



Full wwPDB EM Validation Report ⓘ

Jun 19, 2026 – 04:23 am BST

PDB ID : 8RCL / pdb_00008rcl
EMDB ID : EMD-19054
Title : Escherichia coli paused disome complex (Non-rotated disome interface class 1)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-12-06
Resolution : 3.49 Å(reported)
Based on initial model : 7N1P

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:

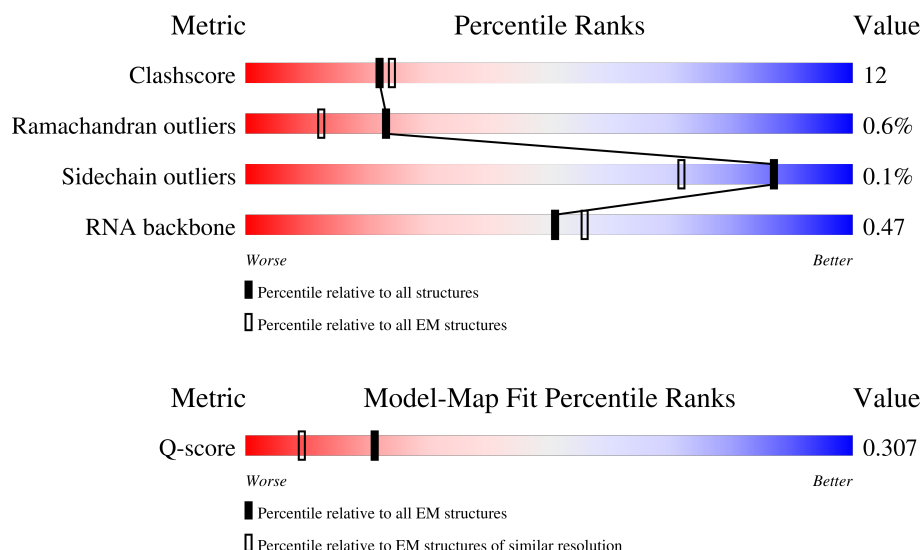
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.49 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	13600 (2.99 - 3.99)

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	12	78	
2	32	59	
3	4	70	

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Mol	Chain	Length	Quality of chain
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	
7	A1	1542	
7	A2	1542	
8	B	241	
8	B2	241	
9	C1	233	
9	C2	233	
10	D1	206	
10	D2	206	
11	E1	167	
11	E2	167	
12	F1	135	
12	F2	135	
13	G1	179	
13	G2	179	
14	H1	130	
14	H2	130	
15	I1	130	
15	I2	130	
16	J1	103	
16	J2	103	
17	K1	129	

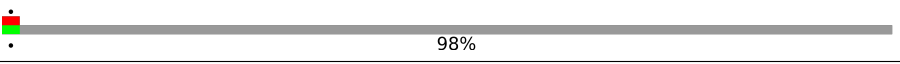
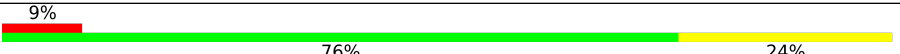
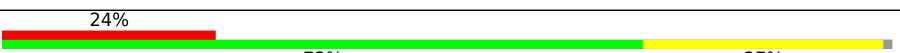
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Mol	Chain	Length	Quality of chain
17	K2	129	
18	L1	124	
18	L2	124	
19	M1	118	
19	M2	118	
20	N1	101	
20	N2	101	
21	O1	89	
21	O2	89	
22	P1	82	
23	Q1	84	
23	Q2	84	
24	R1	75	
24	R2	75	
25	S1	92	
25	S2	92	
26	T1	87	
27	U1	71	
27	U2	71	
28	V2	64	
29	W	76	
30	W1	76	
31	X2	77	
32	Y1	76	
33	Y2	76	

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Mol	Chain	Length	Quality of chain
34	Z1	557	
35	a2	234	
36	b2	273	
37	e2	179	
38	g2	55	
39	h2	136	
40	i2	149	
41	l2	46	
42	o2	144	
43	p	10	
44	r2	117	
45	z2	85	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 188653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	30	Total	C	N	O	P	0	0
			644	288	119	207	30		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

- Molecule 29 is a RNA chain called tRNA-Trp (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	2		

- Molecule 31 is a RNA chain called tRNA-Arg (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	X2	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

- Molecule 32 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Y1	36	Total	C	N	O	P		0	0
			778	348	142	252	36			

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Y2	76	Total	C	N	O	P		0	0
			1628	726	293	533	76			

- Molecule 34 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 37 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 38 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 40 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 41 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 42 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 43 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 44 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r2	116	Total	C	N	O	0	0
			891	552	178	161		

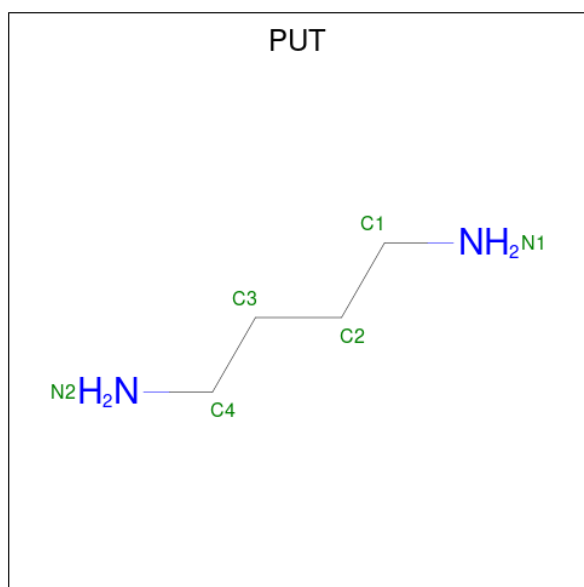
- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

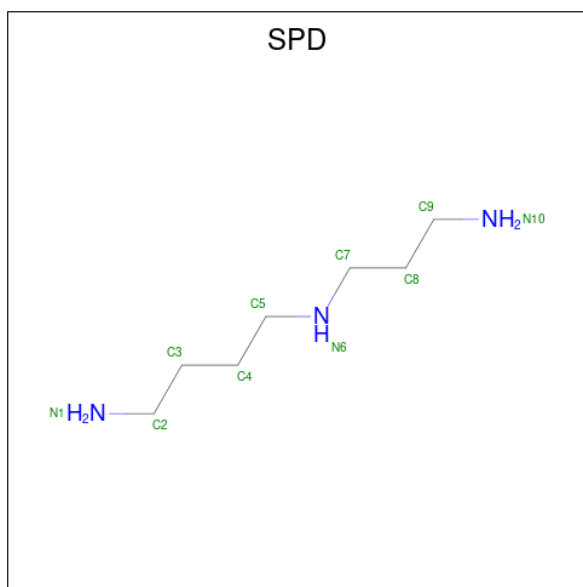
Mol	Chain	Residues	Atoms		AltConf
46	4	1	Total	Zn	0
			1	1	
46	B	1	Total	Zn	0
			1	1	

- Molecule 47 is 1,4-DIAMINOBTUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			6	4	2	
47	72	1	Total	C	N	0
			6	4	2	

- Molecule 48 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
48	72	1	Total	C	N	0
			10	7	3	

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

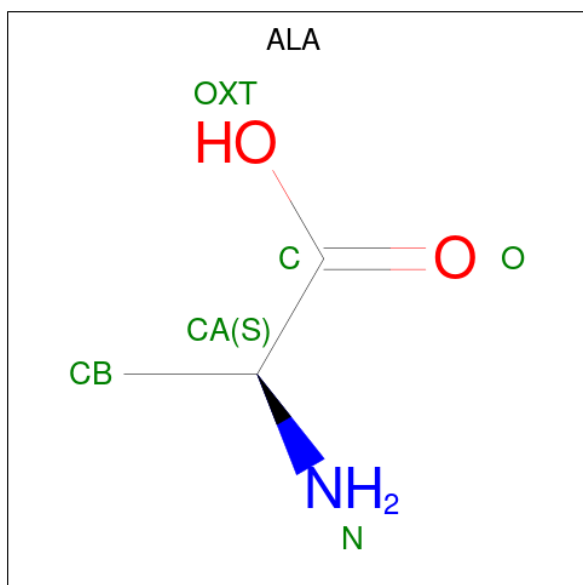
Mol	Chain	Residues	Atoms		AltConf
49	72	189	Total	Mg	0
			189	189	
49	82	1	Total	Mg	0
			1	1	
49	A1	59	Total	Mg	0
			59	59	
49	A2	42	Total	Mg	0
			42	42	
49	V2	1	Total	Mg	0
			1	1	
49	W	1	Total	Mg	0
			1	1	
49	Y2	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
49	b2	1	Total	Mg	0
			1	1	
49	o2	1	Total	Mg	0
			1	1	

- Molecule 50 is ALANINE (CCD ID: ALA) (formula: $C_3H_7NO_2$).

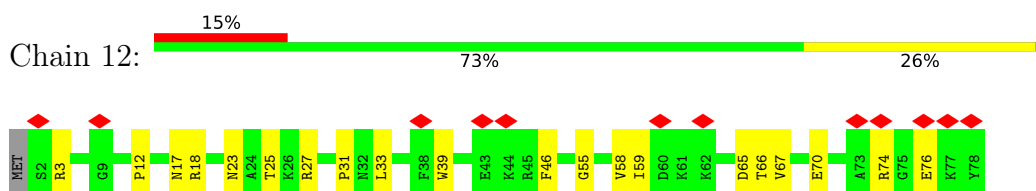


Mol	Chain	Residues	Atoms				AltConf
50	Y2	1	Total	C	N	O	0
			5	3	1	1	

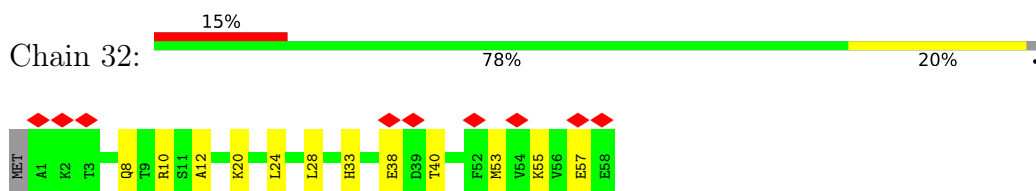
3 Residue-property plots [i](#)

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

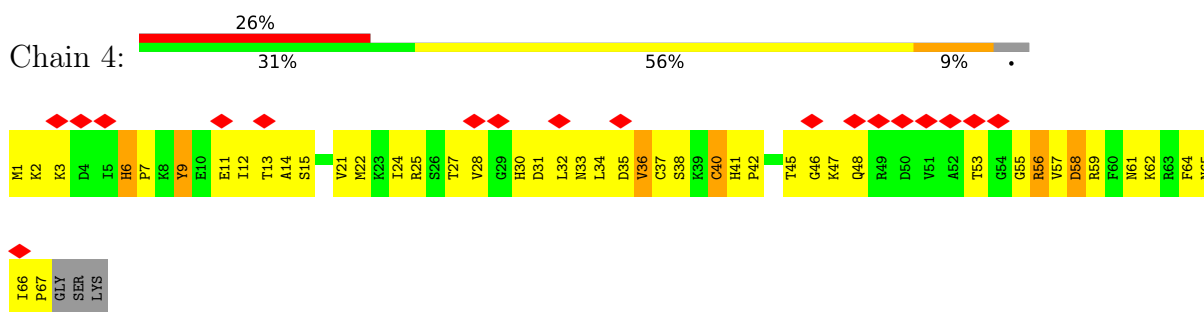
- Molecule 1: 50S ribosomal protein L28



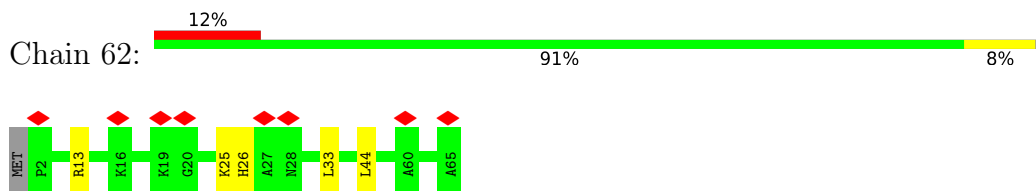
- Molecule 2: 50S ribosomal protein L30



- Molecule 3: Large ribosomal subunit protein bL31



- Molecule 4: 50S ribosomal protein L35

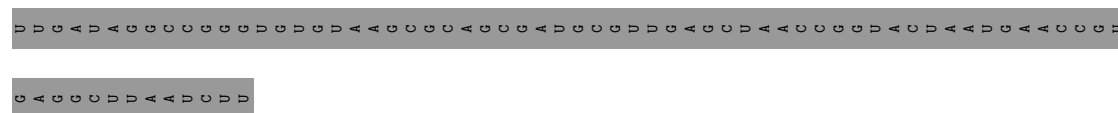


- Molecule 5: 23S ribosomal RNA



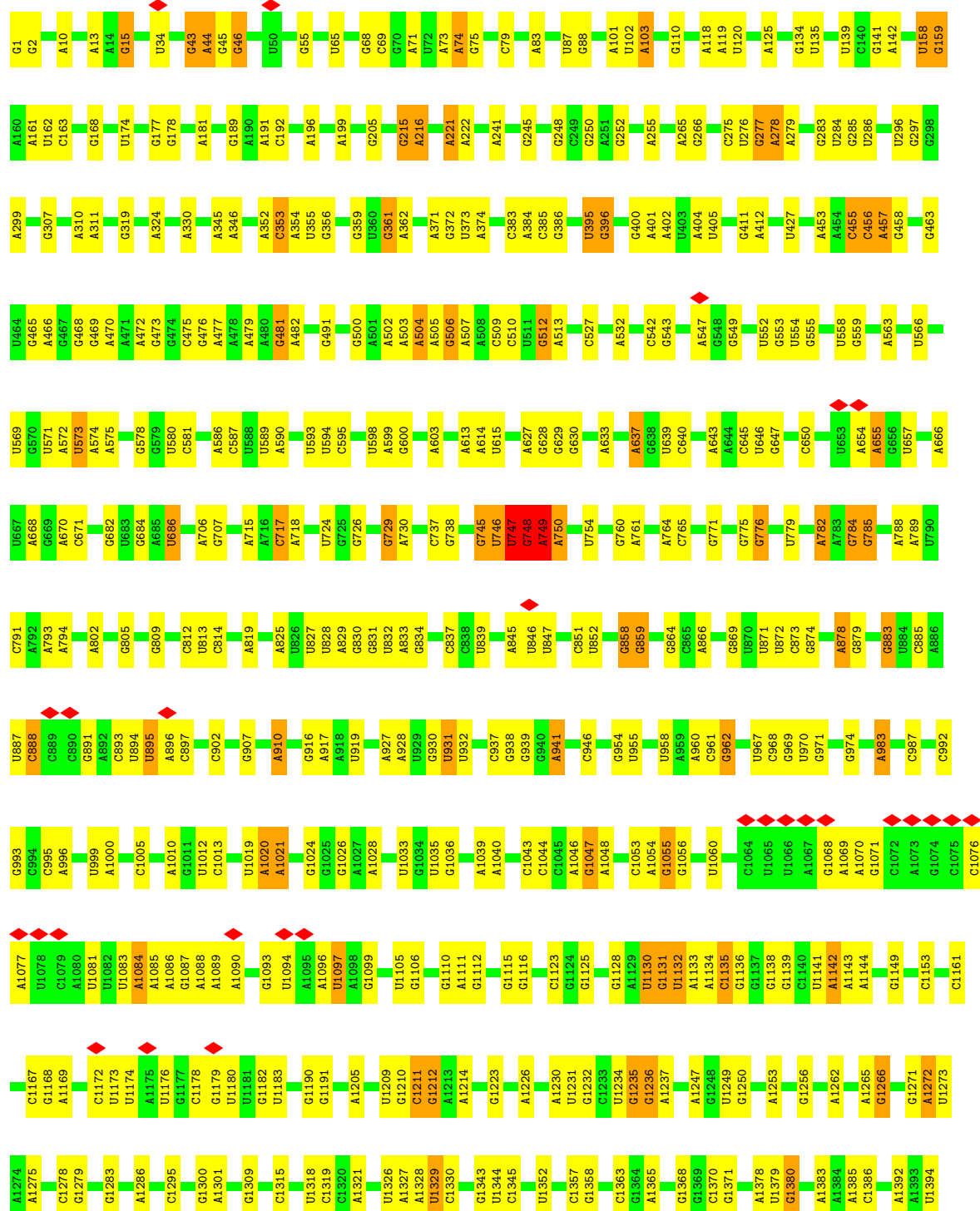






Molecule 5: 23S ribosomal RNA

Chain 72: 66% 28% 5%



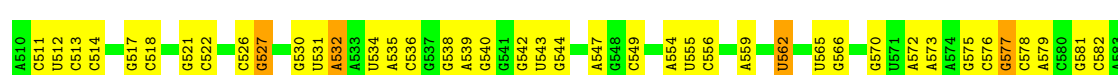
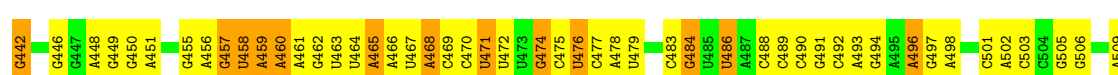
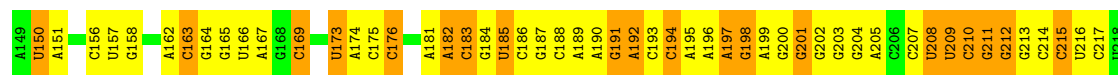
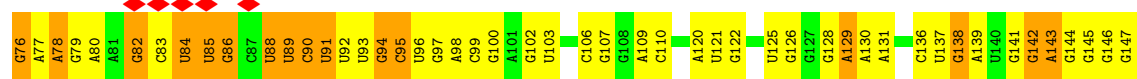
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A2726	G2581	C2498	A2392	U2291	U2181	G2115	G2010	A1783	C1646	U1396
G2732	G2582	C2499	U2393	U2292	U2182	G2116	A2013	A1784	U1405	U1405
A2733	G2583	U2500	C2394	U2293	A2184	A2117	U2022	A1785	G1514	U1406
U2740	U2585	C2501	C2395	A2298	U2185	U2118	U2023	A1786	G1416	G1416
U2743	U2586	G2502	C2396	G2304	G2186	G2120	G2024	A1789	C1417	G1417
G2744	A2590	A2503	C2403	U2305	U2187	G2124	C2025	C1790	G1418	G1418
G2747	G2591	G2504	A2406	G2308	A2198	G2125	A1913	A1791	G1419	G1419
A2748	G2592	G2505	G2410	A2309	G2201	A2126	3TD1915	G1914	A1527	A1420
G2751	G2595	U2506	G2421	G2310	U2202	G2127	C1920	A1677	A1530	A1427
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G2765	G2608	U2519	A2426	A2321	U2213	A2134	G2040	A1802	C1536	A1432
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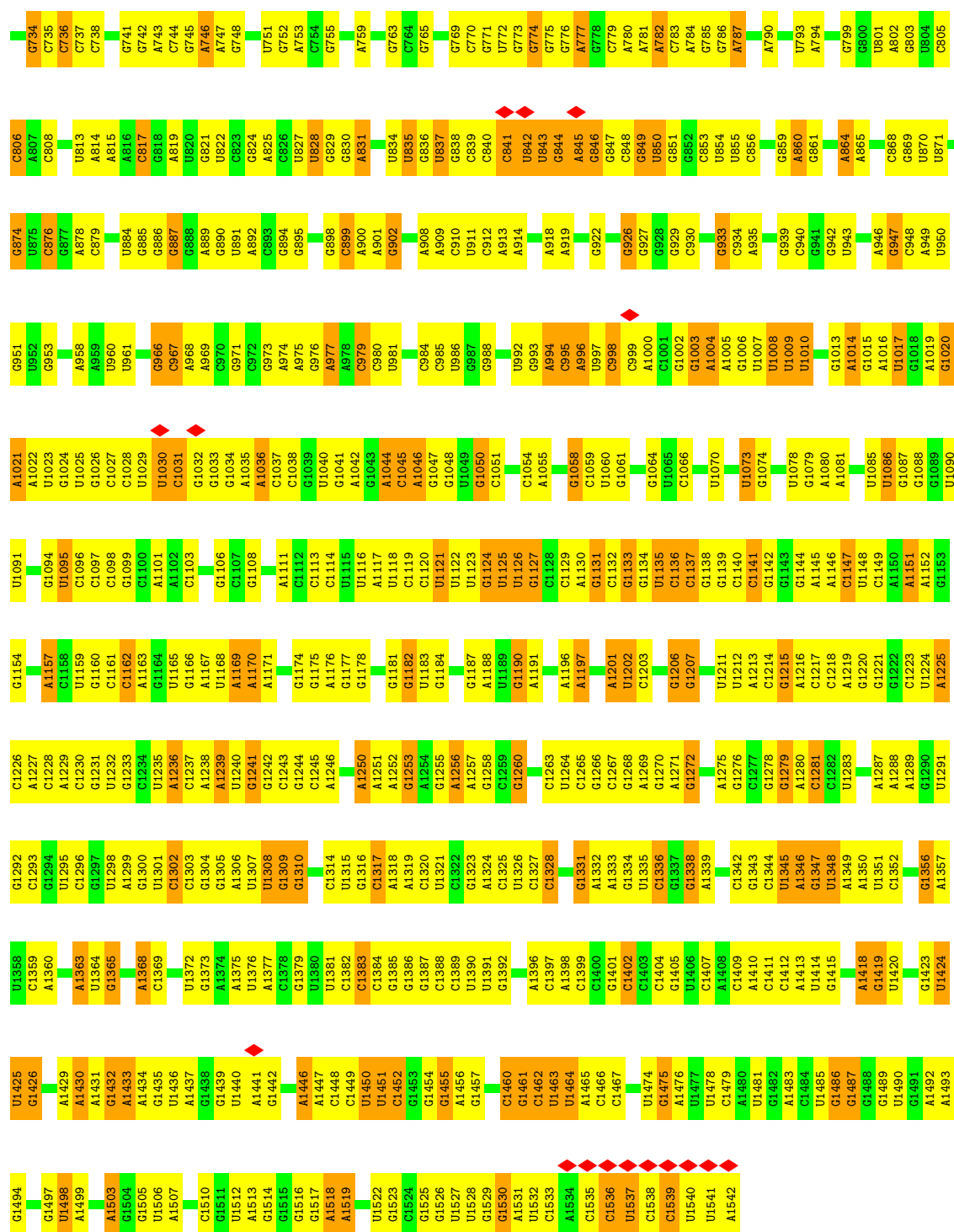


• Molecule 6: 5S ribosomal RNA

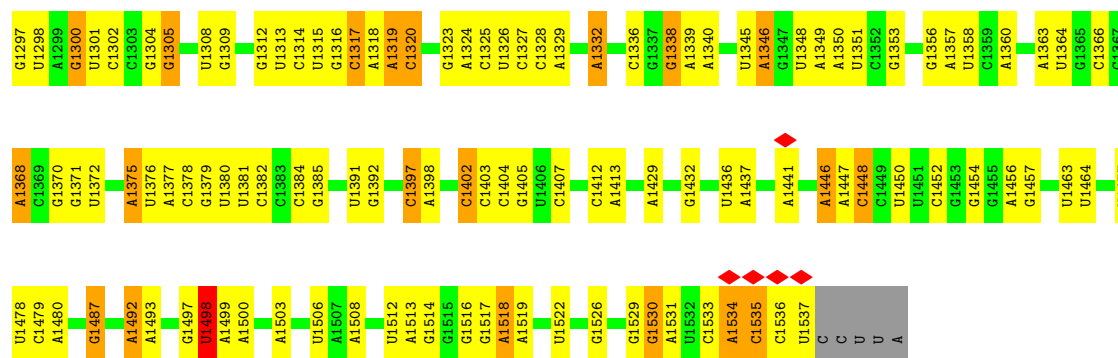


• Molecule 7: 16S ribosomal RNA

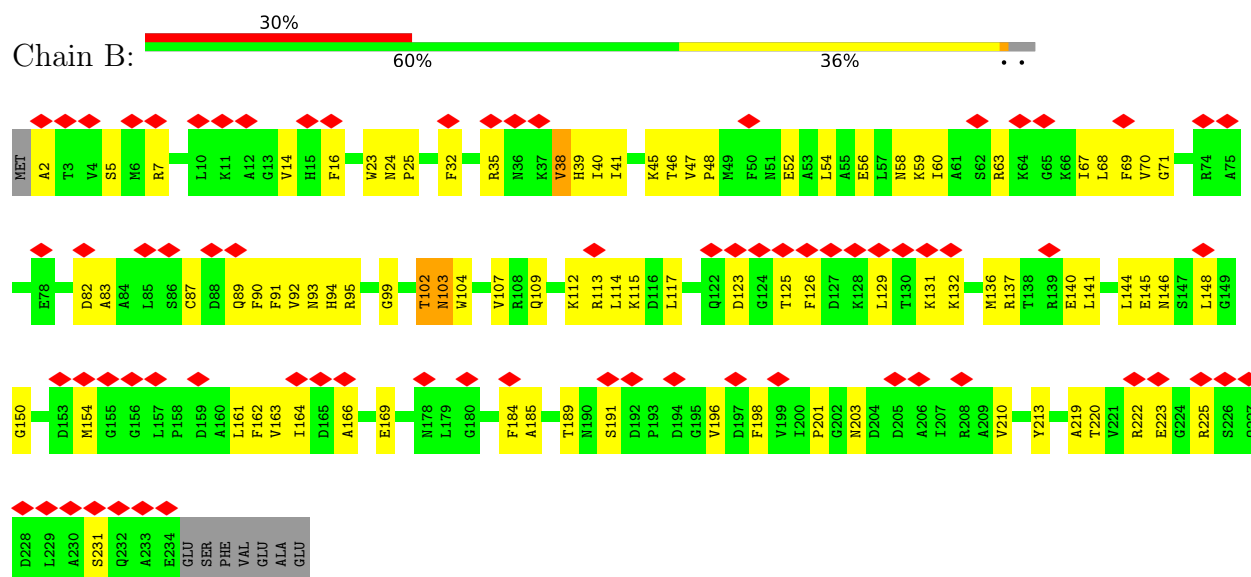




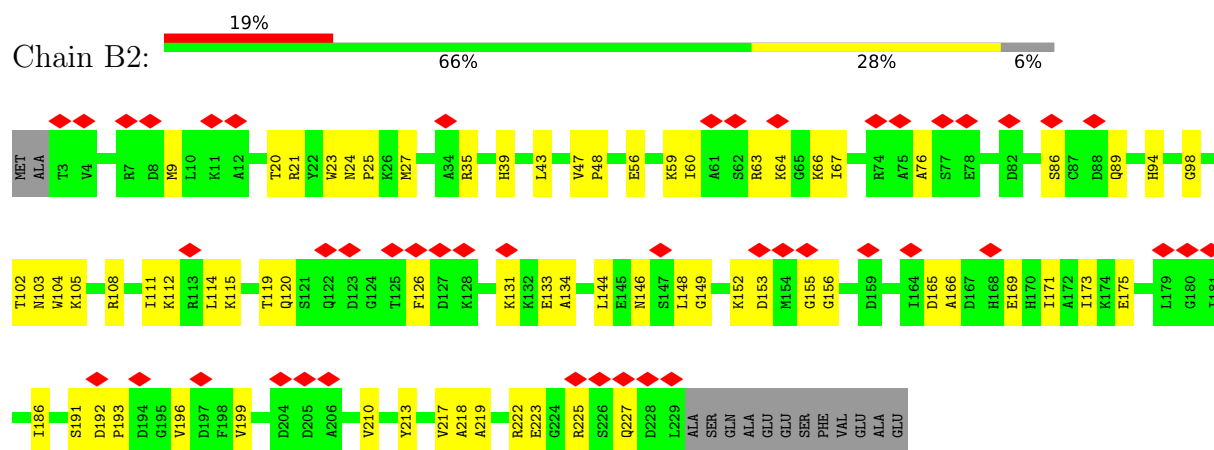




• Molecule 8: Small ribosomal subunit protein uS2

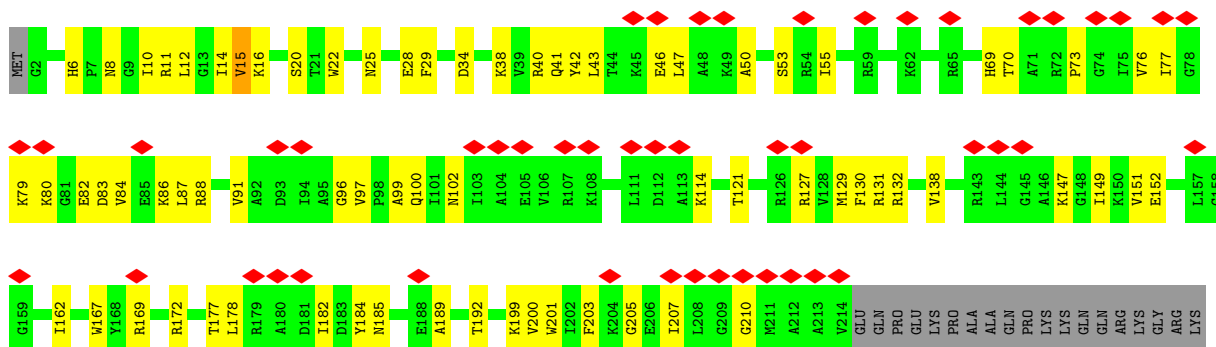


• Molecule 8: Small ribosomal subunit protein uS2

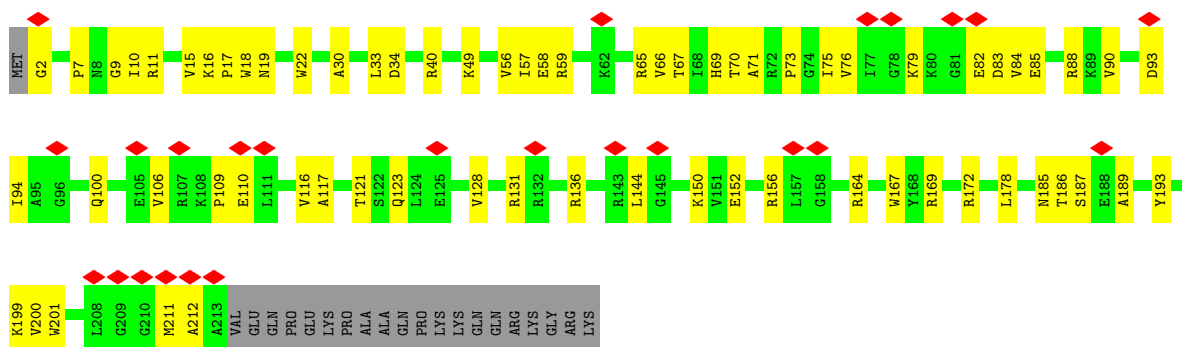


• Molecule 9: Small ribosomal subunit protein uS3

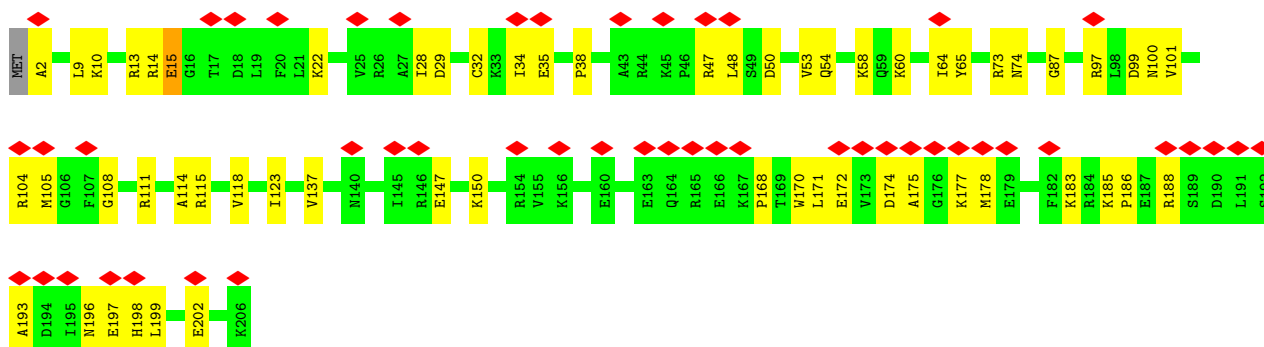
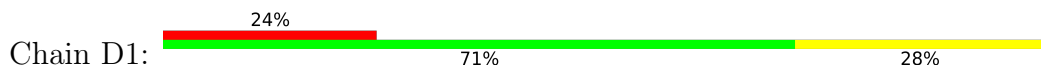




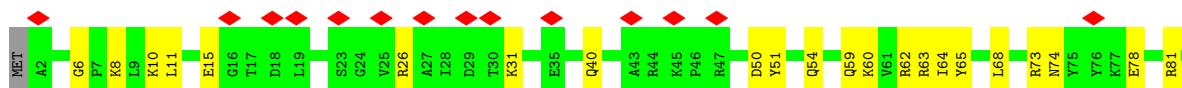
• Molecule 9: Small ribosomal subunit protein uS3

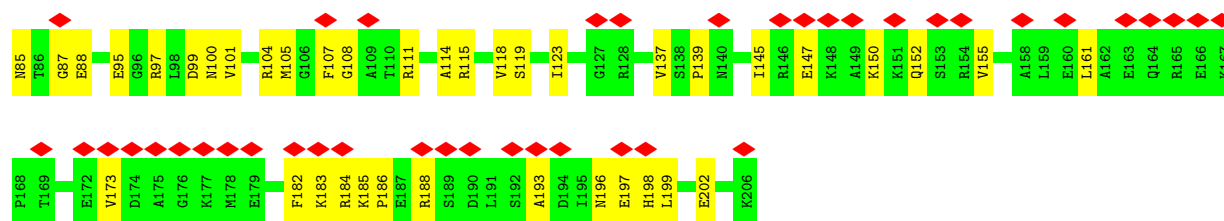


• Molecule 10: Small ribosomal subunit protein uS4

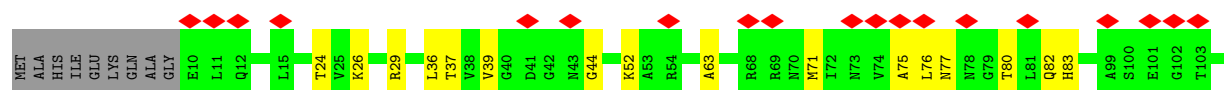
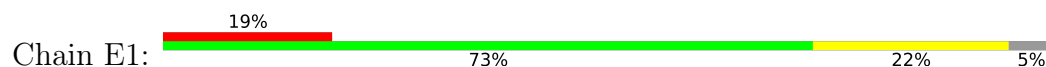


• Molecule 10: Small ribosomal subunit protein uS4

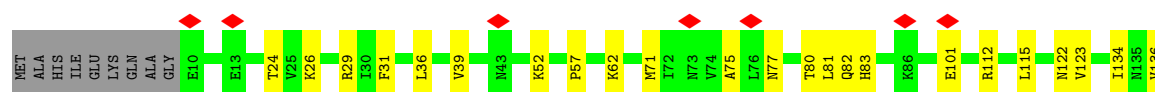
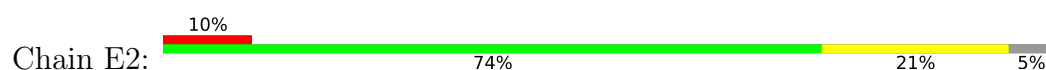




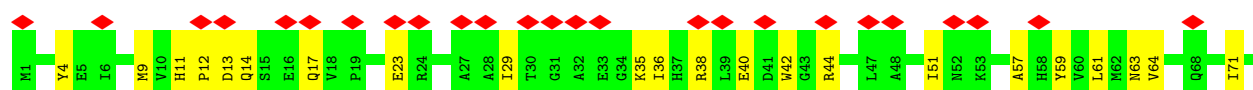
- Molecule 11: Small ribosomal subunit protein uS5



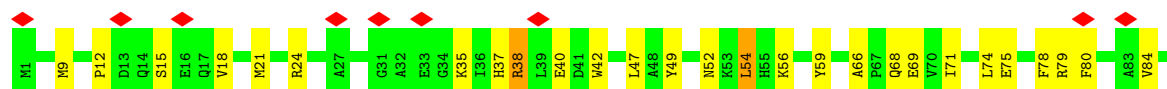
- Molecule 11: Small ribosomal subunit protein uS5

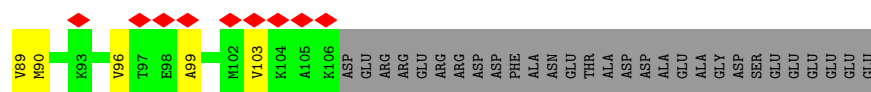


- Molecule 12: 30S ribosomal protein S6

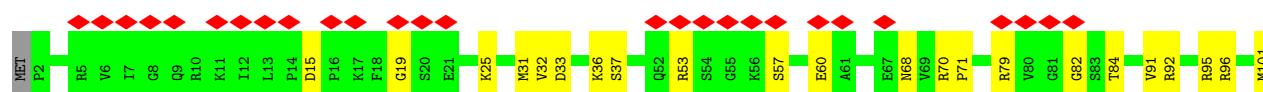


- Molecule 12: 30S ribosomal protein S6

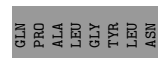
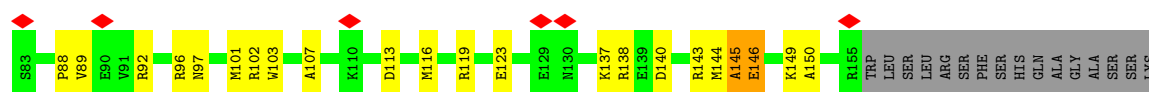
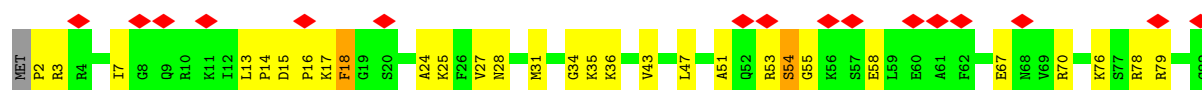




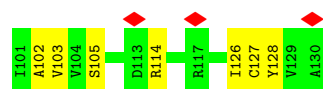
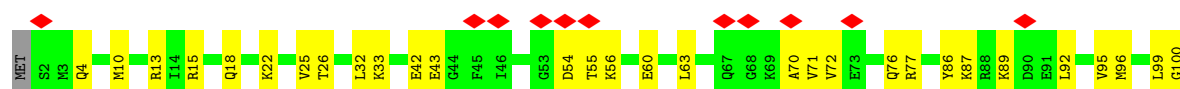
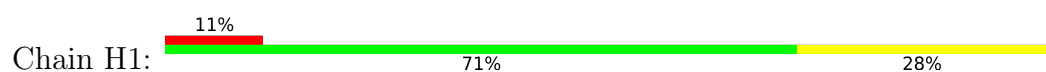
- Molecule 13: 30S ribosomal protein S7



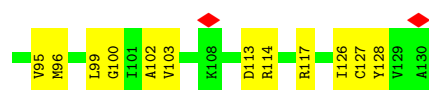
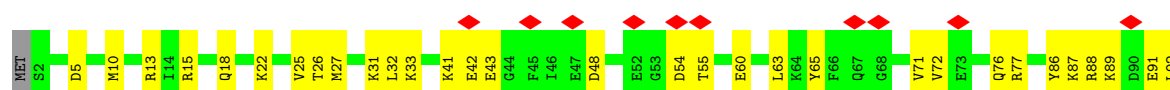
- Molecule 13: 30S ribosomal protein S7



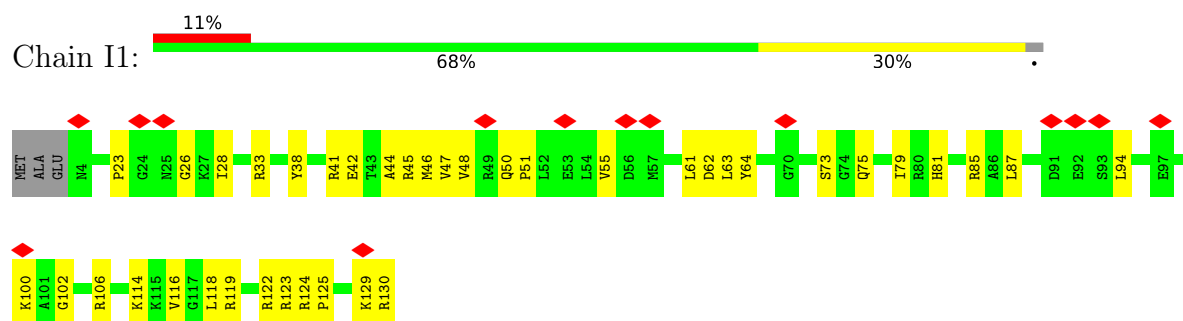
- Molecule 14: Small ribosomal subunit protein uS8



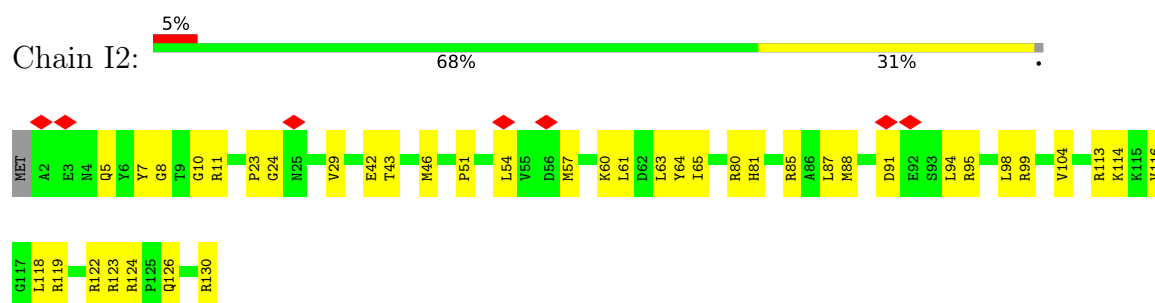
- Molecule 14: Small ribosomal subunit protein uS8



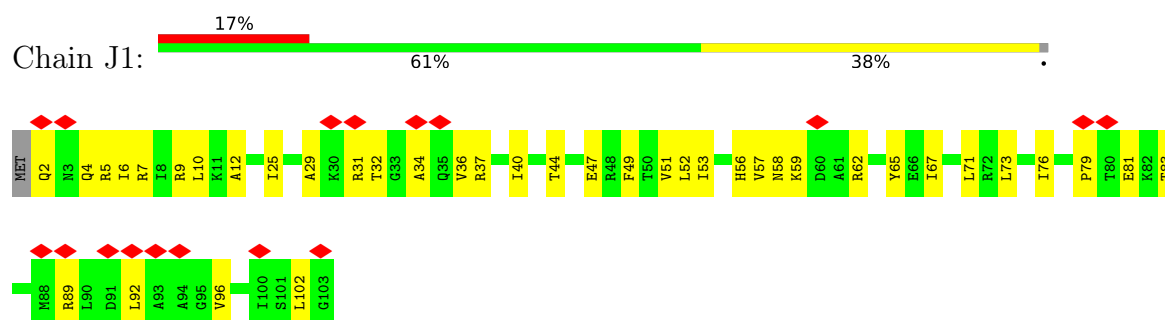
- Molecule 15: Small ribosomal subunit protein uS9



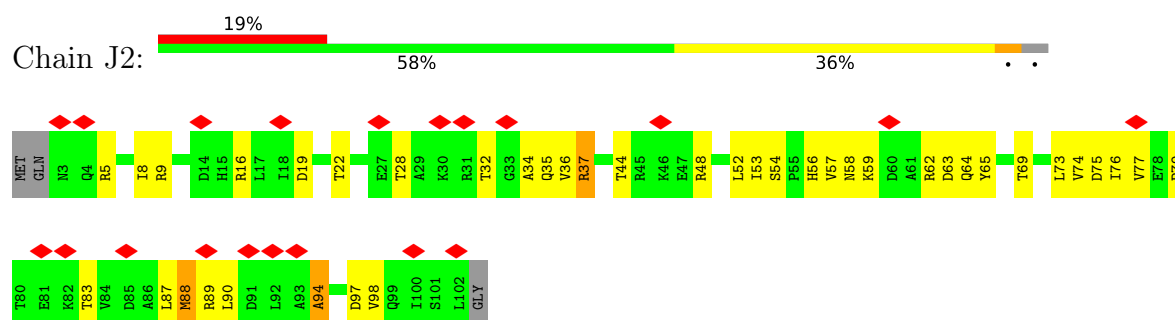
- Molecule 15: Small ribosomal subunit protein uS9



- Molecule 16: 30S ribosomal protein S10

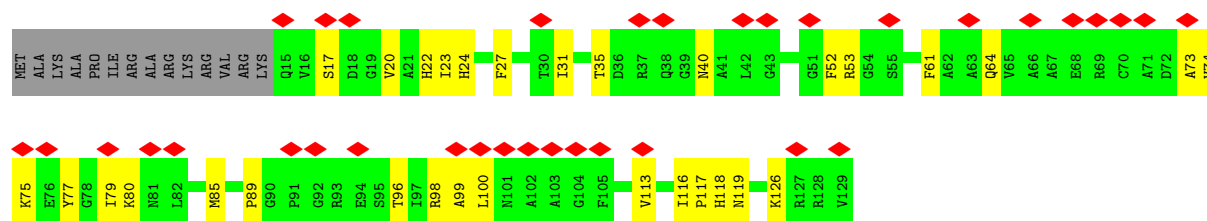


- Molecule 16: 30S ribosomal protein S10

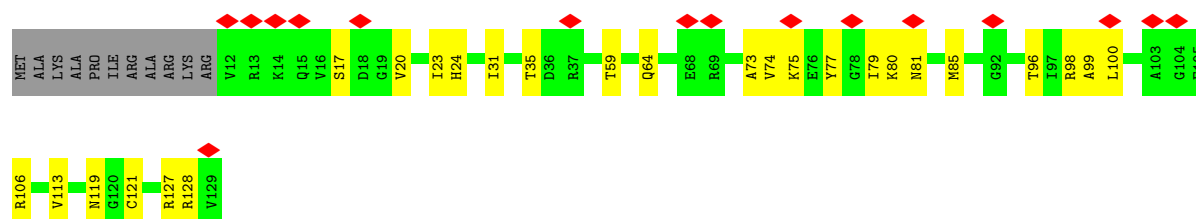
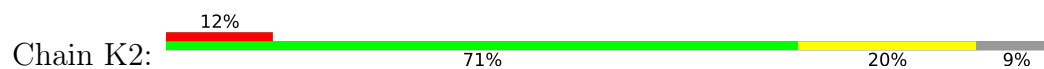


- Molecule 17: Small ribosomal subunit protein uS11

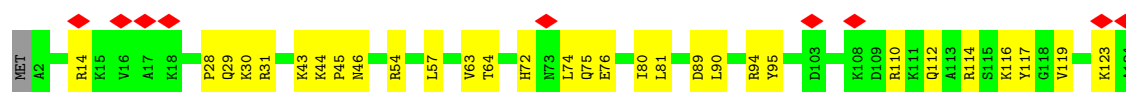
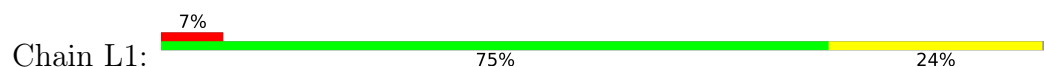




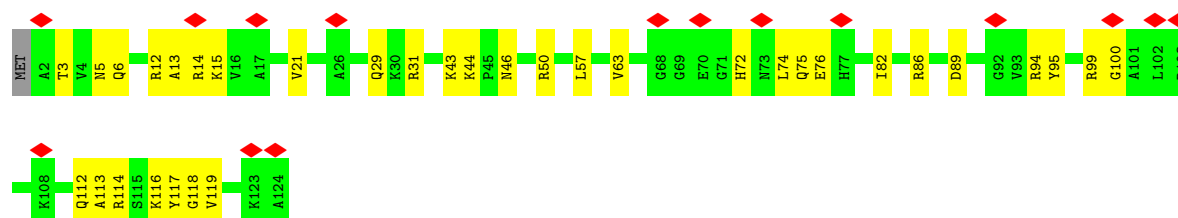
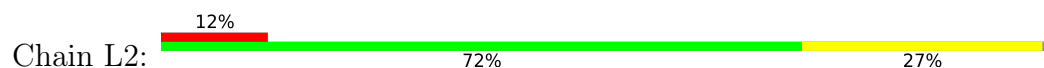
- Molecule 17: Small ribosomal subunit protein uS11



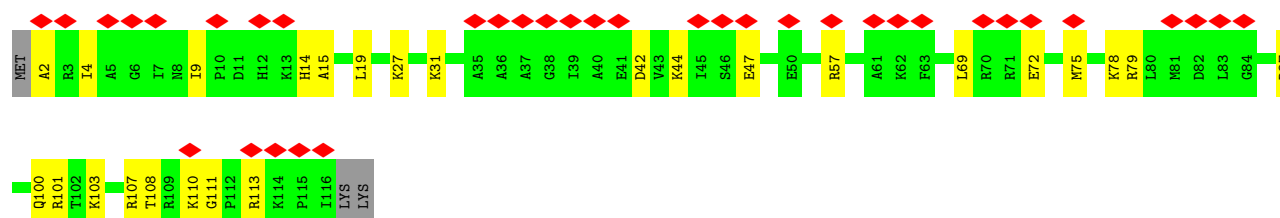
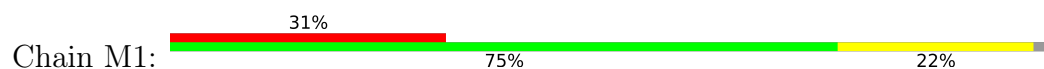
- Molecule 18: Small ribosomal subunit protein uS12



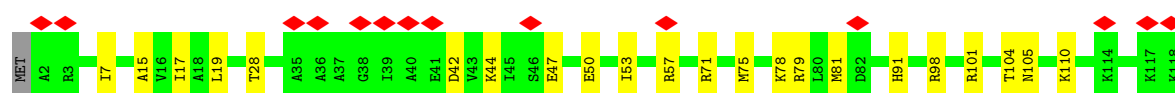
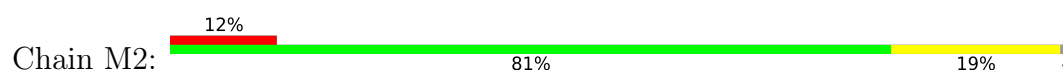
- Molecule 18: Small ribosomal subunit protein uS12



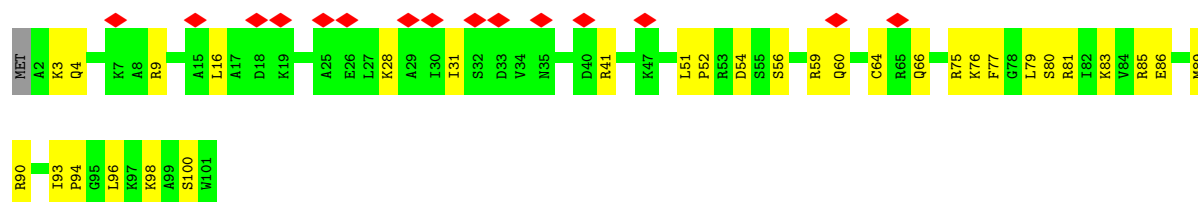
- Molecule 19: Small ribosomal subunit protein uS13



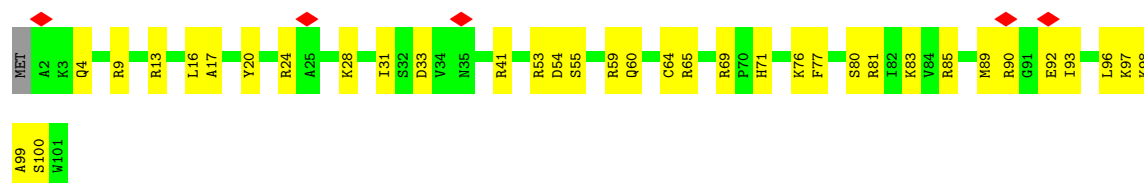
- Molecule 19: Small ribosomal subunit protein uS13



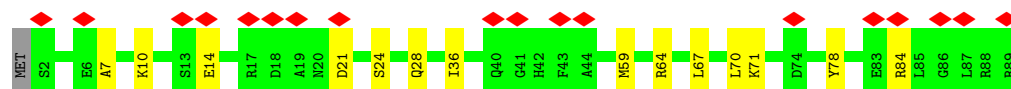
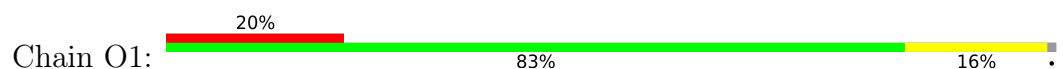
- Molecule 20: Small ribosomal subunit protein uS14



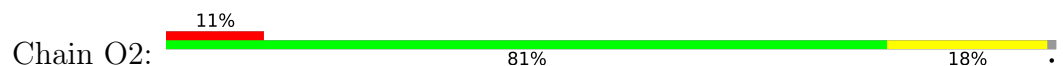
- Molecule 20: Small ribosomal subunit protein uS14



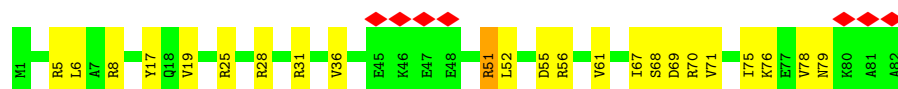
- Molecule 21: 30S ribosomal protein S15



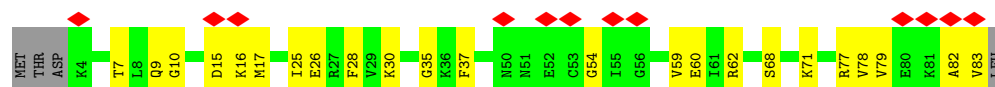
- Molecule 21: 30S ribosomal protein S15



- Molecule 22: 30S ribosomal protein S16



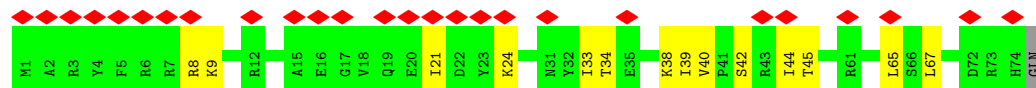
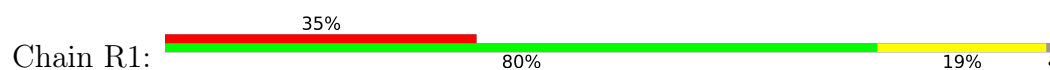
- Molecule 23: Small ribosomal subunit protein uS17



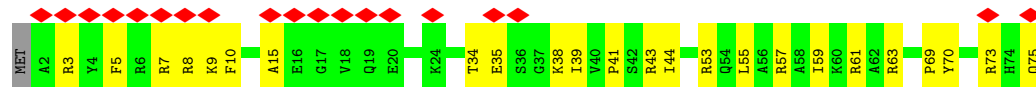
- Molecule 23: Small ribosomal subunit protein uS17



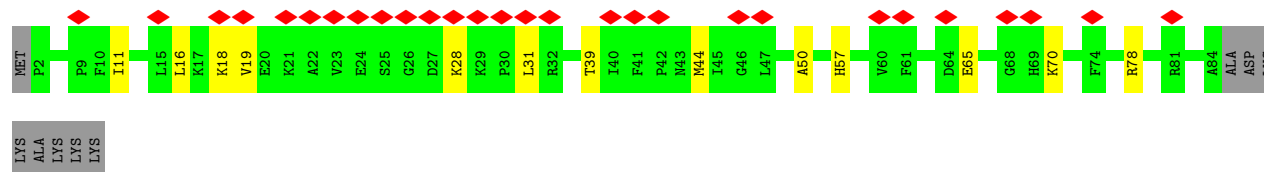
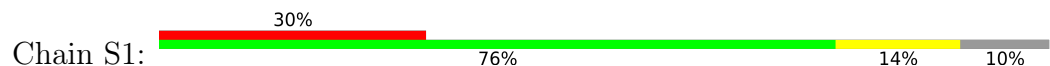
- Molecule 24: Small ribosomal subunit protein bS18



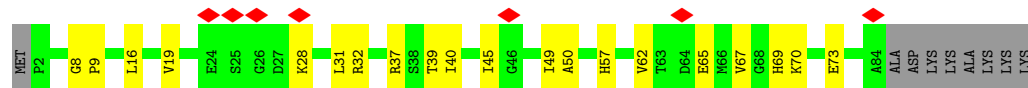
- Molecule 24: Small ribosomal subunit protein bS18



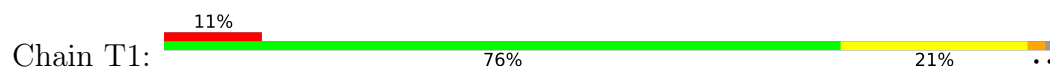
- Molecule 25: Small ribosomal subunit protein uS19

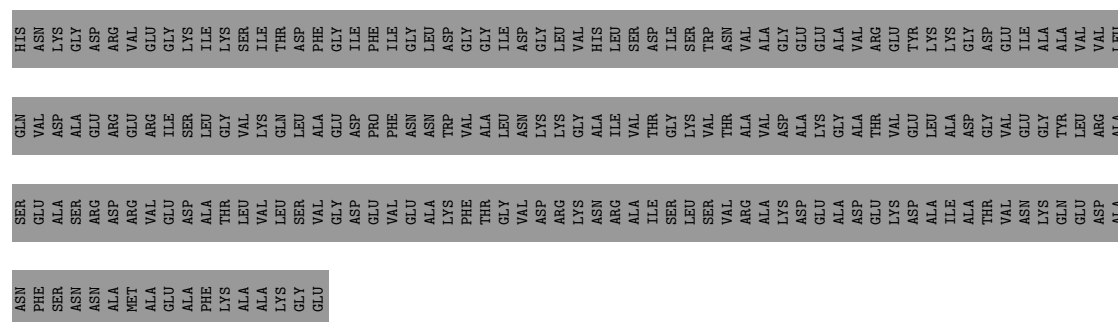


- Molecule 25: Small ribosomal subunit protein uS19

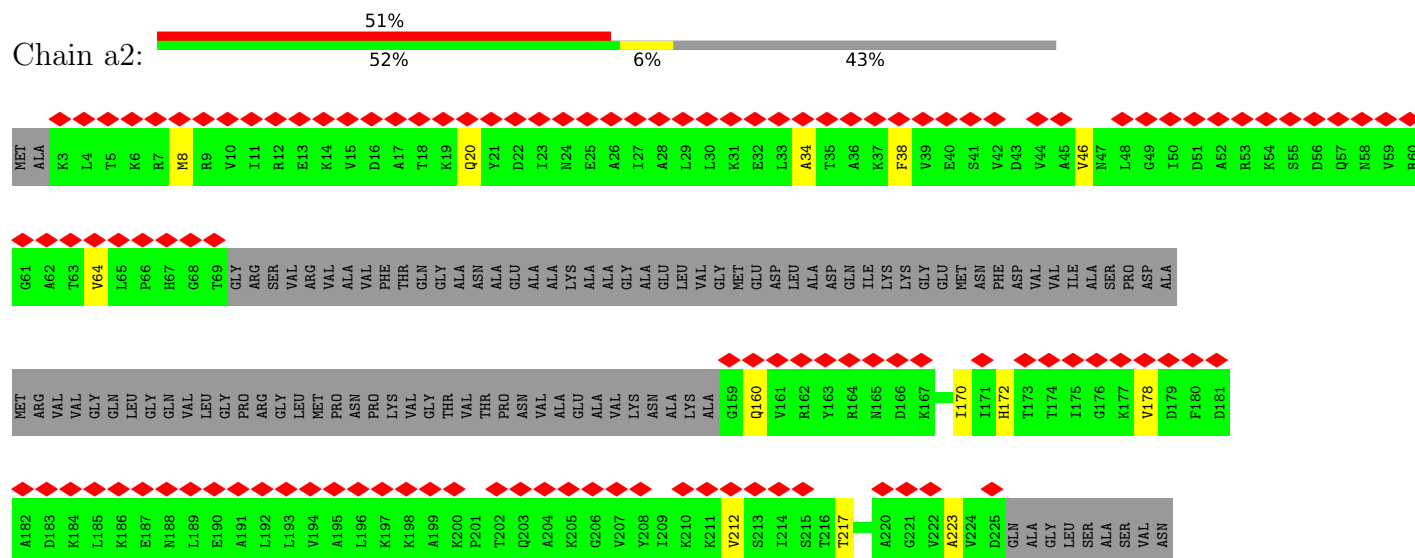


- Molecule 26: Small ribosomal subunit protein bS20

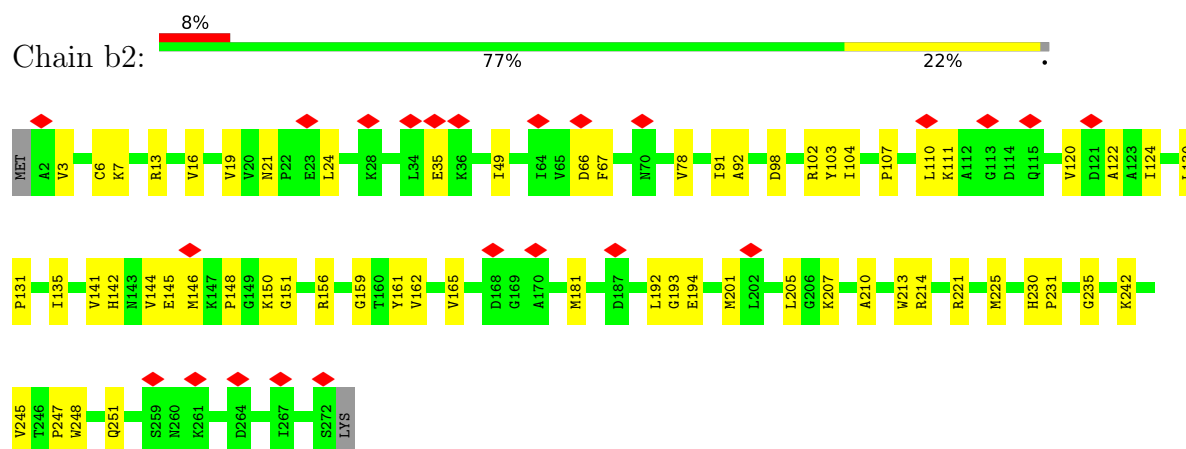




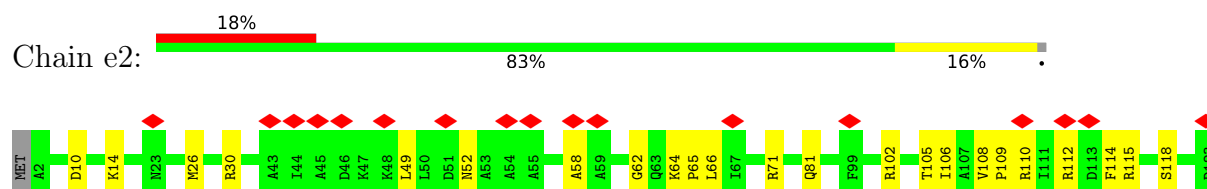
- Molecule 35: Large ribosomal subunit protein uL1

