
33:c:43:SER:O	33:c:47:SER:HB2	2.19	0.43
49:s:28:LYS:HG2	49:s:29:GLN:H	1.84	0.43
1:A:924:U:H2'	1:A:946:G:H22	1.83	0.43
1:A:1082:G:H1	1:A:1165:U:H3	1.67	0.43
1:A:2190:C:H2'	1:A:2191:A:C8	2.53	0.43
1:A:2886:C:H2'	1:A:2887:A:C8	2.54	0.43
6:F:135:GLN:HE21	6:F:146:VAL:HG13	1.84	0.43
14:P:26:LEU:HD12	14:P:86:VAL:HG22	2.00	0.43
31:a:70:G:H1	31:a:99:A:N6	2.17	0.43
39:i:103:LEU:HD23	39:i:103:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:j:23:GLU:HA	40:j:26:VAL:HB	2.01	0.43
1:A:1474:C:O2'	1:A:1617:A:OP2	2.33	0.43
1:A:1831:A:OP2	1:A:1844:A:N6	2.46	0.43
1:A:2320:U:H2'	1:A:2321:U:C6	2.54	0.43
5:E:54:ARG:HD2	5:E:81:PRO:HD3	2.00	0.43
17:S:50:VAL:HG11	17:S:103:ILE:HG22	2.01	0.43
18:T:52:ASP:HB2	18:T:84:THR:HG22	2.00	0.43
31:a:136:U:H1'	46:p:63:GLY:HA3	2.01	0.43
31:a:429:U:H1'	33:c:126:ARG:HH22	1.84	0.43
31:a:960:U:H2'	31:a:961:G:C8	2.52	0.43
31:a:1237:C:OP2	43:m:107:ARG:NH1	2.49	0.43
31:a:1443:A:H61	31:a:1477:G:H1'	1.84	0.43
32:b:20:THR:OG1	32:b:21:ARG:N	2.49	0.43
38:h:18:ASN:HD21	38:h:74:ILE:HB	1.84	0.43
40:j:8:ILE:HG23	40:j:98:ILE:HG13	2.01	0.43
46:p:49:VAL:HG21	46:p:73:LEU:HD22	2.00	0.43
1:A:1532:A:H2'	1:A:1533:A:C8	2.54	0.42
1:A:2046:U:O3'	24:0:6:ARG:NH1	2.51	0.42
3:C:243:ARG:NE	3:C:247:MET:SD	2.91	0.42
31:a:19:U:H2'	31:a:20:C:C6	2.54	0.42
31:a:224:U:H2'	31:a:225:A:C8	2.54	0.42
42:l:127:ARG:HH11	42:l:134:LYS:HA	1.84	0.42
50:t:45:ASP:OD1	50:t:45:ASP:N	2.51	0.42
1:A:613:U:H5''	1:A:868:A:C2	2.54	0.42
4:D:22:LEU:HA	4:D:22:LEU:HD23	1.84	0.42
13:O:10:ALA:O	13:O:14:ARG:HD3	2.19	0.42
14:P:39:ARG:NH2	31:a:353:C:H5''	2.34	0.42
15:Q:103:LEU:HD13	15:Q:107:ASN:HD21	1.85	0.42
17:S:6:VAL:HG12	17:S:8:ARG:HG3	2.01	0.42
24:0:30:CYS:SG	24:0:37:LYS:HB2	2.59	0.42
31:a:798:U:O2'	31:a:800:G:N7	2.45	0.42
31:a:1358:A:H5''	39:i:123:ARG:HG3	2.01	0.42
37:g:75:VAL:HG12	37:g:86:GLN:HB3	2.00	0.42
1:A:898:U:H2'	1:A:899:C:H6	1.84	0.42
1:A:1019:A:OP2	16:R:80:LYS:HE3	2.19	0.42
1:A:1546:G:N2	3:C:98:ASP:O	2.35	0.42
1:A:1819:C:H2'	1:A:1820:A:C5	2.54	0.42
1:A:1825:U:H2'	1:A:1826:C:C6	2.54	0.42
1:A:2917:G:H8	1:A:2917:G:OP2	2.02	0.42
2:B:25:A:OP1	13:O:39:HIS:NE2	2.46	0.42
4:D:108:VAL:HG21	4:D:176:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:GLY:O	4:D:163:ARG:HA	2.19	0.42
8:J:57:ILE:HD12	8:J:125:VAL:HG22	2.00	0.42
31:a:53:A:N7	31:a:112:U:O2'	2.51	0.42
31:a:514:G:H2'	31:a:515:G:C8	2.54	0.42
31:a:1106:C:H2'	31:a:1107:C:C6	2.54	0.42
31:a:1332:G:H2'	31:a:1333:A:C8	2.54	0.42
34:d:26:LEU:HD12	34:d:30:PRO:HA	2.02	0.42
42:l:55:PRO:HD3	42:l:63:ARG:HG2	2.01	0.42
1:A:518:A:OP1	5:E:84:ARG:NH1	2.40	0.42
1:A:1074:A:N6	1:A:1171:G:H2'	2.35	0.42
1:A:2644:U:C2	24:0:4:PRO:HA	2.54	0.42
1:A:2695:C:H5	7:G:153:ARG:HH22	1.66	0.42
3:C:62:TYR:HA	3:C:86:ASN:HD21	1.85	0.42
18:T:12:VAL:HG12	18:T:14:THR:HG23	2.02	0.42
20:W:83:ASP:OD1	20:W:83:ASP:N	2.51	0.42
31:a:80:G:H2'	31:a:81:A:H8	1.85	0.42
31:a:1171:C:H2'	31:a:1172:G:C8	2.55	0.42
42:l:112:ARG:HB3	42:l:130:TYR:HA	2.02	0.42
43:m:86:TYR:HA	43:m:89:ILE:HD12	2.00	0.42
1:A:575:A:H5'	1:A:576:G:C5	2.54	0.42
1:A:633:U:OP2	10:L:16:ARG:NH2	2.42	0.42
1:A:685:U:H2'	1:A:686:C:C6	2.54	0.42
1:A:1038:C:H2'	1:A:1039:G:H8	1.85	0.42
1:A:1302:A:OP1	17:S:99:ARG:NH1	2.41	0.42
9:K:104:ARG:HG2	9:K:121:VAL:HG12	2.01	0.42
31:a:75:G:H8	31:a:75:G:OP2	2.03	0.42
31:a:554:C:OP2	34:d:55:GLN:NE2	2.52	0.42
31:a:979:A:OP1	40:j:57:LYS:NZ	2.44	0.42
51:x:74:C:H2'	51:x:75:G:C8	2.54	0.42
1:A:860:U:H2'	1:A:861:C:C6	2.55	0.42
1:A:1382:G:H5'	1:A:1643:C:OP2	2.18	0.42
1:A:2390:A:OP1	27:3:27:ALA:N	2.41	0.42
6:F:65:PRO:HB2	6:F:87:ALA:HB1	2.01	0.42
9:K:8:LEU:HD22	9:K:82:ASN:HB3	2.02	0.42
31:a:471:U:H3	31:a:479:G:H1	1.68	0.42
31:a:509:G:H2'	31:a:510:C:C6	2.53	0.42
31:a:518:A:N3	31:a:552:G:O2'	2.47	0.42
31:a:1072:U:H2'	31:a:1073:C:C6	2.55	0.42
33:c:123:LEU:HD13	33:c:195:LEU:HD13	2.01	0.42
51:x:15:A:H2'	51:x:70:G:H1	1.84	0.42
1:A:419:G:O2'	1:A:447:G:O6	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:C:H2'	1:A:758:A:H8	1.85	0.42
1:A:1133:G:H2'	1:A:1134:A:H4'	2.02	0.42
1:A:1821:G:H1	1:A:1856:U:H3	1.68	0.42
4:D:14:GLN:HE21	4:D:22:LEU:HD13	1.84	0.42
31:a:960:U:H2'	31:a:961:G:H8	1.85	0.42
34:d:162:PRO:HD2	34:d:165:LEU:HD12	2.02	0.42
39:i:52:LEU:HG	39:i:57:THR:HB	2.01	0.42
40:j:52:LEU:HD21	40:j:59:LYS:HD2	2.02	0.42
43:m:83:ILE:HD12	49:s:66:MET:HG2	2.01	0.42
49:s:37:ARG:H	49:s:37:ARG:HG2	1.54	0.42
50:t:71:THR:HG22	50:t:74:ARG:HE	1.84	0.42
1:A:1138:C:H2'	1:A:1139:G:C8	2.54	0.42
1:A:2818:C:H2'	1:A:2819:A:C8	2.55	0.42
1:A:2823:C:H2'	1:A:2824:G:C8	2.54	0.42
2:B:64:A:N6	2:B:106:C:OP2	2.52	0.42
15:Q:105:ALA:HB1	16:R:40:PHE:CZ	2.55	0.42
31:a:140:A:H8	31:a:140:A:OP2	2.02	0.42
31:a:343:C:O2'	31:a:1442:A:N3	2.53	0.42
31:a:1463:A:H2'	31:a:1464:G:C8	2.55	0.42
33:c:68:HIS:HB3	33:c:105:ILE:HD11	2.01	0.42
36:f:86:ILE:HG22	36:f:87:ARG:HG2	2.02	0.42
42:l:64:LYS:HG2	42:l:80:ILE:HB	2.02	0.42
43:m:72:GLU:OE2	43:m:76:ASN:ND2	2.49	0.42
1:A:506:U:H2'	1:A:507:A:H8	1.85	0.42
1:A:745:C:O2'	1:A:781:A:N6	2.46	0.42
1:A:2121:U:OP1	1:A:2228:A:O2'	2.25	0.42
1:A:2177:G:H2'	1:A:2178:C:C6	2.55	0.42
1:A:2381:A:N6	1:A:2394:G:O2'	2.53	0.42
3:C:108:LYS:HB3	3:C:194:GLN:HB3	2.02	0.42
6:F:69:ARG:HA	6:F:84:PRO:HA	2.01	0.42
6:F:140:GLU:HA	29:6:28:LYS:HE3	2.02	0.42
7:G:160:GLY:H	7:G:172:ARG:HH22	1.67	0.42
8:J:18:VAL:HG13	8:J:58:ILE:HD12	2.01	0.42
8:J:38:ARG:NH2	8:J:111:PRO:HD3	2.34	0.42
8:J:108:GLY:O	8:J:112:LYS:NZ	2.52	0.42
24:0:16:ARG:HE	24:0:16:ARG:HB2	1.63	0.42
31:a:398:C:H2'	31:a:399:G:H8	1.85	0.42
31:a:1330:U:O2'	49:s:78:ARG:NH2	2.52	0.42
1:A:1042:A:H2'	1:A:1043:G:C8	2.55	0.42
1:A:1363:G:H1'	1:A:1661:A:N6	2.35	0.42
1:A:1817:C:H3'	1:A:1818:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2164:A:O4'	1:A:2188:G:O2'	2.37	0.42
3:C:96:TYR:HE2	3:C:102:ARG:HD2	1.85	0.42
15:Q:61:TRP:HA	15:Q:97:ASP:OD2	2.20	0.42
31:a:767:G:H4'	31:a:890:C:H4'	2.02	0.42
35:e:14:ARG:HG2	35:e:117:LEU:HD11	2.01	0.42
1:A:46:C:OP2	1:A:218:G:H8	2.03	0.41
1:A:1049:G:O2'	1:A:1056:A:N1	2.52	0.41
1:A:1676:G:N2	1:A:1679:A:OP2	2.34	0.41
1:A:2100:A:H2'	1:A:2101:G:H8	1.85	0.41
1:A:2369:A:H2'	1:A:2370:G:H8	1.84	0.41
5:E:17:ILE:HD12	5:E:125:VAL:HG11	2.01	0.41
9:K:71:ARG:HE	9:K:77:ILE:HD11	1.85	0.41
31:a:69:C:H2'	31:a:70:G:C8	2.54	0.41
31:a:307:G:N2	31:a:574:U:O2	2.53	0.41
31:a:359:G:H8	31:a:359:G:OP2	2.03	0.41
38:h:21:ARG:CZ	38:h:70:ASN:HB3	2.50	0.41
39:i:113:ARG:HG3	39:i:115:LYS:HZ3	1.85	0.41
50:t:32:ILE:HG23	50:t:79:LEU:HD21	2.01	0.41
1:A:1555:A:H2'	1:A:1556:A:C8	2.55	0.41
1:A:2275:G:H2'	1:A:2276:A:C8	2.54	0.41
31:a:746:C:H2'	31:a:747:U:H6	1.84	0.41
31:a:1235:C:OP2	43:m:90:ARG:NH1	2.47	0.41
34:d:17:ILE:HD12	34:d:17:ILE:HA	1.85	0.41
1:A:116:G:OP2	1:A:118:A:O2'	2.24	0.41
1:A:1102:G:OP2	1:A:1102:G:H2'	2.19	0.41
1:A:1364:C:OP1	1:A:1692:U:O2'	2.38	0.41
1:A:1991:C:O2'	1:A:1992:C:O5'	2.37	0.41
31:a:901:U:H2'	31:a:902:A:H8	1.85	0.41
1:A:40:U:H2'	1:A:41:A:H8	1.85	0.41
1:A:500:A:N3	1:A:504:A:O2'	2.53	0.41
1:A:751:G:H2'	1:A:773:G:H22	1.84	0.41
1:A:2177:G:H2'	1:A:2178:C:H6	1.84	0.41
1:A:2207:C:H5''	1:A:2208:C:OP2	2.20	0.41
1:A:2535:U:OP2	1:A:2605:G:N1	2.48	0.41
3:C:93:LEU:HD12	3:C:103:TYR:CZ	2.56	0.41
6:F:102:LYS:O	6:F:107:SER:N	2.49	0.41
10:L:3:LEU:HA	10:L:6:LEU:HG	2.02	0.41
15:Q:83:LEU:HD23	15:Q:113:ALA:HB2	2.02	0.41
28:4:16:VAL:HG22	28:4:25:VAL:HG22	2.03	0.41
31:a:262:G:O2'	47:q:20:ASP:O	2.37	0.41
31:a:580:U:H5''	31:a:828:A:C5	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:109:ASP:O	33:c:140:THR:HG22	2.20	0.41
33:c:150:THR:HG22	33:c:199:VAL:HG13	2.02	0.41
37:g:75:VAL:HA	37:g:88:PRO:HA	2.02	0.41
15:Q:49:ASP:HA	15:Q:52:GLN:HB2	2.03	0.41
19:U:36:GLU:HA	19:U:60:GLU:HG2	2.02	0.41
29:6:49:PHE:O	29:6:53:ASP:HB2	2.20	0.41
31:a:698:C:H5''	41:k:33:ILE:HD11	2.02	0.41
31:a:1294:A:H4'	31:a:1295:C:H5''	2.02	0.41
34:d:138:THR:HG22	34:d:175:THR:HG22	2.02	0.41
35:e:36:LEU:HD11	35:e:137:ILE:HD12	2.02	0.41
42:l:42:GLN:HA	42:l:95:ILE:O	2.21	0.41
49:s:11:VAL:HA	49:s:38:SER:HB2	2.01	0.41
50:t:32:ILE:HG23	50:t:79:LEU:HD11	2.02	0.41
1:A:2:G:H2'	1:A:3:U:C6	2.56	0.41
1:A:74:U:H3'	22:Y:44:ARG:HH22	1.86	0.41
1:A:193:A:N3	1:A:726:C:O2'	2.52	0.41
1:A:2061:G:N2	1:A:2601:A:OP2	2.52	0.41
1:A:2087:A:C2	52:A:3001:TEL:H241	2.55	0.41
1:A:2144:G:N2	1:A:2148:A:OP1	2.54	0.41
