Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2023 – 02:54 PM EDT

PDB ID	:	6MPF
Title	:	Structure of the Thermus thermophilus 30S ribosomal subunit complexed with a 2-thiocytidine (s2C32) and inosine (I34) modified anticodon stem loop (ASL) of Escherichia coli transfer RNA Arginine 1 (TRNAARG1) bound to an mRNA with an CGC-codon in the A-site and paromomycin
Authors	:	Cantara, W.A.; DeMirci, H.; Agris, P.F.
Deposited on	:	2018-10-05
Resolution	:	3.33 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

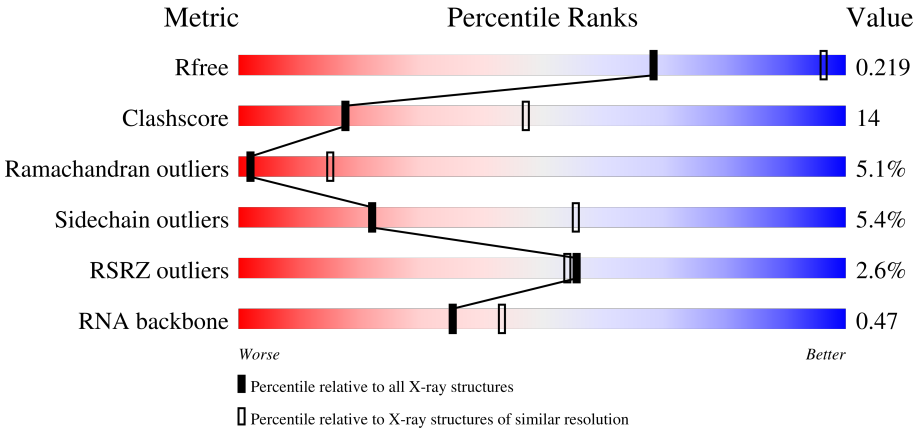
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.33 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)
RNA backbone	3102	1129 (3.78-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1508	39% 39% 18% ·
2	B	234	5% 50% 43% 6% ·
3	C	206	3% 53% 38% 8%
4	D	208	3% 58% 39% ·

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Mol	Chain	Length	Quality of chain
5	E	150	65% 33%
6	F	101	55% 44%
7	G	155	59% 37%
8	H	138	64% 33%
9	I	127	5% 54% 43%
10	J	98	23% 44% 51% 5%
11	K	119	3% 57% 39%
12	L	124	4% 58% 35% 6%
13	M	125	14% 56% 41%
14	N	60	57% 42%
15	O	88	63% 33% 5%
16	P	83	57% 39% 5%
17	Q	104	5% 46% 49% 5%
18	R	73	4% 62% 33% 5%
19	S	80	42% 50% 6%
20	T	99	58% 36%
21	V	24	71% 29%
22	W	4	100%
23	X	11	36% 36% 18% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1602	-	-	-	X
25	MG	A	1606	-	-	-	X
25	MG	A	1611	-	-	-	X
25	MG	A	1612	-	-	-	X
25	MG	A	1613	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	MG	A	1617	-	-	-	X
25	MG	A	1628	-	-	-	X
25	MG	A	1634	-	-	-	X
25	MG	A	1648	-	-	-	X
25	MG	A	1653	-	-	-	X
25	MG	A	1664	-	-	-	X
25	MG	A	1675	-	-	-	X
25	MG	A	1676	-	-	-	X
25	MG	A	1679	-	-	-	X
25	MG	A	1683	-	-	-	X
25	MG	A	1685	-	-	-	X
25	MG	A	1686	-	-	-	X
25	MG	A	1687	-	-	-	X
25	MG	A	1691	-	-	-	X
25	MG	A	1692	-	-	-	X
25	MG	A	1698	-	-	-	X
25	MG	A	1699	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52108 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1508	32415	14427	6005	10475	1508	22	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	234	1900	1213	341	341	5	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	206	1612	1016	314	281	1	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	208	1703	1066	339	291	7	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	150	1146	724	217	201	4	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

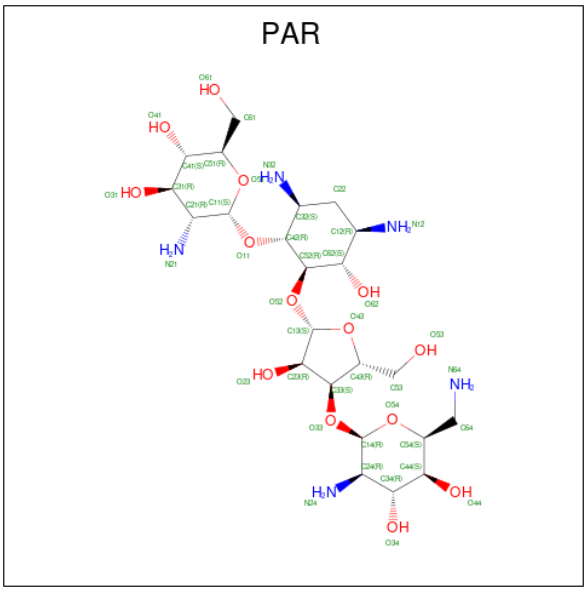
- Molecule 22 is a RNA chain called mRNA A-site fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	W	4	Total	C	N	O	P	0	0	0
			82	38	16	25	3			

- Molecule 23 is a RNA chain called tRNA ASL Escherichia coli Arg1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	X	11	Total	C	N	O	P	S	0	0	0
			232	105	43	73	10	1			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	98	Total	Mg	0	0
			98	98		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	E	1	Total Mg 1 1	0	0
25	J	2	Total Mg 2 2	0	0
25	W	1	Total Mg 1 1	0	0
25	X	1	Total Mg 1 1	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

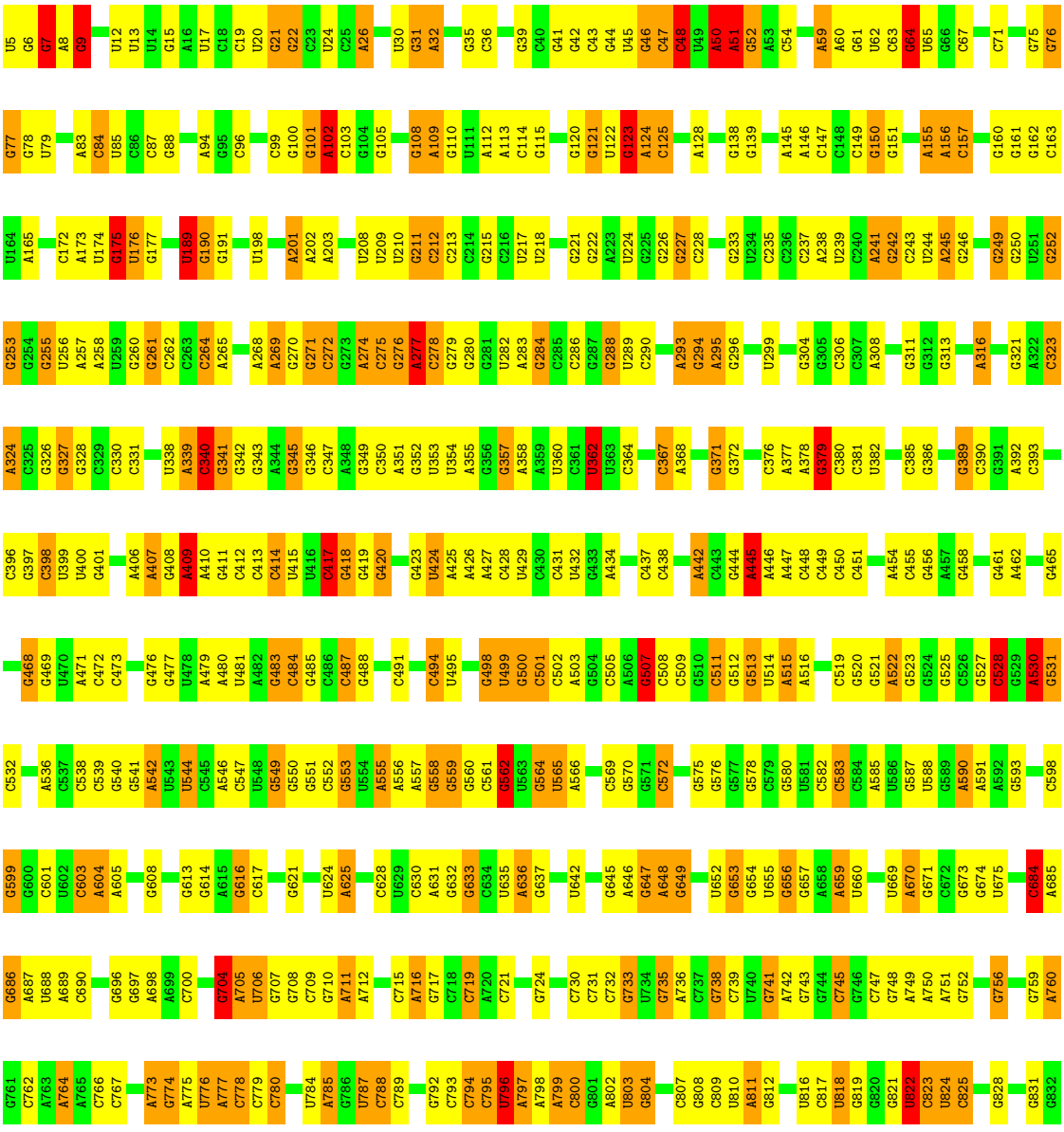
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	D	1	Total Zn 1 1	0	0
26	N	1	Total Zn 1 1	0	0

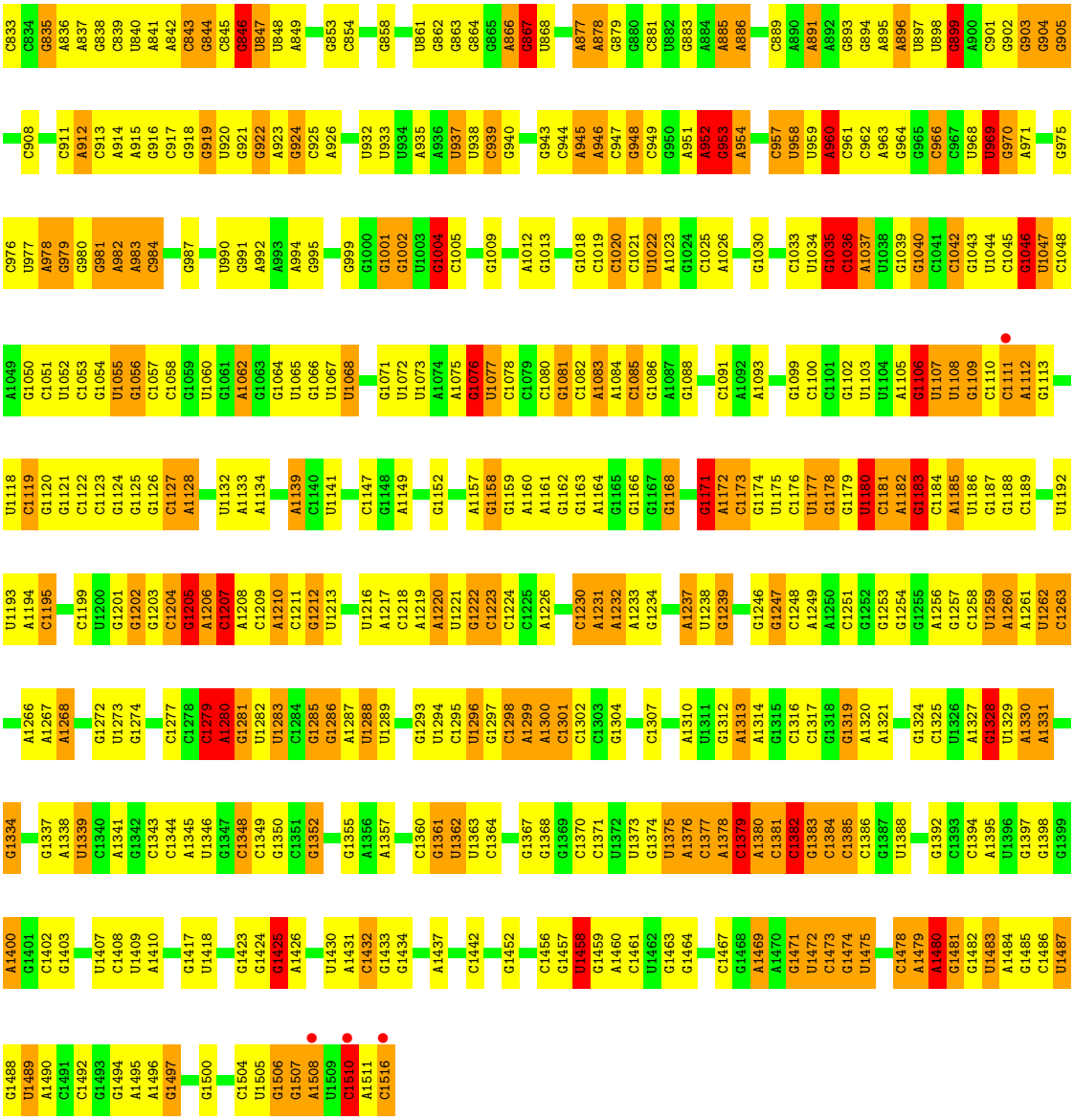
3 Residue-property plots (i)

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: 16S rRNA

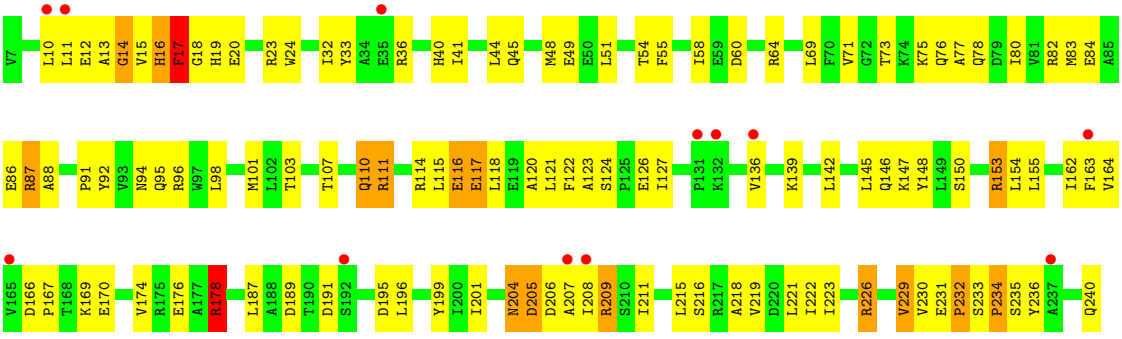
Chain A:



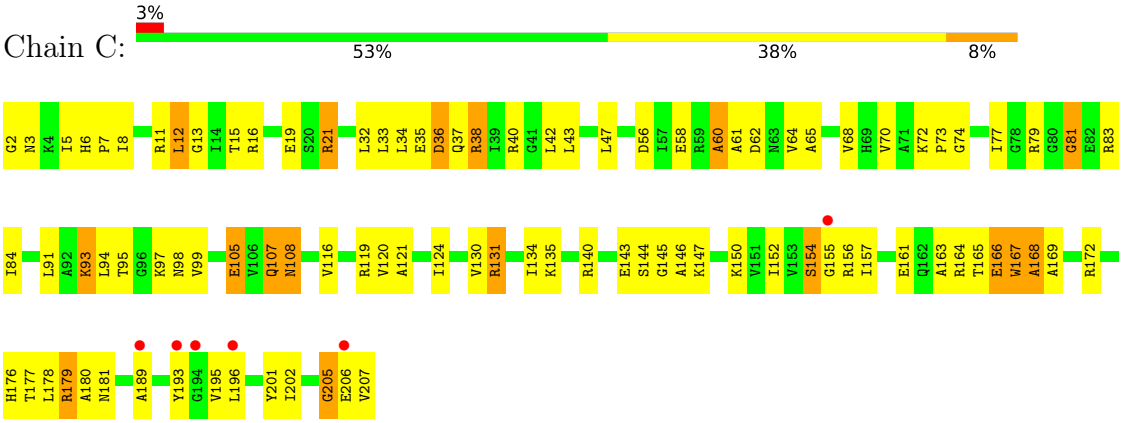


• Molecule 2: 30S ribosomal protein S2

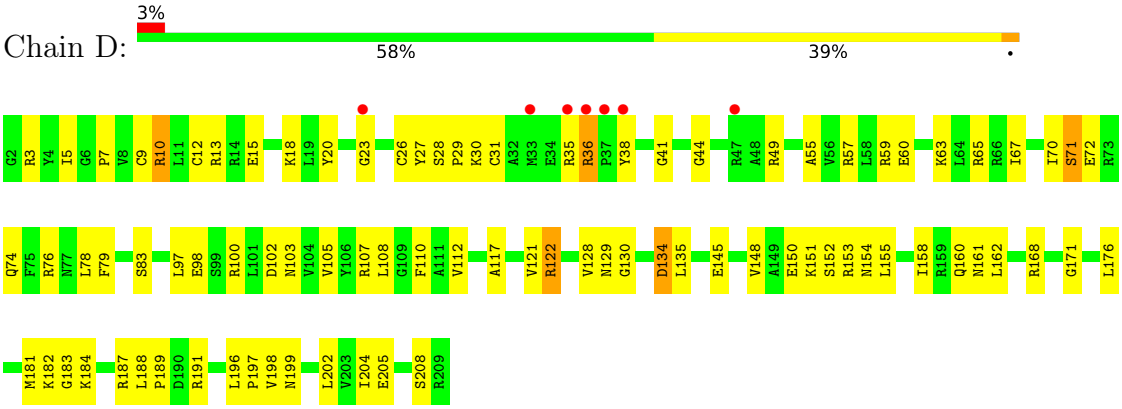
Chain B:



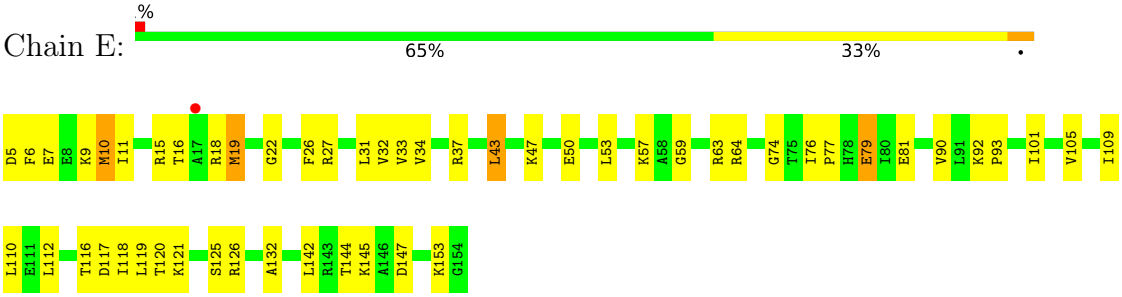
• Molecule 3: 30S ribosomal protein S3



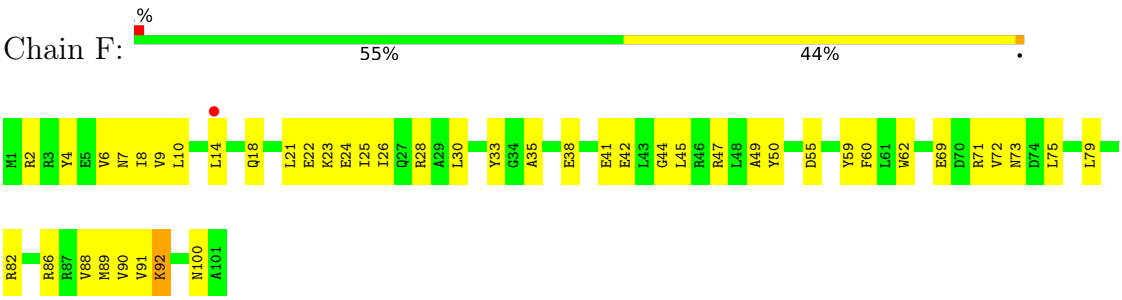
• Molecule 4: 30S ribosomal protein S4



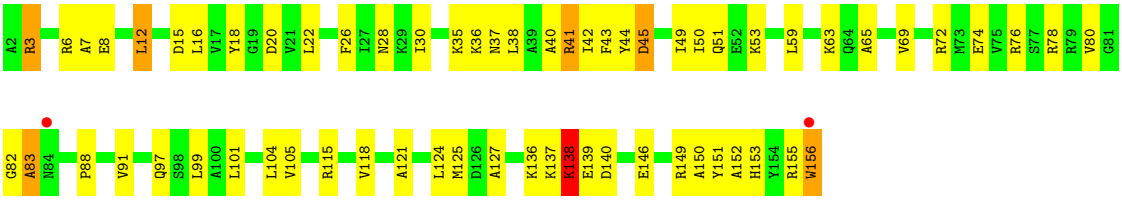
• Molecule 5: 30S ribosomal protein S5



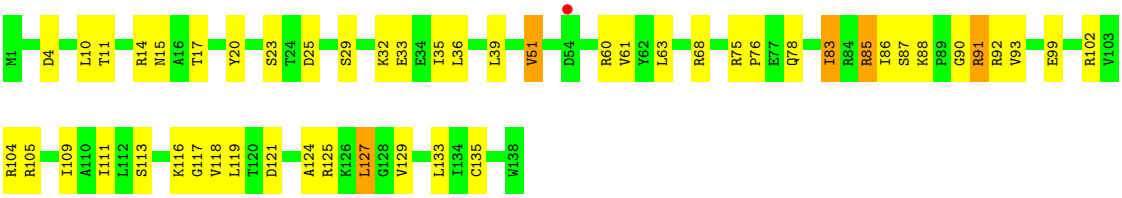
• Molecule 6: 30S ribosomal protein S6



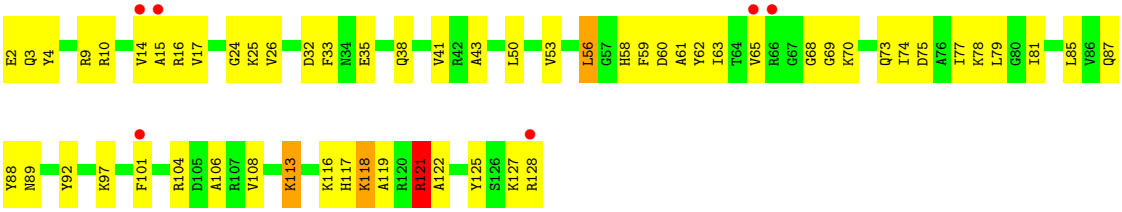
• Molecule 7: 30S ribosomal protein S7



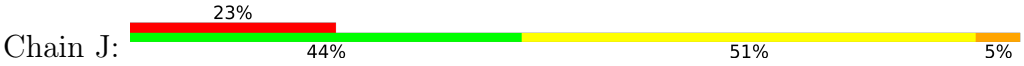
• Molecule 8: 30S ribosomal protein S8

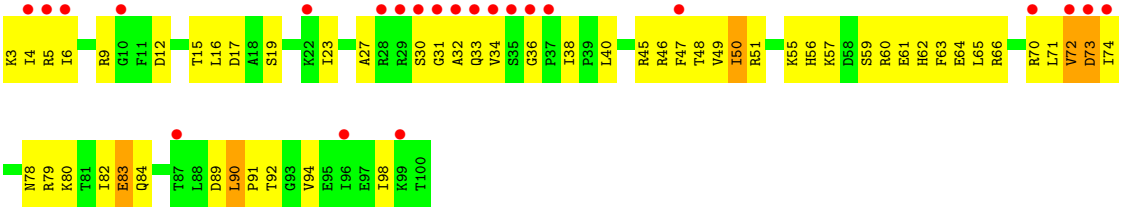


• Molecule 9: 30S ribosomal protein S9

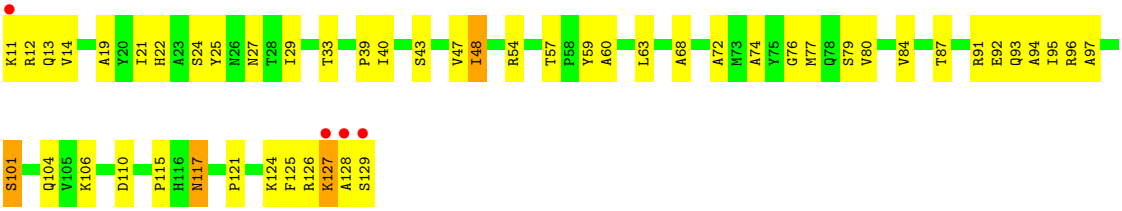


• Molecule 10: 30S ribosomal protein S10



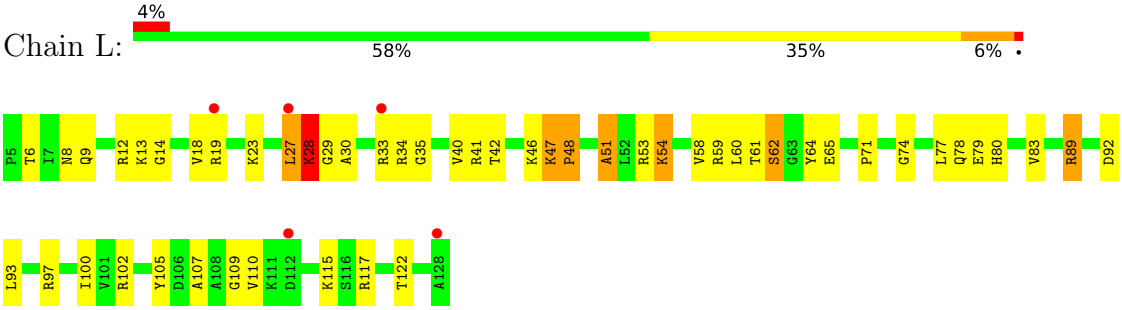


• Molecule 11: 30S ribosomal protein S11



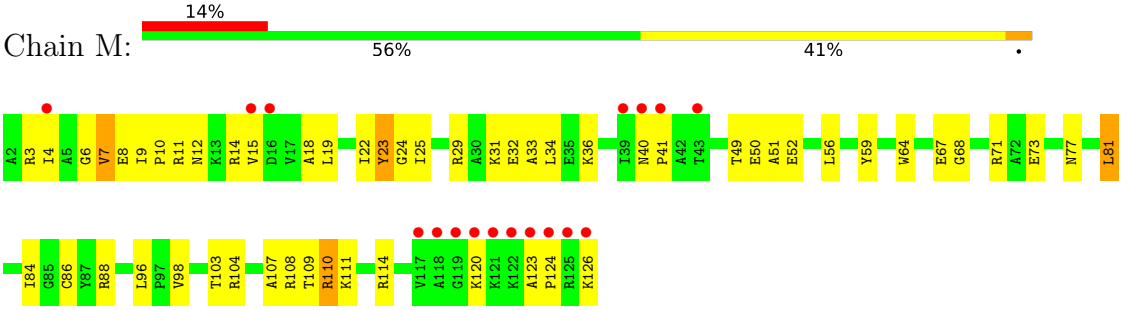
• Molecule 12: 30S ribosomal protein S12