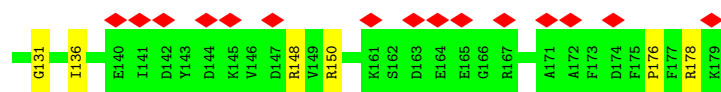


- Molecule 36: 50S ribosomal protein L2

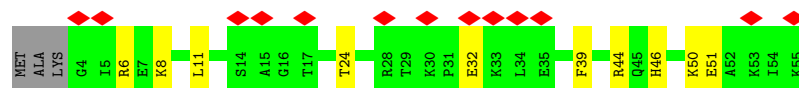
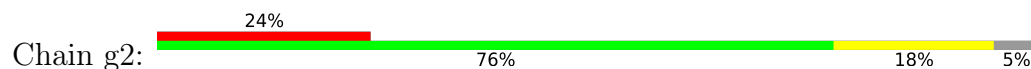


- Molecule 37: 50S ribosomal protein L5

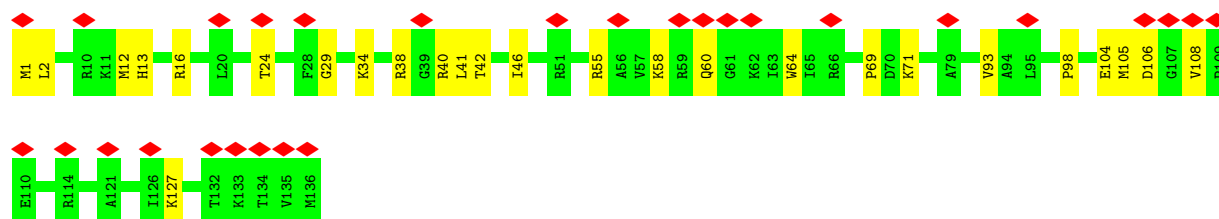
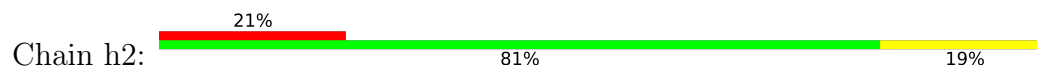




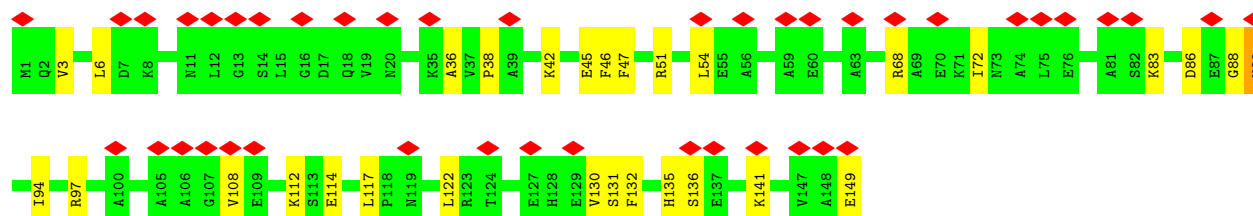
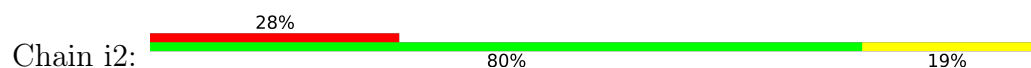
- Molecule 38: Large ribosomal subunit protein bL33



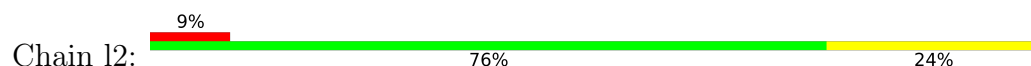
- Molecule 39: 50S ribosomal protein L16



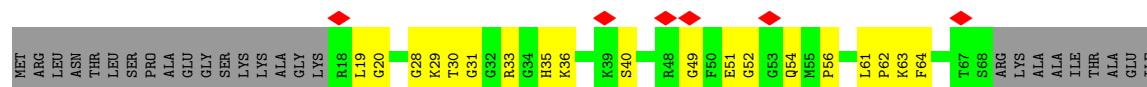
- Molecule 40: 50S ribosomal protein L9

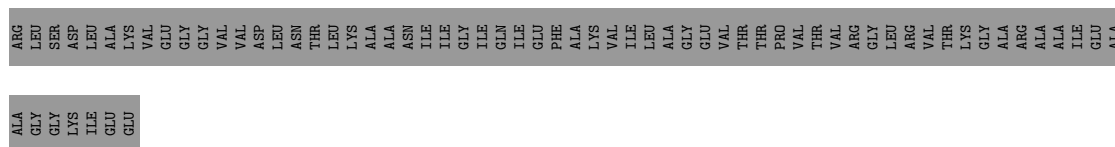


- Molecule 41: 50S ribosomal protein L34



- Molecule 42: 50S ribosomal protein L15

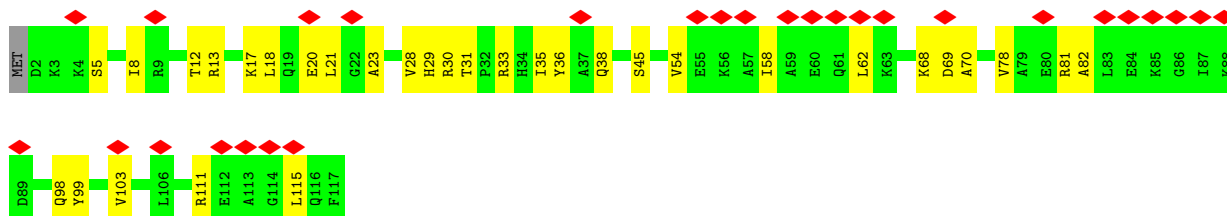
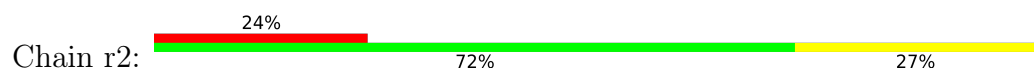




• Molecule 43: Nascent chain



• Molecule 44: 50S ribosomal protein L18



• Molecule 45: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39441	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	24.615	Depositor
Minimum map value	-5.965	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.974	Depositor
Recommended contour level	5.5	Depositor
Map size (Å)	744.12, 744.12, 744.12	wwPDB
Map dimensions	468, 468, 468	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.59, 1.59, 1.59	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CM0, H2U, OMU, PUT, 3AU, OMC, MIA, 2MG, SPD, 5MC, RSP, G7M, UR3, 5MU, 4SU, 2MA, ZN, 4OC, OMG, 1MG, 3TD, 6MZ, PSU, 7MG, MG, MA6

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	12	0.10	0/635	0.32	0/848
2	32	0.09	0/453	0.32	0/605
3	4	0.93	0/539	1.18	0/721
4	62	0.09	0/513	0.31	0/676
5	71	0.10	0/696	0.25	0/1081
5	72	0.11	0/69306	0.24	12/108116 (0.0%)
6	82	0.16	1/2872 (0.0%)	0.27	0/4478
7	A1	0.17	0/36794	0.33	0/57392
7	A2	0.16	0/36681	0.29	0/57217
8	B	0.14	0/1846	0.45	0/2488
8	B2	0.13	0/1807	0.39	0/2435
9	C1	0.12	0/1692	0.38	0/2280
9	C2	0.13	0/1685	0.36	0/2270
10	D1	0.11	0/1665	0.36	0/2227
10	D2	0.10	0/1665	0.31	0/2227
11	E1	0.12	0/1179	0.33	0/1584
11	E2	0.13	0/1179	0.33	0/1584
12	F1	0.09	0/881	0.28	0/1189
12	F2	0.12	0/881	0.39	0/1189
13	G1	0.10	0/1246	0.32	0/1672
13	G2	0.12	0/1230	0.43	0/1649
14	H1	0.11	0/989	0.33	0/1326
14	H2	0.12	0/989	0.33	0/1326
15	I1	0.11	0/1034	0.35	0/1375
15	I2	0.12	0/1048	0.35	0/1394
16	J1	0.16	0/827	0.40	0/1117
16	J2	0.16	0/813	0.47	0/1100
17	K1	0.10	0/873	0.33	0/1180
17	K2	0.12	0/900	0.33	0/1215
18	L1	0.12	0/969	0.35	0/1300
18	L2	0.12	0/969	0.35	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M1	0.10	0/900	0.31	0/1204
19	M2	0.11	0/919	0.33	0/1226
20	N1	0.13	0/817	0.38	0/1088
20	N2	0.12	0/817	0.38	0/1088
21	O1	0.10	0/722	0.32	0/964
21	O2	0.11	0/722	0.36	0/964
22	P1	0.13	0/659	0.33	0/884
23	Q1	0.13	0/657	0.38	0/881
23	Q2	0.13	0/657	0.39	0/881
24	R1	0.12	0/635	0.33	0/849
24	R2	0.14	0/637	0.44	0/851
25	S1	0.11	0/680	0.31	0/915
25	S2	0.12	0/680	0.33	0/915
26	T1	0.14	0/676	0.39	0/895
27	U1	0.13	0/598	0.41	0/792
27	U2	0.13	0/592	0.38	0/785
28	V2	0.21	0/1552	0.46	0/2419
29	W	0.29	0/1604	0.42	1/2496 (0.0%)
30	W1	0.28	0/747	0.28	0/1161
31	X2	0.41	2/1628 (0.1%)	0.39	0/2526
32	Y1	0.14	0/786	0.34	0/1216
33	Y2	0.26	0/1725	0.42	2/2687 (0.1%)
34	Z1	0.09	0/76	0.23	0/101
35	a2	0.07	0/1033	0.22	0/1387
36	b2	0.12	0/2121	0.34	0/2852
37	e2	0.09	0/1444	0.27	0/1937
38	g2	0.09	0/434	0.32	0/576
39	h2	0.09	0/1104	0.28	0/1474
40	i2	0.12	0/1122	0.38	0/1515
41	l2	0.09	0/380	0.27	0/498
42	o2	0.12	0/383	0.41	0/501
43	p	0.82	0/77	1.11	0/104
44	r2	0.10	0/901	0.35	0/1209
45	z2	0.09	0/589	0.29	0/779
All	All	0.15	3/203930 (0.0%)	0.31	15/307181 (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	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	D1	0	2
10	D2	0	1
15	I2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X2	35	I	C5-C6	7.33	1.54	1.39
31	X2	35	I	N3-C4	7.04	1.50	1.35
6	82	120	U	C1'-N1	6.11	1.57	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2584	U	P-O3'-C3'	-10.97	103.75	120.20
5	72	2585	U	P-O3'-C3'	-10.18	104.93	120.20
5	72	1939	5MU	P-O3'-C3'	-9.81	105.48	120.20
5	72	747	5MU	P-O3'-C3'	-9.25	106.33	120.20
5	72	749	A	P-O3'-C3'	-8.84	106.94	120.20
33	Y2	52	G	P-O3'-C3'	-8.21	107.89	120.20
5	72	748	G	P-O3'-C3'	-8.05	108.13	120.20
33	Y2	74	C	P-O3'-C3'	-7.73	108.61	120.20
5	72	2585	U	C2'-C3'-O3'	-7.56	98.16	109.50
5	72	2585	U	C3'-C2'-C1'	-6.61	94.89	101.50
29	W	76	A	C3'-C2'-O2'	-5.68	106.07	114.60
5	72	749	A	C2'-C3'-O3'	-5.66	105.20	113.70
5	72	2583	G	P-O3'-C3'	-5.60	111.79	120.20
5	72	748	G	C4'-C3'-O3'	5.51	117.67	109.40
5	72	1937	A	P-O3'-C3'	-5.28	112.28	120.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	56	ARG	Sidechain
3	4	59	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain
15	I2	113	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain
17	K1	98	ARG	Sidechain
17	K2	98	ARG	Sidechain
21	O2	84	ARG	Sidechain
22	P1	51	ARG	Sidechain
43	p	35	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	12	625	0	652	14	0
2	32	449	0	491	10	0
3	4	529	0	527	43	0
4	62	504	0	572	6	0
5	71	644	0	328	4	0
5	72	62355	0	31381	488	0
6	82	2569	0	1301	27	0
7	A1	33092	0	16676	768	0
7	A2	32990	0	16623	563	0
8	B	1815	0	1836	72	0
8	B2	1776	0	1802	47	0
9	C1	1665	0	1741	57	0
9	C2	1658	0	1732	56	0
10	D1	1643	0	1707	42	0
10	D2	1643	0	1707	39	0
11	E1	1166	0	1212	28	0
11	E2	1166	0	1212	34	0
12	F1	862	0	864	20	0
12	F2	862	0	864	28	0
13	G1	1228	0	1277	22	0
13	G2	1214	0	1267	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	H1	979	0	1031	35	0
14	H2	979	0	1031	38	0
15	I1	1022	0	1070	30	0
15	I2	1036	0	1081	37	0
16	J1	817	0	853	31	0
16	J2	803	0	842	29	0
17	K1	857	0	861	23	0
17	K2	884	0	896	16	0
18	L1	955	0	1016	22	0
18	L2	955	0	1016	28	0
19	M1	891	0	952	25	0
19	M2	910	0	978	21	0
20	N1	805	0	844	33	0
20	N2	805	0	844	36	0
21	O1	714	0	734	9	0
21	O2	714	0	734	10	0
22	P1	649	0	666	17	0
23	Q1	648	0	691	17	0
23	Q2	648	0	691	17	0
24	R1	624	0	652	9	0
24	R2	626	0	648	22	0
25	S1	663	0	688	8	0
25	S2	663	0	688	15	0
26	T1	670	0	719	17	0
27	U1	590	0	629	18	0
27	U2	584	0	618	10	0
28	V2	1382	0	694	49	0
29	W	1630	0	840	32	0
30	W1	781	0	405	9	0
31	X2	1654	0	849	30	0
32	Y1	778	0	399	11	0
33	Y2	1628	0	828	20	0
34	Z1	75	0	65	0	0
35	a2	1026	0	1092	7	0
36	b2	2082	0	2154	52	0
37	e2	1420	0	1457	26	0
38	g2	427	0	464	8	0
39	h2	1085	0	1169	16	0
40	i2	1111	0	1148	17	0
41	l2	377	0	418	9	0
42	o2	377	0	389	17	0
43	p	76	0	75	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	r2	891	0	923	20	0
45	z2	582	0	599	19	0
46	4	1	0	0	0	0
46	B	1	0	0	0	0
47	72	12	0	24	0	0
48	72	10	0	19	1	0
49	72	189	0	0	0	0
49	82	1	0	0	0	0
49	A1	59	0	0	0	0
49	A2	42	0	0	0	0
49	V2	1	0	0	0	0
49	W	1	0	0	0	0
49	Y2	1	0	0	0	0
49	b2	1	0	0	0	0
49	o2	1	0	0	0	0
50	Y2	5	0	4	1	0
All	All	188653	0	121260	2962	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 12.