1:A:2163:A:C5	1:A:2185:G:N2	2.88	0.41
1:A:2859:G:OP1	4:D:59:LYS:NZ	2.46	0.41
5:E:54:ARG:HE	5:E:80:SER:HA	1.86	0.41
31:a:180:G:H1	31:a:208:A:H2'	1.84	0.41
31:a:521:U:H2'	31:a:522:A:C8	2.56	0.41
31:a:1418:C:H2'	31:a:1419:A:C8	2.56	0.41
43:m:85:SER:O	43:m:88:GLY:N	2.44	0.41
1:A:31:C:O2'	1:A:1278:G:OP1	2.36	0.41
1:A:1177:G:H4'	8:J:85:LEU:HD13	2.03	0.41
1:A:1199:C:H5'	15:Q:76:TYR:HE2	1.85	0.41
1:A:1497:G:N2	1:A:1499:A:N1	2.66	0.41
1:A:1683:C:O3'	1:A:2738:G:N2	2.52	0.41
1:A:2324:C:P	13:O:14:ARG:HE	2.43	0.41
17:S:86:ARG:HD3	17:S:87:PRO:HD2	2.02	0.41
31:a:225:A:OP1	31:a:472:C:O2'	2.33	0.41
31:a:1169:G:H1	31:a:1185:A:N6	2.18	0.41
31:a:1359:A:P	39:i:123:ARG:HD2	2.60	0.41
34:d:200:ARG:HE	34:d:200:ARG:HB3	1.69	0.41
36:f:37:ILE:HG23	36:f:63:VAL:HG13	2.02	0.41
37:g:13:LEU:HD13	37:g:21:LYS:HD3	2.02	0.41
42:l:99:ARG:NH1	42:l:107:ARG:HE	2.18	0.41
1:A:1377:G:O2'	1:A:1432:A:N1	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2135:G:N1	1:A:2212:C:C2	2.89	0.41
1:A:2139:G:O6	1:A:2207:C:N4	2.54	0.41
1:A:2143:A:H5''	1:A:2144:G:OP2	2.20	0.41
1:A:2275:G:H2'	1:A:2276:A:H8	1.86	0.41
1:A:2456:C:H5''	1:A:2458:G:H5'	2.03	0.41
1:A:2822:C:H5'	1:A:2823:C:OP2	2.20	0.41
5:E:24:PHE:HB3	5:E:118:VAL:HG21	2.03	0.41
5:E:202:VAL:HA	5:E:205:VAL:HG12	2.01	0.41
13:O:33:VAL:HG11	13:O:106:VAL:HG22	2.03	0.41
13:O:77:VAL:HG13	13:O:109:LEU:HD21	2.02	0.41
20:W:54:TYR:OH	20:W:84:ARG:NH1	2.53	0.41
31:a:156:G:H2'	31:a:157:G:H8	1.85	0.41
31:a:746:C:H2'	31:a:747:U:C6	2.55	0.41
36:f:3:LYS:HA	36:f:65:VAL:O	2.20	0.41
36:f:35:ALA:HB1	36:f:65:VAL:HG13	2.03	0.41
1:A:161:A:N3	1:A:2237:C:O2'	2.49	0.41
1:A:612:U:H5'	1:A:613:U:OP2	2.20	0.41
1:A:1068:G:N2	1:A:1069:U:O4	2.54	0.41
1:A:1171:G:H4'	28:4:5:PRO:HB3	2.03	0.41
1:A:1263:G:H2'	1:A:1265:A:OP2	2.21	0.41
1:A:2125:U:H2'	1:A:2126:G:C8	2.56	0.41
1:A:2274:U:O2'	1:A:2465:G:OP2	2.36	0.41
1:A:2487:U:O2'	1:A:2489:U:O4	2.36	0.41
4:D:23:ILE:HG23	4:D:189:LYS:HG3	2.01	0.41
5:E:49:HIS:ND1	5:E:92:PRO:HB2	2.36	0.41
6:F:74:ILE:HG22	6:F:77:PHE:H	1.85	0.41
6:F:91:LEU:HB3	6:F:96:MET:CG	2.51	0.41
7:G:27:VAL:HG12	7:G:80:VAL:HG21	2.02	0.41
7:G:28:LYS:HA	7:G:33:GLU:HG2	2.03	0.41
9:K:77:ILE:H	9:K:77:ILE:HG13	1.73	0.41
18:T:55:ASN:O	18:T:79:ALA:HA	2.21	0.41
31:a:274:G:H1'	31:a:276:U:OP2	2.20	0.41
31:a:547:U:OP2	42:l:125:GLN:HB2	2.21	0.41
31:a:887:C:H5''	38:h:82:LYS:HG2	2.03	0.41
31:a:901:U:H2'	31:a:902:A:C8	2.55	0.41
31:a:975:A:OP2	31:a:975:A:H8	2.03	0.41
31:a:1006:A:H8	31:a:1006:A:OP2	2.03	0.41
31:a:1317:C:H2'	31:a:1318:G:C8	2.55	0.41
31:a:1460:U:N3	31:a:1461:U:O3'	2.54	0.41
37:g:76:LYS:HG2	37:g:77:ALA:H	1.86	0.41
38:h:8:ALA:O	38:h:12:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:i:114:LYS:HA	39:i:121:ALA:HB2	2.03	0.41
51:x:56:G:H2'	51:x:57:C:C6	2.56	0.41
1:A:30:G:O2'	1:A:1254:A:N3	2.44	0.41
1:A:38:A:H2'	1:A:39:C:O4'	2.20	0.41
1:A:193:A:H5''	1:A:207:A:N6	2.36	0.41
1:A:1823:U:H2'	1:A:1824:C:C6	2.56	0.41
1:A:2028:C:H2'	1:A:2029:G:C8	2.56	0.41
1:A:2295:A:H4'	1:A:2296:A:OP2	2.21	0.41
3:C:245:SER:O	3:C:247:MET:HG3	2.20	0.41
4:D:192:VAL:HG12	4:D:200:ILE:HD13	2.03	0.41
17:S:58:ALA:O	17:S:63:GLU:N	2.54	0.41
19:U:64:HIS:CD2	19:U:66:SER:H	2.39	0.41
31:a:435:C:H2'	31:a:436:G:H21	1.86	0.41
31:a:500:A:H2'	31:a:501:A:C8	2.55	0.41
31:a:1444:G:H2'	31:a:1445:U:C6	2.56	0.41
37:g:49:ILE:HD12	37:g:117:GLU:HG2	2.03	0.41
1:A:302:A:H2'	1:A:303:G:C8	2.56	0.40
1:A:957:A:H2'	1:A:958:A:C8	2.56	0.40
1:A:1115:A:H2'	1:A:1118:C:OP2	2.21	0.40
1:A:1812:A:H5''	1:A:2637:G:H4'	2.03	0.40
3:C:53:HIS:CG	3:C:219:THR:HG22	2.56	0.40
7:G:149:ILE:HG22	7:G:163:ILE:HG21	2.03	0.40
16:R:40:PHE:HA	16:R:47:LYS:HA	2.02	0.40
19:U:9:VAL:HG21	19:U:23:ILE:HD11	2.02	0.40
31:a:477:A:H5'	31:a:478:G:N7	2.36	0.40
31:a:733:G:OP1	31:a:841:G:N2	2.55	0.40
31:a:1236:A:OP2	43:m:95:LEU:HD21	2.20	0.40
32:b:218:ALA:HA	32:b:221:ILE:HG12	2.03	0.40
36:f:33:ASN:HD22	36:f:67:SER:HB2	1.86	0.40
44:n:21:TYR:HE2	44:n:23:ARG:HE	1.69	0.40
1:A:557:U:O2'	1:A:1255:G:N2	2.52	0.40
1:A:872:C:H4'	1:A:2457:G:C5	2.56	0.40
1:A:1711:G:O2'	9:K:6:THR:HG22	2.20	0.40
1:A:2421:A:OP2	1:A:2453:C:N4	2.54	0.40
1:A:2467:U:O3'	1:A:2468:A:H3'	2.21	0.40
1:A:2721:C:H2'	1:A:2722:A:H8	1.86	0.40
31:a:98:U:H1'	31:a:99:A:H2	1.86	0.40
31:a:591:C:OP2	31:a:767:G:N1	2.53	0.40
31:a:952:G:O6	31:a:1350:U:O2	2.39	0.40
31:a:1323:C:H2'	31:a:1324:U:C6	2.57	0.40
32:b:166:PRO:HG3	32:b:187:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:t:28:MET:HE3	50:t:58:ILE:HG12	2.03	0.40
1:A:407:A:H2'	1:A:408:G:H8	1.87	0.40
1:A:547:A:H2'	1:A:548:A:C8	2.56	0.40
1:A:2516:G:H2'	1:A:2517:A:H8	1.84	0.40
31:a:371:A:C6	42:l:41:PRO:HD2	2.56	0.40
31:a:1436:C:H2'	31:a:1437:A:C8	2.56	0.40
33:c:3:GLN:HB3	33:c:4:LYS:H	1.70	0.40
33:c:33:HIS:NE2	44:n:38:LYS:HB3	2.37	0.40
37:g:113:GLU:N	37:g:119:ARG:HD2	2.36	0.40
38:h:24:LYS:HA	38:h:62:VAL:O	2.21	0.40
45:o:25:PRO:HB3	45:o:66:LEU:HD22	2.03	0.40
50:t:46:LYS:HA	50:t:49:THR:HG22	2.04	0.40
1:A:444:U:P	21:X:32:ASN:H	2.43	0.40
1:A:776:G:OP2	3:C:207:LYS:HE2	2.22	0.40
1:A:2133:C:N4	1:A:2215:U:O4	2.53	0.40
9:K:65:THR:OG1	9:K:67:SER:O	2.35	0.40
18:T:31:ASP:N	18:T:31:ASP:OD1	2.52	0.40
31:a:418:G:H2'	31:a:437:U:C5	2.57	0.40
31:a:1196:G:H5'	39:i:115:LYS:HZ2	1.86	0.40
31:a:1289:A:H5'	40:j:42:LEU:HD21	2.03	0.40
31:a:1338:G:H5''	43:m:26:GLY:H	1.86	0.40
43:m:34:LEU:HB3	43:m:39:VAL:HG22	2.03	0.40
1:A:352:G:N2	1:A:524:A:N7	2.69	0.40
1:A:478:U:H2'	1:A:479:A:H8	1.85	0.40
1:A:936:C:N4	51:x:49:C:O2'	2.48	0.40
1:A:2343:A:OP1	6:F:88:LYS:NZ	2.41	0.40
3:C:165:LEU:HD11	3:C:175:ARG:HB2	2.03	0.40
8:J:102:LEU:HA	8:J:102:LEU:HD23	1.88	0.40
23:Z:6:ILE:HD12	23:Z:37:HIS:HD2	1.86	0.40
29:6:16:CYS:SG	29:6:17:ALA:N	2.95	0.40
31:a:69:C:O2'	31:a:170:A:N3	2.52	0.40
31:a:968:A:C4	49:s:55:ARG:HD3	2.57	0.40
33:c:8:VAL:O	33:c:12:ILE:HG13	2.21	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	
3	C	270/277 (98%)	253 (94%)	17 (6%)	0	100	100
4	D	204/209 (98%)	194 (95%)	10 (5%)	0	100	100
5	E	203/207 (98%)	187 (92%)	16 (8%)	0	100	100
6	F	174/179 (97%)	158 (91%)	16 (9%)	0	100	100
7	G	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	9	34
9	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	L	144/146 (99%)	138 (96%)	6 (4%)	0	100	100
11	M	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
12	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
13	O	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
14	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
15	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	7	30
16	R	99/102 (97%)	83 (84%)	15 (15%)	1 (1%)	12	41
17	S	107/113 (95%)	91 (85%)	14 (13%)	2 (2%)	6	27
18	T	88/95 (93%)	83 (94%)	5 (6%)	0	100	100
19	U	99/103 (96%)	86 (87%)	13 (13%)	0	100	100
20	W	80/94 (85%)	70 (88%)	10 (12%)	0	100	100
21	X	56/62 (90%)	46 (82%)	10 (18%)	0	100	100
22	Y	63/66 (96%)	61 (97%)	2 (3%)	0	100	100
23	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
24	0	52/59 (88%)	50 (96%)	1 (2%)	1 (2%)	6	27
25	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
26	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
27	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
29	6	61/63 (97%)	51 (84%)	9 (15%)	1 (2%)	7	30
32	b	216/246 (88%)	185 (86%)	27 (12%)	4 (2%)	6	27
33	c	204/218 (94%)	185 (91%)	19 (9%)	0	100	100
34	d	193/200 (96%)	173 (90%)	18 (9%)	2 (1%)	12	41
35	e	162/166 (98%)	152 (94%)	10 (6%)	0	100	100
36	f	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
37	g	147/156 (94%)	134 (91%)	12 (8%)	1 (1%)	18	49
38	h	129/132 (98%)	108 (84%)	19 (15%)	2 (2%)	7	30
39	i	123/130 (95%)	104 (85%)	18 (15%)	1 (1%)	16	47
40	j	93/102 (91%)	83 (89%)	9 (10%)	1 (1%)	11	39
41	k	112/131 (86%)	102 (91%)	10 (9%)	0	100	100
42	l	134/138 (97%)	115 (86%)	18 (13%)	1 (1%)	18	49
43	m	106/121 (88%)	93 (88%)	12 (11%)	1 (1%)	14	44
44	n	58/61 (95%)	47 (81%)	10 (17%)	1 (2%)	7	30
45	o	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	10	37
46	p	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	16
47	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
48	r	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
49	s	76/92 (83%)	66 (87%)	10 (13%)	0	100	100
50	t	81/88 (92%)	76 (94%)	3 (4%)	2 (2%)	4	21
All	All	5207/5515 (94%)	4721 (91%)	457 (9%)	29 (1%)	23	52