Chain L:



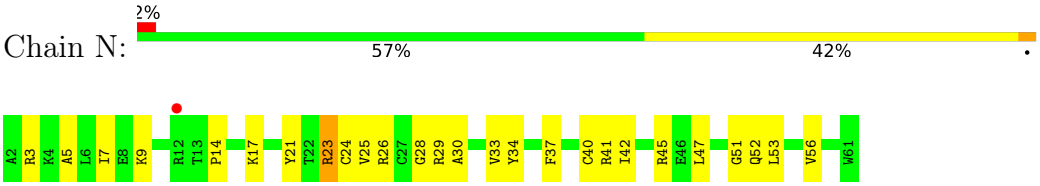
• Molecule 13: 30S ribosomal protein S13

Chain M:



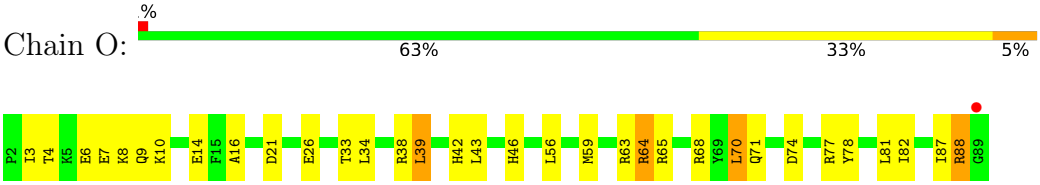
• Molecule 14: 30S ribosomal protein S14 type Z

Chain N:



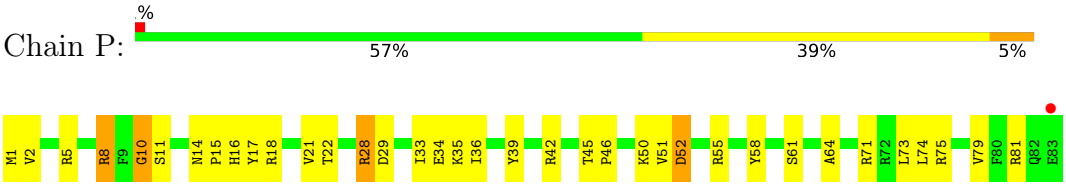
• Molecule 15: 30S ribosomal protein S15

Chain O:



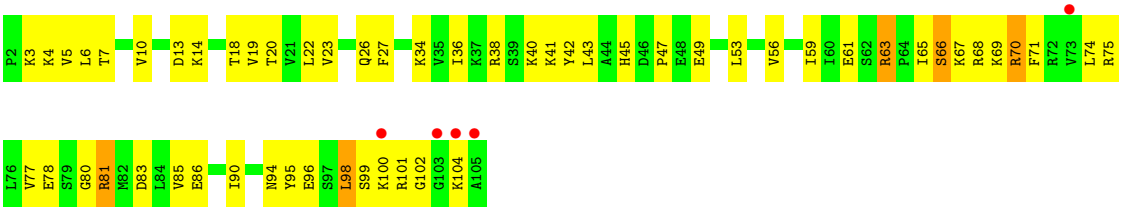
• Molecule 16: 30S ribosomal protein S16

Chain P:

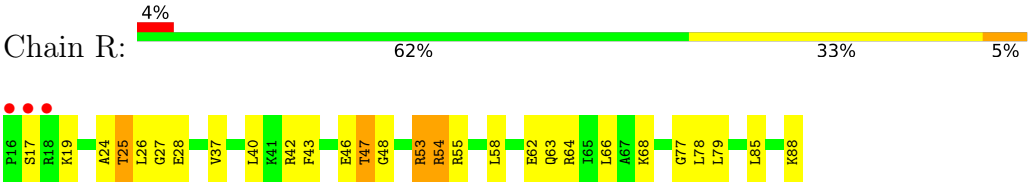


• Molecule 17: 30S ribosomal protein S17

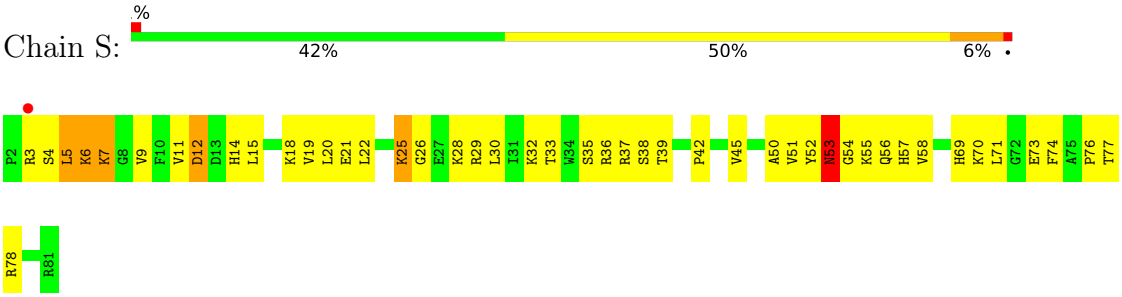
Chain Q:



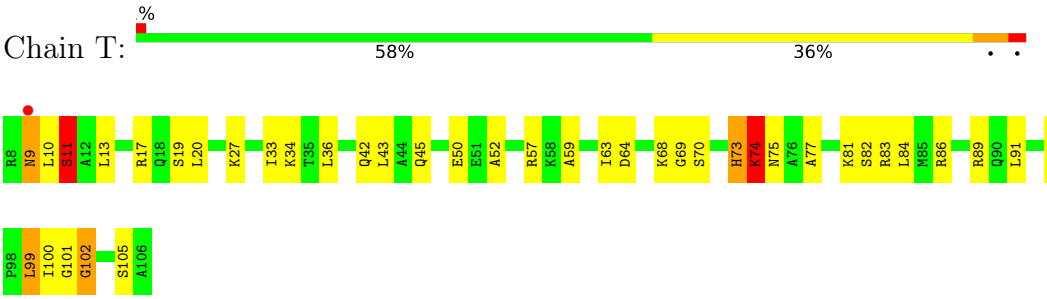
• Molecule 18: 30S ribosomal protein S18



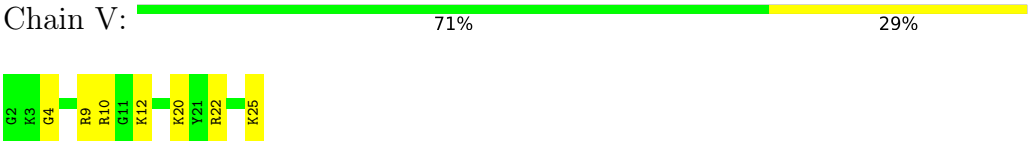
• Molecule 19: 30S ribosomal protein S19



• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein Thx



• Molecule 22: mRNA A-site fragment

There are no outlier residues recorded for this chain.

• Molecule 23: tRNA ASL Escherichia coli Arg1

Chain X:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.33Å 402.33Å 176.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 3.33 49.56 – 3.33	Depositor EDS
% Data completeness (in resolution range)	92.9 (49.56-3.33) 92.1 (49.56-3.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.178 , 0.219 0.178 , 0.219	Depositor DCC
R_{free} test set	1895 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	118.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 101.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52108	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.05	59/36285 (0.2%)	1.70	908/56631 (1.6%)
2	B	0.46	0/1935	0.66	0/2609
3	C	0.50	0/1636	0.69	0/2205
4	D	0.49	0/1733	0.70	0/2318
5	E	0.64	0/1162	0.81	1/1564 (0.1%)
6	F	0.46	0/856	0.65	0/1154
7	G	0.47	0/1276	0.65	1/1709 (0.1%)
8	H	0.67	0/1136	0.82	2/1527 (0.1%)
9	I	0.48	0/1029	0.70	1/1379 (0.1%)
10	J	0.48	0/807	0.70	0/1085
11	K	0.52	0/900	0.72	0/1213
12	L	0.68	0/986	0.90	1/1320 (0.1%)
13	M	0.47	0/1008	0.68	0/1347
14	N	0.50	0/501	0.68	0/664
15	O	0.50	0/745	0.75	1/992 (0.1%)
16	P	0.62	0/716	0.81	0/963
17	Q	0.72	0/870	0.81	1/1159 (0.1%)
18	R	0.54	0/604	0.67	0/801
19	S	0.43	0/661	0.66	0/890
20	T	0.56	0/765	0.87	3/1007 (0.3%)
21	V	0.47	0/212	0.68	0/277
22	W	0.97	0/91	1.62	0/140
23	X	0.95	0/235	1.52	4/360 (1.1%)
All	All	0.90	59/56149 (0.1%)	1.47	923/83314 (1.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	2
8	H	0	1
9	I	0	1
12	L	0	1
14	N	0	1
17	Q	0	1
18	R	0	1
19	S	0	1
20	T	0	1
All	All	0	10

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	G	N1-C2	17.96	1.52	1.37
1	A	564	G	C5-C6	-15.25	1.27	1.42
1	A	564	G	C6-N1	12.96	1.48	1.39
1	A	564	G	N9-C8	11.08	1.45	1.37
1	A	564	G	N7-C5	-10.97	1.32	1.39
1	A	5	U	OP3-P	-9.91	1.49	1.61
1	A	846	G	N9-C8	8.57	1.43	1.37
1	A	274	A	N9-C4	-8.30	1.32	1.37
1	A	1352	G	C6-O6	8.26	1.31	1.24
1	A	1208	A	N9-C4	-8.03	1.33	1.37
1	A	846	G	N7-C5	7.75	1.44	1.39
1	A	564	G	C5-C4	7.70	1.43	1.38
1	A	886	A	N9-C4	-7.20	1.33	1.37
1	A	308	A	N9-C4	-7.13	1.33	1.37
1	A	1479	A	C5-C6	-7.05	1.34	1.41
1	A	22	G	N3-C4	-6.99	1.30	1.35
1	A	564	G	C8-N7	6.96	1.35	1.30
1	A	564	G	N9-C4	-6.55	1.32	1.38
1	A	1479	A	N7-C5	-6.52	1.35	1.39
1	A	1490	A	C5-C6	-6.49	1.35	1.41
1	A	835	G	C6-N1	6.46	1.44	1.39
1	A	1479	A	N9-C4	-6.29	1.34	1.37
1	A	558	G	N9-C8	-6.26	1.33	1.37
1	A	846	G	N9-C4	-6.20	1.32	1.38
1	A	547	C	N1-C6	-6.11	1.33	1.37
1	A	306	C	C4-C5	-5.86	1.38	1.43
1	A	1280	A	N7-C5	-5.80	1.35	1.39
1	A	1058	C	N1-C6	-5.79	1.33	1.37
1	A	261	G	N9-C4	-5.79	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	846	G	C8-N7	5.76	1.34	1.30
1	A	293	A	N3-C4	-5.71	1.31	1.34
1	A	128	A	N3-C4	-5.70	1.31	1.34
1	A	101	G	N9-C4	-5.68	1.33	1.38
1	A	1280	A	N3-C4	-5.61	1.31	1.34
1	A	1479	A	N3-C4	-5.53	1.31	1.34
1	A	924	G	N9-C8	-5.49	1.34	1.37
1	A	914	A	N9-C4	-5.49	1.34	1.37
1	A	800	C	N1-C6	-5.47	1.33	1.37
1	A	125	C	N3-C4	-5.41	1.30	1.33
1	A	274	A	C5-C6	-5.40	1.36	1.41
1	A	862	G	N9-C8	-5.37	1.34	1.37
1	A	1036	C	P-O5'	5.35	1.65	1.59
1	A	559	G	N3-C4	-5.32	1.31	1.35
1	A	835	G	N1-C2	5.32	1.42	1.37
1	A	896	A	N9-C4	-5.32	1.34	1.37
1	A	553	G	N3-C4	-5.31	1.31	1.35
1	A	1280	A	N9-C4	-5.17	1.34	1.37
1	A	1492	C	N1-C6	-5.14	1.34	1.37
1	A	1381	C	N1-C6	-5.13	1.34	1.37
1	A	570	G	N3-C4	-5.11	1.31	1.35
1	A	647	G	N7-C5	-5.09	1.36	1.39
1	A	5	U	N1-C2	5.08	1.43	1.38
1	A	799	A	N9-C4	-5.08	1.34	1.37
1	A	1352	G	C6-N1	5.07	1.43	1.39
1	A	1352	G	N1-C2	5.07	1.41	1.37
1	A	863	G	N9-C8	-5.07	1.34	1.37
1	A	846	G	C6-N1	5.06	1.43	1.39
1	A	1500	G	N3-C4	-5.05	1.31	1.35
1	A	843	C	N3-C4	-5.02	1.30	1.33