All (2962) 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)
28:V2:49:G:H1	31:X2:36:C:H42	1.11	0.91
7:A1:1217:C:H5'	20:N1:9:ARG:HH21	1.37	0.89
7:A1:1419:G:N1	7:A1:1481:U:O2	2.09	0.86
7:A1:375:U:H4'	22:P1:6:LEU:HD11	1.58	0.85
7:A2:74:A:H61	7:A2:96:U:H3	1.18	0.85
7:A1:1178:G:N2	7:A1:1181:G:OP2	2.10	0.84
7:A1:1305:G:H2'	7:A1:1331:G:H21	1.43	0.84
5:72:1478:G:H1	5:72:1513:U:H3	1.26	0.83
7:A1:94:G:H4'	7:A1:95:C:H5'	1.59	0.82
3:4:34:LEU:HD22	37:e2:106:ILE:HD12	1.61	0.81
9:C2:79:LYS:HA	9:C2:83:ASP:HB2	1.62	0.81
20:N2:93:ILE:HG21	20:N2:96:LEU:HD12	1.62	0.81
7:A1:1338:G:H21	30:W1:41:C:H1'	1.44	0.81
3:4:41:HIS:HB2	37:e2:109:PRO:HB3	1.61	0.80
12:F2:42:TRP:HD1	12:F2:59:TYR:HB3	1.44	0.80
7:A2:501:C:OP1	18:L2:114:ARG:NH2	2.15	0.80
7:A1:1229:A:OP2	19:M1:113:ARG:NH2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:677:U:H3	7:A2:713:G:H22	1.29	0.79
7:A1:664:G:H22	7:A1:741:G:H1	1.29	0.79
28:V2:41:G:H2'	28:V2:42:G:H4'	1.64	0.79
5:72:1779:U:OP2	5:72:1784:A:N6	2.16	0.79
16:J1:57:VAL:HG12	16:J1:58:ASN:H	1.48	0.79
7:A1:409:U:H3	7:A1:433:G:H1	1.31	0.78
7:A2:672:U:H5'	12:F2:79:ARG:HH22	1.48	0.78
29:W:11:U:H3	29:W:24:G:H1	1.31	0.78
5:72:1800:C:HO2'	5:72:1818:U:H3	1.29	0.78
7:A1:1045:C:H3'	7:A1:1046:A:H5''	1.65	0.77
26:T1:35:VAL:HG22	26:T1:50:ALA:HB1	1.67	0.77
7:A2:416:G:H1	7:A2:427:U:H3	1.33	0.77
8:B:38:VAL:HG12	8:B:39:HIS:H	1.51	0.76
7:A1:254:G:H1'	23:Q1:17:MET:HE2	1.68	0.76
8:B:47:VAL:HG13	8:B:48:PRO:HD3	1.68	0.76
15:I1:28:ILE:HD12	15:I1:63:LEU:HB2	1.64	0.76
20:N2:54:ASP:HA	20:N2:59:ARG:HG2	1.66	0.76
7:A1:90:C:O2'	7:A1:91:U:H5'	1.86	0.76
7:A1:427:U:OP1	10:D1:13:ARG:NH2	2.18	0.76
7:A2:1081:A:N7	11:E2:52:LYS:NZ	2.33	0.76
10:D2:62:ARG:HH21	10:D2:68:LEU:HA	1.51	0.76
2:32:12:ALA:O	2:32:20:LYS:NZ	2.19	0.76
10:D2:85:ASN:HD21	11:E2:101:GLU:HG3	1.49	0.75
7:A2:459:A:N6	7:A2:474:G:N3	2.34	0.75
9:C2:10:ILE:HG23	9:C2:11:ARG:HD3	1.67	0.75
7:A2:664:G:H22	7:A2:741:G:H1	1.35	0.75
10:D1:54:GLN:HA	10:D1:199:LEU:HD21	1.67	0.75
7:A2:459:A:H61	7:A2:473:U:H3	1.34	0.75
14:H1:13:ARG:NH1	14:H1:26:THR:O	2.20	0.75
3:4:66:ILE:O	3:4:67:PRO:O	2.05	0.74
7:A1:1349:A:H5''	15:I1:123:ARG:HG2	1.67	0.74
24:R1:9:LYS:NZ	24:R1:44:ILE:O	2.21	0.74
8:B:94:HIS:HD2	8:B:95:ARG:HG2	1.53	0.74
7:A1:1373:G:OP2	15:I1:73:SER:OG	2.05	0.74
7:A2:1030:U:O2	7:A2:1032:G:N2	2.20	0.74
7:A1:1130:A:H2'	7:A1:1131:G:C8	2.23	0.73
7:A2:427:U:H3'	7:A2:428:G:H5''	1.68	0.73
7:A2:562:U:O2'	18:L2:14:ARG:NH2	2.21	0.73
13:G2:28:ASN:HA	13:G2:31:MET:HE3	1.68	0.73
7:A1:1088:G:H21	7:A1:1167:A:H61	1.36	0.73
8:B:67:ILE:HB	8:B:89:GLN:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:1800:C:H3'	36:b2:146:MET:HE1	1.70	0.73
19:M1:4:ILE:HG13	19:M1:57:ARG:HG2	1.69	0.73
16:J2:53:ILE:HD13	16:J2:63:ASP:HB2	1.71	0.72
5:72:2251:OMG:N2	29:W:75:C:O2	2.15	0.72
27:U1:28:VAL:HG13	27:U1:29:LEU:HD22	1.72	0.72
7:A1:231:U:H2'	7:A1:232:G:H8	1.55	0.72
7:A2:83:C:H2'	7:A2:84:U:H3'	1.72	0.72
10:D2:15:GLU:OE2	10:D2:63:ARG:NH2	2.22	0.72
5:72:2:G:H1	5:72:2901:U:H3	1.37	0.72
7:A1:211:G:C5	7:A1:212:G:H1'	2.23	0.72
18:L1:72:HIS:HB2	18:L1:74:LEU:HD23	1.71	0.72
5:72:1528:A:N6	5:72:1543:G:O2'	2.22	0.72
10:D2:54:GLN:HA	10:D2:199:LEU:HD21	1.72	0.71
36:b2:231:PRO:O	36:b2:242:LYS:NZ	2.20	0.71
13:G2:88:PRO:HG3	13:G2:149:LYS:HA	1.72	0.71
8:B2:219:ALA:HA	8:B2:222:ARG:HE	1.54	0.71
5:72:825:A:O2'	42:o2:54:GLN:OE1	2.08	0.71
7:A2:1073:U:OP2	11:E2:62:LYS:NZ	2.23	0.71
5:72:1211:C:H4'	5:72:1212:G:OP2	1.90	0.71
13:G2:70:ARG:H	13:G2:138:ARG:HH21	1.39	0.70
7:A2:570:G:O6	7:A2:865:A:N6	2.24	0.70
7:A2:483:C:H2'	7:A2:484:G:C8	2.25	0.70
17:K1:27:PHE:HE1	17:K1:89:PRO:HG2	1.57	0.70
18:L1:46:ASN:ND2	18:L1:89:ASP:OD2	2.23	0.70
5:72:1936:A:H2	5:72:1943:U:H3	1.39	0.70
7:A1:1537:U:H3	28:V2:13:C:H42	1.35	0.70
11:E2:156:LYS:NZ	14:H2:71:VAL:O	2.22	0.70
7:A1:891:U:H2'	7:A1:892:A:H8	1.57	0.70
36:b2:21:ASN:HB3	36:b2:24:LEU:HD23	1.73	0.70
7:A2:1010:U:H3	7:A2:1019:A:H61	1.38	0.70
8:B:87:CYS:SG	8:B:225:ARG:NH1	2.64	0.70
11:E2:157:ARG:NH1	14:H2:99:LEU:O	2.24	0.70
7:A1:83:C:H2'	7:A1:84:U:H3'	1.74	0.70
7:A1:562:U:O2'	18:L1:14:ARG:NH2	2.24	0.70
10:D1:100:ASN:OD1	10:D1:111:ARG:NH1	2.25	0.70
7:A1:390:U:H4'	22:P1:28:ARG:HH21	1.57	0.69
10:D2:100:ASN:OD1	10:D2:111:ARG:NH1	2.25	0.69
5:72:1044:C:O2'	5:72:1111:A:N1	2.24	0.69
10:D1:65:TYR:O	10:D1:97:ARG:NH1	2.24	0.69
7:A1:128:G:O2'	7:A1:129:A:H5'	1.92	0.69
7:A2:501:C:H6	7:A2:501:C:H5'	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M1:107:ARG:NH1	19:M1:111:GLY:O	2.25	0.69
37:e2:10:ASP:O	37:e2:14:LYS:NZ	2.25	0.69
5:72:1789:A:OP2	36:b2:221:ARG:NH1	2.25	0.69
11:E1:159:LYS:NZ	14:H1:42:GLU:O	2.23	0.69
15:I2:57:MET:HE3	16:J1:89:ARG:HH21	1.55	0.69
5:72:475:C:H4'	5:72:510:C:H5'	1.74	0.69
5:72:1791:A:N6	5:72:1828:G:O2'	2.26	0.69
5:72:2062:A:N6	43:p:31:VAL:O	2.25	0.69
7:A1:413:G:O3'	7:A1:428:G:N2	2.24	0.69
7:A2:455:G:H1	7:A2:477:C:H42	1.41	0.69
7:A2:898:G:N2	7:A2:901:A:OP2	2.26	0.69
8:B2:24:ASN:HD22	8:B2:192:ASP:HA	1.58	0.69
17:K1:24:HIS:HB3	17:K1:31:ILE:HB	1.74	0.69
32:Y1:15:G:N2	32:Y1:48:C:O2	2.25	0.69
8:B:92:VAL:HG12	8:B:93:ASN:H	1.58	0.68
14:H2:96:MET:HB3	14:H2:100:GLY:H	1.58	0.68
7:A1:1106:G:H5''	9:C1:172:ARG:HG2	1.74	0.68
7:A1:1236:A:H4'	7:A1:1304:G:H4'	1.74	0.68
7:A2:454:G:H1	7:A2:478:A:H2	1.40	0.68
7:A2:553:A:H5''	18:L2:21:VAL:HG21	1.76	0.68
7:A2:1009:U:H3	7:A2:1020:G:H1	1.42	0.68
6:82:3:C:O2'	6:82:4:C:OP1	2.12	0.68
7:A1:1310:G:OP2	19:M1:87:ARG:NH2	2.26	0.68
10:D1:172:GLU:HG3	10:D1:183:LYS:HD2	1.75	0.68
12:F1:99:ALA:O	12:F1:104:LYS:NZ	2.26	0.68
7:A2:1316:G:N1	7:A2:1319:A:OP2	2.27	0.68
18:L2:72:HIS:HB2	18:L2:74:LEU:HD23	1.75	0.68
7:A2:380:G:N2	7:A2:383:A:OP2	2.27	0.67
13:G2:150:ALA:HB1	17:K2:59:THR:HG21	1.76	0.67
4:62:13:ARG:HG2	42:o2:63:LYS:HA	1.75	0.67
5:72:2134:A:H1'	5:72:2159:G:H1'	1.76	0.67
7:A1:532:A:N6	7:A1:1206:G:O2'	2.28	0.67
5:72:960:A:H2'	5:72:962:G:H5''	1.77	0.67
5:72:2108:A:H2	5:72:2181:U:H3	1.42	0.67
7:A1:503:C:OP1	18:L1:116:LYS:NZ	2.27	0.67
5:72:45:G:H5'	5:72:46:G:H5'	1.75	0.67
16:J1:52:LEU:HB2	20:N1:81:ARG:HD2	1.76	0.67
5:72:858:G:N2	5:72:2269:G:OP2	2.28	0.67
3:4:14:ALA:HB3	3:4:22:MET:HB2	1.75	0.66
7:A1:1230:C:H2'	7:A1:1231:G:H8	1.59	0.66
7:A2:502:A:H61	7:A2:543:U:H3	1.40	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:706:A:OP1	36:b2:7:LYS:NZ	2.29	0.66
5:72:745:1MG:N7	5:72:746:PSU:N1	2.44	0.66
7:A1:1059:C:H4'	20:N1:85:ARG:HH22	1.60	0.66
7:A1:1536:C:H42	28:V2:14:G:H1	1.44	0.66
7:A1:1540:U:H2'	28:V2:6:A:H5''	1.76	0.66
8:B2:114:LEU:HD13	8:B2:148:LEU:HD22	1.78	0.66
7:A1:93:U:H5''	7:A1:94:G:OP2	1.94	0.66
6:82:30:C:H1'	6:82:57:A:H61	1.58	0.66
7:A1:1308:U:OP2	19:M1:100:GLN:NE2	2.29	0.66
10:D1:97:ARG:NH2	10:D1:99:ASP:OD2	2.29	0.66
16:J1:52:LEU:HD21	16:J1:59:LYS:HG3	1.77	0.66
13:G1:82:GLY:HA3	28:V2:17:G:H4'	1.78	0.66
27:U1:66:ARG:HD3	27:U1:66:ARG:H	1.60	0.66
37:e2:110:ARG:NH2	37:e2:136:ILE:O	2.28	0.66
7:A2:1349:A:H5''	15:I2:123:ARG:HG2	1.76	0.65
23:Q2:68:SER:HB3	23:Q2:71:LYS:HB2	1.78	0.65
7:A1:836:G:H3'	7:A1:837:U:H5''	1.78	0.65
7:A1:950:U:H2'	7:A1:951:G:H8	1.61	0.65
5:72:463:G:N2	5:72:466:A:OP2	2.19	0.65
5:72:1309:G:H4'	41:I2:7:PRO:HB2	1.78	0.65
5:72:1427:A:N6	5:72:1571:A:OP2	2.21	0.65
5:72:2688:G:N1	5:72:2720:U:OP2	2.18	0.65
5:72:1800:C:O2'	5:72:1818:U:N3	2.21	0.65
7:A2:1059:C:O3'	20:N2:85:ARG:NH1	2.30	0.65
7:A2:75:G:H1	7:A2:95:C:H42	1.45	0.65
13:G2:34:GLY:O	13:G2:36:LYS:N	2.30	0.65
16:J2:34:ALA:HB2	16:J2:83:THR:HG21	1.77	0.65
5:72:910:A:N3	5:72:2264:C:O2'	2.27	0.65
7:A1:713:G:H2'	7:A1:714:G:C8	2.31	0.65
8:B:70:VAL:HG23	8:B:161:LEU:HD11	1.78	0.65
5:72:2522:U:O2'	5:72:2647:U:OP1	2.14	0.65
41:I2:18:PHE:HB2	41:I2:43:THR:HG21	1.77	0.65
7:A1:742:G:O2'	7:A1:743:A:H5'	1.96	0.65
7:A2:408:A:H61	7:A2:434:U:H3	1.43	0.64
11:E2:75:ALA:O	11:E2:82:GLN:NE2	2.25	0.64
2:32:10:ARG:NH1	5:72:1000:A:O2'	2.22	0.64
5:72:958:U:OP1	39:h2:40:ARG:NH2	2.30	0.64
7:A1:1019:A:H3'	7:A1:1020:G:H5''	1.79	0.64
7:A1:337:G:H2'	7:A1:338:A:C8	2.31	0.64
7:A1:1045:C:C3'	7:A1:1046:A:H5''	2.27	0.64
8:B:231:SER:H	8:B2:35:ARG:HG2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G1:68:ASN:O	13:G1:138:ARG:NH2	2.30	0.64
7:A2:1356:G:H2'	7:A2:1357:A:C8	2.33	0.64
9:C2:18:TRP:HZ3	20:N2:97:LYS:HE3	1.62	0.64
17:K2:24:HIS:HB3	17:K2:31:ILE:HB	1.78	0.64
8:B:196:VAL:HG12	8:B:198:PHE:H	1.62	0.64
14:H1:96:MET:HB3	14:H1:100:GLY:H	1.62	0.64
9:C2:15:VAL:HG23	9:C2:16:LYS:H	1.63	0.64
9:C2:131:ARG:HH12	28:V2:62:C:H5''	1.62	0.64
36:b2:3:VAL:HG12	36:b2:19:VAL:HG12	1.80	0.64
5:72:1040:A:H61	5:72:1115:G:H1	1.44	0.64
18:L2:46:ASN:ND2	18:L2:89:ASP:OD2	2.31	0.64
20:N2:64:CYS:HB2	20:N2:80:SER:HB3	1.80	0.64
31:X2:23:G:H2'	31:X2:24:A:H8	1.61	0.64
3:4:41:HIS:CE1	37:e2:114:PHE:HD2	2.15	0.64
7:A1:1304:G:H21	7:A1:1333:A:H62	1.45	0.64
15:I2:91:ASP:O	16:J1:31:ARG:NH1	2.31	0.64
7:A2:476:U:H2'	7:A2:477:C:C6	2.33	0.63
7:A2:503:C:OP1	18:L2:116:LYS:NZ	2.31	0.63
11:E2:157:ARG:HH21	14:H2:43:GLU:HB3	1.62	0.63
33:Y2:9:A:N6	33:Y2:23:A:N7	2.46	0.63
7:A1:201:G:H21	7:A1:469:C:H1'	1.63	0.63
7:A1:83:C:N3	7:A1:86:G:N2	2.47	0.63
7:A1:838:G:H22	7:A1:849:G:H1'	1.64	0.63
7:A2:1115:U:H3	7:A2:1185:G:H1	1.44	0.63
26:T1:54:MET:SD	26:T1:55:GLN:N	2.71	0.63
7:A2:202:G:H1	7:A2:215:C:H42	1.46	0.63
10:D2:65:TYR:O	10:D2:97:ARG:NH1	2.28	0.63
7:A1:1539:C:H42	28:V2:10:G:H1	1.45	0.63
10:D1:174:ASP:HB3	10:D1:177:LYS:HB3	1.79	0.63
7:A2:1368:A:H5''	15:I2:114:LYS:HB3	1.81	0.63
27:U1:62:ARG:O	27:U1:66:ARG:NH1	2.32	0.63
37:e2:108:VAL:HG11	37:e2:176:PRO:HG3	1.80	0.63
5:72:476:G:H22	5:72:479:A:H5''	1.63	0.63
5:72:1537:G:N2	5:72:1537:G:OP2	2.30	0.63
7:A2:363:A:H5'	18:L2:31:ARG:HB2	1.80	0.63
10:D2:101:VAL:HG21	10:D2:137:VAL:HG21	1.80	0.63
16:J2:35:GLN:HE22	16:J2:77:VAL:HB	1.64	0.63
21:O1:14:GLU:HB2	21:O1:84:ARG:HH22	1.62	0.63
7:A1:694:A:N1	7:A1:787:A:O2'	2.31	0.62
7:A1:1008:U:H2'	7:A1:1009:U:C6	2.34	0.62
7:A1:1342:C:H2'	7:A1:1343:G:C8	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:195:A:H2'	7:A2:196:A:C8	2.34	0.62
41:l2:24:THR:HG23	41:l2:27:GLY:H	1.63	0.62
3:4:7:PRO:HG2	37:e2:62:GLY:C	2.23	0.62
5:72:1047:G:HO2'	5:72:1110:G:H1	1.45	0.62
7:A1:258:G:H1	7:A1:268:U:H3	1.47	0.62
7:A1:401:C:O2'	7:A1:621:A:N3	2.32	0.62
7:A1:693:G:H3'	7:A1:694:A:H8	1.63	0.62
7:A2:70:U:H3	7:A2:98:A:H61	1.45	0.62
14:H1:10:MET:HE1	14:H1:33:LYS:HA	1.82	0.62
18:L2:100:GLY:HA3	18:L2:118:GLY:HA3	1.81	0.62
7:A1:501:C:OP1	18:L1:114:ARG:NH2	2.31	0.62
7:A2:1077:G:N2	7:A2:1080:A:OP2	2.29	0.62
44:r2:31:THR:HG22	44:r2:33:ARG:H	1.65	0.62
4:62:13:ARG:NH2	5:72:250:G:OP2	2.33	0.62
7:A1:1404:C:H42	7:A1:1497:G:H1	1.47	0.62
7:A2:1142:G:H3'	7:A2:1143:G:H8	1.64	0.62
8:B:59:LYS:HE2	8:B:63:ARG:HH21	1.64	0.62
16:J1:51:VAL:HG23	20:N1:81:ARG:HG3	1.82	0.62
16:J1:56:HIS:ND1	16:J1:57:VAL:HG23	2.15	0.62
7:A2:54:C:H2'	7:A2:352:C:H41	1.65	0.62
9:C2:150:LYS:HG3	9:C2:169:ARG:HB3	1.82	0.62
12:F2:42:TRP:CD1	12:F2:59:TYR:HB3	2.32	0.62
5:72:1378:A:O2'	5:72:1380:G:OP2	2.18	0.62
11:E1:156:LYS:NZ	14:H1:71:VAL:O	2.26	0.62
12:F1:81:ASN:HB3	12:F1:84:VAL:HG12	1.80	0.62
5:72:481:G:O2'	5:72:507:A:N1	2.31	0.62
7:A1:151:A:OP2	7:A1:169:C:N4	2.33	0.62
10:D1:14:ARG:O	10:D1:15:GLU:HG2	1.99	0.62
11:E2:159:LYS:NZ	14:H2:42:GLU:O	2.27	0.62
16:J2:54:SER:HB3	16:J2:58:ASN:HB3	1.81	0.62
5:72:2788:C:O2'	5:72:2809:A:N3	2.28	0.61
7:A1:490:C:H2'	7:A1:491:G:C8	2.35	0.61
7:A1:1425:U:H2'	7:A1:1426:G:H5''	1.81	0.61
14:H2:13:ARG:NH1	14:H2:26:THR:O	2.33	0.61
25:S2:50:ALA:HB1	25:S2:57:HIS:HB3	1.81	0.61
5:72:2330:G:O3'	45:z2:44:LYS:NZ	2.31	0.61
7:A2:671:G:O2'	12:F2:79:ARG:NH2	2.33	0.61
16:J1:53:ILE:HD12	20:N1:85:ARG:HD3	1.83	0.61
7:A1:404:G:P	10:D1:115:ARG:HH12	2.23	0.61
7:A1:1216:A:OP1	20:N1:3:LYS:NZ	2.33	0.61
7:A1:1256:A:H5'	7:A1:1258:G:H1'	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:109:GLN:HA	8:B:112:LYS:HD2	1.80	0.61
17:K1:126:LYS:HE3	27:U1:37:PHE:HB3	1.80	0.61
33:Y2:34:G:H2'	33:Y2:35:G:C8	2.35	0.61
7:A2:404:G:OP2	10:D2:115:ARG:NH1	2.26	0.61
5:72:65:U:O2'	5:72:456:C:N3	2.32	0.61
5:72:707:G:H1	5:72:724:U:H3	1.49	0.61
7:A1:746:A:H2'	7:A1:747:A:C8	2.36	0.61
19:M2:81:MET:HE2	19:M2:91:HIS:HB3	1.81	0.61
5:72:1664:A:H61	5:72:1996:C:H42	1.47	0.61
5:72:2470:G:O6	5:72:2481:G:N2	2.33	0.61
7:A1:662:U:H2'	7:A1:663:A:C8	2.35	0.61
7:A2:397:A:N7	7:A2:547:A:O2'	2.32	0.61
7:A2:999:C:H2'	7:A2:1000:A:H8	1.66	0.61
13:G2:16:PRO:HA	15:I2:46:MET:HG3	1.83	0.61
24:R2:63:ARG:HB3	24:R2:70:TYR:CZ	2.35	0.61
29:W:54:5MU:H3'	29:W:55:PSU:H6	1.66	0.61
7:A1:1448:C:H2'	7:A1:1449:C:C6	2.36	0.61
8:B:35:ARG:HB3	8:B:40:ILE:HD11	1.81	0.61
16:J2:52:LEU:HD11	20:N2:81:ARG:HD2	1.83	0.61
7:A1:269:C:H2'	7:A1:270:A:H8	1.64	0.61
7:A1:1003:G:H21	7:A1:1005:A:H5'	1.66	0.61
7:A2:33:A:O2'	18:L2:29:GLN:NE2	2.34	0.61
7:A1:1460:C:H3'	7:A1:1461:G:H5''	1.83	0.61
20:N2:16:LEU:HD23	20:N2:54:ASP:HB2	1.83	0.61
7:A2:902:G:OP1	7:A2:902:G:H4'	2.00	0.60
18:L1:114:ARG:HG2	18:L1:119:VAL:HB	1.83	0.60
5:72:1131:G:N2	5:72:1132:U:O4	2.33	0.60
5:72:2554:U:H3	33:Y2:74:C:H42	1.49	0.60
6:82:66:A:H61	6:82:107:G:H2'	1.65	0.60
7:A1:269:C:H2'	7:A1:270:A:C8	2.35	0.60
7:A1:407:U:H2'	7:A1:408:A:C8	2.35	0.60
7:A1:1296:C:H5'	19:M1:14:HIS:HE2	1.66	0.60
8:B:14:VAL:O	8:B:203:ASN:ND2	2.34	0.60
12:F2:42:TRP:HZ3	12:F2:103:VAL:HG13	1.67	0.60
31:X2:19:G:H22	31:X2:56:PSU:HN3	1.49	0.60
5:72:2336:A:H61	45:z2:43:THR:HG21	1.67	0.60
7:A1:404:G:OP1	10:D1:115:ARG:NH1	2.35	0.60
7:A1:927:G:O2'	7:A1:1503:A:N7	2.31	0.60
7:A2:642:A:O3'	14:H2:31:LYS:NZ	2.33	0.60
7:A2:246:A:N7	7:A2:281:G:N2	2.48	0.60
7:A2:414:A:H3'	7:A2:415:A:H8	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N1:64:CYS:HB2	20:N1:80:SER:HB3	1.82	0.60
5:72:1475:G:O2'	5:72:1476:U:O5'	2.17	0.60
7:A1:1345:U:O5'	15:I1:122:ARG:NH1	2.32	0.60
7:A2:942:G:N2	15:I2:126:GLN:OE1	2.34	0.60
7:A2:1261:A:N6	7:A2:1274:A:O2'	2.35	0.60
15:I2:130:ARG:NH1	29:W:35:C:OP1	2.34	0.60
5:72:2500:U:O2'	5:72:2504:PSU:OP1	2.19	0.60
7:A1:626:G:O3'	22:P1:51:ARG:NH2	2.32	0.60
10:D2:185:LYS:HG3	10:D2:186:PRO:HD2	1.84	0.60
7:A1:1391:U:H2'	7:A1:1392:G:C8	2.37	0.60
12:F1:40:GLU:HB2	12:F1:61:LEU:HB3	1.84	0.60
12:F2:66:ALA:HB3	12:F2:71:ILE:HD11	1.84	0.60
7:A1:142:G:H3'	7:A1:143:A:H8	1.66	0.60
7:A2:181:A:H61	7:A2:194:C:H3'	1.67	0.60
7:A2:1030:U:H2'	7:A2:1032:G:H1	1.66	0.60
27:U2:31:GLU:OE2	27:U2:34:ARG:NH2	2.35	0.60
25:S1:50:ALA:HB1	25:S1:57:HIS:HB3	1.83	0.60
29:W:9:A:H5'	29:W:46:G7M:H8	1.84	0.60
2:32:8:GLN:HB2	2:32:28:LEU:HD13	1.84	0.59
5:72:1580:A:O2'	5:72:1581:G:OP1	2.18	0.59
7:A1:770:C:H2'	7:A1:771:G:H8	1.66	0.59
7:A1:999:C:H2'	7:A1:1000:A:C8	2.36	0.59
7:A1:1187:G:N3	20:N1:100:SER:OG	2.35	0.59
42:o2:19:LEU:HB2	42:o2:31:GLY:HA2	1.84	0.59
5:72:1416:G:O2'	5:72:1417:C:OP2	2.15	0.59
5:72:2114:A:H62	5:72:2115:G:H21	1.48	0.59
9:C1:138:VAL:HA	9:C1:149:ILE:HD13	1.84	0.59
23:Q1:9:GLN:NE2	23:Q1:60:GLU:OE1	2.35	0.59
31:X2:19:G:N2	31:X2:56:PSU:HN3	1.99	0.59
5:72:686:U:O4	41:I2:12:ARG:NH1	2.28	0.59
7:A2:74:A:H3'	7:A2:75:G:H8	1.66	0.59
7:A2:1255:G:O2'	7:A2:1258:G:N3	2.34	0.59
10:D1:196:ASN:HB2	10:D1:198:HIS:CE1	2.37	0.59
10:D2:97:ARG:NH2	10:D2:99:ASP:OD2	2.35	0.59
15:I1:23:PRO:HA	15:I1:61:LEU:HA	1.84	0.59
6:82:75:G:H2'	6:82:76:G:H8	1.67	0.59
7:A1:1206:G:H2'	7:A1:1207:2MG:C8	2.36	0.59
7:A2:376:G:H2'	7:A2:377:G:H8	1.67	0.59
36:b2:130:LEU:HB2	36:b2:135:ILE:HD11	1.84	0.59
7:A1:1124:G:H3'	16:J1:37:ARG:HH21	1.66	0.59
7:A2:501:C:H1'	7:A2:549:C:H1'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C1:40:ARG:NH2	9:C1:55:ILE:O	2.36	0.59
12:F1:12:PRO:O	12:F1:44:ARG:NH2	2.36	0.59
13:G1:150:ALA:HA	17:K1:61:PHE:HB3	1.82	0.59
19:M2:75:MET:HA	19:M2:78:LYS:HE3	1.84	0.59
7:A1:1346:A:H2	7:A1:1375:A:H62	1.50	0.59
9:C2:85:GLU:HA	9:C2:88:ARG:HD3	1.85	0.59
11:E1:77:ASN:HB2	11:E1:82:GLN:HG2	1.82	0.59
39:h2:58:LYS:O	39:h2:60:GLN:NE2	2.35	0.59
40:i2:6:LEU:HD23	40:i2:36:ALA:HA	1.83	0.59
7:A1:67:C:H2'	7:A1:68:G:C8	2.37	0.59
7:A1:441:A:H2'	7:A1:442:G:H5''	1.85	0.59
7:A1:633:G:H2'	7:A1:634:C:C6	2.38	0.59
7:A1:995:C:H2'	7:A1:996:A:H8	1.68	0.59
7:A2:269:C:H2'	7:A2:270:A:H8	1.67	0.59
9:C1:88:ARG:NH1	9:C1:99:ALA:O	2.36	0.59
10:D1:147:GLU:CD	10:D1:147:GLU:H	2.11	0.59
10:D2:6:GLY:O	10:D2:8:LYS:NZ	2.33	0.59
37:e2:26:MET:O	37:e2:30:ARG:NH2	2.35	0.59
3:4:24:ILE:HG23	37:e2:102:ARG:HD3	1.83	0.59
3:4:38:SER:HB3	37:e2:105:THR:HA	1.83	0.59
5:72:512:G:OP1	5:72:1234:U:O2'	2.19	0.59
9:C1:151:VAL:HG23	9:C1:200:VAL:HG22	1.84	0.59
15:I1:129:LYS:NZ	30:W1:33:U:OP1	2.35	0.59
7:A1:974:A:OP2	20:N1:81:ARG:NE	2.33	0.59
7:A2:87:C:H2'	7:A2:88:U:H4'	1.84	0.59
7:A2:808:C:OP2	21:O2:48:LYS:NZ	2.29	0.59
7:A2:1011:C:H2'	7:A2:1012:A:C8	2.37	0.59
13:G2:67:GLU:O	13:G2:138:ARG:NH2	2.36	0.59
36:b2:66:ASP:OD2	36:b2:102:ARG:NH1	2.34	0.59
5:72:1852:U:OP1	31:X2:72:G:O2'	2.20	0.59
5:72:2258:C:O2'	5:72:2427:C:OP2	2.19	0.59
7:A1:1412:C:H2'	7:A1:1413:A:C8	2.38	0.59
7:A2:56:U:H2'	7:A2:57:G:C8	2.37	0.59
7:A2:975:A:N1	7:A2:1366:C:O2'	2.32	0.59
7:A2:1071:C:H2'	7:A2:1072:G:H8	1.67	0.59
9:C1:10:ILE:HG23	9:C1:11:ARG:HG3	1.85	0.59
9:C1:73:PRO:O	9:C1:77:ILE:HG12	2.02	0.59
10:D1:185:LYS:HG3	10:D1:186:PRO:HD2	1.84	0.59
15:I1:47:VAL:HA	15:I1:50:GLN:HG2	1.84	0.59
5:72:566:U:H5''	42:o2:29:LYS:HE3	1.85	0.58
5:72:2141:G:H2'	5:72:2142:A:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:33:A:H1'	18:L2:29:GLN:HE22	1.67	0.58
7:A2:541:G:O2'	10:D2:40:GLN:OE1	2.21	0.58
17:K2:73:ALA:HB1	17:K2:77:TYR:HD2	1.68	0.58
18:L2:114:ARG:HG2	18:L2:119:VAL:HB	1.84	0.58
36:b2:107:PRO:HD2	36:b2:110:LEU:HD22	1.84	0.58
44:r2:20:GLU:HG2	44:r2:21:LEU:HD12	1.85	0.58
3:4:30:HIS:CE1	3:4:32:LEU:HB3	2.38	0.58
5:72:643:A:N1	5:72:2369:A:O2'	2.36	0.58
7:A1:490:C:H2'	7:A1:491:G:H8	1.67	0.58
7:A1:538:G:H2'	7:A1:539:A:H8	1.68	0.58
7:A1:1462:C:H2'	7:A1:1463:U:H5'	1.85	0.58
22:P1:55:ASP:OD1	22:P1:56:ARG:N	2.36	0.58
20:N1:31:ILE:O	20:N1:41:ARG:NH1	2.36	0.58
7:A1:200:G:H1	7:A1:217:C:H42	1.51	0.58
7:A1:603:U:H2'	7:A1:604:G:C8	2.38	0.58
7:A2:1216:A:O2'	20:N2:9:ARG:NH2	2.35	0.58
7:A1:736:C:H2'	7:A1:737:C:C6	2.39	0.58
7:A2:1309:G:N7	19:M2:98:ARG:NH2	2.52	0.58
9:C2:88:ARG:HH12	9:C2:100:GLN:HG3	1.69	0.58
12:F2:49:TYR:OH	24:R2:63:ARG:O	2.17	0.58
7:A2:477:C:H3'	7:A2:478:A:H8	1.69	0.58
9:C2:110:GLU:HB2	9:C2:144:LEU:HD12	1.85	0.58
5:72:2585:U:O4	50:Y2:102:ALA:N	2.37	0.58
7:A1:70:U:O2'	7:A1:72:A:N6	2.30	0.58
7:A1:830:G:H2'	7:A1:831:A:C8	2.39	0.58
7:A1:1160:G:H4'	8:B:131:LYS:HE2	1.84	0.58
7:A2:150:U:H2'	7:A2:151:A:H8	1.67	0.58
7:A2:269:C:H2'	7:A2:270:A:C8	2.39	0.58
9:C1:82:GLU:OE1	9:C1:82:GLU:N	2.36	0.58
12:F1:38:ARG:HB3	12:F1:63:ASN:HB2	1.85	0.58
7:A1:413:G:H1	10:D1:32:CYS:HA	1.69	0.58
7:A1:1133:G:H2'	7:A1:1134:G:C8	2.39	0.58
7:A1:1321:U:O2'	25:S1:78:ARG:NH2	2.37	0.58
7:A2:1534:A:H1'	7:A2:1535:C:H5''	1.86	0.58
9:C2:152:GLU:HG3	9:C2:199:LYS:HB2	1.85	0.58
10:D2:73:ARG:NH2	10:D2:74:ASN:OD1	2.35	0.58
5:72:684:G:OP1	41:l2:21:ARG:NH1	2.27	0.58
5:72:2645:G:OP2	5:72:2645:G:N2	2.25	0.58
7:A1:82:G:H3'	7:A1:83:C:H6	1.69	0.58
7:A1:1333:A:H3'	7:A1:1334:G:H8	1.68	0.58
7:A2:1397:C:OP2	11:E2:29:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H2:10:MET:HE1	14:H2:33:LYS:HA	1.86	0.58
5:72:574:A:N6	5:72:2034:U:OP1	2.37	0.57
5:72:1394:U:H4'	5:72:1603:A:H4'	1.86	0.57
5:72:2127:G:H2'	5:72:2128:G:O4'	2.04	0.57
5:72:2305:U:H5''	37:e2:131:GLY:HA3	1.86	0.57
7:A1:477:C:H2'	7:A1:478:A:C8	2.38	0.57
7:A2:203:G:O2'	7:A2:465:A:N1	2.36	0.57
17:K2:20:VAL:HG13	17:K2:35:THR:HG23	1.86	0.57
32:Y1:9:A:H1'	32:Y1:45:G:H2'	1.85	0.57
5:72:1138:G:H2'	5:72:1139:G:O4'	2.04	0.57
7:A1:219:U:H2'	7:A1:220:G:C8	2.39	0.57
7:A2:1106:G:O2'	9:C2:169:ARG:NH1	2.37	0.57
13:G1:140:ASP:OD1	13:G1:143:ARG:NH2	2.32	0.57
29:W:7:G:O2'	29:W:49:G:O5'	2.22	0.57
5:72:831:G:N2	42:o2:52:GLY:O	2.36	0.57
5:72:1056:G:H4'	5:72:1086:A:H8	1.70	0.57
5:72:1447:C:O2'	5:72:1544:A:N3	2.35	0.57
7:A1:71:A:H61	7:A1:99:C:H1'	1.68	0.57
7:A1:841:C:C4	7:A1:843:U:H5'	2.40	0.57
7:A1:926:G:H22	28:V2:20:C:H3'	1.68	0.57
7:A2:438:U:H4'	7:A2:439:U:O5'	2.03	0.57
7:A2:835:U:OP1	24:R2:53:ARG:NH1	2.38	0.57
10:D1:105:MET:HE1	10:D1:171:LEU:HD22	1.87	0.57
15:I2:51:PRO:HD3	15:I2:80:ARG:HG3	1.85	0.57
7:A1:1086:U:H3	7:A1:1099:G:N2	2.02	0.57
7:A1:1360:A:OP2	20:N1:75:ARG:NH2	2.35	0.57
5:72:278:A:OP2	5:72:361:G:N1	2.37	0.57
7:A1:827:U:O3'	14:H1:22:LYS:NZ	2.37	0.57
7:A2:972:C:OP2	16:J2:59:LYS:NZ	2.36	0.57
15:I1:119:ARG:HH12	15:I1:125:PRO:HA	1.70	0.57
36:b2:92:ALA:N	36:b2:104:ILE:O	2.32	0.57
38:g2:39:PHE:HB2	38:g2:46:HIS:CE1	2.38	0.57
7:A1:195:A:H2'	7:A1:196:A:C8	2.39	0.57
7:A2:154:U:H2'	7:A2:155:A:C8	2.40	0.57
7:A2:382:A:H2'	7:A2:383:A:C8	2.40	0.57
8:B:38:VAL:HG12	8:B:39:HIS:N	2.19	0.57
6:82:49:C:H2'	6:82:50:A:C8	2.40	0.57
7:A1:207:C:O2	7:A1:212:G:N1	2.38	0.57
7:A1:1316:G:N1	7:A1:1319:A:OP2	2.35	0.57
7:A2:663:A:O3'	24:R2:53:ARG:NH2	2.36	0.57
10:D2:196:ASN:HB2	10:D2:198:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:L1:44:LYS:HB3	18:L1:45:PRO:HD3	1.86	0.57
7:A1:458:U:H3	7:A1:474:G:H1	1.50	0.57
9:C1:127:ARG:HH21	9:C1:192:THR:HG21	1.69	0.57
3:4:9:TYR:HB3	3:4:25:ARG:HG2	1.87	0.57
7:A1:1162:C:H2'	7:A1:1163:A:C8	2.40	0.57
7:A2:297:G:N2	7:A2:300:A:OP2	2.33	0.57
8:B2:153:ASP:OD1	8:B2:153:ASP:N	2.33	0.57
44:r2:78:VAL:HA	44:r2:81:ARG:HD2	1.86	0.57
5:72:2655:G:O2'	5:72:2664:G:O6	2.20	0.57
7:A1:715:A:H2'	7:A1:716:A:C8	2.40	0.57
7:A2:203:G:H1'	7:A2:465:A:H61	1.69	0.57
7:A2:859:G:OP2	7:A2:869:G:N1	2.25	0.57
8:B:117:LEU:HG	8:B:141:LEU:HD22	1.86	0.57
17:K1:73:ALA:O	17:K1:77:TYR:N	2.32	0.57
29:W:16:H2U:C4	29:W:59:G:H22	2.18	0.57
5:72:1094:U:H1'	5:72:1097:U:H5	1.70	0.56
5:72:1826:G:O2'	5:72:1971:U:OP2	2.23	0.56
7:A1:588:G:H2'	7:A1:589:U:C6	2.40	0.56
7:A1:598:U:H4'	14:H1:86:TYR:CD2	2.39	0.56
8:B2:67:ILE:HG12	8:B2:89:GLN:HE21	1.70	0.56
9:C1:14:ILE:O	9:C1:15:VAL:HB	2.05	0.56
11:E1:75:ALA:O	11:E1:82:GLN:NE2	2.25	0.56
13:G1:53:ARG:HH12	13:G1:121:ALA:HB1	1.70	0.56
14:H2:18:GLN:HE21	14:H2:72:VAL:H	1.53	0.56
5:72:324:A:OP2	5:72:1205:A:N6	2.37	0.56
7:A1:401:C:H2'	7:A1:402:G:H8	1.69	0.56
7:A1:649:A:C3'	7:A1:650:G:H5''	2.35	0.56
7:A1:948:C:H2'	7:A1:949:A:H8	1.70	0.56
5:72:858:G:N3	5:72:2268:A:H2'	2.20	0.56
5:72:1028:A:N3	5:72:2486:C:O2'	2.34	0.56
6:82:75:G:H2'	6:82:76:G:C8	2.41	0.56
7:A1:696:A:N3	7:A1:786:G:O2'	2.33	0.56
7:A1:908:A:H2'	7:A1:909:A:C8	2.40	0.56
7:A1:1404:C:H2'	7:A1:1405:G:C8	2.40	0.56
7:A2:67:C:O2'	7:A2:171:A:N3	2.36	0.56
7:A2:483:C:O2'	7:A2:484:G:OP1	2.22	0.56
7:A2:1060:U:H2'	7:A2:1061:G:H8	1.69	0.56
7:A2:1175:G:H2'	7:A2:1176:A:C8	2.40	0.56
10:D2:108:GLY:HA3	10:D2:114:ALA:HB2	1.88	0.56
17:K2:73:ALA:O	17:K2:77:TYR:N	2.28	0.56
18:L2:43:LYS:HG2	18:L2:44:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:M1:75:MET:HG3	19:M1:78:LYS:HE3	1.87	0.56
29:W:16:H2U:P	29:W:16:H2U:H62	2.45	0.56
3:4:36:VAL:HG23	3:4:40:CYS:HB3	1.87	0.56
7:A1:58:C:H2'	7:A1:59:A:H8	1.69	0.56
7:A2:1060:U:OP1	20:N2:85:ARG:NH2	2.30	0.56
7:A1:603:U:H2'	7:A1:604:G:H8	1.69	0.56
7:A1:1356:G:H2'	7:A1:1357:A:C8	2.40	0.56
7:A2:358:U:H2'	7:A2:359:G:C8	2.41	0.56
8:B:104:TRP:HA	8:B:107:VAL:HG22	1.87	0.56
8:B:113:ARG:HH12	8:B:117:LEU:HB2	1.70	0.56
17:K2:64:GLN:HG3	17:K2:99:ALA:HB2	1.88	0.56
20:N1:51:LEU:HD12	20:N1:52:PRO:HD2	1.87	0.56
7:A1:911:U:OP2	18:L1:94:ARG:NH2	2.39	0.56
7:A1:1058:G:H2'	7:A1:1059:C:C6	2.40	0.56
7:A1:1323:G:H2'	7:A1:1324:A:C8	2.41	0.56
7:A1:1513:A:H2'	7:A1:1514:G:H8	1.70	0.56
14:H1:103:VAL:HG12	14:H1:126:ILE:HD13	1.86	0.56
15:I2:54:LEU:HD12	15:I2:98:LEU:HD23	1.88	0.56
39:h2:1:MET:HG2	39:h2:2:LEU:H	1.69	0.56
5:72:1537:G:H3'	5:72:1538:G:O4'	2.06	0.56
7:A1:584:G:H2'	7:A1:585:G:C8	2.41	0.56
7:A2:212:G:H2'	7:A2:213:G:C8	2.41	0.56
7:A2:923:A:OP1	11:E2:26:LYS:NZ	2.31	0.56
7:A2:1371:G:H2'	7:A2:1372:U:C6	2.40	0.56
16:J1:65:TYR:HB3	20:N1:96:LEU:HD22	1.88	0.56
28:V2:31:U:O2'	28:V2:32:U:OP1	2.20	0.56
7:A1:1317:C:OP2	20:N1:28:LYS:NZ	2.26	0.56
7:A2:1326:U:H2'	7:A2:1327:C:C6	2.41	0.56
9:C1:6:HIS:CE1	9:C1:8:ASN:HB3	2.41	0.56
16:J1:6:ILE:HA	16:J1:102:LEU:HA	1.88	0.56
31:X2:23:G:H2'	31:X2:24:A:C8	2.40	0.56
5:72:1039:A:H2	5:72:1116:G:H22	1.53	0.56
7:A1:202:G:H1	7:A1:215:C:H42	1.52	0.56
7:A1:1229:A:H2'	7:A1:1230:C:C6	2.41	0.56
7:A2:562:U:H1'	18:L2:12:ARG:HD2	1.86	0.56
7:A2:1218:C:H2'	7:A2:1219:A:H8	1.70	0.56
7:A2:1268:G:N3	7:A2:1326:U:O2'	2.39	0.56
5:72:1130:U:O2'	5:72:1131:G:OP1	2.23	0.56
5:72:468:G:OP2	41:I2:37:LYS:NZ	2.34	0.55
7:A1:467:U:H5'	7:A1:468:A:H5'	1.86	0.55
7:A2:1106:G:H5''	9:C2:172:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1130:A:O2'	15:I2:5:GLN:NE2	2.35	0.55
22:P1:6:LEU:HD13	22:P1:17:TYR:CD1	2.41	0.55
7:A1:691:G:O6	17:K1:53:ARG:NH2	2.39	0.55
7:A1:784:A:H2'	7:A1:785:G:H8	1.71	0.55
7:A1:1086:U:H3	7:A1:1099:G:H22	1.53	0.55
7:A2:532:A:N6	7:A2:1206:G:O2'	2.39	0.55
7:A2:855:U:OP2	7:A2:871:U:N3	2.30	0.55
10:D2:118:VAL:HG22	10:D2:123:ILE:HG13	1.88	0.55
3:4:64:PHE:CG	25:S2:9:PRO:HD3	2.41	0.55
5:72:79:C:O2'	5:72:346:A:N3	2.37	0.55
5:72:858:G:O2'	5:72:859:G:O4'	2.19	0.55
5:72:910:A:H62	39:h2:12:MET:HA	1.72	0.55
5:72:931:U:O2	5:72:1167:C:O2'	2.24	0.55
5:72:2585:U:C4	43:p:36:TRP:HB2	2.41	0.55
7:A1:450:G:H1	7:A1:483:C:H42	1.55	0.55
7:A2:1218:C:H2'	7:A2:1219:A:C8	2.41	0.55
7:A2:1308:U:H2'	7:A2:1309:G:H8	1.70	0.55
10:D2:11:LEU:HD23	10:D2:63:ARG:HG2	1.88	0.55
24:R2:5:PHE:HD1	24:R2:43:ARG:HG2	1.72	0.55
5:72:455:C:H3'	5:72:456:C:H5''	1.89	0.55
7:A1:166:U:H2'	7:A1:167:A:H8	1.71	0.55
7:A1:185:U:H2'	7:A1:186:C:C6	2.42	0.55
7:A1:370:C:H2'	7:A1:371:A:C8	2.41	0.55
7:A1:1263:C:H2'	7:A1:1264:U:C6	2.42	0.55
7:A1:1376:U:H2'	7:A1:1377:A:C8	2.41	0.55
7:A2:389:A:H3'	7:A2:390:U:H6	1.72	0.55
7:A2:963:G:H21	16:J2:57:VAL:HG11	1.72	0.55
8:B:91:PHE:HE2	8:B:93:ASN:HD21	1.55	0.55
15:I1:116:VAL:HG21	16:J1:62:ARG:HB2	1.88	0.55
28:V2:26:G:H22	32:Y1:34:CM0:H3	1.53	0.55
39:h2:64:TRP:HB2	39:h2:104:GLU:HB2	1.88	0.55
5:72:355:U:H2'	5:72:356:G:H8	1.72	0.55
5:72:630:G:N2	5:72:633:A:OP2	2.31	0.55
5:72:668:A:H2'	5:72:670:A:H62	1.72	0.55
5:72:987:C:O2'	5:72:1000:A:N3	2.40	0.55
7:A1:448:A:H3'	7:A1:449:G:H8	1.70	0.55
7:A1:662:U:O2'	7:A1:836:G:O5'	2.25	0.55
7:A1:1397:C:OP2	11:E1:29:ARG:NH2	2.40	0.55
7:A2:880:C:H3'	18:L2:6:GLN:HE21	1.72	0.55
5:72:2393:U:H5''	42:o2:62:PRO:HB3	1.89	0.55
7:A1:1041:G:H2'	7:A1:1042:A:C8	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:109:A:H2'	7:A2:326:G:H21	1.71	0.55
10:D1:50:ASP:O	10:D1:53:VAL:HG22	2.07	0.55
19:M1:75:MET:HA	19:M1:78:LYS:HE3	1.89	0.55
5:72:371:A:N6	5:72:402:A:OP2	2.35	0.55
7:A1:591:U:H2'	7:A1:592:G:C8	2.42	0.55
7:A2:362:G:N2	7:A2:365:U:OP2	2.40	0.55
7:A2:452:A:H61	7:A2:480:U:H3	1.53	0.55
7:A2:1040:U:H2'	7:A2:1041:G:H8	1.70	0.55
2:32:24:LEU:HD11	5:72:930:G:H1'	1.88	0.55
5:72:1604:C:O2'	5:72:1610:A:N1	2.39	0.55
7:A2:606:G:N2	7:A2:632:U:OP1	2.28	0.55
7:A2:1193:G:O6	9:C2:2:GLY:N	2.39	0.55
8:B2:67:ILE:H	8:B2:89:GLN:NE2	2.04	0.55
11:E1:157:ARG:HH21	14:H1:43:GLU:HB3	1.72	0.55
5:72:717:C:H3'	5:72:718:A:H8	1.72	0.55
5:72:2554:U:O4	33:Y2:74:C:N4	2.40	0.55
7:A1:538:G:H2'	7:A1:539:A:C8	2.41	0.55
7:A1:666:G:H5'	7:A1:726:C:H1'	1.87	0.55
7:A2:37:U:HO2'	7:A2:500:G:HO2'	1.51	0.55
7:A1:10:A:H2'	7:A1:11:G:H8	1.72	0.55
7:A1:386:C:H2'	7:A1:387:U:H5''	1.89	0.55
7:A1:948:C:H2'	7:A1:949:A:C8	2.42	0.55
7:A2:643:C:H5'	14:H2:32:LEU:HD21	1.88	0.55
7:A2:1492:A:H2'	7:A2:1493:A:C4	2.42	0.55
9:C2:73:PRO:O	9:C2:76:VAL:HG22	2.07	0.55
14:H2:76:GLN:NE2	14:H2:77:ARG:O	2.39	0.55
36:b2:78:VAL:HG21	36:b2:110:LEU:HD21	1.89	0.55
7:A1:77:A:H2'	7:A1:78:A:C8	2.42	0.54
7:A1:1005:A:H3'	7:A1:1006:G:H8	1.72	0.54
7:A2:40:C:H2'	7:A2:41:G:C8	2.41	0.54
7:A2:1137:C:O2	7:A2:1138:G:N2	2.40	0.54
30:W1:43:C:H2'	30:W1:44:G:C8	2.42	0.54
5:72:276:U:H2'	5:72:277:G:C2	2.42	0.54
5:72:839:U:H3	5:72:939:G:H1	1.54	0.54
5:72:1363:C:O2'	5:72:1809:A:N3	2.36	0.54
7:A1:1244:G:H1	7:A1:1293:C:H42	1.55	0.54
7:A1:1455:G:H3'	7:A1:1456:A:H8	1.72	0.54
16:J1:34:ALA:HB2	16:J1:83:THR:HG21	1.89	0.54
5:72:954:G:OP2	39:h2:16:ARG:NH1	2.37	0.54
5:72:1167:C:H2'	5:72:1168:G:C8	2.41	0.54
5:72:2166:U:H2'	5:72:2167:U:H5'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:31:G:O2'	7:A1:48:C:N4	2.40	0.54
7:A1:82:G:H3'	7:A1:83:C:C6	2.42	0.54
7:A1:476:U:H2'	7:A1:477:C:C6	2.43	0.54
7:A1:584:G:H2'	7:A1:585:G:H8	1.73	0.54
7:A1:599:C:H2'	7:A1:600:A:H8	1.72	0.54
25:S2:39:THR:HA	25:S2:70:LYS:HA	1.90	0.54
3:4:6:HIS:CE1	37:e2:64:LYS:H	2.25	0.54
7:A2:1247:U:H2'	7:A2:1248:A:H5''	1.88	0.54
7:A2:1323:G:H2'	7:A2:1324:A:C8	2.43	0.54
10:D2:188:ARG:HH22	10:D2:193:ALA:HA	1.72	0.54
12:F1:14:GLN:HB3	12:F1:17:GLN:HE21	1.73	0.54
22:P1:61:VAL:HG22	22:P1:67:ILE:HD11	1.90	0.54
23:Q1:68:SER:HB3	23:Q1:71:LYS:HB2	1.90	0.54
30:W1:37:MIA:N1	30:W1:37:MIA:H131	2.22	0.54
33:Y2:20:G:N2	33:Y2:59:U:OP1	2.40	0.54
42:o2:20:GLY:HA2	42:o2:28:GLY:HA2	1.88	0.54
5:72:2512:C:H2'	5:72:2513:A:O4'	2.08	0.54
7:A1:59:A:H3'	7:A1:331:G:H22	1.71	0.54
7:A1:1250:A:H2'	7:A1:1251:A:C8	2.43	0.54
7:A1:1324:A:H2'	7:A1:1325:C:C6	2.42	0.54
7:A2:1029:U:H2'	7:A2:1030:U:H6	1.73	0.54
7:A2:1040:U:H2'	7:A2:1041:G:C8	2.43	0.54
8:B2:86:SER:OG	8:B2:222:ARG:NH1	2.41	0.54
23:Q2:59:VAL:HG12	23:Q2:78:VAL:HG22	1.89	0.54
7:A1:401:C:H2'	7:A1:402:G:C8	2.42	0.54
7:A1:539:A:H2'	7:A1:540:G:C8	2.43	0.54
7:A1:876:C:P	14:H1:15:ARG:HH12	2.31	0.54
8:B2:59:LYS:HG2	8:B2:63:ARG:HH12	1.71	0.54
9:C1:100:GLN:NE2	9:C1:102:ASN:OD1	2.38	0.54
15:I1:45:ARG:O	15:I1:48:VAL:HG22	2.07	0.54
20:N2:60:GLN:OE1	20:N2:60:GLN:N	2.40	0.54
5:72:458:G:O2'	5:72:469:G:O6	2.25	0.54
7:A1:746:A:H2'	7:A1:747:A:H8	1.72	0.54
7:A2:358:U:H2'	7:A2:359:G:H8	1.72	0.54
7:A2:1162:C:H2'	7:A2:1163:A:C8	2.43	0.54
36:b2:107:PRO:HG2	36:b2:110:LEU:HB2	1.88	0.54
5:72:2070:A:H2'	5:72:2071:A:O4'	2.08	0.54
5:72:2859:G:H2'	5:72:2860:A:C8	2.43	0.54
7:A1:187:G:N2	7:A1:190:A:OP2	2.40	0.54
7:A1:1170:A:H2'	7:A1:1171:A:O4'	2.08	0.54
7:A2:1124:G:N2	7:A2:1125:U:O4	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C2:40:ARG:NH1	20:N2:92:GLU:OE1	2.41	0.54
15:I2:88:MET:SD	15:I2:95:ARG:NE	2.80	0.54
16:J2:65:TYR:HB3	20:N2:96:LEU:HD22	1.88	0.54
44:r2:28:VAL:HG11	44:r2:103:VAL:HG13	1.90	0.54
45:z2:21:LEU:HD21	45:z2:41:ARG:HG2	1.89	0.54
7:A1:1047:G:HO2'	7:A1:1215:G:HO2'	1.55	0.54
19:M1:107:ARG:NH1	19:M1:113:ARG:HD2	2.23	0.54
44:r2:99:TYR:OH	44:r2:111:ARG:NH2	2.41	0.54
6:82:49:C:H2'	6:82:50:A:H8	1.72	0.54
7:A1:350:G:H2'	7:A1:351:G:C8	2.43	0.54
7:A1:1118:U:H4'	15:I1:85:ARG:HH22	1.73	0.54
7:A1:1267:C:H3'	7:A1:1268:G:C8	2.43	0.54
7:A2:180:U:O2	7:A2:196:A:N6	2.40	0.54
8:B2:131:LYS:C	8:B2:133:GLU:H	2.16	0.54
9:C1:15:VAL:HG12	9:C1:16:LYS:N	2.21	0.54
9:C1:53:SER:N	9:C1:69:HIS:O	2.41	0.54
10:D2:95:GLU:O	10:D2:100:ASN:ND2	2.40	0.54
37:e2:71:ARG:O	37:e2:81:GLN:NE2	2.40	0.54
45:z2:75:LYS:HB2	45:z2:77:ARG:HG3	1.88	0.54
4:62:13:ARG:NH1	42:o2:61:LEU:O	2.35	0.53
7:A1:977:A:H8	7:A1:1223:C:C2	2.26	0.53
7:A1:1081:A:N7	11:E1:52:LYS:NZ	2.55	0.53
7:A1:1513:A:H2'	7:A1:1514:G:C8	2.43	0.53
7:A2:150:U:H2'	7:A2:151:A:C8	2.43	0.53
11:E2:115:LEU:HD13	11:E2:123:VAL:HG11	1.89	0.53
12:F2:68:GLN:CD	12:F2:68:GLN:H	2.16	0.53
13:G1:79:ARG:HG2	13:G1:84:THR:HB	1.91	0.53
26:T1:55:GLN:HB3	26:T1:56:PRO:HD3	1.90	0.53
28:V2:46:C:H4'	28:V2:47:G:OP1	2.04	0.53
5:72:1105:U:H2'	5:72:1106:G:C8	2.44	0.53
5:72:1190:G:OP1	42:o2:30:THR:OG1	2.21	0.53
5:72:1326:U:O2'	5:72:2010:G:O2'	2.22	0.53
5:72:1786:A:H1'	5:72:1938:A:N6	2.23	0.53
5:72:2251:OMG:N1	29:W:75:C:N3	2.49	0.53
7:A1:150:U:H2'	7:A1:151:A:H8	1.72	0.53
7:A1:830:G:H2'	7:A1:831:A:H8	1.72	0.53
7:A1:1015:G:H2'	7:A1:1016:A:C8	2.43	0.53
7:A2:999:C:H2'	7:A2:1000:A:C8	2.42	0.53
7:A2:1060:U:H3	7:A2:1197:A:H61	1.55	0.53
7:A2:1404:C:H2'	7:A2:1405:G:C8	2.42	0.53
21:O2:70:LEU:HD22	21:O2:78:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S2:32:ARG:HH21	25:S2:57:HIS:CE1	2.26	0.53
30:W1:10:G:O2'	30:W1:11:C:OP1	2.24	0.53
3:4:27:THR:O	3:4:28:VAL:C	2.52	0.53
7:A1:649:A:H3'	7:A1:650:G:H5''	1.91	0.53
7:A1:677:U:H2'	7:A1:678:U:C6	2.43	0.53
7:A1:1266:G:N2	7:A1:1269:A:OP2	2.37	0.53
7:A2:160:A:H2'	7:A2:161:A:O4'	2.08	0.53
7:A2:598:U:H4'	14:H2:86:TYR:CD2	2.43	0.53
1:12:58:VAL:HG12	5:72:372:G:H2'	1.91	0.53
5:72:754:U:O2'	5:72:1272:A:N1	2.41	0.53
5:72:2595:G:N2	5:72:2598:A:OP2	2.37	0.53
7:A1:73:C:H2'	7:A1:74:A:C8	2.44	0.53
7:A1:781:A:H5''	7:A1:782:A:C8	2.43	0.53
7:A1:1414:U:H2'	7:A1:1415:G:C8	2.44	0.53
7:A2:147:G:H2'	7:A2:148:G:C8	2.43	0.53
7:A2:191:G:H3'	7:A2:192:A:H8	1.74	0.53
7:A2:203:G:H1	7:A2:214:C:H42	1.55	0.53
8:B:162:PHE:HD1	8:B:184:PHE:HB2	1.73	0.53
31:X2:18:G:H1'	31:X2:62:C:H5'	1.89	0.53
3:4:64:PHE:CD1	25:S2:8:GLY:HA2	2.43	0.53
5:72:1024:G:O2'	5:72:1144:A:O2'	2.25	0.53
5:72:1594:U:H2'	5:72:1595:C:C6	2.44	0.53
5:72:2175:C:H2'	5:72:2176:A:H8	1.73	0.53
7:A1:19:A:H2'	7:A1:20:U:C6	2.43	0.53
7:A1:555:U:H2'	7:A1:556:C:C6	2.44	0.53
7:A1:1088:G:N2	7:A1:1167:A:H61	2.05	0.53
7:A1:1256:A:O2'	7:A1:1278:G:O6	2.24	0.53
7:A2:43:C:H2'	7:A2:44:A:C8	2.44	0.53
11:E1:149:SER:OG	11:E1:152:MET:HE3	2.09	0.53
17:K1:89:PRO:HB3	27:U1:32:VAL:HG11	1.91	0.53
21:O2:21:ASP:OD1	21:O2:24:SER:HB3	2.09	0.53
27:U2:68:THR:HG22	27:U2:70:LEU:H	1.74	0.53
5:72:788:A:OP1	5:72:791:C:N4	2.34	0.53
5:72:2447:G:N2	5:72:2450:A:N7	2.57	0.53
7:A2:231:U:H2'	7:A2:232:G:H8	1.74	0.53
7:A2:514:C:H2'	7:A2:515:G:H8	1.74	0.53
13:G2:13:LEU:HD12	13:G2:14:PRO:HD2	1.89	0.53
18:L1:54:ARG:HH11	18:L1:64:THR:HB	1.73	0.53
28:V2:26:G:H1	32:Y1:34:CM0:H3	1.56	0.53
29:W:54:5MU:H3'	29:W:55:PSU:C6	2.43	0.53
6:82:42:C:C5	37:e2:66:LEU:HD22	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:166:U:H2'	7:A1:167:A:C8	2.44	0.53
7:A1:591:U:H2'	7:A1:592:G:H8	1.73	0.53
7:A1:783:C:H2'	7:A1:784:A:C8	2.44	0.53
7:A2:235:C:H2'	7:A2:236:A:C8	2.43	0.53
7:A2:385:C:H2'	7:A2:386:C:C6	2.44	0.53
7:A2:1251:A:H2'	7:A2:1252:A:C8	2.43	0.53
3:4:12:ILE:N	3:4:24:ILE:O	2.41	0.53
5:72:571:U:O2	5:72:2030:6MZ:O2'	2.18	0.53
5:72:1278:C:H2'	5:72:1279:G:C8	2.43	0.53
7:A1:1267:C:H3'	7:A1:1268:G:H8	1.73	0.53
7:A2:418:C:H2'	7:A2:419:C:C6	2.44	0.53
7:A2:1149:C:H2'	7:A2:1150:A:C8	2.44	0.53
9:C1:147:LYS:HD2	9:C1:205:GLY:HA2	1.90	0.53
38:g2:39:PHE:HA	38:g2:46:HIS:HA	1.91	0.53
5:72:776:G:N7	5:72:793:A:O2'	2.41	0.53
7:A1:335:C:H2'	7:A1:336:A:H8	1.73	0.53
7:A1:542:G:OP1	10:D1:10:LYS:NZ	2.41	0.53
7:A1:1048:G:H2'	7:A1:1050:G:H8	1.73	0.53
7:A1:1512:U:H2'	7:A1:1513:A:C8	2.44	0.53
7:A2:17:U:H2'	7:A2:18:C:C6	2.43	0.53
9:C2:57:ILE:HG12	9:C2:66:VAL:HG13	1.90	0.53
10:D1:13:ARG:HH21	10:D1:38:PRO:HA	1.74	0.53
12:F1:29:ILE:HD13	12:F1:64:VAL:HG11	1.91	0.53
14:H2:18:GLN:NE2	14:H2:72:VAL:H	2.06	0.53
29:W:50:G:H1	29:W:64:U:H3	1.57	0.53
44:r2:8:ILE:O	44:r2:12:THR:OG1	2.26	0.53
5:72:2262:U:OP2	45:z2:16:SER:OG	2.21	0.53
7:A1:512:U:H2'	7:A1:513:C:C6	2.44	0.53
7:A1:908:A:H2'	7:A1:909:A:H8	1.74	0.53
7:A1:1314:C:H2'	7:A1:1315:U:C6	2.44	0.53
7:A1:1474:U:H2'	7:A1:1475:G:C8	2.44	0.53
7:A2:58:C:O2'	7:A2:388:G:N7	2.42	0.53
7:A2:932:C:H5''	13:G2:3:ARG:HG2	1.91	0.53
9:C2:164:ARG:HD3	28:V2:60:A:O2'	2.09	0.53
17:K2:81:ASN:HA	17:K2:106:ARG:HB2	1.90	0.53
5:72:1754:A:N1	5:72:2716:C:O2'	2.40	0.52
7:A1:410:G:N2	7:A1:431:A:N7	2.57	0.52
7:A1:690:G:H2'	7:A1:691:G:C8	2.45	0.52
7:A1:712:A:H2'	7:A1:713:G:C8	2.43	0.52
7:A1:1144:G:N2	7:A1:1146:A:H62	2.06	0.52
7:A2:979:C:OP1	7:A2:1223:C:N4	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1345:U:H5''	15:I2:122:ARG:HH11	1.73	0.52
7:A2:1497:G:H2'	7:A2:1498:UR3:H6	1.91	0.52
13:G2:113:ASP:H	13:G2:119:ARG:HE	1.57	0.52
44:r2:29:HIS:HB3	44:r2:36:TYR:HB2	1.91	0.52
5:72:503:A:H5''	5:72:504:A:H3'	1.90	0.52
5:72:858:G:OP2	45:z2:78:LYS:NZ	2.42	0.52
5:72:2162:G:H3'	5:72:2163:A:H8	1.73	0.52
7:A1:17:U:H2'	7:A1:18:C:C6	2.45	0.52
7:A1:1305:G:H4'	7:A1:1332:A:H62	1.74	0.52
7:A1:1390:U:O2'	7:A1:1391:U:H5'	2.09	0.52
7:A2:1314:C:H2'	7:A2:1315:U:C6	2.44	0.52
9:C1:114:LYS:HA	9:C1:185:ASN:ND2	2.24	0.52
14:H1:18:GLN:HE21	14:H1:72:VAL:H	1.55	0.52
19:M2:71:ARG:HD3	37:e2:115:ARG:HD2	1.90	0.52
29:W:50:G:H22	29:W:64:U:H3	1.56	0.52
3:4:53:THR:HG22	19:M2:75:MET:HE3	1.91	0.52
5:72:1939:5MU:H3'	5:72:1940:U:H5'	1.92	0.52
5:72:2646:C:OP2	5:72:2732:G:O2'	2.25	0.52
7:A1:10:A:H2'	7:A1:11:G:C8	2.44	0.52
7:A1:376:G:O3'	22:P1:5:ARG:NH1	2.38	0.52
7:A2:1317:C:O2	25:S2:37:ARG:NH1	2.41	0.52
9:C1:42:TYR:HD2	9:C1:43:LEU:HD12	1.74	0.52
10:D1:101:VAL:HG21	10:D1:137:VAL:HG21	1.90	0.52
26:T1:28:MET:HE1	26:T1:58:VAL:HA	1.91	0.52
7:A1:894:G:H2'	7:A1:895:G:H8	1.74	0.52
7:A2:96:U:H2'	7:A2:97:G:C8	2.45	0.52
7:A2:376:G:H1	7:A2:387:U:H3	1.57	0.52
14:H1:76:GLN:NE2	14:H1:77:ARG:O	2.42	0.52
20:N1:60:GLN:OE1	20:N1:60:GLN:N	2.42	0.52
24:R2:34:THR:HG22	24:R2:38:LYS:H	1.74	0.52
29:W:43:G:H2'	29:W:44:G:C8	2.45	0.52
5:72:829:A:N7	5:72:2247:A:O2'	2.42	0.52
5:72:888:C:OP2	5:72:888:C:H4'	2.10	0.52
7:A1:714:G:H2'	7:A1:715:A:C8	2.44	0.52
7:A1:834:U:H2'	7:A1:835:U:C6	2.45	0.52
7:A1:1489:G:H2'	7:A1:1490:U:C6	2.45	0.52
7:A2:126:G:OP1	7:A2:605:U:O2'	2.20	0.52
7:A2:183:C:O2'	7:A2:184:G:H5'	2.09	0.52
7:A2:377:G:H2'	7:A2:378:G:H8	1.74	0.52
7:A2:545:C:O2'	7:A2:549:C:H5'	2.10	0.52
9:C1:15:VAL:HG13	9:C1:207:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C1:46:GLU:HB2	9:C1:47:LEU:HD12	1.91	0.52
16:J1:36:VAL:HG12	16:J1:76:ILE:CG1	2.39	0.52
23:Q2:60:GLU:HG2	23:Q2:77:ARG:HH21	1.73	0.52
43:p:31:VAL:C	43:p:33:ASN:H	2.18	0.52
7:A2:254:G:H2'	7:A2:255:G:H8	1.74	0.52
7:A2:1413:A:H2	7:A2:1487:G:H22	1.56	0.52
8:B2:149:GLY:HA2	8:B2:152:LYS:HE3	1.92	0.52
9:C2:76:VAL:HA	9:C2:79:LYS:HD2	1.92	0.52
24:R2:41:PRO:HG2	24:R2:44:ILE:HG12	1.91	0.52
1:12:65:ASP:OD1	1:12:66:THR:N	2.42	0.52
5:72:747:5MU:H3'	5:72:748:G:C5'	2.40	0.52
7:A1:1166:G:H22	7:A1:1169:A:H5''	1.74	0.52
7:A2:655:A:H2'	7:A2:656:G:H8	1.75	0.52
16:J1:36:VAL:HG12	16:J1:76:ILE:HG13	1.90	0.52
3:4:11:GLU:HA	3:4:25:ARG:HA	1.91	0.52
7:A1:181:A:H61	7:A1:194:C:H3'	1.75	0.52
7:A1:999:C:H2'	7:A1:1000:A:H8	1.74	0.52
7:A2:361:G:H2'	7:A2:362:G:O4'	2.09	0.52
7:A2:993:G:H2'	7:A2:995:C:H41	1.75	0.52
8:B:163:VAL:HG22	8:B:164:ILE:H	1.74	0.52
12:F2:21:MET:HA	12:F2:24:ARG:HH11	1.75	0.52
14:H2:87:LYS:HG2	14:H2:92:LEU:HA	1.92	0.52
20:N2:4:GLN:N	20:N2:4:GLN:OE1	2.41	0.52
5:72:1791:A:H4'	36:b2:205:LEU:HD11	1.91	0.52
7:A1:191:G:H3'	7:A1:192:A:H8	1.75	0.52
7:A1:742:G:H2'	7:A1:743:A:H8	1.75	0.52
7:A1:1130:A:H5''	15:I1:64:TYR:HE2	1.75	0.52
7:A2:21:G:H2'	7:A2:22:G:C8	2.45	0.52
7:A2:769:G:H4'	7:A2:1513:A:H4'	1.92	0.52
9:C1:47:LEU:HB3	9:C1:50:ALA:HB3	1.92	0.52
10:D1:28:ILE:HD12	10:D1:29:ASP:N	2.24	0.52
10:D1:118:VAL:HG22	10:D1:123:ILE:HG13	1.91	0.52
5:72:2135:A:C5	5:72:2136:G:H1'	2.46	0.52
7:A1:685:G:N1	7:A1:704:A:OP2	2.43	0.52
7:A1:1237:C:H3'	7:A1:1336:C:H41	1.74	0.52
13:G2:15:ASP:OD1	13:G2:15:ASP:N	2.43	0.52
13:G2:16:PRO:HB2	15:I2:42:GLU:HG2	1.92	0.52
14:H2:41:LYS:HE2	14:H2:48:ASP:HA	1.92	0.52
5:72:1167:C:H2'	5:72:1168:G:H8	1.75	0.51
7:A1:1021:A:H3'	7:A1:1022:A:H8	1.75	0.51
7:A1:1157:A:H1'	7:A1:1181:G:N2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:1391:U:H2'	7:A1:1392:G:H8	1.73	0.51
7:A2:946:A:H2'	7:A2:947:G:C8	2.45	0.51
7:A2:1118:U:H4'	15:I2:85:ARG:HH22	1.74	0.51
11:E1:157:ARG:NH1	14:H1:99:LEU:O	2.43	0.51
11:E1:166:GLY:HA3	14:H1:114:ARG:HH22	1.76	0.51
21:O1:70:LEU:HD22	21:O1:78:TYR:HB2	1.91	0.51
7:A1:54:C:H2'	7:A1:352:C:H41	1.75	0.51
7:A2:200:G:H2'	7:A2:201:G:H8	1.74	0.51
11:E2:149:SER:OG	11:E2:152:MET:HE3	2.10	0.51
13:G2:24:ALA:O	13:G2:27:VAL:HG22	2.10	0.51
17:K1:27:PHE:CE1	17:K1:89:PRO:HG2	2.40	0.51
19:M1:107:ARG:HH21	19:M1:110:LYS:HE3	1.75	0.51
45:z2:50:ASN:HB2	45:z2:82:ILE:HB	1.91	0.51
3:4:37:CYS:H	3:4:40:CYS:HB2	1.76	0.51
7:A1:1304:G:H2'	7:A1:1305:G:O4'	2.10	0.51
13:G2:145:ALA:O	13:G2:149:LYS:N	2.43	0.51
40:i2:3:VAL:HG12	40:i2:38:PRO:HA	1.92	0.51
45:z2:21:LEU:HD23	45:z2:40:GLN:HA	1.93	0.51
5:72:2469:A:H61	5:72:2481:G:H1'	1.76	0.51
6:82:88:C:H4'	6:82:89:U:OP1	2.09	0.51
7:A1:837:U:O2	7:A1:849:G:N2	2.44	0.51
7:A1:1275:A:H2'	7:A1:1276:G:O4'	2.11	0.51
7:A1:1327:C:H2'	7:A1:1328:C:H6	1.76	0.51
7:A2:173:U:H5''	7:A2:197:A:O4'	2.10	0.51
7:A2:1412:C:H2'	7:A2:1413:A:C8	2.45	0.51
8:B2:223:GLU:O	8:B2:227:GLN:HG2	2.10	0.51
10:D1:188:ARG:HH22	10:D1:193:ALA:HA	1.74	0.51
14:H2:54:ASP:OD1	14:H2:55:THR:N	2.43	0.51
17:K1:74:VAL:HG23	17:K1:75:LYS:H	1.76	0.51
17:K2:17:SER:HA	17:K2:79:ILE:HA	1.92	0.51
20:N2:13:ARG:NH1	20:N2:54:ASP:OD2	2.44	0.51
21:O2:24:SER:O	21:O2:28:GLN:HG2	2.11	0.51
36:b2:145:GLU:OE2	36:b2:150:LYS:N	2.44	0.51
7:A1:250:A:H4'	7:A1:251:G:O5'	2.10	0.51
7:A1:404:G:H2'	7:A1:405:U:C6	2.45	0.51
7:A1:853:C:H2'	7:A1:854:U:C6	2.45	0.51
7:A1:1130:A:H2'	7:A1:1131:G:H8	1.74	0.51
7:A2:144:G:H2'	7:A2:145:G:C8	2.46	0.51
7:A2:414:A:OP2	7:A2:428:G:N2	2.44	0.51
7:A2:1185:G:H2'	7:A2:1186:G:C8	2.46	0.51
10:D2:50:ASP:OD1	10:D2:51:TYR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:71:1918:A:O2'	5:71:1920:C:N4	2.44	0.51
5:72:1935:G:H3'	5:72:1962:5MC:HN41	1.75	0.51
5:72:2505:G:OP2	43:p:35:ARG:NH2	2.43	0.51
7:A1:304:U:H2'	7:A1:305:G:C8	2.45	0.51
7:A1:405:U:O4	10:D1:2:ALA:N	2.43	0.51
7:A1:1181:G:H1'	7:A1:1182:G:C8	2.46	0.51
7:A1:1540:U:H4'	27:U1:21:ARG:CZ	2.40	0.51
7:A2:236:A:H2'	7:A2:237:G:C8	2.46	0.51
7:A2:1319:A:O2'	7:A2:1323:G:N7	2.36	0.51
24:R1:39:ILE:H	24:R1:39:ILE:HD12	1.74	0.51
5:72:2059:A:H2'	5:72:2503:2MA:HM22	1.93	0.51
7:A1:578:C:H2'	7:A1:579:A:H8	1.76	0.51
7:A2:519:C:H3'	7:A2:520:A:H8	1.76	0.51
9:C1:34:ASP:OD1	20:N1:66:GLN:NE2	2.44	0.51
9:C2:75:ILE:HG13	9:C2:79:LYS:HE3	1.92	0.51
10:D1:150:LYS:HE2	10:D1:178:MET:HB2	1.92	0.51
24:R1:39:ILE:HG22	24:R1:40:VAL:H	1.76	0.51
24:R1:42:SER:HA	24:R1:45:THR:HG22	1.91	0.51
30:W1:9:A:H5'	30:W1:46:G7M:H8	1.93	0.51
43:p:31:VAL:HG12	43:p:33:ASN:H	1.75	0.51
5:72:307:G:N1	5:72:310:A:OP2	2.43	0.51
7:A1:613:C:H2'	7:A1:614:C:C6	2.46	0.51
7:A1:745:G:H2'	7:A1:746:A:C8	2.45	0.51
7:A1:1064:G:H21	7:A1:1190:G:H8	1.59	0.51
7:A1:1356:G:H2'	7:A1:1357:A:H8	1.75	0.51
7:A1:1464:U:H2'	7:A1:1465:A:H8	1.75	0.51
7:A1:1540:U:C4	28:V2:7:A:H5'	2.46	0.51
7:A2:377:G:H2'	7:A2:378:G:C8	2.46	0.51
7:A2:553:A:H2'	7:A2:554:A:C8	2.45	0.51
7:A2:876:C:P	14:H2:15:ARG:HH12	2.33	0.51
13:G2:107:ALA:HB3	13:G2:123:GLU:OE2	2.11	0.51
28:V2:12:A:H2'	28:V2:13:C:C6	2.45	0.51
40:i2:97:ARG:NH2	40:i2:112:LYS:HD3	2.25	0.51
40:i2:130:VAL:HG12	40:i2:131:SER:H	1.75	0.51
5:72:1859:U:H2'	5:72:1860:G:C8	2.46	0.51
5:72:2523:G:HO2'	5:72:2764:A:HO2'	1.50	0.51
7:A1:1046:A:H2'	7:A1:1047:G:H5'	1.93	0.51
7:A2:1015:G:N2	7:A2:1218:C:O2	2.39	0.51
7:A2:1121:U:H2'	7:A2:1122:U:C6	2.46	0.51
9:C1:11:ARG:NH1	9:C1:178:LEU:HA	2.26	0.51
9:C2:212:ALA:H	16:J2:16:ARG:HH12	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:J2:88:MET:C	16:J2:90:LEU:H	2.19	0.51
17:K1:116:ILE:HD12	17:K1:117:PRO:HD2	1.91	0.51
35:a2:46:VAL:HG22	35:a2:212:VAL:HG13	1.93	0.51
3:4:12:ILE:HB	3:4:31:ASP:HA	1.93	0.51
5:72:1478:G:N2	5:72:1513:U:O2	2.32	0.51
5:72:2277:G:OP2	45:z2:12:ASN:ND2	2.34	0.51
7:A1:129:A:HO2'	7:A1:130:A:H2'	1.75	0.51
7:A1:256:U:H3	7:A1:270:A:H61	1.59	0.51
7:A1:268:U:H2'	7:A1:269:C:C6	2.46	0.51
7:A1:538:G:OP2	18:L1:110:ARG:NH2	2.44	0.51
7:A1:784:A:H2'	7:A1:785:G:C8	2.46	0.51
7:A1:853:C:H2'	7:A1:854:U:H6	1.76	0.51
7:A2:382:A:H2'	7:A2:383:A:H8	1.76	0.51
7:A2:474:G:H2'	7:A2:475:C:C2	2.46	0.51
9:C2:34:ASP:OD2	20:N2:65:ARG:NH2	2.44	0.51
14:H1:95:VAL:HG21	14:H1:102:ALA:HB2	1.92	0.51
24:R2:39:ILE:H	24:R2:39:ILE:HD12	1.76	0.51
1:12:70:GLU:OE1	1:12:74:ARG:NH2	2.44	0.50
5:72:2149:U:H2'	5:72:2150:C:C6	2.46	0.50
5:72:2451:A:N3	29:W:76:A:O2'	2.45	0.50
7:A1:201:G:H1	7:A1:216:U:H3	1.57	0.50
7:A1:602:A:H2'	7:A1:603:U:C6	2.45	0.50
7:A1:709:U:H2'	7:A1:710:G:C8	2.45	0.50
7:A1:1348:U:H2'	7:A1:1349:A:H8	1.76	0.50
7:A2:58:C:H2'	7:A2:59:A:H8	1.76	0.50
7:A2:1162:C:H2'	7:A2:1163:A:H8	1.76	0.50
8:B:82:ASP:OD1	8:B:83:ALA:N	2.44	0.50
8:B2:111:ILE:HG12	8:B2:148:LEU:HD21	1.91	0.50
22:P1:71:VAL:O	22:P1:75:ILE:HG13	2.11	0.50
29:W:37:MIA:N1	29:W:37:MIA:H131	2.26	0.50
33:Y2:58:A:O2'	33:Y2:60:C:OP2	2.25	0.50
44:r2:69:ASP:OD1	44:r2:70:ALA:N	2.44	0.50
5:72:1820:U:C4	36:b2:159:GLY:HA3	2.46	0.50
7:A1:845:A:H61	24:R1:8:ARG:HB2	1.76	0.50
7:A1:1418:A:H3'	7:A1:1419:G:H5''	1.92	0.50
7:A2:451:A:H62	7:A2:481:G:H5'	1.76	0.50
8:B:54:LEU:HB3	8:B:220:THR:HG21	1.94	0.50
17:K2:74:VAL:HG23	17:K2:75:LYS:H	1.76	0.50
23:Q1:82:ALA:O	23:Q1:83:VAL:HG12	2.11	0.50
26:T1:73:ALA:HA	26:T1:76:LYS:HD3	1.92	0.50
35:a2:170:ILE:HB	35:a2:172:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e2:118:SER:HA	37:e2:178:ARG:NE	2.26	0.50
5:72:68:G:N2	5:72:74:A:O5'	2.43	0.50
5:72:299:A:N3	5:72:319:G:O2'	2.40	0.50
7:A1:76:G:H2'	7:A1:77:A:C8	2.46	0.50
7:A1:488:C:O2'	7:A1:489:C:H5'	2.11	0.50
7:A1:666:G:H2'	7:A1:667:G:C8	2.46	0.50
7:A1:769:G:H4'	7:A1:1513:A:H4'	1.93	0.50
7:A2:154:U:H2'	7:A2:155:A:H8	1.77	0.50
7:A2:188:C:H3'	7:A2:189:A:H8	1.76	0.50
7:A2:218:U:H2'	7:A2:219:U:C6	2.46	0.50
8:B2:47:VAL:HB	8:B2:48:PRO:HD3	1.93	0.50
11:E2:57:PRO:HD3	28:V2:62:C:H4'	1.94	0.50
5:72:593:U:H2'	5:72:594:U:C6	2.47	0.50
5:72:1818:U:OP2	36:b2:156:ARG:NE	2.42	0.50
5:72:2142:A:N6	5:72:2148:G:H1	2.09	0.50
7:A1:407:U:H2'	7:A1:408:A:H8	1.76	0.50
7:A1:505:G:H2'	7:A1:506:G:H8	1.77	0.50
7:A1:1126:U:H5	16:J1:7:ARG:HH22	1.59	0.50
7:A2:254:G:H1'	23:Q2:17:MET:HE2	1.92	0.50
7:A2:486:U:H2'	7:A2:487:A:H8	1.76	0.50
7:A2:494:G:H2'	7:A2:496:A:H8	1.76	0.50
32:Y1:28:C:H42	32:Y1:42:G:H1	1.58	0.50
36:b2:91:ILE:HD12	36:b2:103:TYR:CD1	2.47	0.50
7:A1:12:U:H2'	7:A1:13:U:H5''	1.94	0.50
7:A1:138:G:H2'	7:A1:139:A:C8	2.47	0.50
7:A1:578:C:H2'	7:A1:579:A:C8	2.46	0.50
7:A1:1448:C:H2'	7:A1:1449:C:H6	1.75	0.50
7:A1:1522:U:H2'	7:A1:1523:G:C8	2.47	0.50
7:A2:1:A:OP1	7:A2:3:A:N6	2.45	0.50
7:A2:360:G:O2'	7:A2:361:G:H5'	2.12	0.50
14:H1:54:ASP:OD1	14:H1:55:THR:N	2.44	0.50
25:S1:19:VAL:HG21	25:S1:44:MET:HG2	1.93	0.50
36:b2:245:VAL:HG12	36:b2:251:GLN:HA	1.92	0.50
5:72:2162:G:H2'	5:72:2162:G:N3	2.27	0.50
5:72:2165:C:H3'	5:72:2166:U:H5''	1.94	0.50
7:A1:979:C:H1'	7:A1:1317:C:H41	1.77	0.50
7:A1:1271:A:H2'	7:A1:1272:G:C8	2.47	0.50
7:A1:1437:A:H5''	26:T1:29:ARG:HH12	1.76	0.50
7:A2:200:G:H2'	7:A2:201:G:C8	2.46	0.50
7:A2:376:G:H2'	7:A2:377:G:C8	2.45	0.50
7:A2:1166:G:O2'	7:A2:1169:A:N6	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1199:U:H4'	16:J2:56:HIS:CD2	2.47	0.50
10:D2:59:GLN:O	10:D2:63:ARG:NE	2.41	0.50
11:E2:83:HIS:NE2	11:E2:147:MET:HG3	2.27	0.50
12:F2:42:TRP:CZ3	12:F2:103:VAL:HG13	2.45	0.50
13:G1:15:ASP:OD1	13:G1:19:GLY:N	2.45	0.50
24:R1:65:LEU:HB3	24:R1:67:LEU:HD13	1.92	0.50
37:e2:49:LEU:HA	37:e2:52:ASN:HD21	1.77	0.50
45:z2:25:ARG:HH21	45:z2:29:GLU:HB3	1.77	0.50
3:4:15:SER:HA	3:4:21:VAL:HA	1.92	0.50
5:72:746:PSU:O4'	5:72:748:G:N2	2.44	0.50
5:72:1230:A:H2'	5:72:1231:U:C6	2.47	0.50
5:72:2583:G:C6	5:72:2584:U:N3	2.80	0.50
7:A1:102:G:H2'	7:A1:103:U:H6	1.77	0.50
7:A1:335:C:H2'	7:A1:336:A:C8	2.46	0.50
7:A1:643:C:H5''	14:H1:32:LEU:HD21	1.92	0.50
7:A1:1304:G:H1'	7:A1:1334:G:N2	2.27	0.50
7:A2:575:G:O2'	7:A2:821:G:H5'	2.12	0.50
10:D1:87:GLY:HA3	10:D1:197:GLU:OE1	2.12	0.50
26:T1:29:ARG:O	26:T1:32:ILE:HG22	2.10	0.50
28:V2:8:A:H4'	28:V2:9:A:OP1	2.10	0.50
40:i2:94:ILE:HD12	40:i2:122:LEU:HB3	1.93	0.50
5:72:1275:A:OP2	5:72:1646:C:N4	2.43	0.50
5:72:2523:G:O2'	5:72:2764:A:O2'	2.26	0.50
5:72:2554:U:H2'	5:72:2555:U:C6	2.47	0.50
7:A1:162:A:C5	7:A1:163:C:H1'	2.47	0.50
7:A1:310:G:H2'	7:A1:311:C:H6	1.77	0.50
7:A1:1079:G:P	11:E1:138:ARG:HH22	2.34	0.50
7:A2:461:A:H2'	7:A2:462:G:H8	1.77	0.50
7:A2:1115:U:O2	7:A2:1185:G:N2	2.42	0.50
14:H2:22:LYS:O	14:H2:65:TYR:OH	2.24	0.50
28:V2:16:U:H1'	28:V2:17:G:C4	2.46	0.50
44:r2:13:ARG:HG2	44:r2:17:LYS:HZ2	1.77	0.50
7:A1:34:C:H2'	7:A1:35:G:C8	2.47	0.50
7:A1:219:U:H2'	7:A1:220:G:H8	1.76	0.50
7:A1:850:U:N3	7:A1:851:G:N7	2.60	0.50
7:A1:859:G:OP2	7:A1:869:G:N1	2.30	0.50
7:A1:1327:C:H2'	7:A1:1328:C:C6	2.47	0.50
7:A2:453:G:H2'	7:A2:454:G:C8	2.47	0.50
7:A2:766:A:OP2	7:A2:812:G:N2	2.45	0.50
7:A2:1010:U:H3	7:A2:1019:A:N6	2.08	0.50
7:A2:1238:A:H2'	7:A2:1239:A:H5''	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C2:56:VAL:HB	9:C2:67:THR:HB	1.93	0.50
12:F1:36:ILE:HG13	12:F1:64:VAL:HG12	1.94	0.50
31:X2:35:I:H3'	31:X2:36:C:H6	1.77	0.50
6:82:13:G:N7	6:82:70:C:H4'	2.27	0.49
7:A1:918:A:H2'	7:A1:919:A:C8	2.47	0.49
8:B:70:VAL:HG11	8:B:169:GLU:HG2	1.94	0.49
9:C2:22:TRP:HB2	9:C2:59:ARG:HB2	1.94	0.49
15:I2:119:ARG:HH21	15:I2:123:ARG:NH2	2.09	0.49
18:L1:75:GLN:NE2	18:L1:76:GLU:O	2.44	0.49
7:A1:461:A:H2'	7:A1:462:G:C8	2.47	0.49
7:A1:864:A:H2'	7:A1:865:A:C8	2.46	0.49
7:A1:901:A:C5	7:A1:902:G:H1'	2.46	0.49
7:A2:493:A:H2'	7:A2:494:G:O4'	2.12	0.49
7:A2:552:U:H2'	7:A2:553:A:H8	1.76	0.49
7:A2:1236:A:H4'	7:A2:1304:G:H4'	1.95	0.49
7:A2:1402:4OC:O5'	7:A2:1402:4OC:H6	2.11	0.49
8:B2:66:LYS:HD2	8:B2:155:GLY:HA2	1.93	0.49
9:C1:25:ASN:O	9:C1:29:PHE:HB2	2.12	0.49
1:12:17:ASN:OD1	1:12:27:ARG:HD2	2.12	0.49
3:4:7:PRO:HG3	37:e2:58:ALA:O	2.13	0.49
3:4:65:ASN:O	3:4:66:ILE:C	2.55	0.49
5:72:748:G:C4	5:72:750:A:C6	3.00	0.49
5:72:833:A:H2'	5:72:834:G:C8	2.47	0.49
5:72:1681:G:O2'	5:72:1762:A:N3	2.45	0.49
5:72:1759:A:HO2'	5:72:2714:G:HO2'	1.42	0.49
7:A1:157:U:H2'	7:A1:158:G:C8	2.46	0.49
7:A1:252:U:H2'	7:A1:253:A:H8	1.77	0.49
7:A1:666:G:H2'	7:A1:667:G:H8	1.76	0.49
7:A1:1368:A:OP2	15:I1:114:LYS:NZ	2.35	0.49
7:A2:56:U:H2'	7:A2:57:G:H8	1.77	0.49
8:B2:56:GLU:O	8:B2:60:ILE:HG13	2.12	0.49
11:E1:153:VAL:HG21	14:H1:99:LEU:HD23	1.94	0.49
24:R2:55:LEU:O	24:R2:59:ILE:HG12	2.11	0.49
26:T1:54:MET:HE3	26:T1:79:LEU:HD21	1.94	0.49
7:A1:230:G:OP1	22:P1:31:ARG:NH2	2.45	0.49
7:A1:744:C:H2'	7:A1:745:G:H8	1.77	0.49
7:A1:1040:U:H2'	7:A1:1041:G:C8	2.47	0.49
7:A1:1303:C:H2'	7:A1:1304:G:O4'	2.11	0.49
7:A1:1382:C:H2'	7:A1:1383:C:C6	2.48	0.49
7:A2:1245:C:H2'	7:A2:1246:A:C8	2.47	0.49
5:72:158:U:O2'	5:72:159:G:OP1	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:320:A:H2'	7:A1:321:A:C8	2.47	0.49
7:A1:505:G:H5'	7:A1:534:U:H2'	1.93	0.49
7:A1:947:G:H2'	7:A1:948:C:C6	2.47	0.49
7:A2:1188:A:O3'	20:N2:98:LYS:HE2	2.12	0.49
7:A2:1219:A:H2'	7:A2:1220:G:C8	2.47	0.49
10:D1:73:ARG:NH2	10:D1:74:ASN:OD1	2.39	0.49
12:F2:78:PHE:HA	12:F2:84:VAL:HG21	1.94	0.49
15:I1:33:ARG:HH21	15:I1:38:TYR:HA	1.76	0.49
16:J1:2:GLN:HB2	16:J1:5:ARG:HG2	1.95	0.49
16:J2:64:GLN:O	20:N2:99:ALA:N	2.39	0.49
23:Q1:7:THR:HG22	23:Q1:62:ARG:HB3	1.93	0.49
23:Q1:59:VAL:HG12	23:Q1:78:VAL:HG22	1.95	0.49
26:T1:54:MET:HE1	26:T1:76:LYS:HG2	1.95	0.49
5:72:453:A:N3	5:72:457:A:O2'	2.45	0.49
5:72:1801:A:N6	5:72:2201:G:O2'	2.46	0.49
5:72:2124:G:H3'	5:72:2125:G:H8	1.77	0.49
7:A1:57:G:H2'	7:A1:58:C:C6	2.48	0.49
7:A1:722:G:H2'	7:A1:724:G:C8	2.47	0.49
7:A2:1:A:H2'	7:A2:1:A:N3	2.27	0.49
7:A2:137:U:H3	7:A2:226:G:H1	1.61	0.49
7:A2:974:A:OP1	20:N2:69:ARG:NH1	2.39	0.49
8:B:99:GLY:O	8:B:103:ASN:HB2	2.13	0.49
9:C1:42:TYR:O	9:C1:46:GLU:HG2	2.11	0.49
11:E1:44:GLY:HA2	11:E1:76:LEU:HG	1.95	0.49
19:M1:107:ARG:NH2	19:M1:110:LYS:HE3	2.26	0.49
25:S1:39:THR:HA	25:S1:70:LYS:HA	1.93	0.49
5:72:83:A:O2'	5:72:103:A:N6	2.45	0.49
7:A1:1236:A:H2'	7:A1:1237:C:C6	2.48	0.49
7:A1:1291:U:H2'	7:A1:1292:G:H8	1.78	0.49
7:A1:1342:C:H2'	7:A1:1343:G:H8	1.75	0.49
7:A2:202:G:H21	7:A2:466:A:H61	1.61	0.49
7:A2:299:G:H2'	7:A2:300:A:C8	2.47	0.49
7:A2:559:A:H4'	7:A2:560:A:H3'	1.93	0.49
7:A2:1292:G:H2'	7:A2:1293:C:C6	2.47	0.49
7:A2:1308:U:H2'	7:A2:1309:G:C8	2.47	0.49
9:C1:178:LEU:HD23	9:C1:178:LEU:H	1.77	0.49
13:G1:70:ARG:HG2	13:G1:96:ARG:HE	1.78	0.49
13:G1:92:ARG:O	13:G1:96:ARG:HG3	2.13	0.49
20:N2:69:ARG:CZ	20:N2:81:ARG:HH21	2.25	0.49
5:72:383:C:H2'	5:72:385:C:H41	1.76	0.49
5:72:776:G:O2'	5:72:2241:A:OP1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:1071:G:N3	5:72:1089:A:O2'	2.45	0.49
7:A1:900:A:H2'	7:A1:901:A:C8	2.47	0.49
7:A1:1414:U:H2'	7:A1:1415:G:H8	1.78	0.49
7:A1:1449:C:H2'	7:A1:1450:U:O4'	2.12	0.49
7:A2:643:C:H5''	14:H2:32:LEU:HD11	1.94	0.49
7:A2:1228:C:H2'	7:A2:1229:A:C8	2.47	0.49
15:I1:87:LEU:HB3	15:I1:94:LEU:HD12	1.94	0.49
23:Q2:15:ASP:OD2	23:Q2:54:GLY:HA2	2.12	0.49
5:72:682:G:O6	5:72:794:A:N6	2.46	0.49
5:72:2175:C:H2'	5:72:2176:A:C8	2.47	0.49
7:A1:190:A:H3'	7:A1:191:G:H8	1.78	0.49
7:A1:543:U:H2'	7:A1:544:G:H8	1.77	0.49
7:A1:899:C:H2'	7:A1:900:A:O4'	2.13	0.49
7:A1:1002:G:H3'	7:A1:1003:G:H8	1.78	0.49
7:A2:1176:A:H2'	7:A2:1177:G:C8	2.48	0.49
7:A2:1219:A:H2'	7:A2:1220:G:H8	1.78	0.49
12:F2:52:ASN:C	12:F2:54:LEU:H	2.21	0.49
18:L1:28:PRO:HB2	18:L1:29:GLN:OE1	2.13	0.49
24:R2:35:GLU:CD	24:R2:35:GLU:H	2.21	0.49
28:V2:32:U:H1'	28:V2:33:A:C4	2.48	0.49
7:A1:71:A:N1	7:A1:99:C:O2'	2.44	0.49
7:A1:581:G:N1	7:A1:759:A:OP2	2.38	0.49
7:A2:109:A:H2'	7:A2:326:G:N2	2.28	0.49
7:A2:448:A:H3'	7:A2:449:G:H8	1.78	0.49
7:A2:552:U:H2'	7:A2:553:A:C8	2.48	0.49
7:A2:655:A:H2'	7:A2:656:G:C8	2.48	0.49
7:A2:1175:G:H2'	7:A2:1176:A:H8	1.78	0.49
7:A2:1375:A:OP1	13:G2:28:ASN:ND2	2.46	0.49
9:C2:79:LYS:HB3	9:C2:84:VAL:HB	1.95	0.49
9:C2:150:LYS:O	9:C2:201:TRP:N	2.46	0.49
5:72:1709:U:O2'	5:72:2859:G:N3	2.46	0.48
7:A1:311:C:H2'	7:A1:312:C:C6	2.47	0.48
7:A1:1006:G:H2'	7:A1:1007:U:C6	2.48	0.48
7:A1:1372:U:H2'	7:A1:1373:G:O4'	2.13	0.48
7:A1:1409:C:H2'	7:A1:1410:A:H8	1.78	0.48
7:A2:1043:G:H2'	7:A2:1044:A:H8	1.78	0.48
7:A2:1120:C:H2'	7:A2:1121:U:C6	2.48	0.48
8:B:166:ALA:HB2	8:B:185:ALA:HB1	1.94	0.48
19:M1:44:LYS:HB2	19:M1:47:GLU:OE1	2.13	0.48
36:b2:13:ARG:O	36:b2:16:VAL:HG22	2.13	0.48
37:e2:52:ASN:OD1	37:e2:150:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:9:TYR:OH	37:e2:102:ARG:NH2	2.44	0.48
5:72:1212:G:O2'	5:72:1236:G:N1	2.28	0.48
5:72:1357:C:H2'	5:72:1358:G:O4'	2.13	0.48
5:72:1682:G:OP2	5:72:1699:G:N2	2.45	0.48
7:A1:670:G:H2'	7:A1:671:G:C8	2.48	0.48
7:A1:773:G:H2'	7:A1:774:G:O4'	2.13	0.48
7:A1:783:C:H2'	7:A1:784:A:H8	1.78	0.48
7:A1:842:U:H3'	7:A1:843:U:H4'	1.95	0.48
7:A1:986:U:H3	7:A1:1219:A:H61	1.61	0.48
7:A1:1238:A:N7	7:A1:1299:A:N6	2.61	0.48
7:A1:1435:G:H2'	7:A1:1436:U:C6	2.47	0.48
7:A1:1436:U:H2'	7:A1:1437:A:C8	2.49	0.48
7:A2:128:G:H2'	7:A2:129:A:C8	2.48	0.48
7:A2:197:A:H4'	7:A2:198:G:O5'	2.12	0.48
7:A2:1057:G:H2'	7:A2:1058:G:O4'	2.13	0.48
8:B:70:VAL:HB	8:B:163:VAL:HG23	1.95	0.48
9:C1:83:ASP:O	9:C1:87:LEU:HG	2.13	0.48
9:C2:58:GLU:OE2	16:J2:94:ALA:HB1	2.12	0.48
28:V2:60:A:H2'	28:V2:60:A:N3	2.27	0.48
5:72:69:C:O2	5:72:73:A:O2'	2.27	0.48
5:72:1141:U:H4'	5:72:1142:A:O4'	2.13	0.48
7:A1:313:A:H2'	7:A1:314:C:C6	2.48	0.48
7:A1:785:G:H2'	7:A1:786:G:H8	1.78	0.48
7:A1:984:C:H2'	7:A1:985:C:C6	2.48	0.48
7:A1:1087:G:N2	7:A1:1099:G:H1'	2.28	0.48
7:A1:1418:A:H2'	7:A1:1419:G:H5''	1.94	0.48
7:A2:1144:G:N2	7:A2:1146:A:H62	2.11	0.48
7:A2:1149:C:OP2	15:I2:11:ARG:NH2	2.41	0.48
8:B:23:TRP:CH2	8:B:25:PRO:HA	2.48	0.48
8:B:47:VAL:CG1	8:B:48:PRO:HD3	2.41	0.48
9:C2:58:GLU:O	9:C2:65:ARG:N	2.46	0.48
29:W:36:A:H2'	29:W:37:MIA:O4'	2.12	0.48
5:72:587:C:O2	42:o2:33:ARG:NH1	2.47	0.48
5:72:1130:U:O2'	5:72:1131:G:P	2.70	0.48
5:72:1664:A:H61	5:72:1996:C:N4	2.11	0.48
7:A1:1060:U:H3	7:A1:1197:A:H61	1.62	0.48
7:A1:1397:C:H41	28:V2:27:A:H2'	1.78	0.48
7:A1:1410:A:H2'	7:A1:1411:C:C6	2.49	0.48
7:A1:1419:G:H2'	7:A1:1420:U:C6	2.48	0.48
7:A1:1525:G:H2'	7:A1:1526:G:H8	1.78	0.48
7:A2:94:G:H4'	7:A2:95:C:H5'	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:235:C:H2'	7:A2:236:A:H8	1.78	0.48
8:B:70:VAL:HA	8:B:92:VAL:HB	1.95	0.48
11:E1:83:HIS:NE2	11:E1:147:MET:HG3	2.29	0.48
11:E2:153:VAL:HG21	14:H2:99:LEU:HD23	1.95	0.48
28:V2:35:A:H2'	28:V2:36:A:C8	2.48	0.48
2:32:12:ALA:HB2	2:32:53:MET:HE1	1.95	0.48
5:72:554:U:H2'	5:72:555:G:O4'	2.13	0.48
7:A1:471:U:H2'	7:A1:472:U:C6	2.49	0.48
7:A1:513:C:H2'	7:A1:514:C:C6	2.47	0.48
7:A1:718:A:C8	17:K1:118:HIS:HB3	2.49	0.48
7:A1:1304:G:H1'	7:A1:1334:G:H22	1.78	0.48
7:A2:151:A:H2'	7:A2:152:A:H8	1.78	0.48
7:A2:494:G:H2'	7:A2:496:A:C8	2.49	0.48
7:A2:1287:A:H5''	7:A2:1287:A:H8	1.79	0.48
8:B:60:ILE:HG12	8:B:63:ARG:HH12	1.77	0.48
11:E1:136:VAL:O	11:E1:140:THR:HG23	2.13	0.48
11:E2:136:VAL:O	11:E2:140:THR:HG23	2.12	0.48
15:I1:33:ARG:NH2	15:I1:38:TYR:HA	2.28	0.48
15:I2:116:VAL:HG23	16:J2:62:ARG:HH11	1.78	0.48
19:M2:44:LYS:HB2	19:M2:47:GLU:OE1	2.14	0.48
23:Q2:46:VAL:HG11	23:Q2:61:ILE:HD12	1.95	0.48
3:4:56:ARG:HD2	19:M2:79:ARG:NH1	2.29	0.48
5:72:1808:A:H3'	5:72:1809:A:C8	2.49	0.48
5:72:2394:C:H5''	42:o2:63:LYS:HD3	1.95	0.48
7:A1:436:C:H2'	7:A1:437:U:C6	2.49	0.48
7:A1:457:G:H5'	7:A1:458:U:OP2	2.13	0.48
7:A1:1404:C:H2'	7:A1:1405:G:H8	1.78	0.48
7:A1:1415:G:H1	7:A1:1485:U:H3	1.62	0.48
7:A2:88:U:O2'	7:A2:89:U:O5'	2.28	0.48
7:A2:323:U:H2'	7:A2:324:G:O4'	2.14	0.48
7:A2:1317:C:O5'	20:N2:28:LYS:NZ	2.44	0.48
9:C1:77:ILE:HA	9:C1:84:VAL:HG23	1.93	0.48
9:C2:82:GLU:HG2	9:C2:85:GLU:HB3	1.94	0.48
10:D2:60:LYS:O	10:D2:64:ILE:HD12	2.13	0.48
11:E1:83:HIS:ND1	14:H1:96:MET:HE1	2.29	0.48
20:N1:79:LEU:HB3	20:N1:83:LYS:HB3	1.95	0.48
20:N2:31:ILE:O	20:N2:41:ARG:NH1	2.47	0.48
31:X2:35:I:H3'	31:X2:36:C:C6	2.49	0.48
1:12:55:GLY:O	1:12:59:ILE:HG12	2.13	0.48
3:4:66:ILE:C	3:4:67:PRO:O	2.55	0.48
5:72:2140:G:H2'	5:72:2141:G:O4'	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:2285:C:OP2	38:g2:6:ARG:NH2	2.46	0.48
6:82:33:G:H1	6:82:49:C:H42	1.60	0.48
7:A1:599:C:H2'	7:A1:600:A:C8	2.49	0.48
7:A1:1409:C:H2'	7:A1:1410:A:C8	2.49	0.48
7:A1:1411:C:H2'	7:A1:1412:C:C6	2.49	0.48
7:A1:1456:A:H2'	7:A1:1457:G:O4'	2.13	0.48
7:A2:142:G:H3'	7:A2:143:A:H8	1.79	0.48
7:A2:461:A:H2'	7:A2:462:G:C8	2.48	0.48
7:A2:1250:A:H2'	7:A2:1251:A:C8	2.49	0.48
7:A2:1268:G:H2'	7:A2:1269:A:C8	2.47	0.48
8:B2:186:ILE:HG21	8:B2:213:TYR:CE2	2.48	0.48
13:G1:32:VAL:HG22	13:G1:33:ASP:OD2	2.14	0.48
29:W:10:G:H2'	29:W:11:U:C6	2.49	0.48
5:72:1105:U:H2'	5:72:1106:G:H8	1.77	0.48
5:72:1329:U:H5''	5:72:1330:C:H5	1.78	0.48
7:A1:1218:C:H2'	7:A1:1219:A:C8	2.48	0.48
7:A1:1264:U:H2'	7:A1:1265:C:C6	2.48	0.48
7:A1:1512:U:H2'	7:A1:1513:A:H8	1.79	0.48
7:A1:1532:U:H2'	7:A1:1533:C:O4'	2.13	0.48
7:A2:831:A:H2'	7:A2:832:G:H8	1.78	0.48
7:A2:1302:C:C6	19:M2:17:ILE:HG13	2.48	0.48
7:A2:1328:C:H2'	7:A2:1329:A:C8	2.49	0.48
8:B:114:LEU:HD13	8:B:148:LEU:HD23	1.96	0.48
9:C1:79:LYS:HD2	9:C1:80:LYS:HZ3	1.77	0.48
15:I2:60:LYS:HG2	15:I2:61:LEU:HD12	1.95	0.48
17:K1:22:HIS:HA	17:K1:85:MET:HB2	1.96	0.48
23:Q2:56:GLY:O	23:Q2:82:ALA:HB2	2.14	0.48
5:72:221:A:N1	5:72:265:A:O2'	2.42	0.48
5:72:962:G:H5'	5:72:962:G:H8	1.79	0.48
5:72:1504:A:H2'	5:72:1505:A:C8	2.49	0.48
5:72:1915:3TD:O5'	5:72:1915:3TD:H6	2.14	0.48
5:72:2039:U:H2'	5:72:2040:G:C8	2.48	0.48
5:72:2470:G:OP1	39:h2:55:ARG:NH2	2.37	0.48
7:A1:539:A:OP2	18:L1:112:GLN:NE2	2.47	0.48
7:A1:691:G:H2'	7:A1:692:U:C6	2.48	0.48
7:A1:708:C:H2'	7:A1:709:U:C6	2.49	0.48
7:A1:1060:U:H2'	7:A1:1061:G:H8	1.78	0.48
7:A1:1268:G:H21	7:A1:1326:U:H1'	1.78	0.48
7:A2:105:G:H2'	7:A2:106:C:C6	2.49	0.48
7:A2:337:G:H2'	7:A2:338:A:C8	2.49	0.48
7:A2:537:G:O2'	7:A2:538:G:OP1	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D2:147:GLU:HA	10:D2:150:LYS:HG2	1.94	0.48
12:F1:14:GLN:HB3	12:F1:17:GLN:NE2	2.29	0.48
13:G1:31:MET:SD	13:G1:36:LYS:HG2	2.54	0.48
13:G2:97:ASN:O	13:G2:101:MET:HG3	2.13	0.48
14:H2:10:MET:HA	14:H2:27:MET:HE1	1.95	0.48
15:I1:26:GLY:N	15:I1:62:ASP:OD1	2.46	0.48
15:I2:87:LEU:HB3	15:I2:94:LEU:HD12	1.95	0.48
23:Q2:57:ASP:OD1	23:Q2:82:ALA:N	2.43	0.48
5:72:1789:A:OP1	36:b2:221:ARG:HG3	2.14	0.48
5:72:2474:U:OP2	5:72:2475:C:N4	2.39	0.48
7:A1:1279:G:H4'	7:A1:1281:C:H5	1.77	0.48
7:A2:399:G:H2'	7:A2:400:C:C6	2.49	0.48
7:A2:1084:G:O2'	7:A2:1103:C:N4	2.41	0.48
9:C1:20:SER:HB3	9:C1:22:TRP:NE1	2.29	0.48
14:H2:103:VAL:HG12	14:H2:126:ILE:HD13	1.96	0.48
23:Q1:77:ARG:HH12	23:Q1:79:VAL:HG22	1.78	0.48
3:4:58:ASP:O	3:4:62:LYS:HG2	2.14	0.47
5:72:1019:U:OP1	5:72:1035:U:O2'	2.22	0.47
5:72:1055:G:O2'	5:72:1084:A:N6	2.46	0.47
7:A1:1074:G:H4'	8:B:102:THR:HB	1.96	0.47
7:A1:1177:G:H2'	7:A1:1178:G:O4'	2.14	0.47
7:A1:1382:C:H1'	13:G1:79:ARG:HD2	1.95	0.47
7:A2:309:A:H2'	7:A2:310:G:H8	1.78	0.47
7:A2:421:U:C3'	7:A2:422:C:H5'	2.44	0.47
13:G2:78:ARG:HA	13:G2:78:ARG:HD3	1.68	0.47
19:M1:79:ARG:HH11	25:S1:65:GLU:HB3	1.79	0.47
33:Y2:10:G:O6	33:Y2:45:G:N2	2.47	0.47
7:A1:72:A:H2'	7:A1:73:C:C6	2.49	0.47
7:A1:88:U:O2'	7:A1:89:U:O5'	2.31	0.47
7:A1:640:A:H2'	7:A1:641:U:O4'	2.14	0.47
7:A1:1225:A:H2'	7:A1:1225:A:N3	2.29	0.47
7:A1:1346:A:O2'	7:A1:1347:G:H4'	2.14	0.47
7:A2:107:G:OP1	7:A2:325:A:N6	2.43	0.47
7:A2:459:A:H2'	7:A2:460:A:O4'	2.13	0.47
7:A2:1086:U:H3	7:A2:1099:G:H22	1.61	0.47
9:C1:29:PHE:HZ	20:N1:94:PRO:HD2	1.79	0.47
9:C1:184:TYR:HE1	9:C1:199:LYS:HB3	1.78	0.47
36:b2:35:GLU:OE1	36:b2:35:GLU:N	2.47	0.47
41:I2:22:MET:HG3	41:I2:28:ARG:HG2	1.96	0.47
2:32:10:ARG:HA	2:32:10:ARG:HD3	1.66	0.47
5:72:245:G:O2'	5:72:384:A:N1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:748:G:C8	5:72:750:A:C5	3.02	0.47
5:72:793:A:OP2	5:72:2071:A:O2'	2.28	0.47
5:72:1818:U:H5	36:b2:156:ARG:HH22	1.62	0.47
5:72:2357:G:N2	5:72:2360:G:OP2	2.41	0.47
6:82:95:U:H2'	6:82:96:G:H8	1.79	0.47
7:A1:33:A:H2'	7:A1:34:C:C6	2.48	0.47
7:A1:210:C:H1'	7:A1:211:G:C2	2.49	0.47
7:A2:1073:U:O2	8:B2:103:ASN:ND2	2.47	0.47
8:B2:114:LEU:HD12	8:B2:144:LEU:HB3	1.95	0.47
16:J2:37:ARG:HB2	16:J2:75:ASP:HB2	1.95	0.47
21:O1:24:SER:O	21:O1:28:GLN:HG2	2.14	0.47
2:32:38:GLU:HG2	2:32:40:THR:HG23	1.96	0.47
3:4:45:THR:HG22	3:4:47:LYS:HG2	1.95	0.47
5:72:1:G:H2'	5:72:2:G:H8	1.79	0.47
5:72:1056:G:H4'	5:72:1086:A:C8	2.49	0.47
7:A1:147:G:H2'	7:A1:148:G:C8	2.50	0.47
7:A1:669:G:H2'	7:A1:670:G:C8	2.50	0.47
7:A2:1312:G:H2'	7:A2:1313:U:C6	2.49	0.47
8:B:102:THR:C	8:B:104:TRP:H	2.22	0.47
8:B2:169:GLU:N	8:B2:169:GLU:OE1	2.48	0.47
14:H1:18:GLN:NE2	14:H1:72:VAL:H	2.12	0.47
31:X2:8:4SU:O2'	31:X2:22:A:N1	2.32	0.47
5:72:779:U:OP1	36:b2:49:ILE:HD12	2.14	0.47
5:72:1043:C:O2'	5:72:1048:A:O2'	2.29	0.47
6:82:95:U:H2'	6:82:96:G:C8	2.50	0.47
7:A1:595:A:H61	7:A1:641:U:H2'	1.79	0.47
7:A1:988:G:H4'	7:A1:1014:A:H61	1.80	0.47
7:A2:19:A:H2'	7:A2:20:U:C6	2.49	0.47
7:A2:246:A:N1	7:A2:278:G:O2'	2.37	0.47
7:A2:824:G:H2'	7:A2:825:A:C8	2.50	0.47
7:A2:946:A:H2'	7:A2:947:G:H8	1.80	0.47
7:A2:1500:A:H5''	7:A2:1508:A:H5''	1.97	0.47
9:C1:83:ASP:O	9:C1:86:LYS:HG2	2.15	0.47
12:F1:11:HIS:ND1	12:F1:13:ASP:OD1	2.48	0.47
13:G2:51:ALA:O	13:G2:55:GLY:N	2.44	0.47
18:L1:63:VAL:HG21	18:L1:95:TYR:CE2	2.50	0.47
20:N1:86:GLU:O	20:N1:90:ARG:HG3	2.14	0.47
5:72:878:A:H3'	5:72:879:G:H8	1.80	0.47
5:72:2267:A:H5''	5:72:2268:A:H5'	1.97	0.47
5:72:2687:U:H2'	5:72:2688:G:O4'	2.13	0.47
7:A1:173:U:H5''	7:A1:197:A:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:643:C:H2'	7:A1:644:U:C6	2.49	0.47
7:A1:1202:U:H2'	7:A1:1203:C:O4'	2.15	0.47
7:A1:1430:A:H2'	7:A1:1431:A:O4'	2.15	0.47
7:A1:1451:U:H3'	7:A1:1452:C:H6	1.80	0.47
7:A2:428:G:H5'	10:D2:10:LYS:HE3	1.97	0.47
7:A2:1230:C:H41	19:M2:104:THR:HG21	1.79	0.47
7:A2:1402:4OC:HM23	7:A2:1402:4OC:H1'	1.57	0.47
8:B:68:LEU:HD12	8:B:69:PHE:H	1.79	0.47
9:C2:70:THR:O	9:C2:106:VAL:N	2.46	0.47
12:F1:9:MET:HE2	12:F1:86:ARG:HB3	1.97	0.47
14:H1:18:GLN:HB3	14:H1:70:ALA:HB1	1.97	0.47
20:N1:4:GLN:OE1	20:N1:4:GLN:N	2.42	0.47
25:S2:31:LEU:HB2	25:S2:49:ILE:HG13	1.96	0.47
38:g2:11:LEU:HD23	38:g2:51:GLU:HA	1.96	0.47
5:71:1916:A:H2'	5:71:1917:U:O4'	2.15	0.47
5:72:191:A:H2'	5:72:192:C:C6	2.49	0.47
5:72:411:G:OP2	5:72:2406:A:O2'	2.31	0.47
5:72:500:G:N1	5:72:503:A:OP2	2.45	0.47
5:72:586:A:N1	5:72:809:G:O2'	2.42	0.47
5:72:717:C:H2'	5:72:718:A:O4'	2.14	0.47
5:72:1416:G:HO2'	5:72:1417:C:P	2.37	0.47
5:72:1432:G:H2'	5:72:1433:A:C8	2.50	0.47
5:72:1936:A:OP2	5:72:1962:5MC:N4	2.42	0.47
5:72:2109:U:H2'	5:72:2110:G:C8	2.49	0.47
5:72:2394:C:N3	31:X2:77:A:O2'	2.44	0.47
7:A1:220:G:H2'	7:A1:221:C:H6	1.79	0.47
7:A1:501:C:H2'	7:A1:502:A:C8	2.49	0.47
7:A1:735:C:H2'	7:A1:736:C:C6	2.49	0.47
7:A1:1036:A:H3'	7:A1:1037:C:C6	2.49	0.47
7:A1:1111:A:N1	9:C1:177:THR:OG1	2.43	0.47
7:A1:1288:A:H2'	7:A1:1289:A:H8	1.80	0.47
7:A1:1402:4OC:HM23	7:A1:1402:4OC:H1'	1.57	0.47
7:A1:1539:C:N4	28:V2:10:G:H1	2.12	0.47
7:A2:41:G:H2'	7:A2:42:G:H8	1.80	0.47
7:A2:123:U:H5''	7:A2:311:C:O2'	2.15	0.47
7:A2:553:A:H2'	7:A2:554:A:H8	1.80	0.47
7:A2:1187:G:N3	20:N2:100:SER:OG	2.40	0.47
7:A2:1403:C:N4	28:V2:53:G:OP1	2.48	0.47
7:A2:1535:C:H5'	24:R2:3:ARG:HE	1.79	0.47
8:B:90:PHE:CD2	8:B:154:MET:HG2	2.50	0.47
9:C2:19:ASN:ND2	20:N2:90:ARG:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:D1:10:LYS:HG3	10:D1:38:PRO:HG2	1.95	0.47
11:E2:156:LYS:HE2	14:H2:71:VAL:HA	1.96	0.47
14:H2:88:ARG:NH2	14:H2:91:GLU:OE2	2.48	0.47
16:J2:28:THR:O	16:J2:32:THR:HG22	2.15	0.47
17:K1:17:SER:HA	17:K1:79:ILE:HA	1.95	0.47
19:M1:42:ASP:OD1	19:M1:42:ASP:N	2.47	0.47
20:N1:54:ASP:HA	20:N1:59:ARG:HG2	1.96	0.47
23:Q2:11:ARG:O	23:Q2:12:VAL:C	2.57	0.47
24:R2:7:ARG:HE	24:R2:9:LYS:HE2	1.80	0.47
27:U1:34:ARG:HD3	27:U1:35:ARG:NH1	2.29	0.47
27:U2:13:ASP:OD1	27:U2:14:VAL:N	2.47	0.47
29:W:23:A:H2'	29:W:24:G:C8	2.49	0.47
31:X2:15:G:N2	31:X2:49:C:O2	2.47	0.47
40:i2:135:HIS:CG	40:i2:136:SER:H	2.33	0.47
44:r2:82:ALA:HB3	44:r2:115:LEU:HD21	1.97	0.47
5:72:569:U:O2'	5:72:983:A:N1	2.47	0.47
5:72:1570:A:H2'	5:72:1571:A:C8	2.50	0.47
5:72:1753:G:N2	5:72:1756:G:O5'	2.45	0.47
5:72:1971:U:OP2	5:72:1971:U:H4'	2.14	0.47
7:A1:634:C:H2'	7:A1:635:A:C8	2.49	0.47
7:A2:178:C:H2'	7:A2:179:A:H8	1.80	0.47
7:A2:502:A:H5'	18:L2:113:ALA:HA	1.97	0.47
7:A2:1140:C:O2'	7:A2:1141:C:H6	1.98	0.47
7:A2:1320:C:OP1	25:S2:70:LYS:NZ	2.32	0.47
8:B:112:LYS:O	8:B:115:LYS:HG2	2.15	0.47
9:C2:17:PRO:HA	9:C2:211:MET:HE1	1.97	0.47
9:C2:167:TRP:HZ3	9:C2:169:ARG:HG2	1.79	0.47
13:G2:92:ARG:O	13:G2:96:ARG:HG3	2.15	0.47
17:K1:113:VAL:HG12	17:K1:113:VAL:O	2.15	0.47
24:R2:57:ARG:HD3	24:R2:61:ARG:HH22	1.80	0.47
30:W1:37:MIA:H112	30:W1:38:A:H1'	1.96	0.47
1:12:74:ARG:HD2	1:12:76:GLU:HB2	1.96	0.47
5:72:2604:PSU:H2'	5:72:2605:PSU:C6	2.49	0.47
7:A1:412:A:O2'	7:A1:413:G:H5'	2.15	0.47
7:A1:671:G:H2'	7:A1:672:U:H5'	1.96	0.47
7:A1:1147:C:H2'	7:A1:1148:U:H6	1.79	0.47
7:A1:1478:U:H2'	7:A1:1479:C:C6	2.50	0.47
7:A2:263:A:H2'	7:A2:264:C:C6	2.50	0.47
7:A2:354:G:O2'	7:A2:389:A:OP1	2.27	0.47
7:A2:375:U:H3	7:A2:389:A:H61	1.62	0.47
7:A2:666:G:H5'	7:A2:726:C:H1'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1095:U:H2'	7:A2:1096:C:C6	2.49	0.47
7:A2:1477:U:H2'	7:A2:1478:U:C6	2.49	0.47
8:B2:102:THR:HG23	8:B2:175:GLU:HB3	1.97	0.47
11:E2:83:HIS:CE1	14:H2:96:MET:HE1	2.50	0.47
15:I2:7:TYR:CG	15:I2:8:GLY:N	2.83	0.47