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	133	HIS
15	Q	93	LYS
17	S	40	PRO
32	b	18	HIS
32	b	19	GLN
34	d	32	ALA
38	h	99	ASN
46	p	47	ALA
50	t	69	LYS

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Mol	Chain	Res	Type
8	J	132	PRO
15	Q	92	ARG
34	d	33	PRO
38	h	4	THR
44	n	32	SER
29	6	60	ASN
32	b	67	ILE
43	m	105	ASN
46	p	48	GLU
17	S	39	THR
24	0	51	GLY
32	b	66	LYS
37	g	115	THR
42	l	135	PRO
50	t	68	HIS
46	p	46	PRO
16	R	50	ASN
45	o	25	PRO
39	i	125	PRO
40	j	79	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	220/225 (98%)	220 (100%)	0	100	100
4	D	167/170 (98%)	165 (99%)	2 (1%)	63	78
5	E	169/170 (99%)	167 (99%)	2 (1%)	63	78
6	F	151/154 (98%)	149 (99%)	2 (1%)	61	77
7	G	148/151 (98%)	147 (99%)	1 (1%)	76	82
8	J	120/123 (98%)	117 (98%)	3 (2%)	42	69
9	K	101/101 (100%)	100 (99%)	1 (1%)	68	79
10	L	110/110 (100%)	109 (99%)	1 (1%)	70	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	109/116 (94%)	107 (98%)	2 (2%)	51	73
12	N	99/100 (99%)	98 (99%)	1 (1%)	68	79
13	O	93/93 (100%)	93 (100%)	0	100	100
14	P	100/100 (100%)	100 (100%)	0	100	100
15	Q	96/98 (98%)	96 (100%)	0	100	100
16	R	83/84 (99%)	83 (100%)	0	100	100
17	S	90/93 (97%)	87 (97%)	3 (3%)	33	63
18	T	81/85 (95%)	81 (100%)	0	100	100
19	U	85/87 (98%)	85 (100%)	0	100	100
20	W	64/74 (86%)	64 (100%)	0	100	100
21	X	47/50 (94%)	47 (100%)	0	100	100
22	Y	56/57 (98%)	56 (100%)	0	100	100
23	Z	52/53 (98%)	52 (100%)	0	100	100
24	0	48/53 (91%)	46 (96%)	2 (4%)	26	58
25	1	46/47 (98%)	46 (100%)	0	100	100
26	2	39/39 (100%)	39 (100%)	0	100	100
27	3	54/56 (96%)	52 (96%)	2 (4%)	30	61
28	4	35/35 (100%)	35 (100%)	0	100	100
29	6	53/53 (100%)	53 (100%)	0	100	100
32	b	189/212 (89%)	187 (99%)	2 (1%)	65	78
33	c	168/178 (94%)	167 (99%)	1 (1%)	78	83
34	d	169/173 (98%)	165 (98%)	4 (2%)	43	69
35	e	128/130 (98%)	125 (98%)	3 (2%)	44	70
36	f	81/84 (96%)	80 (99%)	1 (1%)	63	78
37	g	125/132 (95%)	125 (100%)	0	100	100
38	h	111/112 (99%)	110 (99%)	1 (1%)	70	80
39	i	98/102 (96%)	96 (98%)	2 (2%)	48	72
40	j	86/92 (94%)	85 (99%)	1 (1%)	63	78
41	k	86/100 (86%)	84 (98%)	2 (2%)	44	70
42	l	114/116 (98%)	114 (100%)	0	100	100
43	m	94/104 (90%)	94 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	n	53/54 (98%)	53 (100%)	0	100	100
45	o	80/83 (96%)	80 (100%)	0	100	100
46	p	74/76 (97%)	74 (100%)	0	100	100
47	q	77/80 (96%)	76 (99%)	1 (1%)	61	77
48	r	56/64 (88%)	56 (100%)	0	100	100
49	s	70/81 (86%)	70 (100%)	0	100	100
50	t	66/70 (94%)	66 (100%)	0	100	100
All	All	4441/4620 (96%)	4401 (99%)	40 (1%)	68	80

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	108	VAL
4	D	199	LEU
5	E	192	LEU
5	E	194	ILE
6	F	4	LEU
6	F	136	LEU
7	G	108	VAL
8	J	26	LEU
8	J	49	VAL
8	J	123	LEU
9	K	19	VAL
10	L	4	HIS
11	M	27	VAL
11	M	94	VAL
12	N	117	ILE
17	S	29	VAL
17	S	46	ILE
17	S	104	THR
24	0	22	LEU
24	0	38	LEU
27	3	32	LEU
27	3	62	LEU
32	b	179	LEU
32	b	199	VAL
33	c	71	LYS
34	d	22	THR
34	d	26	LEU
34	d	150	ILE

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Mol	Chain	Res	Type
34	d	172	LEU
35	e	36	LEU
35	e	46	VAL
35	e	95	LEU
36	f	85	ILE
38	h	103	ILE
39	i	65	VAL
39	i	113	ARG
40	j	25	ILE
41	k	25	ILE
41	k	52	LEU
47	q	40	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	86	ASN
3	C	177	ASN
3	C	232	HIS
4	D	33	ASN
4	D	128	GLN
4	D	172	GLN
5	E	9	GLN
5	E	10	ASN
5	E	29	ASN
5	E	46	GLN
5	E	75	GLN
6	F	27	GLN
6	F	135	GLN
7	G	66	HIS
8	J	81	HIS
9	K	34	ASN
10	L	27	ASN
10	L	35	HIS
10	L	78	ASN
10	L	126	ASN
11	M	13	HIS
12	N	61	GLN
13	O	15	HIS
13	O	37	ASN
14	P	36	ASN
15	Q	29	HIS

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Mol	Chain	Res	Type
15	Q	37	GLN
15	Q	66	ASN
15	Q	107	ASN
18	T	55	ASN
19	U	64	HIS
20	W	37	GLN
21	X	17	ASN
21	X	23	ASN
22	Y	31	GLN
24	0	40	HIS
24	0	55	ASN
25	1	22	ASN
25	1	26	ASN
32	b	18	HIS
32	b	24	ASN
32	b	36	ASN
32	b	123	ASN
32	b	203	ASN
34	d	96	ASN
34	d	118	HIS
35	e	45	HIS
35	e	83	HIS
36	f	33	ASN
37	g	19	ASN
37	g	84	ASN
37	g	142	HIS
38	h	22	HIS
38	h	57	GLN
39	i	68	HIS
39	i	81	HIS
41	k	24	HIS
41	k	121	ASN
42	l	42	GLN
42	l	85	HIS
42	l	90	HIS
42	l	109	HIS
43	m	105	ASN
44	n	10	GLN
45	o	5	GLN
45	o	13	ASN
45	o	28	GLN
45	o	42	HIS

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Mol	Chain	Res	Type
45	o	46	HIS
45	o	51	HIS
50	t	20	HIS
50	t	68	HIS
50	t	70	ASN
50	t	84	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2928 (98%)	867 (30%)	89 (3%)
2	B	111/112 (99%)	40 (36%)	3 (2%)
30	7	2/3 (66%)	0	0
31	a	1532/1554 (98%)	412 (26%)	0
51	x	86/87 (98%)	25 (29%)	0
All	All	4610/4684 (98%)	1344 (29%)	92 (1%)