All (923) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	G	N1-C6-O6	42.19	145.22	119.90
1	A	564	G	C5-C6-O6	-33.26	108.64	128.60
1	A	564	G	C4-C5-N7	27.13	121.65	110.80
1	A	564	G	N3-C2-N2	-25.32	102.17	119.90
1	A	564	G	C5-N7-C8	-23.55	92.52	104.30
1	A	564	G	C6-C5-N7	-23.48	116.31	130.40
1	A	835	G	N1-C6-O6	23.11	133.76	119.90
1	A	564	G	N3-C4-C5	22.26	139.73	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	564	G	C2-N3-C4	-22.03	100.89	111.90
1	A	564	G	N1-C2-N2	19.24	133.51	116.20
1	A	835	G	C5-C6-O6	-18.31	117.62	128.60
1	A	564	G	N7-C8-N9	16.91	121.56	113.10
1	A	846	G	C5-N7-C8	-16.31	96.14	104.30
1	A	564	G	N3-C4-N9	-15.53	116.68	126.00
1	A	835	G	C5-N7-C8	-15.05	96.77	104.30
1	A	110	G	N1-C6-O6	14.78	128.77	119.90
1	A	835	G	C4-C5-N7	14.73	116.69	110.80
1	A	1352	G	C5-C6-N1	-14.53	104.24	111.50
1	A	835	G	C6-C5-N7	-14.46	121.72	130.40
1	A	564	G	C8-N9-C4	-14.32	100.67	106.40
1	A	846	G	N3-C4-C5	13.84	135.52	128.60
1	A	1479	A	N1-C6-N6	13.22	126.53	118.60
1	A	1479	A	C6-C5-N7	-13.10	123.13	132.30
1	A	110	G	C6-C5-N7	-13.07	122.56	130.40
1	A	1497	G	O5'-P-OP2	-12.86	94.13	105.70
1	A	1471	G	O5'-P-OP2	-12.64	94.32	105.70
1	A	101	G	C5-N7-C8	-12.60	98.00	104.30
1	A	846	G	C4-C5-N7	12.47	115.79	110.80
1	A	101	G	N1-C6-O6	12.40	127.34	119.90
1	A	1036	C	O4'-C1'-N1	12.38	118.10	108.20
1	A	564	G	C5-C6-N1	-12.22	105.39	111.50
1	A	101	G	C4-C5-N7	12.09	115.64	110.80
1	A	274	A	C2-N3-C4	-11.93	104.64	110.60
1	A	835	G	N7-C8-N9	11.78	118.99	113.10
1	A	564	G	C8-N9-C1'	11.64	142.13	127.00
1	A	1479	A	C5-N7-C8	-11.58	98.11	103.90
1	A	1479	A	C2-N3-C4	-11.36	104.92	110.60
1	A	953	G	C5-C6-N1	-11.30	105.85	111.50
1	A	261	G	C5-N7-C8	-11.28	98.66	104.30
1	A	1383	G	O5'-P-OP2	-11.22	95.61	105.70
1	A	110	G	C5-C6-O6	-11.21	121.87	128.60
1	A	1504	C	C6-N1-C2	11.17	124.77	120.30
1	A	1384	C	N3-C4-C5	-10.89	117.54	121.90
1	A	7	G	C8-N9-C4	10.84	110.74	106.40
1	A	1479	A	C4-C5-N7	10.79	116.09	110.70
1	A	799	A	C2-N3-C4	-10.75	105.23	110.60
1	A	357	G	N1-C6-O6	10.72	126.33	119.90
1	A	846	G	N3-C4-N9	-10.70	119.58	126.00
1	A	835	G	N3-C2-N2	-10.66	112.44	119.90
1	A	947	C	O5'-P-OP1	-10.60	96.16	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	846	G	C4-C5-C6	-10.43	112.54	118.80
1	A	1504	C	N3-C4-C5	10.34	126.04	121.90
1	A	1352	G	N3-C2-N2	-10.28	112.71	119.90
1	A	21	G	C8-N9-C4	10.23	110.49	106.40
1	A	101	G	C2-N3-C4	-10.13	106.84	111.90
1	A	465	G	N1-C6-O6	10.07	125.94	119.90
1	A	113	A	N1-C6-N6	9.85	124.51	118.60
1	A	674	G	N1-C6-O6	9.83	125.80	119.90
1	A	948	G	C8-N9-C4	9.72	110.29	106.40
1	A	1352	G	C4-C5-N7	-9.71	106.91	110.80
1	A	113	A	C5-C6-N6	-9.69	115.95	123.70
1	A	846	G	C8-N9-C1'	9.58	139.46	127.00
1	A	846	G	N7-C8-N9	9.57	117.89	113.10
1	A	1036	C	C6-N1-C2	-9.55	116.48	120.30
1	A	101	G	N3-C4-C5	9.50	133.35	128.60
1	A	101	G	C6-C5-N7	-9.49	124.70	130.40
1	A	1056	G	C5-C6-N1	-9.40	106.80	111.50
1	A	274	A	C5-N7-C8	-9.38	99.21	103.90
1	A	1398	G	N1-C6-O6	9.35	125.51	119.90
1	A	1207	C	O5'-P-OP2	-9.33	97.30	105.70
1	A	952	A	N7-C8-N9	9.30	118.45	113.80
1	A	261	G	N7-C8-N9	9.29	117.75	113.10
1	A	1480	A	C8-N9-C4	-9.27	102.09	105.80
1	A	1487	U	C6-N1-C2	9.21	126.53	121.00
1	A	48	C	O5'-P-OP1	-8.95	97.64	105.70
1	A	1052	U	O5'-P-OP2	-8.89	97.70	105.70
1	A	505	C	C6-N1-C2	8.87	123.85	120.30
1	A	1479	A	N7-C8-N9	8.85	118.23	113.80
1	A	6	G	N3-C4-N9	8.81	131.29	126.00
1	A	897	U	O5'-P-OP2	-8.75	97.83	105.70
1	A	953	G	N1-C6-O6	8.71	125.13	119.90
1	A	110	G	N9-C4-C5	-8.71	101.92	105.40
1	A	261	G	C4-C5-N7	8.69	114.28	110.80
1	A	509	C	C6-N1-C2	8.61	123.74	120.30
1	A	846	G	C4-N9-C1'	-8.60	115.32	126.50
1	A	925	C	C6-N1-C2	8.58	123.73	120.30
1	A	625	A	O5'-P-OP2	-8.57	97.99	105.70
1	A	64	G	C8-N9-C1'	-8.56	115.87	127.00
1	A	250	G	N1-C6-O6	8.54	125.03	119.90
1	A	1060	U	O5'-P-OP1	-8.48	98.07	105.70
1	A	898	U	C5-C6-N1	-8.43	118.48	122.70
1	A	555	A	N1-C6-N6	-8.43	113.54	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	U	N1-C2-O2	8.41	128.69	122.80
1	A	47	C	N3-C4-C5	8.39	125.26	121.90
1	A	101	G	N7-C8-N9	8.38	117.29	113.10
1	A	1352	G	N1-C6-O6	8.32	124.89	119.90
1	A	47	C	C6-N1-C2	8.26	123.60	120.30
1	A	1370	C	C6-N1-C2	8.21	123.58	120.30
1	A	323	C	C2-N1-C1'	8.19	127.81	118.80
1	A	21	G	N9-C4-C5	-8.18	102.13	105.40
1	A	1280	A	C8-N9-C4	-8.17	102.53	105.80
1	A	551	G	O5'-P-OP2	-8.16	98.36	105.70
1	A	1280	A	N7-C8-N9	8.16	117.88	113.80
20	T	74	LYS	C-N-CA	8.16	142.09	121.70
1	A	1486	C	C5-C6-N1	-8.15	116.93	121.00
1	A	1377	C	C2-N3-C4	-8.14	115.83	119.90
1	A	47	C	C2-N1-C1'	-8.13	109.86	118.80
1	A	1281	G	P-O3'-C3'	8.12	129.44	119.70
1	A	110	G	C4-C5-N7	8.11	114.04	110.80
1	A	1377	C	C6-N1-C2	8.08	123.53	120.30
1	A	22	G	N1-C6-O6	8.06	124.74	119.90
1	A	560	G	C8-N9-C4	8.05	109.62	106.40
1	A	175	G	N3-C4-C5	-8.05	124.58	128.60
1	A	512	G	N1-C6-O6	8.04	124.72	119.90
1	A	1384	C	C5-C4-N4	8.04	125.83	120.20
1	A	1204	C	N1-C2-O2	8.02	123.72	118.90
1	A	947	C	O5'-P-OP2	8.02	120.32	110.70
1	A	274	A	N3-C4-C5	7.98	132.39	126.80
1	A	7	G	N7-C8-N9	-7.91	109.15	113.10
1	A	101	G	C5-C6-O6	-7.89	123.87	128.60
1	A	741	G	N1-C6-O6	7.84	124.60	119.90
1	A	64	G	C4-N9-C1'	7.84	136.69	126.50
1	A	44	G	O5'-P-OP2	-7.83	98.66	105.70
1	A	1478	C	C6-N1-C2	7.81	123.42	120.30
1	A	1475	U	N3-C2-O2	-7.79	116.75	122.20
1	A	274	A	C4-C5-N7	7.74	114.57	110.70
1	A	1379	C	C6-N1-C2	-7.74	117.20	120.30
1	A	22	G	C5-C6-N1	-7.73	107.63	111.50
1	A	795	C	P-O3'-C3'	7.70	128.94	119.70
1	A	795	C	N3-C2-O2	-7.68	116.52	121.90
1	A	64	G	N3-C4-N9	7.68	130.61	126.00
1	A	110	G	C4-C5-C6	7.67	123.40	118.80
1	A	897	U	C5-C4-O4	7.65	130.49	125.90
1	A	1367	G	C8-N9-C4	7.65	109.46	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	735	G	C8-N9-C4	7.64	109.46	106.40
1	A	1377	C	C5-C6-N1	-7.63	117.18	121.00
1	A	1352	G	C4-C5-C6	7.63	123.38	118.80
1	A	367	C	N1-C2-N3	-7.60	113.88	119.20
1	A	952	A	C5-N7-C8	-7.59	100.10	103.90
1	A	1473	C	N3-C4-N4	7.59	123.31	118.00
1	A	274	A	O4'-C1'-N9	-7.58	102.14	108.20
1	A	1171	G	P-O3'-C3'	7.57	128.78	119.70
1	A	538	C	O5'-P-OP2	-7.55	98.90	105.70
1	A	1479	A	C4-C5-C6	7.55	120.77	117.00
1	A	1206	A	N1-C2-N3	7.52	133.06	129.30
1	A	1280	A	C5-N7-C8	-7.51	100.14	103.90
1	A	88	G	O5'-P-OP2	-7.50	98.95	105.70
1	A	371	G	N1-C6-O6	7.50	124.40	119.90
1	A	674	G	C5-C6-N1	-7.50	107.75	111.50
1	A	1328	G	P-O3'-C3'	7.50	128.70	119.70
1	A	711	A	C8-N9-C4	-7.48	102.81	105.80
1	A	371	G	C5-C6-N1	-7.47	107.76	111.50
1	A	1382	C	N1-C2-O2	7.43	123.36	118.90
1	A	1280	A	C2-N3-C4	-7.43	106.89	110.60
1	A	1367	G	N9-C4-C5	-7.42	102.43	105.40
1	A	1386	C	C5-C6-N1	7.39	124.70	121.00
1	A	636	A	C8-N9-C4	-7.39	102.84	105.80
1	A	261	G	N3-C4-C5	7.39	132.29	128.60
1	A	1050	G	C5-N7-C8	-7.38	100.61	104.30
1	A	290	C	C6-N1-C2	7.37	123.25	120.30
1	A	308	A	C8-N9-C4	7.34	108.74	105.80
1	A	1386	C	C4-C5-C6	-7.33	113.73	117.40
1	A	393	C	C6-N1-C2	7.32	123.23	120.30
1	A	530	A	N1-C6-N6	-7.32	114.21	118.60
1	A	500	G	N3-C4-N9	7.29	130.38	126.00
1	A	1352	G	N9-C4-C5	7.29	108.32	105.40
1	A	689	A	C8-N9-C4	7.28	108.71	105.80
1	A	922	G	C4-C5-N7	7.27	113.71	110.80
1	A	1479	A	C5-C6-N1	-7.27	114.06	117.70
1	A	5	U	O5'-P-OP1	-7.27	99.16	105.70
1	A	799	A	N1-C2-N3	7.26	132.93	129.30
1	A	1085	C	C6-N1-C2	7.26	123.20	120.30
1	A	420	G	N1-C6-O6	-7.23	115.56	119.90
1	A	327	G	OP2-P-O3'	7.23	121.10	105.20
1	A	831	G	O5'-P-OP1	-7.23	99.19	105.70
1	A	1442	C	N1-C2-O2	7.22	123.23	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1067	U	C2-N1-C1'	-7.21	109.05	117.70
1	A	313	G	N1-C6-O6	7.21	124.22	119.90
1	A	564	G	C4-N9-C1'	-7.19	117.15	126.50
1	A	560	G	N3-C4-C5	7.18	132.19	128.60
1	A	113	A	C4-C5-N7	7.18	114.29	110.70
1	A	1486	C	C6-N1-C2	7.18	123.17	120.30
1	A	908	C	C5-C6-N1	-7.18	117.41	121.00
1	A	1055	U	C4-C5-C6	7.17	124.00	119.70
1	A	100	G	C4-C5-N7	7.17	113.67	110.80
1	A	1081	G	C5-C6-O6	7.15	132.89	128.60
1	A	1377	C	N3-C4-C5	7.11	124.74	121.90
1	A	598	C	C6-N1-C2	-7.11	117.46	120.30
1	A	845	C	O5'-P-OP2	-7.10	99.31	105.70
1	A	1052	U	OP1-P-OP2	7.09	130.24	119.60
1	A	1183	G	C4-C5-N7	-7.09	107.96	110.80
1	A	1398	G	C5-C6-O6	-7.08	124.35	128.60
1	A	324	A	C2-N3-C4	-7.07	107.06	110.60
1	A	1065	U	N3-C2-O2	7.07	127.15	122.20
1	A	367	C	C6-N1-C2	7.07	123.13	120.30
1	A	1472	U	N1-C2-O2	7.07	127.75	122.80
1	A	536	A	C2-N3-C4	-7.05	107.08	110.60
1	A	261	G	C8-N9-C4	-7.04	103.58	106.40
1	A	1036	C	OP1-P-OP2	-7.04	109.05	119.60
1	A	1035	G	P-O3'-C3'	7.02	128.13	119.70
1	A	101	G	O4'-C1'-N9	7.02	113.82	108.20
1	A	242	G	O5'-P-OP2	-7.02	99.38	105.70
1	A	1206	A	C4-C5-C6	7.01	120.51	117.00
1	A	110	G	N3-C4-N9	7.00	130.20	126.00
1	A	250	G	C6-C5-N7	-7.00	126.20	130.40
1	A	674	G	N3-C2-N2	-6.99	115.01	119.90
1	A	1091	C	C6-N1-C2	6.98	123.09	120.30
1	A	12	U	N3-C4-C5	-6.96	110.42	114.60
1	A	948	G	N7-C8-N9	-6.96	109.62	113.10
1	A	1479	A	N1-C2-N3	6.95	132.77	129.30
1	A	274	A	N1-C6-N6	6.93	122.76	118.60
1	A	12	U	C5-C4-O4	6.93	130.06	125.90
1	A	1247	G	N3-C4-N9	-6.93	121.84	126.00
1	A	1500	G	N3-C2-N2	-6.93	115.05	119.90
1	A	175	G	C8-N9-C4	-6.92	103.63	106.40
1	A	1475	U	C6-N1-C2	-6.91	116.86	121.00
1	A	899	G	C8-N9-C4	6.91	109.16	106.40
1	A	659	A	C8-N9-C4	6.90	108.56	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1352	G	N1-C2-N2	6.90	122.41	116.20
1	A	903	G	C2-N3-C4	-6.90	108.45	111.90
1	A	578	G	N3-C4-N9	6.89	130.13	126.00
1	A	512	G	C5-C6-O6	-6.89	124.47	128.60
1	A	893	G	C8-N9-C4	-6.88	103.65	106.40
1	A	1055	U	C5-C6-N1	-6.88	119.26	122.70
1	A	343	G	C5-C6-O6	-6.88	124.47	128.60
1	A	491	C	O5'-P-OP2	-6.87	99.52	105.70
1	A	555	A	N9-C4-C5	6.87	108.55	105.80
1	A	1281	G	C8-N9-C4	-6.86	103.66	106.40
1	A	1217	A	C8-N9-C4	-6.86	103.06	105.80
1	A	1247	G	C4-N9-C1'	-6.84	117.61	126.50
1	A	741	G	C5-C6-O6	-6.82	124.51	128.60
1	A	500	G	N3-C4-C5	-6.82	125.19	128.60
1	A	1178	G	C4-N9-C1'	6.82	135.36	126.50
1	A	822	U	C2-N1-C1'	6.82	125.88	117.70
1	A	5	U	N3-C2-O2	-6.81	117.43	122.20
1	A	1046	G	N1-C2-N3	6.81	127.99	123.90
1	A	50	A	N9-C4-C5	-6.80	103.08	105.80
1	A	1177	U	C5-C6-N1	6.80	126.10	122.70
1	A	767	C	C6-N1-C2	6.80	123.02	120.30
1	A	1068	U	C5-C6-N1	6.79	126.10	122.70
1	A	690	C	O5'-P-OP2	-6.79	99.58	105.70
1	A	730	C	N3-C4-C5	6.79	124.62	121.90
1	A	261	G	O5'-P-OP2	-6.78	99.60	105.70
1	A	1483	U	O5'-P-OP2	-6.78	99.60	105.70
1	A	507	G	C5-C6-O6	-6.77	124.54	128.60
1	A	1223	C	C6-N1-C2	6.77	123.01	120.30
1	A	802	A	C2-N3-C4	-6.76	107.22	110.60
1	A	741	G	C2-N3-C4	-6.75	108.53	111.90
1	A	1081	G	C4-C5-N7	-6.74	108.10	110.80
1	A	633	G	N1-C6-O6	6.73	123.94	119.90
1	A	793	C	C5-C4-N4	-6.73	115.49	120.20
1	A	1066	G	C8-N9-C4	6.72	109.09	106.40
1	A	544	U	C5-C4-O4	-6.71	121.87	125.90
1	A	110	G	C8-N9-C1'	-6.70	118.29	127.00
1	A	261	G	N3-C4-N9	-6.70	121.98	126.00
1	A	889	C	N3-C4-C5	6.70	124.58	121.90
1	A	1398	G	N9-C4-C5	-6.69	102.72	105.40
1	A	31	G	N3-C2-N2	-6.69	115.22	119.90
1	A	844	G	N3-C4-C5	-6.68	125.26	128.60
1	A	881	C	N3-C4-C5	6.68	124.57	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1508	A	N1-C6-N6	6.68	122.61	118.60
1	A	541	G	N3-C4-N9	6.68	130.01	126.00
1	A	1367	G	C5-C6-O6	-6.68	124.59	128.60
1	A	500	G	P-O3'-C3'	6.67	127.70	119.70
1	A	559	G	N1-C2-N3	6.66	127.90	123.90
1	A	275	C	O5'-P-OP2	-6.65	99.72	105.70
1	A	1480	A	N9-C4-C5	6.64	108.46	105.80
1	A	558	G	O5'-P-OP2	-6.63	99.73	105.70
1	A	835	G	N1-C2-N2	6.63	122.17	116.20
1	A	189	U	P-O3'-C3'	6.63	127.65	119.70
1	A	794	C	N1-C2-O2	-6.62	114.93	118.90
1	A	293	A	O5'-P-OP1	-6.61	99.75	105.70
1	A	1388	U	N1-C2-N3	6.61	118.87	114.90
1	A	105	G	N3-C2-N2	-6.61	115.27	119.90
1	A	1247	G	C8-N9-C1'	6.59	135.57	127.00
1	A	804	G	O5'-P-OP1	-6.59	99.77	105.70
1	A	1147	C	C6-N1-C2	-6.59	117.66	120.30
1	A	323	C	C6-N1-C1'	-6.58	112.91	120.80
1	A	541	G	N1-C2-N2	-6.57	110.29	116.20
1	A	861	U	O5'-P-OP2	-6.57	99.79	105.70
1	A	326	G	N1-C6-O6	6.57	123.84	119.90
1	A	468	G	N3-C4-N9	6.56	129.94	126.00
1	A	1280	A	C6-C5-N7	-6.55	127.72	132.30
1	A	77	G	OP1-P-O3'	6.54	119.59	105.20
1	A	795	C	C2-N3-C4	-6.54	116.63	119.90
1	A	1469	A	O5'-P-OP2	-6.54	99.81	105.70
1	A	175	G	C4-N9-C1'	6.54	135.00	126.50
1	A	739	C	C6-N1-C2	6.52	122.91	120.30
1	A	1281	G	OP2-P-O3'	6.51	119.53	105.20
1	A	1506	G	N3-C2-N2	-6.51	115.34	119.90
1	A	1067	U	C5-C6-N1	-6.51	119.45	122.70
1	A	1504	C	OP1-P-O3'	-6.51	90.89	105.20
1	A	958	U	N3-C4-O4	6.50	123.95	119.40
1	A	716	A	O4'-C1'-N9	6.49	113.39	108.20
1	A	243	C	C6-N1-C2	6.49	122.90	120.30
1	A	1208	A	C2-N3-C4	-6.49	107.36	110.60
1	A	540	G	O5'-P-OP1	6.48	118.48	110.70
1	A	675	U	N3-C4-C5	-6.48	110.71	114.60
1	A	26	A	C8-N9-C4	6.47	108.39	105.80
1	A	952	A	C2-N3-C4	-6.47	107.37	110.60
1	A	113	A	C6-C5-N7	-6.46	127.78	132.30
1	A	558	G	C8-N9-C4	6.45	108.98	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	261	G	C2-N3-C4	-6.45	108.68	111.90
1	A	1209	C	C6-N1-C2	-6.44	117.72	120.30
1	A	553	G	C4-N9-C1'	6.44	134.88	126.50
1	A	1475	U	N1-C2-N3	6.43	118.76	114.90
1	A	560	G	N9-C4-C5	-6.43	102.83	105.40
1	A	669	U	C5-C6-N1	-6.42	119.49	122.70
1	A	398	C	C4-C5-C6	6.42	120.61	117.40
1	A	357	G	C5-N7-C8	-6.41	101.09	104.30
1	A	44	G	C6-C5-N7	-6.41	126.56	130.40
1	A	822	U	C6-N1-C1'	-6.41	112.23	121.20
1	A	580	G	OP1-P-OP2	-6.41	109.99	119.60
1	A	878	A	C2-N3-C4	-6.40	107.40	110.60
1	A	125	C	N3-C2-O2	-6.40	117.42	121.90
1	A	1232	A	C8-N9-C4	-6.40	103.24	105.80
1	A	953	G	C2-N3-C4	-6.39	108.70	111.90
1	A	1257	G	C8-N9-C4	-6.39	103.84	106.40
1	A	1036	C	C5-C6-N1	6.38	124.19	121.00
1	A	1384	C	C4-C5-C6	6.37	120.58	117.40
1	A	952	A	O4'-C1'-N9	-6.37	103.10	108.20
1	A	294	G	C5-C6-N1	-6.36	108.32	111.50
1	A	445	A	C8-N9-C4	-6.36	103.26	105.80
1	A	839	C	C6-N1-C2	6.35	122.84	120.30
1	A	1204	C	N3-C2-O2	-6.35	117.45	121.90
1	A	970	G	C6-C5-N7	-6.34	126.59	130.40
1	A	1050	G	N7-C8-N9	6.34	116.27	113.10
1	A	795	C	N1-C2-O2	6.34	122.70	118.90
1	A	540	G	N3-C4-N9	6.33	129.80	126.00
1	A	759	G	O5'-P-OP2	-6.33	100.00	105.70
1	A	952	A	N1-C6-N6	6.33	122.40	118.60
1	A	21	G	N3-C2-N2	6.32	124.33	119.90
1	A	598	C	C5-C6-N1	6.32	124.16	121.00
1	A	1180	U	N3-C4-C5	-6.32	110.81	114.60
1	A	1472	U	C2-N3-C4	6.32	130.79	127.00
1	A	84	C	OP1-P-O3'	6.31	119.08	105.20
1	A	237	C	N1-C2-O2	-6.30	115.12	118.90
1	A	833	C	N1-C2-O2	-6.30	115.12	118.90
1	A	103	C	C6-N1-C2	6.29	122.82	120.30
1	A	583	C	C2-N1-C1'	6.29	125.72	118.80
1	A	1220	A	P-O3'-C3'	6.29	127.25	119.70
1	A	1205	G	P-O3'-C3'	6.29	127.25	119.70
1	A	1505	U	N1-C2-N3	-6.29	111.13	114.90
1	A	1065	U	C5-C4-O4	-6.29	122.13	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	905	G	N1-C6-O6	6.29	123.67	119.90
23	X	30	G	N3-C4-C5	-6.28	125.46	128.60
1	A	1424	G	N3-C4-N9	6.27	129.76	126.00
1	A	50	A	N1-C6-N6	6.26	122.35	118.60
1	A	1262	U	C5-C6-N1	6.26	125.83	122.70
1	A	389	G	N3-C4-N9	-6.25	122.25	126.00
1	A	6	G	N3-C4-C5	-6.24	125.48	128.60
1	A	1053	C	O5'-P-OP2	-6.23	100.09	105.70
1	A	500	G	C4-N9-C1'	6.23	134.60	126.50
1	A	864	G	C8-N9-C4	6.23	108.89	106.40
1	A	24	U	C5-C6-N1	-6.23	119.59	122.70
1	A	752	G	C5-C6-O6	-6.22	124.86	128.60
1	A	719	C	O5'-P-OP2	-6.22	100.10	105.70
1	A	1490	A	C5-C6-N6	-6.22	118.72	123.70
1	A	766	C	N3-C4-C5	6.22	124.39	121.90
1	A	102	A	O5'-P-OP1	-6.21	100.11	105.70
1	A	1313	A	N1-C6-N6	6.21	122.33	118.60
1	A	1107	U	C5-C6-N1	6.21	125.81	122.70
9	I	56	LEU	CA-CB-CG	6.21	129.58	115.30
1	A	269	A	O5'-P-OP2	-6.20	100.12	105.70
1	A	795	C	C5-C6-N1	-6.20	117.90	121.00
1	A	750	A	N1-C2-N3	6.19	132.40	129.30
1	A	252	G	C5-C6-N1	-6.18	108.41	111.50
1	A	1487	U	N3-C2-O2	6.18	126.53	122.20
1	A	278	C	C6-N1-C2	-6.18	117.83	120.30
1	A	272	C	C2-N1-C1'	-6.18	112.00	118.80
1	A	323	C	O5'-P-OP2	-6.18	100.14	105.70
1	A	379	G	OP1-P-OP2	6.18	128.87	119.60
1	A	747	C	C6-N1-C2	6.18	122.77	120.30
1	A	1180	U	C5-C4-O4	6.18	129.61	125.90
1	A	1279	C	P-O3'-C3'	6.18	127.11	119.70
1	A	1004	G	C4-N9-C1'	6.17	134.53	126.50
1	A	1490	A	N1-C6-N6	6.16	122.30	118.60
1	A	706	U	N1-C2-O2	6.16	127.11	122.80
1	A	800	C	C2-N3-C4	-6.16	116.82	119.90
1	A	885	A	N1-C6-N6	6.16	122.29	118.60
1	A	846	G	C5-C6-O6	-6.14	124.91	128.60
1	A	970	G	N3-C4-N9	6.14	129.69	126.00
1	A	328	G	N1-C6-O6	6.14	123.58	119.90
1	A	598	C	C2-N1-C1'	6.14	125.55	118.80
1	A	1478	C	C5-C6-N1	-6.14	117.93	121.00
1	A	541	G	N3-C2-N2	6.13	124.19	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1370	C	C5-C6-N1	-6.12	117.94	121.00
1	A	894	G	O5'-P-OP2	-6.12	100.19	105.70
1	A	919	G	N1-C6-O6	6.11	123.57	119.90
1	A	253	G	C6-C5-N7	-6.11	126.73	130.40
1	A	222	G	C8-N9-C4	6.10	108.84	106.40
1	A	241	A	O4'-C1'-N9	6.10	113.08	108.20
1	A	293	A	C5-C6-N1	-6.10	114.65	117.70
1	A	706	U	N3-C2-O2	-6.10	117.93	122.20
1	A	1352	G	C8-N9-C4	-6.09	103.96	106.40
1	A	1036	C	O5'-P-OP2	6.09	118.01	110.70
1	A	121	G	C5-C6-N1	6.09	114.54	111.50
1	A	787	U	C5-C4-O4	6.08	129.55	125.90
1	A	1208	A	N3-C4-C5	6.08	131.06	126.80
1	A	905	G	N9-C4-C5	-6.08	102.97	105.40
1	A	569	C	C6-N1-C2	6.07	122.73	120.30
20	T	20	LEU	CA-CB-CG	-6.07	101.34	115.30
1	A	750	A	C6-N1-C2	-6.07	114.96	118.60
1	A	1212	G	N1-C6-O6	6.06	123.54	119.90
1	A	1507	G	C8-N9-C4	6.06	108.82	106.40
1	A	794	C	O5'-P-OP1	-6.06	100.25	105.70
1	A	1036	C	N1-C1'-C2'	-6.06	105.34	112.00
1	A	1072	U	C5-C4-O4	6.05	129.53	125.90
1	A	1082	C	O5'-P-OP2	6.05	117.96	110.70
1	A	343	G	N1-C2-N2	6.05	121.64	116.20
1	A	785	A	N1-C2-N3	6.04	132.32	129.30
1	A	51	A	C6-C5-N7	-6.04	128.07	132.30
1	A	250	G	C5-C6-O6	-6.04	124.97	128.60
1	A	282	U	O5'-P-OP1	-6.04	100.26	105.70
1	A	553	G	OP1-P-O3'	6.03	118.47	105.20
1	A	822	U	N1-C2-O2	6.03	127.02	122.80
1	A	1312	G	N9-C4-C5	6.03	107.81	105.40
1	A	19	C	C4-C5-C6	6.03	120.42	117.40
1	A	1171	G	N3-C2-N2	-6.03	115.68	119.90
1	A	286	C	OP1-P-O3'	6.03	118.46	105.20
1	A	913	C	C6-N1-C2	6.03	122.71	120.30
1	A	468	G	N3-C4-C5	-6.02	125.59	128.60
1	A	741	G	C6-C5-N7	-6.02	126.79	130.40
1	A	840	U	C5-C4-O4	-6.01	122.29	125.90
1	A	1247	G	N3-C4-C5	6.01	131.60	128.60
1	A	889	C	C6-N1-C2	6.01	122.70	120.30
1	A	1392	G	N1-C6-O6	-6.00	116.30	119.90
1	A	926	A	N9-C4-C5	-6.00	103.40	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1497	G	C4-C5-C6	6.00	122.40	118.80
1	A	1379	C	OP2-P-O3'	6.00	118.39	105.20
1	A	952	A	C6-C5-N7	-6.00	128.10	132.30
1	A	1106	G	N3-C4-C5	-6.00	125.60	128.60
1	A	1206	A	O5'-P-OP1	-6.00	100.30	105.70
1	A	544	U	N3-C4-O4	5.99	123.60	119.40
1	A	270	G	C8-N9-C1'	-5.99	119.21	127.00
1	A	945	A	C8-N9-C4	5.99	108.20	105.80
1	A	541	G	C6-C5-N7	-5.98	126.81	130.40
1	A	235	C	C2-N3-C4	-5.98	116.91	119.90
1	A	288	G	O5'-P-OP2	-5.97	100.32	105.70
1	A	512	G	C6-C5-N7	-5.97	126.82	130.40
1	A	836	A	O5'-P-OP1	-5.97	100.33	105.70
1	A	1076	G	O5'-P-OP2	-5.97	100.33	105.70
1	A	357	G	N7-C8-N9	5.96	116.08	113.10
1	A	389	G	C5-C6-N1	-5.96	108.52	111.50
1	A	64	G	N3-C4-C5	-5.96	125.62	128.60
1	A	123	G	P-O3'-C3'	5.95	126.84	119.70
1	A	47	C	N3-C2-O2	5.95	126.06	121.90
1	A	498	G	N1-C6-O6	5.94	123.47	119.90
1	A	912	A	N1-C6-N6	-5.94	115.03	118.60
1	A	465	G	N3-C2-N2	-5.94	115.75	119.90
1	A	1257	G	N7-C8-N9	5.94	116.07	113.10
1	A	21	G	C8-N9-C1'	-5.93	119.29	127.00
1	A	1046	G	C8-N9-C4	-5.93	104.03	106.40
1	A	175	G	C4-C5-C6	5.92	122.36	118.80
1	A	465	G	C5-C6-O6	-5.92	125.05	128.60
1	A	278	C	C5-C6-N1	5.92	123.96	121.00
1	A	357	G	C5-C6-O6	-5.91	125.05	128.60
1	A	939	C	C6-N1-C2	5.91	122.66	120.30
1	A	1475	U	C2-N1-C1'	5.91	124.79	117.70
1	A	99	C	OP2-P-O3'	5.91	118.19	105.20
1	A	1487	U	C2-N1-C1'	-5.91	110.61	117.70
1	A	1516	C	C6-N1-C2	-5.91	117.94	120.30
1	A	946	A	C8-N9-C4	5.90	108.16	105.80