28:V2:54:G:N2	33:Y2:36:C:O2	2.41	0.47
40:i2:42:LYS:O	40:i2:45:GLU:HG2	2.14	0.47
5:72:1223:G:N2	5:72:1226:A:OP2	2.42	0.47
7:A1:382:A:H2'	7:A1:383:A:C8	2.49	0.47
7:A1:461:A:H2'	7:A1:462:G:H8	1.80	0.47
7:A1:505:G:H2'	7:A1:506:G:C8	2.49	0.47
7:A1:688:G:H2'	7:A1:689:C:O4'	2.15	0.47
7:A1:996:A:H2'	7:A1:997:U:C6	2.50	0.47
7:A1:1216:A:O2'	20:N1:9:ARG:NH2	2.48	0.47
7:A1:1512:U:H3	7:A1:1523:G:H1	1.61	0.47
7:A2:486:U:H2'	7:A2:487:A:C8	2.50	0.47
7:A2:1220:G:P	20:N2:53:ARG:HH12	2.37	0.47
7:A2:1328:C:H2'	7:A2:1329:A:H8	1.80	0.47
8:B:68:LEU:HD22	8:B:154:MET:HE1	1.96	0.47
15:I1:42:GLU:O	15:I1:46:MET:HG2	2.15	0.47
15:I1:118:LEU:HB3	15:I1:123:ARG:O	2.14	0.47
16:J1:4:GLN:HB2	16:J1:79:PRO:HG3	1.96	0.47
17:K1:64:GLN:HG3	17:K1:99:ALA:HB2	1.96	0.47
18:L1:63:VAL:HG21	18:L1:95:TYR:HE2	1.79	0.47
31:X2:9:A:O2'	31:X2:46:G:N3	2.44	0.47
5:72:784:G:H5'	5:72:785:G:OP1	2.15	0.46
7:A1:224:U:H2'	7:A1:225:C:C6	2.50	0.46
7:A1:390:U:H2'	7:A1:391:G:H8	1.80	0.46
7:A1:543:U:H2'	7:A1:544:G:C8	2.51	0.46
7:A1:844:G:H3'	7:A1:845:A:H3'	1.95	0.46
7:A1:912:C:H2'	7:A1:913:A:C8	2.50	0.46
7:A1:1326:U:H2'	7:A1:1327:C:H6	1.79	0.46
7:A2:161:A:H2'	7:A2:162:A:C8	2.51	0.46
7:A2:206:C:OP2	7:A2:207:C:N4	2.48	0.46
7:A2:1245:C:H2'	7:A2:1246:A:H8	1.80	0.46
10:D1:99:ASP:OD1	10:D1:100:ASN:N	2.48	0.46
12:F2:15:SER:HA	12:F2:18:VAL:HG23	1.97	0.46
19:M2:7:ILE:HB	37:e2:112:ARG:HH12	1.80	0.46
20:N1:98:LYS:HE2	20:N1:98:LYS:HB2	1.74	0.46
26:T1:51:PHE:O	26:T1:54:MET:HG3	2.14	0.46
31:X2:16:C:H2'	31:X2:60:A:H61	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:2127:G:N2	5:72:2162:G:O4'	2.41	0.46
5:72:2291:U:H2'	5:72:2292:U:C6	2.50	0.46
7:A1:109:A:H5'	7:A1:110:C:H5	1.79	0.46
7:A1:1382:C:H2'	7:A1:1383:C:H6	1.80	0.46
7:A2:1149:C:P	15:I2:11:ARG:HH21	2.38	0.46
7:A2:1346:A:P	15:I2:122:ARG:HH12	2.38	0.46
7:A2:1384:C:H2'	7:A2:1385:G:C8	2.50	0.46
8:B:132:LYS:O	8:B:136:MET:HG2	2.15	0.46
8:B:137:ARG:NH2	8:B:140:GLU:OE2	2.48	0.46
9:C1:207:ILE:HG22	9:C1:210:GLY:HA3	1.96	0.46
12:F2:35:LYS:HD2	12:F2:37:HIS:HB3	1.97	0.46
31:X2:16:C:H2'	31:X2:60:A:N6	2.31	0.46
5:72:1580:A:HO2'	5:72:1581:G:P	2.37	0.46
5:72:1798:U:O2'	5:72:1802:A:N3	2.46	0.46
5:72:2175:C:H5''	35:a2:8:MET:HE3	1.96	0.46
5:72:2370:G:H4'	38:g2:44:ARG:NH2	2.31	0.46
6:82:66:A:N6	6:82:107:G:H2'	2.29	0.46
7:A1:570:G:O6	7:A1:865:A:N6	2.48	0.46
7:A1:837:U:H2'	7:A1:838:G:C8	2.49	0.46
7:A1:886:G:H2'	7:A1:887:G:O4'	2.16	0.46
7:A1:995:C:H2'	7:A1:996:A:H5'	1.97	0.46
7:A1:1387:G:H2'	7:A1:1388:C:C6	2.50	0.46
7:A2:501:C:O2	7:A2:549:C:O2'	2.33	0.46
7:A2:1327:C:H2'	7:A2:1328:C:C6	2.49	0.46
7:A2:1530:G:H2'	7:A2:1531:A:C8	2.50	0.46
9:C1:38:LYS:O	9:C1:41:GLN:HG2	2.15	0.46
10:D1:60:LYS:O	10:D1:64:ILE:HG13	2.15	0.46
11:E2:31:PHE:H	28:V2:60:A:N6	2.14	0.46
21:O1:36:ILE:HD11	21:O1:59:MET:HG3	1.97	0.46
23:Q1:30:LYS:HE3	23:Q1:35:GLY:HA2	1.96	0.46
27:U2:17:ARG:NH2	28:V2:38:A:N3	2.63	0.46
29:W:23:A:H2'	29:W:24:G:H8	1.80	0.46
31:X2:19:G:N2	31:X2:59:A:OP2	2.47	0.46
39:h2:13:HIS:O	39:h2:71:LYS:NZ	2.48	0.46
5:72:241:A:N1	5:72:255:A:H5''	2.30	0.46
5:72:1417:C:HO2'	5:72:1587:G:HO2'	1.59	0.46
5:72:1909:C:H2'	5:72:1910:G:H8	1.80	0.46
5:72:2105:U:H2'	5:72:2106:U:C6	2.50	0.46
7:A1:71:A:H2'	7:A1:72:A:C8	2.50	0.46
7:A1:202:G:H1	7:A1:215:C:N4	2.13	0.46
7:A1:728:A:H2'	7:A1:729:A:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:994:A:N6	7:A1:1215:G:O2'	2.48	0.46
7:A1:1023:U:H2'	7:A1:1024:G:C8	2.50	0.46
7:A1:1252:A:H2'	7:A1:1253:G:O4'	2.15	0.46
7:A2:21:G:H2'	7:A2:22:G:H8	1.79	0.46
7:A2:997:U:H2'	7:A2:998:C:C6	2.50	0.46
7:A2:1114:C:H2'	7:A2:1115:U:H6	1.81	0.46
7:A2:1239:A:H61	7:A2:1296:C:H2'	1.80	0.46
8:B:52:GLU:O	8:B:56:GLU:HG2	2.14	0.46
8:B2:9:MET:HB2	8:B2:43:LEU:HD21	1.97	0.46
10:D1:168:PRO:HB3	10:D1:170:TRP:CH2	2.51	0.46
12:F1:44:ARG:HA	12:F1:57:ALA:O	2.13	0.46
14:H2:95:VAL:HG21	14:H2:102:ALA:HB2	1.97	0.46
25:S2:28:LYS:HA	25:S2:28:LYS:HE3	1.98	0.46
33:Y2:9:A:N7	33:Y2:23:A:N6	2.63	0.46
35:a2:20:GLN:HA	35:a2:223:ALA:HB3	1.97	0.46
5:72:782:A:C2	36:b2:225:MET:HG2	2.50	0.46
5:72:1343:G:H1'	5:72:1597:A:C4	2.50	0.46
5:72:1597:A:H5''	5:72:1598:A:H5'	1.96	0.46
5:72:2047:C:O2'	5:72:2823:A:N1	2.46	0.46
5:72:2482:A:H4'	33:Y2:64:C:OP1	2.15	0.46
7:A1:1396:A:H2	11:E1:24:THR:HG21	1.79	0.46
7:A2:43:C:H2'	7:A2:44:A:H8	1.79	0.46
7:A2:1060:U:H2'	7:A2:1061:G:C8	2.49	0.46
7:A2:1338:G:H2'	7:A2:1339:A:C8	2.50	0.46
8:B:38:VAL:CG1	8:B:39:HIS:H	2.24	0.46
8:B2:24:ASN:ND2	8:B2:192:ASP:HA	2.29	0.46
10:D2:87:GLY:HA3	10:D2:197:GLU:OE1	2.16	0.46
16:J1:31:ARG:NH2	16:J1:32:THR:OG1	2.49	0.46
32:Y1:39:G:H2'	32:Y1:40:G:C8	2.50	0.46
36:b2:161:TYR:HB3	36:b2:194:GLU:HG3	1.97	0.46
5:72:1209:U:O2'	5:72:1237:A:N1	2.42	0.46
5:72:1210:G:H4'	5:72:1211:C:H5''	1.98	0.46
7:A1:263:A:H2'	7:A1:264:C:C6	2.50	0.46
7:A1:715:A:H2'	7:A1:716:A:H8	1.81	0.46
7:A1:950:U:OP2	19:M1:101:ARG:NE	2.39	0.46
7:A1:1007:U:H2'	7:A1:1008:U:C6	2.50	0.46
7:A1:1135:U:O4	7:A1:1138:G:N2	2.48	0.46
7:A2:320:A:H2'	7:A2:321:A:C8	2.50	0.46
7:A2:922:G:H1'	11:E2:24:THR:HG23	1.96	0.46
7:A2:998:C:H42	7:A2:1042:A:H61	1.62	0.46
7:A2:1043:G:H2'	7:A2:1044:A:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1380:U:O2	7:A2:1382:C:N4	2.48	0.46
8:B:24:ASN:N	8:B:189:THR:O	2.43	0.46
9:C1:29:PHE:CZ	20:N1:94:PRO:HD2	2.50	0.46
9:C2:121:THR:HG22	9:C2:189:ALA:HB2	1.97	0.46
12:F2:9:MET:HE1	12:F2:47:LEU:HD11	1.98	0.46
15:I2:60:LYS:HE3	15:I2:61:LEU:HD11	1.96	0.46
24:R2:57:ARG:HG3	24:R2:61:ARG:HH12	1.80	0.46
5:72:296:U:H2'	5:72:297:G:C8	2.51	0.46
5:72:598:U:H2'	5:72:599:A:C8	2.50	0.46
5:72:1786:A:C4	5:72:1938:A:C6	3.04	0.46
5:72:2150:C:H5'	5:72:2172:U:O2	2.16	0.46
5:72:2449:H2U:H4'	5:72:2450:A:OP1	2.16	0.46
7:A1:67:C:H2'	7:A1:68:G:H8	1.80	0.46
7:A1:255:G:H2'	7:A1:256:U:C6	2.51	0.46
7:A1:409:U:OP1	10:D1:22:LYS:HG3	2.15	0.46
7:A1:465:A:H2'	7:A1:466:A:C8	2.51	0.46
7:A1:682:G:H2'	7:A1:683:G:C8	2.50	0.46
7:A1:1013:G:N2	7:A1:1015:G:H3'	2.31	0.46
7:A1:1016:A:H3'	7:A1:1017:U:H6	1.80	0.46
7:A1:1025:U:O3'	7:A1:1026:G:H8	1.98	0.46
7:A1:1486:G:H2'	7:A1:1487:G:C8	2.51	0.46
7:A2:372:C:H4'	7:A2:373:A:OP1	2.14	0.46
7:A2:413:G:N2	7:A2:428:G:O2'	2.49	0.46
7:A2:908:A:H2'	7:A2:909:A:C8	2.51	0.46
7:A2:953:G:H2'	7:A2:954:G:O4'	2.15	0.46
7:A2:1478:U:H2'	7:A2:1479:C:C6	2.51	0.46
9:C2:186:THR:HG22	9:C2:199:LYS:HG2	1.97	0.46
10:D1:202:GLU:HB2	11:E1:112:ARG:HH22	1.80	0.46
16:J2:97:ASP:OD1	16:J2:98:VAL:N	2.47	0.46
19:M1:27:LYS:HG3	19:M1:31:LYS:NZ	2.31	0.46
20:N1:16:LEU:HD23	20:N1:54:ASP:HB2	1.98	0.46
29:W:51:G:H1	29:W:63:C:H42	1.63	0.46
36:b2:205:LEU:HD13	36:b2:210:ALA:HB3	1.97	0.46
2:32:10:ARG:NH2	5:72:1000:A:O3'	2.44	0.46
5:72:221:A:O2'	5:72:266:G:N7	2.49	0.46
5:72:1475:G:H4'	5:72:1476:U:H5'	1.96	0.46
5:72:2391:G:C6	5:72:2427:C:H1'	2.50	0.46
5:72:2584:U:O5'	5:72:2584:U:H6	1.99	0.46
7:A1:125:U:H2'	7:A1:126:G:C8	2.51	0.46
7:A1:413:G:H1'	7:A1:428:G:H21	1.81	0.46
7:A1:634:C:H2'	7:A1:635:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:668:G:H2'	7:A1:669:G:H8	1.81	0.46
7:A1:979:C:H2'	7:A1:980:C:H5'	1.97	0.46
7:A1:1113:C:H2'	7:A1:1114:C:C6	2.50	0.46
7:A2:222:C:H2'	7:A2:223:A:H8	1.80	0.46
7:A2:369:G:H2'	7:A2:370:C:C6	2.51	0.46
7:A2:1513:A:H2'	7:A2:1514:G:C8	2.50	0.46
8:B2:60:ILE:O	8:B2:63:ARG:HG2	2.15	0.46
9:C1:162:ILE:HG21	28:V2:29:A:H8	1.80	0.46
13:G1:57:SER:HB2	13:G1:60:GLU:HG2	1.97	0.46
20:N1:96:LEU:HD23	20:N1:96:LEU:HA	1.85	0.46
28:V2:26:G:N2	32:Y1:34:CM0:H3	2.14	0.46
3:4:35:ASP:HB3	19:M2:57:ARG:NH1	2.30	0.46
7:A1:844:G:H8	7:A1:845:A:HO2'	1.63	0.46
7:A1:1126:U:O2'	7:A1:1127:G:H5'	2.16	0.46
7:A2:328:C:H4'	7:A2:329:A:H5''	1.97	0.46
7:A2:1244:G:H2'	7:A2:1245:C:C6	2.51	0.46
11:E2:166:GLY:HA3	14:H2:114:ARG:HH22	1.80	0.46
13:G1:71:PRO:O	13:G1:96:ARG:NE	2.49	0.46
16:J2:8:ILE:HB	16:J2:74:VAL:HG23	1.98	0.46
5:72:465:G:O2'	41:I2:21:ARG:NH2	2.49	0.46
5:72:859:G:N2	5:72:916:G:H2'	2.30	0.46
5:72:2514:U:H2'	5:72:2515:C:C6	2.51	0.46
7:A1:185:U:H2'	7:A1:186:C:H6	1.81	0.46
7:A1:303:A:C2'	7:A1:304:U:H5'	2.46	0.46
7:A1:310:G:H2'	7:A1:311:C:C6	2.51	0.46
7:A1:801:U:H2'	7:A1:802:A:C8	2.51	0.46
7:A1:1073:U:H2'	7:A1:1074:G:C8	2.51	0.46
9:C1:50:ALA:HB1	9:C1:76:VAL:HG22	1.97	0.46
9:C2:16:LYS:HD3	9:C2:17:PRO:HD2	1.98	0.46
16:J1:29:ALA:HB3	16:J1:36:VAL:HG11	1.97	0.46
18:L2:75:GLN:NE2	18:L2:76:GLU:O	2.49	0.46
20:N1:85:ARG:O	20:N1:89:MET:N	2.38	0.46
20:N2:17:ALA:HA	20:N2:55:SER:HA	1.98	0.46
22:P1:51:ARG:O	22:P1:52:LEU:HD23	2.16	0.46
44:r2:5:SER:O	44:r2:8:ILE:HG22	2.17	0.46
3:4:41:HIS:HE1	37:e2:114:PHE:HD2	1.63	0.45
3:4:57:VAL:HG12	3:4:61:ASN:HD21	1.80	0.45
5:72:1796:U:H2'	5:72:1797:G:C8	2.50	0.45
5:72:2101:A:H2'	5:72:2102:G:C8	2.51	0.45
5:72:2830:C:O2'	5:72:2883:A:N1	2.41	0.45
6:82:44:G:H1'	6:82:47:C:H42	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:489:C:H2'	7:A1:490:C:C6	2.51	0.45
7:A1:933:G:H8	7:A1:933:G:OP2	1.99	0.45
7:A1:1245:C:H2'	7:A1:1246:A:H8	1.81	0.45
7:A1:1418:A:C3'	7:A1:1419:G:H5''	2.46	0.45
7:A2:37:U:O2'	7:A2:500:G:O2'	2.23	0.45
7:A2:824:G:H2'	7:A2:825:A:H8	1.80	0.45
7:A2:951:G:OP2	19:M2:101:ARG:NH2	2.49	0.45
7:A2:1030:U:O2	7:A2:1030:U:H2'	2.14	0.45
7:A2:1450:U:H2'	7:A2:1452:C:C5	2.51	0.45
8:B2:166:ALA:HB3	8:B2:191:SER:HB3	1.98	0.45
8:B2:169:GLU:O	8:B2:173:ILE:HG13	2.16	0.45
11:E1:36:LEU:HD22	11:E1:134:ILE:HG22	1.98	0.45
15:I1:45:ARG:HB2	15:I1:46:MET:HE2	1.97	0.45
36:b2:124:ILE:HG13	36:b2:124:ILE:O	2.16	0.45
5:72:158:U:H3	5:72:168:G:H1	1.63	0.45
5:72:927:A:H2'	5:72:928:A:C8	2.51	0.45
5:72:2087:G:H2'	5:72:2088:A:H8	1.80	0.45
6:82:29:A:O2'	6:82:58:A:N1	2.45	0.45
7:A1:265:G:N2	7:A1:267:C:O4'	2.49	0.45
7:A1:431:A:H2'	7:A1:432:A:O4'	2.17	0.45
7:A1:590:U:H2'	7:A1:591:U:C6	2.51	0.45
7:A1:1015:G:H8	7:A1:1015:G:O5'	1.98	0.45
7:A1:1325:C:H2'	7:A1:1326:U:C6	2.51	0.45
7:A2:41:G:H2'	7:A2:42:G:C8	2.50	0.45
7:A2:337:G:H2'	7:A2:338:A:H8	1.82	0.45
7:A2:401:C:O2'	7:A2:621:A:N3	2.46	0.45
7:A2:1172:C:H2'	7:A2:1173:U:C6	2.52	0.45
7:A2:1326:U:H2'	7:A2:1327:C:H6	1.80	0.45
8:B:219:ALA:HA	8:B:222:ARG:HD2	1.98	0.45
13:G2:25:LYS:HB3	13:G2:101:MET:HE1	1.97	0.45
4:62:26:HIS:HB3	4:62:44:LEU:HD22	1.99	0.45
5:72:1428:C:N4	5:72:1570:A:OP2	2.36	0.45
5:72:1791:A:H5''	36:b2:205:LEU:HD11	1.97	0.45
5:72:2251:OMG:H1'	5:72:2251:OMG:HM23	1.67	0.45
7:A1:208:U:O2'	7:A1:209:U:H6	1.99	0.45
7:A1:587:G:H4'	14:H1:4:GLN:HB3	1.97	0.45
7:A1:1010:U:H3	7:A1:1019:A:H61	1.63	0.45
7:A1:1384:C:H2'	7:A1:1385:G:C8	2.51	0.45
7:A2:214:C:H2'	7:A2:215:C:H6	1.82	0.45
7:A2:431:A:H2'	7:A2:432:A:C8	2.52	0.45
7:A2:489:C:H2'	7:A2:490:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:539:A:H2'	7:A2:540:G:C8	2.52	0.45
7:A2:718:A:H5'	17:K2:119:ASN:OD1	2.16	0.45
7:A2:1064:G:N2	7:A2:1190:G:H1'	2.31	0.45
8:B:46:THR:HG23	8:B:201:PRO:HG2	1.99	0.45
9:C2:90:VAL:O	9:C2:94:ILE:HG13	2.17	0.45
11:E2:77:ASN:HB2	11:E2:82:GLN:HG2	1.98	0.45
13:G2:116:MET:HA	13:G2:119:ARG:HD2	1.98	0.45
17:K2:23:ILE:N	17:K2:85:MET:O	2.46	0.45
32:Y1:23:A:H2'	32:Y1:24:G:C8	2.51	0.45
38:g2:8:LYS:HA	38:g2:24:THR:HG22	1.98	0.45
44:r2:30:ARG:HA	44:r2:35:ILE:HD12	1.99	0.45
5:72:629:G:H5''	5:72:650:C:O2'	2.16	0.45
6:82:49:C:H5''	44:r2:68:LYS:HE3	1.98	0.45
7:A1:229:U:H2'	7:A1:230:G:C8	2.52	0.45
7:A1:312:C:H2'	7:A1:313:A:C8	2.51	0.45
7:A1:411:A:N6	7:A1:428:G:N3	2.64	0.45
7:A2:481:G:O2'	7:A2:483:C:N4	2.46	0.45
7:A2:673:A:H2'	7:A2:674:G:C8	2.52	0.45
7:A2:1119:C:H2'	7:A2:1120:C:H6	1.82	0.45
9:C2:117:ALA:HB1	9:C2:187:SER:HB3	1.98	0.45
28:V2:49:G:H8	28:V2:49:G:O5'	2.00	0.45
36:b2:165:VAL:HG21	36:b2:181:MET:HE1	1.97	0.45
39:h2:29:GLY:HA2	39:h2:106:ASP:OD2	2.17	0.45
45:z2:34:GLY:N	45:z2:61:ALA:O	2.36	0.45
5:72:639:U:H2'	5:72:640:C:C6	2.52	0.45
5:72:747:5MU:C4	5:72:2613:U:C4	3.04	0.45
5:72:1418:G:H1'	5:72:1580:A:H61	1.82	0.45
5:72:2144:G:H8	5:72:2144:G:O5'	2.00	0.45
7:A1:148:G:H1'	7:A1:1447:A:H1'	1.97	0.45
7:A1:414:A:P	7:A1:428:G:H22	2.39	0.45
7:A1:855:U:H2'	7:A1:856:C:C6	2.51	0.45
7:A1:1305:G:H4'	7:A1:1332:A:N6	2.31	0.45
7:A2:236:A:H2'	7:A2:237:G:H8	1.81	0.45
7:A2:1273:C:H2'	7:A2:1274:A:O4'	2.16	0.45
7:A2:1492:A:H2'	7:A2:1493:A:C5	2.51	0.45
8:B2:126:PHE:HD2	8:B2:134:ALA:HB1	1.82	0.45
15:I1:42:GLU:HG3	15:I1:46:MET:HE3	1.99	0.45
25:S1:18:LYS:HD3	25:S1:31:LEU:HD12	1.98	0.45
29:W:17:H2U:H3'	29:W:17:H2U:H61	1.98	0.45
36:b2:142:HIS:ND1	36:b2:193:GLY:O	2.45	0.45
5:72:573:U:N3	5:72:2031:A:OP1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:1028:A:N6	5:72:1125:G:H2'	2.31	0.45
5:72:1880:U:H2'	5:72:1881:C:C6	2.52	0.45
7:A1:1044:A:C4	7:A1:1045:C:H1'	2.51	0.45
7:A1:1079:G:H2'	7:A1:1080:A:C8	2.51	0.45
7:A1:1483:A:H8	7:A1:1483:A:O5'	2.00	0.45
7:A1:1527:U:H2'	7:A1:1528:U:C6	2.52	0.45
7:A2:67:C:H2'	7:A2:68:G:H8	1.81	0.45
7:A2:80:A:H2'	7:A2:81:A:O4'	2.16	0.45
7:A2:398:U:H2'	7:A2:399:G:C8	2.51	0.45
7:A2:1044:A:C5	7:A2:1045:C:H1'	2.52	0.45
8:B2:64:LYS:HE2	8:B2:225:ARG:HG3	1.99	0.45
9:C1:152:GLU:HG3	9:C1:199:LYS:HB2	1.98	0.45
10:D2:99:ASP:OD1	10:D2:100:ASN:N	2.49	0.45
27:U1:39:GLU:HG3	27:U1:44:GLU:HB2	1.99	0.45
5:72:2129:C:O2'	5:72:2159:G:N1	2.49	0.45
5:72:2304:G:H22	5:72:2312:U:H3	1.63	0.45
6:82:9:G:HO2'	44:r2:45:SER:HG	1.61	0.45
7:A1:32:A:H2'	7:A1:33:A:C8	2.52	0.45
7:A1:188:C:H3'	7:A1:189:A:H8	1.82	0.45
7:A1:706:A:H2'	7:A1:707:U:C6	2.51	0.45
7:A1:1073:U:H2'	7:A1:1074:G:H8	1.82	0.45
7:A1:1423:G:H2'	7:A1:1424:U:C6	2.51	0.45
7:A2:371:A:O2'	7:A2:373:A:N7	2.48	0.45
7:A2:1080:A:OP1	11:E2:52:LYS:HE2	2.16	0.45
7:A2:1174:G:H2'	7:A2:1175:G:H8	1.82	0.45
12:F2:75:GLU:HG2	12:F2:89:VAL:HG21	1.98	0.45
27:U1:42:THR:HG23	27:U1:43:THR:H	1.82	0.45
36:b2:67:PHE:CE1	36:b2:156:ARG:HD2	2.51	0.45
39:h2:41:LEU:HD23	39:h2:41:LEU:HA	1.75	0.45
5:72:871:U:H2'	5:72:872:U:C6	2.52	0.45
5:72:1542:U:H2'	5:72:1543:G:O4'	2.17	0.45
5:72:2115:G:H4'	5:72:2166:U:H3	1.82	0.45
5:72:2599:G:OP2	36:b2:235:GLY:HA2	2.17	0.45
7:A1:175:C:C2'	7:A1:176:C:H5'	2.46	0.45
7:A1:220:G:H2'	7:A1:221:C:C6	2.52	0.45
7:A1:275:G:H2'	7:A1:276:G:C8	2.51	0.45
7:A1:381:C:H2'	7:A1:382:A:O4'	2.16	0.45
7:A1:1004:A:O2'	7:A1:1036:A:N6	2.44	0.45
9:C1:53:SER:HA	9:C1:114:LYS:HG2	1.97	0.45
13:G1:91:VAL:HG13	13:G1:96:ARG:HG2	1.98	0.45
29:W:10:G:HO2'	29:W:11:U:P	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:482:A:N6	5:72:506:G:O2'	2.50	0.45
5:72:1020:A:H1'	5:72:1021:A:OP2	2.17	0.45
5:72:2153:C:H2'	5:72:2154:A:C8	2.52	0.45
5:72:2328:A:H2'	5:72:2329:U:C6	2.52	0.45
7:A1:950:U:H2'	7:A1:951:G:C8	2.47	0.45
7:A1:1141:C:O2'	7:A1:1142:G:H8	1.99	0.45
7:A1:1456:A:H3'	7:A1:1457:G:H8	1.82	0.45
7:A1:1530:G:H2'	7:A1:1531:A:C8	2.52	0.45
7:A2:982:U:H4'	7:A2:983:A:O5'	2.17	0.45
8:B:125:THR:O	8:B:129:LEU:HB2	2.17	0.45
8:B:162:PHE:CD1	8:B:184:PHE:HB2	2.50	0.45
9:C2:33:LEU:HD22	20:N2:93:ILE:HD13	1.99	0.45
14:H1:87:LYS:HG2	14:H1:92:LEU:HA	1.99	0.45
45:z2:40:GLN:OE1	45:z2:44:LYS:HB2	2.17	0.45
5:72:1315:C:O2'	5:72:1392:A:N3	2.39	0.45
5:72:2788:C:H2'	5:72:2789:C:C6	2.52	0.45
5:72:2834:G:H2'	5:72:2879:A:N6	2.32	0.45
7:A1:84:U:H4'	7:A1:85:U:H3'	1.99	0.45
7:A1:637:C:H2'	7:A1:638:U:C6	2.51	0.45
7:A1:725:G:H2'	7:A1:726:C:C6	2.52	0.45
7:A1:946:A:H2'	7:A1:947:G:C8	2.52	0.45
7:A1:1122:U:H2'	7:A1:1123:U:C6	2.52	0.45
7:A1:1239:A:H1'	7:A1:1241:G:C4	2.52	0.45
7:A1:1498:UR3:O5'	7:A1:1498:UR3:H6	2.16	0.45
7:A2:522:C:H41	18:L2:50:ARG:NH2	2.14	0.45
7:A2:1027:C:H2'	7:A2:1028:C:C6	2.52	0.45
13:G1:108:ALA:O	13:G1:119:ARG:HD3	2.16	0.45
13:G2:27:VAL:HG12	13:G2:43:VAL:HG11	1.99	0.45
21:O1:71:LYS:HE2	21:O1:78:TYR:CE2	2.52	0.45
28:V2:40:A:H5''	28:V2:41:G:C8	2.52	0.45
31:X2:59:A:O2'	31:X2:61:U:H2'	2.17	0.45
39:h2:46:ILE:HD12	39:h2:69:PRO:HG3	1.99	0.45
5:72:1272:A:C5	5:72:1618:6MZ:H1'	2.52	0.44
5:72:1527:G:N1	5:72:1544:A:OP2	2.46	0.44
5:72:1566:A:H5'	36:b2:214:ARG:CZ	2.47	0.44
5:72:1586:A:H2'	5:72:1587:G:O4'	2.17	0.44
5:72:2087:G:H2'	5:72:2088:A:C8	2.52	0.44
5:72:2116:G:H5''	5:72:2117:A:OP1	2.17	0.44
5:72:2144:G:C2	5:72:2146:C:H1'	2.52	0.44
5:72:2540:C:O2'	5:72:2740:A:N3	2.47	0.44
7:A1:369:G:OP2	7:A1:388:G:N1	2.40	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:418:C:H2'	7:A1:419:C:C6	2.51	0.44
7:A1:463:U:C4	7:A1:467:U:H2'	2.52	0.44
7:A1:1015:G:H2'	7:A1:1016:A:H8	1.82	0.44
7:A2:502:A:OP1	18:L2:114:ARG:N	2.51	0.44
7:A2:555:U:H2'	7:A2:556:C:C6	2.53	0.44
7:A2:949:A:N7	19:M2:105:ASN:ND2	2.65	0.44
7:A2:1391:U:H2'	7:A2:1392:G:C8	2.52	0.44
8:B:24:ASN:ND2	8:B:191:SER:O	2.50	0.44
11:E2:39:VAL:HG23	11:E2:71:MET:HE1	1.99	0.44
13:G1:113:ASP:HB2	13:G1:119:ARG:CG	2.48	0.44
16:J1:40:ILE:HD11	16:J1:73:LEU:HD23	1.98	0.44
17:K2:113:VAL:O	17:K2:113:VAL:HG12	2.17	0.44
21:O1:64:ARG:HD2	21:O1:67:LEU:HD21	1.98	0.44
24:R2:8:ARG:HB3	24:R2:10:PHE:HE1	1.82	0.44
27:U1:29:LEU:HD12	27:U1:33:ARG:HH12	1.82	0.44
27:U2:38:TYR:CG	27:U2:39:GLU:N	2.85	0.44
42:o2:19:LEU:HD13	42:o2:31:GLY:HA3	2.00	0.44
5:72:158:U:HO2'	5:72:159:G:P	2.40	0.44
5:72:372:G:O2'	5:72:400:G:O6	2.30	0.44
5:72:1035:U:H2'	5:72:1036:G:H8	1.81	0.44
5:72:1214:A:H62	5:72:1235:G:H21	1.65	0.44
5:72:1278:C:H2'	5:72:1279:G:H8	1.82	0.44
5:72:1827:U:OP2	36:b2:221:ARG:NE	2.50	0.44
5:72:2138:G:H1	5:72:2153:C:H42	1.65	0.44
5:72:2329:U:H2'	5:72:2330:G:C8	2.52	0.44
7:A1:70:U:H2'	7:A1:94:G:N7	2.32	0.44
7:A1:275:G:H5'	23:Q1:16:LYS:HD2	1.99	0.44
7:A1:1413:A:H2	7:A1:1487:G:H22	1.65	0.44
7:A1:1526:G:H2'	7:A1:1527:U:C6	2.53	0.44
7:A2:148:G:O2'	7:A2:1446:A:N3	2.49	0.44
7:A2:360:G:C2'	7:A2:361:G:H5'	2.48	0.44
7:A2:451:A:OP1	7:A2:481:G:N2	2.51	0.44
7:A2:509:A:N3	7:A2:543:U:O2'	2.50	0.44
7:A2:1157:A:H4'	7:A2:1158:C:O5'	2.17	0.44
7:A2:1377:A:C6	13:G2:7:ILE:HD12	2.52	0.44
8:B2:20:THR:HG23	8:B2:21:ARG:H	1.81	0.44
9:C2:79:LYS:HD3	9:C2:84:VAL:HB	1.99	0.44
12:F2:69:GLU:H	12:F2:69:GLU:CD	2.26	0.44
15:I1:51:PRO:O	15:I1:55:VAL:HG22	2.17	0.44
18:L1:44:LYS:NZ	28:V2:25:U:O3'	2.44	0.44
28:V2:28:C:H2'	28:V2:29:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b2:141:VAL:HG12	36:b2:192:LEU:HD13	1.99	0.44
1:12:23:ASN:OD1	5:72:2079:U:O2'	2.34	0.44
3:4:3:LYS:N	3:4:3:LYS:HD2	2.33	0.44
5:72:2547:A:H2'	5:72:2548:U:C6	2.52	0.44
7:A1:182:A:O2'	7:A1:183:C:H5''	2.17	0.44
7:A1:323:U:H2'	7:A1:324:G:O4'	2.18	0.44
7:A1:324:G:N2	7:A1:326:G:H3'	2.32	0.44
7:A1:460:A:H61	7:A1:472:U:H3	1.66	0.44
7:A1:929:G:H2'	7:A1:930:C:C6	2.52	0.44
7:A1:984:C:H2'	7:A1:985:C:H6	1.80	0.44
7:A1:1041:G:H2'	7:A1:1042:A:H8	1.83	0.44
7:A1:1048:G:H5''	20:N1:3:LYS:HZ2	1.83	0.44
7:A1:1255:G:O2'	7:A1:1258:G:N3	2.37	0.44
7:A2:342:C:H2'	7:A2:343:U:C6	2.53	0.44
7:A2:432:A:H3'	7:A2:433:G:H8	1.82	0.44
7:A2:838:G:H2'	7:A2:839:C:C6	2.52	0.44
8:B2:112:LYS:HA	8:B2:115:LYS:HE2	1.99	0.44
13:G2:16:PRO:HB3	15:I2:43:THR:HA	1.98	0.44
17:K1:73:ALA:HB1	17:K1:77:TYR:HD2	1.81	0.44
29:W:17:H2U:H62	29:W:17:H2U:O5'	2.17	0.44
33:Y2:11:C:N4	33:Y2:24:G:O6	2.39	0.44
42:o2:49:GLY:O	42:o2:56:PRO:HB3	2.17	0.44
5:71:1904:G:O2'	5:71:1928:A:N1	2.50	0.44
5:72:395:U:O2'	5:72:396:G:N7	2.43	0.44
5:72:558:U:H2'	5:72:559:G:H8	1.81	0.44
5:72:1019:U:H3	5:72:1142:A:H62	1.64	0.44
5:72:1528:A:OP2	5:72:1543:G:N2	2.50	0.44
5:72:2233:U:H2'	5:72:2234:G:C8	2.53	0.44
5:72:2271:G:OP1	45:z2:18:ALA:HB1	2.16	0.44
5:72:2519:U:O4'	5:72:2542:A:N6	2.50	0.44
7:A1:408:A:H2'	7:A1:409:U:C6	2.52	0.44
7:A1:459:A:H2'	7:A1:460:A:C8	2.52	0.44
7:A1:651:C:N4	7:A1:753:A:OP2	2.48	0.44
7:A1:878:A:H2'	7:A1:879:C:C6	2.52	0.44
7:A1:1535:C:H3'	7:A1:1536:C:C6	2.52	0.44
7:A2:188:C:H3'	7:A2:189:A:C8	2.53	0.44
7:A2:421:U:O2'	7:A2:422:C:H5'	2.17	0.44
7:A2:713:G:H2'	7:A2:714:G:C8	2.52	0.44
7:A2:974:A:O4'	20:N2:71:HIS:ND1	2.49	0.44
7:A2:1227:A:H5'	19:M2:110:LYS:NZ	2.33	0.44
7:A2:1258:G:H2'	7:A2:1259:C:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1447:A:OP1	7:A2:1448:C:N4	2.42	0.44
11:E1:115:LEU:HD13	11:E1:123:VAL:HG11	2.00	0.44
14:H2:92:LEU:HD11	14:H2:117:ARG:HB2	2.00	0.44
15:I1:44:ALA:O	15:I1:48:VAL:HG13	2.17	0.44
22:P1:76:LYS:C	22:P1:78:VAL:H	2.25	0.44
1:12:17:ASN:HB2	1:12:25:THR:OG1	2.17	0.44
1:12:59:ILE:HD12	1:12:67:VAL:HG21	2.00	0.44
5:72:2039:U:H2'	5:72:2040:G:H8	1.82	0.44
7:A1:40:C:H2'	7:A1:41:G:H8	1.82	0.44
7:A1:647:C:H2'	7:A1:648:A:H8	1.82	0.44
7:A1:772:U:H2'	7:A1:773:G:C8	2.53	0.44
7:A1:1037:C:H2'	7:A1:1038:C:C6	2.52	0.44
7:A1:1257:A:H8	7:A1:1257:A:O5'	2.01	0.44
7:A2:67:C:H2'	7:A2:68:G:C8	2.53	0.44
7:A2:389:A:H3'	7:A2:390:U:C6	2.52	0.44
9:C2:116:VAL:HG21	9:C2:200:VAL:HG11	1.99	0.44
11:E2:83:HIS:CE1	11:E2:147:MET:HG3	2.53	0.44
12:F1:14:GLN:O	12:F1:17:GLN:NE2	2.51	0.44
14:H2:96:MET:HB3	14:H2:100:GLY:N	2.28	0.44
15:I1:75:GLN:O	15:I1:79:ILE:HG13	2.17	0.44
15:I2:130:ARG:HH12	29:W:35:C:P	2.41	0.44
22:P1:19:VAL:HG12	22:P1:36:VAL:HG23	1.99	0.44
25:S2:45:ILE:HD13	25:S2:62:VAL:HG12	1.99	0.44
3:4:28:VAL:HG21	3:4:32:LEU:HD23	2.00	0.44
5:72:87:U:H5'	5:72:88:G:H5''	2.00	0.44
5:72:715:A:H61	21:O2:53:ARG:NH2	2.16	0.44
5:72:1130:U:HO2'	5:72:1131:G:P	2.41	0.44
5:72:2107:G:H2'	5:72:2108:A:O4'	2.17	0.44
5:72:2646:C:H2'	5:72:2647:U:O4'	2.18	0.44
7:A1:231:U:H2'	7:A1:232:G:C8	2.44	0.44
7:A1:894:G:H2'	7:A1:895:G:C8	2.52	0.44
7:A1:1097:C:H2'	7:A1:1098:C:C6	2.52	0.44
7:A1:1121:U:H2'	7:A1:1122:U:H6	1.83	0.44
7:A2:458:U:H2'	7:A2:474:G:N2	2.33	0.44
7:A2:1142:G:H3'	7:A2:1143:G:C8	2.48	0.44
27:U1:13:ASP:O	27:U1:17:ARG:HG2	2.18	0.44
27:U1:51:SER:O	27:U1:55:ARG:HG3	2.18	0.44
28:V2:30:A:O2'	28:V2:31:U:O4'	2.36	0.44
33:Y2:45:G:H3'	33:Y2:46:G7M:H5''	2.00	0.44
35:a2:64:VAL:HG22	35:a2:160:GLN:HG3	1.99	0.44
1:12:3:ARG:O	1:12:12:PRO:HD3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:1:G:H2'	5:72:2:G:C8	2.53	0.44
5:72:1010:A:N3	5:72:1153:C:H1'	2.32	0.44
5:72:1847:A:HO2'	5:72:1848:A:P	2.40	0.44
5:72:2352:A:N1	45:z2:34:GLY:HA3	2.32	0.44
7:A1:337:G:H2'	7:A1:338:A:H8	1.80	0.44
7:A1:653:U:C2	14:H1:56:LYS:HG2	2.52	0.44
7:A1:671:G:C2'	7:A1:672:U:H5'	2.48	0.44
7:A1:718:A:H5'	17:K1:119:ASN:ND2	2.32	0.44
7:A1:771:G:H2'	7:A1:772:U:C6	2.52	0.44
7:A1:860:A:H2'	7:A1:861:G:O4'	2.17	0.44
7:A2:116:A:H2'	7:A2:117:G:O4'	2.17	0.44
7:A2:434:U:H2'	7:A2:435:A:C8	2.52	0.44
7:A2:990:C:H2'	7:A2:991:U:C6	2.52	0.44
8:B:123:ASP:HA	8:B:126:PHE:CE2	2.53	0.44
11:E2:156:LYS:HZ1	14:H2:71:VAL:C	2.18	0.44
13:G2:76:LYS:HG2	13:G2:89:VAL:HB	1.99	0.44
14:H1:87:LYS:HE2	14:H1:87:LYS:HB2	1.70	0.44
16:J1:32:THR:O	16:J1:32:THR:HG22	2.18	0.44
21:O2:7:ALA:O	21:O2:10:LYS:HG2	2.18	0.44
28:V2:48:C:H2'	28:V2:49:G:C8	2.53	0.44
3:4:2:LYS:NZ	6:82:40:U:O2'	2.51	0.44
5:72:1265:A:H4'	5:72:1266:G:H4'	2.00	0.44
5:72:2182:U:H2'	5:72:2183:A:C8	2.53	0.44
5:72:2186:G:H2'	5:72:2187:U:O4'	2.17	0.44
5:72:2591:C:H2'	5:72:2592:G:C8	2.52	0.44
7:A1:35:G:H2'	7:A1:36:C:C6	2.53	0.44
7:A1:109:A:H5'	7:A1:110:C:C5	2.53	0.44
7:A1:165:G:H2'	7:A1:166:U:C6	2.53	0.44
7:A1:188:C:H3'	7:A1:189:A:C8	2.52	0.44
7:A1:578:C:O2'	7:A1:728:A:N3	2.45	0.44
7:A1:604:G:H2'	7:A1:605:U:O4'	2.18	0.44
7:A1:898:G:N2	7:A1:901:A:OP2	2.51	0.44
7:A1:1106:G:O2'	9:C1:169:ARG:NH2	2.51	0.44
7:A1:1431:A:H2'	7:A1:1432:G:C8	2.53	0.44
7:A2:252:U:O4	7:A2:253:A:N6	2.50	0.44
7:A2:1301:U:O2'	7:A2:1302:C:H3'	2.18	0.44
7:A2:1324:A:H2'	7:A2:1325:C:C6	2.53	0.44
9:C1:114:LYS:HD2	9:C1:185:ASN:ND2	2.33	0.44
13:G1:37:SER:HB3	15:I1:41:ARG:NH1	2.33	0.44
18:L1:123:LYS:HA	18:L1:123:LYS:HE3	2.00	0.44
22:P1:69:ASP:OD1	22:P1:70:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S1:28:LYS:HA	25:S1:28:LYS:HE3	1.99	0.44
28:V2:36:A:O2'	28:V2:37:A:O5'	2.36	0.44
40:i2:83:LYS:HA	40:i2:149:GLU:HB2	1.99	0.44
40:i2:141:LYS:HE2	40:i2:141:LYS:HB2	1.84	0.44
45:z2:25:ARG:NH2	45:z2:29:GLU:HB3	2.33	0.44
5:72:13:A:O2'	5:72:15:G:N7	2.51	0.44
5:72:894:U:H2'	5:72:895:U:O4'	2.18	0.44
5:72:1231:U:H2'	5:72:1232:G:H8	1.81	0.44
5:72:2131:U:H5'	5:72:2133:G:H4'	1.99	0.44
5:72:2298:A:H61	5:72:2318:G:H1'	1.83	0.44
5:72:2554:U:H2'	5:72:2555:U:H6	1.83	0.44
7:A1:223:A:H2'	7:A1:224:U:C6	2.52	0.44
7:A1:341:C:H2'	7:A1:342:C:C6	2.53	0.44
7:A1:1090:U:H2'	7:A1:1091:U:C6	2.53	0.44
7:A2:202:G:O2'	7:A2:468:A:N3	2.50	0.44
7:A2:789:U:O2'	7:A2:791:G:N7	2.51	0.44
7:A2:976:G:OP2	7:A2:1358:U:O2'	2.35	0.44
7:A2:1004:A:N6	7:A2:1026:G:H1'	2.33	0.44
7:A2:1032:G:H3'	7:A2:1032:G:N3	2.32	0.44
10:D1:108:GLY:HA3	10:D1:114:ALA:HB2	1.99	0.44
11:E1:83:HIS:CE1	11:E1:147:MET:HG3	2.53	0.44
14:H1:26:THR:HG22	14:H1:60:GLU:OE1	2.18	0.44
14:H1:89:LYS:O	14:H1:92:LEU:HD22	2.17	0.44
14:H2:89:LYS:O	14:H2:92:LEU:HD22	2.18	0.44
23:Q1:10:GLY:HA3	23:Q1:25:ILE:HD13	1.99	0.44
23:Q1:15:ASP:OD2	23:Q1:54:GLY:HA2	2.18	0.44
5:72:476:G:H22	5:72:479:A:C5'	2.31	0.43
5:72:749:A:N3	5:72:1618:6MZ:H2'	2.33	0.43
5:72:1093:G:H1'	5:72:1099:G:C2	2.53	0.43
5:72:1182:G:H2'	5:72:1183:U:O4'	2.18	0.43
5:72:2230:G:H2'	5:72:2231:U:C6	2.52	0.43
5:72:2532:G:O2'	5:72:2657:A:N1	2.50	0.43
6:82:38:C:H2'	6:82:39:A:H5'	2.00	0.43
7:A1:636:U:H2'	7:A1:637:C:C6	2.53	0.43
7:A1:652:U:O4	7:A1:752:G:O2'	2.27	0.43
7:A1:785:G:H2'	7:A1:786:G:C8	2.53	0.43
7:A1:1013:G:H2'	7:A1:1015:G:OP2	2.18	0.43
7:A1:1478:U:H2'	7:A1:1479:C:H6	1.82	0.43
7:A2:62:U:H2'	7:A2:63:C:C6	2.53	0.43
7:A2:162:A:C5	7:A2:163:C:H1'	2.52	0.43
7:A2:201:G:H2'	7:A2:202:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:262:A:H2'	7:A2:263:A:C8	2.53	0.43
7:A2:363:A:H1'	18:L2:29:GLN:HE21	1.83	0.43
7:A2:373:A:O2'	7:A2:481:G:N2	2.51	0.43
7:A2:778:G:O2'	17:K2:121:CYS:HB3	2.17	0.43
7:A2:1320:C:H1'	25:S2:73:GLU:HG3	2.00	0.43
7:A2:1377:A:N3	13:G2:2:PRO:HG3	2.32	0.43
8:B:92:VAL:HG12	8:B:93:ASN:N	2.28	0.43
10:D1:9:LEU:HD12	10:D1:32:CYS:SG	2.58	0.43
10:D2:78:GLU:OE1	10:D2:81:ARG:HD2	2.18	0.43
13:G2:140:ASP:O	13:G2:144:MET:HG3	2.17	0.43
15:I2:24:GLY:H	15:I2:61:LEU:HA	1.81	0.43
21:O1:21:ASP:OD1	21:O1:24:SER:HB3	2.17	0.43
40:i2:51:ARG:HD3	40:i2:51:ARG:C	2.43	0.43
5:72:1318:U:H2'	5:72:1319:C:C6	2.54	0.43
5:72:1820:U:C2	36:b2:201:MET:SD	3.11	0.43
5:72:2124:G:H3'	5:72:2125:G:C8	2.53	0.43
5:72:2585:U:C5	43:p:36:TRP:HB2	2.53	0.43
7:A1:214:C:H2'	7:A1:215:C:C6	2.53	0.43
7:A1:404:G:O2'	7:A1:498:A:N1	2.50	0.43
7:A1:670:G:H2'	7:A1:671:G:H8	1.82	0.43
7:A1:742:G:H2'	7:A1:743:A:C8	2.53	0.43
7:A1:1036:A:H3'	7:A1:1037:C:H6	1.82	0.43
7:A1:1263:C:H2'	7:A1:1264:U:H6	1.80	0.43
7:A1:1432:G:H8	7:A1:1432:G:OP2	2.01	0.43
7:A1:1433:A:H2'	7:A1:1434:A:O4'	2.18	0.43
7:A2:222:C:H2'	7:A2:223:A:C8	2.53	0.43
7:A2:554:A:H2'	7:A2:555:U:C6	2.53	0.43
7:A2:868:C:H2'	7:A2:869:G:O4'	2.17	0.43
7:A2:1436:U:H2'	7:A2:1437:A:C8	2.52	0.43
9:C2:212:ALA:H	16:J2:16:ARG:NH1	2.15	0.43
15:I2:118:LEU:HB3	15:I2:123:ARG:O	2.17	0.43
16:J1:47:GLU:HG2	16:J1:49:PHE:CE1	2.53	0.43
18:L2:99:ARG:HB2	18:L2:117:TYR:HA	1.99	0.43
19:M1:2:ALA:O	19:M1:9:ILE:HG22	2.19	0.43
19:M2:50:GLU:HA	19:M2:53:ILE:HD12	1.99	0.43
26:T1:54:MET:HE2	26:T1:54:MET:HB2	1.87	0.43
29:W:16:H2U:H3'	29:W:16:H2U:H61	2.00	0.43
36:b2:120:VAL:HG12	36:b2:131:PRO:HG2	2.00	0.43
5:72:1344:U:O2	5:72:1385:A:H5'	2.17	0.43
5:72:1847:A:O2'	5:72:1848:A:O5'	2.30	0.43
5:72:2747:G:O6	5:72:2755:C:H5''	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:681:A:H2'	7:A1:682:G:H8	1.83	0.43
7:A1:1003:G:H2'	7:A1:1003:G:N3	2.32	0.43
7:A1:1237:C:H3'	7:A1:1238:A:H5'	1.99	0.43
7:A2:620:C:H2'	7:A2:621:A:O4'	2.17	0.43
9:C1:130:PHE:CZ	9:C1:131:ARG:HG3	2.53	0.43
12:F2:12:PRO:HD2	12:F2:54:LEU:HD13	2.00	0.43
13:G2:18:PHE:HE2	13:G2:58:GLU:HB2	1.82	0.43
15:I2:123:ARG:NH1	15:I2:124:ARG:O	2.45	0.43
16:J1:12:ALA:HB2	16:J1:96:VAL:HG13	1.99	0.43
23:Q2:60:GLU:N	23:Q2:77:ARG:O	2.45	0.43
37:e2:58:ALA:HB2	37:e2:65:PRO:HD3	1.99	0.43
3:4:1:MET:O	3:4:2:LYS:C	2.60	0.43
5:72:737:C:H2'	5:72:738:G:H8	1.83	0.43
5:72:1475:G:O2'	5:72:1476:U:P	2.77	0.43
5:72:1889:A:H2'	5:72:1890:A:C8	2.53	0.43
5:72:2102:G:C2	5:72:2103:C:H1'	2.53	0.43
5:72:2119:A:C2	5:72:2170:A:H1'	2.54	0.43
7:A1:493:A:H2'	7:A1:494:G:C8	2.54	0.43
7:A1:868:C:H2'	7:A1:869:G:O4'	2.18	0.43
7:A1:1271:A:H2'	7:A1:1272:G:H8	1.84	0.43
7:A1:1359:C:H5	20:N1:75:ARG:HE	1.67	0.43
7:A2:151:A:H2'	7:A2:152:A:C8	2.53	0.43
7:A2:506:G:H2'	7:A2:507:C:C6	2.54	0.43
7:A2:748:G:H2'	7:A2:749:A:C8	2.54	0.43
7:A2:1381:U:H4'	13:G2:79:ARG:NE	2.33	0.43
8:B2:76:ALA:HB1	8:B2:210:VAL:HG21	2.00	0.43
11:E1:37:THR:HG22	11:E1:63:ALA:HB1	2.00	0.43
20:N1:81:ARG:HG2	20:N1:81:ARG:HH11	1.83	0.43
22:P1:25:ARG:HE	22:P1:25:ARG:HB2	1.67	0.43
26:T1:55:GLN:HB3	26:T1:56:PRO:CD	2.48	0.43
39:h2:127:LYS:HE2	39:h2:127:LYS:HB2	1.79	0.43
40:i2:117:LEU:HD13	40:i2:122:LEU:HD23	2.00	0.43
5:72:192:C:O2'	5:72:802:A:N3	2.48	0.43
5:72:1076:C:H2'	5:72:1077:A:C8	2.54	0.43
5:72:1283:G:N1	5:72:1286:A:OP2	2.51	0.43
5:72:1569:A:H2'	5:72:1570:A:C8	2.54	0.43
5:72:1744:A:H3'	5:72:1745:A:H8	1.83	0.43
5:72:1779:U:H5	5:72:1784:A:N7	2.17	0.43
7:A1:4:U:H5'	7:A1:4:U:H6	1.83	0.43
7:A1:669:G:H2'	7:A1:670:G:H8	1.82	0.43
7:A1:681:A:H2'	7:A1:682:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:1264:U:H2'	7:A1:1265:C:H6	1.83	0.43
7:A1:1304:G:N2	7:A1:1333:A:H62	2.14	0.43
7:A2:84:U:H4'	7:A2:85:U:H3'	1.99	0.43
7:A2:440:C:C2	7:A2:441:A:C8	3.06	0.43
7:A2:551:U:H2'	7:A2:552:U:C6	2.54	0.43
10:D2:188:ARG:O	10:D2:188:ARG:NH1	2.48	0.43
11:E2:36:LEU:HD22	11:E2:134:ILE:HG22	2.00	0.43
15:I2:99:ARG:HG3	15:I2:104:VAL:HG21	1.99	0.43
30:W1:10:G:H2'	30:W1:11:C:C6	2.53	0.43
31:X2:9:A:O2'	31:X2:10:G:N7	2.51	0.43
31:X2:70:A:H2'	31:X2:71:U:C6	2.53	0.43
5:72:2602:A:N1	33:Y2:76:A:C8	2.86	0.43
7:A1:56:U:H2'	7:A1:57:G:C8	2.53	0.43
7:A1:90:C:H2'	7:A1:91:U:C6	2.54	0.43
7:A1:143:A:H2	7:A1:220:G:H1	1.66	0.43
7:A1:198:G:H2'	7:A1:199:A:C8	2.53	0.43
7:A1:496:A:H2'	7:A1:497:G:N7	2.34	0.43
7:A1:513:C:H2'	7:A1:514:C:H6	1.83	0.43
7:A1:909:A:H2'	7:A1:910:C:O4'	2.19	0.43
7:A1:1051:C:O2	7:A1:1207:2MG:N1	2.45	0.43
7:A1:1251:A:H2'	7:A1:1252:A:C8	2.54	0.43
7:A1:1323:G:H2'	7:A1:1324:A:H8	1.82	0.43
7:A2:218:U:H2'	7:A2:219:U:H6	1.84	0.43
7:A2:300:A:C6	7:A2:301:G:H1'	2.54	0.43
7:A2:941:G:H4'	7:A2:1350:A:H4'	2.01	0.43
7:A2:1012:A:H2'	7:A2:1013:G:C8	2.52	0.43
8:B2:105:LYS:HA	8:B2:108:ARG:NH1	2.34	0.43
14:H2:26:THR:HG22	14:H2:60:GLU:OE1	2.18	0.43
15:I2:63:LEU:HB3	15:I2:65:ILE:HD11	2.00	0.43
15:I2:130:ARG:HD2	29:W:32:PSU:OP2	2.18	0.43
23:Q1:16:LYS:O	23:Q1:16:LYS:HD3	2.18	0.43
37:e2:148:ARG:NH1	37:e2:148:ARG:HB2	2.34	0.43
44:r2:18:LEU:HD12	44:r2:23:ALA:HB3	2.01	0.43
5:72:1820:U:N3	36:b2:159:GLY:HA3	2.34	0.43
5:72:1952:A:H2'	5:72:1953:A:C8	2.54	0.43
5:72:2246:G:H2'	5:72:2247:A:C8	2.53	0.43
7:A1:256:U:H2'	7:A1:257:G:C8	2.54	0.43
7:A1:263:A:P	26:T1:74:ARG:HH21	2.41	0.43
7:A1:492:C:H2'	7:A1:493:A:C8	2.53	0.43
7:A1:682:G:H2'	7:A1:683:G:H8	1.83	0.43
7:A1:805:C:H2'	7:A1:806:C:H6	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:1136:C:H5''	7:A1:1137:C:H5	1.84	0.43
7:A1:1388:C:H2'	7:A1:1389:C:C6	2.53	0.43
7:A2:1132:C:H5'	7:A2:1133:G:OP2	2.18	0.43
7:A2:1228:C:H2'	7:A2:1229:A:H8	1.84	0.43
7:A2:1243:C:H42	7:A2:1294:G:H1	1.67	0.43
10:D2:105:MET:SD	10:D2:173:VAL:HG22	2.59	0.43
16:J1:9:ARG:HH22	16:J1:71:LEU:HD12	1.84	0.43
16:J1:25:ILE:HD11	16:J1:92:LEU:HD13	2.01	0.43
16:J2:59:LYS:HZ2	16:J2:62:ARG:NH2	2.17	0.43
17:K1:20:VAL:HG13	17:K1:35:THR:HG23	2.01	0.43
17:K2:96:THR:O	17:K2:100:LEU:HD23	2.18	0.43
33:Y2:9:A:H1'	33:Y2:45:G:O2'	2.19	0.43
5:72:476:G:H4'	5:72:502:A:N1	2.33	0.43
5:72:747:5MU:C5M	5:72:2612:C:H4'	2.49	0.43
5:72:832:U:H2'	5:72:833:A:C8	2.54	0.43
5:72:1909:C:H2'	5:72:1910:G:C8	2.54	0.43
5:72:2590:A:H2'	5:72:2591:C:C6	2.53	0.43
5:72:2857:G:N2	5:72:2860:A:OP2	2.35	0.43
7:A1:175:C:H2'	7:A1:176:C:H5'	2.01	0.43
7:A1:502:A:H2'	7:A1:503:C:O4'	2.19	0.43
7:A1:717:U:H5'	7:A1:734:G:OP2	2.18	0.43
7:A1:1021:A:H3'	7:A1:1022:A:C8	2.54	0.43
7:A1:1539:C:H2'	7:A1:1540:U:C6	2.53	0.43
7:A2:181:A:H2'	7:A2:182:A:C8	2.54	0.43
7:A2:221:C:H2'	7:A2:222:C:C6	2.53	0.43
7:A2:830:G:H2'	7:A2:831:A:C8	2.54	0.43
9:C2:71:ALA:HB1	9:C2:109:PRO:HB3	2.00	0.43
10:D1:34:ILE:HG22	10:D1:35:GLU:N	2.33	0.43
16:J2:56:HIS:ND1	16:J2:57:VAL:HG13	2.33	0.43
16:J2:87:LEU:O	16:J2:90:LEU:HB3	2.19	0.43
19:M2:42:ASP:OD1	19:M2:42:ASP:N	2.48	0.43
22:P1:78:VAL:HG13	22:P1:79:ASN:N	2.33	0.43
33:Y2:31:C:O2	33:Y2:39:G:N2	2.48	0.43
36:b2:247:PRO:HG2	36:b2:248:TRP:CZ3	2.54	0.43
1:12:55:GLY:O	1:12:58:VAL:HG22	2.19	0.43
5:72:552:U:H2'	5:72:553:G:C8	2.54	0.43
5:72:589:U:H2'	5:72:590:A:C8	2.54	0.43
5:72:671:C:N4	42:o2:40:SER:O	2.27	0.43
5:72:992:C:H2'	5:72:993:G:H8	1.84	0.43
5:72:1550:C:H2'	5:72:1551:A:C8	2.54	0.43
5:72:2698:U:H2'	5:72:2699:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:12:U:H4'	7:A1:526:C:H4'	2.00	0.43
7:A1:290:C:H2'	7:A1:291:U:H6	1.84	0.43
7:A1:343:U:H2'	7:A1:345:C:C5	2.54	0.43
7:A1:841:C:C5	7:A1:843:U:H5'	2.54	0.43
7:A1:846:G:H2'	7:A1:847:G:C8	2.53	0.43
7:A1:1030:U:H3'	7:A1:1031:C:H6	1.83	0.43
7:A1:1124:G:H1'	7:A1:1125:U:H5	1.84	0.43
7:A1:1386:G:H2'	7:A1:1387:G:H8	1.83	0.43
7:A1:1388:C:H2'	7:A1:1389:C:H6	1.83	0.43
7:A1:1539:C:O2'	27:U1:21:ARG:HD2	2.18	0.43
7:A2:31:G:C8	7:A2:306:A:H1'	2.54	0.43
7:A2:416:G:N2	7:A2:427:U:O2	2.52	0.43
7:A2:816:A:OP1	7:A2:1526:G:O2'	2.29	0.43
7:A2:1129:C:H1'	7:A2:1130:A:N7	2.33	0.43
7:A2:1264:U:H2'	7:A2:1265:C:C6	2.54	0.43
7:A2:1269:A:H8	7:A2:1269:A:O5'	2.01	0.43
8:B:144:LEU:HD12	8:B:144:LEU:HA	1.78	0.43
9:C1:114:LYS:HA	9:C1:185:ASN:HD22	1.84	0.43
19:M2:17:ILE:HD13	19:M2:17:ILE:HA	1.92	0.43
28:V2:37:A:H4'	28:V2:38:A:H2'	2.01	0.43
33:Y2:5:C:O2	33:Y2:68:G:N2	2.43	0.43
33:Y2:35:G:H2'	33:Y2:36:C:O4'	2.19	0.43
36:b2:111:LYS:HE2	36:b2:111:LYS:HB2	1.85	0.43
5:72:937:C:H2'	5:72:938:G:C8	2.54	0.43
5:72:1674:G:N2	5:72:1677:A:N1	2.67	0.43
6:82:47:C:O3'	44:r2:98:GLN:NE2	2.50	0.43
7:A1:267:C:H2'	7:A1:268:U:C6	2.53	0.43
7:A1:721:G:H4'	7:A1:722:G:O5'	2.19	0.43
7:A1:751:U:H2'	7:A1:752:G:O4'	2.19	0.43
7:A1:1113:C:O4'	9:C1:178:LEU:HD11	2.19	0.43
7:A1:1244:G:H2'	7:A1:1245:C:C6	2.54	0.43
7:A1:1518:MA6:H2'	7:A1:1519:MA6:C8	2.49	0.43
7:A2:202:G:H21	7:A2:466:A:N6	2.17	0.43
7:A2:491:G:O2'	7:A2:492:C:H5'	2.18	0.43
7:A2:1019:A:H5'	7:A2:1020:G:OP2	2.18	0.43
7:A2:1147:C:H2'	7:A2:1148:U:C6	2.54	0.43
7:A2:1305:G:H1'	7:A2:1332:A:N6	2.34	0.43
9:C1:50:ALA:O	9:C1:70:THR:OG1	2.34	0.43
10:D1:170:TRP:CE2	10:D1:186:PRO:HB3	2.54	0.43
18:L1:31:ARG:HE	18:L1:31:ARG:HB3	1.74	0.43
21:O2:3:LEU:HB2	21:O2:35:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:X2:71:U:H2'	31:X2:72:G:O4'	2.19	0.43
36:b2:98:ASP:O	36:b2:98:ASP:OD1	2.36	0.43
5:72:161:A:OP2	5:72:162:U:O2'	2.36	0.42
5:72:265:A:N1	5:72:427:U:O2'	2.47	0.42
5:72:1047:G:O2'	5:72:1110:G:N1	2.42	0.42
5:72:2006:C:O2'	5:72:2823:A:N3	2.52	0.42
5:72:2345:G:N3	5:72:2381:A:H2'	2.34	0.42
7:A1:148:G:O2'	7:A1:1446:A:N3	2.50	0.42
7:A1:577:G:H2'	7:A1:578:C:C6	2.53	0.42
7:A2:106:C:H2'	7:A2:107:G:H8	1.83	0.42
7:A2:448:A:H3'	7:A2:449:G:C8	2.54	0.42
7:A2:454:G:H2'	7:A2:455:G:C8	2.54	0.42
7:A2:578:C:O2'	7:A2:728:A:N3	2.50	0.42
7:A2:1271:A:H2'	7:A2:1272:G:H8	1.83	0.42
7:A2:1376:U:H2'	7:A2:1377:A:H8	1.84	0.42
7:A2:1402:4OC:H2'	7:A2:1403:C:O4'	2.18	0.42
7:A2:1522:U:OP1	17:K2:128:ARG:NH1	2.52	0.42
8:B2:94:HIS:ND1	8:B2:146:ASN:O	2.52	0.42
9:C1:162:ILE:HG21	28:V2:29:A:C8	2.54	0.42
18:L2:57:LEU:HD11	18:L2:82:ILE:HD11	2.01	0.42
19:M2:75:MET:HE2	19:M2:75:MET:HB2	1.89	0.42
28:V2:37:A:H4'	28:V2:38:A:H5'	2.01	0.42
29:W:10:G:O2'	29:W:11:U:OP1	2.27	0.42
39:h2:38:ARG:HB3	39:h2:98:PRO:HD3	2.00	0.42
5:72:580:U:H2'	5:72:581:C:C6	2.54	0.42
5:72:883:G:H1	5:72:893:C:H42	1.65	0.42
5:72:1021:A:O2'	5:72:1123:C:OP1	2.30	0.42
5:72:1265:A:H61	5:72:2013:A:H3'	1.84	0.42
5:72:2506:U:OP2	5:72:2576:G:N1	2.49	0.42
7:A1:198:G:N2	7:A1:219:U:O2	2.52	0.42
7:A1:488:C:H2'	7:A1:489:C:H6	1.83	0.42
7:A1:998:C:H2'	7:A1:999:C:C6	2.53	0.42
7:A1:1116:U:H2'	7:A1:1117:A:C8	2.54	0.42
7:A1:1350:A:H2'	7:A1:1351:U:O4'	2.20	0.42
7:A2:209:U:H3'	7:A2:210:C:H6	1.83	0.42
7:A2:459:A:C6	7:A2:474:G:H1'	2.55	0.42
7:A2:515:G:H3'	7:A2:516:U:H6	1.84	0.42
7:A2:748:G:H2'	7:A2:749:A:H8	1.84	0.42
7:A2:1112:C:C2	9:C2:178:LEU:HD23	2.54	0.42
7:A2:1534:A:O2'	24:R2:3:ARG:NH2	2.52	0.42
8:B:137:ARG:O	8:B:140:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B2:165:ASP:OD1	8:B2:166:ALA:N	2.52	0.42
10:D2:183:LYS:HG2	10:D2:184:ARG:HG2	2.02	0.42
11:E1:39:VAL:HG23	11:E1:71:MET:HE1	2.01	0.42
11:E1:164:ILE:HG13	11:E1:165:LEU:N	2.34	0.42
13:G2:43:VAL:O	13:G2:47:LEU:HD23	2.19	0.42
18:L2:86:ARG:HA	18:L2:94:ARG:HA	2.00	0.42
21:O2:64:ARG:HD2	21:O2:67:LEU:HD21	2.01	0.42
23:Q2:76:VAL:O	23:Q2:77:ARG:HG3	2.19	0.42
24:R2:73:ARG:NH1	24:R2:75:GLN:OE1	2.52	0.42
27:U1:32:VAL:HG12	27:U1:33:ARG:N	2.34	0.42
40:i2:88:GLY:O	40:i2:89:LYS:C	2.62	0.42
4:62:25:LYS:HE3	42:o2:64:PHE:HB3	2.01	0.42
5:72:1135:C:N4	5:72:1138:G:OP2	2.38	0.42
5:72:2131:U:H5'	5:72:2132:U:H2'	2.01	0.42
7:A1:106:C:H2'	7:A1:107:G:C8	2.55	0.42
7:A1:946:A:O2'	7:A1:1333:A:N3	2.47	0.42
7:A1:1009:U:H2'	7:A1:1010:U:C6	2.54	0.42
7:A1:1165:U:H2'	7:A1:1166:G:C8	2.54	0.42
7:A1:1216:A:H2'	7:A1:1217:C:H6	1.84	0.42
7:A1:1296:C:C5'	19:M1:14:HIS:HE2	2.31	0.42
7:A1:1447:A:OP1	7:A1:1448:C:N4	2.45	0.42
7:A1:1518:MA6:H2'	7:A1:1519:MA6:H8	2.01	0.42
7:A2:1254:A:H2'	7:A2:1255:G:C8	2.54	0.42
7:A2:1325:C:H2'	7:A2:1326:U:C6	2.54	0.42
7:A2:1518:MA6:O5'	7:A2:1518:MA6:H8	2.19	0.42
8:B:60:ILE:HG12	8:B:63:ARG:NH1	2.35	0.42
9:C1:167:TRP:HZ3	9:C1:169:ARG:HG2	1.84	0.42
12:F1:42:TRP:HB2	12:F1:59:TYR:HB2	2.01	0.42
12:F2:79:ARG:HG2	12:F2:80:PHE:CE1	2.55	0.42
14:H1:95:VAL:CG2	14:H1:102:ALA:HB2	2.49	0.42
14:H2:5:ASP:CG	14:H2:77:ARG:HH21	2.26	0.42
16:J1:81:GLU:H	16:J1:81:GLU:CD	2.27	0.42
16:J2:19:ASP:HA	16:J2:22:THR:HG22	2.00	0.42
25:S2:16:LEU:O	25:S2:19:VAL:HG12	2.20	0.42
27:U2:59:LYS:O	27:U2:63:GLU:HG2	2.19	0.42
32:Y1:41:A:H2'	32:Y1:42:G:C8	2.55	0.42
2:32:55:LYS:HB3	2:32:55:LYS:HE3	1.70	0.42
3:4:13:THR:N	3:4:31:ASP:OD2	2.52	0.42
5:72:864:G:H21	5:72:866:A:H62	1.68	0.42
5:72:967:U:H2'	5:72:968:C:C6	2.55	0.42
5:72:2110:G:O2'	5:72:2120:G:O4'	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:2262:U:H2'	5:72:2263:C:C6	2.54	0.42
5:72:2271:G:H5''	45:z2:18:ALA:HB3	2.01	0.42
5:72:2574:G:H2'	5:72:2575:C:C6	2.55	0.42
7:A1:352:C:H4'	7:A1:354:G:OP1	2.19	0.42
7:A1:390:U:H2'	7:A1:391:G:C8	2.54	0.42
7:A1:542:G:H2'	7:A1:543:U:C6	2.55	0.42
7:A1:707:U:H2'	7:A1:708:C:C6	2.54	0.42
7:A1:775:G:H2'	7:A1:776:G:C8	2.54	0.42
7:A1:828:U:H2'	7:A1:829:G:O4'	2.20	0.42
7:A2:94:G:H4'	7:A2:95:C:C5'	2.48	0.42
7:A2:404:G:OP1	10:D2:119:SER:OG	2.23	0.42
7:A2:664:G:P	24:R2:53:ARG:HH21	2.42	0.42
7:A2:986:U:H2'	7:A2:987:G:C8	2.54	0.42
7:A2:1530:G:O6	27:U2:46:LYS:NZ	2.39	0.42
8:B:90:PHE:CE2	8:B:154:MET:HG2	2.55	0.42
15:I2:23:PRO:HA	15:I2:61:LEU:HG	2.02	0.42
18:L2:63:VAL:HG21	18:L2:95:TYR:HE2	1.83	0.42
27:U2:10:GLU:O	27:U2:11:PRO:C	2.62	0.42
36:b2:225:MET:SD	36:b2:230:HIS:HB2	2.59	0.42
40:i2:114:GLU:OE2	40:i2:132:PHE:HB3	2.19	0.42
3:4:42:PRO:O	3:4:46:GLY:N	2.52	0.42
5:72:43:G:O2'	5:72:44:A:OP1	2.34	0.42
5:72:590:A:H61	5:72:666:A:H61	1.68	0.42
5:72:729:G:O5'	36:b2:207:LYS:NZ	2.53	0.42
5:72:1068:G:O6	5:72:1069:A:N6	2.53	0.42
5:72:1370:C:H2'	5:72:1371:G:O4'	2.20	0.42
5:72:2659:G:N2	5:72:2662:A:OP2	2.52	0.42
6:82:88:C:O5'	6:82:88:C:H6	2.02	0.42
7:A1:33:A:H2'	7:A1:34:C:H6	1.84	0.42
7:A1:621:A:H2'	7:A1:622:A:C8	2.54	0.42
7:A1:745:G:H2'	7:A1:746:A:H8	1.83	0.42
7:A1:1175:G:H2'	7:A1:1176:A:H8	1.85	0.42
7:A2:1:A:H3'	7:A2:2:A:C8	2.54	0.42
7:A2:838:G:N2	7:A2:849:G:H1'	2.35	0.42
7:A2:1060:U:P	20:N2:85:ARG:HH22	2.40	0.42
7:A2:1380:U:H1'	7:A2:1382:C:H41	1.85	0.42
7:A2:1512:U:H2'	7:A2:1513:A:C8	2.54	0.42
9:C1:121:THR:HG22	9:C1:189:ALA:HB2	2.01	0.42
9:C2:90:VAL:HA	9:C2:93:ASP:OD2	2.19	0.42
11:E2:80:THR:HG23	11:E2:122:ASN:O	2.19	0.42
11:E2:83:HIS:CG	14:H2:96:MET:HE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F2:80:PHE:HB3	36:b2:124:ILE:HD11	2.01	0.42
15:I2:57:MET:SD	15:I2:60:LYS:HE2	2.59	0.42
19:M1:15:ALA:O	19:M1:19:LEU:HD23	2.20	0.42
27:U1:54:LYS:HE3	27:U1:54:LYS:HB2	1.89	0.42
33:Y2:43:G:H2'	33:Y2:44:A:H8	1.85	0.42
5:72:590:A:N6	5:72:666:A:H61	2.17	0.42
5:72:969:G:H2'	5:72:970:U:C6	2.54	0.42
5:72:1645:G:H5''	5:72:1646:C:H5'	2.01	0.42
5:72:1796:U:H2'	5:72:1797:G:H8	1.84	0.42
5:72:1838:C:H4'	5:72:1839:G:C8	2.54	0.42
5:72:2182:U:H2'	5:72:2183:A:N7	2.35	0.42
7:A1:34:C:H2'	7:A1:35:G:H8	1.84	0.42
7:A1:142:G:H2'	7:A1:142:G:N3	2.33	0.42
7:A1:673:A:H61	7:A1:716:A:N6	2.18	0.42
7:A1:997:U:O2'	7:A1:998:C:H5'	2.20	0.42
7:A1:1145:A:H4'	7:A1:1146:A:H5''	2.02	0.42
7:A2:190:A:H3'	7:A2:191:G:H8	1.85	0.42
7:A2:202:G:H1	7:A2:215:C:N4	2.15	0.42
7:A2:518:C:H4'	7:A2:519:C:H5''	2.01	0.42
7:A2:845:A:OP1	24:R2:15:ALA:HA	2.20	0.42
7:A2:1114:C:H2'	7:A2:1115:U:C6	2.54	0.42
8:B:164:ILE:C	8:B:166:ALA:H	2.27	0.42
10:D1:14:ARG:HG3	10:D1:15:GLU:N	2.35	0.42
10:D2:202:GLU:OE1	11:E2:112:ARG:NH2	2.50	0.42
11:E1:26:LYS:HE3	11:E1:26:LYS:HB3	1.80	0.42
16:J1:10:LEU:O	16:J1:71:LEU:HA	2.20	0.42
19:M1:69:LEU:HD12	19:M1:72:GLU:OE2	2.19	0.42
25:S2:40:ILE:N	25:S2:69:HIS:O	2.36	0.42
27:U2:7:ARG:HB2	27:U2:10:GLU:HB2	2.01	0.42
31:X2:19:G:H21	31:X2:59:A:P	2.43	0.42
31:X2:47:G7M:O2'	31:X2:48:3AU:H5'A	2.19	0.42
31:X2:48:3AU:O4	31:X2:48:3AU:N40	2.52	0.42
36:b2:6:CYS:SG	36:b2:13:ARG:NH2	2.93	0.42
36:b2:135:ILE:HD12	36:b2:192:LEU:HD21	2.01	0.42
4:62:33:LEU:HD23	4:62:33:LEU:H	1.85	0.42
5:72:627:A:O4'	5:72:637:A:N6	2.52	0.42
7:A1:362:G:N2	7:A1:365:U:OP2	2.41	0.42
7:A1:677:U:O2	7:A1:777:A:O2'	2.36	0.42
7:A1:691:G:H22	7:A1:695:A:H3'	1.85	0.42
7:A1:824:G:H2'	7:A1:825:A:C8	2.54	0.42
7:A1:1133:G:H2'	7:A1:1134:G:H8	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:1288:A:H2'	7:A1:1289:A:C8	2.53	0.42
7:A1:1363:A:O2'	7:A1:1365:G:N7	2.45	0.42
7:A2:165:G:H2'	7:A2:166:U:C6	2.55	0.42
7:A2:497:G:N2	7:A2:498:A:N1	2.68	0.42
8:B2:126:PHE:CD2	8:B2:134:ALA:HB1	2.54	0.42
8:B2:213:TYR:O	8:B2:217:VAL:HG22	2.20	0.42
10:D2:26:ARG:HD3	10:D2:31:LYS:HD2	2.02	0.42
10:D2:85:ASN:HB3	10:D2:88:GLU:OE1	2.19	0.42
10:D2:161:LEU:HD23	10:D2:161:LEU:HA	1.89	0.42
11:E1:107:ALA:HB1	11:E1:111:MET:HE3	2.01	0.42
14:H2:25:VAL:HG13	14:H2:63:LEU:HD11	2.01	0.42
19:M1:107:ARG:NE	19:M1:107:ARG:HA	2.35	0.42
3:4:58:ASP:N	3:4:58:ASP:OD1	2.52	0.42
5:72:971:G:O2'	5:72:983:A:N3	2.49	0.42
5:72:1327:A:H2'	5:72:1328:A:O4'	2.20	0.42
5:72:1440:U:H2'	5:72:1441:G:C8	2.54	0.42
5:72:1469:A:H2'	5:72:1470:A:C8	2.55	0.42
5:72:1720:U:H2'	5:72:1721:G:O4'	2.20	0.42
5:72:1847:A:O2'	5:72:1848:A:P	2.78	0.42
5:72:2794:C:H2'	5:72:2795:C:C6	2.54	0.42
7:A1:72:A:H2'	7:A1:73:C:H6	1.84	0.42
7:A1:97:G:H2'	7:A1:98:A:O4'	2.19	0.42
7:A1:270:A:H2'	7:A1:271:C:O4'	2.20	0.42
7:A1:398:U:H2'	7:A1:399:G:C8	2.54	0.42
7:A1:824:G:H2'	7:A1:825:A:H8	1.84	0.42
7:A2:90:C:H1'	7:A2:91:U:H5'	2.02	0.42
7:A2:471:U:H2'	7:A2:472:U:C6	2.55	0.42
7:A2:945:G:N3	7:A2:945:G:H2'	2.34	0.42
7:A2:966:2MG:H2'	7:A2:967:5MC:C6	2.55	0.42
9:C2:123:GLN:HB3	9:C2:128:VAL:HB	2.01	0.42
9:C2:136:ARG:HA	9:C2:136:ARG:HD3	1.71	0.42
15:I1:81:HIS:CE1	15:I1:106:ARG:HG2	2.55	0.42
17:K1:89:PRO:CB	27:U1:32:VAL:HG11	2.50	0.42
29:W:35:C:H2'	29:W:36:A:H8	1.85	0.42
31:X2:51:G:H2'	31:X2:52:A:H8	1.85	0.42
39:h2:24:THR:O	39:h2:34:LYS:NZ	2.52	0.42
39:h2:105:MET:SD	39:h2:108:VAL:HG21	2.60	0.42
44:r2:58:ILE:HG13	44:r2:58:ILE:O	2.19	0.42
2:32:55:LYS:HD2	2:32:57:GLU:OE2	2.19	0.42
3:4:48:GLN:HG3	3:4:48:GLN:O	2.19	0.42
5:72:215:G:H4'	5:72:216:A:H4'	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:355:U:H2'	5:72:356:G:C8	2.53	0.42
5:72:1486:U:H2'	5:72:1487:U:C6	2.54	0.42
5:72:1677:A:H2'	5:72:1678:A:C8	2.54	0.42
5:72:2137:U:H2'	5:72:2138:G:O4'	2.20	0.42
5:72:2263:C:N4	45:z2:15:ASP:OD1	2.53	0.42
7:A1:96:U:H2'	7:A1:97:G:H8	1.85	0.42
7:A1:302:G:H2'	7:A1:303:A:H8	1.85	0.42
7:A1:1148:U:H2'	7:A1:1149:C:O4'	2.20	0.42
7:A1:1418:A:C2'	7:A1:1419:G:H5''	2.50	0.42
7:A2:601:G:H2'	7:A2:602:A:C8	2.54	0.42
7:A2:1479:C:H2'	7:A2:1480:A:C8	2.55	0.42
9:C2:22:TRP:HB3	9:C2:59:ARG:H	1.85	0.42
12:F1:51:ILE:O	12:F1:51:ILE:HG13	2.19	0.42
14:H1:25:VAL:HG13	14:H1:63:LEU:HD11	2.02	0.42
14:H1:96:MET:HB3	14:H1:100:GLY:N	2.31	0.42
15:I1:44:ALA:O	15:I1:47:VAL:HG12	2.20	0.42
16:J1:57:VAL:HG12	16:J1:58:ASN:N	2.25	0.42
20:N2:83:LYS:HA	20:N2:83:LYS:HE3	2.00	0.42
23:Q1:26:GLU:HG2	23:Q1:26:GLU:O	2.20	0.42
28:V2:19:G:H8	28:V2:19:G:OP2	2.03	0.42
28:V2:33:A:H2'	28:V2:34:A:C8	2.54	0.42
36:b2:144:VAL:HG21	36:b2:162:VAL:HG11	2.02	0.42
44:r2:54:VAL:HG23	44:r2:54:VAL:O	2.19	0.42
3:4:56:ARG:HD3	25:S2:65:GLU:O	2.20	0.42
5:71:1913:A:C8	7:A1:1494:G:H4'	2.54	0.42
5:72:189:G:H2'	5:72:205:G:N2	2.35	0.42
5:72:833:A:H2'	5:72:834:G:H8	1.83	0.42
7:A1:302:G:H2'	7:A1:303:A:C8	2.55	0.42
7:A1:398:U:H2'	7:A1:399:G:H8	1.85	0.42
7:A1:839:C:H2'	7:A1:840:C:C6	2.55	0.42
7:A1:1086:U:H2'	7:A1:1087:G:H8	1.84	0.42
7:A1:1113:C:H42	7:A1:1187:G:H1	1.67	0.42
7:A1:1251:A:H2'	7:A1:1252:A:O4'	2.20	0.42
7:A1:1257:A:H5''	7:A1:1258:G:C8	2.55	0.42
7:A2:106:C:H2'	7:A2:107:G:C8	2.55	0.42
7:A2:243:A:H62	7:A2:281:G:H1'	1.84	0.42
7:A2:334:C:H2'	7:A2:335:C:C6	2.55	0.42
7:A2:715:A:H2'	7:A2:716:A:C8	2.55	0.42
7:A2:776:G:O2'	7:A2:777:A:H8	2.03	0.42
7:A2:1125:U:O2'	7:A2:1126:U:H3'	2.19	0.42
8:B:32:PHE:HD2	8:B:40:ILE:HB	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:210:VAL:HA	8:B:213:TYR:CD2	2.55	0.42
9:C2:185:ASN:CG	9:C2:186:THR:H	2.24	0.42
10:D2:107:PHE:CG	10:D2:145:ILE:HD11	2.54	0.42
11:E2:164:ILE:HG13	11:E2:165:LEU:N	2.35	0.42
12:F2:80:PHE:CG	36:b2:124:ILE:HD11	2.55	0.42
15:I1:123:ARG:NH1	15:I1:124:ARG:O	2.46	0.42
15:I2:95:ARG:HD3	15:I2:95:ARG:HA	1.86	0.42
16:J2:44:THR:HG23	16:J2:69:THR:O	2.20	0.42
17:K1:23:ILE:N	17:K1:85:MET:O	2.48	0.42
18:L2:43:LYS:CG	18:L2:44:LYS:H	2.32	0.42
20:N2:76:LYS:HG3	20:N2:77:PHE:CD2	2.53	0.42
23:Q2:30:LYS:HE3	23:Q2:35:GLY:HA2	2.02	0.42
27:U1:49:LYS:HE2	27:U1:49:LYS:HB2	1.77	0.42
42:o2:51:GLU:HG3	42:o2:51:GLU:O	2.19	0.42
5:72:455:C:N3	5:72:472:A:H2'	2.35	0.41
5:72:749:A:OP2	48:72:3003:SPD:N1	2.53	0.41
5:72:813:U:H2'	5:72:814:C:C6	2.55	0.41
5:72:2061:G:H5'	5:72:2503:2MA:C2	2.50	0.41
7:A1:62:U:H2'	7:A1:63:C:C6	2.55	0.41
7:A1:189:A:H2'	7:A1:190:A:O4'	2.20	0.41
7:A1:684:U:H1'	17:K1:40:ASN:HA	2.02	0.41
7:A1:745:G:H1'	7:A1:836:G:O2'	2.21	0.41
7:A1:751:U:H4'	21:O1:24:SER:HA	2.01	0.41
7:A1:776:G:H22	7:A1:802:A:P	2.42	0.41
7:A1:1118:U:H2'	7:A1:1119:C:C6	2.54	0.41
7:A1:1296:C:O4'	7:A1:1302:C:N4	2.52	0.41
7:A1:1306:A:H2'	7:A1:1307:U:O4'	2.20	0.41
7:A1:1450:U:O2'	7:A1:1451:U:H2'	2.20	0.41
7:A2:158:G:H2'	7:A2:159:G:H8	1.85	0.41
7:A2:321:A:H2'	7:A2:322:C:C6	2.55	0.41
7:A2:322:C:H2'	7:A2:323:U:C6	2.55	0.41
7:A2:434:U:H2'	7:A2:435:A:H8	1.85	0.41
7:A2:728:A:H2'	7:A2:729:A:C8	2.55	0.41
7:A2:1170:A:H2'	7:A2:1171:A:O4'	2.21	0.41
7:A2:1312:G:H2'	7:A2:1313:U:H6	1.85	0.41
8:B:5:SER:C	8:B:7:ARG:H	2.27	0.41
8:B:71:GLY:HA3	8:B:93:ASN:O	2.20	0.41
8:B:90:PHE:HB3	8:B:150:GLY:O	2.20	0.41
16:J2:36:VAL:HG12	16:J2:76:ILE:HG13	2.02	0.41
29:W:51:G:O2'	29:W:52:A:H5'	2.20	0.41
33:Y2:18:G:H1	33:Y2:55:PSU:H1'	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:b2:122:ALA:O	36:b2:130:LEU:HD21	2.20	0.41
5:72:1487:U:H2'	5:72:1488:C:C6	2.55	0.41
5:72:2183:A:H2'	5:72:2184:A:C8	2.55	0.41
6:82:7:G:O2'	44:r2:38:GLN:OE1	2.37	0.41
6:82:38:C:C2'	6:82:39:A:H5'	2.50	0.41
6:82:41:G:P	6:82:43:C:H41	2.43	0.41
7:A1:70:U:H1'	7:A1:71:A:N7	2.35	0.41
7:A1:188:C:H2'	7:A1:189:A:O4'	2.20	0.41
7:A1:891:U:H2'	7:A1:892:A:C8	2.46	0.41
7:A1:1134:G:H3'	7:A1:1135:U:H5''	2.03	0.41
7:A1:1489:G:H2'	7:A1:1490:U:H6	1.84	0.41
7:A2:33:A:H2'	7:A2:34:C:C6	2.55	0.41
7:A2:59:A:H3'	7:A2:331:G:H22	1.85	0.41
7:A2:279:A:H5''	7:A2:281:G:O4'	2.20	0.41
7:A2:496:A:O2'	7:A2:497:G:H3'	2.21	0.41
7:A2:736:C:H2'	7:A2:737:C:C6	2.55	0.41
7:A2:1011:C:H2'	7:A2:1012:A:H8	1.79	0.41
7:A2:1144:G:H21	7:A2:1146:A:H62	1.66	0.41
7:A2:1247:U:C2'	7:A2:1248:A:H5''	2.49	0.41
7:A2:1258:G:H2'	7:A2:1259:C:H6	1.85	0.41
7:A2:1463:U:H2'	7:A2:1464:U:C6	2.55	0.41
8:B:16:PHE:O	8:B:203:ASN:ND2	2.53	0.41
8:B:58:ASN:ND2	8:B:223:GLU:OE1	2.53	0.41
8:B2:98:GLY:HA2	8:B2:171:ILE:HD11	2.02	0.41
9:C1:184:TYR:CE1	9:C1:199:LYS:HB3	2.56	0.41
12:F1:35:LYS:HE3	12:F1:35:LYS:HB3	1.86	0.41
12:F2:40:GLU:OE2	12:F2:99:ALA:HA	2.20	0.41
13:G2:145:ALA:O	13:G2:146:GLU:C	2.63	0.41
14:H1:105:SER:HB2	14:H1:126:ILE:HD11	2.02	0.41
16:J2:5:ARG:HG2	16:J2:77:VAL:HA	2.01	0.41
18:L1:110:ARG:HD3	18:L1:117:TYR:CD2	2.55	0.41
23:Q1:7:THR:OG1	23:Q1:60:GLU:OE2	2.30	0.41
28:V2:48:C:H42	31:X2:37:G:H1	1.67	0.41
32:Y1:43:G:H3'	32:Y1:44:G:H8	1.85	0.41
5:72:873:C:H2'	5:72:874:G:C8	2.55	0.41
5:72:1094:U:O2'	5:72:1096:A:N7	2.46	0.41
5:72:1190:G:H2'	5:72:1191:G:H8	1.85	0.41
5:72:1497:U:H5''	5:72:1498:C:H5	1.85	0.41
5:72:2167:U:N3	5:72:2170:A:OP2	2.46	0.41
5:72:2526:G:H1	5:72:2537:U:H3	1.68	0.41
5:72:2583:G:C5	5:72:2584:U:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:38:G:N1	7:A1:397:A:OP1	2.40	0.41
7:A1:929:G:H2'	7:A1:930:C:H6	1.85	0.41
7:A1:1119:C:H2'	7:A1:1120:C:C6	2.54	0.41
7:A1:1169:A:H3'	7:A1:1170:A:H8	1.85	0.41
7:A1:1187:G:H2'	7:A1:1188:A:H8	1.85	0.41
7:A2:187:G:N2	7:A2:189:A:H3'	2.35	0.41
7:A2:409:U:H2'	7:A2:410:G:O4'	2.21	0.41
7:A2:693:G:OP1	17:K2:127:ARG:NH2	2.48	0.41
7:A2:865:A:H5'	7:A2:1078:U:C5	2.55	0.41
7:A2:1271:A:H2'	7:A2:1272:G:C8	2.56	0.41
9:C2:7:PRO:HG3	9:C2:201:TRP:HE1	1.85	0.41
14:H1:127:CYS:SG	14:H1:128:TYR:N	2.93	0.41
18:L1:30:LYS:HB3	18:L1:57:LEU:HD12	2.02	0.41
23:Q2:28:PHE:CE2	23:Q2:37:PHE:HB3	2.56	0.41
24:R1:33:ILE:HD12	24:R1:33:ILE:HA	1.93	0.41
24:R2:5:PHE:HA	24:R2:43:ARG:HB3	2.02	0.41
35:a2:34:ALA:HB2	35:a2:178:VAL:HG21	2.02	0.41
36:b2:145:GLU:OE2	36:b2:151:GLY:N	2.32	0.41
3:4:57:VAL:HG22	25:S2:67:VAL:HG21	2.03	0.41
5:72:558:U:H2'	5:72:559:G:C8	2.55	0.41
5:72:760:G:H2'	5:72:761:A:O4'	2.20	0.41
5:72:1047:G:N2	5:72:1110:G:O2'	2.53	0.41
5:72:1385:A:H1'	5:72:1386:C:C6	2.55	0.41
5:72:2660:A:H2'	5:72:2661:G:O4'	2.20	0.41
7:A1:210:C:H1'	7:A1:211:G:N2	2.35	0.41
7:A1:409:U:H2'	7:A1:410:G:O4'	2.19	0.41
7:A1:436:C:H2'	7:A1:437:U:H6	1.85	0.41
7:A1:1201:A:H4'	7:A1:1202:U:O5'	2.19	0.41
7:A1:1292:G:H2'	7:A1:1293:C:C6	2.56	0.41
7:A1:1307:U:H1'	19:M1:108:THR:HG21	2.01	0.41
7:A1:1309:G:H2'	7:A1:1310:G:O4'	2.19	0.41
7:A1:1381:U:H2'	7:A1:1382:C:O4'	2.20	0.41
7:A1:1537:U:H1'	7:A1:1538:C:C5	2.55	0.41
7:A2:341:C:H2'	7:A2:342:C:C6	2.55	0.41
7:A2:410:G:H2'	7:A2:429:U:C4	2.56	0.41
7:A2:432:A:H2'	7:A2:433:G:O4'	2.20	0.41
7:A2:950:U:H2'	7:A2:951:G:C8	2.55	0.41
7:A2:1005:A:H2'	7:A2:1006:G:O4'	2.19	0.41
8:B:102:THR:OG1	8:B:103:ASN:N	2.53	0.41
8:B2:196:VAL:HG11	8:B2:199:VAL:HG23	2.01	0.41
9:C1:12:LEU:HD23	9:C1:12:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C1:132:ARG:HE	28:V2:34:A:N6	2.18	0.41
10:D2:152:GLN:HB3	10:D2:155:VAL:HG23	2.03	0.41
24:R2:57:ARG:O	24:R2:61:ARG:HG3	2.20	0.41
26:T1:82:GLN:O	26:T1:85:LYS:HG3	2.19	0.41
28:V2:21:U:H2'	28:V2:22:U:C6	2.54	0.41
40:i2:72:ILE:HB	40:i2:108:VAL:HG11	2.03	0.41
5:72:542:C:H2'	5:72:543:G:C8	2.55	0.41
5:72:600:G:H1	5:72:657:U:H3	1.68	0.41
5:72:851:C:H2'	5:72:852:U:C6	2.56	0.41
5:72:873:C:H2'	5:72:874:G:H8	1.84	0.41
5:72:1864:U:OP1	5:72:2410:G:O2'	2.36	0.41
7:A1:283:U:H2'	7:A1:284:C:C6	2.56	0.41
7:A1:370:C:H2'	7:A1:371:A:H8	1.81	0.41
7:A1:488:C:H2'	7:A1:489:C:C6	2.56	0.41
7:A1:1116:U:H3	7:A1:1184:G:H1	1.68	0.41
7:A1:1121:U:H2'	7:A1:1122:U:C6	2.56	0.41
7:A2:501:C:H2'	7:A2:502:A:O4'	2.21	0.41
7:A2:519:C:H2'	7:A2:520:A:O4'	2.21	0.41
7:A2:1029:U:H2'	7:A2:1030:U:C6	2.53	0.41
7:A2:1078:U:H4'	11:E2:138:ARG:NH1	2.35	0.41
7:A2:1227:A:OP2	19:M2:110:LYS:NZ	2.53	0.41
11:E1:80:THR:HG23	11:E1:122:ASN:O	2.20	0.41
14:H2:10:MET:HG3	14:H2:27:MET:HE1	2.02	0.41
14:H2:127:CYS:SG	14:H2:128:TYR:N	2.93	0.41
15:I2:29:VAL:HG13	15:I2:64:TYR:HA	2.02	0.41
18:L2:112:GLN:OE1	18:L2:112:GLN:N	2.54	0.41
23:Q2:16:LYS:O	23:Q2:16:LYS:HD3	2.19	0.41
40:i2:68:ARG:H	40:i2:68:ARG:HG2	1.71	0.41
5:72:1416:G:O2'	5:72:1417:C:P	2.79	0.41
5:72:1417:C:H42	5:72:1581:G:H1	1.69	0.41
5:72:1447:C:H2'	5:72:1448:G:C8	2.55	0.41
5:72:1869:G:H2'	5:72:1871:A:N7	2.35	0.41
5:72:2148:G:H8	5:72:2148:G:OP2	2.03	0.41
5:72:2204:G:O2'	36:b2:148:PRO:O	2.35	0.41
5:72:2395:C:H2'	5:72:2396:G:C8	2.55	0.41
7:A1:1146:A:H3'	7:A1:1147:C:H6	1.86	0.41
7:A2:400:C:H2'	7:A2:401:C:O4'	2.21	0.41
7:A2:454:G:H1'	7:A2:479:U:C4	2.55	0.41
7:A2:634:C:H2'	7:A2:635:A:C8	2.56	0.41
7:A2:831:A:H2'	7:A2:832:G:C8	2.55	0.41
7:A2:995:C:H2'	7:A2:996:A:H5''	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A2:1021:A:H2'	7:A2:1022:A:H5''	2.02	0.41
7:A2:1132:C:H3'	7:A2:1133:G:H8	1.86	0.41
7:A2:1147:C:H4'	15:I2:7:TYR:CE2	2.56	0.41
7:A2:1436:U:H2'	7:A2:1437:A:H8	1.86	0.41
8:B:117:LEU:HD23	8:B:141:LEU:HD13	2.02	0.41
8:B:145:GLU:O	8:B:146:ASN:C	2.63	0.41
8:B2:23:TRP:CZ3	8:B2:25:PRO:HA	2.56	0.41
9:C2:49:LYS:HE2	9:C2:49:LYS:HB3	1.90	0.41
10:D1:34:ILE:HG22	10:D1:35:GLU:H	1.86	0.41
13:G2:103:TRP:CG	13:G2:137:LYS:HD3	2.56	0.41
15:I2:10:GLY:HA2	15:I2:81:HIS:ND1	2.36	0.41
23:Q1:77:ARG:CZ	23:Q1:77:ARG:HB3	2.51	0.41
23:Q2:54:GLY:O	23:Q2:57:ASP:HB2	2.21	0.41
31:X2:37:G:H2'	31:X2:38:2MA:O4'	2.20	0.41
39:h2:42:THR:HG22	39:h2:93:VAL:HG12	2.03	0.41
5:72:371:A:OP1	5:72:371:A:H3'	2.21	0.41
5:72:749:A:C8	5:72:1618:6MZ:C6	3.03	0.41
5:72:1838:C:H4'	5:72:1839:G:H8	1.86	0.41
7:A1:321:A:H2'	7:A1:322:C:C6	2.56	0.41
7:A1:412:A:O2'	7:A1:413:G:C5'	2.68	0.41
7:A1:455:G:H2'	7:A1:456:A:C8	2.56	0.41
7:A1:675:A:H2'	7:A1:676:A:O4'	2.21	0.41
7:A1:899:C:H6	7:A1:899:C:O5'	2.04	0.41
7:A1:1157:A:H1'	7:A1:1181:G:H22	1.84	0.41
7:A1:1232:U:H2'	7:A1:1233:G:H8	1.85	0.41
7:A1:1245:C:H2'	7:A1:1246:A:C8	2.56	0.41
7:A2:202:G:H2'	7:A2:203:G:O4'	2.20	0.41
7:A2:911:U:H2'	7:A2:912:C:C6	2.56	0.41
7:A2:1128:C:C2'	7:A2:1129:C:H5'	2.50	0.41
7:A2:1323:G:H2'	7:A2:1324:A:H8	1.85	0.41
8:B:67:ILE:HG22	8:B:68:LEU:N	2.36	0.41
9:C1:28:GLU:H	9:C1:28:GLU:CD	2.28	0.41
9:C2:11:ARG:HD2	9:C2:178:LEU:HA	2.02	0.41
10:D1:58:LYS:HE3	10:D1:58:LYS:HB3	1.96	0.41
11:E2:81:LEU:HD12	11:E2:123:VAL:HG23	2.02	0.41
17:K1:52:PHE:O	17:K1:53:ARG:HD2	2.20	0.41
18:L2:3:THR:HG22	18:L2:5:ASN:H	1.86	0.41
19:M1:4:ILE:HD13	19:M1:19:LEU:HD11	2.03	0.41
20:N1:76:LYS:HG3	20:N1:77:PHE:CD2	2.56	0.41
26:T1:58:VAL:HG23	26:T1:59:ASP:N	2.36	0.41
38:g2:32:GLU:OE1	38:g2:32:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:o2:35:HIS:C	42:o2:36:LYS:HG2	2.46	0.41
5:72:1703:G:H2'	5:72:1704:C:C6	2.56	0.41
7:A1:295:C:H2'	7:A1:296:U:H6	1.85	0.41
7:A1:1242:G:N2	7:A1:1295:U:C2	2.89	0.41
7:A2:528:C:H3'	7:A2:529:G:H8	1.85	0.41
7:A2:543:U:H2'	7:A2:544:G:H8	1.84	0.41
7:A2:543:U:H2'	7:A2:544:G:C8	2.55	0.41
7:A2:574:A:H1'	7:A2:883:C:H1'	2.03	0.41
7:A2:846:G:O2'	7:A2:847:G:H5'	2.21	0.41
7:A2:1025:U:O5'	7:A2:1025:U:H6	2.03	0.41
7:A2:1105:A:H2'	7:A2:1106:G:H8	1.86	0.41
9:C2:9:GLY:HA3	20:N2:89:MET:SD	2.61	0.41
12:F2:21:MET:HA	12:F2:24:ARG:HD3	2.03	0.41
15:I1:100:LYS:C	15:I1:102:GLY:H	2.28	0.41
19:M1:107:ARG:CZ	19:M1:113:ARG:HH11	2.33	0.41
23:Q1:28:PHE:CE2	23:Q1:37:PHE:HB3	2.55	0.41
29:W:35:C:H2'	29:W:36:A:C8	2.55	0.41
31:X2:5:C:H2'	31:X2:6:C:C6	2.56	0.41
31:X2:15:G:H5'	31:X2:17:H2U:N3	2.36	0.41
45:z2:25:ARG:NH1	45:z2:31:VAL:HG12	2.36	0.41
1:12:39:TRP:HB2	1:12:46:PHE:CE1	2.56	0.41
5:72:373:U:H2'	5:72:374:A:H8	1.84	0.41
5:72:1053:C:H2'	5:72:1054:A:C8	2.55	0.41
5:72:2162:G:H4'	5:72:2173:A:C4	2.55	0.41
5:72:2421:G:H2'	31:X2:77:A:N6	2.36	0.41
5:72:2469:A:N6	5:72:2481:G:H1'	2.36	0.41
5:72:2557:G:H2'	5:72:2558:C:C6	2.56	0.41
6:82:33:G:C2	6:82:34:A:H1'	2.56	0.41
6:82:78:A:H2'	6:82:79:G:O4'	2.20	0.41
7:A1:52:C:H42	7:A1:359:G:H1	1.69	0.41
7:A1:93:U:H6	7:A1:93:U:O5'	2.04	0.41
7:A1:97:G:C2	7:A1:98:A:H1'	2.56	0.41
7:A1:129:A:O2'	7:A1:130:A:H2'	2.21	0.41
7:A1:254:G:C2	7:A1:255:G:C8	3.09	0.41
7:A1:295:C:H2'	7:A1:296:U:C6	2.56	0.41
7:A1:403:C:H2'	7:A1:404:G:C8	2.55	0.41
7:A1:439:U:C4	7:A1:440:C:C4	3.09	0.41
7:A1:738:C:OP1	12:F1:4:TYR:OH	2.33	0.41
7:A1:813:U:H2'	7:A1:814:A:H8	1.85	0.41
7:A1:828:U:P	14:H1:22:LYS:HZ1	2.44	0.41
7:A1:1009:U:H2'	7:A1:1010:U:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:1013:G:H21	7:A1:1015:G:H3'	1.85	0.41
7:A1:1119:C:H2'	7:A1:1120:C:H6	1.86	0.41
7:A1:1260:G:O2'	7:A1:1283:U:H4'	2.21	0.41
7:A1:1333:A:H3'	7:A1:1334:G:C8	2.53	0.41
7:A1:1486:G:H2'	7:A1:1487:G:H8	1.86	0.41
7:A2:87:C:C4	7:A2:88:U:H1'	2.56	0.41
7:A2:140:U:H3'	7:A2:141:G:H5''	2.02	0.41
7:A2:143:A:H2	7:A2:220:G:H1	1.68	0.41
7:A2:158:G:H2'	7:A2:159:G:C8	2.56	0.41
7:A2:266:G:H1'	7:A2:268:U:OP2	2.21	0.41
7:A2:522:C:H1'	7:A2:536:C:H5''	2.03	0.41
7:A2:1161:C:H42	7:A2:1175:G:H1	1.68	0.41
7:A2:1173:U:H2'	7:A2:1174:G:O4'	2.21	0.41
8:B:41:ILE:H	8:B:41:ILE:HD12	1.84	0.41
8:B:45:LYS:HD3	8:B:45:LYS:HA	1.88	0.41
8:B:231:SER:N	8:B2:35:ARG:HG2	2.30	0.41
9:C1:184:TYR:HB2	9:C1:201:TRP:CD1	2.56	0.41
10:D1:47:ARG:NE	28:V2:32:U:OP1	2.53	0.41
10:D1:48:LEU:HD23	10:D1:53:VAL:HG12	2.03	0.41
11:E1:156:LYS:HE2	14:H1:71:VAL:HA	2.02	0.41
12:F1:4:TYR:CD2	12:F1:71:ILE:HG13	2.55	0.41
12:F1:23:GLU:OE1	12:F1:23:GLU:N	2.41	0.41
13:G1:146:GLU:HA	13:G1:146:GLU:OE1	2.21	0.41
16:J2:9:ARG:HG3	16:J2:73:LEU:HD13	2.02	0.41
16:J2:52:LEU:CD1	20:N2:81:ARG:HD2	2.50	0.41
16:J2:63:ASP:OD1	20:N2:98:LYS:HG3	2.20	0.41
18:L1:80:ILE:HG22	18:L1:81:LEU:N	2.36	0.41
18:L1:89:ASP:C	18:L1:90:LEU:HD22	2.46	0.41
18:L2:13:ALA:O	18:L2:15:LYS:NZ	2.50	0.41
18:L2:63:VAL:HG21	18:L2:95:TYR:CE2	2.56	0.41
21:O2:3:LEU:HD23	21:O2:8:THR:HG22	2.02	0.41
22:P1:68:SER:HB3	22:P1:71:VAL:HG22	2.01	0.41
23:Q1:71:LYS:HB3	23:Q1:71:LYS:HE2	1.79	0.41
26:T1:64:LYS:HB3	26:T1:66:LEU:HD13	2.03	0.41
28:V2:8:A:H2'	28:V2:8:A:N3	2.35	0.41
43:p:32:ARG:C	43:p:34:ALA:N	2.79	0.41
44:r2:62:LEU:HD12	44:r2:62:LEU:O	2.21	0.41
5:72:572:A:H5''	5:72:573:U:OP2	2.21	0.41
5:72:627:A:H4'	5:72:628:G:H5'	2.03	0.41
5:72:1139:G:O2'	5:72:1143:A:N1	2.44	0.41
5:72:1275:A:N1	5:72:1295:C:O2'	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:72:1429:G:H2'	5:72:1430:G:H8	1.86	0.41
5:72:1723:G:H2'	5:72:1724:G:O4'	2.21	0.41
5:72:1853:A:N1	5:72:2087:G:H1'	2.36	0.41
7:A1:588:G:H2'	7:A1:589:U:H6	1.85	0.41
7:A1:730:G:N2	7:A1:765:G:H5''	2.36	0.41
7:A1:821:G:H2'	7:A1:822:U:C6	2.56	0.41
7:A1:953:G:O6	19:M1:103:LYS:HE2	2.21	0.41
7:A1:967:5MC:H3'	7:A1:968:A:H2'	2.03	0.41
7:A1:1048:G:H2'	7:A1:1050:G:C8	2.53	0.41
7:A1:1095:U:H2'	7:A1:1096:C:C6	2.56	0.41
7:A1:1151:A:H5''	16:J1:44:THR:H	1.86	0.41
7:A1:1466:C:H2'	7:A1:1467:C:O4'	2.21	0.41
7:A2:604:G:H2'	7:A2:605:U:O4'	2.22	0.41
7:A2:939:G:O5'	13:G2:102:ARG:NH1	2.54	0.41
8:B2:20:THR:O	8:B2:21:ARG:C	2.64	0.41
8:B2:27:MET:HG2	8:B2:193:PRO:HD3	2.02	0.41
9:C2:169:ARG:HE	9:C2:169:ARG:HB2	1.74	0.41
12:F2:90:MET:HE2	12:F2:90:MET:HB3	1.96	0.41
13:G2:53:ARG:O	13:G2:54:SER:HB2	2.21	0.41
19:M2:15:ALA:O	19:M2:19:LEU:HD23	2.21	0.41
20:N1:93:ILE:HA	20:N1:94:PRO:HD3	1.86	0.41
22:P1:8:ARG:HG3	22:P1:17:TYR:CE1	2.56	0.41
35:a2:38:PHE:HZ	35:a2:217:THR:HG21	1.85	0.41
40:i2:54:LEU:HD13	40:i2:54:LEU:HA	1.93	0.41
45:z2:71:VAL:HG13	45:z2:77:ARG:O	2.21	0.41
5:72:594:U:H2'	5:72:595:C:C6	2.56	0.40
5:72:1405:U:H2'	5:72:1406:U:C6	2.56	0.40
5:72:2142:A:H61	5:72:2148:G:H1	1.68	0.40
7:A1:212:G:H3'	7:A1:213:G:H8	1.86	0.40
7:A1:554:A:H2'	7:A1:555:U:C6	2.57	0.40
7:A1:643:C:H5''	14:H1:32:LEU:HD11	2.03	0.40
7:A1:802:A:H3'	7:A1:803:G:H8	1.85	0.40
7:A1:1005:A:H3'	7:A1:1006:G:C8	2.55	0.40
7:A1:1343:G:H2'	7:A1:1344:C:O4'	2.22	0.40
7:A1:1348:U:H2'	7:A1:1349:A:C8	2.53	0.40
7:A2:368:U:H6	7:A2:368:U:H2'	1.67	0.40
7:A2:420:U:H1'	7:A2:424:G:N2	2.36	0.40
7:A2:427:U:C4	7:A2:428:G:C5	3.10	0.40
7:A2:1073:U:H2'	7:A2:1074:G:O4'	2.20	0.40
7:A2:1377:A:H4'	7:A2:1378:C:H5	1.87	0.40
8:B:2:ALA:HB1	8:B:54:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B2:104:TRP:CZ2	8:B2:156:GLY:HA2	2.56	0.40
8:B2:210:VAL:HA	8:B2:213:TYR:CD2	2.56	0.40
8:B2:218:ALA:O	8:B2:222:ARG:HG2	2.21	0.40
9:C1:96:GLY:O	9:C1:97:VAL:HB	2.21	0.40
9:C2:30:ALA:HA	9:C2:33:LEU:HD12	2.03	0.40
12:F2:56:LYS:HE2	12:F2:56:LYS:HB3	1.93	0.40
16:J1:49:PHE:HE2	16:J1:67:ILE:HG12	1.85	0.40
23:Q2:60:GLU:HG2	23:Q2:77:ARG:NH2	2.35	0.40
3:4:34:LEU:CD2	37:e2:106:ILE:HD12	2.42	0.40
5:72:749:A:H5'	5:72:749:A:H8	1.86	0.40
5:72:1128:G:N7	5:72:2489:U:O2'	2.55	0.40
5:72:1747:U:H2'	5:72:1748:C:C6	2.56	0.40
5:72:1935:G:N2	5:72:1964:G:H5'	2.37	0.40
5:72:1999:C:H2'	5:72:2000:C:C6	2.56	0.40
7:A1:1024:G:H2'	7:A1:1025:U:O4'	2.22	0.40
7:A1:1317:C:OP1	20:N1:56:SER:OG	2.28	0.40
7:A1:1398:A:H5''	7:A1:1401:G:H4'	2.03	0.40
7:A2:380:G:N2	7:A2:384:G:N7	2.70	0.40
7:A2:427:U:C3'	7:A2:428:G:H5''	2.46	0.40
7:A2:512:U:H2'	7:A2:513:C:C6	2.57	0.40
7:A2:1088:G:H21	7:A2:1167:A:H61	1.69	0.40
7:A2:1300:G:N2	7:A2:1301:U:O4	2.53	0.40
8:B:115:LYS:HB3	8:B:115:LYS:HE2	1.90	0.40
8:B2:20:THR:HA	8:B2:39:HIS:NE2	2.36	0.40
9:C1:182:ILE:HG22	9:C1:203:PHE:HA	2.04	0.40
9:C2:156:ARG:HD3	9:C2:193:TYR:O	2.21	0.40
20:N2:33:ASP:O	20:N2:41:ARG:NH1	2.52	0.40
21:O2:4:SER:O	21:O2:8:THR:HG23	2.20	0.40
24:R2:8:ARG:HB3	24:R2:10:PHE:CE1	2.56	0.40
26:T1:49:LYS:HE3	26:T1:49:LYS:HB3	1.77	0.40
29:W:2:G:H2'	29:W:3:G:H8	1.86	0.40
29:W:16:H2U:O4	29:W:59:G:N2	2.53	0.40
32:Y1:9:A:H2'	32:Y1:11:C:H41	1.85	0.40
33:Y2:18:G:O2'	33:Y2:57:G:N2	2.43	0.40
36:b2:210:ALA:HA	36:b2:213:TRP:CE3	2.56	0.40
38:g2:50:LYS:HE2	38:g2:50:LYS:HB2	1.88	0.40
1:12:31:PRO:HB2	1:12:33:LEU:HG	2.03	0.40
3:4:30:HIS:HE1	3:4:32:LEU:HB3	1.85	0.40
5:72:837:C:N3	5:72:941:A:N6	2.69	0.40
5:72:1131:G:C8	5:72:2025:C:H4'	2.56	0.40
5:72:1214:A:H62	5:72:1235:G:N2	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A1:90:C:HO2'	7:A1:91:U:H5'	1.86	0.40
7:A1:299:G:N2	7:A1:565:U:O2	2.54	0.40
7:A1:689:C:H2'	7:A1:690:G:O4'	2.21	0.40
7:A1:779:C:H2'	7:A1:780:A:C8	2.57	0.40
7:A1:781:A:H3'	7:A1:782:A:H8	1.85	0.40
7:A1:817:C:N4	7:A1:819:A:N3	2.70	0.40
7:A1:1176:A:H2'	7:A1:1177:G:O4'	2.21	0.40
7:A1:1326:U:H2'	7:A1:1327:C:C6	2.56	0.40
7:A1:1338:G:H2'	7:A1:1339:A:C8	2.56	0.40
7:A1:1402:4OC:HN4	28:V2:23:C:P	2.44	0.40
7:A2:144:G:H2'	7:A2:145:G:H8	1.85	0.40
7:A2:446:G:C2	7:A2:489:C:C2	3.10	0.40
7:A2:983:A:N1	7:A2:1222:G:N2	2.70	0.40
7:A2:1317:C:OP1	20:N2:24:ARG:NH1	2.55	0.40
7:A2:1328:C:OP1	19:M2:28:THR:HG21	2.21	0.40
9:C2:69:HIS:O	9:C2:70:THR:OG1	2.31	0.40
12:F1:88:MET:HE2	12:F1:90:MET:SD	2.62	0.40
13:G1:25:LYS:HB3	13:G1:101:MET:HE1	2.02	0.40
13:G1:136:LYS:HA	13:G1:139:GLU:OE1	2.22	0.40
15:I1:130:ARG:NH2	30:W1:35:A:OP2	2.35	0.40
17:K1:96:THR:O	17:K1:100:LEU:HD23	2.20	0.40
23:Q2:26:GLU:O	23:Q2:26:GLU:HG2	2.21	0.40
27:U2:28:VAL:O	27:U2:32:VAL:HG23	2.21	0.40
28:V2:40:A:H5''	28:V2:41:G:H8	1.86	0.40
40:i2:46:PHE:HD1	40:i2:47:PHE:CD1	2.39	0.40
5:72:655:A:H8	5:72:655:A:OP1	2.05	0.40
5:72:1871:A:O2'	5:72:1872:A:H8	2.04	0.40
5:72:2202:U:O2'	5:72:2204:G:OP1	2.30	0.40
7:A1:203:G:H1	7:A1:214:C:H42	1.70	0.40
7:A1:404:G:H2'	7:A1:405:U:H6	1.85	0.40
7:A1:484:G:C5	7:A1:486:U:H1'	2.56	0.40
7:A1:1026:G:H1	7:A1:1035:A:H61	1.68	0.40
7:A1:1087:G:C2	7:A1:1099:G:H1'	2.57	0.40
7:A1:1317:C:H3'	7:A1:1318:A:H8	1.86	0.40
7:A1:1510:C:H42	7:A1:1525:G:H1	1.69	0.40
7:A2:402:G:O2'	7:A2:403:C:H5'	2.21	0.40
7:A2:1456:A:H2'	7:A2:1457:G:O4'	2.22	0.40
8:B:163:VAL:HG22	8:B:164:ILE:N	2.36	0.40
8:B2:119:THR:HG23	8:B2:120:GLN:H	1.87	0.40
10:D1:22:LYS:HD2	10:D1:22:LYS:HA	1.85	0.40
10:D2:202:GLU:HB2	11:E2:112:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:G1:92:ARG:HG3	13:G1:95:ARG:H	1.86	0.40
13:G2:18:PHE:CE2	13:G2:58:GLU:HB2	2.56	0.40
20:N2:20:TYR:HB2	20:N2:55:SER:HB2	2.03	0.40
24:R1:34:THR:HG22	24:R1:38:LYS:H	1.87	0.40
1:12:18:ARG:HD3	1:12:18:ARG:HA	1.84	0.40
5:72:353:C:H2'	5:72:354:A:C8	2.57	0.40
5:72:477:A:N6	5:72:500:G:O3'	2.54	0.40
5:72:771:G:OP1	41:12:14:ARG:HD2	2.22	0.40
5:72:2446:G:H21	5:72:2449:H2U:C2	2.31	0.40
7:A1:501:C:H1'	7:A1:549:C:H1'	2.04	0.40
7:A1:685:G:H2'	7:A1:686:U:C6	2.57	0.40
7:A1:772:U:H2'	7:A1:773:G:H8	1.86	0.40
7:A1:843:U:H6	7:A1:843:U:H2'	1.70	0.40
7:A1:861:G:O2'	7:A1:874:G:O2'	2.31	0.40
7:A1:995:C:C2'	7:A1:996:A:H5'	2.51	0.40
7:A1:1219:A:H2'	7:A1:1220:G:C8	2.56	0.40
7:A2:1004:A:H2'	7:A2:1005:A:O4'	2.21	0.40
7:A2:1090:U:H2'	7:A2:1091:U:C6	2.57	0.40
7:A2:1226:C:H4'	7:A2:1227:A:OP1	2.22	0.40
7:A2:1241:G:H2'	7:A2:1242:G:C8	2.56	0.40
7:A2:1267:C:H3'	7:A2:1268:G:H8	1.87	0.40
7:A2:1325:C:H2'	7:A2:1326:U:H6	1.85	0.40
9:C1:87:LEU:O	9:C1:91:VAL:HG12	2.20	0.40
10:D2:139:PRO:HA	10:D2:182:PHE:HD2	1.87	0.40
12:F2:12:PRO:HG3	12:F2:56:LYS:O	2.21	0.40
12:F2:38:ARG:HH12	12:F2:96:VAL:HG12	1.86	0.40
12:F2:74:LEU:HD13	12:F2:74:LEU:HA	1.93	0.40
13:G2:143:ARG:NH2	31:X2:42:G:O2'	2.54	0.40
14:H2:102:ALA:HB3	14:H2:113:ASP:HB3	2.03	0.40
21:O1:7:ALA:O	21:O1:10:LYS:HG2	2.21	0.40
24:R1:24:LYS:HE2	24:R1:24:LYS:HB2	1.93	0.40
25:S1:11:ILE:HD13	25:S1:16:LEU:HD13	2.03	0.40
27:U1:40:LYS:NZ	27:U1:41:PRO:HD2	2.37	0.40
37:e2:114:PHE:CZ	37:e2:176:PRO:HB2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	6	34
3	4	65/70 (93%)	54 (83%)	10 (15%)	1 (2%)	8	37
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	35 (15%)	3 (1%)	9	39
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	186 (88%)	23 (11%)	2 (1%)	14	47
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100	100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	24	57
10	D2	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	79 (76%)	23 (22%)	2 (2%)	6	33
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2	20
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	116 (91%)	11 (9%)	0	100	100
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100
16	J2	98/103 (95%)	86 (88%)	8 (8%)	4 (4%)	2	19
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	47
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14	47
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	85 (87%)	13 (13%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	74 (92%)	6 (8%)	0	100	100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	9	39
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	38
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	38
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	4	29
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100	100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3	26
34	Z1	7/557 (1%)	7 (100%)	0	0	100	100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
38	g2	50/55 (91%)	50 (100%)	0	0	100	100
39	h2	135/136 (99%)	135 (100%)	0	0	100	100
40	i2	147/149 (99%)	116 (79%)	29 (20%)	2 (1%)	9	38
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	z2	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
All	All	6102/7240 (84%)	5611 (92%)	457 (8%)	34 (1%)	23	54