All (1344) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	U
1	A	10	A
1	A	13	A
1	A	18	C
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	C
1	A	55	G
1	A	60	G
1	A	61	A
1	A	62	C
1	A	63	G
1	A	64	A
1	A	65	A
1	A	66	C
1	A	71	A
1	A	74	U

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Mol	Chain	Res	Type
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C
1	A	83	G
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	99	U
1	A	100	U
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	126	A
1	A	127	C
1	A	134	C
1	A	141	U
1	A	156	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	167	U
1	A	174	U
1	A	175	G
1	A	176	A
1	A	177	G
1	A	178	A
1	A	179	A
1	A	182	C
1	A	184	G
1	A	187	C
1	A	188	C

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Mol	Chain	Res	Type
1	A	196	U
1	A	199	A
1	A	202	A
1	A	207	A
1	A	216	A
1	A	218	G
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	234	C
1	A	236	A
1	A	237	U
1	A	244	A
1	A	247	A
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	255	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	275	A
1	A	282	G
1	A	283	G
1	A	284	C
1	A	285	U
1	A	286	U
1	A	290	U
1	A	291	C
1	A	298	U
1	A	299	U
1	A	301	U

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Mol	Chain	Res	Type
1	A	302	A
1	A	308	C
1	A	309	U
1	A	310	C
1	A	337	A
1	A	345	A
1	A	346	G
1	A	348	U
1	A	349	C
1	A	352	G
1	A	354	A
1	A	360	C
1	A	361	G
1	A	366	A
1	A	367	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	382	G
1	A	389	A
1	A	395	C
1	A	396	G
1	A	398	U
1	A	409	U
1	A	411	G
1	A	412	A
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	430	C
1	A	433	G
1	A	434	U
1	A	436	A
1	A	442	C
1	A	444	U
1	A	445	C
1	A	453	G
1	A	458	G
1	A	459	A
1	A	469	A
1	A	471	G

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Mol	Chain	Res	Type
1	A	482	C
1	A	483	C
1	A	489	G
1	A	490	A
1	A	494	A
1	A	498	U
1	A	502	C
1	A	503	C
1	A	504	A
1	A	506	U
1	A	508	C
1	A	511	U
1	A	524	A
1	A	526	A
1	A	527	A
1	A	528	G
1	A	529	C
1	A	548	A
1	A	550	G
1	A	551	A
1	A	552	G
1	A	554	U
1	A	555	C
1	A	556	C
1	A	558	G
1	A	568	G
1	A	573	C
1	A	575	A
1	A	577	U
1	A	578	A
1	A	583	G
1	A	584	A
1	A	590	U
1	A	591	U
1	A	592	A
1	A	593	A
1	A	595	G
1	A	599	G
1	A	607	G
1	A	613	U
1	A	617	G
1	A	618	A

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Mol	Chain	Res	Type
1	A	619	A
1	A	622	A
1	A	630	A
1	A	632	U
1	A	646	A
1	A	647	A
1	A	648	G
1	A	649	G
1	A	655	C
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	668	G
1	A	673	A
1	A	680	G
1	A	683	A
1	A	686	C
1	A	689	A
1	A	690	A
1	A	691	U
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	702	A
1	A	703	G
1	A	715	A
1	A	716	G
1	A	717	A
1	A	718	C
1	A	733	U
1	A	741	U
1	A	749	G
1	A	764	C
1	A	765	A
1	A	766	C
1	A	777	C
1	A	787	C
1	A	788	G
1	A	790	A
1	A	794	U

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Mol	Chain	Res	Type
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	837	U
1	A	839	G
1	A	847	A
1	A	852	G
1	A	853	C
1	A	858	U
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	878	G
1	A	890	G
1	A	891	G
1	A	892	U
1	A	893	A
1	A	906	G
1	A	908	A
1	A	913	A
1	A	914	C
1	A	916	G
1	A	919	U
1	A	923	C
1	A	928	G
1	A	929	G
1	A	931	C
1	A	933	C
1	A	934	U
1	A	935	A
1	A	936	C
1	A	937	C
1	A	939	G

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Mol	Chain	Res	Type
1	A	940	G
1	A	941	U
1	A	942	U
1	A	943	A
1	A	944	C
1	A	948	A
1	A	953	G
1	A	954	U
1	A	957	A
1	A	958	A
1	A	959	C
1	A	962	C
1	A	964	A
1	A	970	A
1	A	973	G
1	A	975	C
1	A	977	U
1	A	980	C
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1006	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1026	A
1	A	1029	A
1	A	1031	C
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1058	U
1	A	1059	A
1	A	1067	A
1	A	1068	G
1	A	1069	U
1	A	1071	G
1	A	1072	A

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Mol	Chain	Res	Type
1	A	1073	A
1	A	1079	U
1	A	1090	U
1	A	1091	U
1	A	1101	G
1	A	1102	G
1	A	1103	A
1	A	1106	U
1	A	1110	C
1	A	1111	U
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1119	A
1	A	1120	G
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1125	C
1	A	1126	A
1	A	1127	U
1	A	1128	U
1	A	1134	A
1	A	1142	A
1	A	1143	U
1	A	1145	G
1	A	1146	C
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A
1	A	1173	A
1	A	1174	A
1	A	1176	U
1	A	1178	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1182	G
1	A	1185	G

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Mol	Chain	Res	Type
1	A	1188	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1210	A
1	A	1221	A
1	A	1226	U
1	A	1227	G
1	A	1235	A
1	A	1236	G
1	A	1244	A
1	A	1245	G
1	A	1248	C
1	A	1249	U
1	A	1250	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1261	C
1	A	1270	C
1	A	1276	G
1	A	1278	G
1	A	1280	G
1	A	1281	C
1	A	1282	U
1	A	1290	G
1	A	1293	A
1	A	1294	A
1	A	1295	U
1	A	1296	G
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1323	A
1	A	1325	A
1	A	1326	A
1	A	1330	C

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Mol	Chain	Res	Type
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C
1	A	1344	C
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1354	C
1	A	1362	G
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1369	C
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1422	C
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1443	C
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1457	U

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Mol	Chain	Res	Type
1	A	1459	U
1	A	1460	G
1	A	1464	A
1	A	1465	A
1	A	1467	G
1	A	1472	G
1	A	1473	A
1	A	1475	G
1	A	1481	G
1	A	1487	G
1	A	1489	U
1	A	1490	A
1	A	1494	G
1	A	1499	A
1	A	1500	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1522	U
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1544	C
1	A	1545	C
1	A	1549	U
1	A	1550	C
1	A	1551	C
1	A	1553	A
1	A	1556	A
1	A	1557	G

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Mol	Chain	Res	Type
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1562	A
1	A	1563	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1573	C
1	A	1602	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1613	C
1	A	1617	A
1	A	1622	C
1	A	1626	U
1	A	1628	G
1	A	1631	A
1	A	1632	G
1	A	1645	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1661	A
1	A	1672	A
1	A	1679	A
1	A	1680	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1694	G
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1708	U
1	A	1709	A

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Mol	Chain	Res	Type
1	A	1712	G
1	A	1717	C
1	A	1719	G
1	A	1720	C
1	A	1727	A
1	A	1738	U
1	A	1740	G
1	A	1745	A
1	A	1746	A
1	A	1748	G
1	A	1750	G
1	A	1752	G
1	A	1753	C
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1762	G
1	A	1766	C
1	A	1768	A
1	A	1771	C
1	A	1776	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1781	C
1	A	1782	G
1	A	1783	C
1	A	1785	G
1	A	1789	A
1	A	1790	U
1	A	1792	G
1	A	1793	G
1	A	1797	A
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1812	A
1	A	1813	A
1	A	1814	A
1	A	1815	A
1	A	1829	C

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Mol	Chain	Res	Type
1	A	1830	G
1	A	1831	A
1	A	1833	G
1	A	1839	A
1	A	1843	G
1	A	1845	A
1	A	1846	G
1	A	1849	U
1	A	1858	A
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1895	A
1	A	1899	U
1	A	1902	G
1	A	1904	G
1	A	1932	G
1	A	1935	G
1	A	1941	A
1	A	1942	A
1	A	1943	C
1	A	1944	U
1	A	1946	U
1	A	1952	U
1	A	1956	A
1	A	1958	G
1	A	1959	G
1	A	1966	A
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1970	C
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1992	C
1	A	1993	G

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Mol	Chain	Res	Type
1	A	1995	A
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2004	G
1	A	2010	A
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2033	G
1	A	2050	G
1	A	2051	U
1	A	2052	A
1	A	2053	C
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2065	C
1	A	2068	G
1	A	2070	U
1	A	2072	C
1	A	2079	C
1	A	2080	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2098	G
1	A	2101	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2131	U
1	A	2134	A
1	A	2135	G

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Mol	Chain	Res	Type
1	A	2136	C
1	A	2139	G
1	A	2140	U
1	A	2145	G
1	A	2146	A
1	A	2147	U
1	A	2149	G
1	A	2156	G
1	A	2160	U
1	A	2161	G
1	A	2162	G
1	A	2166	C
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2177	G
1	A	2185	G
1	A	2187	A
1	A	2198	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2208	C
1	A	2210	G
1	A	2212	C
1	A	2213	U
1	A	2217	U
1	A	2219	G
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2241	A
1	A	2242	U
1	A	2244	G
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A

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Mol	Chain	Res	Type
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2267	G
1	A	2268	G
1	A	2295	A
1	A	2296	A
1	A	2307	A
1	A	2308	G
1	A	2311	G
1	A	2312	C
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2324	C
1	A	2325	U
1	A	2327	A
1	A	2328	G
1	A	2331	U
1	A	2332	G
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2340	A
1	A	2341	U
1	A	2342	C
1	A	2343	A
1	A	2344	U
1	A	2345	U
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2351	A
1	A	2354	G
1	A	2356	A
1	A	2357	A
1	A	2363	C
1	A	2364	A
1	A	2368	G
1	A	2374	G

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Mol	Chain	Res	Type
1	A	2376	C
1	A	2379	C
1	A	2381	A
1	A	2387	A
1	A	2390	A
1	A	2401	G
1	A	2406	A
1	A	2408	G
1	A	2412	G
1	A	2413	G
1	A	2414	C
1	A	2418	G
1	A	2420	G
1	A	2431	U
1	A	2432	C
1	A	2435	C
1	A	2448	U
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2456	C
1	A	2457	G
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2497	A
1	A	2505	A
1	A	2506	C
1	A	2507	A
1	A	2511	A
1	A	2523	G
1	A	2524	G
1	A	2525	C

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Mol	Chain	Res	Type
1	A	2527	C
1	A	2531	G
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2547	A
1	A	2554	G
1	A	2558	G
1	A	2563	C
1	A	2564	G
1	A	2570	A
1	A	2583	U
1	A	2593	A
1	A	2595	A
1	A	2596	G
1	A	2598	G
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2612	G
1	A	2613	U
1	A	2615	C
1	A	2631	A
1	A	2632	G
1	A	2638	U
1	A	2642	U
1	A	2644	U
1	A	2654	G
1	A	2659	G
1	A	2660	G
1	A	2667	G
1	A	2674	G
1	A	2675	C
1	A	2689	A
1	A	2692	G
1	A	2696	C
1	A	2702	G
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G

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Mol	Chain	Res	Type
1	A	2747	G
1	A	2753	U
1	A	2755	U
1	A	2760	G
1	A	2762	A
1	A	2764	G
1	A	2765	G
1	A	2766	G
1	A	2773	G
1	A	2777	A
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2789	C
1	A	2794	A
1	A	2795	G
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2821	U
1	A	2822	C
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2828	G
1	A	2831	A
1	A	2832	G
1	A	2833	U
1	A	2843	G
1	A	2855	G
1	A	2859	G
1	A	2860	A
1	A	2862	A
1	A	2866	C
1	A	2868	G
1	A	2874	G
1	A	2886	C
1	A	2891	G
1	A	2892	G
1	A	2897	G
1	A	2899	C