1	A	468	G	C4-N9-C1'	5.90	134.17	126.50
1	A	487	C	N1-C2-O2	-5.90	115.36	118.90
1	A	893	G	N3-C4-C5	-5.90	125.65	128.60
1	A	1424	G	C4-N9-C1'	5.90	134.17	126.50
1	A	271	G	C8-N9-C4	5.90	108.76	106.40
1	A	389	G	N3-C4-C5	5.89	131.55	128.60
1	A	511	C	N3-C2-O2	5.89	126.03	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1505	U	C6-N1-C2	5.89	124.54	121.00
1	A	914	A	C2-N3-C4	-5.88	107.66	110.60
1	A	1348	C	N1-C2-O2	5.88	122.43	118.90
1	A	100	G	N1-C6-O6	5.88	123.43	119.90
1	A	1504	C	OP2-P-O3'	5.88	118.13	105.20
1	A	1504	C	C5-C6-N1	-5.88	118.06	121.00
1	A	1489	U	OP2-P-O3'	5.88	118.12	105.20
1	A	113	A	C5-N7-C8	-5.87	100.96	103.90
1	A	673	G	C8-N9-C4	5.87	108.75	106.40
1	A	1232	A	N9-C4-C5	5.87	108.15	105.80
1	A	1367	G	C4-C5-N7	5.87	113.15	110.80
1	A	877	A	O5'-P-OP2	5.86	117.73	110.70
1	A	898	U	C4-C5-C6	5.86	123.22	119.70
1	A	367	C	C2-N3-C4	5.86	122.83	119.90
1	A	227	G	N1-C6-O6	5.85	123.41	119.90
1	A	835	G	C2-N3-C4	-5.85	108.97	111.90
1	A	684	C	P-O3'-C3'	5.85	126.72	119.70
1	A	1286	G	C5-C6-N1	-5.85	108.58	111.50
1	A	494	C	P-O3'-C3'	5.84	126.71	119.70
1	A	277	A	C8-N9-C4	-5.84	103.46	105.80
1	A	789	C	N3-C4-C5	5.84	124.24	121.90
1	A	105	G	N3-C4-C5	5.84	131.52	128.60
1	A	105	G	N3-C4-N9	-5.84	122.50	126.00
1	A	603	C	N3-C4-C5	5.83	124.23	121.90
1	A	299	U	C5-C4-O4	5.83	129.40	125.90
1	A	295	A	N1-C6-N6	5.83	122.10	118.60
1	A	500	G	C8-N9-C1'	-5.83	119.43	127.00
1	A	9	G	O5'-P-OP2	-5.82	100.46	105.70
1	A	1046	G	P-O3'-C3'	5.82	126.68	119.70
1	A	895	A	C6-N1-C2	-5.82	115.11	118.60
1	A	1178	G	C8-N9-C1'	-5.82	119.44	127.00
1	A	1398	G	C8-N9-C4	5.82	108.73	106.40
1	A	587	G	C8-N9-C4	5.81	108.72	106.40
1	A	1364	C	C6-N1-C2	-5.81	117.98	120.30
1	A	1078	C	N3-C4-C5	5.81	124.22	121.90
1	A	901	C	OP2-P-O3'	5.80	117.97	105.20
1	A	1054	G	N3-C4-C5	-5.80	125.70	128.60
1	A	1247	G	C6-C5-N7	5.80	133.88	130.40
1	A	1379	C	C5-C6-N1	5.79	123.90	121.00
1	A	1285	G	C4-C5-C6	5.79	122.27	118.80
1	A	926	A	C8-N9-C4	5.79	108.11	105.80
1	A	840	U	N3-C2-O2	5.79	126.25	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	G	C6-C5-N7	-5.78	126.93	130.40
1	A	409	A	C8-N9-C4	-5.78	103.49	105.80
1	A	1218	C	O5'-P-OP2	-5.78	100.50	105.70
1	A	1371	C	C6-N1-C2	5.78	122.61	120.30
1	A	343	G	N1-C6-O6	5.77	123.36	119.90
1	A	357	G	C5-C6-N1	-5.77	108.62	111.50
1	A	883	G	N1-C6-O6	5.77	123.36	119.90
1	A	591	A	OP1-P-O3'	5.76	117.88	105.20
1	A	835	G	C5-C6-N1	-5.76	108.62	111.50
1	A	1263	C	N3-C2-O2	-5.76	117.87	121.90
1	A	540	G	N3-C4-C5	-5.75	125.72	128.60
1	A	624	U	N3-C2-O2	-5.75	118.17	122.20
1	A	649	G	O5'-P-OP2	-5.75	100.52	105.70
1	A	59	A	O5'-P-OP2	-5.75	100.53	105.70
1	A	807	C	N3-C4-C5	5.74	124.20	121.90
1	A	505	C	C5-C6-N1	-5.74	118.13	121.00
1	A	1357	A	N9-C4-C5	5.74	108.09	105.80
1	A	760	A	O5'-P-OP1	-5.74	100.54	105.70
1	A	800	C	C5-C6-N1	-5.74	118.13	121.00
1	A	1479	A	N9-C4-C5	-5.73	103.51	105.80
1	A	87	C	OP2-P-O3'	5.73	117.81	105.20
1	A	100	G	C6-C5-N7	-5.73	126.96	130.40
1	A	426	A	OP1-P-OP2	-5.73	111.01	119.60
1	A	30	U	C6-N1-C2	5.72	124.44	121.00
1	A	578	G	N3-C4-C5	-5.72	125.74	128.60
1	A	1064	G	C4-C5-N7	5.72	113.09	110.80
1	A	624	U	N1-C2-N3	5.72	118.33	114.90
1	A	797	A	N1-C6-N6	5.72	122.03	118.60
1	A	381	C	C2-N3-C4	-5.72	117.04	119.90
1	A	215	G	O5'-P-OP2	-5.71	100.56	105.70
1	A	745	C	N3-C4-C5	5.71	124.19	121.90
1	A	867	G	P-O3'-C3'	5.71	126.56	119.70
1	A	1368	G	C4-C5-N7	-5.71	108.52	110.80
1	A	19	C	N1-C2-O2	-5.71	115.48	118.90
23	X	40	C	N1-C2-O2	5.70	122.32	118.90
1	A	585	A	C2-N3-C4	-5.70	107.75	110.60
1	A	1382	C	C6-N1-C1'	-5.70	113.96	120.80
1	A	15	G	C4-C5-N7	5.70	113.08	110.80
1	A	795	C	C4-C5-C6	5.69	120.25	117.40
1	A	326	G	OP1-P-O3'	5.69	117.71	105.20
1	A	558	G	OP1-P-O3'	5.68	117.70	105.20
1	A	802	A	C4-C5-C6	5.68	119.84	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1064	G	C2-N3-C4	-5.68	109.06	111.90
1	A	1181	C	N1-C2-O2	5.68	122.31	118.90
1	A	952	A	C8-N9-C4	-5.68	103.53	105.80
1	A	244	U	C5-C4-O4	5.67	129.30	125.90
5	E	47	LYS	CD-CE-NZ	5.67	124.75	111.70
1	A	1432	C	C6-N1-C2	5.67	122.57	120.30
1	A	1036	C	N3-C4-C5	-5.67	119.63	121.90
1	A	275	C	C6-N1-C2	5.66	122.56	120.30
1	A	46	G	N1-C6-O6	5.66	123.30	119.90
1	A	227	G	C8-N9-C1'	-5.66	119.64	127.00
1	A	294	G	C4-C5-N7	-5.66	108.54	110.80
1	A	484	C	OP1-P-O3'	5.66	117.65	105.20
1	A	21	G	N7-C8-N9	-5.66	110.27	113.10
1	A	276	G	C6-C5-N7	-5.65	127.01	130.40
1	A	710	G	C5-C6-O6	5.65	131.99	128.60
1	A	1357	A	N1-C6-N6	-5.65	115.21	118.60
1	A	937	U	C2-N1-C1'	5.65	124.48	117.70
1	A	903	G	C5-C6-N1	-5.64	108.68	111.50
1	A	1424	G	C4-C5-N7	5.63	113.05	110.80
1	A	85	U	OP1-P-O3'	5.63	117.58	105.20
1	A	250	G	C8-N9-C1'	-5.63	119.68	127.00
1	A	549	G	N3-C2-N2	5.63	123.84	119.90
1	A	1473	C	C5-C4-N4	-5.63	116.26	120.20
1	A	505	C	N3-C4-C5	5.62	124.15	121.90
1	A	274	A	N3-C4-N9	-5.62	122.90	127.40
1	A	908	C	C2-N1-C1'	-5.62	112.61	118.80
1	A	110	G	C4-N9-C1'	5.62	133.81	126.50
1	A	762	C	N3-C4-C5	5.61	124.14	121.90
1	A	970	G	C4-N9-C1'	5.61	133.80	126.50
1	A	698	A	O5'-P-OP1	5.61	117.43	110.70
1	A	1230	C	N1-C2-O2	5.61	122.26	118.90
1	A	1385	C	C6-N1-C2	-5.61	118.06	120.30
1	A	903	G	N3-C4-C5	5.60	131.40	128.60
1	A	1106	G	C8-N9-C4	-5.60	104.16	106.40
1	A	264	C	C5-C6-N1	-5.60	118.20	121.00
1	A	511	C	N3-C4-C5	5.60	124.14	121.90
1	A	1288	U	O5'-P-OP2	-5.60	100.66	105.70
1	A	52	G	N1-C6-O6	-5.60	116.54	119.90
1	A	921	G	C5-C6-O6	5.60	131.96	128.60
1	A	751	A	N1-C2-N3	5.59	132.10	129.30
1	A	1208	A	N3-C4-N9	-5.59	122.93	127.40
1	A	704	G	OP1-P-OP2	5.59	127.99	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	202	A	N1-C6-N6	5.59	121.95	118.60
1	A	730	C	C5-C4-N4	-5.59	116.29	120.20
1	A	789	C	C6-N1-C2	5.59	122.53	120.30
1	A	113	A	N9-C4-C5	-5.58	103.57	105.80
1	A	847	U	P-O3'-C3'	5.58	126.40	119.70
1	A	1475	U	C4-C5-C6	5.58	123.05	119.70
1	A	752	G	OP1-P-OP2	-5.57	111.24	119.60
1	A	1467	C	O5'-P-OP2	5.57	117.39	110.70
1	A	1510	C	C6-N1-C2	-5.57	118.07	120.30
1	A	656	G	N1-C6-O6	5.57	123.24	119.90
1	A	1423	G	C4-C5-C6	5.57	122.14	118.80
1	A	283	A	C2-N3-C4	-5.56	107.82	110.60
1	A	264	C	C6-N1-C2	5.56	122.52	120.30
1	A	717	G	OP1-P-OP2	5.56	127.94	119.60
1	A	499	U	C6-N1-C2	-5.56	117.67	121.00
1	A	1382	C	C2-N1-C1'	5.55	124.91	118.80
1	A	560	G	C2-N3-C4	-5.55	109.12	111.90
1	A	767	C	N3-C4-C5	5.55	124.12	121.90
1	A	1072	U	N3-C4-C5	-5.55	111.27	114.60
1	A	1076	G	P-O3'-C3'	5.55	126.36	119.70
23	X	30	G	N3-C4-N9	5.55	129.33	126.00
23	X	35	C	O5'-P-OP1	-5.54	100.71	105.70
1	A	802	A	N1-C2-N3	5.54	132.07	129.30
1	A	382	U	O5'-P-OP2	-5.53	100.72	105.70
1	A	538	C	O5'-P-OP1	5.53	117.33	110.70
1	A	804	G	C5-N7-C8	5.53	107.06	104.30
1	A	15	G	N9-C4-C5	-5.53	103.19	105.40
1	A	796	U	O5'-P-OP1	-5.53	100.73	105.70
1	A	926	A	C2-N3-C4	-5.53	107.84	110.60
1	A	788	C	N3-C4-C5	5.52	124.11	121.90
1	A	895	A	N1-C2-N3	5.52	132.06	129.30
1	A	6	G	C8-N9-C1'	-5.52	119.83	127.00
1	A	858	G	C5-C6-O6	-5.52	125.29	128.60
1	A	101	G	N3-C4-N9	-5.51	122.69	126.00
1	A	249	G	C8-N9-C4	5.51	108.61	106.40
1	A	367	C	N1-C2-O2	5.51	122.21	118.90
1	A	24	U	C6-N1-C2	5.51	124.31	121.00
1	A	270	G	C4-N9-C1'	5.51	133.66	126.50
1	A	357	G	C6-C5-N7	-5.51	127.09	130.40
1	A	1062	A	N1-C6-N6	-5.51	115.29	118.60
1	A	1495	A	C5-C6-N1	-5.51	114.94	117.70
1	A	1507	G	N3-C4-C5	5.51	131.35	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1317	C	C6-N1-C2	5.51	122.50	120.30
1	A	670	A	C8-N9-C4	5.51	108.00	105.80
1	A	1424	G	C8-N9-C1'	-5.51	119.84	127.00
1	A	528	C	N3-C2-O2	-5.50	118.05	121.90
1	A	774	G	N3-C4-N9	5.50	129.30	126.00
1	A	918	G	OP1-P-O3'	5.50	117.29	105.20
1	A	731	C	C6-N1-C2	5.49	122.50	120.30
1	A	389	G	C2-N3-C4	-5.49	109.16	111.90
1	A	398	C	C5-C6-N1	-5.49	118.26	121.00
1	A	628	C	N3-C4-C5	5.49	124.09	121.90
1	A	105	G	C5-N7-C8	-5.48	101.56	104.30
1	A	1067	U	C6-N1-C2	5.48	124.29	121.00
1	A	1430	U	OP1-P-O3'	5.48	117.26	105.20
1	A	280	G	N1-C2-N3	5.48	127.19	123.90
1	A	1183	G	C5-C6-O6	5.48	131.89	128.60
1	A	891	A	N9-C4-C5	5.47	107.99	105.80
1	A	797	A	C2-N3-C4	-5.47	107.86	110.60
1	A	557	A	OP1-P-OP2	-5.47	111.40	119.60
1	A	1310	A	OP1-P-O3'	5.46	117.22	105.20
1	A	1313	A	C5-C6-N6	-5.46	119.33	123.70
1	A	555	A	C4-C5-N7	-5.46	107.97	110.70
1	A	764	A	N1-C6-N6	5.45	121.87	118.60
1	A	840	U	N1-C2-O2	-5.45	118.98	122.80
1	A	1458	U	C5-C4-O4	5.45	129.17	125.90
1	A	1500	G	C5-C6-N1	-5.45	108.77	111.50
1	A	255	G	C6-C5-N7	-5.45	127.13	130.40
1	A	1385	C	C5-C6-N1	5.45	123.72	121.00
1	A	793	C	N3-C4-N4	5.44	121.81	118.00
1	A	1507	G	N9-C4-C5	-5.44	103.22	105.40
1	A	227	G	N3-C4-N9	5.44	129.26	126.00
1	A	1042	C	C5-C6-N1	5.44	123.72	121.00
1	A	50	A	C4-C5-N7	5.44	113.42	110.70
1	A	926	A	N1-C6-N6	5.44	121.86	118.60
1	A	323	C	N3-C2-O2	-5.43	118.09	121.90
1	A	326	G	C6-C5-N7	-5.43	127.14	130.40
1	A	803	U	C2-N1-C1'	-5.43	111.18	117.70
1	A	1257	G	C6-C5-N7	-5.43	127.14	130.40
1	A	1173	C	N1-C2-O2	-5.43	115.64	118.90
1	A	1497	G	C6-C5-N7	-5.43	127.14	130.40
1	A	6	G	N9-C4-C5	-5.43	103.23	105.40
1	A	31	G	N1-C6-O6	5.43	123.16	119.90
1	A	101	G	C5-C6-N1	-5.42	108.79	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	293	A	C4-C5-C6	5.42	119.71	117.00
1	A	261	G	C6-C5-N7	-5.42	127.15	130.40
1	A	110	G	C2-N3-C4	-5.41	109.19	111.90
1	A	540	G	N1-C2-N2	-5.41	111.33	116.20
1	A	924	G	C8-N9-C4	5.41	108.56	106.40
1	A	1177	U	N3-C4-O4	5.41	123.19	119.40
1	A	514	U	N1-C2-O2	5.41	126.58	122.80
1	A	922	G	C5-C6-O6	-5.41	125.36	128.60
1	A	1473	C	N1-C2-O2	-5.40	115.66	118.90
1	A	213	C	C6-N1-C2	5.39	122.46	120.30
1	A	1206	A	C8-N9-C4	-5.39	103.64	105.80
1	A	736	A	C6-N1-C2	-5.39	115.37	118.60
1	A	835	G	N9-C4-C5	-5.39	103.24	105.40
1	A	1202	G	N1-C6-O6	5.39	123.13	119.90
1	A	125	C	C6-N1-C2	-5.38	118.15	120.30
1	A	674	G	N3-C4-C5	5.38	131.29	128.60
1	A	1050	G	O5'-P-OP2	-5.38	100.86	105.70
1	A	1479	A	C5-C6-N6	-5.38	119.40	123.70
1	A	669	U	OP1-P-OP2	5.37	127.65	119.60
1	A	862	G	N1-C2-N3	5.36	127.12	123.90
1	A	1040	G	C5-N7-C8	5.36	106.98	104.30
1	A	7	G	C2-N3-C4	-5.35	109.23	111.90
1	A	1081	G	N9-C4-C5	5.35	107.54	105.40
1	A	360	U	N3-C4-O4	5.35	123.14	119.40
1	A	553	G	C8-N9-C1'	-5.34	120.05	127.00
1	A	227	G	N9-C4-C5	-5.34	103.26	105.40
1	A	1423	G	C6-C5-N7	-5.34	127.19	130.40
1	A	1232	A	C4-C5-C6	5.34	119.67	117.00
1	A	110	G	N1-C2-N3	5.34	127.10	123.90
1	A	553	G	C4-C5-C6	5.34	122.00	118.80
1	A	1260	A	C5-N7-C8	-5.33	101.23	103.90
1	A	922	G	C5-N7-C8	-5.33	101.63	104.30
1	A	1166	G	N1-C6-O6	5.33	123.10	119.90
1	A	835	G	C8-N9-C4	-5.33	104.27	106.40
1	A	970	G	C8-N9-C1'	-5.33	120.07	127.00
1	A	191	G	N9-C4-C5	-5.33	103.27	105.40
1	A	698	A	N1-C2-N3	5.33	131.96	129.30
1	A	1423	G	C5-C6-N1	-5.33	108.83	111.50
1	A	1065	U	N3-C4-O4	5.33	123.13	119.40
1	A	1495	A	C2-N3-C4	-5.33	107.94	110.60
1	A	468	G	P-O3'-C3'	5.33	126.09	119.70
1	A	99	C	C6-N1-C2	5.32	122.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1050	G	C4-C5-N7	5.32	112.93	110.80
1	A	1286	G	C2-N3-C4	-5.32	109.24	111.90
1	A	360	U	N3-C2-O2	5.32	125.92	122.20
1	A	1280	A	N9-C1'-C2'	5.32	120.92	114.00
1	A	539	C	C5-C6-N1	-5.32	118.34	121.00
1	A	731	C	N3-C4-C5	5.32	124.03	121.90
1	A	1504	C	C2-N3-C4	-5.31	117.24	119.90
1	A	583	C	C6-N1-C1'	-5.31	114.43	120.80
1	A	773	A	C8-N9-C4	5.31	107.92	105.80
1	A	1184	C	C4-C5-C6	5.31	120.05	117.40
1	A	862	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1033	C	N3-C4-C5	-5.30	119.78	121.90
1	A	177	G	N7-C8-N9	5.30	115.75	113.10
1	A	326	G	C5-N7-C8	-5.30	101.65	104.30
1	A	578	G	C6-C5-N7	-5.30	127.22	130.40
1	A	1222	G	N1-C6-O6	5.30	123.08	119.90
1	A	417	C	P-O3'-C3'	5.30	126.06	119.70
1	A	674	G	OP2-P-O3'	5.30	116.86	105.20
1	A	957	C	N1-C2-O2	5.30	122.08	118.90
1	A	558	G	N3-C4-N9	5.30	129.18	126.00
1	A	863	G	C8-N9-C1'	-5.30	120.11	127.00
1	A	896	A	C2-N3-C4	-5.30	107.95	110.60
1	A	897	U	N3-C4-C5	-5.30	111.42	114.60
1	A	392	A	C8-N9-C4	-5.29	103.68	105.80
1	A	420	G	C6-C5-N7	5.29	133.57	130.40
1	A	1057	C	C5-C4-N4	-5.29	116.50	120.20
1	A	546	A	N1-C6-N6	-5.29	115.43	118.60
1	A	917	C	C6-N1-C2	5.29	122.42	120.30
1	A	46	G	N3-C2-N2	-5.29	116.20	119.90
1	A	1425	G	C2-N3-C4	5.29	114.54	111.90
1	A	1367	G	N1-C6-O6	5.28	123.07	119.90
1	A	818	U	C5-C4-O4	-5.28	122.73	125.90
1	A	687	A	C8-N9-C4	5.28	107.91	105.80
1	A	1178	G	C6-C5-N7	-5.28	127.23	130.40
1	A	343	G	N1-C2-N3	-5.27	120.74	123.90
1	A	794	C	C5-C4-N4	-5.27	116.51	120.20
20	T	84	LEU	CA-CB-CG	5.27	127.43	115.30
1	A	601	C	O5'-P-OP2	-5.27	100.96	105.70
1	A	924	G	N3-C4-N9	5.27	129.16	126.00
1	A	1285	G	C6-C5-N7	-5.27	127.24	130.40
1	A	284	G	C5-N7-C8	-5.27	101.67	104.30
1	A	1177	U	C6-N1-C2	-5.27	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1424	G	N9-C4-C5	-5.26	103.29	105.40
1	A	862	G	C2-N3-C4	-5.26	109.27	111.90
1	A	864	G	N7-C8-N9	-5.26	110.47	113.10
1	A	1217	A	N7-C8-N9	5.26	116.43	113.80
1	A	1285	G	C5-C6-N1	-5.26	108.87	111.50
1	A	674	G	N3-C4-N9	-5.26	122.85	126.00
1	A	743	G	C5-N7-C8	5.26	106.93	104.30
1	A	139	G	C6-C5-N7	-5.25	127.25	130.40
1	A	243	C	C5-C6-N1	-5.25	118.37	121.00
1	A	1479	A	OP1-P-O3'	5.25	116.74	105.20
1	A	112	A	N1-C2-N3	5.24	131.92	129.30
1	A	780	C	OP1-P-OP2	5.23	127.44	119.60
1	A	1331	A	N1-C6-N6	-5.23	115.46	118.60
1	A	839	C	C5-C6-N1	-5.22	118.39	121.00
1	A	1209	C	N3-C2-O2	-5.22	118.24	121.90
1	A	1216	U	C5-C6-N1	-5.22	120.09	122.70
1	A	241	A	O5'-P-OP2	-5.22	101.00	105.70
1	A	1210	A	C8-N9-C4	-5.21	103.72	105.80
1	A	1272	G	O5'-P-OP2	-5.21	101.01	105.70
1	A	468	G	C8-N9-C1'	-5.21	120.23	127.00
1	A	792	G	C8-N9-C4	5.21	108.48	106.40
1	A	1339	U	C5-C6-N1	-5.21	120.10	122.70
1	A	743	G	N7-C8-N9	-5.21	110.50	113.10
1	A	284	G	C5-C6-O6	-5.20	125.48	128.60
1	A	488	G	OP1-P-OP2	5.20	127.40	119.60
1	A	1223	C	N3-C4-C5	5.20	123.98	121.90
12	L	92	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	76	G	OP1-P-OP2	-5.20	111.81	119.60
1	A	784	U	O5'-P-OP2	5.20	116.94	110.70
1	A	1232	A	N3-C4-C5	-5.20	123.16	126.80
1	A	1378	A	C6-N1-C2	-5.19	115.48	118.60
1	A	572	C	OP2-P-O3'	5.19	116.62	105.20
1	A	921	G	C5-C6-N1	-5.19	108.91	111.50
1	A	862	G	N1-C6-O6	5.19	123.01	119.90
1	A	1386	C	N3-C4-C5	5.19	123.97	121.90
1	A	32	A	O5'-P-OP1	5.19	116.92	110.70
1	A	316	A	OP2-P-O3'	5.18	116.61	105.20
1	A	564	G	C4-C5-C6	5.18	121.91	118.80
8	H	127	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	51	A	C5-N7-C8	-5.18	101.31	103.90
1	A	952	A	C5-C6-N1	-5.18	115.11	117.70
1	A	286	C	C5-C6-N1	-5.17	118.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	812	G	N3-C4-C5	5.17	131.19	128.60
1	A	1035	G	C6-C5-N7	5.17	133.50	130.40
1	A	1397	G	C6-C5-N7	-5.17	127.30	130.40
1	A	546	A	O5'-P-OP2	-5.16	101.05	105.70
1	A	190	G	C8-N9-C4	-5.16	104.34	106.40
1	A	7	G	N9-C4-C5	-5.16	103.34	105.40
1	A	304	G	N1-C6-O6	5.16	122.99	119.90
1	A	803	U	C6-N1-C1'	5.15	128.41	121.20
1	A	1497	G	N3-C4-N9	5.15	129.09	126.00
1	A	881	C	N3-C4-N4	-5.15	114.39	118.00
1	A	115	G	C5-C6-N1	-5.15	108.93	111.50
1	A	367	C	C5-C4-N4	-5.15	116.60	120.20
1	A	897	U	C4-C5-C6	5.15	122.79	119.70
1	A	853	G	C4-C5-N7	5.15	112.86	110.80
1	A	883	G	C4-C5-N7	5.15	112.86	110.80
7	G	12	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	741	G	C4-C5-N7	5.14	112.86	110.80
1	A	821	G	C5-C6-N1	-5.14	108.93	111.50
1	A	233	G	N1-C6-O6	-5.14	116.81	119.90
1	A	294	G	C5-C6-O6	5.14	131.69	128.60
1	A	1247	G	C4-C5-C6	-5.14	115.72	118.80
1	A	1487	U	N1-C2-N3	-5.14	111.82	114.90
1	A	840	U	C2-N3-C4	-5.13	123.92	127.00
1	A	120	G	C8-N9-C4	5.13	108.45	106.40
1	A	71	C	C6-N1-C2	5.13	122.35	120.30
1	A	250	G	N9-C4-C5	-5.13	103.35	105.40
1	A	891	A	C8-N9-C4	-5.13	103.75	105.80
1	A	275	C	N3-C4-C5	5.13	123.95	121.90
1	A	711	A	N7-C8-N9	5.13	116.36	113.80
1	A	1208	A	C5-N7-C8	-5.13	101.34	103.90
1	A	1483	U	OP1-P-O3'	5.13	116.48	105.20
1	A	362	U	OP2-P-O3'	5.13	116.48	105.20
1	A	797	A	C8-N9-C4	5.13	107.85	105.80
1	A	1375	U	OP1-P-OP2	5.13	127.29	119.60
1	A	124	A	O5'-P-OP1	-5.12	101.09	105.70
1	A	272	C	N3-C4-C5	5.12	123.95	121.90
1	A	637	G	C8-N9-C4	-5.12	104.35	106.40
1	A	1177	U	N3-C4-C5	-5.12	111.53	114.60
1	A	853	G	C5-N7-C8	-5.12	101.74	104.30
1	A	1171	G	N3-C4-N9	-5.12	122.93	126.00
1	A	636	A	N9-C4-C5	5.12	107.85	105.80
1	A	953	G	C8-N9-C4	5.12	108.45	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1216	U	C4-C5-C6	5.12	122.77	119.70
1	A	898	U	O5'-P-OP2	-5.11	101.10	105.70
1	A	5	U	C2-N1-C1'	5.11	123.83	117.70
1	A	1398	G	C2-N3-C4	-5.11	109.35	111.90
1	A	1486	C	C2-N3-C4	-5.11	117.35	119.90
8	H	91	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	572	C	C2-N1-C1'	-5.10	113.19	118.80
1	A	284	G	C4-C5-N7	5.10	112.84	110.80
1	A	1035	G	OP1-P-O3'	-5.10	93.99	105.20
1	A	1036	C	N1-C2-O2	5.09	121.96	118.90
1	A	1500	G	N1-C6-O6	5.09	122.96	119.90
1	A	881	C	C6-N1-C2	5.09	122.34	120.30
1	A	1507	G	N1-C6-O6	5.09	122.95	119.90
1	A	51	A	N1-C6-N6	5.09	121.65	118.60
1	A	177	G	C8-N9-C4	-5.09	104.36	106.40
1	A	1181	C	C5-C6-N1	5.09	123.55	121.00
1	A	1328	G	OP2-P-O3'	5.09	116.39	105.20
1	A	578	G	C4-C5-C6	5.08	121.85	118.80
1	A	1040	G	N7-C8-N9	-5.08	110.56	113.10
1	A	1081	G	N3-C4-N9	-5.08	122.95	126.00
1	A	1181	C	C2-N1-C1'	5.08	124.39	118.80
1	A	669	U	O5'-P-OP1	-5.08	101.13	105.70
1	A	908	C	C2-N3-C4	-5.08	117.36	119.90
1	A	1424	G	C6-C5-N7	-5.08	127.35	130.40
1	A	886	A	C5-N7-C8	-5.08	101.36	103.90
1	A	970	G	N9-C4-C5	-5.08	103.37	105.40
1	A	340	C	P-O3'-C3'	5.07	125.79	119.70
1	A	367	C	N3-C4-N4	5.07	121.55	118.00
1	A	590	A	C6-N1-C2	5.07	121.64	118.60
1	A	604	A	O5'-P-OP2	5.07	116.79	110.70
1	A	653	G	C8-N9-C4	5.07	108.43	106.40
1	A	1280	A	C5-C6-N1	-5.07	115.16	117.70
1	A	1497	G	N1-C2-N3	5.07	126.94	123.90
1	A	588	U	N3-C4-C5	-5.07	111.56	114.60
1	A	766	C	C5-C6-N1	-5.07	118.47	121.00
1	A	1065	U	N1-C2-O2	-5.07	119.25	122.80
1	A	1398	G	C6-C5-N7	-5.07	127.36	130.40
1	A	1463	G	N1-C6-O6	5.07	122.94	119.90
1	A	588	U	C4-C5-C6	5.06	122.74	119.70
1	A	546	A	N7-C8-N9	-5.06	111.27	113.80
1	A	101	G	C5'-C4'-O4'	5.06	115.17	109.10
1	A	1171	G	OP2-P-O3'	5.06	116.33	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1497	G	N3-C4-C5	-5.06	126.07	128.60
1	A	1099	G	C4-C5-N7	5.06	112.82	110.80
1	A	1195	C	C6-N1-C1'	-5.05	114.73	120.80
1	A	1497	G	C4-N9-C1'	5.05	133.07	126.50
1	A	735	G	N7-C8-N9	-5.05	110.58	113.10
1	A	1280	A	N1-C6-N6	5.05	121.63	118.60
1	A	1487	U	C5-C6-N1	-5.05	120.17	122.70
1	A	13	U	OP2-P-O3'	5.05	116.30	105.20
1	A	308	A	N3-C4-C5	5.05	130.33	126.80
1	A	670	A	P-O3'-C3'	5.04	125.75	119.70
1	A	99	C	OP1-P-O3'	-5.04	94.11	105.20
1	A	749	A	C2-N3-C4	-5.04	108.08	110.60
1	A	756	G	C8-N9-C4	-5.04	104.38	106.40
1	A	960	A	C8-N9-C4	-5.04	103.78	105.80
17	Q	98	LEU	CB-CG-CD2	5.04	119.57	111.00
1	A	511	C	OP2-P-O3'	5.03	116.27	105.20
1	A	798	A	N1-C6-N6	5.03	121.62	118.60
1	A	799	A	N3-C4-C5	5.03	130.32	126.80
1	A	1385	C	OP2-P-O3'	5.03	116.26	105.20
1	A	272	C	C6-N1-C2	5.03	122.31	120.30
1	A	558	G	N7-C8-N9	-5.03	110.59	113.10
1	A	1158	G	N1-C6-O6	5.02	122.91	119.90
1	A	1178	G	OP1-P-O3'	5.02	116.25	105.20
1	A	1480	A	OP2-P-O3'	5.01	116.23	105.20
1	A	189	U	OP1-P-O3'	5.01	116.23	105.20
1	A	899	G	O5'-P-OP2	-5.01	101.19	105.70
1	A	327	G	OP1-P-O3'	-5.01	94.18	105.20
1	A	562	G	N1-C6-O6	5.01	122.91	119.90
1	A	343	G	C4-C5-N7	5.00	112.80	110.80
1	A	742	A	C6-N1-C2	-5.00	115.60	118.60
1	A	969	U	P-O3'-C3'	5.00	125.70	119.70
1	A	1497	G	C8-N9-C1'	-5.00	120.50	127.00
15	O	70	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	THR	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
9	I	117	HIS	Peptide