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	54	SER
13	G2	146	GLU
23	Q2	12	VAL
10	D1	175	ALA
12	F2	38	ARG
13	G2	17	LYS
13	G2	145	ALA
16	J2	89	ARG
16	J2	94	ALA
40	i2	89	LYS
43	p	30	ALA
8	B	102	THR
8	B	103	ASN
17	K1	80	LYS
17	K2	80	LYS
18	L1	43	LYS
24	R1	21	ILE
26	T1	55	GLN
2	32	33	HIS
9	C1	129	MET
3	4	55	GLY
12	F2	54	LEU
16	J2	88	MET
40	i2	86	ASP
16	J2	79	PRO
8	B	38	VAL
26	T1	56	PRO
27	U2	6	VAL
43	p	31	VAL
27	U2	11	PRO
24	R2	69	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	
1	12	67/68 (98%)	67 (100%)	0	100	100
2	32	48/49 (98%)	48 (100%)	0	100	100
3	4	60/62 (97%)	54 (90%)	6 (10%)	7	28
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	189 (100%)	0	100	100
9	C1	173/190 (91%)	173 (100%)	0	100	100
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	172 (100%)	0	100	100
10	D2	172/173 (99%)	172 (100%)	0	100	100
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	91 (100%)	0	100	100
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	83 (100%)	0	100	100
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	64 (100%)	0	100	100
24	R2	64/65 (98%)	64 (100%)	0	100	100
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	65 (100%)	0	100	100
27	U1	60/61 (98%)	60 (100%)	0	100	100
27	U2	59/61 (97%)	59 (100%)	0	100	100
34	Z1	8/461 (2%)	8 (100%)	0	100	100
35	a2	110/181 (61%)	110 (100%)	0	100	100
36	b2	216/218 (99%)	216 (100%)	0	100	100
37	e2	149/150 (99%)	149 (100%)	0	100	100
38	g2	47/49 (96%)	47 (100%)	0	100	100
39	h2	110/109 (101%)	110 (100%)	0	100	100
40	i2	114/114 (100%)	114 (100%)	0	100	100
41	l2	38/38 (100%)	38 (100%)	0	100	100
42	o2	35/103 (34%)	35 (100%)	0	100	100
43	p	5/5 (100%)	4 (80%)	1 (20%)	1	7
44	r2	86/87 (99%)	86 (100%)	0	100	100
45	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5107/5932 (86%)	5100 (100%)	7 (0%)	87	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	4	6	HIS
3	4	9	TYR
3	4	33	ASN
3	4	36	VAL
3	4	40	CYS
3	4	58	ASP
43	p	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	12	20	HIS
3	4	6	HIS
3	4	33	ASN
3	4	41	HIS
3	4	61	ASN
8	B	58	ASN
8	B	93	ASN
8	B	94	HIS
8	B2	89	GLN
8	B2	177	ASN
9	C1	8	ASN
9	C1	185	ASN
9	C2	190	HIS
10	D1	59	GLN
10	D2	85	ASN
10	D2	116	GLN
11	E2	89	HIS
11	E2	122	ASN
12	F1	52	ASN
12	F2	46	GLN
13	G1	9	GLN
13	G2	97	ASN
15	I1	110	GLN
15	I1	126	GLN
15	I2	75	GLN
16	J2	35	GLN
17	K2	22	HIS
17	K2	38	GLN
18	L2	6	GLN
18	L2	29	GLN
20	N2	43	ASN
23	Q1	51	ASN
24	R2	52	GLN
36	b2	243	HIS
39	h2	13	HIS
40	i2	43	ASN
40	i2	133	GLN
40	i2	135	HIS
45	z2	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	75/76 (98%)	26 (34%)	4 (5%)
30	W1	34/76 (44%)	9 (26%)	2 (5%)
31	X2	74/77 (96%)	27 (36%)	5 (6%)
32	Y1	34/76 (44%)	5 (14%)	2 (5%)
33	Y2	75/76 (98%)	23 (30%)	2 (2%)
5	71	29/2904 (0%)	4 (13%)	0
5	72	2903/2904 (99%)	464 (15%)	33 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1541/1542 (99%)	450 (29%)	36 (2%)
7	A2	1536/1542 (99%)	401 (26%)	33 (2%)
All	All	6483/9457 (68%)	1472 (22%)	129 (1%)