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Mol	Chain	Res	Type
1	A	2900	A
1	A	2901	G
1	A	2905	C
1	A	2908	A
1	A	2916	A
1	A	2917	G
2	B	10	G
2	B	12	U
2	B	15	C
2	B	22	G
2	B	23	U
2	B	28	C
2	B	31	G
2	B	32	U
2	B	33	U
2	B	34	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	47	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	62	U
2	B	63	C
2	B	64	A
2	B	65	G
2	B	66	C
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A
2	B	101	U

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Mol	Chain	Res	Type
2	B	106	C
2	B	107	G
2	B	110	G
2	B	114	A
31	a	9	G
31	a	10	A
31	a	11	G
31	a	24	G
31	a	32	C
31	a	33	G
31	a	34	A
31	a	41	G
31	a	46	G
31	a	49	C
31	a	50	C
31	a	51	U
31	a	52	A
31	a	53	A
31	a	60	C
31	a	65	C
31	a	66	G
31	a	72	A
31	a	75	G
31	a	77	U
31	a	80	G
31	a	84	U
31	a	85	U
31	a	86	G
31	a	87	C
31	a	88	U
31	a	89	C
31	a	90	C
31	a	92	U
31	a	93	G
31	a	99	A
31	a	113	G
31	a	114	A
31	a	117	A
31	a	118	A
31	a	119	C
31	a	120	A
31	a	128	A

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Mol	Chain	Res	Type
31	a	129	A
31	a	130	C
31	a	136	U
31	a	137	G
31	a	140	A
31	a	141	G
31	a	142	A
31	a	144	U
31	a	153	U
31	a	154	C
31	a	158	G
31	a	162	C
31	a	167	G
31	a	172	U
31	a	176	G
31	a	181	G
31	a	182	U
31	a	189	A
31	a	190	A
31	a	193	G
31	a	194	C
31	a	197	G
31	a	207	U
31	a	208	A
31	a	209	A
31	a	211	A
31	a	218	U
31	a	219	U
31	a	220	C
31	a	221	G
31	a	222	G
31	a	249	G
31	a	253	U
31	a	255	G
31	a	259	G
31	a	262	G
31	a	274	G
31	a	275	C
31	a	277	C
31	a	280	C
31	a	287	A
31	a	288	C

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Mol	Chain	Res	Type
31	a	297	G
31	a	306	A
31	a	314	A
31	a	316	C
31	a	321	A
31	a	329	A
31	a	336	C
31	a	337	A
31	a	338	C
31	a	340	G
31	a	352	A
31	a	353	C
31	a	355	G
31	a	357	A
31	a	359	G
31	a	360	C
31	a	362	G
31	a	371	A
31	a	373	U
31	a	375	U
31	a	380	C
31	a	383	U
31	a	385	G
31	a	390	A
31	a	392	G
31	a	396	G
31	a	400	G
31	a	406	C
31	a	414	G
31	a	419	A
31	a	420	U
31	a	421	G
31	a	426	U
31	a	429	U
31	a	430	C
31	a	432	G
31	a	436	G
31	a	437	U
31	a	438	A
31	a	439	A
31	a	442	C
31	a	447	U

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Mol	Chain	Res	Type
31	a	456	A
31	a	457	A
31	a	459	A
31	a	460	A
31	a	461	C
31	a	465	U
31	a	466	G
31	a	467	C
31	a	473	G
31	a	474	A
31	a	476	U
31	a	477	A
31	a	478	G
31	a	480	G
31	a	483	G
31	a	484	U
31	a	485	A
31	a	487	C
31	a	488	U
31	a	490	G
31	a	491	A
31	a	494	G
31	a	506	A
31	a	508	A
31	a	518	A
31	a	519	A
31	a	520	C
31	a	526	G
31	a	527	C
31	a	530	G
31	a	533	G
31	a	536	G
31	a	539	G
31	a	540	U
31	a	541	A
31	a	542	A
31	a	553	G
31	a	554	C
31	a	556	A
31	a	563	U
31	a	564	C
31	a	568	A

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Mol	Chain	Res	Type
31	a	571	U
31	a	573	U
31	a	575	G
31	a	581	A
31	a	582	A
31	a	585	G
31	a	586	G
31	a	588	U
31	a	591	C
31	a	597	G
31	a	616	A
31	a	627	C
31	a	628	U
31	a	629	C
31	a	641	G
31	a	642	U
31	a	643	C
31	a	648	G
31	a	650	A
31	a	661	U
31	a	662	U
31	a	670	G
31	a	674	A
31	a	694	G
31	a	696	A
31	a	704	A
31	a	727	A
31	a	732	U
31	a	733	G
31	a	740	G
31	a	742	G
31	a	745	U
31	a	756	U
31	a	757	A
31	a	758	A
31	a	762	A
31	a	764	G
31	a	768	A
31	a	787	G
31	a	802	U
31	a	803	A
31	a	806	C

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Mol	Chain	Res	Type
31	a	815	C
31	a	821	G
31	a	824	A
31	a	826	C
31	a	828	A
31	a	829	U
31	a	841	G
31	a	845	G
31	a	849	G
31	a	853	C
31	a	855	G
31	a	856	C
31	a	861	U
31	a	880	U
31	a	884	G
31	a	885	C
31	a	895	G
31	a	899	A
31	a	909	C
31	a	924	A
31	a	932	G
31	a	936	G
31	a	944	C
31	a	945	A
31	a	952	G
31	a	964	G
31	a	966	U
31	a	967	U
31	a	968	A
31	a	970	U
31	a	975	A
31	a	976	G
31	a	978	A
31	a	979	A
31	a	981	G
31	a	984	A
31	a	985	A
31	a	986	G
31	a	987	A
31	a	992	U
31	a	993	A
31	a	999	U

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Mol	Chain	Res	Type
31	a	1000	C
31	a	1002	U
31	a	1003	G
31	a	1006	A
31	a	1008	C
31	a	1009	C
31	a	1010	U
31	a	1011	C
31	a	1012	U
31	a	1013	G
31	a	1014	A
31	a	1015	C
31	a	1017	A
31	a	1019	C
31	a	1020	C
31	a	1023	G
31	a	1024	A
31	a	1027	U
31	a	1028	A
31	a	1030	G
31	a	1031	A
31	a	1033	G
31	a	1035	C
31	a	1036	C
31	a	1039	U
31	a	1040	U
31	a	1041	C
31	a	1042	G
31	a	1043	G
31	a	1046	G
31	a	1047	C
31	a	1050	A
31	a	1051	G
31	a	1052	U
31	a	1053	G
31	a	1056	A
31	a	1058	G
31	a	1060	G
31	a	1064	C
31	a	1071	G
31	a	1074	G
31	a	1075	U

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Mol	Chain	Res	Type
31	a	1095	U
31	a	1102	A
31	a	1104	G
31	a	1105	U
31	a	1110	C
31	a	1111	A
31	a	1112	A
31	a	1114	G
31	a	1118	G
31	a	1124	C
31	a	1128	A
31	a	1134	G
31	a	1136	U
31	a	1140	A
31	a	1141	G
31	a	1142	C
31	a	1143	A
31	a	1145	U
31	a	1148	G
31	a	1149	U
31	a	1150	U
31	a	1151	G
31	a	1153	G
31	a	1155	A
31	a	1163	G
31	a	1166	A
31	a	1167	C
31	a	1168	U
31	a	1169	G
31	a	1170	C
31	a	1176	A
31	a	1177	C
31	a	1178	A
31	a	1180	A
31	a	1190	G
31	a	1192	U
31	a	1193	G
31	a	1205	A
31	a	1206	A
31	a	1209	C
31	a	1211	U
31	a	1214	U

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Mol	Chain	Res	Type
31	a	1221	U
31	a	1222	A
31	a	1224	G
31	a	1233	U
31	a	1236	A
31	a	1237	C
31	a	1238	A
31	a	1239	C
31	a	1245	A
31	a	1247	A
31	a	1248	A
31	a	1258	C
31	a	1259	A
31	a	1265	C
31	a	1266	A
31	a	1267	G
31	a	1269	G
31	a	1279	G
31	a	1288	A
31	a	1289	A
31	a	1291	C
31	a	1294	A
31	a	1295	C
31	a	1296	A
31	a	1299	U
31	a	1307	C
31	a	1308	A
31	a	1309	G
31	a	1311	U
31	a	1312	C
31	a	1313	G
31	a	1314	G
31	a	1323	C
31	a	1326	C
31	a	1329	C
31	a	1331	C
31	a	1332	G
31	a	1336	G
31	a	1340	G
31	a	1345	U
31	a	1347	G
31	a	1349	A

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Mol	Chain	Res	Type
31	a	1354	U
31	a	1355	A
31	a	1362	G
31	a	1366	A
31	a	1371	C
31	a	1372	A
31	a	1373	U
31	a	1377	G
31	a	1379	G
31	a	1387	C
31	a	1403	A
31	a	1406	C
31	a	1407	A
31	a	1413	C
31	a	1428	G
31	a	1435	A
31	a	1451	A
31	a	1452	G
31	a	1455	A
31	a	1461	U
31	a	1462	U
31	a	1463	A
31	a	1464	G
31	a	1478	A
31	a	1494	U
31	a	1496	G
31	a	1497	G
31	a	1500	U
31	a	1502	A
31	a	1503	A
31	a	1507	G
31	a	1513	A
31	a	1516	U
31	a	1517	A
31	a	1527	G
31	a	1529	A
31	a	1539	G
31	a	1540	G
51	x	7	G
51	x	8	U
51	x	9	G
51	x	13	G

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Mol	Chain	Res	Type
51	x	16	U
51	x	17	U
51	x	18	G
51	x	19	G
51	x	20	U
51	x	21	A
51	x	22	G
51	x	23	A
51	x	24	C
51	x	26	C
51	x	27	G
51	x	42	U
51	x	44	G
51	x	50	A
51	x	52	U
51	x	54	G
51	x	58	U
51	x	67	C
51	x	68	A
51	x	72	C
51	x	87	A

All (92) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	C
1	A	88	G
1	A	92	G
1	A	118	A
1	A	163	U
1	A	181	G
1	A	199	A
1	A	236	A
1	A	252	C
1	A	347	G
1	A	410	G
1	A	411	G
1	A	441	C
1	A	455	G
1	A	458	G
1	A	459	A
1	A	482	C

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Mol	Chain	Res	Type
1	A	490	A
1	A	525	A
1	A	549	A
1	A	554	U
1	A	576	G
1	A	594	C
1	A	666	G
1	A	689	A
1	A	702	A
1	A	732	A
1	A	756	U
1	A	810	G
1	A	831	U
1	A	848	G
1	A	855	G
1	A	933	C
1	A	1028	C
1	A	1032	C
1	A	1036	A
1	A	1041	C
1	A	1172	A
1	A	1187	U
1	A	1210	A
1	A	1226	U
1	A	1243	A
1	A	1250	G
1	A	1260	A
1	A	1266	A
1	A	1269	A
1	A	1294	A
1	A	1305	A
1	A	1325	A
1	A	1339	A
1	A	1351	U
1	A	1448	U
1	A	1464	A
1	A	1507	U
1	A	1525	G
1	A	1529	G
1	A	1530	G
1	A	1535	U
1	A	1543	U

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Mol	Chain	Res	Type
1	A	1565	U
1	A	1570	U
1	A	1631	A
1	A	1671	G
1	A	1726	G
1	A	1751	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1844	A
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1991	C
1	A	2009	G
1	A	2127	U
1	A	2139	G
1	A	2155	A
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2356	A
1	A	2454	A
1	A	2456	C
1	A	2468	A
1	A	2531	G
1	A	2631	A
1	A	2710	C
1	A	2805	A
1	A	2904	A
2	B	37	A
2	B	48	G
2	B	49	G