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Mol	Chain	Res	Type	Group
12	L	14	GLY	Peptide
14	N	7	ILE	Peptide
17	Q	66	SER	Peptide
18	R	46	GLU	Peptide
19	S	53	ASN	Peptide
20	T	11	SER	Peptide

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	A	32415	0	16360	502	0
2	B	1900	0	1951	89	0
3	C	1612	0	1677	90	0
4	D	1703	0	1763	60	0
5	E	1146	0	1207	35	0
6	F	843	0	857	34	0
7	G	1257	0	1296	42	0
8	H	1116	0	1177	40	0
9	I	1010	0	1037	42	0
10	J	794	0	840	51	1
11	K	885	0	904	33	0
12	L	970	0	1057	39	0
13	M	997	0	1072	41	0
14	N	492	0	529	31	0
15	O	734	0	771	29	0
16	P	700	0	720	25	0
17	Q	857	0	928	39	0
18	R	598	0	670	31	0
19	S	647	0	673	43	0
20	T	763	0	860	32	0
21	V	208	0	221	6	0
22	W	82	0	46	0	0
23	X	232	0	121	6	0
24	A	42	0	45	1	0
25	A	98	0	0	0	0
25	E	1	0	0	0	0
25	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	1	0	0	0	0
25	X	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
All	All	52108	0	36782	1183	1

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 14.