All (1472) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A
5	72	46	G
5	72	55	G
5	72	71	A
5	72	74	A
5	72	75	G
5	72	101	A
5	72	102	U
5	72	103	A
5	72	110	G
5	72	118	A
5	72	119	A
5	72	120	U
5	72	125	A
5	72	135	U
5	72	139	U
5	72	141	G
5	72	142	A

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Mol	Chain	Res	Type
5	72	159	G
5	72	163	C
5	72	174	U
5	72	177	G
5	72	178	G
5	72	181	A
5	72	196	A
5	72	199	A
5	72	215	G
5	72	216	A
5	72	221	A
5	72	222	A
5	72	248	G
5	72	252	G
5	72	275	C
5	72	277	G
5	72	278	A
5	72	279	A
5	72	283	G
5	72	284	U
5	72	285	G
5	72	286	U
5	72	311	A
5	72	330	A
5	72	345	A
5	72	353	C
5	72	359	G
5	72	361	G
5	72	362	A
5	72	386	G
5	72	395	U
5	72	396	G
5	72	401	A
5	72	405	U
5	72	412	A
5	72	455	C
5	72	456	C
5	72	457	A
5	72	470	A
5	72	473	G
5	72	481	G
5	72	491	G

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Mol	Chain	Res	Type
5	72	505	A
5	72	506	G
5	72	509	C
5	72	513	A
5	72	527	C
5	72	532	A
5	72	547	A
5	72	549	G
5	72	563	A
5	72	573	U
5	72	575	A
5	72	578	G
5	72	603	A
5	72	613	A
5	72	614	A
5	72	615	U
5	72	637	A
5	72	645	C
5	72	646	U
5	72	647	G
5	72	654	A
5	72	655	A
5	72	686	U
5	72	717	C
5	72	726	G
5	72	729	G
5	72	730	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	750	A
5	72	764	A
5	72	765	C
5	72	775	G
5	72	776	G
5	72	782	A
5	72	784	G
5	72	785	G
5	72	789	A
5	72	805	G
5	72	812	C
5	72	819	A

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Mol	Chain	Res	Type
5	72	827	U
5	72	828	U
5	72	830	G
5	72	845	A
5	72	846	U
5	72	847	U
5	72	858	G
5	72	859	G
5	72	869	G
5	72	878	A
5	72	883	G
5	72	885	C
5	72	887	U
5	72	888	C
5	72	891	G
5	72	895	U
5	72	896	A
5	72	897	C
5	72	902	C
5	72	907	G
5	72	910	A
5	72	917	A
5	72	919	U
5	72	931	U
5	72	932	U
5	72	941	A
5	72	946	C
5	72	961	C
5	72	962	G
5	72	974	G
5	72	983	A
5	72	995	C
5	72	996	A
5	72	999	U
5	72	1005	C
5	72	1012	U
5	72	1013	C
5	72	1021	A
5	72	1026	G
5	72	1033	U
5	72	1046	A
5	72	1047	G

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Mol	Chain	Res	Type
5	72	1055	G
5	72	1060	U
5	72	1070	A
5	72	1081	U
5	72	1083	U
5	72	1084	A
5	72	1085	A
5	72	1087	G
5	72	1088	A
5	72	1090	A
5	72	1097	U
5	72	1112	G
5	72	1130	U
5	72	1131	G
5	72	1132	U
5	72	1133	A
5	72	1134	A
5	72	1135	C
5	72	1136	G
5	72	1142	A
5	72	1149	G
5	72	1161	C
5	72	1169	A
5	72	1172	C
5	72	1173	U
5	72	1174	U
5	72	1176	U
5	72	1178	C
5	72	1179	G
5	72	1180	U
5	72	1212	G
5	72	1235	G
5	72	1236	G
5	72	1247	A
5	72	1249	U
5	72	1250	G
5	72	1253	A
5	72	1256	G
5	72	1262	A
5	72	1271	G
5	72	1272	A
5	72	1273	U

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Mol	Chain	Res	Type
5	72	1300	G
5	72	1301	A
5	72	1321	A
5	72	1329	U
5	72	1345	C
5	72	1352	U
5	72	1365	A
5	72	1368	G
5	72	1379	U
5	72	1380	G
5	72	1383	A
5	72	1395	A
5	72	1396	U
5	72	1416	G
5	72	1417	C
5	72	1419	A
5	72	1420	A
5	72	1428	C
5	72	1434	A
5	72	1452	G
5	72	1453	A
5	72	1461	C
5	72	1476	U
5	72	1482	G
5	72	1488	C
5	72	1490	A
5	72	1491	G
5	72	1493	C
5	72	1494	A
5	72	1497	U
5	72	1503	A
5	72	1508	A
5	72	1509	A
5	72	1515	A
5	72	1524	G
5	72	1532	A
5	72	1539	U
5	72	1566	A
5	72	1569	A
5	72	1578	U
5	72	1581	G
5	72	1583	A

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Mol	Chain	Res	Type
5	72	1584	U
5	72	1608	A
5	72	1610	A
5	72	1618	6MZ
5	72	1619	G
5	72	1647	U
5	72	1648	U
5	72	1649	G
5	72	1674	G
5	72	1715	G
5	72	1727	C
5	72	1729	U
5	72	1730	C
5	72	1731	G
5	72	1738	G
5	72	1764	C
5	72	1773	A
5	72	1782	U
5	72	1784	A
5	72	1786	A
5	72	1791	A
5	72	1799	G
5	72	1800	C
5	72	1801	A
5	72	1807	G
5	72	1808	A
5	72	1816	C
5	72	1848	A
5	72	1870	C
5	72	1872	A
5	72	1873	G
5	72	1901	A
5	72	1906	G
5	72	1907	G
5	72	1913	A
5	72	1920	C
5	72	1929	G
5	72	1930	G
5	72	1937	A
5	72	1939	5MU
5	72	1940	U
5	72	1955	U

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Mol	Chain	Res	Type
5	72	1956	U
5	72	1960	A
5	72	1963	U
5	72	1964	G
5	72	1966	A
5	72	1967	C
5	72	1970	A
5	72	1971	U
5	72	1972	G
5	72	1975	G
5	72	1982	U
5	72	1991	U
5	72	1993	U
5	72	1997	C
5	72	2022	U
5	72	2023	C
5	72	2030	6MZ
5	72	2031	A
5	72	2032	G
5	72	2033	A
5	72	2043	C
5	72	2055	C
5	72	2056	G
5	72	2059	A
5	72	2060	A
5	72	2061	G
5	72	2062	A
5	72	2069	G7M
5	72	2072	C
5	72	2093	G
5	72	2098	U
5	72	2100	G
5	72	2101	A
5	72	2104	C
5	72	2109	U
5	72	2110	G
5	72	2111	U
5	72	2112	G
5	72	2113	U
5	72	2114	A
5	72	2115	G
5	72	2116	G

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Mol	Chain	Res	Type
5	72	2117	A
5	72	2118	U
5	72	2119	A
5	72	2120	G
5	72	2126	A
5	72	2130	U
5	72	2131	U
5	72	2132	U
5	72	2133	G
5	72	2134	A
5	72	2139	U
5	72	2140	G
5	72	2141	G
5	72	2145	C
5	72	2146	C
5	72	2149	U
5	72	2154	A
5	72	2158	A
5	72	2161	C
5	72	2162	G
5	72	2164	C
5	72	2165	C
5	72	2166	U
5	72	2167	U
5	72	2170	A
5	72	2171	A
5	72	2172	U
5	72	2173	A
5	72	2179	C
5	72	2182	U
5	72	2183	A
5	72	2198	A
5	72	2204	G
5	72	2211	A
5	72	2225	A
5	72	2238	G
5	72	2239	G
5	72	2243	U
5	72	2251	OMG
5	72	2268	A
5	72	2278	A
5	72	2279	G

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Mol	Chain	Res	Type
5	72	2283	C
5	72	2287	A
5	72	2305	U
5	72	2308	G
5	72	2309	A
5	72	2311	A
5	72	2312	U
5	72	2319	G
5	72	2321	U
5	72	2322	A
5	72	2325	G
5	72	2333	A
5	72	2336	A
5	72	2345	G
5	72	2347	C
5	72	2350	C
5	72	2361	G
5	72	2372	U
5	72	2375	G
5	72	2379	G
5	72	2383	G
5	72	2385	C
5	72	2391	G
5	72	2402	U
5	72	2403	C
5	72	2406	A
5	72	2410	G
5	72	2423	U
5	72	2425	A
5	72	2429	G
5	72	2430	A
5	72	2431	U
5	72	2441	U
5	72	2448	A
5	72	2457	PSU
5	72	2464	G
5	72	2475	C
5	72	2476	A
5	72	2478	A
5	72	2482	A
5	72	2484	G
5	72	2491	U

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Mol	Chain	Res	Type
5	72	2494	G
5	72	2498	OMC
5	72	2502	G
5	72	2503	2MA
5	72	2505	G
5	72	2507	C
5	72	2514	U
5	72	2518	A
5	72	2529	G
5	72	2535	G
5	72	2537	U
5	72	2547	A
5	72	2549	G
5	72	2554	U
5	72	2556	C
5	72	2566	A
5	72	2567	G
5	72	2571	U
5	72	2572	A
5	72	2573	C
5	72	2581	G
5	72	2582	G
5	72	2585	U
5	72	2586	U
5	72	2602	A
5	72	2608	G
5	72	2609	U
5	72	2613	U
5	72	2614	A
5	72	2615	U
5	72	2629	U
5	72	2630	G
5	72	2663	G
5	72	2689	U
5	72	2690	U
5	72	2714	G
5	72	2726	A
5	72	2732	G
5	72	2733	A
5	72	2743	U
5	72	2744	G
5	72	2748	A

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Mol	Chain	Res	Type
5	72	2751	G
5	72	2757	A
5	72	2765	A
5	72	2778	A
5	72	2779	U
5	72	2798	U
5	72	2800	A
5	72	2818	U
5	72	2820	A
5	72	2821	A
5	72	2832	U
5	72	2835	A
5	72	2861	U
5	72	2867	G
5	72	2873	A
5	72	2879	A
5	72	2880	C
5	72	2883	A
5	72	2884	U
5	72	2885	G
5	72	2886	A
5	72	2891	U
5	72	2904	U
6	82	4	C
6	82	9	G
6	82	13	G
6	82	33	G
6	82	34	A
6	82	35	C
6	82	37	C
6	82	40	U
6	82	41	G
6	82	45	A
6	82	48	U
6	82	50	A
6	82	51	G
6	82	66	A
6	82	67	G
6	82	87	U
6	82	89	U
6	82	90	C
6	82	91	C

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Mol	Chain	Res	Type
6	82	99	A
6	82	109	A
7	A1	4	U
7	A1	5	U
7	A1	6	G
7	A1	7	A
7	A1	8	A
7	A1	9	G
7	A1	26	A
7	A1	28	A
7	A1	32	A
7	A1	33	A
7	A1	39	G
7	A1	47	C
7	A1	48	C
7	A1	50	A
7	A1	51	A
7	A1	52	C
7	A1	54	C
7	A1	58	C
7	A1	70	U
7	A1	71	A
7	A1	72	A
7	A1	75	G
7	A1	76	G
7	A1	78	A
7	A1	79	G
7	A1	80	A
7	A1	82	G
7	A1	84	U
7	A1	85	U
7	A1	86	G
7	A1	88	U
7	A1	89	U
7	A1	90	C
7	A1	91	U
7	A1	92	U
7	A1	94	G
7	A1	95	C
7	A1	100	G
7	A1	120	A
7	A1	121	U

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Mol	Chain	Res	Type
7	A1	122	G
7	A1	129	A
7	A1	131	A
7	A1	136	C
7	A1	137	U
7	A1	138	G
7	A1	141	G
7	A1	142	G
7	A1	143	A
7	A1	144	G
7	A1	145	G
7	A1	146	G
7	A1	150	U
7	A1	156	C
7	A1	163	C
7	A1	164	G
7	A1	169	C
7	A1	173	U
7	A1	174	A
7	A1	176	C
7	A1	182	A
7	A1	183	C
7	A1	184	G
7	A1	185	U
7	A1	191	G
7	A1	192	A
7	A1	193	C
7	A1	194	C
7	A1	197	A
7	A1	198	G
7	A1	201	G
7	A1	204	G
7	A1	205	A
7	A1	208	U
7	A1	209	U
7	A1	210	C
7	A1	211	G
7	A1	212	G
7	A1	215	C
7	A1	222	C
7	A1	239	U
7	A1	240	G

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Mol	Chain	Res	Type
7	A1	245	U
7	A1	247	G
7	A1	251	G
7	A1	252	U
7	A1	253	A
7	A1	259	G
7	A1	261	U
7	A1	264	C
7	A1	266	G
7	A1	267	C
7	A1	275	G
7	A1	281	G
7	A1	289	G
7	A1	294	U
7	A1	298	A
7	A1	301	G
7	A1	306	A
7	A1	315	A
7	A1	316	C
7	A1	323	U
7	A1	328	C
7	A1	329	A
7	A1	330	C
7	A1	345	C
7	A1	351	G
7	A1	352	C
7	A1	354	G
7	A1	363	A
7	A1	367	U
7	A1	372	C
7	A1	373	A
7	A1	384	G
7	A1	387	U
7	A1	388	G
7	A1	406	G
7	A1	407	U
7	A1	411	A
7	A1	412	A
7	A1	413	G
7	A1	414	A
7	A1	415	A
7	A1	421	U

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Mol	Chain	Res	Type
7	A1	422	C
7	A1	423	G
7	A1	424	G
7	A1	428	G
7	A1	429	U
7	A1	438	U
7	A1	442	G
7	A1	446	G
7	A1	451	A
7	A1	457	G
7	A1	458	U
7	A1	459	A
7	A1	460	A
7	A1	464	U
7	A1	465	A
7	A1	468	A
7	A1	470	C
7	A1	471	U
7	A1	474	G
7	A1	475	C
7	A1	476	U
7	A1	479	U
7	A1	484	G
7	A1	486	U
7	A1	496	A
7	A1	509	A
7	A1	511	C
7	A1	517	G
7	A1	518	C
7	A1	521	G
7	A1	522	C
7	A1	527	G7M
7	A1	530	G
7	A1	531	U
7	A1	532	A
7	A1	536	C
7	A1	547	A
7	A1	559	A
7	A1	562	U
7	A1	566	G
7	A1	572	A
7	A1	573	A

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Mol	Chain	Res	Type
7	A1	575	G
7	A1	576	C
7	A1	577	G
7	A1	582	C
7	A1	596	A
7	A1	611	C
7	A1	633	G
7	A1	639	G
7	A1	640	A
7	A1	641	U
7	A1	643	C
7	A1	649	A
7	A1	650	G
7	A1	652	U
7	A1	653	U
7	A1	654	G
7	A1	661	G
7	A1	664	G
7	A1	665	A
7	A1	668	G
7	A1	672	U
7	A1	674	G
7	A1	675	A
7	A1	684	U
7	A1	686	U
7	A1	687	A
7	A1	690	G
7	A1	693	G
7	A1	694	A
7	A1	702	A
7	A1	703	G
7	A1	704	A
7	A1	705	G
7	A1	709	U
7	A1	712	A
7	A1	717	U
7	A1	720	C
7	A1	721	G
7	A1	723	U
7	A1	724	G
7	A1	725	G
7	A1	731	G

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Mol	Chain	Res	Type
7	A1	734	G
7	A1	736	C
7	A1	746	A
7	A1	748	G
7	A1	755	G
7	A1	763	G
7	A1	774	G
7	A1	777	A
7	A1	782	A
7	A1	787	A
7	A1	790	A
7	A1	793	U
7	A1	794	A
7	A1	799	G
7	A1	806	C
7	A1	808	C
7	A1	815	A
7	A1	817	C
7	A1	828	U
7	A1	831	A
7	A1	835	U
7	A1	837	U
7	A1	841	C
7	A1	842	U
7	A1	843	U
7	A1	844	G
7	A1	845	A
7	A1	846	G
7	A1	848	C
7	A1	849	G
7	A1	850	U
7	A1	860	A
7	A1	864	A
7	A1	870	U
7	A1	871	U
7	A1	874	G
7	A1	876	C
7	A1	884	U
7	A1	885	G
7	A1	887	G
7	A1	889	A
7	A1	890	G

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Mol	Chain	Res	Type
7	A1	899	C
7	A1	902	G
7	A1	914	A
7	A1	922	G
7	A1	926	G
7	A1	933	G
7	A1	934	C
7	A1	935	A
7	A1	939	G
7	A1	940	C
7	A1	942	G
7	A1	943	U
7	A1	947	G
7	A1	958	A
7	A1	960	U
7	A1	961	U
7	A1	966	2MG
7	A1	969	A
7	A1	971	G
7	A1	973	G
7	A1	975	A
7	A1	976	G
7	A1	977	A
7	A1	979	C
7	A1	981	U
7	A1	992	U
7	A1	993	G
7	A1	994	A
7	A1	995	C
7	A1	996	A
7	A1	998	C
7	A1	1003	G
7	A1	1004	A
7	A1	1008	U
7	A1	1009	U
7	A1	1010	U
7	A1	1014	A
7	A1	1017	U
7	A1	1020	G
7	A1	1021	A
7	A1	1027	C
7	A1	1028	C

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Mol	Chain	Res	Type
7	A1	1029	U
7	A1	1030	U
7	A1	1031	C
7	A1	1032	G
7	A1	1033	G
7	A1	1034	G
7	A1	1036	A
7	A1	1044	A
7	A1	1045	C
7	A1	1046	A
7	A1	1050	G
7	A1	1054	C
7	A1	1055	A
7	A1	1058	G
7	A1	1066	C
7	A1	1070	U
7	A1	1073	U
7	A1	1078	U
7	A1	1085	U
7	A1	1086	U
7	A1	1094	G
7	A1	1095	U
7	A1	1101	A
7	A1	1103	C
7	A1	1108	G
7	A1	1121	U
7	A1	1124	G
7	A1	1125	U
7	A1	1126	U
7	A1	1127	G
7	A1	1129	C
7	A1	1131	G
7	A1	1132	C
7	A1	1133	G
7	A1	1135	U
7	A1	1136	C
7	A1	1137	C
7	A1	1139	G
7	A1	1140	C
7	A1	1141	C
7	A1	1147	C
7	A1	1151	A

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Mol	Chain	Res	Type
7	A1	1152	A
7	A1	1154	G
7	A1	1157	A
7	A1	1159	U
7	A1	1161	C
7	A1	1162	C
7	A1	1168	U
7	A1	1169	A
7	A1	1170	A
7	A1	1174	G
7	A1	1182	G
7	A1	1183	U
7	A1	1190	G
7	A1	1191	A
7	A1	1196	A
7	A1	1197	A
7	A1	1201	A
7	A1	1202	U
7	A1	1206	G
7	A1	1211	U
7	A1	1212	U
7	A1	1213	A
7	A1	1214	C
7	A1	1215	G
7	A1	1221	G
7	A1	1224	U
7	A1	1225	A
7	A1	1226	C
7	A1	1227	A
7	A1	1228	C
7	A1	1235	U
7	A1	1236	A
7	A1	1239	A
7	A1	1240	U
7	A1	1241	G
7	A1	1243	C
7	A1	1250	A
7	A1	1253	G
7	A1	1256	A
7	A1	1260	G
7	A1	1270	G
7	A1	1272	G

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Mol	Chain	Res	Type
7	A1	1279	G
7	A1	1280	A
7	A1	1281	C
7	A1	1287	A
7	A1	1298	U
7	A1	1300	G
7	A1	1301	U
7	A1	1302	C
7	A1	1308	U
7	A1	1309	G
7	A1	1310	G
7	A1	1317	C
7	A1	1320	C
7	A1	1328	C
7	A1	1331	G
7	A1	1335	U
7	A1	1336	C
7	A1	1338	G
7	A1	1345	U
7	A1	1346	A
7	A1	1347	G
7	A1	1348	U
7	A1	1352	C
7	A1	1356	G
7	A1	1363	A
7	A1	1364	U
7	A1	1365	G
7	A1	1368	A
7	A1	1369	C
7	A1	1379	G
7	A1	1383	C
7	A1	1399	C
7	A1	1418	A
7	A1	1419	G
7	A1	1424	U
7	A1	1425	U
7	A1	1426	G
7	A1	1429	A
7	A1	1430	A
7	A1	1432	G
7	A1	1433	A
7	A1	1439	G

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Mol	Chain	Res	Type
7	A1	1440	U
7	A1	1441	A
7	A1	1442	G
7	A1	1446	A
7	A1	1450	U
7	A1	1451	U
7	A1	1452	C
7	A1	1454	G
7	A1	1455	G
7	A1	1460	C
7	A1	1461	G
7	A1	1462	C
7	A1	1464	U
7	A1	1475	G
7	A1	1476	A
7	A1	1486	G
7	A1	1487	G
7	A1	1492	A
7	A1	1493	A
7	A1	1499	A
7	A1	1503	A
7	A1	1505	G
7	A1	1506	U
7	A1	1507	A
7	A1	1517	G
7	A1	1529	G
7	A1	1530	G
7	A1	1536	C
7	A1	1537	U
7	A1	1539	C
7	A1	1541	U
7	A1	1542	A
7	A2	2	A
7	A2	4	U
7	A2	7	A
7	A2	8	A
7	A2	9	G
7	A2	16	A
7	A2	26	A
7	A2	30	U
7	A2	31	G
7	A2	32	A

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Mol	Chain	Res	Type
7	A2	39	G
7	A2	40	C
7	A2	47	C
7	A2	48	C
7	A2	51	A
7	A2	64	G
7	A2	70	U
7	A2	71	A
7	A2	72	A
7	A2	73	C
7	A2	74	A
7	A2	75	G
7	A2	76	G
7	A2	78	A
7	A2	82	G
7	A2	85	U
7	A2	86	G
7	A2	88	U
7	A2	90	C
7	A2	91	U
7	A2	94	G
7	A2	95	C
7	A2	97	G
7	A2	98	A
7	A2	116	A
7	A2	120	A
7	A2	121	U
7	A2	129	A
7	A2	131	A
7	A2	137	U
7	A2	138	G
7	A2	141	G
7	A2	143	A
7	A2	148	G
7	A2	150	U
7	A2	155	A
7	A2	163	C
7	A2	164	G
7	A2	173	U
7	A2	174	A
7	A2	176	C
7	A2	177	G

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Mol	Chain	Res	Type
7	A2	182	A
7	A2	183	C
7	A2	184	G
7	A2	186	C
7	A2	187	G
7	A2	188	C
7	A2	193	C
7	A2	195	A
7	A2	197	A
7	A2	199	A
7	A2	202	G
7	A2	204	G
7	A2	205	A
7	A2	207	C
7	A2	208	U
7	A2	209	U
7	A2	210	C
7	A2	215	C
7	A2	216	U
7	A2	218	U
7	A2	224	U
7	A2	240	G
7	A2	245	U
7	A2	247	G
7	A2	250	A
7	A2	251	G
7	A2	252	U
7	A2	253	A
7	A2	257	G
7	A2	262	A
7	A2	263	A
7	A2	266	G
7	A2	267	C
7	A2	269	C
7	A2	275	G
7	A2	276	G
7	A2	278	G
7	A2	279	A
7	A2	281	G
7	A2	282	A
7	A2	289	G
7	A2	301	G

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Mol	Chain	Res	Type
7	A2	305	G
7	A2	316	C
7	A2	323	U
7	A2	328	C
7	A2	329	A
7	A2	330	C
7	A2	331	G
7	A2	347	G
7	A2	351	G
7	A2	352	C
7	A2	354	G
7	A2	355	C
7	A2	356	A
7	A2	361	G
7	A2	367	U
7	A2	368	U
7	A2	370	C
7	A2	372	C
7	A2	373	A
7	A2	374	A
7	A2	375	U
7	A2	387	U
7	A2	388	G
7	A2	391	G
7	A2	393	A
7	A2	397	A
7	A2	398	U
7	A2	405	U
7	A2	406	G
7	A2	408	A
7	A2	409	U
7	A2	411	A
7	A2	412	A
7	A2	413	G
7	A2	414	A
7	A2	415	A
7	A2	416	G
7	A2	422	C
7	A2	423	G
7	A2	424	G
7	A2	426	U
7	A2	428	G

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Mol	Chain	Res	Type
7	A2	429	U
7	A2	431	A
7	A2	437	U
7	A2	439	U
7	A2	440	C
7	A2	442	G
7	A2	443	C
7	A2	444	G
7	A2	445	G
7	A2	448	A
7	A2	450	G
7	A2	452	A
7	A2	456	A
7	A2	457	G
7	A2	458	U
7	A2	459	A
7	A2	460	A
7	A2	461	A
7	A2	462	G
7	A2	464	U
7	A2	465	A
7	A2	466	A
7	A2	467	U
7	A2	468	A
7	A2	469	C
7	A2	472	U
7	A2	473	U
7	A2	474	G
7	A2	475	C
7	A2	478	A
7	A2	479	U
7	A2	480	U
7	A2	481	G
7	A2	482	A
7	A2	484	G
7	A2	492	C
7	A2	495	A
7	A2	496	A
7	A2	497	G
7	A2	498	A
7	A2	499	A
7	A2	501	C

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Mol	Chain	Res	Type
7	A2	506	G
7	A2	511	C
7	A2	512	U
7	A2	513	C
7	A2	516	U
7	A2	518	C
7	A2	520	A
7	A2	521	G
7	A2	524	G
7	A2	527	G7M
7	A2	529	G
7	A2	530	G
7	A2	531	U
7	A2	532	A
7	A2	533	A
7	A2	534	U
7	A2	536	C
7	A2	538	G
7	A2	539	A
7	A2	542	G
7	A2	547	A
7	A2	549	C
7	A2	551	U
7	A2	558	G
7	A2	559	A
7	A2	562	U
7	A2	572	A
7	A2	573	A
7	A2	575	G
7	A2	576	C
7	A2	577	G
7	A2	633	G
7	A2	653	U
7	A2	665	A
7	A2	703	G
7	A2	717	U
7	A2	718	A
7	A2	721	G
7	A2	723	U
7	A2	724	G
7	A2	731	G
7	A2	733	G

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Mol	Chain	Res	Type
7	A2	734	G
7	A2	735	C
7	A2	748	G
7	A2	755	G
7	A2	777	A
7	A2	788	U
7	A2	790	A
7	A2	793	U
7	A2	794	A
7	A2	815	A
7	A2	817	C
7	A2	821	G
7	A2	829	G
7	A2	841	C
7	A2	842	U
7	A2	843	U
7	A2	844	G
7	A2	845	A
7	A2	846	G
7	A2	902	G
7	A2	914	A
7	A2	926	G
7	A2	933	G
7	A2	934	C
7	A2	935	A
7	A2	945	G
7	A2	953	G
7	A2	960	U
7	A2	961	U
7	A2	966	2MG
7	A2	968	A
7	A2	969	A
7	A2	972	C
7	A2	974	A
7	A2	975	A
7	A2	976	G
7	A2	977	A
7	A2	989	U
7	A2	991	U
7	A2	992	U
7	A2	993	G
7	A2	994	A

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Mol	Chain	Res	Type
7	A2	996	A
7	A2	1004	A
7	A2	1006	G
7	A2	1008	U
7	A2	1009	U
7	A2	1011	C
7	A2	1014	A
7	A2	1017	U
7	A2	1018	G
7	A2	1019	A
7	A2	1020	G
7	A2	1021	A
7	A2	1022	A
7	A2	1023	U
7	A2	1029	U
7	A2	1030	U
7	A2	1031	C
7	A2	1032	G
7	A2	1033	G
7	A2	1034	G
7	A2	1044	A
7	A2	1046	A
7	A2	1056	U
7	A2	1063	C
7	A2	1064	G
7	A2	1065	U
7	A2	1067	A
7	A2	1074	G
7	A2	1081	A
7	A2	1085	U
7	A2	1086	U
7	A2	1094	G
7	A2	1095	U
7	A2	1098	C
7	A2	1101	A
7	A2	1102	A
7	A2	1108	G
7	A2	1113	C
7	A2	1124	G
7	A2	1125	U
7	A2	1127	G
7	A2	1128	C

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Mol	Chain	Res	Type
7	A2	1129	C
7	A2	1130	A
7	A2	1131	G
7	A2	1133	G
7	A2	1134	G
7	A2	1136	C
7	A2	1137	C
7	A2	1138	G
7	A2	1139	G
7	A2	1140	C
7	A2	1141	C
7	A2	1146	A
7	A2	1152	A
7	A2	1157	A
7	A2	1158	C
7	A2	1159	U
7	A2	1160	G
7	A2	1168	U
7	A2	1169	A
7	A2	1182	G
7	A2	1184	G
7	A2	1185	G
7	A2	1191	A
7	A2	1196	A
7	A2	1197	A
7	A2	1201	A
7	A2	1202	U
7	A2	1206	G
7	A2	1212	U
7	A2	1213	A
7	A2	1215	G
7	A2	1217	C
7	A2	1218	C
7	A2	1225	A
7	A2	1226	C
7	A2	1227	A
7	A2	1238	A
7	A2	1241	G
7	A2	1248	A
7	A2	1249	C
7	A2	1253	G
7	A2	1256	A

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Mol	Chain	Res	Type
7	A2	1268	G
7	A2	1270	G
7	A2	1271	A
7	A2	1279	G
7	A2	1280	A
7	A2	1281	C
7	A2	1282	C
7	A2	1286	U
7	A2	1287	A
7	A2	1291	U
7	A2	1297	G
7	A2	1298	U
7	A2	1300	G
7	A2	1305	G
7	A2	1317	C
7	A2	1318	A
7	A2	1319	A
7	A2	1320	C
7	A2	1332	A
7	A2	1336	C
7	A2	1338	G
7	A2	1340	A
7	A2	1346	A
7	A2	1348	U
7	A2	1351	U
7	A2	1353	G
7	A2	1360	A
7	A2	1363	A
7	A2	1364	U
7	A2	1368	A
7	A2	1370	G
7	A2	1375	A
7	A2	1379	G
7	A2	1397	C
7	A2	1398	A
7	A2	1429	A
7	A2	1432	G
7	A2	1441	A
7	A2	1446	A
7	A2	1448	C
7	A2	1454	G
7	A2	1487	G

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Mol	Chain	Res	Type
7	A2	1492	A
7	A2	1498	UR3
7	A2	1499	A
7	A2	1503	A
7	A2	1506	U
7	A2	1517	G
7	A2	1529	G
7	A2	1530	G
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
7	A2	1536	C
7	A2	1537	U
28	V2	6	A
28	V2	8	A
28	V2	9	A
28	V2	10	G
28	V2	11	G
28	V2	14	G
28	V2	15	G
28	V2	16	U
28	V2	17	G
28	V2	18	A
28	V2	19	G
28	V2	20	C
28	V2	21	U
28	V2	23	C
28	V2	24	G
28	V2	30	A
28	V2	32	U
28	V2	33	A
28	V2	34	A
28	V2	35	A
28	V2	37	A
28	V2	38	A
28	V2	39	A
28	V2	40	A
28	V2	41	G
28	V2	42	G
28	V2	43	U
28	V2	45	U
28	V2	46	C

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Mol	Chain	Res	Type
28	V2	47	G
28	V2	48	C
28	V2	50	C
28	V2	53	G
28	V2	54	G
28	V2	57	A
28	V2	58	A
28	V2	61	U
28	V2	62	C
28	V2	63	G
28	V2	64	A
28	V2	66	A
28	V2	67	A
29	W	2	G
29	W	4	G
29	W	8	4SU
29	W	11	U
29	W	15	A
29	W	16	H2U
29	W	17	H2U
29	W	18	G
29	W	19	G
29	W	20	H2U
29	W	22	G
29	W	34	C
29	W	44	G
29	W	46	G7M
29	W	47	U
29	W	48	U
29	W	49	G
29	W	52	A
29	W	53	G
29	W	54	5MU
29	W	55	PSU
29	W	58	A
29	W	59	G
29	W	60	U
29	W	72	U
29	W	76	A
30	W1	11	C
30	W1	15	G
30	W1	22	G

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Mol	Chain	Res	Type
30	W1	35	A
30	W1	37	MIA
30	W1	44	G
30	W1	46	G7M
30	W1	47	U
30	W1	48	C
31	X2	2	C
31	X2	3	A
31	X2	8	4SU
31	X2	9	A
31	X2	13	C
31	X2	15	G
31	X2	16	C
31	X2	18	G
31	X2	20	A
31	X2	21	H2U
31	X2	22	A
31	X2	23	G
31	X2	33	RSP
31	X2	38	2MA
31	X2	47	G7M
31	X2	48	3AU
31	X2	49	C
31	X2	50	G
31	X2	55	5MU
31	X2	60	A
31	X2	66	C
31	X2	71	U
31	X2	72	G
31	X2	73	C
31	X2	74	A
31	X2	76	C
31	X2	77	A
32	Y1	10	G
32	Y1	11	C
32	Y1	46	7MG
32	Y1	47	U
32	Y1	48	C
33	Y2	15	G
33	Y2	16	C
33	Y2	17	H2U
33	Y2	18	G

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Mol	Chain	Res	Type
33	Y2	19	G
33	Y2	20	G
33	Y2	21	A
33	Y2	22	G
33	Y2	34	G
33	Y2	36	C
33	Y2	39	G
33	Y2	45	G
33	Y2	46	G7M
33	Y2	48	C
33	Y2	49	A
33	Y2	54	5MU
33	Y2	56	C
33	Y2	64	C
33	Y2	72	C
33	Y2	73	A
33	Y2	74	C
33	Y2	75	C
33	Y2	76	A

All (129) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	72	43	G
5	72	134	G
5	72	158	U
5	72	277	G
5	72	285	G
5	72	352	A
5	72	404	A
5	72	504	A
5	72	512	G
5	72	613	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	784	G
5	72	827	U
5	72	1020	A
5	72	1046	A
5	72	1130	U
5	72	1211	C

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Mol	Chain	Res	Type
5	72	1266	G
5	72	1416	G
5	72	1475	G
5	72	1490	A
5	72	1580	A
5	72	1847	A
5	72	1940	U
5	72	2061	G
5	72	2118	U
5	72	2172	U
5	72	2430	A
5	72	2581	G
5	72	2585	U
5	72	2756	U
6	82	3	C
6	82	15	A
6	82	39	A
6	82	88	C
7	A1	5	U
7	A1	7	A
7	A1	51	A
7	A1	70	U
7	A1	129	A
7	A1	173	U
7	A1	197	A
7	A1	209	U
7	A1	251	G
7	A1	274	A
7	A1	372	C
7	A1	412	A
7	A1	421	U
7	A1	428	G
7	A1	438	U
7	A1	535	A
7	A1	559	A
7	A1	575	G
7	A1	653	U
7	A1	686	U
7	A1	870	U
7	A1	884	U
7	A1	992	U
7	A1	993	G

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Mol	Chain	Res	Type
7	A1	1054	C
7	A1	1085	U
7	A1	1182	G
7	A1	1190	G
7	A1	1201	A
7	A1	1302	C
7	A1	1335	U
7	A1	1432	G
7	A1	1440	U
7	A1	1452	C
7	A1	1463	U
7	A1	1536	C
7	A2	7	A
7	A2	13	U
7	A2	30	U
7	A2	70	U
7	A2	183	C
7	A2	208	U
7	A2	209	U
7	A2	251	G
7	A2	367	U
7	A2	411	A
7	A2	428	G
7	A2	438	U
7	A2	532	A
7	A2	537	G
7	A2	717	U
7	A2	845	A
7	A2	992	U
7	A2	993	G
7	A2	1085	U
7	A2	1101	A
7	A2	1129	C
7	A2	1136	C
7	A2	1140	C
7	A2	1168	U
7	A2	1190	G
7	A2	1201	A
7	A2	1256	A
7	A2	1281	C
7	A2	1297	G
7	A2	1319	A

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Mol	Chain	Res	Type
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
28	V2	8	A
28	V2	23	C
28	V2	31	U
28	V2	36	A
28	V2	37	A
28	V2	39	A
28	V2	46	C
28	V2	53	G
29	W	10	G
29	W	18	G
29	W	19	G
29	W	43	G
30	W1	10	G
30	W1	43	C
31	X2	15	G
31	X2	22	A
31	X2	47	G7M
31	X2	49	C
31	X2	73	C
32	Y1	10	G
32	Y1	47	U
33	Y2	17	H2U
33	Y2	63	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.07	9 (31%)
7	MA6	A1	1518	7	23,26,27	1.36	3 (13%)	34,38,41	3.31	14 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MA6	A2	1519	7	23,26,27	1.36	3 (13%)	34,38,41	3.33	14 (41%)
5	PSU	72	2504	5,49	18,21,22	4.67	8 (44%)	22,30,33	1.92	5 (22%)
29	MIA	W	37	29	28,31,32	2.41	5 (17%)	40,44,47	2.69	17 (42%)
7	2MG	A2	966	7	23,26,27	3.10	8 (34%)	32,38,41	2.53	11 (34%)
7	4OC	A1	1402	7	20,23,24	3.22	8 (40%)	26,32,35	0.93	1 (3%)
30	G7M	W1	46	30	23,26,27	2.85	8 (34%)	35,39,42	1.93	8 (22%)
5	2MG	72	1835	5	23,26,27	3.07	8 (34%)	32,38,41	2.52	11 (34%)
5	3TD	72	1915	5	19,22,23	4.03	7 (36%)	21,32,35	1.78	3 (14%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
7	5MC	A2	1407	7	18,22,23	4.00	7 (38%)	26,32,35	0.97	2 (7%)
5	1MG	72	745	5	22,26,27	2.72	5 (22%)	33,39,42	2.31	8 (24%)
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.29	3 (9%)
31	2MA	X2	38	31	22,25,26	4.13	8 (36%)	33,37,40	3.42	11 (33%)
7	UR3	A2	1498	7	19,22,23	2.73	8 (42%)	26,32,35	1.29	2 (7%)
7	2MG	A1	1516	7	23,26,27	3.11	8 (34%)	32,38,41	2.51	11 (34%)
5	PSU	72	746	5	18,21,22	0.99	2 (11%)	22,30,33	0.95	1 (4%)
5	5MU	72	747	5	19,22,23	0.34	0	28,32,35	0.58	0
29	H2U	W	16	29	18,21,22	3.05	5 (27%)	21,30,33	1.98	5 (23%)
5	3TD	71	1915	5	19,22,23	4.09	7 (36%)	21,32,35	1.70	2 (9%)
7	MA6	A2	1518	7	23,26,27	1.37	3 (13%)	34,38,41	3.32	14 (41%)
31	G7M	X2	47	31	23,26,27	2.85	8 (34%)	35,39,42	1.93	8 (22%)
33	G7M	Y2	46	33	23,26,27	2.84	9 (39%)	35,39,42	1.75	8 (22%)
5	5MU	72	1939	5	19,22,23	0.74	0	28,32,35	1.27	2 (7%)
5	OMG	72	2251	5,29	23,26,27	2.57	7 (30%)	33,38,41	2.42	10 (30%)
5	PSU	72	2605	5	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
7	4OC	A2	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.90	1 (3%)
5	6MZ	72	1618	5	22,25,26	2.76	4 (18%)	30,36,39	2.52	10 (33%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
33	PSU	Y2	55	33	18,21,22	0.88	1 (5%)	22,30,33	0.64	0
31	PSU	X2	56	31	18,21,22	0.87	1 (5%)	22,30,33	0.49	0
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.04	5 (23%)
7	G7M	A1	527	7	23,26,27	2.84	9 (39%)	35,39,42	1.74	9 (25%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.21	4 (15%)
29	5MU	W	54	29	19,22,23	0.25	0	28,32,35	0.39	0
7	2MG	A2	1516	7	23,26,27	3.08	8 (34%)	32,38,41	2.48	11 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	OMC	72	2498	5,49	19,22,23	3.29	8 (42%)	26,31,34	0.76	0
30	PSU	W1	39	30	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
33	5MU	Y2	54	33	19,22,23	0.24	0	28,32,35	0.24	0
7	G7M	A2	527	7	23,26,27	2.82	9 (39%)	35,39,42	1.73	9 (25%)
7	UR3	A1	1498	7	19,22,23	2.75	8 (42%)	26,32,35	1.29	3 (11%)
29	H2U	W	20	29	18,21,22	3.04	5 (27%)	21,30,33	2.02	5 (23%)
29	G7M	W	46	29	23,26,27	2.83	8 (34%)	35,39,42	1.93	8 (22%)
29	H2U	W	17	29	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
7	2MG	A1	1207	7	23,26,27	3.10	8 (34%)	32,38,41	2.51	11 (34%)
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
7	5MC	A1	967	7	18,22,23	4.03	7 (38%)	26,32,35	1.01	2 (7%)
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.27	4 (15%)
32	6MZ	Y1	37	32	22,25,26	2.81	4 (18%)	30,36,39	2.46	12 (40%)
7	2MG	A1	966	7	23,26,27	3.10	8 (34%)	32,38,41	2.56	11 (34%)
32	CM0	Y1	34	32	23,26,27	3.73	6 (26%)	27,37,40	1.52	2 (7%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
33	H2U	Y2	17	33	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
5	2MG	72	2445	5	23,26,27	3.09	8 (34%)	32,38,41	2.52	12 (37%)
5	H2U	72	2449	5,49	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
31	RSP	X2	33	31	17,21,22	4.13	7 (41%)	22,30,33	0.78	0
29	PSU	W	55	29	18,21,22	0.85	1 (5%)	22,30,33	0.79	1 (4%)
30	MIA	W1	37	30	28,31,32	2.42	5 (17%)	40,44,47	2.81	15 (37%)
7	2MG	A2	1207	7	23,26,27	3.12	8 (34%)	32,38,41	2.53	11 (34%)
29	PSU	W	32	29	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
5	G7M	72	2069	5	23,26,27	2.82	9 (39%)	35,39,42	1.75	9 (25%)
7	MA6	A1	1519	7	23,26,27	1.34	3 (13%)	34,38,41	3.36	13 (38%)
5	PSU	72	2604	5	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
31	5MU	X2	55	31	19,22,23	0.25	0	28,32,35	0.18	0
29	4SU	W	8	29	18,21,22	3.77	7 (38%)	26,30,33	2.26	5 (19%)
7	5MC	A2	967	7	18,22,23	4.01	7 (38%)	26,32,35	1.00	2 (7%)
5	5MC	72	1962	5	18,22,23	4.01	7 (38%)	26,32,35	1.06	2 (7%)
31	H2U	X2	17	31	18,21,22	3.09	5 (27%)	21,30,33	1.95	5 (23%)
5	2MA	72	2503	5	22,25,26	4.06	8 (36%)	33,37,40	3.50	11 (33%)
7	5MC	A1	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6MZ	72	2030	5	22,25,26	2.84	4 (18%)	30,36,39	2.42	11 (36%)