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	TEL	A	3001	-	60,62,62	1.35	6 (10%)	78,92,92	1.97	17 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	TEL	A	3001	-	1/1/19/19	17/73/108/108	0/4/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	3001	TEL	O5-C10	5.77	1.45	1.35
52	A	3001	TEL	O9-C15	5.03	1.45	1.34
52	A	3001	TEL	C40-N41	-3.25	1.35	1.38
52	A	3001	TEL	O5-C2	-2.75	1.43	1.47
52	A	3001	TEL	C36-N31	-2.28	1.34	1.37
52	A	3001	TEL	O9-C4	-2.02	1.43	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	3001	TEL	O9-C15-C21	9.44	120.25	110.93
52	A	3001	TEL	C17-C11-N6	-5.47	104.95	113.25
52	A	3001	TEL	N31-C37-N41	-4.48	108.78	112.35
52	A	3001	TEL	C36-N31-C37	3.93	108.64	106.71
52	A	3001	TEL	C4-O9-C15	-3.76	111.64	118.20
52	A	3001	TEL	O20-C15-C21	-3.15	120.57	124.65
52	A	3001	TEL	C8-C4-C2	-3.12	110.94	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A	3001	TEL	C28-C24-C19	-3.08	111.08	116.10
52	A	3001	TEL	C43-C40-N41	2.85	126.41	122.45
52	A	3001	TEL	C1-C2-C3	-2.80	111.17	116.36
52	A	3001	TEL	O9-C15-O20	-2.64	119.18	123.95
52	A	3001	TEL	C56-N52-C47	2.47	121.18	116.85
52	A	3001	TEL	C42-O39-C34	-2.43	112.12	116.26
52	A	3001	TEL	C24-C19-C13	-2.36	109.37	113.32
52	A	3001	TEL	C37-N41-C40	2.31	107.80	105.94
52	A	3001	TEL	C43-C40-C36	-2.23	126.24	129.65
52	A	3001	TEL	C54-C49-N53	-2.18	109.45	115.59

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
52	A	3001	TEL	C21

All (17) torsion outliers are listed below:

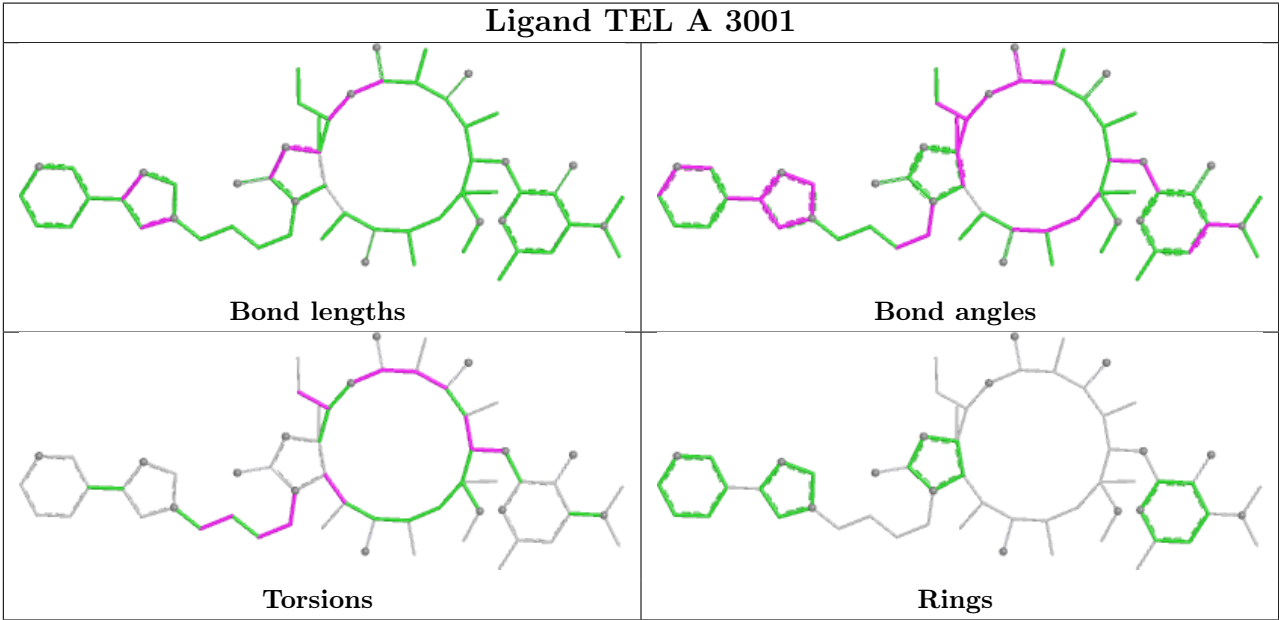
Mol	Chain	Res	Type	Atoms
52	A	3001	TEL	C15-C21-C26-O29
52	A	3001	TEL	C15-C21-C26-C30
52	A	3001	TEL	C21-C15-O9-C4
52	A	3001	TEL	O20-C15-O9-C4
52	A	3001	TEL	O9-C4-C8-C14
52	A	3001	TEL	N6-C3-C7-C12
52	A	3001	TEL	O20-C15-C21-C25
52	A	3001	TEL	O9-C15-C21-C25
52	A	3001	TEL	C17-C22-C27-N31
52	A	3001	TEL	O9-C15-C21-C26
52	A	3001	TEL	C2-C4-C8-C14
52	A	3001	TEL	C35-C30-C34-C28
52	A	3001	TEL	C17-C11-N6-C10
52	A	3001	TEL	C30-C34-O39-C42
52	A	3001	TEL	O20-C15-C21-C26
52	A	3001	TEL	C2-C3-C7-C12
52	A	3001	TEL	N6-C11-C17-C22

There are no ring outliers.

1 monomer is involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	A	3001	TEL	20	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	182:C	O3'	183:A	P	6.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1449:C	O3'	1450:C	P	4.07
1	A	1451:U	O3'	1452:C	P	3.36
1	A	1452:C	O3'	1453:A	P	3.32
1	A	183:A	O3'	184:G	P	3.31

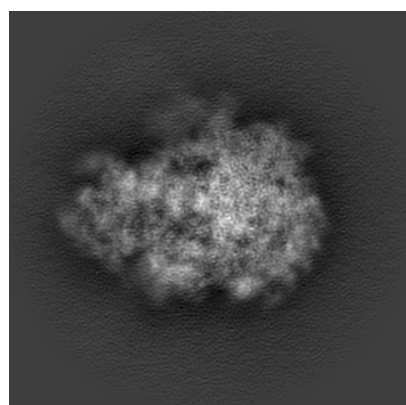
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0176. These allow visual inspection of the internal detail of the map and identification of artifacts.

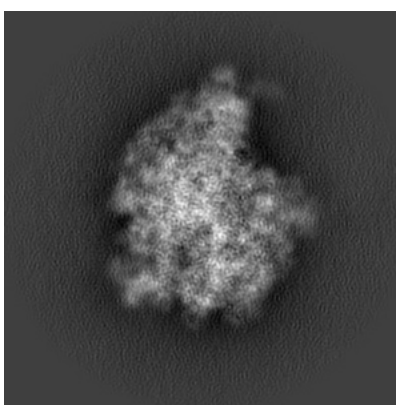
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

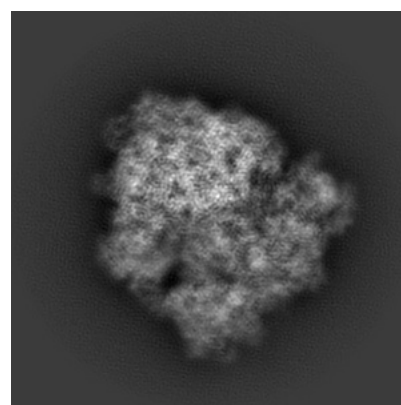
6.1.1 Primary map



X



Y

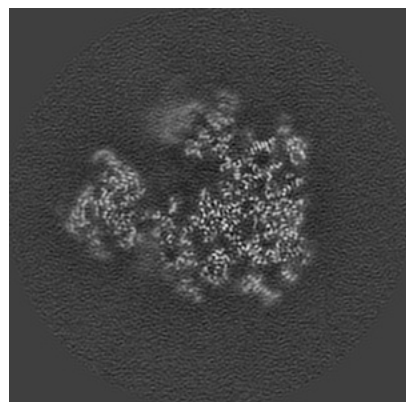


Z

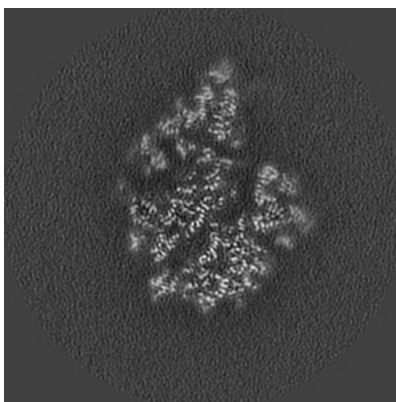
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

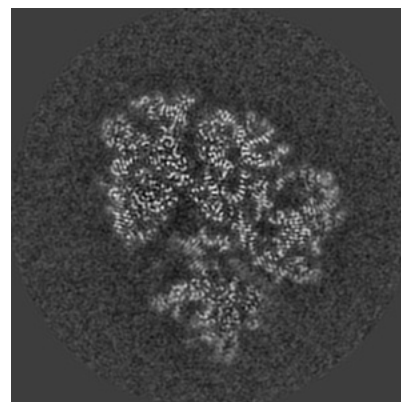
6.2.1 Primary map



X Index: 180



Y Index: 180

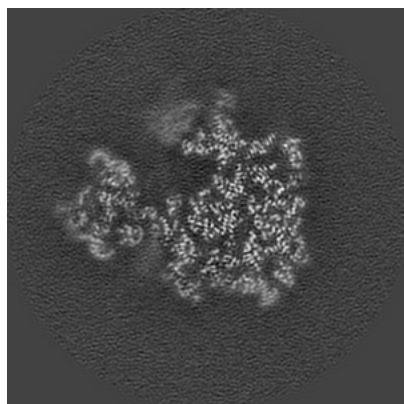


Z Index: 180

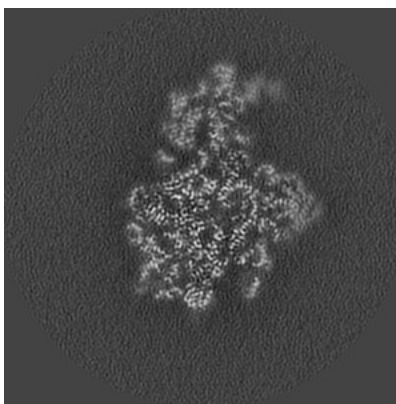
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

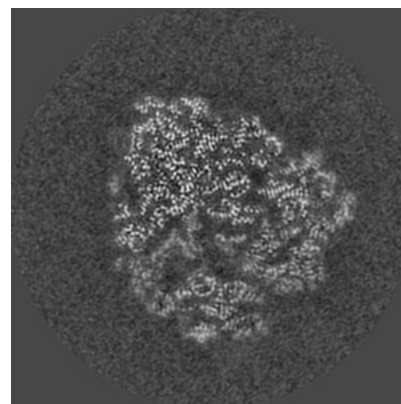
6.3.1 Primary map



X Index: 184



Y Index: 190

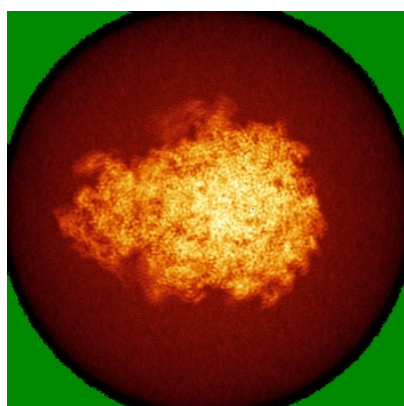


Z Index: 190

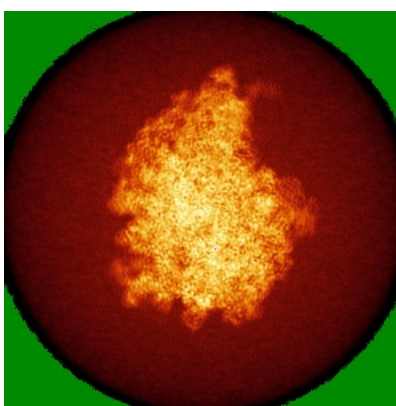
The images above show the largest variance slices of the map in three orthogonal directions.