All (1183) 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)
18:R:54:ARG:HH12	18:R:55:ARG:CG	1.67	1.07
2:B:178:ARG:HH21	2:B:196:LEU:C	1.56	1.06
18:R:54:ARG:NH1	18:R:55:ARG:HG2	1.70	1.05
2:B:178:ARG:NH2	2:B:196:LEU:O	1.88	1.05
3:C:107:GLN:OE1	3:C:108:ASN:HB2	1.55	1.04
1:A:1110:C:H4'	9:I:16:ARG:HH22	1.30	0.97
1:A:1202:G:OP2	19:S:37:ARG:NH2	1.97	0.97
19:S:33:THR:HG22	19:S:35:SER:H	1.30	0.95
1:A:530:A:OP2	4:D:3:ARG:NH1	2.02	0.93
1:A:1258:C:HO2'	1:A:1260:A:H8	1.17	0.92
1:A:1300:A:OP1	19:S:5:LEU:HD11	1.68	0.92
18:R:54:ARG:HH12	18:R:55:ARG:HG3	1.32	0.92
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.51	0.91
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.53	0.89
1:A:1093:A:N1	3:C:177:THR:HG22	1.86	0.89
18:R:54:ARG:NH1	18:R:55:ARG:CG	2.29	0.89
2:B:32:ILE:HD12	2:B:40:HIS:HB3	1.53	0.89
8:H:121:ASP:HB2	8:H:125:ARG:HH21	1.38	0.89
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.37	0.89
1:A:653:G:H21	6:F:73:ASN:HD21	1.18	0.86
1:A:1479:A:H2	1:A:1482:G:H1	1.23	0.86
1:A:969:U:H3	1:A:1026:A:H62	1.20	0.85
12:L:89:ARG:HE	12:L:97:ARG:HG2	1.42	0.85
1:A:564:G:C6	1:A:741:G:N7	2.45	0.85
1:A:1381:C:H4'	1:A:1382:C:H5"	1.59	0.85
2:B:54:THR:HG22	2:B:199:TYR:HB3	1.59	0.85
5:E:33:VAL:HG11	5:E:109:ILE:HG12	1.60	0.84
1:A:952:A:H5'	1:A:952:A:H8	1.42	0.83
4:D:71:SER:OG	4:D:72:GLU:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:C:H41	19:S:4:SER:HB3	1.44	0.82
10:J:6:ILE:HG22	10:J:98:ILE:HG22	1.60	0.82
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.62	0.82
1:A:1348:C:O2'	10:J:60:ARG:NH2	2.13	0.81
3:C:12:LEU:HD21	14:N:51:GLY:HA2	1.64	0.80
2:B:207:ALA:O	2:B:209:ARG:N	2.13	0.79
1:A:201:A:H4'	20:T:68:LYS:HE2	1.63	0.79
19:S:53:ASN:HB3	19:S:55:LYS:H	1.47	0.78
2:B:15:VAL:HG21	2:B:209:ARG:HB3	1.67	0.77
1:A:980:G:H22	1:A:1021:C:H1'	1.50	0.77
1:A:952:A:H4'	1:A:953:G:H5"	1.67	0.76
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.68	0.76
17:Q:104:LYS:HD2	17:Q:104:LYS:O	1.84	0.76
10:J:90:LEU:H	10:J:91:PRO:HD2	1.50	0.76
2:B:189:ASP:HB3	2:B:205:ASP:OD2	1.85	0.76
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.65	0.75
12:L:74:GLY:O	12:L:102:ARG:NH2	2.20	0.75
1:A:647:G:H22	1:A:724:G:H1	1.34	0.75
1:A:96:C:OP1	20:T:17:ARG:NH1	2.20	0.75
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.68	0.75
1:A:1118:U:H5"	1:A:1119:C:OP2	1.86	0.74
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.69	0.74
15:O:87:ILE:HG22	15:O:88:ARG:H	1.52	0.74
3:C:143:GLU:O	3:C:145:GLY:N	2.21	0.74
2:B:174:VAL:O	2:B:178:ARG:HD3	1.87	0.73
7:G:136:LYS:O	7:G:138:LYS:N	2.21	0.73
2:B:32:ILE:CD1	2:B:40:HIS:HB3	2.18	0.73
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.68	0.73
4:D:70:ILE:HD11	4:D:100:ARG:HD2	1.69	0.73
1:A:992:A:H4'	19:S:14:HIS:NE2	2.03	0.73
11:K:22:HIS:HB3	11:K:29:ILE:HG23	1.71	0.73
1:A:1106:G:HO2'	1:A:1127:C:N4	1.87	0.73
18:R:54:ARG:CZ	18:R:55:ARG:HG2	2.18	0.73
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.22	0.73
1:A:272:C:H5'	17:Q:68:ARG:HH12	1.53	0.73
16:P:22:THR:HA	16:P:33:ILE:HG13	1.71	0.73
1:A:905:G:O2'	1:A:1510:C:OP1	2.08	0.72
1:A:1106:G:O2'	1:A:1127:C:N4	2.23	0.72
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.72	0.72
11:K:124:LYS:HE3	11:K:125:PHE:CE1	2.24	0.72
2:B:73:THR:HB	2:B:170:GLU:OE2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LEU:HB2	2:B:142:LEU:HD13	1.72	0.72
6:F:100:ASN:ND2	18:R:26:LEU:O	2.23	0.72
3:C:6:HIS:HD2	3:C:8:ILE:H	1.33	0.72
5:E:10:MET:HA	5:E:32:VAL:HA	1.70	0.72
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.24	0.72
1:A:660:U:H3	1:A:696:G:H22	1.38	0.71
18:R:47:THR:HG22	18:R:48:GLY:H	1.55	0.71
1:A:503:A:OP2	12:L:51:ALA:HB1	1.91	0.71
3:C:93:LYS:HG3	3:C:94:LEU:HD23	1.71	0.71
8:H:116:LYS:HE3	8:H:127:LEU:HD12	1.71	0.71
2:B:178:ARG:NH2	2:B:196:LEU:C	2.38	0.71
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.73	0.71
1:A:818:U:OP1	18:R:64:ARG:NH2	2.25	0.70
1:A:923:A:H2'	1:A:924:G:C8	2.26	0.70
1:A:1487:U:H2'	1:A:1488:G:C8	2.26	0.70
11:K:127:LYS:O	11:K:129:SER:N	2.24	0.70
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.55	0.70
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.74	0.70
1:A:572:C:H42	1:A:633:G:H1	1.39	0.70
12:L:59:ARG:HG3	12:L:65:GLU:HG3	1.72	0.69
20:T:89:ARG:NH2	20:T:105:SER:O	2.23	0.69
1:A:1093:A:C6	3:C:177:THR:HG22	2.26	0.69
2:B:178:ARG:CZ	2:B:196:LEU:O	2.41	0.69
7:G:15:ASP:HB3	7:G:20:ASP:H	1.58	0.69
3:C:179:ARG:HD3	3:C:207:VAL:HG22	1.75	0.69
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.75	0.68
12:L:27:LEU:O	12:L:29:GLY:N	2.25	0.68
1:A:1093:A:H61	3:C:177:THR:HG22	1.57	0.68
10:J:57:LYS:O	10:J:60:ARG:NH1	2.25	0.68
6:F:49:ALA:N	18:R:77:GLY:O	2.22	0.68
4:D:145:GLU:HB2	4:D:184:LYS:HE2	1.76	0.68
8:H:25:ASP:OD1	8:H:60:ARG:NE	2.21	0.68
1:A:1047:U:OP2	1:A:1171:G:N2	2.27	0.68
10:J:50:ILE:HD12	10:J:50:ILE:H	1.58	0.68
3:C:33:LEU:HD21	14:N:53:LEU:CD2	2.23	0.68
1:A:1093:A:N6	3:C:177:THR:HG22	2.09	0.68
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.07	0.68
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.25	0.67
1:A:642:U:OP2	15:O:8:LYS:NZ	2.27	0.67
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.76	0.67
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:ARG:HH11	2:B:145:LEU:HD21	1.58	0.67
3:C:179:ARG:NH1	3:C:206:GLU:OE1	2.28	0.67
1:A:952:A:N6	1:A:1348:C:O2'	2.28	0.67
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.26	0.67
1:A:294:G:H2'	1:A:295:A:C8	2.29	0.67
12:L:27:LEU:C	12:L:29:GLY:H	1.98	0.67
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.77	0.67
2:B:146:GLN:O	2:B:150:SER:OG	2.13	0.66
1:A:981:G:H2'	1:A:982:A:H4'	1.78	0.66
3:C:107:GLN:OE1	3:C:107:GLN:C	2.34	0.66
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.25	0.66
3:C:32:LEU:O	3:C:36:ASP:HB2	1.95	0.65
7:G:37:ASN:OD1	9:I:41:VAL:HG22	1.96	0.65
1:A:1046:G:H1'	1:A:1171:G:N2	2.12	0.65
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.78	0.65
12:L:110:VAL:H	12:L:122:THR:HG22	1.60	0.65
2:B:178:ARG:NE	2:B:196:LEU:O	2.30	0.65
9:I:32:ASP:OD1	9:I:33:PHE:N	2.29	0.65
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.79	0.65
12:L:71:PRO:O	12:L:102:ARG:NH1	2.29	0.65
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.65
1:A:778:C:H5"	1:A:779:C:OP2	1.97	0.65
1:A:1298:C:H5"	1:A:1299:A:OP2	1.97	0.65
1:A:1417:G:H2'	1:A:1418:U:C6	2.31	0.65
1:A:835:G:O6	1:A:846:G:C8	2.50	0.65
4:D:187:ARG:NH1	4:D:188:LEU:HB2	2.12	0.65
20:T:57:ARG:NE	20:T:102:GLY:HA3	2.12	0.65
1:A:9:G:OP2	5:E:121:LYS:NZ	2.20	0.65
2:B:223:ILE:HA	2:B:226:ARG:HB2	1.77	0.65
7:G:38:LEU:HA	7:G:41:ARG:HB3	1.78	0.65
1:A:963:A:H1'	19:S:54:GLY:O	1.97	0.64
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.79	0.64
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.79	0.64
1:A:521:G:H2'	1:A:522:A:C8	2.32	0.64
1:A:652:U:H2'	1:A:653:G:C8	2.32	0.64
8:H:35:ILE:HG23	8:H:111:ILE:HD13	1.79	0.64
10:J:65:LEU:HD13	14:N:56:VAL:HG22	1.79	0.64
3:C:154:SER:OG	3:C:155:GLY:N	2.28	0.64
16:P:10:GLY:HA3	16:P:14:ASN:O	1.98	0.64
19:S:53:ASN:HB2	19:S:56:GLN:O	1.98	0.64
1:A:1112:A:O2'	9:I:3:GLN:OE1	2.08	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:VAL:O	3:C:124:ILE:HG12	1.97	0.64
12:L:78:GLN:O	12:L:80:HIS:N	2.29	0.63
11:K:11:LYS:HG3	11:K:12:ARG:HH22	1.63	0.63
1:A:1295:C:H41	19:S:4:SER:CB	2.12	0.63
6:F:24:GLU:OE2	6:F:28:ARG:NH2	2.32	0.63
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.29	0.63
2:B:32:ILE:HD12	2:B:40:HIS:CB	2.28	0.63
11:K:11:LYS:HG3	11:K:12:ARG:NH2	2.13	0.63
1:A:1185:A:H5'	1:A:1186:U:OP2	1.99	0.63
1:A:520:G:H2'	1:A:521:G:H8	1.62	0.63
1:A:1093:A:N1	3:C:177:THR:CG2	2.60	0.63
1:A:1036:C:O2'	1:A:1037:A:P	2.56	0.62
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.79	0.62
20:T:33:ILE:HD13	20:T:63:ILE:HG12	1.81	0.62
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.32	0.62
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.10	0.62
1:A:338:U:O2'	1:A:341:G:O6	2.17	0.62
2:B:147:LYS:HD2	2:B:148:TYR:CE1	2.34	0.62
2:B:189:ASP:O	2:B:191:ASP:N	2.31	0.62
1:A:385:C:O3'	16:P:28:ARG:NH2	2.33	0.62
1:A:1294:U:O4	19:S:4:SER:OG	2.10	0.62
1:A:1183:G:H1'	14:N:29:ARG:HD3	1.80	0.62
4:D:145:GLU:OE2	4:D:182:LYS:HD2	1.99	0.62
10:J:48:THR:O	14:N:34:TYR:OH	2.18	0.62
18:R:54:ARG:NH1	18:R:55:ARG:HG3	2.08	0.62
4:D:187:ARG:HH12	4:D:188:LEU:HB2	1.65	0.62
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.33	0.62
1:A:608:G:H4'	16:P:16:HIS:CD2	2.35	0.61
1:A:1472:U:H2'	1:A:1473:C:H6	1.64	0.61
1:A:1334:G:OP1	21:V:10:ARG:NH2	2.32	0.61
6:F:23:LYS:HE3	6:F:42:GLU:OE2	2.00	0.61
4:D:160:GLN:HG3	4:D:161:ASN:HD22	1.64	0.61
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.83	0.61
1:A:520:G:H2'	1:A:521:G:C8	2.36	0.61
3:C:73:PRO:HG3	3:C:105:GLU:HG2	1.82	0.61
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.82	0.61
13:M:33:ALA:HA	13:M:59:TYR:HE2	1.66	0.61
20:T:59:ALA:O	20:T:63:ILE:HG13	2.01	0.61
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.83	0.61
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.82	0.61
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:74:LYS:HB3	20:T:75:ASN:OD1	2.01	0.61
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.83	0.60
12:L:40:VAL:HG21	12:L:77:LEU:O	1.99	0.60
1:A:1001:G:N7	1:A:1002:G:N2	2.49	0.60
1:A:1204:C:OP2	19:S:78:ARG:NH2	2.33	0.60
3:C:107:GLN:OE1	3:C:107:GLN:O	2.18	0.60
5:E:11:ILE:HD12	5:E:31:LEU:HD13	1.83	0.60
2:B:121:LEU:O	2:B:127:ILE:HG22	2.02	0.60
3:C:11:ARG:NH1	3:C:177:THR:O	2.35	0.60
4:D:63:LYS:O	4:D:67:ILE:HG13	2.01	0.60
20:T:82:SER:O	20:T:86:ARG:HG3	2.01	0.60
1:A:952:A:H5'	1:A:952:A:C8	2.31	0.60
1:A:376:C:H2'	1:A:377:A:O4'	2.00	0.60
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.83	0.60
1:A:8:A:N6	4:D:205:GLU:O	2.35	0.60
1:A:521:G:H2'	1:A:522:A:H8	1.66	0.60
1:A:1172:A:OP2	3:C:3:ASN:ND2	2.35	0.60
13:M:11:ARG:HG2	13:M:12:ASN:N	2.16	0.60
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.83	0.60
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	1.84	0.60
7:G:69:VAL:O	7:G:138:LYS:HG3	2.02	0.59
1:A:992:A:H4'	19:S:14:HIS:CE1	2.37	0.59
3:C:119:ARG:HG2	3:C:140:ARG:HH22	1.67	0.59
1:A:1042:C:HO2'	10:J:56:HIS:HD1	1.51	0.59
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.83	0.59
1:A:1337:G:H2'	1:A:1338:A:C8	2.38	0.59
1:A:1383:G:C2	1:A:1384:C:H1'	2.37	0.59
18:R:53:ARG:C	18:R:55:ARG:H	2.06	0.59
1:A:1472:U:H2'	1:A:1473:C:C6	2.37	0.59
4:D:38:TYR:HB2	4:D:44:GLY:O	2.02	0.59
12:L:89:ARG:NH2	12:L:97:ARG:HE	2.01	0.59
1:A:437:C:H2'	1:A:438:C:C6	2.38	0.59
3:C:33:LEU:CD2	14:N:53:LEU:HD22	2.33	0.59
1:A:257:A:H5'	20:T:74:LYS:HD3	1.84	0.59
1:A:1111:C:H5'	9:I:62:TYR:CZ	2.38	0.59
1:A:1431:A:OP2	1:A:1432:C:H5	1.85	0.59
6:F:44:GLY:O	6:F:60:PHE:N	2.31	0.59
1:A:155:A:H2'	1:A:156:A:C8	2.38	0.58
1:A:345:G:H8	1:A:345:G:H5"	1.68	0.58
1:A:1328:G:N2	1:A:1355:G:H2'	2.18	0.58
3:C:43:LEU:HD21	3:C:91:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LEU:HD13	14:N:56:VAL:CG2	2.34	0.58
17:Q:86:GLU:O	17:Q:90:ILE:HG13	2.02	0.58
2:B:19:HIS:CD2	2:B:204:ASN:HD21	2.21	0.58
3:C:131:ARG:NH1	5:E:50:GLU:HG2	2.19	0.58
16:P:51:VAL:O	16:P:52:ASP:HB3	2.04	0.58
1:A:175:G:H4'	1:A:176:U:C5'	2.34	0.58
1:A:1183:G:C1'	14:N:29:ARG:HD3	2.33	0.58
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.84	0.58
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.84	0.58
1:A:272:C:OP1	17:Q:68:ARG:NH2	2.37	0.58
1:A:721:C:OP2	6:F:92:LYS:NZ	2.30	0.58
1:A:979:G:H2'	1:A:980:G:C8	2.38	0.58
5:E:7:GLU:O	5:E:34:VAL:HA	2.03	0.58
1:A:437:C:H2'	1:A:438:C:H6	1.67	0.58
1:A:198:U:H4'	20:T:57:ARG:HD3	1.85	0.58
1:A:173:A:H2'	1:A:174:U:C6	2.39	0.58
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.38	0.58
1:A:1111:C:H5'	9:I:62:TYR:CE2	2.39	0.58
2:B:136:VAL:HA	2:B:139:LYS:HE2	1.85	0.58
1:A:444:G:H5"	1:A:445:A:H3'	1.86	0.57
1:A:1379:C:H4'	1:A:1380:A:OP2	2.03	0.57
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.04	0.57
1:A:1055:U:OP2	5:E:57:LYS:NZ	2.24	0.57
12:L:8:ASN:O	12:L:12:ARG:HG3	2.04	0.57
1:A:78:G:H5"	1:A:79:U:OP2	2.03	0.57
1:A:564:G:N1	1:A:741:G:C8	2.72	0.57
1:A:1479:A:H2	1:A:1482:G:N1	1.98	0.57
2:B:11:LEU:HD23	2:B:48:MET:HG3	1.85	0.57
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.19	0.57
1:A:264:C:H2'	1:A:265:A:C8	2.39	0.57
1:A:431:C:H2'	1:A:432:U:C6	2.39	0.57
1:A:1036:C:C6	23:X:34:I:H4'	2.40	0.57
4:D:102:ASP:OD1	4:D:103:ASN:N	2.38	0.57
13:M:49:THR:HG22	13:M:51:ALA:H	1.68	0.57
13:M:120:LYS:HD3	13:M:123:ALA:HB3	1.86	0.57
23:X:34:I:H2'	23:X:35:C:H6	1.69	0.57
1:A:35:G:H2'	1:A:36:C:C6	2.40	0.57
1:A:35:G:H2'	1:A:36:C:H6	1.69	0.57
1:A:249:G:OP1	17:Q:67:LYS:O	2.22	0.57
1:A:696:G:H2'	1:A:697:G:C8	2.40	0.57
1:A:719:C:OP2	18:R:68:LYS:NZ	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:G:N2	1:A:1171:G:O2'	2.38	0.57
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.86	0.57
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.05	0.57
11:K:79:SER:OG	11:K:106:LYS:HD2	2.05	0.57
13:M:24:GLY:O	13:M:29:ARG:NH1	2.35	0.57
1:A:238:A:H4'	1:A:239:U:H5"	1.86	0.56
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.40	0.56
1:A:816:U:H2'	1:A:817:C:C6	2.40	0.56
1:A:1021:C:H2'	1:A:1022:U:C6	2.40	0.56
12:L:33:ARG:HD2	12:L:62:SER:HB3	1.85	0.56
15:O:10:LYS:O	15:O:14:GLU:HB2	2.04	0.56
1:A:966:C:HO2'	1:A:995:G:HO2'	1.47	0.56
1:A:1109:G:N2	1:A:1128:A:H62	2.02	0.56
3:C:3:ASN:OD1	3:C:3:ASN:N	2.36	0.56
12:L:47:LYS:HB3	12:L:48:PRO:CD	2.29	0.56
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.21	0.56
15:O:6:GLU:O	15:O:10:LYS:HG3	2.05	0.56
16:P:11:SER:O	16:P:14:ASN:N	2.35	0.56
18:R:37:VAL:HG22	18:R:78:LEU:HB3	1.87	0.56
2:B:12:GLU:OE2	2:B:14:GLY:N	2.39	0.56
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.85	0.56
1:A:21:G:H2'	1:A:22:G:C8	2.40	0.56
1:A:1204:C:P	19:S:78:ARG:HH21	2.28	0.56
10:J:89:ASP:OD1	10:J:91:PRO:HD2	2.06	0.56
11:K:43:SER:HB3	11:K:68:ALA:HB2	1.88	0.56
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.40	0.56
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.05	0.56
1:A:450:C:H2'	1:A:451:C:H6	1.70	0.56
1:A:603:C:H2'	1:A:604:A:O4'	2.05	0.56
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.38	0.56
1:A:656:G:H2'	1:A:657:G:C8	2.41	0.56
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.86	0.56
11:K:33:THR:HG22	11:K:39:PRO:HA	1.87	0.56
1:A:175:G:H4'	1:A:176:U:H5'	1.88	0.56
1:A:652:U:H2'	1:A:653:G:H8	1.69	0.56
1:A:1456:C:H2'	1:A:1457:G:H8	1.70	0.56
4:D:152:SER:O	4:D:158:ILE:HD11	2.06	0.56
1:A:531:G:H2'	1:A:532:C:C6	2.41	0.55
1:A:653:G:N2	6:F:73:ASN:HD21	1.98	0.55
1:A:1297:G:H22	1:A:1300:A:H5"	1.69	0.55
1:A:1437:A:OP1	20:T:27:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:O	10:J:83:GLU:HG3	2.07	0.55
2:B:17:PHE:HB3	2:B:44:LEU:HD21	1.88	0.55
1:A:704:G:H4'	1:A:705:A:H5'	1.87	0.55
3:C:178:LEU:O	3:C:180:ALA:N	2.35	0.55
8:H:102:ARG:HE	8:H:125:ARG:NH1	2.05	0.55
11:K:121:PRO:HG2	11:K:126:ARG:HB3	1.89	0.55
5:E:43:LEU:HD11	5:E:132:ALA:HB1	1.87	0.55
1:A:525:G:OP1	4:D:10:ARG:NH2	2.34	0.55
1:A:1110:C:C4'	9:I:16:ARG:HH22	2.11	0.55
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.88	0.55
11:K:57:THR:HG23	11:K:60:ALA:H	1.71	0.55
1:A:575:G:H2'	1:A:576:G:H8	1.72	0.55
1:A:957:C:H5"	1:A:958:U:C5	2.42	0.55
16:P:8:ARG:HG2	16:P:17:TYR:CE1	2.42	0.55
3:C:43:LEU:O	3:C:47:LEU:HB2	2.07	0.55
3:C:157:ILE:HD13	3:C:166:GLU:HB2	1.89	0.55
5:E:101:ILE:O	5:E:120:THR:HB	2.06	0.55
10:J:50:ILE:H	10:J:50:ILE:CD1	2.18	0.55
2:B:229:VAL:HG12	2:B:230:VAL:O	2.06	0.54
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.90	0.54
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.89	0.54
10:J:90:LEU:H	10:J:91:PRO:CD	2.20	0.54
1:A:1224:C:OP1	21:V:10:ARG:HG3	2.06	0.54
3:C:6:HIS:CD2	3:C:8:ILE:H	2.21	0.54
23:X:34:I:H2'	23:X:35:C:C6	2.41	0.54
8:H:102:ARG:HG3	8:H:125:ARG:HH12	1.70	0.54
1:A:522:A:H2'	1:A:523:G:C8	2.42	0.54
1:A:1182:A:O2'	1:A:1183:G:OP2	2.24	0.54
3:C:119:ARG:HG2	3:C:140:ARG:NH2	2.22	0.54
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.89	0.54
8:H:86:ILE:HG21	8:H:133:LEU:HD22	1.90	0.54
1:A:748:G:N2	1:A:796:U:OP2	2.39	0.54
3:C:154:SER:O	3:C:165:THR:HA	2.08	0.54
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.54
3:C:64:VAL:HG21	3:C:95:THR:HG21	1.89	0.54
1:A:866:A:H4'	1:A:867:G:OP1	2.07	0.54
1:A:952:A:H62	10:J:60:ARG:HH21	1.56	0.54
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.89	0.54
16:P:39:TYR:CD2	16:P:73:LEU:HD11	2.43	0.54
1:A:824:U:H3'	1:A:825:C:O4'	2.07	0.54
1:A:842:A:O2'	1:A:843:C:H5'	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:G:O2'	1:A:1036:C:OP2	2.19	0.54
1:A:1110:C:H42	1:A:1125:G:H1	1.54	0.54
1:A:238:A:C2	1:A:241:A:C8	2.96	0.54
1:A:271:G:O2'	17:Q:68:ARG:NH1	2.41	0.54
1:A:1004:G:H5'	1:A:1005:C:OP2	2.07	0.54
1:A:935:A:N3	1:A:962:C:O2'	2.37	0.54
1:A:984:C:OP2	1:A:1020:C:O2'	2.20	0.54
1:A:1036:C:O2'	1:A:1037:A:O5'	2.26	0.54
1:A:275:C:O2	17:Q:38:ARG:HG3	2.08	0.53
1:A:502:C:H2'	1:A:503:A:C8	2.43	0.53
1:A:1249:A:N3	1:A:1307:C:O2'	2.40	0.53
2:B:18:GLY:HA3	2:B:41:ILE:HD13	1.90	0.53
11:K:19:ALA:HB2	11:K:80:VAL:HG11	1.90	0.53
1:A:7:G:O2'	5:E:120:THR:O	2.26	0.53
1:A:647:G:OP1	18:R:64:ARG:NH1	2.35	0.53
3:C:72:LYS:O	3:C:74:GLY:N	2.42	0.53
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.43	0.53
1:A:525:G:P	4:D:10:ARG:HH22	2.30	0.53
1:A:944:C:O3'	9:I:128:ARG:NH2	2.41	0.53
1:A:1374:G:H21	1:A:1479:A:H8	1.57	0.53
1:A:854:C:H5"	8:H:88:LYS:HD3	1.90	0.53
1:A:1237:A:H5'	1:A:1239:G:H1'	1.90	0.53