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
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
7	MA6	A1	1518	7	-	3/11/29/30	0/3/3/3
7	MA6	A2	1519	7	-	2/11/29/30	0/3/3/3
5	PSU	72	2504	5,49	-	1/7/25/26	0/2/2/2
29	MIA	W	37	29	-	1/15/33/34	0/3/3/3
7	2MG	A2	966	7	-	0/9/27/28	0/3/3/3
7	4OC	A1	1402	7	-	2/9/29/30	0/2/2/2
30	G7M	W1	46	30	-	4/7/25/26	0/3/3/3
5	2MG	72	1835	5	-	0/9/27/28	0/3/3/3
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
5	PSU	72	2457	5	-	2/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
5	1MG	72	745	5	-	0/7/25/26	0/3/3/3
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
31	2MA	X2	38	31	-	5/7/25/26	0/3/3/3
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
7	2MG	A1	1516	7	-	0/9/27/28	0/3/3/3
5	PSU	72	746	5	-	1/7/25/26	0/2/2/2
5	5MU	72	747	5	-	0/7/25/26	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
7	MA6	A2	1518	7	-	0/11/29/30	0/3/3/3
31	G7M	X2	47	31	-	3/7/25/26	0/3/3/3
33	G7M	Y2	46	33	-	2/7/25/26	0/3/3/3
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
5	OMG	72	2251	5,29	-	3/9/27/28	0/3/3/3
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
5	6MZ	72	1618	5	-	4/9/27/28	0/3/3/3
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PSU	X2	56	31	-	2/7/25/26	0/2/2/2
31	H2U	X2	21	31	-	3/7/38/39	0/2/2/2
7	G7M	A1	527	7	-	1/7/25/26	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/9/27/28	0/3/3/3
5	OMC	72	2498	5,49	-	2/9/27/28	0/2/2/2
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
7	G7M	A2	527	7	-	3/7/25/26	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
29	G7M	W	46	29	-	5/7/25/26	0/3/3/3
29	H2U	W	17	29	-	1/7/38/39	0/2/2/2
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
7	2MG	A1	1207	7	-	0/9/27/28	0/3/3/3
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/9/27/28	0/3/3/3
7	2MG	A1	966	7	-	0/9/27/28	0/3/3/3
32	CM0	Y1	34	32	-	2/12/30/31	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
5	2MG	72	2445	5	-	0/9/27/28	0/3/3/3
5	H2U	72	2449	5,49	-	1/7/38/39	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
29	PSU	W	55	29	-	3/7/25/26	0/2/2/2
30	MIA	W1	37	30	-	6/15/33/34	0/3/3/3
7	2MG	A2	1207	7	-	0/9/27/28	0/3/3/3
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2
5	G7M	72	2069	5	-	2/7/25/26	0/3/3/3
7	MA6	A1	1519	7	-	6/11/29/30	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
5	2MA	72	2503	5	-	0/7/25/26	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
5	6MZ	72	2030	5	-	3/9/27/28	0/3/3/3

All (446) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	34	CM0	C6-C5	12.87	1.48	1.34
5	71	1915	3TD	C6-C5	12.74	1.50	1.35
31	X2	38	2MA	C4-N3	12.55	1.50	1.34
5	72	1915	3TD	C6-C5	12.52	1.49	1.35
5	72	2503	2MA	C4-N3	12.22	1.49	1.34
5	72	2504	PSU	C6-C5	12.20	1.49	1.35
5	72	955	PSU	C6-C5	12.17	1.49	1.35
5	72	2457	PSU	C6-C5	12.13	1.49	1.35
30	W1	32	PSU	C6-C5	12.13	1.49	1.35
30	W1	39	PSU	C6-C5	12.12	1.49	1.35
29	W	32	PSU	C6-C5	12.10	1.49	1.35
5	72	2605	PSU	C6-C5	12.09	1.49	1.35
5	72	2580	PSU	C6-C5	12.06	1.49	1.35
5	72	2604	PSU	C6-C5	12.06	1.49	1.35
5	72	2030	6MZ	C6-N6	12.00	1.47	1.34
32	Y1	37	6MZ	C6-N6	11.87	1.47	1.34
31	X2	33	RSP	C2-N3	11.76	1.48	1.36
5	72	1618	6MZ	C6-N6	11.70	1.46	1.34
32	Y1	46	7MG	C8-N9	9.99	1.51	1.46
7	A1	967	5MC	C6-C5	9.98	1.51	1.34
7	A1	1407	5MC	C6-C5	9.89	1.50	1.34
5	72	1962	5MC	C6-C5	9.89	1.50	1.34
7	A2	967	5MC	C6-C5	9.87	1.50	1.34
7	A2	1407	5MC	C6-C5	9.84	1.50	1.34
5	72	2504	PSU	C2-N1	9.63	1.49	1.36
31	X2	17	H2U	C2-N1	9.62	1.49	1.35
5	72	955	PSU	C2-N1	9.58	1.49	1.36
5	72	2580	PSU	C2-N1	9.56	1.49	1.36
30	W1	32	PSU	C2-N1	9.55	1.49	1.36
5	72	2604	PSU	C2-N1	9.54	1.49	1.36
30	W1	39	PSU	C2-N1	9.53	1.49	1.36
5	72	2457	PSU	C2-N1	9.53	1.49	1.36
5	72	2605	PSU	C2-N1	9.52	1.49	1.36
29	W	32	PSU	C2-N1	9.49	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	17	H2U	C2-N1	9.46	1.49	1.35
31	X2	21	H2U	C2-N1	9.44	1.49	1.35
33	Y2	17	H2U	C2-N1	9.42	1.49	1.35
29	W	16	H2U	C2-N1	9.39	1.49	1.35
5	72	2449	H2U	C2-N1	9.36	1.49	1.35
29	W	20	H2U	C2-N1	9.34	1.49	1.35
30	W1	8	4SU	C4-N3	8.98	1.47	1.37
5	71	1915	3TD	C2-N1	8.86	1.48	1.37
29	W	8	4SU	C4-N3	8.85	1.47	1.37
5	72	1915	3TD	C2-N1	8.85	1.48	1.37
31	X2	8	4SU	C4-N3	8.83	1.47	1.37
5	72	2504	PSU	C2-N3	8.24	1.51	1.37
5	72	955	PSU	C2-N3	8.23	1.51	1.37
7	A1	1516	2MG	C2-N3	8.23	1.47	1.31
7	A2	1207	2MG	C2-N3	8.22	1.47	1.31
30	W1	32	PSU	C2-N3	8.21	1.51	1.37
29	W	32	PSU	C2-N3	8.21	1.51	1.37
7	A2	966	2MG	C2-N3	8.21	1.47	1.31
7	A1	1207	2MG	C2-N3	8.20	1.47	1.31
5	72	2605	PSU	C2-N3	8.20	1.51	1.37
5	72	2580	PSU	C2-N3	8.19	1.51	1.37
5	72	2604	PSU	C2-N3	8.19	1.51	1.37
5	72	2457	PSU	C2-N3	8.19	1.51	1.37
5	72	2445	2MG	C2-N3	8.17	1.47	1.31
7	A2	1516	2MG	C2-N3	8.17	1.47	1.31
30	W1	39	PSU	C2-N3	8.14	1.51	1.37
31	X2	48	3AU	C2-N1	8.13	1.50	1.38
7	A1	966	2MG	C2-N3	8.13	1.47	1.31
30	W1	37	MIA	C6-N6	8.11	1.47	1.34
5	72	1835	2MG	C2-N3	8.06	1.47	1.31
31	X2	38	2MA	C2-N3	8.05	1.48	1.34
29	W	37	MIA	C6-N6	7.98	1.47	1.34
32	Y1	46	7MG	C5-N7	7.90	1.44	1.35
5	72	2503	2MA	C2-N3	7.85	1.48	1.34
30	W1	37	MIA	C2-S10	7.71	1.82	1.75
29	W	37	MIA	C2-S10	7.69	1.82	1.75
5	72	1962	5MC	C4-N3	7.46	1.46	1.34
7	A2	967	5MC	C4-N3	7.45	1.46	1.34
7	A1	967	5MC	C4-N3	7.44	1.46	1.34
32	Y1	34	CM0	C2-N1	7.39	1.50	1.38
7	A1	1407	5MC	C4-N3	7.35	1.46	1.34
7	A2	1407	5MC	C4-N3	7.30	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2251	OMG	C2-N2	7.18	1.51	1.34
7	A2	1402	4OC	C4-N3	7.12	1.45	1.32
7	A1	1498	UR3	C2-N1	7.04	1.48	1.38
5	72	2498	OMC	C2-N3	7.00	1.50	1.36
7	A2	1498	UR3	C2-N1	6.98	1.48	1.38
32	Y1	34	CM0	C2-N3	6.98	1.50	1.38
5	72	2445	2MG	C4-N3	6.97	1.50	1.34
5	72	2552	OMU	C2-N3	6.97	1.50	1.38
7	A1	1407	5MC	C2-N3	6.96	1.50	1.36
7	A1	966	2MG	C4-N3	6.96	1.50	1.34
7	A1	1402	4OC	C4-N3	6.95	1.44	1.32
7	A1	1516	2MG	C4-N3	6.94	1.50	1.34
7	A1	967	5MC	C2-N3	6.94	1.50	1.36
7	A2	1207	2MG	C4-N3	6.93	1.50	1.34
5	72	745	1MG	C2-N3	6.92	1.47	1.34
7	A2	967	5MC	C2-N3	6.92	1.50	1.36
30	W1	8	4SU	C2-N3	6.91	1.50	1.38
5	72	1962	5MC	C2-N3	6.90	1.50	1.36
7	A2	1407	5MC	C2-N3	6.90	1.50	1.36
7	A2	966	2MG	C4-N3	6.89	1.50	1.34
5	72	1835	2MG	C4-N3	6.88	1.50	1.34
31	X2	8	4SU	C2-N3	6.86	1.50	1.38
5	72	2503	2MA	C6-N1	6.85	1.44	1.35
7	A1	1207	2MG	C4-N3	6.84	1.50	1.34
29	W	8	4SU	C2-N3	6.82	1.50	1.38
31	X2	38	2MA	C6-N1	6.82	1.44	1.35
7	A2	1516	2MG	C4-N3	6.80	1.50	1.34
30	W1	46	G7M	C4-N3	6.76	1.50	1.34
31	X2	47	G7M	C4-N3	6.75	1.50	1.34
31	X2	33	RSP	C6-C5	6.72	1.50	1.35
29	W	46	G7M	C4-N3	6.70	1.50	1.34
31	X2	33	RSP	C4-N4	6.65	1.49	1.33
33	Y2	46	G7M	C4-N3	6.63	1.50	1.34
33	Y2	46	G7M	C2-N2	6.61	1.49	1.34
31	X2	47	G7M	C2-N2	6.59	1.49	1.34
29	W	46	G7M	C2-N2	6.58	1.49	1.34
5	72	2069	G7M	C2-N2	6.58	1.49	1.34
30	W1	46	G7M	C2-N2	6.56	1.49	1.34
7	A2	527	G7M	C2-N2	6.55	1.49	1.34
7	A2	1207	2MG	C2-N2	6.54	1.47	1.33
7	A1	527	G7M	C2-N2	6.53	1.49	1.34
5	72	2552	OMU	C2-N1	6.53	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2069	G7M	C4-N3	6.52	1.49	1.34
7	A2	527	G7M	C4-N3	6.52	1.49	1.34
29	W	17	H2U	C2-N3	6.52	1.49	1.38
5	72	745	1MG	C4-N3	6.50	1.49	1.34
7	A1	527	G7M	C4-N3	6.50	1.49	1.34
31	X2	17	H2U	C2-N3	6.49	1.49	1.38
33	Y2	17	H2U	C2-N3	6.49	1.49	1.38
7	A1	1516	2MG	C2-N2	6.48	1.47	1.33
31	X2	21	H2U	C2-N3	6.47	1.49	1.38
7	A1	966	2MG	C2-N2	6.47	1.47	1.33
29	W	20	H2U	C2-N3	6.46	1.49	1.38
7	A1	1207	2MG	C2-N2	6.45	1.47	1.33
7	A2	966	2MG	C2-N2	6.45	1.47	1.33
7	A1	1402	4OC	C6-C5	6.43	1.50	1.35
5	72	1835	2MG	C2-N2	6.43	1.47	1.33
29	W	16	H2U	C2-N3	6.42	1.49	1.38
7	A2	1516	2MG	C2-N2	6.41	1.47	1.33
5	72	745	1MG	C2-N2	6.41	1.45	1.34
5	72	2449	H2U	C2-N3	6.40	1.49	1.38
31	X2	48	3AU	C2-N3	6.38	1.50	1.38
5	72	2445	2MG	C2-N2	6.38	1.47	1.33
7	A2	1402	4OC	C6-C5	6.36	1.49	1.35
7	A2	1402	4OC	C2-N3	6.33	1.49	1.36
7	A1	1402	4OC	C2-N3	6.21	1.48	1.36
31	X2	38	2MA	C2-N1	6.20	1.45	1.34
5	72	2503	2MA	C2-N1	6.17	1.45	1.34
7	A1	1498	UR3	C6-C5	6.16	1.49	1.35
7	A2	1498	UR3	C6-C5	6.13	1.49	1.35
5	72	2498	OMC	C6-C5	6.11	1.49	1.35
31	X2	8	4SU	C4-S4	-6.07	1.56	1.68
31	X2	48	3AU	C6-C5	6.04	1.49	1.35
29	W	8	4SU	C4-S4	-5.96	1.57	1.68
5	72	2251	OMG	C4-N3	5.93	1.48	1.34
30	W1	8	4SU	C4-S4	-5.93	1.57	1.68
32	Y1	46	7MG	C2-N3	5.92	1.47	1.33
33	Y2	46	G7M	C2-N3	5.88	1.47	1.33
31	X2	8	4SU	C2-N1	5.86	1.47	1.38
30	W1	46	G7M	C2-N3	5.85	1.47	1.33
7	A1	527	G7M	C2-N3	5.85	1.47	1.33
30	W1	8	4SU	C6-C5	5.84	1.48	1.35
5	72	955	PSU	C6-N1	5.83	1.45	1.36
30	W1	8	4SU	C2-N1	5.83	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	8	4SU	C6-C5	5.82	1.48	1.35
30	W1	39	PSU	C6-N1	5.82	1.45	1.36
31	X2	8	4SU	C6-C5	5.82	1.48	1.35
5	72	2457	PSU	C6-N1	5.80	1.45	1.36
5	72	2580	PSU	C6-N1	5.79	1.45	1.36
31	X2	47	G7M	C2-N3	5.79	1.47	1.33
7	A2	527	G7M	C2-N3	5.79	1.47	1.33
5	72	2069	G7M	C2-N3	5.79	1.47	1.33
29	W	46	G7M	C2-N3	5.79	1.47	1.33
5	72	2504	PSU	C6-N1	5.79	1.45	1.36
30	W1	32	PSU	C6-N1	5.77	1.45	1.36
5	72	2605	PSU	C6-N1	5.77	1.45	1.36
5	72	2604	PSU	C6-N1	5.76	1.45	1.36
29	W	32	PSU	C6-N1	5.73	1.45	1.36
29	W	8	4SU	C2-N1	5.72	1.47	1.38
32	Y1	46	7MG	C4-N9	5.67	1.44	1.37
7	A1	967	5MC	C4-N4	5.66	1.48	1.34
7	A1	1407	5MC	C4-N4	5.66	1.48	1.34
7	A2	1407	5MC	C4-N4	5.64	1.48	1.34
7	A2	967	5MC	C4-N4	5.63	1.48	1.34
5	72	1962	5MC	C4-N4	5.62	1.48	1.34
7	A1	1407	5MC	C6-N1	5.61	1.47	1.38
32	Y1	46	7MG	C4-N3	5.59	1.47	1.34
7	A2	1407	5MC	C6-N1	5.53	1.47	1.38
5	71	1915	3TD	C6-N1	5.53	1.45	1.36
5	72	2498	OMC	C4-N3	5.51	1.45	1.34
7	A1	967	5MC	C6-N1	5.49	1.47	1.38
5	72	1915	3TD	C6-N1	5.49	1.45	1.36
5	72	1962	5MC	C6-N1	5.47	1.47	1.38
5	72	2552	OMU	C6-C5	5.47	1.47	1.35
7	A2	967	5MC	C6-N1	5.44	1.47	1.38
7	A1	1207	2MG	C2-N1	5.42	1.45	1.36
31	X2	33	RSP	C4-N3	5.41	1.45	1.34
7	A1	966	2MG	C2-N1	5.40	1.45	1.36
7	A2	1207	2MG	C2-N1	5.40	1.45	1.36
7	A2	966	2MG	C2-N1	5.39	1.45	1.36
7	A1	1516	2MG	C2-N1	5.38	1.45	1.36
7	A2	1516	2MG	C2-N1	5.36	1.45	1.36
31	X2	38	2MA	C5-C6	5.35	1.55	1.41
5	72	2445	2MG	C2-N1	5.29	1.45	1.36
5	72	2503	2MA	C5-C6	5.27	1.55	1.41
5	72	1835	2MG	C2-N1	5.24	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2251	OMG	C2-N3	5.23	1.45	1.33
5	72	2498	OMC	C4-N4	5.21	1.46	1.33
7	A1	1498	UR3	C2-N3	5.13	1.48	1.39
7	A2	1402	4OC	C4-N4	5.12	1.46	1.35
7	A1	1402	4OC	C4-N4	5.09	1.46	1.35
7	A2	1498	UR3	C2-N3	5.03	1.48	1.39
29	W	20	H2U	C4-N3	4.97	1.46	1.37
29	W	17	H2U	C4-N3	4.97	1.46	1.37
31	X2	21	H2U	C4-N3	4.92	1.46	1.37
31	X2	17	H2U	C4-N3	4.92	1.46	1.37
5	72	2449	H2U	C4-N3	4.90	1.45	1.37
33	Y2	17	H2U	C4-N3	4.90	1.45	1.37
29	W	16	H2U	C4-N3	4.86	1.45	1.37
32	Y1	46	7MG	C2-N2	4.74	1.45	1.34
5	72	2552	OMU	C4-N3	4.64	1.46	1.38
7	A2	967	5MC	C2-N1	4.56	1.49	1.40
7	A1	1407	5MC	C2-N1	4.56	1.49	1.40
5	72	1962	5MC	C2-N1	4.55	1.49	1.40
32	Y1	34	CM0	C6-N1	4.53	1.45	1.38
7	A1	967	5MC	C2-N1	4.52	1.49	1.40
5	72	2552	OMU	O4-C4	-4.49	1.15	1.24
7	A2	1407	5MC	C2-N1	4.48	1.49	1.40
5	72	2498	OMC	C2-N1	4.45	1.49	1.40
5	72	2504	PSU	C4-N3	4.40	1.47	1.38
5	72	2580	PSU	C4-N3	4.39	1.47	1.38
30	W1	32	PSU	C4-N3	4.38	1.47	1.38
5	72	955	PSU	C4-N3	4.35	1.46	1.38
5	72	2605	PSU	C4-N3	4.34	1.46	1.38
5	72	2457	PSU	C4-N3	4.33	1.46	1.38
30	W1	39	PSU	C4-N3	4.32	1.46	1.38
29	W	32	PSU	C4-N3	4.32	1.46	1.38
31	X2	47	G7M	C5-N7	-4.31	1.34	1.39
29	W	46	G7M	C5-N7	-4.31	1.34	1.39
30	W1	46	G7M	C5-N7	-4.30	1.34	1.39
7	A1	527	G7M	C5-N7	-4.30	1.34	1.39
5	72	2604	PSU	C4-N3	4.28	1.46	1.38
7	A2	1402	4OC	C2-N1	4.26	1.49	1.40
7	A2	527	G7M	C5-N7	-4.23	1.34	1.39
5	71	1915	3TD	C2-N3	4.21	1.47	1.38
7	A1	1402	4OC	C2-N1	4.20	1.49	1.40
5	72	2069	G7M	C5-N7	-4.18	1.34	1.39
5	72	1915	3TD	C2-N3	4.18	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2498	OMC	O2-C2	-4.13	1.16	1.23
33	Y2	46	G7M	C5-N7	-4.05	1.34	1.39
30	W1	46	G7M	C5-C6	3.98	1.54	1.43
7	A1	1402	4OC	C5-C4	3.97	1.49	1.40
31	X2	47	G7M	C5-C6	3.96	1.54	1.43
29	W	46	G7M	C5-C6	3.93	1.54	1.43
7	A1	527	G7M	C5-C6	3.93	1.54	1.43
33	Y2	46	G7M	C5-C6	3.92	1.54	1.43
7	A2	1402	4OC	C5-C4	3.86	1.49	1.40
5	72	2069	G7M	C5-C6	3.85	1.54	1.43
7	A2	527	G7M	C5-C6	3.84	1.54	1.43
32	Y1	46	7MG	C2-N1	3.84	1.47	1.37
7	A2	1518	MA6	C6-N6	3.83	1.48	1.36
7	A2	1519	MA6	C6-N6	3.81	1.48	1.36
7	A1	1518	MA6	C6-N6	3.81	1.48	1.36
5	72	2498	OMC	C6-N1	3.79	1.47	1.38
7	A1	1519	MA6	C6-N6	3.76	1.47	1.36
32	Y1	34	CM0	C4-N3	3.71	1.45	1.38
5	72	2552	OMU	C6-N1	3.70	1.46	1.38
31	X2	38	2MA	C5-N7	-3.60	1.32	1.39
5	72	2552	OMU	O2-C2	-3.57	1.16	1.23
31	X2	48	3AU	C4-N3	3.57	1.46	1.40
31	X2	33	RSP	C5-C4	3.56	1.51	1.42
5	72	2503	2MA	C5-N7	-3.54	1.32	1.39
32	Y1	46	7MG	C5-C6	3.52	1.52	1.43
29	W	8	4SU	C5-C4	3.49	1.47	1.42
30	W1	8	4SU	C6-N1	3.48	1.46	1.38
30	W1	8	4SU	C5-C4	3.48	1.47	1.42
31	X2	8	4SU	C5-C4	3.47	1.47	1.42
32	Y1	46	7MG	C6-N1	3.44	1.45	1.38
5	72	745	1MG	C5-C6	3.43	1.54	1.45
33	Y2	55	PSU	C6-C5	3.43	1.39	1.35
31	X2	38	2MA	C8-N7	3.40	1.38	1.31
5	72	2503	2MA	C8-N7	3.39	1.38	1.31
31	X2	8	4SU	C6-N1	3.38	1.46	1.38
29	W	8	4SU	C6-N1	3.38	1.46	1.38
31	X2	56	PSU	C6-C5	3.34	1.39	1.35
5	72	2251	OMG	C2-N1	3.30	1.45	1.37
7	A1	1402	4OC	C6-N1	3.28	1.45	1.38
31	X2	48	3AU	C6-N1	3.27	1.45	1.38
29	W	55	PSU	C6-C5	3.25	1.39	1.35
5	72	955	PSU	O4-C4	-3.24	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	W1	32	PSU	O4-C4	-3.22	1.17	1.23
30	W1	39	PSU	O4-C4	-3.21	1.17	1.23
5	72	2604	PSU	O4-C4	-3.21	1.17	1.23
7	A2	1402	4OC	C6-N1	3.21	1.45	1.38
29	W	32	PSU	O4-C4	-3.18	1.17	1.23
5	72	2605	PSU	O4-C4	-3.18	1.17	1.23
5	72	2457	PSU	O4-C4	-3.17	1.17	1.23
31	X2	33	RSP	C2-S2	-3.17	1.59	1.67
5	72	2580	PSU	O4-C4	-3.15	1.17	1.23
5	72	2504	PSU	O4-C4	-3.13	1.17	1.23
31	X2	33	RSP	C6-N1	3.10	1.45	1.38
33	Y2	46	G7M	C2-N1	3.09	1.45	1.37
33	Y2	46	G7M	C6-N1	3.06	1.44	1.38
5	72	746	PSU	C6-C5	3.06	1.38	1.35
7	A1	1498	UR3	C6-N1	3.03	1.45	1.38
31	X2	48	3AU	C11-C10	3.03	1.59	1.52
5	72	2069	G7M	C2-N1	3.02	1.45	1.37
7	A1	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	1498	UR3	C6-N1	2.99	1.45	1.38
7	A1	527	G7M	C6-N1	2.99	1.44	1.38
30	W1	46	G7M	C2-N1	2.97	1.45	1.37
29	W	46	G7M	C2-N1	2.97	1.45	1.37
30	W1	46	G7M	C6-N1	2.95	1.44	1.38
31	X2	47	G7M	C2-N1	2.95	1.45	1.37
5	72	2069	G7M	C6-N1	2.94	1.44	1.38
29	W	46	G7M	C6-N1	2.93	1.44	1.38
7	A2	966	2MG	C5-C6	2.93	1.55	1.44
7	A2	527	G7M	C6-N1	2.92	1.44	1.38
31	X2	47	G7M	C6-N1	2.92	1.44	1.38
7	A1	966	2MG	C5-C6	2.90	1.55	1.44
5	72	2445	2MG	C5-C6	2.89	1.55	1.44
5	72	1835	2MG	C5-C6	2.89	1.55	1.44
7	A2	1207	2MG	C5-C6	2.88	1.55	1.44
7	A1	1207	2MG	C5-C6	2.88	1.55	1.44
7	A1	1516	2MG	C5-C6	2.87	1.55	1.44
7	A2	1516	2MG	C5-C6	2.86	1.55	1.44
5	72	1835	2MG	C5-N7	-2.83	1.33	1.39
7	A2	1207	2MG	C5-N7	-2.83	1.33	1.39
5	72	2498	OMC	C5-C4	2.81	1.49	1.42
7	A1	1402	4OC	O2-C2	-2.81	1.18	1.23
7	A1	966	2MG	C6-N1	2.80	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2580	PSU	C1'-C5	2.79	1.56	1.50
5	72	2604	PSU	C1'-C5	2.78	1.56	1.50
5	72	2445	2MG	C5-N7	-2.78	1.33	1.39
5	72	2605	PSU	C1'-C5	2.76	1.56	1.50
7	A2	1516	2MG	C5-N7	-2.76	1.33	1.39
7	A1	1207	2MG	C5-N7	-2.76	1.33	1.39
7	A2	1516	2MG	C6-N1	2.76	1.44	1.38
7	A2	966	2MG	C6-N1	2.75	1.43	1.38
7	A1	1516	2MG	C5-N7	-2.74	1.33	1.39
30	W1	32	PSU	C1'-C5	2.74	1.56	1.50
5	72	2457	PSU	C1'-C5	2.73	1.56	1.50
7	A1	966	2MG	C5-N7	-2.73	1.33	1.39
7	A2	1402	4OC	O2-C2	-2.72	1.18	1.23
31	X2	48	3AU	C5-C4	2.72	1.50	1.43
5	72	955	PSU	C1'-C5	2.72	1.56	1.50
7	A1	1516	2MG	C6-N1	2.72	1.43	1.38
5	72	2445	2MG	C6-N1	2.71	1.43	1.38
5	72	2504	PSU	C1'-C5	2.70	1.56	1.50
7	A2	966	2MG	C5-N7	-2.70	1.33	1.39
7	A2	1207	2MG	C6-N1	2.69	1.43	1.38
5	72	1835	2MG	C6-N1	2.68	1.43	1.38
30	W1	39	PSU	C1'-C5	2.67	1.56	1.50
7	A1	1207	2MG	C6-N1	2.66	1.43	1.38
5	72	2604	PSU	O2-C2	-2.65	1.17	1.23
5	72	745	1MG	C5-N7	-2.65	1.33	1.39
5	72	955	PSU	O2-C2	-2.65	1.17	1.23
30	W1	37	MIA	C5-N7	-2.65	1.34	1.39
29	W	32	PSU	C1'-C5	2.64	1.56	1.50
5	72	1618	6MZ	C5-N7	-2.64	1.34	1.39
29	W	37	MIA	C5-N7	-2.62	1.34	1.39
30	W1	39	PSU	O2-C2	-2.61	1.17	1.23
29	W	32	PSU	O2-C2	-2.61	1.17	1.23
5	71	1915	3TD	C1'-C5	2.61	1.56	1.50
32	Y1	34	CM0	O5-C7	-2.60	1.38	1.44
5	72	2580	PSU	O2-C2	-2.60	1.17	1.23
5	72	2030	6MZ	C5-N7	-2.60	1.34	1.39
5	72	2457	PSU	O2-C2	-2.59	1.18	1.23
5	72	2605	PSU	O2-C2	-2.59	1.18	1.23
5	72	2504	PSU	O2-C2	-2.58	1.18	1.23
30	W1	32	PSU	O2-C2	-2.57	1.18	1.23
29	W	37	MIA	C5-C4	-2.55	1.34	1.39
30	W1	46	G7M	O6-C6	-2.52	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	71	1915	3TD	C4-N3	2.52	1.45	1.40
32	Y1	37	6MZ	C5-N7	-2.50	1.34	1.39
5	72	1915	3TD	C4-N3	2.50	1.45	1.40
7	A2	527	G7M	O6-C6	-2.50	1.18	1.23
31	X2	47	G7M	O6-C6	-2.49	1.18	1.23
7	A1	527	G7M	O6-C6	-2.46	1.18	1.23
32	Y1	46	7MG	O6-C6	-2.46	1.18	1.23
29	W	46	G7M	O6-C6	-2.43	1.19	1.23
5	72	746	PSU	C4-C5	-2.43	1.37	1.44
5	72	1915	3TD	C1'-C5	2.43	1.55	1.50
5	72	2069	G7M	O6-C6	-2.42	1.19	1.23
33	Y2	46	G7M	O6-C6	-2.39	1.19	1.23
7	A2	1207	2MG	O6-C6	-2.39	1.19	1.23
30	W1	37	MIA	C5-C4	-2.37	1.34	1.39
5	72	2251	OMG	C5-C6	2.37	1.53	1.44
7	A1	1207	2MG	O6-C6	-2.37	1.19	1.23
5	72	1835	2MG	O6-C6	-2.36	1.19	1.23
7	A2	1519	MA6	C5-C4	-2.36	1.34	1.39
7	A2	1407	5MC	O2-C2	-2.35	1.19	1.23
7	A1	1516	2MG	O6-C6	-2.35	1.19	1.23
7	A2	1516	2MG	O6-C6	-2.34	1.19	1.23
5	72	2445	2MG	O6-C6	-2.33	1.19	1.23
7	A2	966	2MG	O6-C6	-2.33	1.19	1.23
7	A1	966	2MG	O6-C6	-2.33	1.19	1.23
5	72	2552	OMU	C5-C4	2.33	1.48	1.43
7	A1	1519	MA6	C5-N7	-2.32	1.34	1.39
7	A2	1518	MA6	C5-N7	-2.31	1.34	1.39
7	A1	1518	MA6	C5-C4	-2.29	1.34	1.39
7	A2	1518	MA6	C5-C4	-2.29	1.34	1.39
29	W	16	H2U	O2-C2	-2.29	1.18	1.23
5	71	1915	3TD	O4-C4	-2.29	1.18	1.23
7	A1	1518	MA6	C5-N7	-2.28	1.34	1.39
5	72	1915	3TD	O4-C4	-2.28	1.18	1.23
31	X2	17	H2U	O2-C2	-2.27	1.18	1.23
7	A2	967	5MC	O2-C2	-2.26	1.19	1.23
7	A1	967	5MC	O2-C2	-2.25	1.19	1.23
29	W	17	H2U	O2-C2	-2.25	1.18	1.23
5	72	2449	H2U	O2-C2	-2.25	1.18	1.23
5	72	1618	6MZ	C6-N1	-2.24	1.31	1.35
5	72	1962	5MC	O2-C2	-2.24	1.19	1.23
33	Y2	17	H2U	O2-C2	-2.24	1.19	1.23
29	W	20	H2U	O2-C2	-2.23	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	1519	MA6	C5-N7	-2.22	1.34	1.39
7	A1	1498	UR3	C5-C4	2.22	1.49	1.43
7	A1	1407	5MC	O2-C2	-2.21	1.19	1.23
7	A1	1519	MA6	C5-C4	-2.21	1.34	1.39
31	X2	21	H2U	O2-C2	-2.20	1.19	1.23
7	A2	1498	UR3	O4-C4	-2.19	1.18	1.23
7	A2	1498	UR3	C5-C4	2.18	1.49	1.43
31	X2	21	H2U	O4-C4	-2.17	1.18	1.23
7	A2	1498	UR3	O2-C2	-2.16	1.18	1.22
32	Y1	37	6MZ	C5-C4	-2.15	1.35	1.39
7	A1	1498	UR3	O4-C4	-2.15	1.18	1.23
7	A1	527	G7M	C8-N7	2.15	1.36	1.33
5	72	2503	2MA	C6-N6	-2.14	1.28	1.34
5	72	2449	H2U	O4-C4	-2.14	1.18	1.23
31	X2	38	2MA	C6-N6	-2.14	1.28	1.34
7	A1	1498	UR3	C4-N3	2.13	1.45	1.40
33	Y2	17	H2U	O4-C4	-2.13	1.18	1.23
33	Y2	46	G7M	C8-N7	2.13	1.36	1.33
5	72	2030	6MZ	C5-C4	-2.12	1.35	1.39
7	A1	1498	UR3	O2-C2	-2.12	1.18	1.22
29	W	17	H2U	O4-C4	-2.12	1.19	1.23
29	W	20	H2U	O4-C4	-2.12	1.19	1.23
29	W	16	H2U	O4-C4	-2.12	1.19	1.23
31	X2	17	H2U	O4-C4	-2.11	1.19	1.23
29	W	37	MIA	C8-N9	-2.11	1.33	1.37
5	72	2030	6MZ	C6-N1	-2.10	1.31	1.35
7	A2	1498	UR3	C4-N3	2.09	1.45	1.40
5	72	1618	6MZ	C5-C4	-2.09	1.35	1.39
32	Y1	37	6MZ	C6-N1	-2.08	1.31	1.35
5	72	2069	G7M	C8-N7	2.06	1.36	1.33
30	W1	37	MIA	C8-N9	-2.06	1.33	1.37
7	A2	527	G7M	C8-N7	2.05	1.36	1.33
5	72	2251	OMG	C8-N7	2.04	1.38	1.32
5	72	2251	OMG	C5-N7	-2.01	1.35	1.39

All (447) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C8	-12.64	98.59	127.14
31	X2	38	2MA	C1'-N9-C8	-12.18	99.63	127.14
7	A2	1519	MA6	N1-C6-N6	-12.11	103.84	117.08
7	A1	1519	MA6	N1-C6-N6	-12.10	103.85	117.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1518	MA6	N1-C6-N6	-11.96	104.00	117.08
7	A1	1518	MA6	N1-C6-N6	-11.72	104.26	117.08
5	72	2503	2MA	C4-N9-C1'	11.04	152.89	126.59
31	X2	38	2MA	C4-N9-C1'	10.78	152.28	126.59
30	W1	37	MIA	C11-S10-C2	10.55	110.15	102.27
29	W	37	MIA	C11-S10-C2	8.92	108.93	102.27
29	W	8	4SU	C4-N3-C2	-7.97	119.60	127.34
31	X2	8	4SU	C4-N3-C2	-7.92	119.65	127.34
30	W1	8	4SU	C4-N3-C2	-7.71	119.85	127.34
31	X2	21	H2U	C4-N3-C2	-7.16	119.85	125.79
5	72	2449	H2U	C4-N3-C2	-7.14	119.87	125.79
29	W	20	H2U	C4-N3-C2	-7.02	119.97	125.79
33	Y2	17	H2U	C4-N3-C2	-7.00	119.98	125.79
5	72	1835	2MG	C2-N3-C4	7.00	120.72	112.04
5	72	2251	OMG	C1'-N9-C8	-6.99	106.81	126.70
30	W1	37	MIA	C5-C4-N3	-6.98	119.34	127.19
5	72	2445	2MG	C2-N3-C4	6.91	120.61	112.04
29	W	17	H2U	C4-N3-C2	-6.89	120.07	125.79
29	W	16	H2U	C4-N3-C2	-6.81	120.15	125.79
5	72	745	1MG	C1'-N9-C4	-6.80	106.32	126.50
31	X2	17	H2U	C4-N3-C2	-6.76	120.18	125.79
7	A1	966	2MG	C2-N3-C4	6.75	120.41	112.04
7	A2	1207	2MG	C2-N3-C4	6.68	120.32	112.04
7	A2	966	2MG	C2-N3-C4	6.60	120.22	112.04
7	A1	1516	2MG	C2-N3-C4	6.56	120.18	112.04
29	W	37	MIA	C5-C4-N3	-6.45	119.93	127.19
5	72	745	1MG	C1'-N9-C8	6.37	144.82	126.70
7	A2	1519	MA6	C5-C6-N6	6.35	136.36	125.30
7	A2	1516	2MG	C2-N3-C4	6.34	119.90	112.04
7	A1	1207	2MG	C2-N3-C4	6.30	119.85	112.04
7	A1	1519	MA6	C5-C6-N6	6.28	136.25	125.30
7	A2	1518	MA6	C5-C6-N6	6.25	136.18	125.30
5	72	1618	6MZ	C5-C4-N3	-6.12	118.76	126.75
7	A1	1518	MA6	C5-C6-N6	6.07	135.88	125.30
31	X2	38	2MA	C5-C4-N3	-6.06	120.37	127.19
7	A1	1207	2MG	C1'-N9-C4	-5.81	109.24	126.50
5	72	2251	OMG	C1'-N9-C4	5.80	143.72	126.50
5	72	1835	2MG	C5-C4-N3	-5.76	119.11	128.46
5	72	2445	2MG	C5-C4-N3	-5.74	119.14	128.46
5	72	2503	2MA	C5-C4-N3	-5.74	120.74	127.19
7	A1	1207	2MG	C1'-N9-C8	5.72	142.99	126.70
7	A2	966	2MG	C1'-N9-C4	-5.66	109.70	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X2	8	4SU	C5-C4-N3	5.64	119.92	114.69
29	W	8	4SU	C5-C4-N3	5.59	119.87	114.69
7	A2	1519	MA6	N1-C2-N3	-5.57	119.89	128.60
7	A2	1516	2MG	C1'-N9-C4	-5.57	109.97	126.50
7	A1	1519	MA6	C1'-N9-C8	-5.56	114.59	127.14
7	A1	966	2MG	C1'-N9-C4	-5.53	110.07	126.50
5	72	1618	6MZ	N1-C2-N3	-5.51	119.98	128.60
7	A1	1518	MA6	C1'-N9-C8	-5.50	114.72	127.14
7	A1	1516	2MG	C1'-N9-C4	-5.50	110.18	126.50
7	A2	1207	2MG	C5-C4-N3	-5.47	119.59	128.46
5	72	1915	3TD	N1-C2-N3	5.47	120.45	116.14
7	A2	1518	MA6	N1-C2-N3	-5.47	120.05	128.60
30	W1	8	4SU	C5-C4-N3	5.45	119.74	114.69
7	A1	1518	MA6	N1-C2-N3	-5.44	120.09	128.60
7	A2	966	2MG	C1'-N9-C8	5.44	142.19	126.70
32	Y1	37	6MZ	N1-C2-N3	-5.43	120.10	128.60
32	Y1	34	CM0	C4-N3-C2	-5.41	120.34	127.35
7	A1	1519	MA6	N1-C2-N3	-5.41	120.14	128.60
5	72	2030	6MZ	N1-C2-N3	-5.39	120.17	128.60
7	A1	966	2MG	C5-C4-N3	-5.37	119.74	128.46
7	A2	1516	2MG	C1'-N9-C8	5.36	141.95	126.70
7	A1	966	2MG	C1'-N9-C8	5.34	141.91	126.70
32	Y1	37	6MZ	C5-C4-N3	-5.31	119.83	126.75
7	A2	1518	MA6	C1'-N9-C8	-5.30	115.16	127.14
5	71	1915	3TD	N1-C2-N3	5.30	120.32	116.14
7	A2	1207	2MG	C1'-N9-C4	-5.29	110.80	126.50
5	72	2030	6MZ	C5-C4-N3	-5.29	119.85	126.75
7	A1	1516	2MG	C1'-N9-C8	5.28	141.72	126.70
7	A1	1516	2MG	C5-C4-N3	-5.26	119.93	128.46
7	A2	1207	2MG	C1'-N9-C8	5.25	141.65	126.70
7	A2	966	2MG	C5-C4-N3	-5.19	120.04	128.46
7	A1	1519	MA6	C5-C4-N3	-5.16	120.02	126.75
7	A2	1516	2MG	C5-C4-N3	-5.07	120.23	128.46
5	72	2552	OMU	C4-N3-C2	-5.06	119.91	126.58
7	A1	1207	2MG	C5-C4-N3	-5.05	120.26	128.46
5	72	745	1MG	C5-C4-N3	-5.05	120.27	128.46
32	Y1	46	7MG	C5-C6-N1	5.01	119.82	110.99
7	A1	1518	MA6	C5-C4-N3	-5.01	120.22	126.75
7	A2	1519	MA6	C1'-N9-C8	-5.01	115.83	127.14
30	W1	37	MIA	C4-C5-C6	4.98	120.67	116.81
30	W1	46	G7M	C2-N3-C4	4.96	121.14	112.30
7	A2	1518	MA6	C5-C4-N3	-4.95	120.30	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	46	G7M	C2-N3-C4	4.90	121.03	112.30
7	A2	1519	MA6	C5-C4-N3	-4.88	120.38	126.75
31	X2	47	G7M	C2-N3-C4	4.87	120.98	112.30
5	72	1835	2MG	C2-N1-C6	-4.77	118.99	124.48
5	72	2445	2MG	C1'-N9-C4	-4.74	112.42	126.50
5	72	955	PSU	C4-N3-C2	-4.74	119.51	126.34
5	72	2445	2MG	C2-N1-C6	-4.74	119.02	124.48
5	72	2504	PSU	C4-N3-C2	-4.71	119.55	126.34
30	W1	46	G7M	C5-C4-N3	-4.70	119.14	128.15
5	72	2445	2MG	C1'-N9-C8	4.70	140.07	126.70
5	72	2251	OMG	C5-C4-N3	-4.70	120.84	128.46
5	72	2503	2MA	N9-C8-N7	-4.68	107.51	113.91
5	72	1618	6MZ	C4-C5-C6	4.68	120.43	116.81
7	A2	1498	UR3	C4-N3-C2	-4.67	120.17	124.56
5	72	2604	PSU	C4-N3-C2	-4.67	119.61	126.34
5	72	1835	2MG	C1'-N9-C4	-4.66	112.66	126.50
29	W	46	G7M	C5-C4-N3	-4.65	119.24	128.15
5	72	2580	PSU	C4-N3-C2	-4.64	119.65	126.34
5	72	2605	PSU	C4-N3-C2	-4.63	119.67	126.34
7	A1	1498	UR3	C4-N3-C2	-4.63	120.21	124.56
5	72	2457	PSU	C4-N3-C2	-4.61	119.69	126.34
7	A2	1519	MA6	N9-C8-N7	-4.61	107.60	113.91
5	72	1835	2MG	C1'-N9-C8	4.59	139.75	126.70
31	X2	47	G7M	C5-C4-N3	-4.55	119.42	128.15
7	A2	1518	MA6	N9-C8-N7	-4.54	107.70	113.91
30	W1	39	PSU	C4-N3-C2	-4.54	119.80	126.34
29	W	32	PSU	C4-N3-C2	-4.53	119.81	126.34
30	W1	32	PSU	C4-N3-C2	-4.51	119.83	126.34
7	A1	1519	MA6	C4-N9-C1'	4.51	137.34	126.59
7	A1	1518	MA6	N9-C8-N7	-4.51	107.75	113.91
7	A1	966	2MG	C2-N1-C6	-4.50	119.30	124.48
32	Y1	46	7MG	C2-N3-C4	4.50	120.31	112.30
7	A2	1207	2MG	C2-N1-C6	-4.48	119.33	124.48
31	X2	38	2MA	N9-C8-N7	-4.41	107.88	113.91
33	Y2	46	G7M	C2-N3-C4	4.41	120.15	112.30
7	A1	527	G7M	C2-N3-C4	4.40	120.14	112.30
7	A1	1516	2MG	C2-N1-C6	-4.39	119.43	124.48
5	72	2069	G7M	C2-N3-C4	4.38	120.10	112.30
7	A2	1516	2MG	C2-N1-C6	-4.36	119.46	124.48
30	W1	37	MIA	N3-C4-N9	4.35	133.03	126.99
5	72	2030	6MZ	C4-C5-C6	4.35	120.18	116.81
5	72	2504	PSU	N1-C2-N3	4.34	120.05	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	966	2MG	C2-N1-C6	-4.34	119.49	124.48
32	Y1	37	6MZ	N9-C8-N7	-4.32	108.00	113.91
29	W	37	MIA	N9-C8-N7	-4.32	108.00	113.91
7	A2	527	G7M	C2-N3-C4	4.30	119.96	112.30
7	A1	1518	MA6	C4-N9-C1'	4.29	136.82	126.59
29	W	37	MIA	C4-C5-C6	4.28	120.12	116.81
7	A1	1519	MA6	N9-C8-N7	-4.28	108.06	113.91
5	72	2251	OMG	C2-N3-C4	4.25	119.87	112.30
7	A1	1207	2MG	C2-N1-C6	-4.25	119.59	124.48
5	72	2030	6MZ	N9-C8-N7	-4.23	108.12	113.91
5	72	2457	PSU	N1-C2-N3	4.20	119.89	115.13
5	72	955	PSU	N1-C2-N3	4.19	119.88	115.13
5	72	2605	PSU	N1-C2-N3	4.19	119.88	115.13
32	Y1	46	7MG	C5-C4-N3	-4.17	120.18	128.13
5	72	1915	3TD	C4-N3-C2	-4.16	120.10	124.61
32	Y1	37	6MZ	C4-C5-C6	4.15	120.03	116.81
7	A2	1518	MA6	C4-N9-C1'	4.15	136.48	126.59
30	W1	39	PSU	N1-C2-N3	4.15	119.83	115.13
29	W	32	PSU	N1-C2-N3	4.14	119.82	115.13
30	W1	46	G7M	C5-C6-N1	4.12	120.40	111.79
32	Y1	37	6MZ	C4-N9-C1'	-4.11	116.79	126.59
5	72	2604	PSU	N1-C2-N3	4.11	119.79	115.13
5	72	2580	PSU	N1-C2-N3	4.11	119.78	115.13
30	W1	32	PSU	N1-C2-N3	4.09	119.76	115.13
29	W	46	G7M	C5-C6-N1	4.08	120.31	111.79
30	W1	37	MIA	N9-C8-N7	-4.08	108.34	113.91
31	X2	47	G7M	C5-C6-N1	4.07	120.29	111.79
5	71	1915	3TD	C4-N3-C2	-4.04	120.22	124.61
33	Y2	46	G7M	C5-C4-N3	-4.02	120.45	128.15
7	A1	527	G7M	C5-C4-N3	-3.99	120.49	128.15
5	72	2030	6MZ	C4-N9-C1'	-3.99	117.09	126.59
7	A2	527	G7M	C5-C6-N1	3.97	120.09	111.79
5	72	2069	G7M	C5-C4-N3	-3.97	120.54	128.15
7	A1	527	G7M	C5-C6-N1	3.95	120.05	111.79
5	72	2069	G7M	C5-C6-N1	3.95	120.03	111.79
33	Y2	46	G7M	C5-C6-N1	3.94	120.01	111.79
30	W1	46	G7M	N9-C4-N3	3.94	133.85	125.94
7	A2	527	G7M	C5-C4-N3	-3.93	120.61	128.15
5	72	1618	6MZ	N3-C4-N9	3.91	133.53	127.08
29	W	46	G7M	N9-C4-N3	3.90	133.77	125.94
5	72	1618	6MZ	C2-N3-C4	3.87	120.89	111.75
5	72	1618	6MZ	N9-C8-N7	-3.87	108.62	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	8	4SU	N3-C2-N1	3.85	120.00	114.89
7	A2	1519	MA6	C4-N9-C1'	3.85	135.76	126.59
31	X2	8	4SU	N3-C2-N1	3.82	119.96	114.89
31	X2	47	G7M	N9-C4-N3	3.81	133.59	125.94
30	W1	8	4SU	N3-C2-N1	3.78	119.90	114.89
5	72	1618	6MZ	C9-N6-C6	-3.77	119.62	122.87
5	72	2552	OMU	N3-C2-N1	3.76	119.89	114.89
31	X2	48	3AU	C4-N3-C2	-3.74	119.94	124.63
29	W	37	MIA	N3-C2-N1	-3.70	120.17	126.95
29	W	37	MIA	N3-C4-N9	3.69	132.12	126.99
30	W1	37	MIA	C12-C13-C14	-3.69	119.96	127.14
5	72	1835	2MG	N9-C4-N3	3.63	133.23	125.94
7	A1	1519	MA6	C4-C5-C6	3.63	119.94	115.88
5	72	745	1MG	C2-N3-C4	3.62	120.11	111.98
7	A1	1518	MA6	C4-C5-C6	3.60	119.91	115.88
32	Y1	34	CM0	N3-C2-N1	3.59	119.65	114.89
7	A2	1519	MA6	C2-N1-C6	3.59	120.22	111.75
30	W1	37	MIA	N3-C2-N1	-3.58	120.38	126.95
5	72	2445	2MG	N9-C4-N3	3.56	133.08	125.94
7	A2	1518	MA6	C2-N1-C6	3.53	120.09	111.75
32	Y1	37	6MZ	C1'-N9-C8	3.53	135.10	127.14
7	A1	1519	MA6	C2-N3-C4	3.51	120.05	111.75
32	Y1	37	6MZ	C2-N3-C4	3.50	120.03	111.75
7	A1	1518	MA6	C2-N1-C6	3.50	120.02	111.75
30	W1	8	4SU	C5-C4-S4	-3.50	119.96	124.47
29	W	37	MIA	C12-C13-C14	-3.49	120.34	127.14
7	A2	1518	MA6	C4-C5-C6	3.49	119.78	115.88
5	72	2251	OMG	N9-C8-N7	-3.48	106.83	113.39
7	A2	1518	MA6	C2-N3-C4	3.48	119.96	111.75
7	A1	1519	MA6	C2-N1-C6	3.47	119.96	111.75
7	A2	1519	MA6	C2-N3-C4	3.47	119.95	111.75
29	W	8	4SU	C5-C4-S4	-3.47	120.00	124.47
5	72	1962	5MC	C5-C6-N1	-3.47	119.77	123.34
7	A2	1519	MA6	C4-C5-C6	3.46	119.76	115.88
7	A1	1518	MA6	C2-N3-C4	3.45	119.91	111.75
31	X2	8	4SU	C5-C4-S4	-3.45	120.02	124.47
29	W	37	MIA	C4-N9-C1'	-3.45	118.37	126.59
5	72	2030	6MZ	C2-N3-C4	3.45	119.89	111.75
29	W	46	G7M	O6-C6-C5	-3.44	120.29	128.06
30	W1	46	G7M	O6-C6-C5	-3.43	120.32	128.06
7	A1	967	5MC	C5-C6-N1	-3.43	119.81	123.34
7	A2	527	G7M	O6-C6-C5	-3.41	120.38	128.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X2	47	G7M	O6-C6-C5	-3.41	120.38	128.06
5	72	2069	G7M	O6-C6-C5	-3.40	120.39	128.06
33	Y2	46	G7M	O6-C6-C5	-3.39	120.41	128.06
5	72	2030	6MZ	C1'-N9-C8	3.39	134.78	127.14
5	72	2504	PSU	C6-C5-C4	3.38	120.56	118.20
7	A1	527	G7M	O6-C6-C5	-3.37	120.45	128.06
29	W	32	PSU	C6-C5-C4	3.37	120.55	118.20
5	72	1939	5MU	O3'-C3'-C2'	-3.34	101.02	111.82
31	X2	48	3AU	C5-C4-N3	3.33	119.89	115.50
5	72	2457	PSU	C6-C5-C4	3.28	120.49	118.20
5	72	2552	OMU	C5-C4-N3	3.27	119.74	114.84
7	A2	1519	MA6	C5-N7-C8	3.26	108.14	103.51
7	A2	1207	2MG	N9-C4-N3	3.26	132.48	125.94
30	W1	39	PSU	C6-C5-C4	3.25	120.47	118.20
7	A1	966	2MG	N9-C4-N3	3.24	132.45	125.94
7	A1	1516	2MG	N9-C4-N3	3.23	132.43	125.94
32	Y1	46	7MG	C4-C5-N7	3.21	109.99	105.53
5	72	2030	6MZ	N3-C4-N9	3.21	132.38	127.08
5	72	2449	H2U	N3-C2-N1	3.21	120.05	116.65
5	72	745	1MG	N9-C4-N3	3.21	132.38	125.94
31	X2	38	2MA	N3-C4-N9	3.20	131.43	126.99
5	72	2503	2MA	C5-N7-C8	3.20	108.06	103.51
7	A2	1518	MA6	C5-N7-C8	3.20	108.05	103.51
32	Y1	37	6MZ	N3-C4-N9	3.19	132.34	127.08
31	X2	21	H2U	N3-C2-N1	3.19	120.02	116.65
29	W	37	MIA	N6-C6-N1	-3.18	114.44	118.50
29	W	17	H2U	N3-C2-N1	3.17	120.01	116.65
29	W	37	MIA	C5-N7-C8	3.17	108.02	103.51
5	72	2069	G7M	N9-C4-N3	3.17	132.30	125.94
29	W	20	H2U	N3-C2-N1	3.16	120.00	116.65
30	W1	46	G7M	C2-N1-C6	-3.15	119.35	125.10
7	A2	967	5MC	C5-C6-N1	-3.15	120.09	123.34
5	72	745	1MG	N9-C8-N7	-3.14	107.47	113.39
29	W	46	G7M	C2-N1-C6	-3.14	119.37	125.10
32	Y1	37	6MZ	C5-N7-C8	3.14	107.97	103.51
31	X2	17	H2U	N3-C2-N1	3.14	119.97	116.65
33	Y2	17	H2U	N3-C2-N1	3.14	119.97	116.65
33	Y2	46	G7M	N9-C4-N3	3.13	132.23	125.94
31	X2	38	2MA	C5-N7-C8	3.13	107.95	103.51
7	A1	1518	MA6	C5-N7-C8	3.13	107.95	103.51
5	72	2580	PSU	C6-C5-C4	3.12	120.38	118.20
7	A1	527	G7M	N9-C4-N3	3.11	132.19	125.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W1	37	MIA	C5-N7-C8	3.10	107.91	103.51
31	X2	38	2MA	N3-C2-N1	-3.09	120.03	125.72
7	A1	1519	MA6	N3-C4-N9	3.09	132.17	127.08
7	A2	966	2MG	N9-C4-N3	3.07	132.11	125.94
5	72	2030	6MZ	C5-N7-C8	3.07	107.87	103.51
5	72	955	PSU	C6-C5-C4	3.07	120.34	118.20
7	A2	527	G7M	N9-C4-N3	3.05	132.06	125.94
7	A1	1518	MA6	N3-C4-N9	3.04	132.09	127.08
5	72	2503	2MA	N3-C2-N1	-3.04	120.13	125.72
31	X2	47	G7M	C2-N1-C6	-3.04	119.56	125.10
5	72	2251	OMG	C2-N1-C6	-3.03	119.56	125.10
7	A1	1519	MA6	C5-N7-C8	3.03	107.81	103.51
7	A2	527	G7M	C2-N1-C6	-3.02	119.60	125.10
7	A1	527	G7M	C2-N1-C6	-3.02	119.60	125.10
5	72	2503	2MA	N3-C4-N9	3.01	131.16	126.99
7	A2	1516	2MG	N9-C4-N3	3.01	131.98	125.94
30	W1	32	PSU	C6-C5-C4	3.00	120.30	118.20
29	W	16	H2U	C5-C4-N3	2.98	119.99	116.65
29	W	16	H2U	N3-C2-N1	2.98	119.80	116.65
5	72	1618	6MZ	C5-N7-C8	2.97	107.73	103.51
5	72	2504	PSU	C6-N1-C2	-2.97	119.65	122.68
5	72	2604	PSU	C6-C5-C4	2.97	120.27	118.20
32	Y1	46	7MG	C5-C4-N9	2.96	110.19	106.35
5	72	2605	PSU	C6-N1-C2	-2.96	119.66	122.68
5	72	2069	G7M	C2-N1-C6	-2.95	119.72	125.10
33	Y2	46	G7M	C2-N1-C6	-2.94	119.73	125.10
30	W1	37	MIA	C2-N3-C4	2.93	120.07	112.35
7	A2	966	2MG	N9-C8-N7	-2.92	107.89	113.39
30	W1	32	PSU	C6-N1-C2	-2.91	119.71	122.68
29	W	37	MIA	S10-C2-N3	2.90	126.03	116.01
5	72	1939	5MU	O2'-C2'-C1'	-2.90	100.34	110.02
5	72	2552	OMU	O4-C4-C5	-2.89	120.08	125.16
7	A1	1407	5MC	C5-C6-N1	-2.89	120.37	123.34
29	W	32	PSU	C6-N1-C2	-2.89	119.73	122.68
5	72	2251	OMG	N9-C4-N3	2.89	131.74	125.94
5	72	2449	H2U	C5-C4-N3	2.88	119.89	116.65
32	Y1	46	7MG	C2-N1-C6	-2.88	119.86	125.10
30	W1	39	PSU	C6-N1-C2	-2.87	119.74	122.68
29	W	37	MIA	C2-N3-C4	2.87	119.91	112.35
7	A1	1516	2MG	N9-C8-N7	-2.86	108.01	113.39
7	A1	966	2MG	N9-C8-N7	-2.86	108.01	113.39
7	A2	1516	2MG	N9-C8-N7	-2.86	108.01	113.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X2	21	H2U	C5-C4-N3	2.85	119.85	116.65
5	72	2457	PSU	C6-N1-C2	-2.85	119.77	122.68
32	Y1	46	7MG	O6-C6-C5	-2.85	120.55	127.54
29	W	37	MIA	C1'-N9-C8	2.85	133.56	127.14
7	A2	1518	MA6	N3-C4-N9	2.84	131.77	127.08
7	A1	1207	2MG	N9-C4-N3	2.84	131.63	125.94
5	72	2605	PSU	C6-C5-C4	2.84	120.18	118.20
29	W	17	H2U	C5-C4-N3	2.82	119.82	116.65
5	72	2445	2MG	C5-C6-N1	2.81	120.33	113.19
5	72	1835	2MG	C5-C6-N1	2.80	120.31	113.19
33	Y2	17	H2U	C5-C4-N3	2.80	119.79	116.65
5	72	1618	6MZ	C4-N9-C1'	-2.80	119.93	126.59
5	72	955	PSU	C6-N1-C2	-2.79	119.83	122.68
29	W	20	H2U	C5-C4-N3	2.79	119.78	116.65
32	Y1	46	7MG	N9-C4-N3	2.78	129.62	125.47
7	A2	1519	MA6	N3-C4-N9	2.77	131.65	127.08
29	W	16	H2U	C5-C6-N1	2.77	120.73	111.61
7	A1	1207	2MG	N9-C8-N7	-2.77	108.18	113.39
7	A1	966	2MG	C5-C6-N1	2.77	120.21	113.19
29	W	46	G7M	CN7-N7-C5	2.76	130.20	126.77
30	W1	37	MIA	S10-C2-N3	2.76	125.54	116.01
29	W	17	H2U	C5-C6-N1	2.75	120.69	111.61
7	A1	1516	2MG	C5-C6-N1	2.75	120.17	113.19
5	72	2251	OMG	C5-C6-N1	2.74	120.14	113.19
31	X2	17	H2U	C5-C4-N3	2.73	119.71	116.65
31	X2	17	H2U	C5-C6-N1	2.72	120.58	111.61
7	A2	966	2MG	C5-C6-N1	2.72	120.10	113.19
7	A2	1207	2MG	C5-C6-N1	2.72	120.10	113.19
30	W1	46	G7M	CN7-N7-C5	2.72	130.14	126.77
7	A2	1407	5MC	C5-C6-N1	-2.71	120.55	123.34
5	72	2580	PSU	C6-N1-C2	-2.70	119.92	122.68
31	X2	47	G7M	CN7-N7-C5	2.68	130.10	126.77
5	72	2604	PSU	C6-N1-C2	-2.67	119.96	122.68
7	A2	1516	2MG	C5-C6-N1	2.66	119.95	113.19
7	A1	1207	2MG	C5-C6-N1	2.65	119.92	113.19
5	72	745	1MG	C5-C6-N1	2.65	120.03	114.91
5	72	2069	G7M	CN7-N7-C5	2.63	130.03	126.77
29	W	20	H2U	C5-C6-N1	2.62	120.26	111.61
33	Y2	17	H2U	C5-C6-N1	2.62	120.24	111.61
7	A2	1207	2MG	N9-C8-N7	-2.61	108.47	113.39
5	72	2449	H2U	C5-C6-N1	2.61	120.20	111.61
7	A2	527	G7M	CN7-N7-C5	2.60	130.00	126.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X2	21	H2U	C5-C6-N1	2.58	120.11	111.61
5	72	1835	2MG	O6-C6-C5	-2.58	119.76	126.60
5	72	2503	2MA	C4-N9-C8	2.58	108.52	105.73
5	72	1835	2MG	N9-C8-N7	-2.57	108.55	113.39
7	A1	1516	2MG	O6-C6-C5	-2.56	119.80	126.60
5	72	2445	2MG	N9-C8-N7	-2.56	108.57	113.39
5	72	2445	2MG	O6-C6-C5	-2.56	119.81	126.60
7	A2	966	2MG	N1-C2-N3	-2.56	120.00	123.95
5	72	2605	PSU	O2-C2-N1	-2.55	119.98	122.79
7	A1	1402	4OC	C6-C5-C4	2.55	120.08	116.96
33	Y2	46	G7M	CN7-N7-C5	2.54	129.93	126.77
29	W	32	PSU	O2-C2-N1	-2.54	119.99	122.79
7	A2	1516	2MG	O6-C6-C5	-2.54	119.87	126.60
29	W	37	MIA	C5-C6-N6	2.54	126.04	121.76
7	A1	966	2MG	O6-C6-C5	-2.53	119.89	126.60
7	A1	1516	2MG	N1-C2-N3	-2.52	120.05	123.95
7	A1	966	2MG	N1-C2-N3	-2.52	120.05	123.95
7	A1	1518	MA6	C4-N9-C8	2.52	108.46	105.73
7	A1	527	G7M	CN7-N7-C5	2.52	129.90	126.77
5	72	955	PSU	O2-C2-N1	-2.51	120.03	122.79
5	72	2457	PSU	O2-C2-N1	-2.51	120.03	122.79
7	A2	966	2MG	O6-C6-C5	-2.51	119.95	126.60
5	72	2504	PSU	O2-C2-N1	-2.50	120.03	122.79
7	A2	1207	2MG	O6-C6-C5	-2.50	119.98	126.60
7	A1	1207	2MG	O6-C6-C5	-2.48	120.01	126.60
5	72	2251	OMG	O6-C6-C5	-2.48	120.02	126.60
30	W1	37	MIA	N6-C6-N1	-2.48	115.33	118.50
29	W	17	H2U	O2-C2-N1	-2.48	120.00	123.11
7	A2	1519	MA6	C4-N9-C8	2.47	108.40	105.73
7	A2	1207	2MG	N1-C2-N3	-2.47	120.14	123.95
7	A1	1207	2MG	N1-C2-N3	-2.45	120.17	123.95
29	W	20	H2U	O2-C2-N1	-2.45	120.03	123.11
7	A2	1518	MA6	C4-N9-C8	2.43	108.36	105.73
32	Y1	46	7MG	N9-C8-N7	2.41	106.83	103.38
5	72	2580	PSU	O2-C2-N1	-2.41	120.14	122.79
33	Y2	17	H2U	O2-C2-N1	-2.41	120.09	123.11
7	A2	1516	2MG	N1-C2-N3	-2.41	120.23	123.95
30	W1	39	PSU	O2-C2-N1	-2.40	120.14	122.79
30	W1	32	PSU	O2-C2-N1	-2.39	120.16	122.79
5	72	2604	PSU	O2-C2-N1	-2.39	120.16	122.79
29	W	16	H2U	O2-C2-N1	-2.39	120.11	123.11
5	72	1835	2MG	N1-C2-N3	-2.39	120.26	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2445	2MG	N1-C2-N3	-2.38	120.27	123.95
29	W	37	MIA	C16-C14-C15	2.37	119.83	114.60
5	72	1618	6MZ	C1'-N9-C8	2.36	132.47	127.14
30	W1	37	MIA	C16-C14-C15	2.36	119.83	114.60
29	W	55	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
7	A2	1402	4OC	C6-C5-C4	2.35	119.83	116.96
5	72	2251	OMG	C8-N7-C5	2.33	108.46	104.24
5	72	1915	3TD	C6-C5-C4	2.32	119.82	118.22
32	Y1	37	6MZ	C9-N6-C6	-2.32	120.88	122.87
5	72	2503	2MA	C4-C5-N7	-2.30	107.81	110.62
31	X2	21	H2U	O2-C2-N1	-2.29	120.23	123.11
5	72	2449	H2U	O2-C2-N1	-2.28	120.25	123.11
7	A2	1519	MA6	C4-C5-N7	-2.24	107.89	110.62
31	X2	38	2MA	C4-C5-N7	-2.24	107.89	110.62
5	72	2503	2MA	CM2-C2-N1	2.23	120.63	117.15
30	W1	37	MIA	C4-N9-C1'	-2.22	121.31	126.59
5	72	2030	6MZ	C4-N9-C8	2.22	108.13	105.73
32	Y1	37	6MZ	C4-N9-C8	2.19	108.10	105.73
7	A2	1518	MA6	C4-C5-N7	-2.18	107.96	110.62
29	W	37	MIA	C4-C5-N7	-2.18	107.96	110.62
5	72	2503	2MA	N6-C6-N1	2.17	120.10	117.03
5	72	746	PSU	C5-C6-N1	-2.17	118.85	122.11
31	X2	38	2MA	C4-N9-C8	2.17	108.08	105.73
7	A1	1519	MA6	C4-N9-C8	2.16	108.07	105.73
29	W	37	MIA	C4-N9-C8	2.16	108.07	105.73
5	72	745	1MG	C8-N7-C5	2.15	108.14	104.24
7	A1	1407	5MC	CM5-C5-C6	-2.15	119.97	122.85
7	A2	966	2MG	C8-N7-C5	2.13	108.10	104.24
7	A2	1407	5MC	CM5-C5-C6	-2.13	120.00	122.85
7	A2	527	G7M	CN7-N7-C8	-2.12	121.56	124.84
5	72	2580	PSU	O4'-C1'-C2'	2.12	108.14	105.14
31	X2	38	2MA	N6-C6-N1	2.12	120.03	117.03
5	72	2552	OMU	O2-C2-N1	-2.12	119.97	122.79
7	A1	1498	UR3	C6-N1-C2	-2.12	119.89	121.79
7	A1	967	5MC	CM5-C5-C6	-2.11	120.03	122.85
7	A1	966	2MG	C8-N7-C5	2.11	108.05	104.24
29	W	8	4SU	O2-C2-N1	-2.09	120.01	122.79
31	X2	47	G7M	CN7-N7-C8	-2.08	121.62	124.84
5	72	2445	2MG	CM2-N2-C2	-2.08	119.26	123.86
7	A1	1498	UR3	C1'-N1-C2	2.08	120.50	116.99
5	72	1962	5MC	CM5-C5-C6	-2.08	120.07	122.85
7	A1	1516	2MG	C8-N7-C5	2.08	108.00	104.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X2	38	2MA	C5-C4-N9	2.07	108.19	105.78
7	A2	1498	UR3	C6-N1-C2	-2.07	119.93	121.79
5	72	2069	G7M	CN7-N7-C8	-2.07	121.64	124.84
29	W	46	G7M	CN7-N7-C8	-2.07	121.64	124.84
32	Y1	37	6MZ	C4-C5-N7	-2.07	108.10	110.62
5	72	2030	6MZ	C4-C5-N7	-2.06	108.10	110.62
7	A1	1207	2MG	C8-N7-C5	2.06	107.97	104.24
5	72	1835	2MG	CM2-N2-C2	-2.06	119.31	123.86
7	A2	1516	2MG	C8-N7-C5	2.06	107.97	104.24
30	W1	46	G7M	CN7-N7-C8	-2.05	121.68	124.84
33	Y2	46	G7M	CN7-N7-C8	-2.05	121.68	124.84
31	X2	48	3AU	C6-N1-C2	-2.04	119.96	121.79
7	A2	527	G7M	N9-C8-N7	-2.03	107.18	112.21
7	A1	527	G7M	CN7-N7-C8	-2.03	121.70	124.84
7	A1	1518	MA6	C4-C5-N7	-2.03	108.15	110.62
7	A1	527	G7M	N9-C8-N7	-2.02	107.20	112.21
30	W1	37	MIA	C5-C6-N6	2.02	125.17	121.76
5	72	2445	2MG	C8-N7-C5	2.02	107.89	104.24
7	A2	967	5MC	CM5-C5-C6	-2.02	120.15	122.85
7	A2	1207	2MG	C8-N7-C5	2.02	107.89	104.24
5	72	2069	G7M	N9-C8-N7	-2.02	107.22	112.21
30	W1	37	MIA	C4-N9-C8	2.01	107.91	105.73
31	X2	17	H2U	O2-C2-N1	-2.01	120.59	123.11

There are no chirality outliers.