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

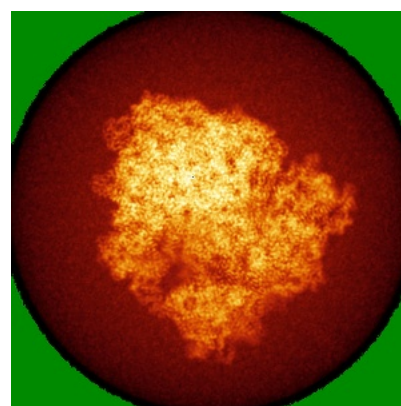
6.4.1 Primary map



X



Y

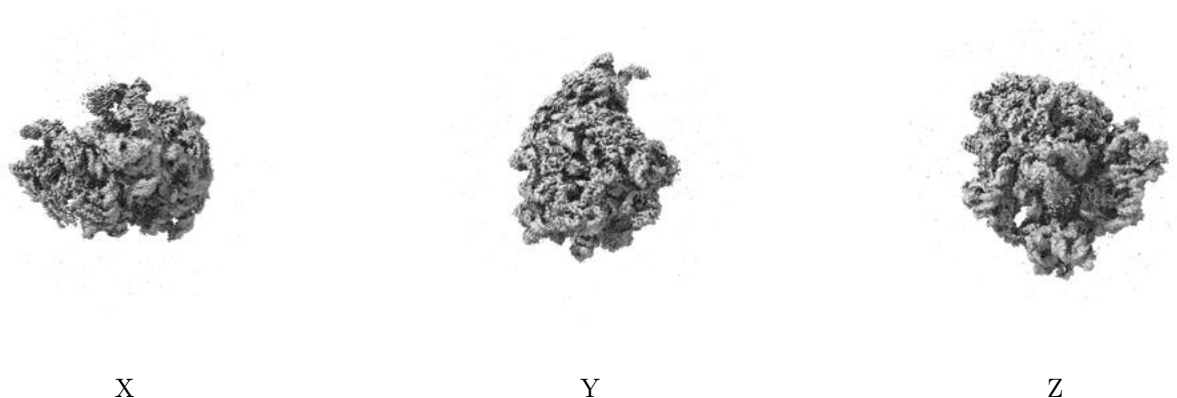


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

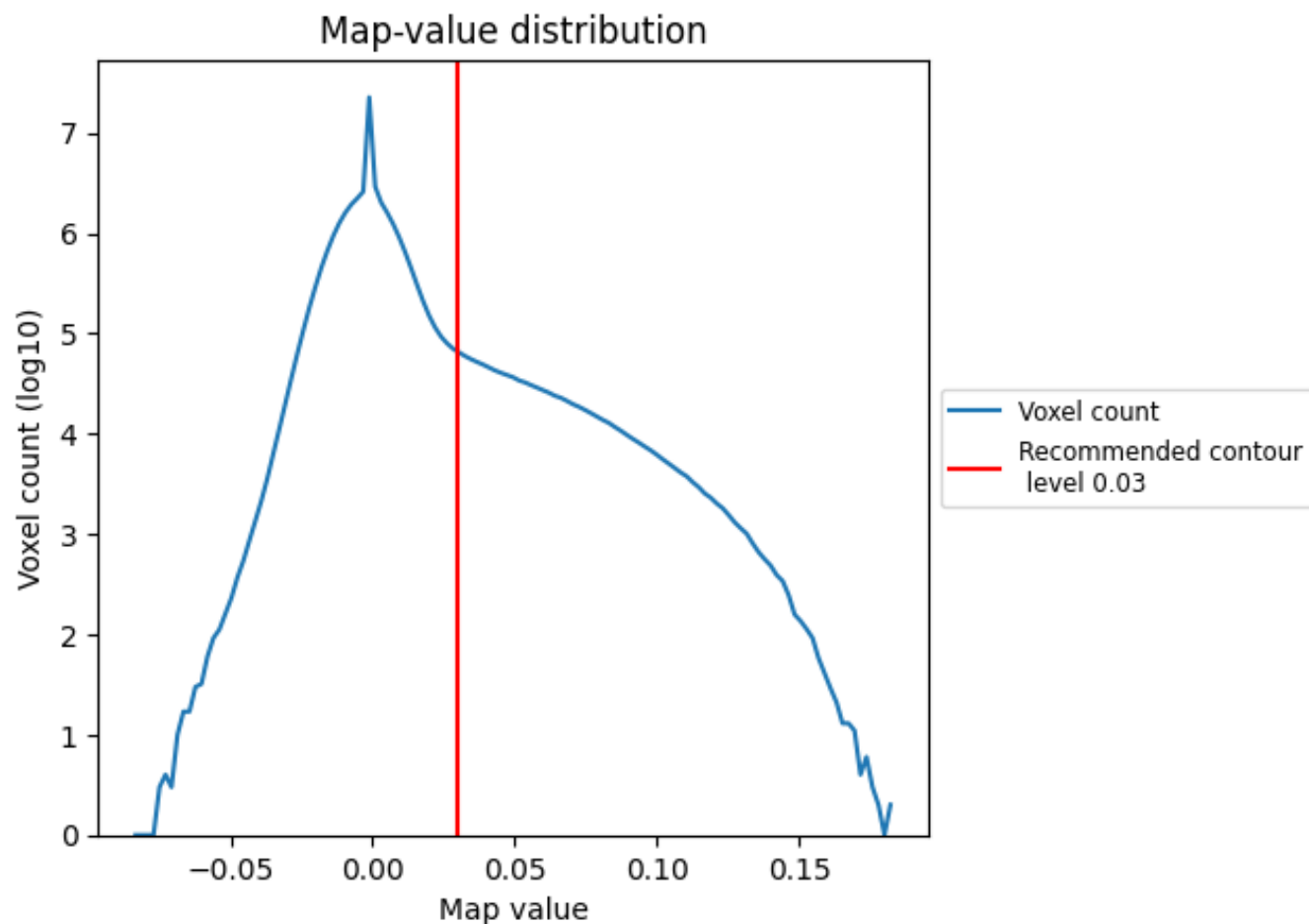
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

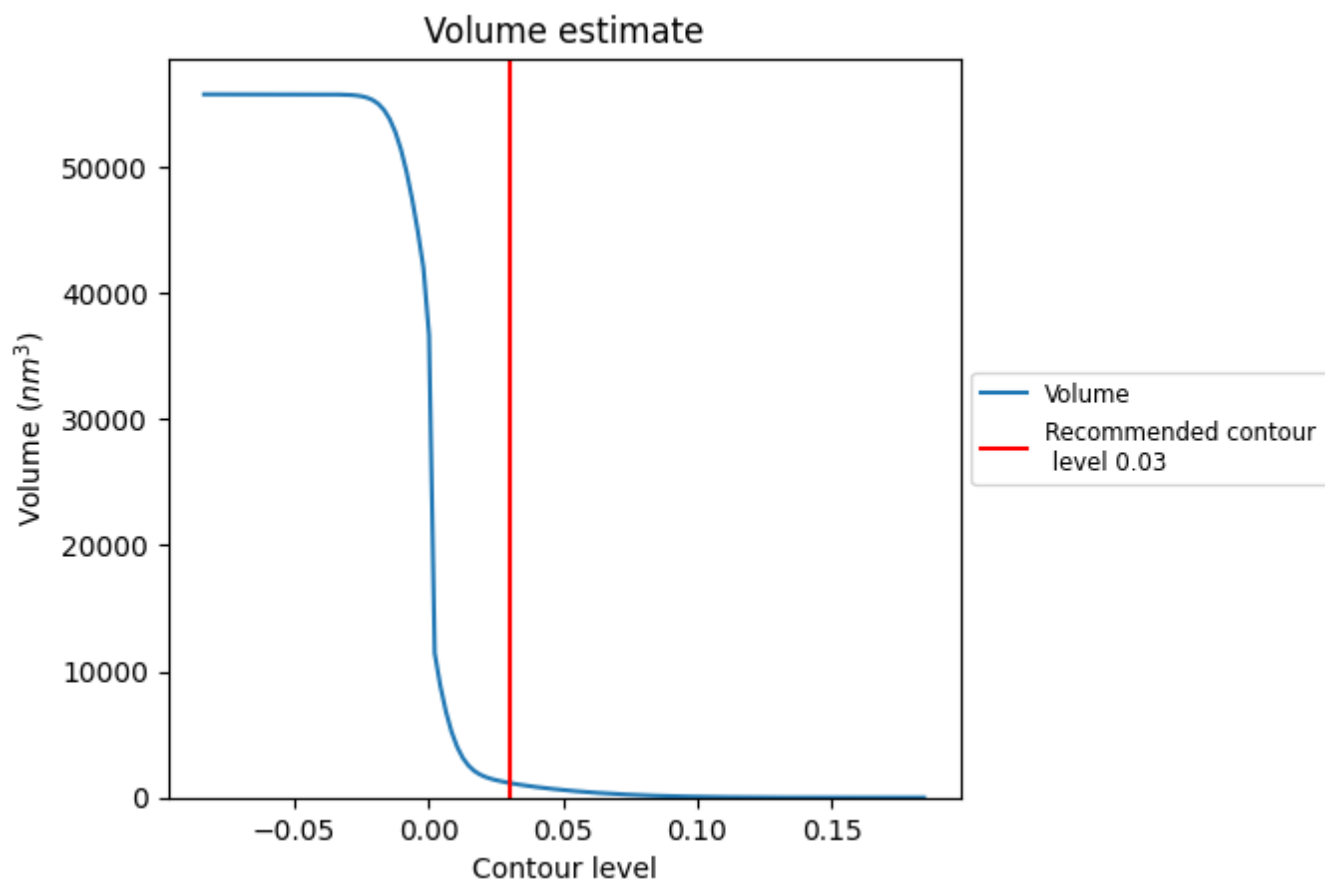
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

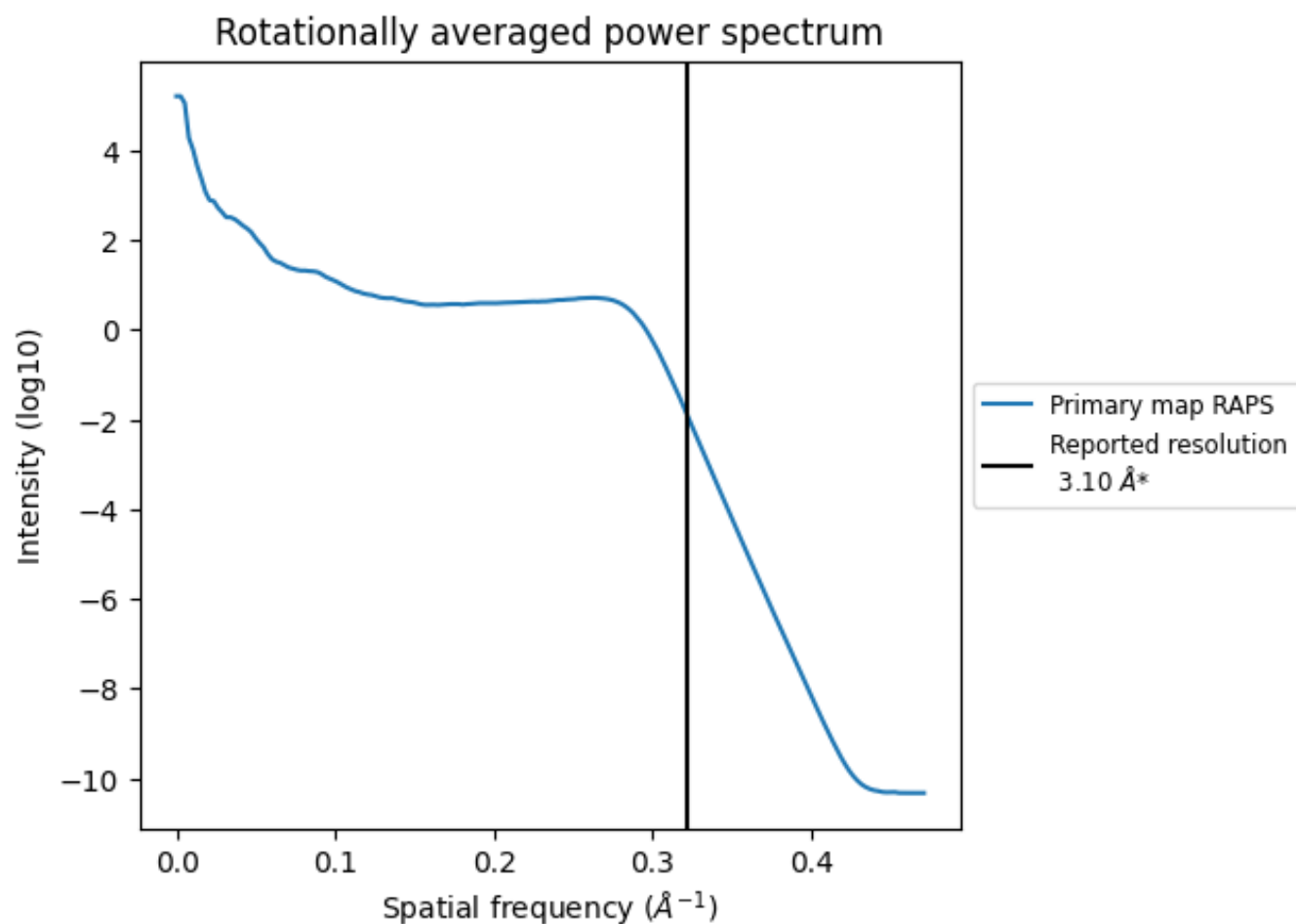
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1164 nm³; this corresponds to an approximate mass of 1051 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 0.323 Å⁻¹