7:G:78:ARG:HB2	7:G:156:TRP:CH2	2.44	0.53
1:A:417:C:O2	1:A:418:G:N2	2.42	0.53
1:A:1076:G:O2'	1:A:1077:U:OP2	2.21	0.53
2:B:60:ASP:O	2:B:64:ARG:HD2	2.08	0.53
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.91	0.53
3:C:156:ARG:HH21	3:C:161:GLU:HA	1.74	0.53
12:L:89:ARG:HH21	12:L:97:ARG:HE	1.57	0.53
12:L:89:ARG:NE	12:L:97:ARG:HG2	2.19	0.53
13:M:6:GLY:O	13:M:8:GLU:N	2.40	0.53
5:E:116:THR:HG23	5:E:117:ASP:OD2	2.09	0.53
16:P:45:THR:HB	16:P:46:PRO:HD2	1.89	0.53
1:A:147:C:H42	1:A:162:G:H1	1.57	0.53
1:A:353:U:H2'	1:A:354:U:C6	2.44	0.53
2:B:84:GLU:OE1	2:B:216:SER:HA	2.09	0.53
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.24	0.53
7:G:121:ALA:O	7:G:125:MET:HG3	2.09	0.53
7:G:151:TYR:OH	11:K:54:ARG:HD3	2.08	0.53
4:D:148:VAL:HG11	4:D:158:ILE:HD12	1.90	0.52
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:C:H2'	1:A:473:C:H6	1.75	0.52
7:G:38:LEU:O	7:G:42:ILE:HG13	2.10	0.52
10:J:46:ARG:NH1	10:J:64:GLU:HB3	2.24	0.52
3:C:64:VAL:HG12	3:C:65:ALA:H	1.75	0.52
1:A:17:U:H1'	1:A:1062:A:N3	2.25	0.52
1:A:1407:U:H2'	1:A:1408:C:C6	2.45	0.52
11:K:126:ARG:O	11:K:129:SER:OXT	2.28	0.52
1:A:427:A:OP2	1:A:428:C:N4	2.39	0.52
6:F:21:LEU:O	6:F:25:ILE:HG13	2.09	0.52
1:A:358:A:C5	12:L:30:ALA:HB1	2.45	0.52
1:A:1480:A:H5'	1:A:1508:A:O4'	2.09	0.52
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.09	0.52
20:T:70:SER:HA	20:T:73:HIS:ND1	2.25	0.52
1:A:1039:G:H2'	1:A:1040:G:O4'	2.10	0.52
1:A:1123:C:H2'	1:A:1124:G:C8	2.45	0.52
1:A:1222:G:H2'	1:A:1223:C:C6	2.44	0.52
1:A:50:A:O5'	1:A:50:A:H8	1.92	0.52
19:S:11:VAL:HG22	19:S:39:THR:HB	1.91	0.52
1:A:75:G:O2'	1:A:76:G:H5'	2.10	0.51
1:A:156:A:C5	1:A:157:C:H1'	2.45	0.51
1:A:412:C:H2'	1:A:413:C:H6	1.75	0.51
8:H:39:LEU:CD1	8:H:111:ILE:HD11	2.40	0.51
13:M:84:ILE:HG13	13:M:86:CYS:H	1.76	0.51
17:Q:65:ILE:HD12	17:Q:65:ILE:N	2.25	0.51
1:A:616:G:H2'	1:A:617:C:C6	2.45	0.51
1:A:1159:G:N7	9:I:97:LYS:NZ	2.57	0.51
4:D:196:LEU:HD23	4:D:197:PRO:HD2	1.92	0.51
1:A:528:C:OP2	4:D:65:ARG:NH1	2.37	0.51
1:A:808:G:N2	8:H:11:THR:HG21	2.26	0.51
1:A:1277:C:H4'	1:A:1283:U:C5	2.45	0.51
1:A:1297:G:H5'	14:N:17:LYS:HE2	1.90	0.51
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.92	0.51
13:M:15:VAL:O	13:M:19:LEU:HG	2.10	0.51
17:Q:66:SER:O	17:Q:70:ARG:NH2	2.44	0.51
1:A:398:C:O3'	4:D:122:ARG:HD2	2.10	0.51
9:I:25:LYS:N	9:I:60:ASP:OD1	2.43	0.51
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.46	0.51
18:R:47:THR:HG22	18:R:48:GLY:N	2.25	0.51
1:A:738:G:OP2	15:O:65:ARG:HD2	2.10	0.51
6:F:10:LEU:N	6:F:59:TYR:O	2.41	0.51
13:M:73:GLU:O	13:M:77:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:42:PRO:O	19:S:45:VAL:HG23	2.10	0.51
1:A:922:G:C2	1:A:923:A:C8	2.99	0.51
3:C:91:LEU:HB2	3:C:99:VAL:HG21	1.93	0.51
8:H:124:ALA:HB1	8:H:129:VAL:O	2.10	0.51
10:J:38:ILE:HB	10:J:71:LEU:CB	2.41	0.51
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.43	0.51
3:C:68:VAL:HG12	3:C:70:VAL:HG13	1.93	0.51
6:F:50:TYR:CE2	18:R:77:GLY:HA2	2.46	0.51
9:I:70:LYS:O	9:I:74:ILE:HG13	2.11	0.51
1:A:648:A:H1'	1:A:716:A:O4'	2.11	0.51
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.92	0.51
3:C:34:LEU:HD22	14:N:25:VAL:HG21	1.92	0.51
1:A:1036:C:O2'	1:A:1037:A:OP2	2.29	0.51
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.46	0.51
1:A:472:C:H2'	1:A:473:C:C6	2.45	0.50
1:A:531:G:H2'	1:A:532:C:H6	1.75	0.50
1:A:904:G:H4'	1:A:1480:A:N7	2.26	0.50
1:A:1036:C:C6	23:X:34:I:H5"	2.46	0.50
11:K:110:ASP:HB2	18:R:88:LYS:HG3	1.92	0.50
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.93	0.50
1:A:1267:A:H2'	1:A:1268:A:H4'	1.92	0.50
4:D:35:ARG:O	4:D:36:ARG:HB2	2.11	0.50
19:S:32:LYS:HD2	19:S:57:HIS:CD2	2.46	0.50
1:A:1425:G:H2'	1:A:1425:G:N3	2.25	0.50
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.92	0.50
6:F:6:VAL:HG22	6:F:90:VAL:HG22	1.93	0.50
1:A:1210:A:OP2	13:M:114:ARG:HD3	2.11	0.50
3:C:179:ARG:HG2	3:C:207:VAL:HA	1.93	0.50
8:H:87:SER:HB2	8:H:93:VAL:HB	1.93	0.50
1:A:353:U:H2'	1:A:354:U:H6	1.76	0.50
1:A:411:G:C5	1:A:412:C:C4	3.00	0.50
1:A:981:G:C8	1:A:981:G:OP2	2.64	0.50
1:A:1088:G:H5"	3:C:172:ARG:HG2	1.94	0.50
2:B:54:THR:O	2:B:58:ILE:HG13	2.12	0.50
11:K:79:SER:HA	11:K:104:GLN:HB2	1.94	0.50
1:A:1394:C:H2'	1:A:1395:A:C8	2.47	0.50
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.77	0.50
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.94	0.50
1:A:123:G:N3	1:A:189:U:H3'	2.27	0.50
1:A:450:C:H2'	1:A:451:C:C6	2.46	0.50
1:A:1157:A:H3'	1:A:1158:G:C8	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:108:LEU:HD13	4:D:183:GLY:HA3	1.93	0.50
10:J:48:THR:OG1	10:J:62:HIS:ND1	2.41	0.50
13:M:4:ILE:HD12	13:M:56:LEU:HB3	1.93	0.50
2:B:103:THR:N	2:B:176:GLU:OE1	2.23	0.50
5:E:10:MET:HB2	5:E:32:VAL:HG23	1.94	0.50
17:Q:94:ASN:O	17:Q:96:GLU:N	2.44	0.50
20:T:99:LEU:C	20:T:101:GLY:N	2.64	0.50
1:A:542:A:OP1	5:E:126:ARG:NH2	2.45	0.49
1:A:564:G:C6	1:A:741:G:C8	3.00	0.49
1:A:1039:G:H5"	3:C:154:SER:CB	2.41	0.49
1:A:1111:C:H5'	9:I:62:TYR:OH	2.12	0.49
2:B:189:ASP:HB3	2:B:205:ASP:CG	2.32	0.49
2:B:195:ASP:O	8:H:68:ARG:NH2	2.44	0.49
19:S:12:ASP:HB2	19:S:38:SER:HB3	1.94	0.49
1:A:1083:A:H4'	1:A:1084:A:O5'	2.12	0.49
1:A:1112:A:O5'	1:A:1113:G:OP2	2.30	0.49
1:A:1381:C:C2	1:A:1383:G:C5	3.00	0.49
2:B:32:ILE:HD12	2:B:40:HIS:CG	2.47	0.49
3:C:135:LYS:HE2	5:E:50:GLU:OE2	2.12	0.49
6:F:45:LEU:HB3	6:F:59:TYR:HD1	1.77	0.49
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.48	0.49
20:T:99:LEU:O	20:T:101:GLY:N	2.45	0.49
9:I:106:ALA:O	9:I:108:VAL:HG13	2.12	0.49
13:M:29:ARG:HG2	13:M:64:TRP:CZ2	2.47	0.49
1:A:1288:U:H2'	1:A:1289:U:C6	2.48	0.49
1:A:1374:G:O2'	1:A:1375:U:H5'	2.13	0.49
1:A:1409:U:H2'	1:A:1410:A:H8	1.78	0.49
10:J:38:ILE:HB	10:J:71:LEU:HB2	1.93	0.49
18:R:17:SER:O	18:R:19:LYS:NZ	2.45	0.49
6:F:100:ASN:HB3	18:R:27:GLY:O	2.13	0.49
10:J:82:ILE:C	10:J:84:GLN:H	2.16	0.49
12:L:27:LEU:C	12:L:29:GLY:N	2.63	0.49
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.13	0.49
19:S:22:LEU:HD22	19:S:28:LYS:H	1.77	0.49
1:A:389:G:H2'	1:A:390:C:C6	2.48	0.49
1:A:982:A:O2'	1:A:1019:C:O2	2.13	0.49
3:C:8:ILE:HG12	3:C:16:ARG:CD	2.43	0.49
1:A:414:C:H5'	1:A:415:U:OP2	2.13	0.49
1:A:564:G:OP2	1:A:564:G:C8	2.66	0.49
1:A:1362:U:C2	7:G:3:ARG:NH1	2.81	0.49
24:A:1601:PAR:N24	24:A:1601:PAR:O44	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:60:GLU:HG3	4:D:198:VAL:HG23	1.93	0.49
5:E:9:LYS:HB2	5:E:112:LEU:HD11	1.95	0.49
7:G:40:ALA:O	7:G:43:PHE:N	2.46	0.49
12:L:54:LYS:HD2	12:L:54:LYS:N	2.27	0.49
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.95	0.49
19:S:4:SER:O	19:S:5:LEU:HB2	2.13	0.49
1:A:108:G:H1'	1:A:109:A:N7	2.27	0.49
1:A:1373:U:H2'	1:A:1374:G:C8	2.48	0.49
1:A:1433:G:H2'	1:A:1434:G:O4'	2.13	0.49
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.43	0.49
14:N:47:LEU:HD12	14:N:52:GLN:HB2	1.95	0.49
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.95	0.49
1:A:952:A:H62	1:A:1348:C:HO2'	1.61	0.48
1:A:1232:A:H2'	1:A:1233:A:O4'	2.13	0.48
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.14	0.48
10:J:80:LYS:HB2	10:J:80:LYS:HE2	1.53	0.48
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.93	0.48
1:A:1085:C:C5'	2:B:98:LEU:HD13	2.43	0.48
1:A:1183:G:C4	14:N:42:ILE:HD13	2.48	0.48
19:S:12:ASP:OD2	19:S:35:SER:OG	2.31	0.48
1:A:409:A:OP2	1:A:423:G:N2	2.42	0.48
3:C:8:ILE:HG12	3:C:16:ARG:HD3	1.95	0.48
7:G:146:GLU:OE2	7:G:149:ARG:NH1	2.46	0.48
1:A:1042:C:C5	3:C:2:GLY:HA2	2.48	0.48
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.96	0.48
1:A:59:A:H2'	1:A:59:A:N3	2.28	0.48
1:A:145:A:H2'	1:A:146:A:O4'	2.14	0.48
1:A:160:G:H2'	1:A:161:G:H8	1.78	0.48
1:A:837:A:H2'	1:A:838:G:O4'	2.14	0.48
2:B:147:LYS:HD2	2:B:148:TYR:CZ	2.48	0.48
3:C:134:ILE:HG21	3:C:167:TRP:O	2.12	0.48
1:A:530:A:H4'	1:A:531:G:H5'	1.95	0.48
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.47	0.48
1:A:648:A:N3	1:A:715:C:H2'	2.29	0.48
1:A:1319:G:C6	1:A:1320:A:C6	3.02	0.48
10:J:78:ASN:O	10:J:82:ILE:HG13	2.12	0.48
11:K:93:GLN:HA	11:K:96:ARG:HD2	1.96	0.48
15:O:3:ILE:HG13	15:O:3:ILE:O	2.14	0.48
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.13	0.48
1:A:1175:U:H2'	1:A:1176:C:H6	1.79	0.48
2:B:80:ILE:HD12	2:B:80:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:6:GLY:C	13:M:8:GLU:H	2.16	0.48
1:A:385:C:H2'	1:A:386:G:C8	2.49	0.48
1:A:613:G:H2'	1:A:614:G:O4'	2.14	0.48
1:A:954:A:N6	1:A:1205:G:O5'	2.47	0.48
1:A:1259:U:H5"	1:A:1260:A:O4'	2.14	0.48
1:A:1409:U:H2'	1:A:1410:A:C8	2.48	0.48
2:B:231:GLU:O	2:B:233:SER:N	2.47	0.48
13:M:49:THR:HB	13:M:52:GLU:HG3	1.96	0.48
13:M:81:LEU:H	13:M:81:LEU:HD23	1.78	0.48
19:S:6:LYS:HB2	19:S:7:LYS:HD3	1.94	0.48
1:A:1100:C:H1'	1:A:1160:A:C4	2.49	0.48
4:D:199:ASN:ND2	4:D:202:LEU:HG	2.29	0.48
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.95	0.48
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.14	0.48
13:M:3:ARG:N	13:M:9:ILE:HG22	2.29	0.48
1:A:409:A:P	1:A:423:G:H22	2.36	0.47
1:A:964:G:H1	1:A:1199:C:H42	1.60	0.47
2:B:103:THR:HG23	2:B:176:GLU:OE1	2.14	0.47
3:C:147:LYS:HE3	3:C:205:GLY:HA2	1.96	0.47
5:E:15:ARG:HD3	5:E:26:PHE:CG	2.48	0.47
17:Q:53:LEU:HD22	17:Q:85:VAL:HG11	1.96	0.47
19:S:71:LEU:HA	19:S:71:LEU:HD23	1.67	0.47
1:A:330:C:H2'	1:A:331:C:C6	2.49	0.47
1:A:483:G:C6	1:A:484:C:N4	2.83	0.47
1:A:1036:C:N1	23:X:34:I:H4'	2.29	0.47
1:A:1187:G:C6	1:A:1188:G:C5	3.02	0.47
7:G:45:ASP:O	7:G:49:ILE:HG13	2.14	0.47
7:G:138:LYS:H	7:G:140:ASP:H	1.62	0.47
1:A:399:U:H2'	1:A:400:U:H6	1.79	0.47
1:A:1036:C:C2'	1:A:1037:A:OP2	2.62	0.47
1:A:1042:C:C4	3:C:2:GLY:HA2	2.49	0.47
2:B:218:ALA:O	2:B:222:ILE:HG12	2.14	0.47
1:A:1056:G:O2'	1:A:1083:A:N1	2.39	0.47
6:F:91:VAL:HG12	6:F:92:LYS:O	2.15	0.47
15:O:3:ILE:HA	15:O:7:GLU:OE1	2.14	0.47
19:S:25:LYS:HG2	19:S:26:GLY:H	1.78	0.47
19:S:51:VAL:O	19:S:58:VAL:HG22	2.14	0.47
1:A:1207:C:H5"	13:M:103:THR:OG1	2.15	0.47
7:G:15:ASP:OD1	7:G:16:LEU:N	2.47	0.47
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.96	0.47
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:69:GLY:O	20:T:73:HIS:CE1	2.67	0.47
1:A:249:G:OP1	17:Q:68:ARG:HB2	2.14	0.47
3:C:60:ALA:O	3:C:62:ASP:N	2.47	0.47
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.50	0.47
11:K:97:ALA:O	11:K:101:SER:HB3	2.14	0.47
18:R:28:GLU:N	18:R:28:GLU:OE1	2.47	0.47
1:A:379:G:H2'	1:A:380:C:H6	1.80	0.47
1:A:732:C:H2'	1:A:733:G:H8	1.79	0.47
3:C:19:GLU:HB3	3:C:40:ARG:HH21	1.80	0.47
17:Q:67:LYS:O	17:Q:69:LYS:N	2.45	0.47
19:S:7:LYS:HD3	19:S:7:LYS:N	2.30	0.47
1:A:67:C:O2'	1:A:165:A:N3	2.38	0.47
1:A:149:C:H2'	1:A:150:G:O4'	2.14	0.47
1:A:823:C:H2'	1:A:823:C:OP2	2.14	0.47
1:A:957:C:H3'	1:A:958:U:H6	1.78	0.47
2:B:114:ARG:HH11	2:B:118:LEU:HD11	1.78	0.47
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.50	0.47
8:H:51:VAL:HG11	8:H:60:ARG:CZ	2.45	0.47
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.95	0.47
1:A:51:A:OP2	1:A:52:G:H5"	2.15	0.47
1:A:549:G:H4'	1:A:550:G:OP1	2.14	0.47
1:A:1212:G:C6	1:A:1213:U:C4	3.03	0.47
7:G:22:LEU:HD23	7:G:22:LEU:HA	1.78	0.47
9:I:50:LEU:HA	9:I:53:VAL:HG22	1.97	0.47
9:I:118:LYS:HB3	9:I:121:ARG:HB2	1.96	0.47
1:A:289:U:OP1	1:A:593:G:O2'	2.24	0.47
1:A:1111:C:H3'	1:A:1112:A:C5'	2.44	0.47
4:D:28:SER:C	4:D:30:LYS:H	2.18	0.47
7:G:65:ALA:O	7:G:69:VAL:HG23	2.15	0.47
11:K:57:THR:CG2	11:K:60:ALA:H	2.28	0.47
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.96	0.47
1:A:340:C:H4'	1:A:341:G:O5'	2.15	0.46
1:A:1039:G:H5"	3:C:154:SER:HB2	1.96	0.46
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.15	0.46
8:H:118:VAL:O	8:H:119:LEU:HD23	2.15	0.46
19:S:18:LYS:HB2	19:S:18:LYS:HE3	1.58	0.46
1:A:257:A:C6	1:A:258:A:C6	3.04	0.46
1:A:354:U:H2'	1:A:355:A:C8	2.50	0.46
1:A:487:C:C2	1:A:525:G:N2	2.83	0.46
1:A:521:G:OP2	12:L:115:LYS:HG3	2.15	0.46
1:A:983:A:H5'	1:A:984:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:HD13	2:B:201:ILE:HG23	1.98	0.46
1:A:981:G:OP2	1:A:981:G:H8	1.96	0.46
1:A:1106:G:H2'	1:A:1127:C:H5	1.80	0.46
1:A:1204:C:OP1	1:A:1205:G:H3'	2.16	0.46
4:D:13:ARG:HB3	4:D:38:TYR:O	2.15	0.46
4:D:79:PHE:HE1	4:D:204:ILE:HG12	1.80	0.46
7:G:80:VAL:HG23	7:G:83:ALA:H	1.81	0.46
17:Q:78:GLU:OE1	17:Q:81:ARG:HD2	2.15	0.46
1:A:252:G:H1	1:A:264:C:H42	1.62	0.46
1:A:278:C:C2	1:A:279:G:C8	3.02	0.46
1:A:1073:U:O2	1:A:1075:A:C8	2.69	0.46
1:A:1348:C:H2'	1:A:1349:C:C6	2.51	0.46
20:T:57:ARG:HH21	20:T:100:ILE:HG23	1.81	0.46
1:A:515:A:H61	3:C:193:TYR:CB	2.29	0.46
1:A:961:C:H2'	1:A:962:C:C6	2.51	0.46
1:A:1171:G:H5'	3:C:176:HIS:CE1	2.51	0.46
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.96	0.46
16:P:51:VAL:O	16:P:52:ASP:CB	2.64	0.46
19:S:53:ASN:CB	19:S:56:GLN:H	2.29	0.46
1:A:953:G:OP2	1:A:1339:U:O2'	2.29	0.46
2:B:215:LEU:O	2:B:219:VAL:HG23	2.15	0.46
3:C:150:LYS:HD3	3:C:152:ILE:HD11	1.97	0.46
4:D:196:LEU:HD23	4:D:196:LEU:HA	1.73	0.46
7:G:18:TYR:HB3	7:G:59:LEU:HD22	1.97	0.46
18:R:53:ARG:C	18:R:55:ARG:N	2.69	0.46
1:A:939:C:H2'	1:A:940:G:O4'	2.16	0.46
9:I:24:GLY:HA2	9:I:59:PHE:O	2.15	0.46
9:I:53:VAL:HB	9:I:92:TYR:CE2	2.51	0.46
13:M:6:GLY:O	13:M:7:VAL:HG22	2.16	0.46
17:Q:26:GLN:O	17:Q:27:PHE:HB3	2.15	0.46
1:A:64:G:H3'	1:A:64:G:OP1	2.14	0.46
1:A:96:C:P	20:T:17:ARG:NH1	2.89	0.46
1:A:1168:G:H5'	9:I:113:LYS:HE2	1.98	0.46
1:A:1374:G:N2	1:A:1479:A:H8	2.13	0.46
8:H:125:ARG:HE	8:H:125:ARG:HB2	1.47	0.46
15:O:88:ARG:HD2	15:O:88:ARG:HA	1.62	0.46
1:A:775:A:H1'	1:A:777:A:N7	2.31	0.46
4:D:18:LYS:HB3	4:D:20:TYR:CE1	2.51	0.46
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.37	0.46
7:G:22:LEU:HD21	7:G:97:GLN:OE1	2.16	0.46
8:H:33:GLU:HA	8:H:36:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:73:HIS:HB3	20:T:74:LYS:HG2	1.96	0.46
1:A:960:A:H2	1:A:961:C:C6	2.34	0.46
3:C:34:LEU:O	3:C:38:ARG:HG2	2.16	0.46
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.97	0.46
10:J:6:ILE:HD11	10:J:72:VAL:HG11	1.98	0.46
10:J:17:ASP:OD1	10:J:70:ARG:NE	2.41	0.46
12:L:41:ARG:HG2	12:L:42:THR:H	1.80	0.46
20:T:36:LEU:HD23	20:T:36:LEU:HA	1.62	0.46
20:T:63:ILE:HG22	20:T:77:ALA:HB1	1.97	0.46
1:A:176:U:H5'	1:A:176:U:H6	1.81	0.45
1:A:211:G:H4'	1:A:212:C:OP1	2.15	0.45
1:A:564:G:C5	1:A:741:G:N7	2.82	0.45
1:A:603:C:C2	4:D:135:LEU:HD22	2.51	0.45
1:A:980:G:N2	1:A:1021:C:H1'	2.25	0.45
6:F:7:ASN:HB2	6:F:89:MET:HB3	1.98	0.45
13:M:96:LEU:O	13:M:110:ARG:NH1	2.48	0.45
16:P:71:ARG:HD3	16:P:75:ARG:NH2	2.31	0.45
20:T:10:LEU:HB3	20:T:11:SER:H	1.36	0.45
1:A:414:C:C2	1:A:420:G:C2	3.04	0.45
1:A:659:A:H1'	11:K:115:PRO:HB3	1.98	0.45
5:E:53:LEU:HA	5:E:53:LEU:HD23	1.70	0.45
1:A:379:G:H2'	1:A:380:C:C6	2.51	0.45
1:A:951:A:OP1	14:N:29:ARG:NH2	2.49	0.45
1:A:1044:U:H2'	1:A:1045:C:C6	2.52	0.45
1:A:1384:C:H2'	1:A:1385:C:O4'	2.17	0.45
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.98	0.45
7:G:136:LYS:HB2	7:G:136:LYS:HE3	1.71	0.45
20:T:13:LEU:HD23	20:T:13:LEU:HA	1.70	0.45
1:A:410:A:C6	1:A:411:G:C6	3.04	0.45
1:A:630:C:H2'	1:A:631:A:H8	1.81	0.45
1:A:1260:A:O2'	1:A:1263:C:N4	2.50	0.45
1:A:1295:C:N4	19:S:4:SER:CB	2.78	0.45
2:B:45:GLN:O	2:B:49:GLU:HG3	2.17	0.45
5:E:5:ASP:CG	5:E:6:PHE:H	2.19	0.45
9:I:53:VAL:HB	9:I:92:TYR:HE2	1.81	0.45
19:S:50:ALA:HA	19:S:58:VAL:O	2.17	0.45
1:A:498:G:C5	1:A:499:U:C5	3.05	0.45
1:A:565:U:H5"	15:O:64:ARG:HH22	1.81	0.45
1:A:1285:G:C6	1:A:1286:G:N1	2.84	0.45
7:G:99:LEU:HA	7:G:99:LEU:HD23	1.73	0.45
1:A:599:G:H1'	1:A:608:G:N2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:A:H4'	1:A:811:A:OP1	2.17	0.45
1:A:1051:C:O2'	1:A:1173:C:H1'	2.17	0.45
1:A:1085:C:H5"	2:B:98:LEU:HD13	1.97	0.45
1:A:1126:G:O5'	1:A:1126:G:H8	1.98	0.45
1:A:1157:A:H3'	1:A:1158:G:H8	1.81	0.45
2:B:82:ARG:HG2	2:B:86:GLU:OE2	2.16	0.45
7:G:15:ASP:OD2	7:G:18:TYR:HB2	2.17	0.45
18:R:19:LYS:HE2	18:R:19:LYS:HB2	1.64	0.45
1:A:277:A:H8	1:A:277:A:OP2	1.99	0.45
1:A:350:C:H2'	1:A:351:A:O4'	2.17	0.45
1:A:803:U:H4'	1:A:804:G:OP2	2.16	0.45
1:A:951:A:OP2	14:N:41:ARG:NH1	2.50	0.45
1:A:1330:A:OP2	9:I:118:LYS:NZ	2.50	0.45
6:F:9:VAL:HG22	6:F:60:PHE:CE1	2.50	0.45
8:H:17:THR:HG22	8:H:63:LEU:HG	1.98	0.45
8:H:104:ARG:O	8:H:105:ARG:C	2.55	0.45
1:A:102:A:C6	1:A:321:G:C6	3.05	0.45
2:B:69:LEU:HD22	2:B:71:VAL:HG13	1.99	0.45
4:D:108:LEU:HD23	4:D:108:LEU:HA	1.73	0.45
5:E:79:GLU:CD	8:H:105:ARG:HE	2.20	0.45
12:L:28:LYS:O	12:L:30:ALA:N	2.49	0.45
12:L:83:VAL:HG11	12:L:100:ILE:HG12	1.98	0.45
1:A:255:G:H2'	1:A:256:U:C6	2.52	0.45
1:A:501:C:OP2	1:A:513:G:H4'	2.17	0.45
1:A:1009:G:N2	1:A:1012:A:OP2	2.50	0.45
1:A:1018:G:H2'	1:A:1019:C:O4'	2.16	0.45
3:C:124:ILE:HD12	3:C:130:VAL:HG22	1.98	0.45
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.99	0.45
17:Q:67:LYS:HA	17:Q:70:ARG:HH21	1.82	0.45
1:A:952:A:H8	1:A:952:A:C5'	2.23	0.45
1:A:960:A:H5'	1:A:961:C:OP2	2.17	0.45
1:A:1109:G:H1	1:A:1126:G:H1	1.64	0.45
1:A:1123:C:H2'	1:A:1124:G:H8	1.81	0.45
2:B:83:MET:SD	2:B:235:SER:HB3	2.57	0.45
9:I:118:LYS:O	9:I:119:ALA:HB3	2.17	0.45
10:J:27:ALA:HB3	10:J:30:SER:H	1.81	0.45
17:Q:90:ILE:HG13	17:Q:90:ILE:H	1.67	0.45
1:A:41:G:H2'	1:A:42:G:C8	2.52	0.44
1:A:64:G:H3'	1:A:64:G:P	2.57	0.44
1:A:371:G:H5"	16:P:5:ARG:HD2	1.99	0.44
1:A:809:C:H2'	1:A:810:U:C6	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:U:H2'	1:A:822:U:O2	2.17	0.44
1:A:1035:G:OP1	1:A:1036:C:C6	2.70	0.44
1:A:1222:G:H2'	1:A:1223:C:H6	1.82	0.44
1:A:1246:G:H2'	1:A:1247:G:O4'	2.17	0.44
1:A:1324:G:OP1	9:I:125:TYR:HE2	2.01	0.44
6:F:18:GLN:O	6:F:22:GLU:HG2	2.17	0.44
21:V:25:LYS:HD2	21:V:25:LYS:HA	1.82	0.44
1:A:50:A:H4'	1:A:51:A:OP2	2.16	0.44
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.65	0.44