All (122) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C5-C6-N6-C10
7	A2	1402	4OC	C1'-C2'-O2'-CM2
5	72	1618	6MZ	N1-C6-N6-C9
5	72	1618	6MZ	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C3'-C4'-C5'-O5'
5	72	1939	5MU	C3'-C4'-C5'-O5'
5	72	1939	5MU	O4'-C4'-C5'-O5'
5	72	2030	6MZ	C5-C6-N6-C9
5	72	2030	6MZ	N1-C6-N6-C9
5	72	2251	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	72	2251	OMG	C1'-C2'-O2'-CM2
30	W1	37	MIA	O4'-C4'-C5'-O5'
30	W1	37	MIA	C3'-C4'-C5'-O5'
30	W1	37	MIA	N1-C2-S10-C11
30	W1	37	MIA	N3-C2-S10-C11
31	X2	8	4SU	C3'-C4'-C5'-O5'
31	X2	8	4SU	O4'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C1'-N1-C6
31	X2	33	RSP	C4'-C5'-O5'-P
31	X2	38	2MA	O4'-C1'-N9-C8
31	X2	38	2MA	O4'-C1'-N9-C4
31	X2	47	G7M	O4'-C4'-C5'-O5'
31	X2	47	G7M	C3'-C4'-C5'-O5'
31	X2	48	3AU	C10-C11-C12-N40
31	X2	55	5MU	C3'-C4'-C5'-O5'
32	Y1	34	CM0	O5-C7-C8-O8
32	Y1	37	6MZ	N1-C6-N6-C9
33	Y2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	17	H2U	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C6
33	Y2	17	H2U	C2'-C1'-N1-C2
33	Y2	17	H2U	C2'-C1'-N1-C6
32	Y1	34	CM0	O5-C7-C8-O9
31	X2	47	G7M	C4'-C5'-O5'-P
7	A1	1498	UR3	O4'-C4'-C5'-O5'
7	A1	1498	UR3	C3'-C4'-C5'-O5'
7	A1	1519	MA6	O4'-C4'-C5'-O5'
7	A2	1498	UR3	O4'-C4'-C5'-O5'
7	A2	1498	UR3	C3'-C4'-C5'-O5'
7	A2	1519	MA6	O4'-C4'-C5'-O5'
5	72	2251	OMG	C3'-C4'-C5'-O5'
5	72	2498	OMC	C3'-C4'-C5'-O5'
5	72	2498	OMC	O4'-C4'-C5'-O5'
29	W	8	4SU	C3'-C4'-C5'-O5'
29	W	8	4SU	O4'-C4'-C5'-O5'
30	W1	8	4SU	O4'-C4'-C5'-O5'
33	Y2	46	G7M	C3'-C4'-C5'-O5'
30	W1	8	4SU	C3'-C4'-C5'-O5'
31	X2	48	3AU	O4'-C4'-C5'-O5'
31	X2	55	5MU	O4'-C4'-C5'-O5'
7	A1	1518	MA6	N1-C6-N6-C10
7	A2	1519	MA6	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	72	1915	3TD	O4'-C4'-C5'-O5'
29	W	54	5MU	C3'-C4'-C5'-O5'
33	Y2	54	5MU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C4'-C5'-O5'-P
29	W	55	PSU	O4'-C4'-C5'-O5'
31	X2	17	H2U	C3'-C4'-C5'-O5'
31	X2	48	3AU	C3'-C4'-C5'-O5'
31	X2	38	2MA	C4'-C5'-O5'-P
7	A1	1519	MA6	C5-C6-N6-C9
31	X2	17	H2U	C4'-C5'-O5'-P
31	X2	21	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C3'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	46	G7M	O4'-C4'-C5'-O5'
33	Y2	54	5MU	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C5-C6-N6-C9
32	Y1	37	6MZ	C5-C6-N6-C9
29	W	46	G7M	C2'-C1'-N9-C4
30	W1	46	G7M	C2'-C1'-N9-C4
30	W1	46	G7M	O4'-C4'-C5'-O5'
7	A1	527	G7M	C4'-C5'-O5'-P
29	W	46	G7M	C4'-C5'-O5'-P
30	W1	46	G7M	C4'-C5'-O5'-P
31	X2	48	3AU	C4'-C5'-O5'-P
32	Y1	46	7MG	C4'-C5'-O5'-P
29	W	54	5MU	O4'-C4'-C5'-O5'
30	W1	37	MIA	C5-C6-N6-C12
7	A2	527	G7M	C3'-C4'-C5'-O5'
7	A2	527	G7M	C4'-C5'-O5'-P
33	Y2	17	H2U	C4'-C5'-O5'-P
30	W1	37	MIA	N1-C6-N6-C12
5	72	2069	G7M	C4'-C5'-O5'-P
29	W	16	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C4'-C5'-O5'-P
29	W	46	G7M	O4'-C4'-C5'-O5'
31	X2	38	2MA	C3'-C4'-C5'-O5'
5	72	1915	3TD	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C2
29	W	37	MIA	N6-C12-C13-C14
5	72	2069	G7M	O4'-C4'-C5'-O5'
5	72	746	PSU	O4'-C1'-C5-C4
5	72	2457	PSU	O4'-C1'-C5-C4

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Mol	Chain	Res	Type	Atoms
5	72	2504	PSU	O4'-C1'-C5-C4
31	X2	56	PSU	O4'-C1'-C5-C4
31	X2	48	3AU	C11-C12-C13-O31
7	A1	1519	MA6	N1-C6-N6-C10
29	W	46	G7M	C2'-C1'-N9-C8
7	A2	527	G7M	O4'-C4'-C5'-O5'
7	A2	967	5MC	O4'-C4'-C5'-O5'
29	W	17	H2U	O4'-C4'-C5'-O5'
30	W1	46	G7M	C3'-C4'-C5'-O5'
31	X2	38	2MA	O4'-C4'-C5'-O5'
31	X2	48	3AU	C11-C12-C13-O30
5	72	2449	H2U	O4'-C1'-N1-C6
5	72	2457	PSU	O4'-C1'-C5-C6
31	X2	21	H2U	O4'-C1'-N1-C6
31	X2	56	PSU	O4'-C1'-C5-C6
29	W	54	5MU	C2'-C1'-N1-C2
31	X2	17	H2U	O4'-C1'-N1-C2
29	W	20	H2U	C4'-C5'-O5'-P
31	X2	17	H2U	C2'-C1'-N1-C2
7	A1	1402	4OC	O4'-C4'-C5'-O5'
5	71	1915	3TD	C3'-C4'-C5'-O5'
5	72	2030	6MZ	O4'-C4'-C5'-O5'
29	W	46	G7M	C3'-C4'-C5'-O5'
31	X2	21	H2U	C2'-C1'-N1-C2

There are no ring outliers.

43 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A1	1518	MA6	2	0
5	72	2504	PSU	1	0
29	W	37	MIA	2	0
7	A2	966	2MG	1	0
7	A1	1402	4OC	2	0
30	W1	46	G7M	1	0
5	72	1915	3TD	1	0
5	72	745	1MG	1	0
31	X2	48	3AU	2	0
31	X2	38	2MA	1	0
7	A2	1498	UR3	1	0
5	72	746	PSU	2	0
5	72	747	5MU	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	W	16	H2U	4	0
7	A2	1518	MA6	1	0
31	X2	47	G7M	1	0
33	Y2	46	G7M	1	0
5	72	1939	5MU	1	0
5	72	2251	OMG	3	0
5	72	2605	PSU	1	0
7	A2	1402	4OC	3	0
5	72	1618	6MZ	3	0
33	Y2	55	PSU	1	0
31	X2	56	PSU	2	0
29	W	54	5MU	2	0
7	A1	1498	UR3	1	0
29	W	46	G7M	1	0
29	W	17	H2U	2	0
7	A1	1207	2MG	2	0
7	A1	967	5MC	1	0
31	X2	8	4SU	1	0
32	Y1	34	CM0	3	0
5	72	2449	H2U	2	0
29	W	55	PSU	2	0
30	W1	37	MIA	2	0
29	W	32	PSU	1	0
7	A1	1519	MA6	2	0
5	72	2604	PSU	1	0
7	A2	967	5MC	1	0
5	72	1962	5MC	2	0
31	X2	17	H2U	1	0
5	72	2503	2MA	2	0
5	72	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 302 ligands modelled in this entry, 298 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
48	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.87	0
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0
47	PUT	72	3002	-	5,5,5	0.24	0	4,4,4	0.56	0
50	ALA	Y2	102	33	3,4,5	0.48	0	2,4,6	2.56	2 (100%)

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
48	SPD	72	3003	-	-	0/7/7/7	-
47	PUT	72	3001	-	-	1/3/3/3	-
47	PUT	72	3002	-	-	0/3/3/3	-
50	ALA	Y2	102	33	-	0/0/2/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
50	Y2	102	ALA	CB-CA-N	-3.01	100.32	109.85
50	Y2	102	ALA	O-C-CA	-2.02	117.88	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	72	3003	SPD	1	0
50	Y2	102	ALA	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

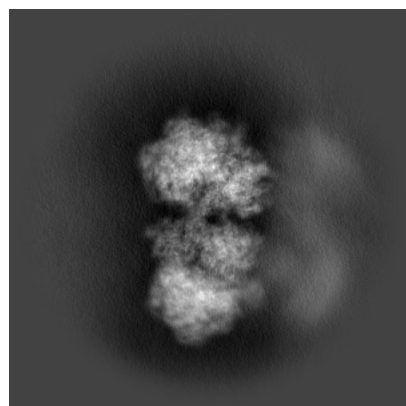
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19054. These allow visual inspection of the internal detail of the map and identification of artifacts.

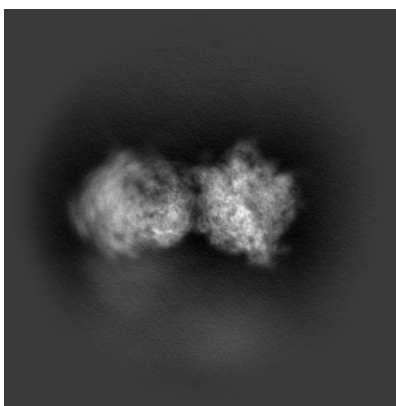
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

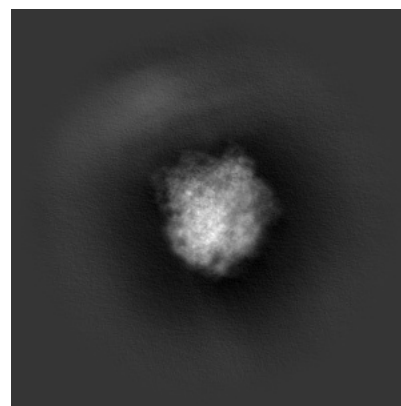
6.1.1 Primary map



X

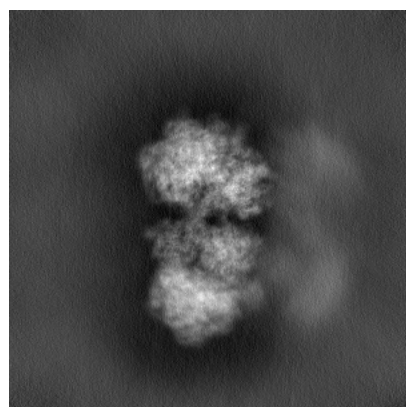


Y

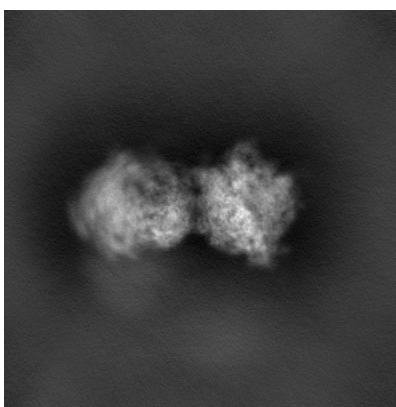


Z

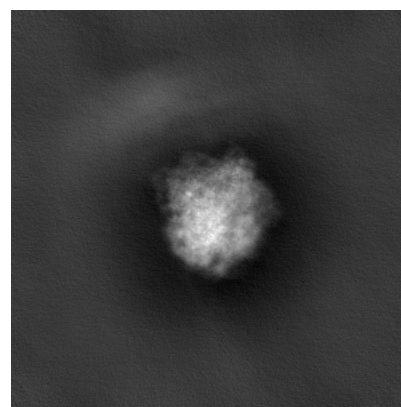
6.1.2 Raw map



X



Y

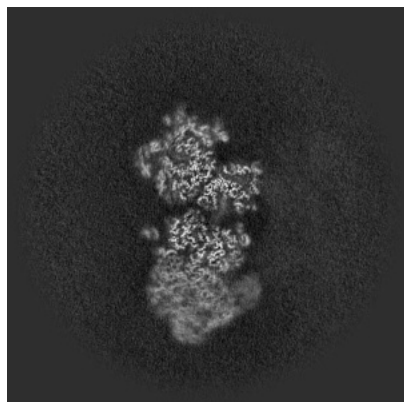


Z

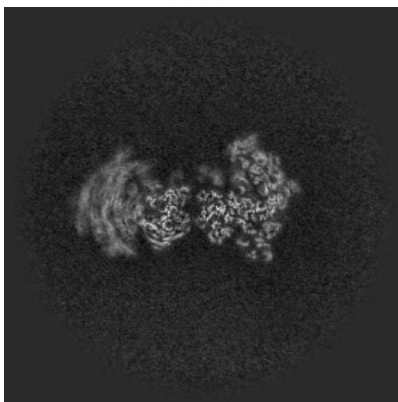
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

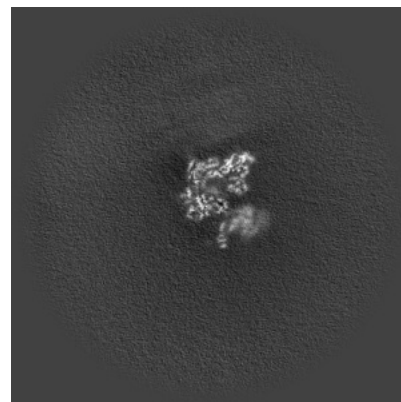
6.2.1 Primary map



X Index: 234

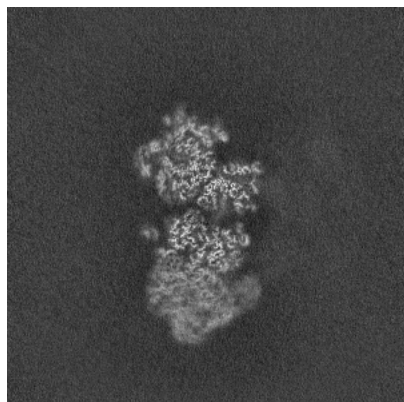


Y Index: 234

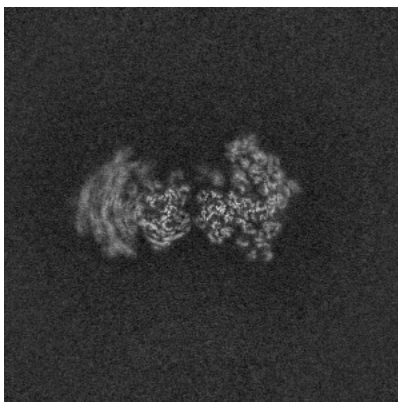


Z Index: 234

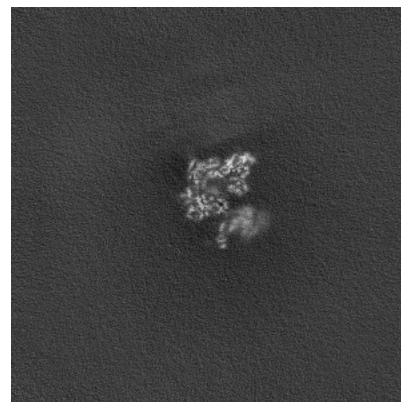
6.2.2 Raw map



X Index: 234



Y Index: 234

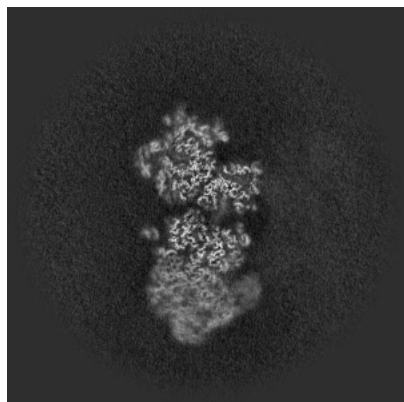


Z Index: 234

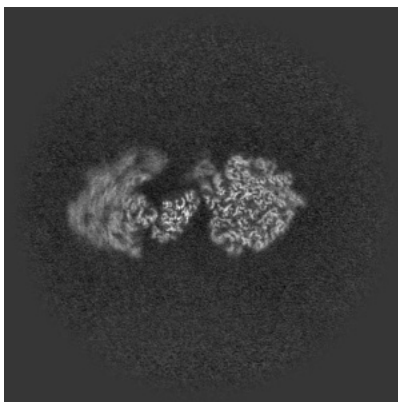
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

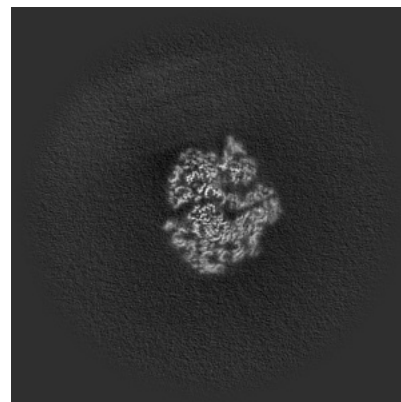
6.3.1 Primary map



X Index: 234

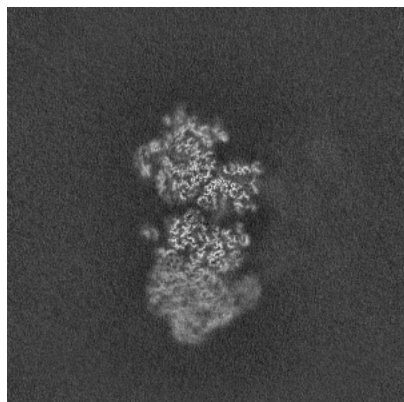


Y Index: 208

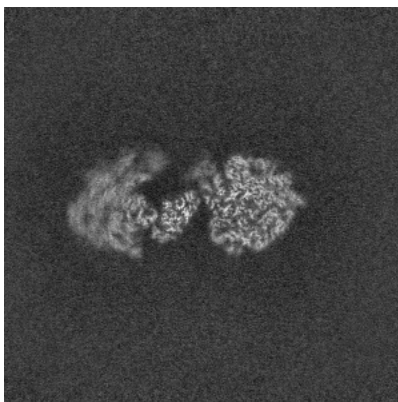


Z Index: 274

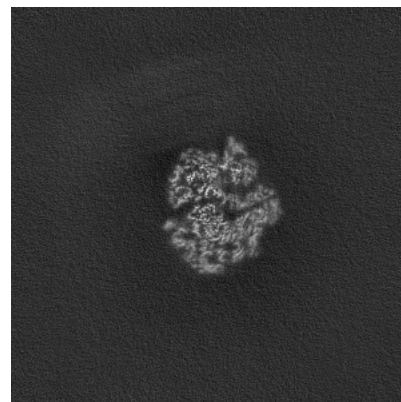
6.3.2 Raw map



X Index: 234



Y Index: 208

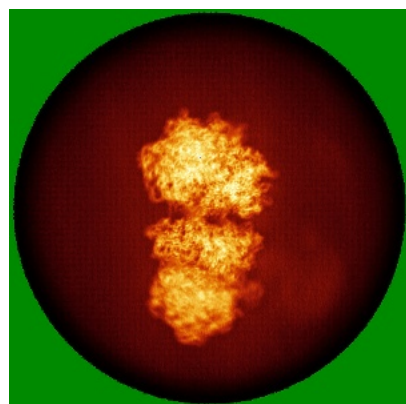


Z Index: 274

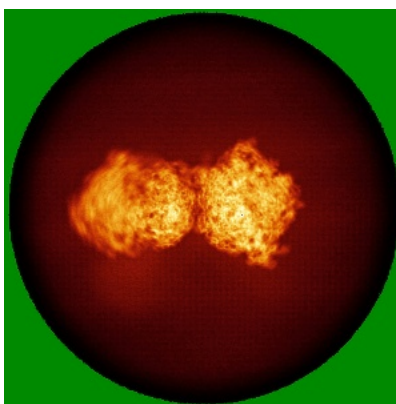
The images above show the largest variance slices of the map in three orthogonal directions.

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

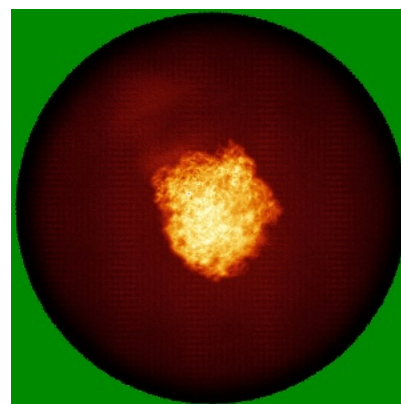
6.4.1 Primary map



X

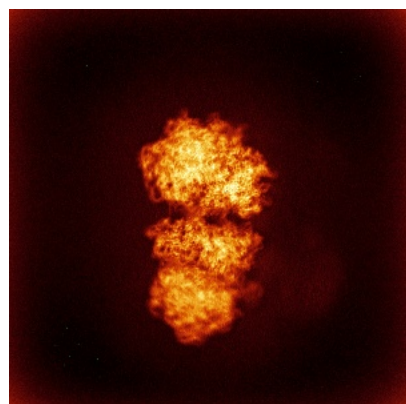


Y

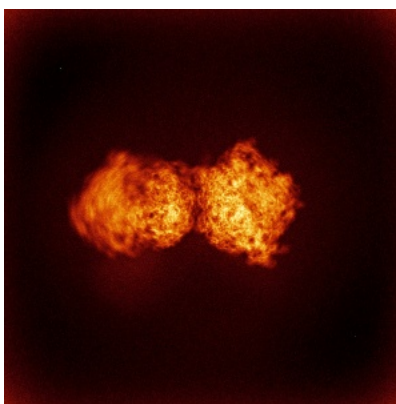


Z

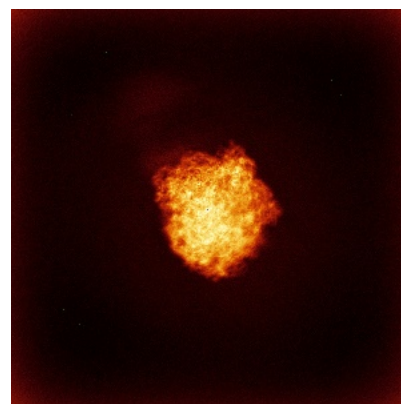
6.4.2 Raw map



X



Y

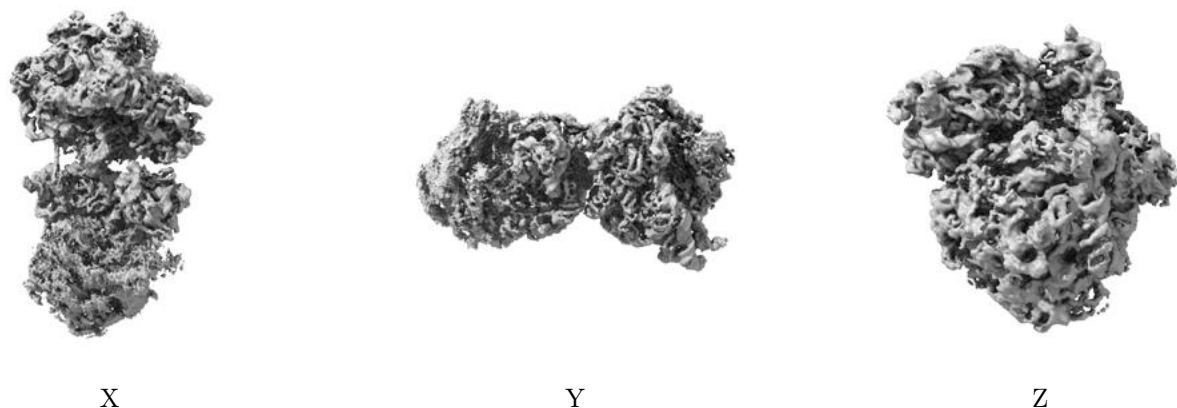


Z

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

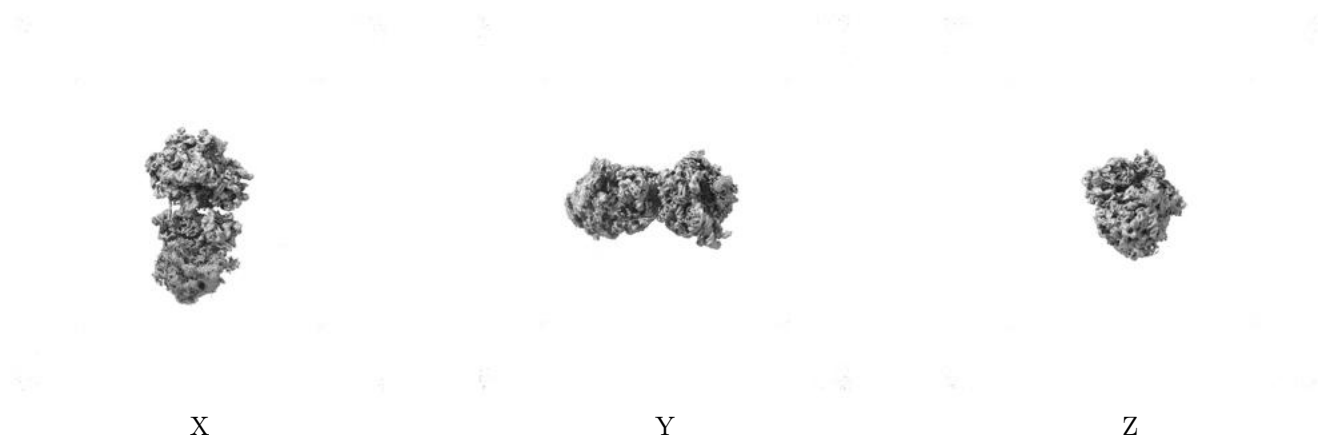
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 5.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

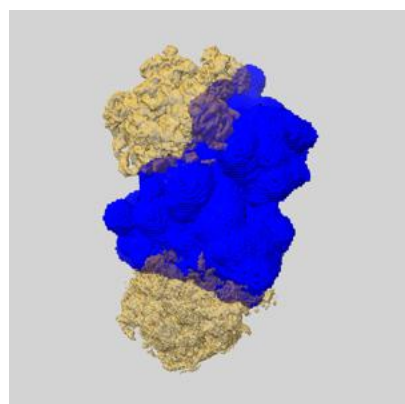
6.6 Mask visualisation [i](#)

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

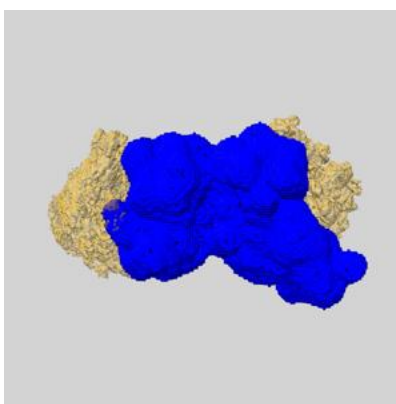
A mask typically either:

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

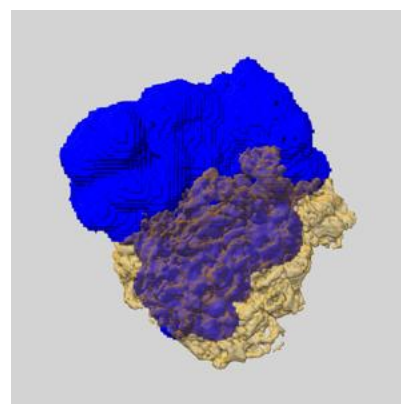
6.6.1 emd_19054_msk_1.map [i](#)



X



Y

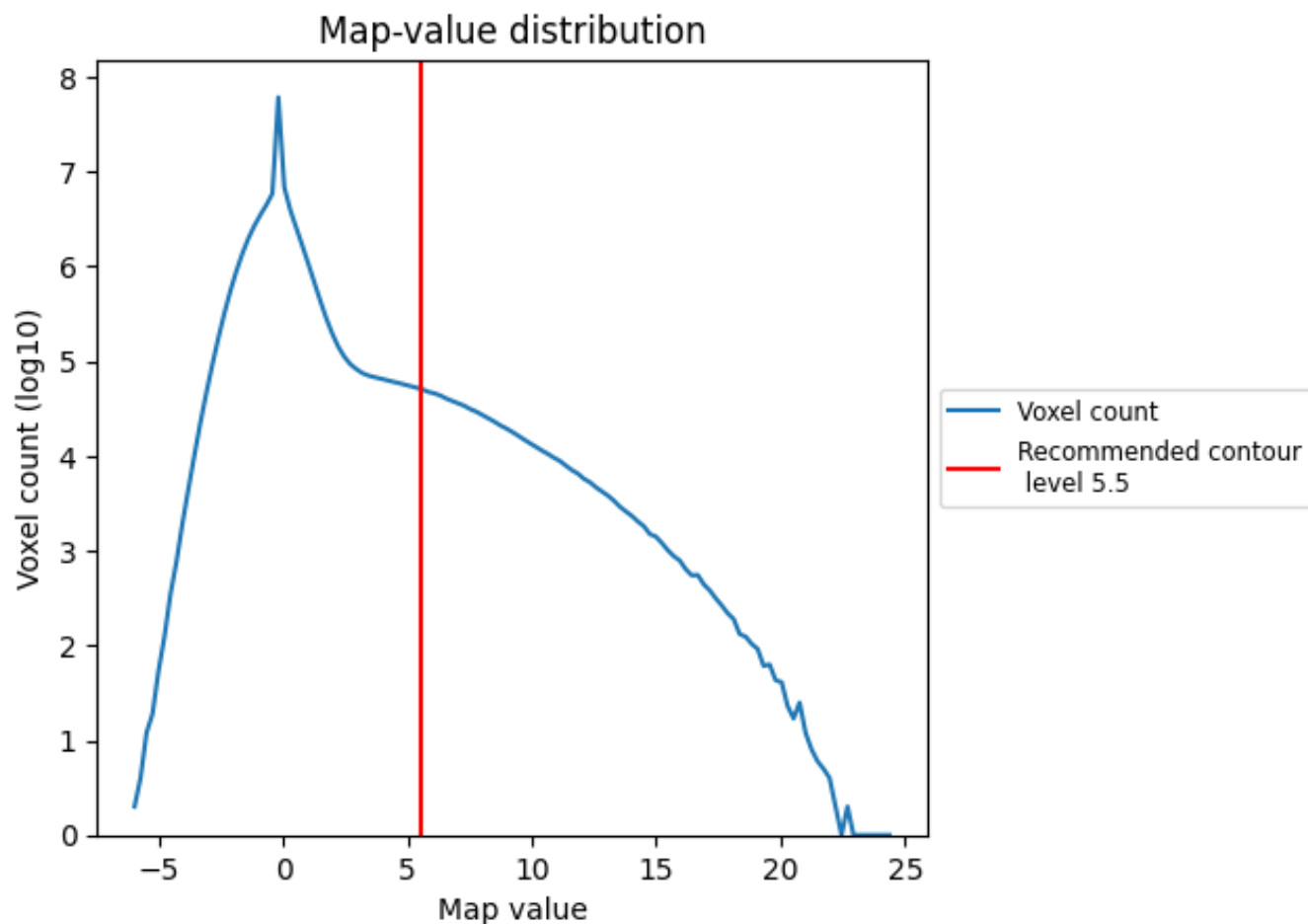


Z

7 Map analysis [i](#)

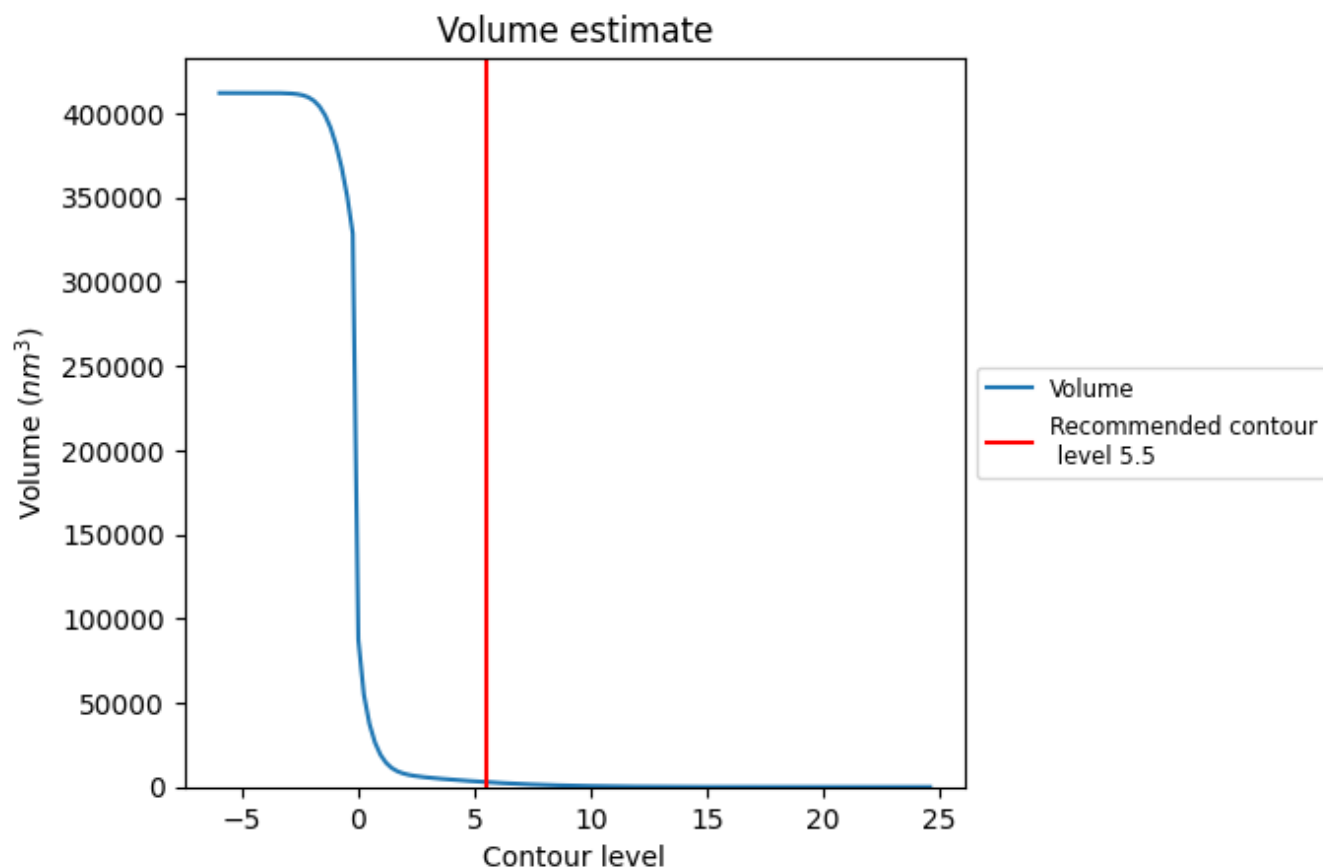
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

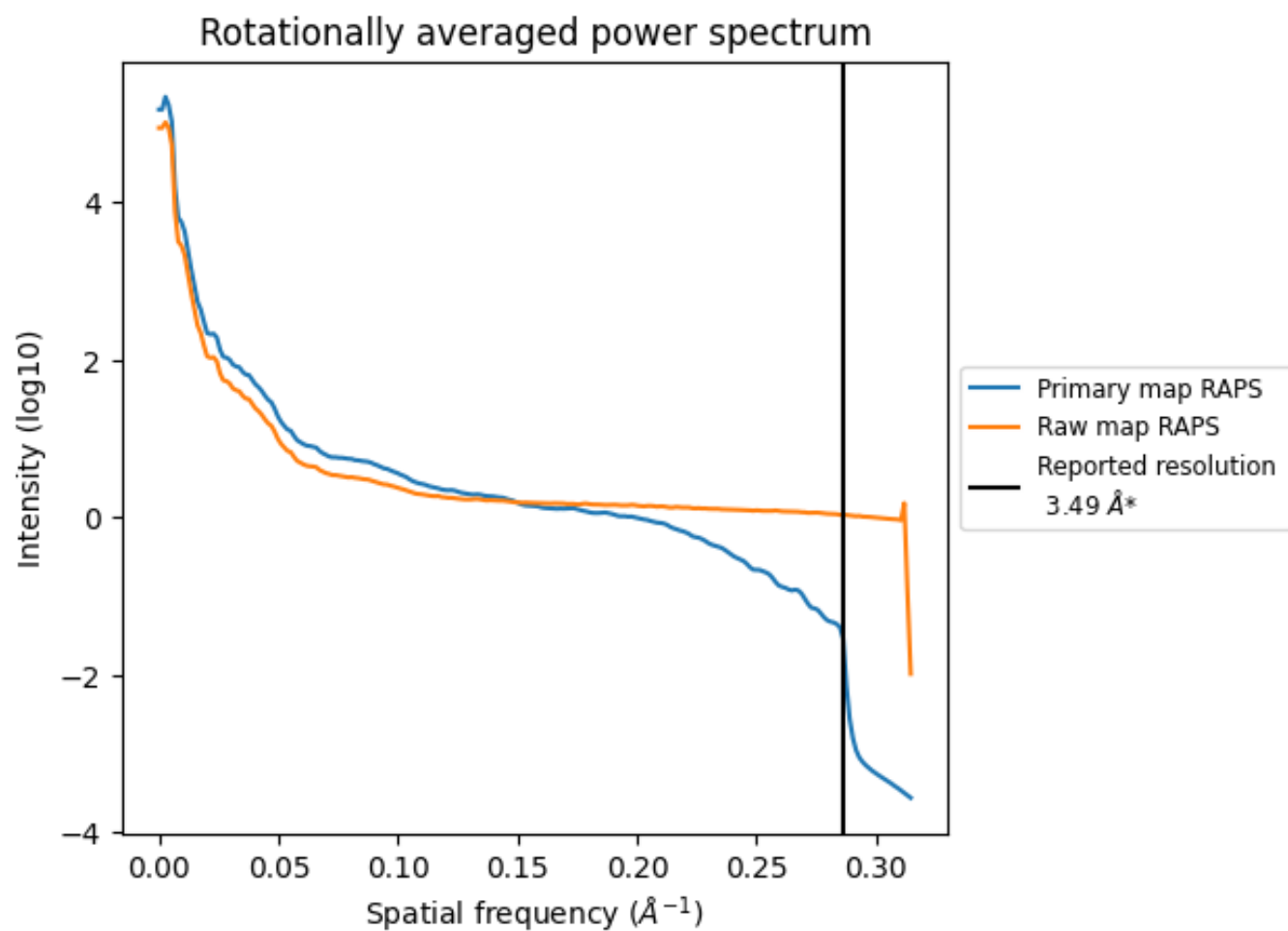
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2896 nm^3 ; this corresponds to an approximate mass of 2616 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 ⓘ

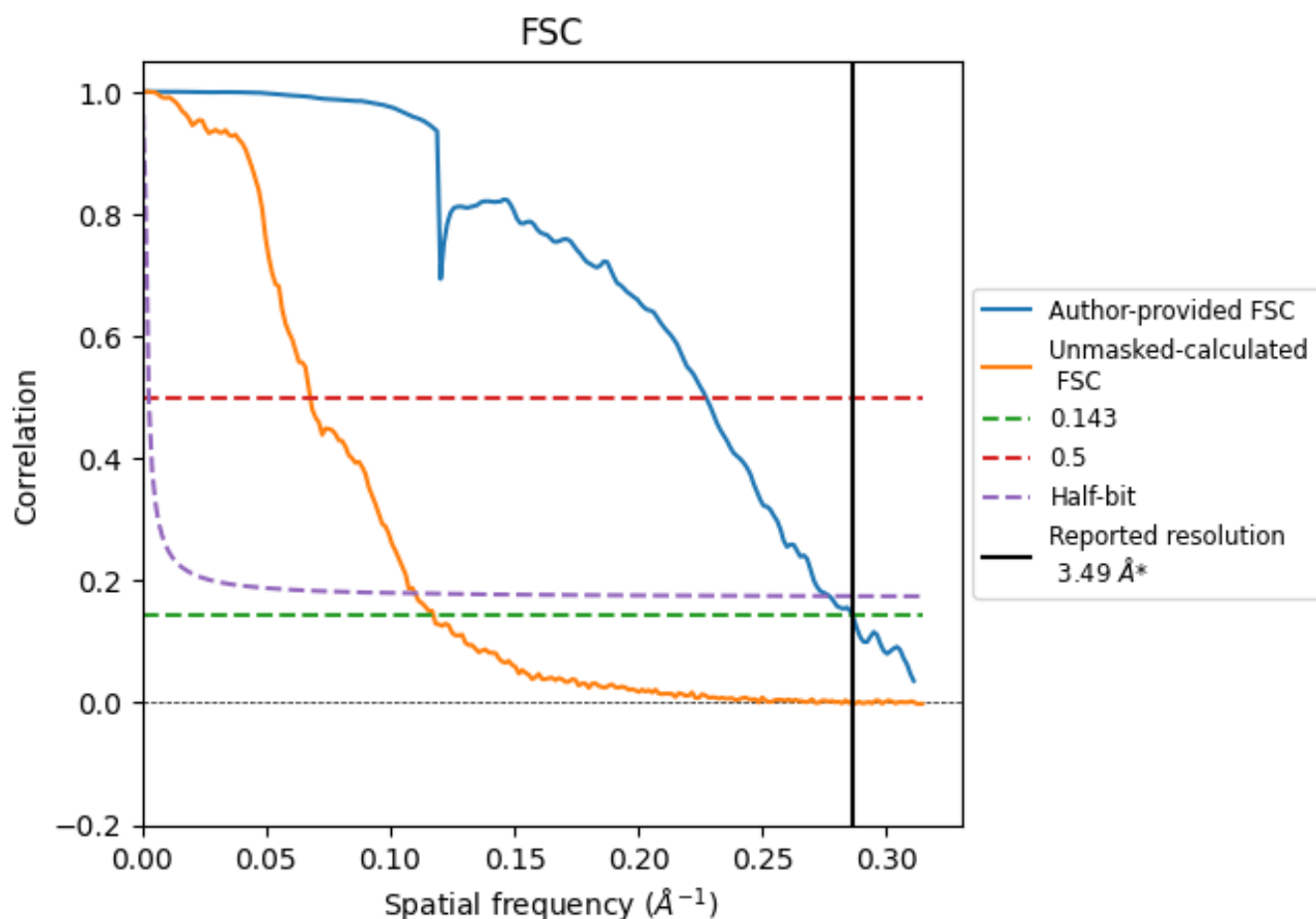


*Reported resolution corresponds to spatial frequency of 0.287 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.287 Å⁻¹

8.2 Resolution estimates [i](#)

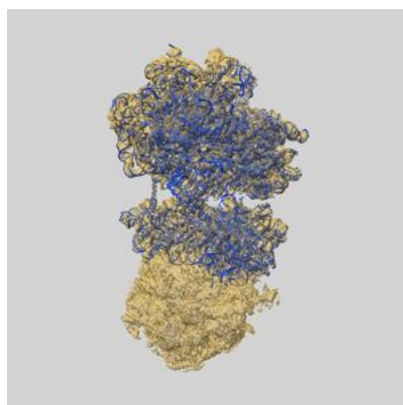
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.49	-	-
Author-provided FSC curve	3.49	4.40	3.61
Unmasked-calculated*	8.52	14.75	9.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.52 differs from the reported value 3.49 by more than 10 %

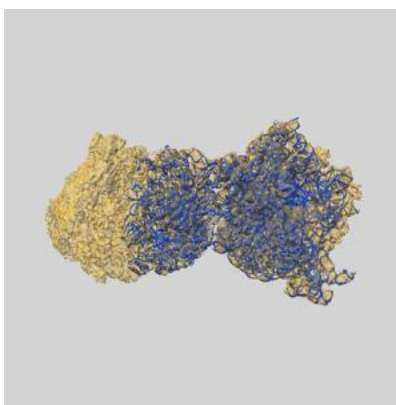
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19054 and PDB model 8RCL. Per-residue inclusion information can be found in section 3 on page 16.

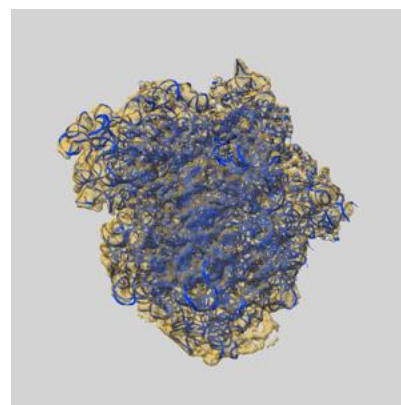
9.1 Map-model overlay [i](#)



X



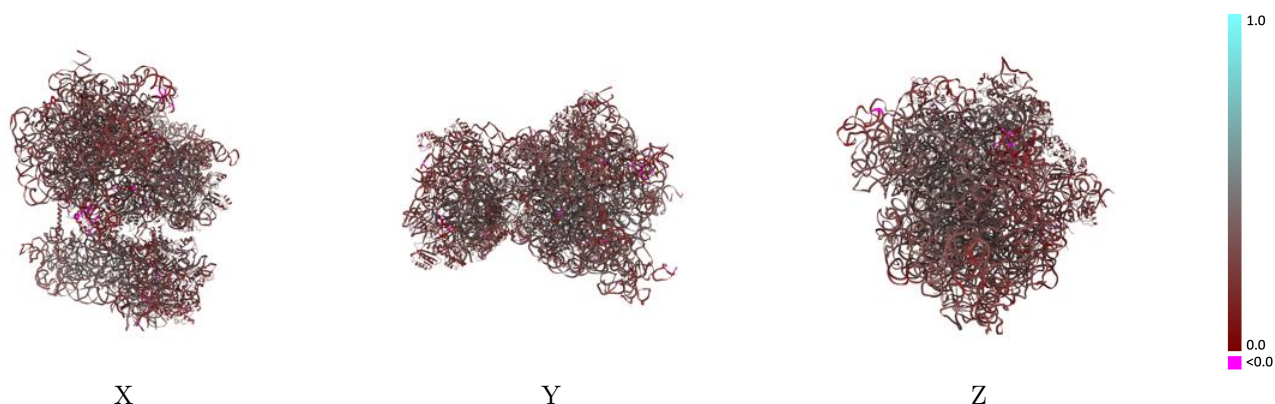
Y



Z

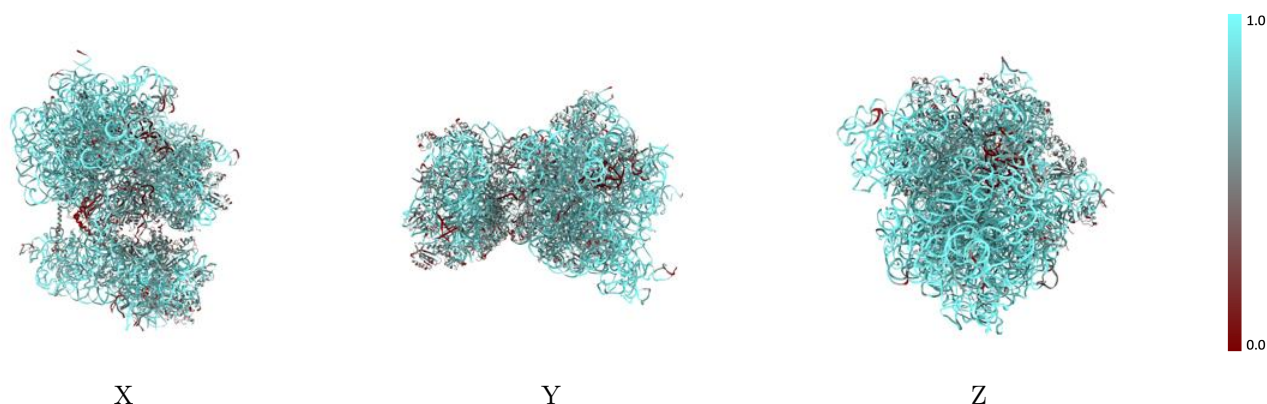
The images above show the 3D surface view of the map at the recommended contour level 5.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



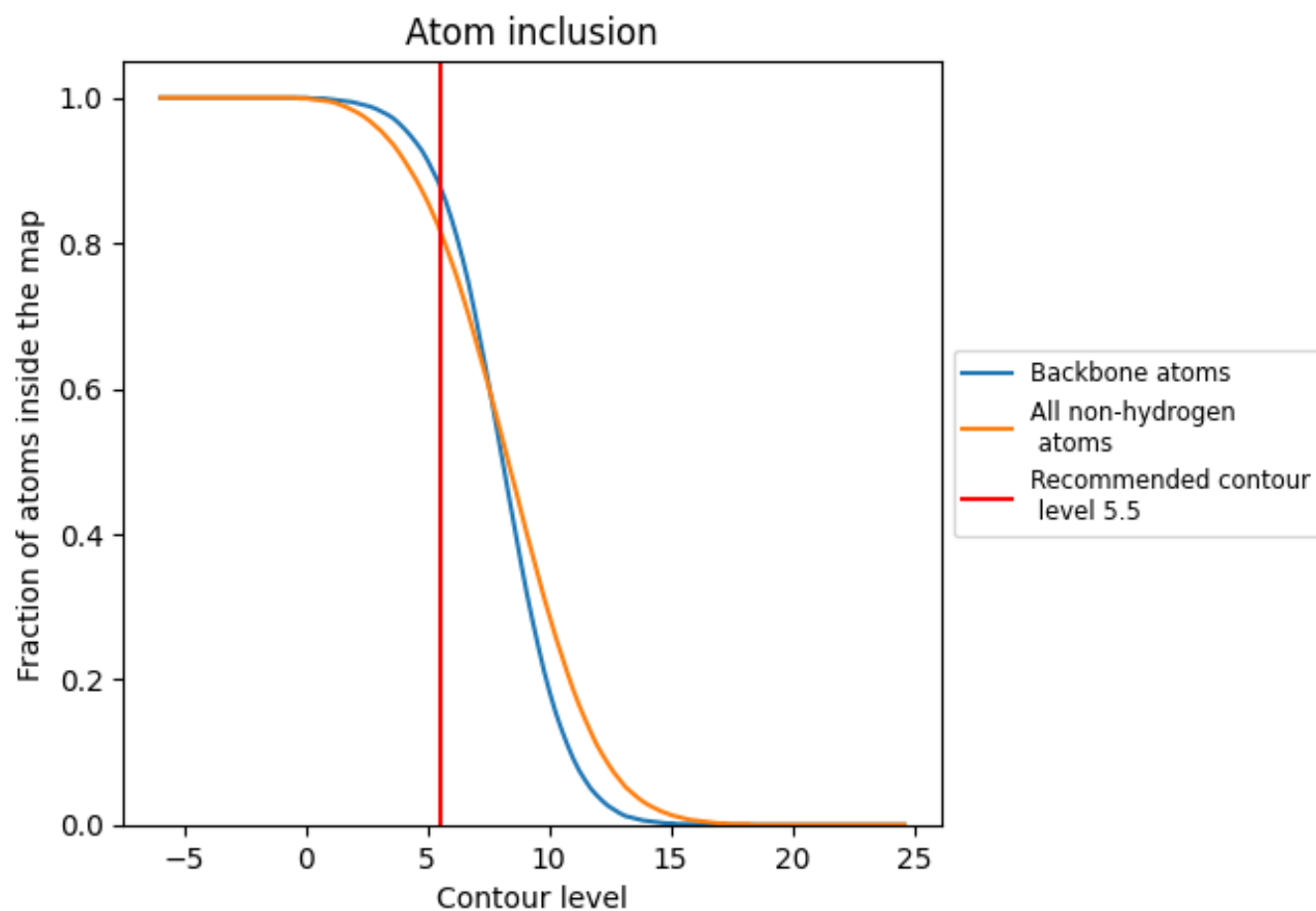
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (5.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.3070
12	 0.5990	 0.2990
32	 0.5950	 0.2170
4	 0.5390	 0.2790
62	 0.6500	 0.2570
71	 0.9210	 0.2890
72	 0.9200	 0.3050
82	 0.8790	 0.2460
A1	 0.9330	 0.3300
A2	 0.9360	 0.3480
B	 0.4920	 0.2480
B2	 0.5520	 0.3030
C1	 0.5530	 0.3100
C2	 0.6350	 0.3220
D1	 0.5610	 0.3160
D2	 0.5160	 0.2670
E1	 0.6000	 0.3100
E2	 0.6380	 0.3470
F1	 0.4210	 0.2320
F2	 0.5910	 0.3360
G1	 0.5310	 0.2340
G2	 0.6120	 0.2960
H1	 0.6220	 0.2890
H2	 0.6310	 0.3190
I1	 0.6230	 0.2570
I2	 0.7020	 0.3240
J1	 0.5780	 0.2960
J2	 0.6170	 0.3170
K1	 0.5380	 0.2640
K2	 0.6220	 0.3420
L1	 0.6840	 0.3460
L2	 0.6830	 0.3310
M1	 0.5310	 0.2140
M2	 0.6480	 0.2890
N1	 0.6330	 0.2480



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Chain	Atom inclusion	Q-score
N2	 0.6960	 0.2940
O1	 0.5910	 0.2410
O2	 0.6390	 0.3030
P1	 0.6860	 0.3380
Q1	 0.6010	 0.3070
Q2	 0.5970	 0.3220
R1	 0.4610	 0.2520
R2	 0.5350	 0.3230
S1	 0.5360	 0.2060
S2	 0.6890	 0.2980
T1	 0.6490	 0.2480
U1	 0.4180	 0.2290
U2	 0.5140	 0.3100
V2	 0.3440	 0.2080
W	 0.8200	 0.2970
W1	 0.7250	 0.2590
X2	 0.4320	 0.1680
Y1	 0.5030	 0.2290
Y2	 0.0520	 0.1910
Z1	 0.0000	 0.1390
a2	 0.1140	 0.1090
b2	 0.6830	 0.3540
e2	 0.5920	 0.2350
g2	 0.5750	 0.2450
h2	 0.5720	 0.2770
i2	 0.5200	 0.2870
l2	 0.7070	 0.2840
o2	 0.7590	 0.2820
p	 0.1130	 0.1230
r2	 0.5890	 0.2110
z2	 0.6470	 0.2260