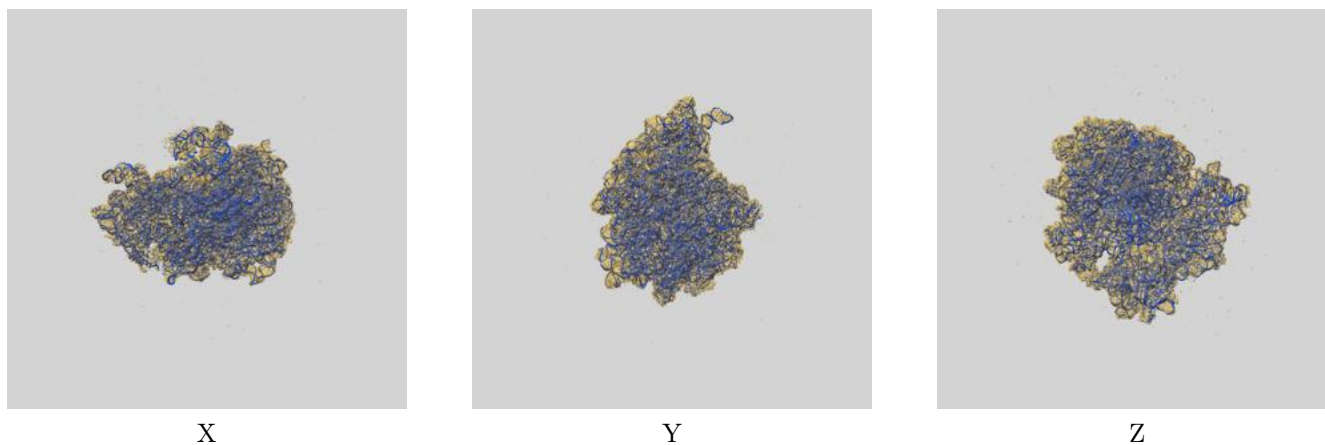
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

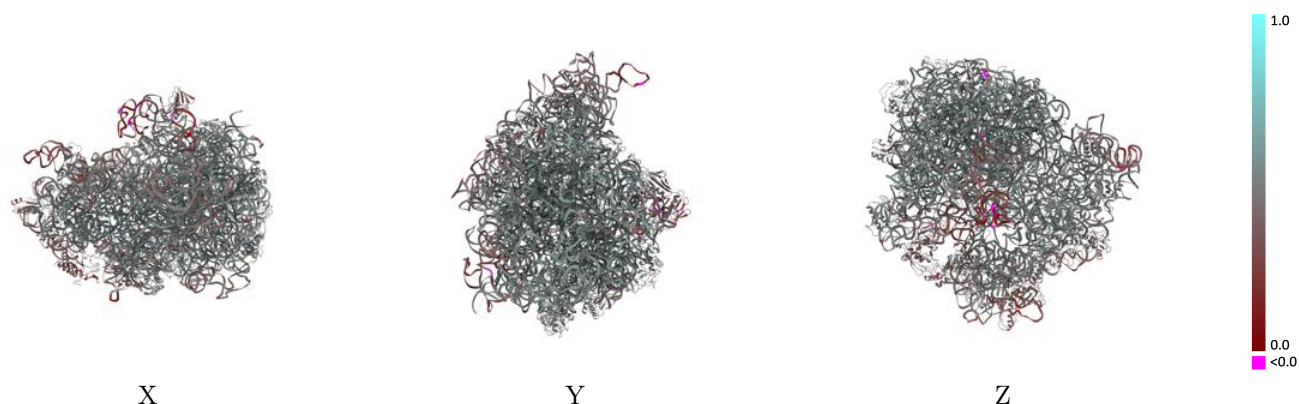
This section contains information regarding the fit between EMDB map EMD-0176 and PDB model 6HA1. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



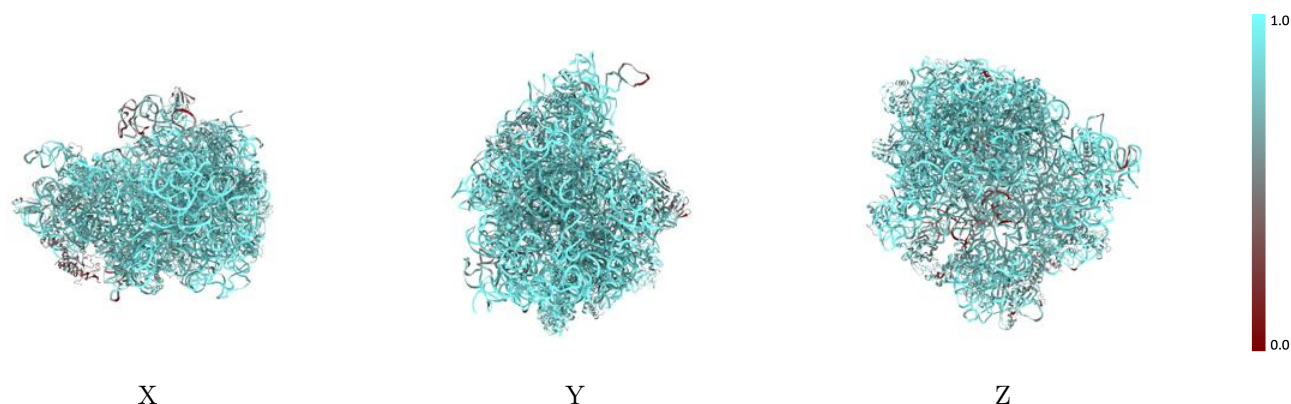
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



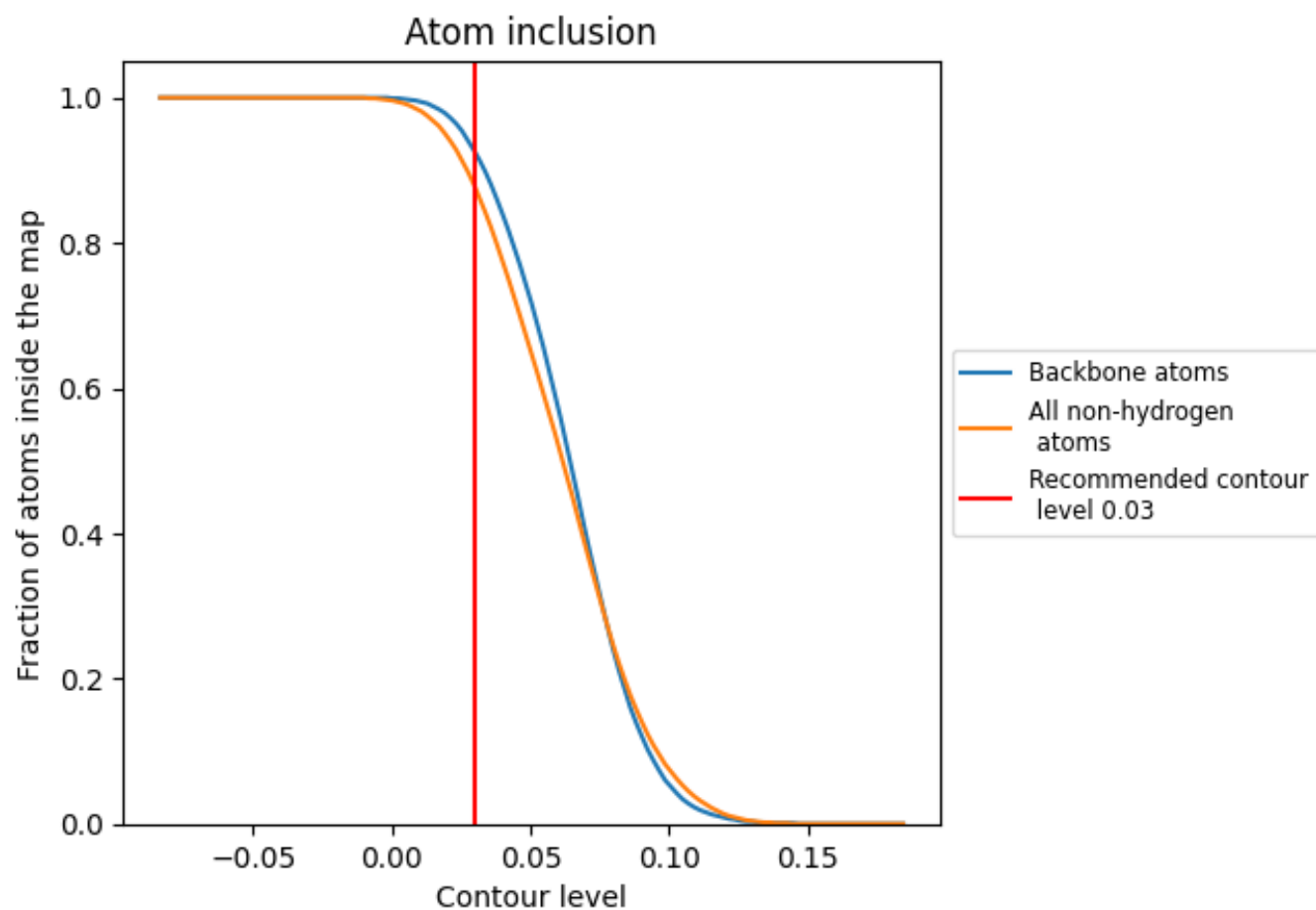
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8770	 0.4800
0	 0.8480	 0.5250
1	 0.8170	 0.4980
2	 0.8610	 0.5440
3	 0.8280	 0.5380
4	 0.7860	 0.5210
6	 0.6480	 0.3300
7	 0.9670	 0.5420
A	 0.9240	 0.4910
B	 0.9570	 0.4680
C	 0.8040	 0.5220
D	 0.8180	 0.5140
E	 0.8240	 0.5020
F	 0.7210	 0.4040
G	 0.6650	 0.3860
J	 0.8100	 0.4980
K	 0.7690	 0.5100
L	 0.8270	 0.5080
M	 0.7940	 0.5120
N	 0.8460	 0.5170
O	 0.7980	 0.4590
P	 0.7880	 0.5040
Q	 0.8460	 0.4980
R	 0.8120	 0.4890
S	 0.8090	 0.5200
T	 0.7830	 0.4850
U	 0.8070	 0.4710
W	 0.8310	 0.5160
X	 0.6500	 0.4710
Y	 0.7700	 0.4290
Z	 0.8090	 0.4840
a	 0.9390	 0.4790
b	 0.3770	 0.3560
c	 0.6990	 0.4430
d	 0.7430	 0.4310



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Chain	Atom inclusion	Q-score
e	 0.7650	 0.4990
f	 0.7380	 0.4540
g	 0.7020	 0.4240
h	 0.7670	 0.4780
i	 0.7510	 0.4310
j	 0.7180	 0.4350
k	 0.7470	 0.4570
l	 0.7480	 0.4780
m	 0.7570	 0.4310
n	 0.7520	 0.4880
o	 0.8050	 0.4490
p	 0.7570	 0.4670
q	 0.7240	 0.4650
r	 0.7430	 0.4400
s	 0.7670	 0.4320
t	 0.7520	 0.4500
x	 0.7450	 0.4170