10:J:4:ILE:HD12	10:J:4:ILE:O	2.17	0.44
16:P:71:ARG:HD3	16:P:75:ARG:HH21	1.82	0.44
18:R:53:ARG:O	18:R:55:ARG:N	2.50	0.44
1:A:648:A:H2'	1:A:715:C:O2	2.17	0.44
1:A:978:A:H2'	1:A:979:G:H8	1.82	0.44
3:C:35:GLU:OE2	3:C:97:LYS:HE2	2.18	0.44
4:D:152:SER:O	4:D:154:ASN:N	2.50	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.60	0.44
1:A:311:G:OP2	1:A:346:G:O2'	2.36	0.44
1:A:981:G:N2	1:A:1020:C:C2	2.85	0.44
1:A:1105:A:H2	1:A:1132:U:H3	1.64	0.44
1:A:1301:C:OP2	19:S:3:ARG:HD3	2.17	0.44
2:B:98:LEU:HB2	2:B:101:MET:HG3	2.00	0.44
3:C:195:VAL:O	3:C:196:LEU:HD12	2.18	0.44
4:D:162:LEU:HD22	4:D:181:MET:HG2	1.99	0.44
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.33	0.44
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.99	0.44
1:A:527:G:C6	1:A:528:C:C4	3.06	0.44
1:A:1171:G:O2'	1:A:1172:A:P	2.75	0.44
1:A:1313:A:C2	1:A:1314:A:C5	3.06	0.44
3:C:107:GLN:O	3:C:107:GLN:CD	2.56	0.44
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.74	0.44
1:A:902:G:C2	1:A:904:G:C8	3.06	0.44
1:A:923:A:H2'	1:A:924:G:H8	1.76	0.44
3:C:77:ILE:HD13	3:C:84:ILE:HD12	2.00	0.44
11:K:29:ILE:HG21	11:K:29:ILE:HD13	1.73	0.44
12:L:78:GLN:C	12:L:80:HIS:H	2.20	0.44
14:N:21:TYR:HE1	14:N:23:ARG:NE	2.16	0.44
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.99	0.44
15:O:78:TYR:O	15:O:82:ILE:HG13	2.17	0.44
1:A:952:A:H4'	1:A:953:G:C5'	2.43	0.44
2:B:55:PHE:CD2	2:B:221:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:58:VAL:O	12:L:65:GLU:HA	2.17	0.44
17:Q:4:LYS:HG2	17:Q:6:LEU:HD21	1.99	0.44
1:A:507:G:H2'	1:A:508:C:C6	2.52	0.44
1:A:794:C:O2'	1:A:878:A:N1	2.49	0.44
1:A:902:G:O2'	1:A:904:G:OP1	2.32	0.44
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.00	0.44
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.17	0.44
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.99	0.44
13:M:33:ALA:HA	13:M:59:TYR:CE2	2.50	0.44
13:M:56:LEU:HA	13:M:56:LEU:HD23	1.76	0.44
15:O:3:ILE:HG21	15:O:34:LEU:HD11	1.99	0.44
19:S:15:LEU:O	19:S:19:VAL:HG12	2.17	0.44
1:A:424:U:O2	1:A:425:A:C8	2.71	0.44
1:A:982:A:H2'	1:A:1018:G:O6	2.18	0.44
1:A:1179:G:H2'	1:A:1180:U:O4'	2.18	0.44
1:A:1211:C:H2'	1:A:1212:G:H8	1.83	0.44
1:A:1288:U:H5'	13:M:109:THR:HG21	1.98	0.44
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.82	0.44
7:G:59:LEU:O	7:G:63:LYS:HG3	2.16	0.44
15:O:6:GLU:HA	15:O:9:GLN:HB2	2.00	0.44
1:A:62:U:H2'	1:A:63:C:C6	2.53	0.43
1:A:245:A:H5'	1:A:245:A:C8	2.52	0.43
1:A:582:C:H2'	1:A:583:C:H6	1.83	0.43
1:A:625:A:N3	8:H:113:SER:OG	2.50	0.43
1:A:957:C:H3'	1:A:958:U:C6	2.52	0.43
2:B:87:ARG:HE	2:B:87:ARG:HB3	1.51	0.43
8:H:29:SER:OG	8:H:32:LYS:HG3	2.19	0.43
11:K:87:THR:HG22	11:K:91:ARG:HH22	1.83	0.43
17:Q:5:VAL:C	17:Q:6:LEU:HD23	2.38	0.43
1:A:483:G:C6	1:A:484:C:C4	3.06	0.43
1:A:616:G:H2'	1:A:617:C:H6	1.83	0.43
1:A:990:U:H2'	1:A:991:G:O4'	2.18	0.43
1:A:1042:C:N4	3:C:2:GLY:HA2	2.34	0.43
1:A:1102:G:H2'	1:A:1103:U:C6	2.53	0.43
1:A:1474:G:C5	1:A:1475:U:C5	3.06	0.43
2:B:114:ARG:NH1	2:B:118:LEU:HD11	2.33	0.43
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.83	0.43
6:F:14:LEU:HB2	6:F:18:GLN:HB2	2.00	0.43
10:J:82:ILE:O	10:J:84:GLN:N	2.51	0.43
14:N:33:VAL:HA	14:N:40:CYS:HA	2.01	0.43
1:A:396:C:H1'	1:A:605:A:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:C:H5'	4:D:72:GLU:HG2	2.00	0.43
1:A:787:U:H5"	1:A:788:C:OP2	2.18	0.43
1:A:1030:G:H5"	14:N:3:ARG:HG2	2.00	0.43
2:B:71:VAL:CG2	2:B:164:VAL:HG22	2.48	0.43
2:B:204:ASN:HD22	2:B:206:ASP:H	1.67	0.43
7:G:50:ILE:HD11	7:G:121:ALA:HA	1.99	0.43
11:K:54:ARG:O	11:K:57:THR:HG22	2.18	0.43
16:P:36:ILE:O	16:P:51:VAL:O	2.36	0.43
19:S:35:SER:O	19:S:38:SER:OG	2.30	0.43
1:A:354:U:H2'	1:A:355:A:H8	1.83	0.43
1:A:1062:A:H5"	5:E:16:THR:HG21	2.01	0.43
1:A:1301:C:OP2	19:S:3:ARG:CD	2.66	0.43
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.01	0.43
18:R:85:LEU:HD23	18:R:88:LYS:HG2	2.00	0.43
1:A:224:U:H5"	16:P:33:ILE:HD13	2.01	0.43
1:A:841:A:H2'	1:A:842:A:C8	2.53	0.43
1:A:1175:U:H2'	1:A:1176:C:C6	2.53	0.43
2:B:13:ALA:HA	2:B:16:HIS:CG	2.53	0.43
3:C:156:ARG:NH2	3:C:161:GLU:HA	2.34	0.43
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.53	0.43
13:M:4:ILE:HD13	13:M:4:ILE:HA	1.85	0.43
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.53	0.43
1:A:77:G:N3	1:A:77:G:H2'	2.34	0.43
1:A:277:A:H5"	1:A:278:C:H5	1.82	0.43
1:A:1279:C:H4'	1:A:1280:A:O4'	2.17	0.43
1:A:1324:G:H2'	1:A:1325:C:C6	2.54	0.43
3:C:11:ARG:O	3:C:13:GLY:N	2.51	0.43
8:H:86:ILE:HG13	8:H:133:LEU:HD22	2.01	0.43
12:L:27:LEU:CB	12:L:62:SER:HB2	2.48	0.43
1:A:245:A:H8	1:A:245:A:OP2	2.01	0.43
1:A:432:U:C5'	4:D:155:LEU:HD22	2.49	0.43
1:A:708:G:C2	1:A:709:C:C6	3.07	0.43
1:A:904:G:C4	1:A:905:G:C8	3.07	0.43
1:A:961:C:H2'	1:A:962:C:H6	1.82	0.43
1:A:1085:C:C4	1:A:1086:G:N7	2.86	0.43
1:A:1273:U:H5'	9:I:38:GLN:NE2	2.34	0.43
1:A:1330:A:H3'	1:A:1331:A:H8	1.84	0.43
3:C:107:GLN:C	3:C:107:GLN:CD	2.78	0.43
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.99	0.43
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.60	0.43
10:J:3:LYS:N	10:J:74:ILE:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:12:ASP:O	10:J:15:THR:HG22	2.18	0.43
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.18	0.43
19:S:20:LEU:HD12	19:S:21:GLU:HG3	2.00	0.43
19:S:74:PHE:O	19:S:76:PRO:HD3	2.18	0.43
1:A:564:G:OP2	1:A:564:G:H8	2.02	0.43
1:A:797:A:N7	1:A:799:A:C4	2.87	0.43
1:A:1188:G:H2'	1:A:1189:C:H6	1.84	0.43
1:A:42:G:H2'	1:A:43:C:O4'	2.18	0.43
1:A:227:G:H2'	1:A:228:C:O4'	2.18	0.43
1:A:952:A:N6	10:J:60:ARG:HH21	2.17	0.43
1:A:1202:G:O3'	19:S:77:THR:HG21	2.19	0.43
1:A:1408:C:H2'	1:A:1409:U:C6	2.54	0.43
3:C:19:GLU:O	3:C:56:ASP:HA	2.19	0.43
4:D:97:LEU:HA	4:D:97:LEU:HD23	1.84	0.43
10:J:12:ASP:HB3	10:J:15:THR:CG2	2.49	0.43
12:L:60:LEU:N	12:L:64:TYR:O	2.46	0.43
21:V:12:LYS:HB3	21:V:22:ARG:HD2	2.01	0.43
1:A:949:C:H4'	10:J:57:LYS:HB3	2.01	0.42
4:D:70:ILE:HD11	4:D:100:ARG:CD	2.44	0.42
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.54	0.42
9:I:16:ARG:O	9:I:63:ILE:HG23	2.19	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
9:I:116:LYS:HD2	9:I:122:ALA:HA	2.00	0.42
1:A:519:C:H2'	1:A:520:G:C8	2.54	0.42
1:A:835:G:H5"	1:A:846:G:O6	2.19	0.42
1:A:1039:G:C4	1:A:1185:A:C2	3.07	0.42
1:A:1287:A:C2	1:A:1313:A:C8	3.07	0.42
8:H:11:THR:HA	8:H:14:ARG:NH1	2.34	0.42
12:L:34:ARG:O	12:L:61:THR:HG23	2.19	0.42
14:N:26:ARG:NE	14:N:47:LEU:HD21	2.35	0.42
1:A:217:U:H2'	1:A:218:U:C6	2.55	0.42
1:A:957:C:C5	1:A:958:U:C2	3.07	0.42
1:A:960:A:N1	1:A:1203:G:N2	2.67	0.42
1:A:983:A:H2	1:A:1004:G:C8	2.37	0.42
1:A:1149:A:OP1	1:A:1149:A:H8	2.01	0.42
1:A:1431:A:OP2	1:A:1432:C:C5	2.68	0.42
2:B:107:THR:HA	2:B:110:GLN:HE21	1.84	0.42
2:B:122:PHE:O	2:B:124:SER:N	2.52	0.42
4:D:13:ARG:HD2	4:D:36:ARG:O	2.19	0.42
6:F:22:GLU:OE2	6:F:22:GLU:HA	2.20	0.42
7:G:88:PRO:HD2	7:G:152:ALA:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:LEU:HD23	13:M:34:LEU:HA	1.67	0.42
15:O:64:ARG:HH21	15:O:68:ARG:HH22	1.66	0.42
1:A:121:G:C6	1:A:122:U:C4	3.07	0.42
1:A:417:C:H1'	1:A:418:G:OP2	2.19	0.42
1:A:608:G:H4'	16:P:16:HIS:CG	2.54	0.42
1:A:653:G:H2'	1:A:654:G:O4'	2.19	0.42
1:A:977:U:H3'	1:A:978:A:H5"	2.02	0.42
2:B:162:ILE:HD13	2:B:162:ILE:HG21	1.75	0.42
2:B:167:PRO:HD3	2:B:187:LEU:O	2.19	0.42
7:G:151:TYR:C	7:G:153:HIS:H	2.23	0.42
8:H:17:THR:C	8:H:78:GLN:HE22	2.20	0.42
17:Q:100:LYS:HB3	17:Q:100:LYS:HE2	1.85	0.42
18:R:24:ALA:C	18:R:26:LEU:H	2.22	0.42
1:A:525:G:H5'	4:D:41:GLY:HA3	2.00	0.42
1:A:564:G:N1	1:A:741:G:N7	2.67	0.42
1:A:1022:U:N3	1:A:1023:A:N7	2.67	0.42
1:A:1042:C:O2'	10:J:56:HIS:ND1	2.43	0.42
1:A:1109:G:H1	1:A:1126:G:N2	2.16	0.42
1:A:1111:C:O5'	1:A:1112:A:H5'	2.19	0.42
1:A:1381:C:H4'	1:A:1382:C:C5'	2.40	0.42
1:A:1402:C:H2'	1:A:1403:G:C8	2.54	0.42
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.84	0.42
3:C:21:ARG:NH1	3:C:56:ASP:OD2	2.48	0.42
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.01	0.42
4:D:187:ARG:HH11	4:D:188:LEU:N	2.17	0.42
10:J:5:ARG:HA	10:J:73:ASP:OD1	2.19	0.42
1:A:399:U:H2'	1:A:400:U:C6	2.54	0.42
1:A:415:U:C2	1:A:419:G:C2	3.07	0.42
1:A:711:A:H2'	1:A:712:A:O4'	2.19	0.42
1:A:835:G:C6	1:A:846:G:C8	3.08	0.42
1:A:1488:G:H2'	1:A:1489:U:O4'	2.20	0.42
2:B:122:PHE:O	2:B:127:ILE:HG21	2.19	0.42
3:C:79:ARG:C	3:C:81:GLY:H	2.23	0.42
4:D:55:ALA:O	4:D:59:ARG:HG2	2.18	0.42
5:E:59:GLY:O	5:E:63:ARG:HG3	2.19	0.42
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.51	0.42
16:P:58:TYR:O	16:P:61:SER:OG	2.27	0.42
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.71	0.42
1:A:256:U:O2	1:A:258:A:C8	2.73	0.42
1:A:745:C:OP1	17:Q:102:GLY:HA3	2.20	0.42
1:A:1207:C:N4	13:M:104:ARG:HG3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1484:A:C2	1:A:1485:G:C4	3.08	0.42
2:B:32:ILE:HD12	2:B:40:HIS:ND1	2.35	0.42
4:D:187:ARG:HH11	4:D:188:LEU:H	1.68	0.42
10:J:19:SER:CB	10:J:91:PRO:HG3	2.47	0.42
10:J:61:GLU:OE1	14:N:45:ARG:HD2	2.19	0.42
11:K:24:SER:OG	11:K:25:TYR:N	2.53	0.42
1:A:428:C:H2'	1:A:429:U:C6	2.55	0.42
1:A:461:G:H2'	1:A:462:A:C8	2.55	0.42
1:A:484:C:H2'	1:A:485:G:C8	2.55	0.42
1:A:511:C:H5"	1:A:511:C:H6	1.85	0.42
2:B:87:ARG:NH1	2:B:234:PRO:HG3	2.34	0.42
2:B:230:VAL:O	2:B:232:PRO:HD3	2.20	0.42
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.01	0.42
9:I:78:LYS:HD3	9:I:101:PHE:HD1	1.84	0.42
10:J:63:PHE:CE2	14:N:45:ARG:HG3	2.55	0.42
11:K:21:ILE:HD12	11:K:94:ALA:HB1	2.01	0.42
2:B:222:ILE:HG22	2:B:226:ARG:HG3	2.00	0.42
5:E:11:ILE:HG21	5:E:105:VAL:HG13	2.01	0.42
6:F:10:LEU:HD23	6:F:10:LEU:HA	1.89	0.42
1:A:448:C:H5"	1:A:449:C:OP2	2.19	0.42
1:A:635:U:C2	1:A:735:G:N2	2.88	0.42
1:A:645:G:H2'	1:A:646:A:C8	2.55	0.42
1:A:775:A:H4'	1:A:776:U:O5'	2.20	0.42
1:A:809:C:O2	8:H:15:ASN:ND2	2.53	0.42
1:A:953:G:H5'	1:A:1339:U:O2'	2.20	0.42
1:A:1019:C:H2'	1:A:1020:C:C6	2.55	0.42
1:A:1248:C:O2	21:V:20:LYS:HD2	2.20	0.42
1:A:1400:A:N6	1:A:1459:G:O2'	2.42	0.42
2:B:91:PRO:HG3	2:B:154:LEU:HB3	2.01	0.42
8:H:23:SER:HA	8:H:61:VAL:O	2.18	0.42
10:J:23:ILE:O	10:J:23:ILE:HG22	2.19	0.42
10:J:78:ASN:OD1	10:J:80:LYS:HB3	2.19	0.42
12:L:77:LEU:HD21	12:L:107:ALA:HB2	2.02	0.42
13:M:6:GLY:O	13:M:8:GLU:HG2	2.20	0.42
1:A:255:G:H2'	1:A:256:U:H6	1.85	0.41
1:A:915:A:C6	1:A:916:G:C5	3.08	0.41
1:A:1338:A:H5"	1:A:1339:U:OP2	2.20	0.41
2:B:91:PRO:HG2	2:B:155:LEU:CD2	2.50	0.41
2:B:223:ILE:HD12	2:B:230:VAL:H	1.85	0.41
6:F:8:ILE:HG12	6:F:88:VAL:HG22	2.02	0.41
7:G:101:LEU:O	7:G:105:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:15:ALA:HA	9:I:65:VAL:HG22	2.02	0.41
12:L:28:LYS:C	12:L:30:ALA:N	2.72	0.41
14:N:23:ARG:NH1	14:N:28:GLY:O	2.50	0.41
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.34	0.41
14:N:37:PHE:CE1	14:N:53:LEU:HD13	2.55	0.41
15:O:3:ILE:HG21	15:O:34:LEU:CD1	2.50	0.41
15:O:64:ARG:NH2	15:O:68:ARG:HH22	2.18	0.41
17:Q:20:THR:HG21	17:Q:41:LYS:HD2	2.01	0.41
1:A:378:A:H5"	1:A:379:G:OP2	2.20	0.41
1:A:1046:G:H5'	1:A:1048:C:H1'	2.01	0.41
1:A:1360:C:C5	1:A:1361:G:C8	3.09	0.41
2:B:115:LEU:CD1	2:B:146:GLN:HG3	2.48	0.41
3:C:6:HIS:CD2	3:C:7:PRO:HD2	2.55	0.41
7:G:12:LEU:HD12	7:G:12:LEU:H	1.86	0.41
8:H:116:LYS:HG3	8:H:129:VAL:HG21	2.02	0.41
11:K:14:VAL:HG21	11:K:40:ILE:HD13	2.01	0.41
19:S:32:LYS:HD3	19:S:50:ALA:HB3	2.03	0.41
20:T:57:ARG:HH21	20:T:100:ILE:CG2	2.33	0.41
1:A:484:C:OP1	12:L:117:ARG:NH2	2.53	0.41
1:A:561:C:H2'	1:A:562:G:O4'	2.21	0.41
1:A:816:U:H2'	1:A:817:C:H6	1.84	0.41
1:A:899:G:H1'	5:E:19:MET:HB3	2.02	0.41
1:A:949:C:H4'	10:J:57:LYS:HD2	2.01	0.41
1:A:1139:A:C5	1:A:1161:A:C6	3.09	0.41
1:A:1226:A:C2	1:A:1274:G:C2	3.08	0.41
3:C:38:ARG:HG2	3:C:38:ARG:H	1.59	0.41
3:C:131:ARG:HH12	5:E:50:GLU:HG2	1.84	0.41
4:D:3:ARG:HA	4:D:3:ARG:HE	1.86	0.41
7:G:150:ALA:HA	11:K:59:TYR:CB	2.50	0.41
18:R:24:ALA:O	18:R:26:LEU:N	2.52	0.41
1:A:45:U:H2'	1:A:46:G:C8	2.56	0.41
1:A:397:G:OP1	4:D:74:GLN:NE2	2.53	0.41
1:A:774:G:C6	1:A:775:A:N7	2.88	0.41
1:A:1068:U:H3	1:A:1081:G:H22	1.68	0.41
6:F:41:GLU:HG2	6:F:62:TRP:CE3	2.55	0.41
8:H:17:THR:O	8:H:78:GLN:NE2	2.46	0.41
12:L:28:LYS:O	12:L:29:GLY:C	2.58	0.41
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.01	0.41
20:T:69:GLY:O	20:T:73:HIS:ND1	2.53	0.41
1:A:293:A:H2'	1:A:294:G:C8	2.56	0.41
1:A:339:A:H5"	1:A:340:C:H5	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:U:O2	1:A:1108:U:H2'	2.19	0.41
1:A:1295:C:O2'	1:A:1296:U:H5'	2.20	0.41
2:B:77:ALA:HA	2:B:80:ILE:HD13	2.03	0.41
3:C:33:LEU:HD11	14:N:53:LEU:HD23	2.03	0.41
3:C:95:THR:O	3:C:97:LYS:N	2.47	0.41
4:D:78:LEU:HD23	4:D:78:LEU:HA	1.67	0.41
4:D:117:ALA:O	4:D:121:VAL:HG23	2.20	0.41
4:D:128:VAL:C	4:D:130:GLY:H	2.24	0.41
7:G:51:GLN:C	7:G:53:LYS:H	2.24	0.41
7:G:104:LEU:HA	7:G:104:LEU:HD23	1.85	0.41
8:H:109:ILE:HD11	8:H:111:ILE:HG13	2.03	0.41
10:J:71:LEU:HA	10:J:71:LEU:HD12	1.76	0.41
1:A:794:C:H4'	1:A:877:A:N6	2.35	0.41
1:A:1478:C:N4	1:A:1481:G:C2	2.88	0.41
2:B:77:ALA:HB2	2:B:211:ILE:HG21	2.03	0.41
3:C:33:LEU:O	3:C:37:GLN:HG2	2.21	0.41
4:D:150:GLU:O	4:D:153:ARG:HG3	2.21	0.41
5:E:7:GLU:CD	5:E:37:ARG:HE	2.24	0.41
7:G:138:LYS:HD3	7:G:139:GLU:N	2.36	0.41
15:O:3:ILE:HG22	15:O:38:ARG:NH1	2.35	0.41
19:S:53:ASN:HB3	19:S:56:GLN:H	1.83	0.41
1:A:458:G:H5"	16:P:81:ARG:CZ	2.50	0.41
1:A:957:C:H5"	1:A:958:U:H5	1.83	0.41
1:A:971:A:C2	14:N:5:ALA:HA	2.55	0.41
1:A:1034:U:H2'	1:A:1037:A:OP2	2.20	0.41
3:C:178:LEU:C	3:C:180:ALA:N	2.74	0.41
10:J:47:PHE:CZ	14:N:37:PHE:CE2	3.08	0.41
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	2.02	0.41
17:Q:74:LEU:HD22	17:Q:75:ARG:HG2	2.02	0.41
1:A:60:A:H4'	1:A:61:G:O5'	2.20	0.41
1:A:773:A:C6	1:A:774:G:C6	3.08	0.41
1:A:819:G:C6	1:A:828:G:C5	3.09	0.41
1:A:1458:U:H2'	1:A:1459:G:C8	2.56	0.41
12:L:27:LEU:HB3	12:L:62:SER:HB2	2.03	0.41
13:M:88:ARG:HG2	13:M:98:VAL:HG13	2.02	0.41
1:A:268:A:N6	1:A:269:A:N6	2.69	0.41
1:A:442:A:C4	1:A:471:A:C2	3.09	0.41
1:A:476:G:H3'	1:A:477:G:H8	1.86	0.41
1:A:684:C:H5"	1:A:686:G:O4'	2.21	0.41
1:A:764:A:C5	1:A:785:A:C2	3.09	0.41
1:A:932:U:H2'	1:A:933:U:H6	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:971:A:H2'	1:A:971:A:N3	2.35	0.41
1:A:1022:U:C2	1:A:1023:A:N7	2.89	0.41
1:A:1286:G:H5"	21:V:4:GLY:HA3	2.03	0.41
2:B:92:TYR:CE2	2:B:94:ASN:HB2	2.56	0.41
3:C:42:LEU:HD12	3:C:42:LEU:HA	1.94	0.41
13:M:22:ILE:HG22	13:M:23:TYR:N	2.36	0.41
13:M:108:ARG:NE	13:M:108:ARG:HA	2.35	0.41
13:M:120:LYS:HD2	13:M:126:LYS:OXT	2.20	0.41
15:O:4:THR:O	15:O:7:GLU:HB2	2.20	0.41
15:O:42:HIS:CE1	15:O:46:HIS:HD2	2.39	0.41
16:P:50:LYS:HB2	16:P:50:LYS:HE2	1.92	0.41
17:Q:18:THR:CG2	17:Q:43:LEU:HD12	2.51	0.41
20:T:33:ILE:O	20:T:34:LYS:C	2.59	0.41
20:T:45:GLN:HA	20:T:91:LEU:HD22	2.02	0.41
23:X:30:G:H2'	23:X:31:G:C8	2.55	0.41
1:A:1022:U:H5'	1:A:1023:A:OP2	2.21	0.41
1:A:1201:G:O3'	19:S:36:ARG:HD3	2.21	0.41
1:A:1253:G:H2'	1:A:1254:G:O4'	2.21	0.41
1:A:1301:C:OP1	19:S:70:LYS:HE3	2.21	0.41
3:C:32:LEU:HD23	3:C:32:LEU:HA	1.91	0.41
3:C:121:ALA:HB1	3:C:189:ALA:HB2	2.01	0.41
5:E:76:ILE:HG23	5:E:142:LEU:HD13	2.03	0.41
7:G:15:ASP:OD2	7:G:18:TYR:N	2.54	0.41
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.39	0.41
11:K:77:MET:CE	11:K:80:VAL:HG22	2.51	0.41
13:M:23:TYR:O	13:M:25:ILE:N	2.48	0.41
15:O:70:LEU:HD12	15:O:78:TYR:HA	2.03	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.21	0.41
16:P:28:ARG:HG3	16:P:29:ASP:OD1	2.21	0.41
20:T:9:ASN:O	20:T:10:LEU:HD23	2.21	0.41
1:A:83:A:H2'	1:A:84:C:O4'	2.21	0.40
1:A:780:C:OP1	11:K:124:LYS:HD3	2.21	0.40
3:C:157:ILE:CD1	3:C:166:GLU:HB2	2.51	0.40
4:D:202:LEU:HD23	4:D:202:LEU:HA	1.89	0.40
5:E:144:THR:O	5:E:147:ASP:N	2.54	0.40
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.76	0.40
10:J:47:PHE:HD1	14:N:34:TYR:CD2	2.39	0.40
10:J:48:THR:OG1	10:J:62:HIS:CE1	2.75	0.40
13:M:77:ASN:O	13:M:81:LEU:HD23	2.21	0.40
13:M:107:ALA:HB3	13:M:111:LYS:HD2	2.03	0.40
18:R:43:PHE:CG	18:R:66:LEU:HD11	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:70:LYS:O	19:S:73:GLU:HB2	2.21	0.40
1:A:352:G:OP1	1:A:362:U:H2'	2.22	0.40
1:A:932:U:H2'	1:A:933:U:C6	2.56	0.40
1:A:1133:A:O2'	1:A:1134:A:H5"	2.21	0.40
2:B:223:ILE:HA	2:B:226:ARG:CB	2.50	0.40
3:C:72:LYS:C	3:C:74:GLY:H	2.24	0.40
4:D:23:GLY:HA3	4:D:112:VAL:HG23	2.03	0.40
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.85	0.40
10:J:16:LEU:CD2	10:J:94:VAL:HG22	2.50	0.40
11:K:84:VAL:HG21	11:K:95:ILE:HD11	2.02	0.40
12:L:46:LYS:HE2	12:L:47:LYS:HB2	2.01	0.40
12:L:53:ARG:HD2	12:L:93:LEU:HD21	2.04	0.40
15:O:71:GLN:HG3	15:O:78:TYR:CD2	2.57	0.40
20:T:43:LEU:HB3	20:T:52:ALA:HB2	2.04	0.40
1:A:162:G:C2	1:A:163:C:C5	3.10	0.40
1:A:189:U:O2	17:Q:63:ARG:NH2	2.54	0.40
1:A:352:G:C2	1:A:353:U:C5	3.09	0.40
1:A:371:G:H2'	1:A:372:G:H8	1.85	0.40
1:A:1080:C:H2'	1:A:1081:G:O4'	2.21	0.40
1:A:1231:A:H4'	9:I:68:GLY:N	2.36	0.40
2:B:117:GLU:O	2:B:120:ALA:HB3	2.21	0.40
8:H:117:GLY:O	8:H:119:LEU:HG	2.21	0.40
17:Q:7:THR:O	17:Q:23:VAL:HG13	2.21	0.40
17:Q:34:LYS:HB2	17:Q:34:LYS:HE2	1.88	0.40
17:Q:36:ILE:HD13	17:Q:36:ILE:HG21	1.70	0.40
18:R:25:THR:O	18:R:42:ARG:NH2	2.53	0.40
1:A:64:G:C2	1:A:67:C:N4	2.90	0.40
1:A:172:C:C2	1:A:173:A:C8	3.09	0.40
1:A:406:A:O2'	1:A:407:A:H4'	2.21	0.40
1:A:630:C:H2'	1:A:631:A:C8	2.56	0.40
1:A:809:C:H2'	1:A:810:U:H6	1.85	0.40
1:A:1302:C:O2'	19:S:78:ARG:NH1	2.54	0.40
1:A:1376:A:H4'	1:A:1377:C:OP2	2.21	0.40
3:C:156:ARG:H	3:C:163:ALA:HA	1.87	0.40
4:D:20:TYR:CE2	4:D:27:TYR:CE1	3.09	0.40
9:I:78:LYS:HD3	9:I:101:PHE:CD1	2.57	0.40
10:J:66:ARG:HE	10:J:66:ARG:HB3	1.63	0.40
11:K:74:ALA:C	11:K:76:GLY:H	2.24	0.40
17:Q:22:LEU:HD13	17:Q:41:LYS:HG3	2.04	0.40
1:A:31:G:O2'	1:A:48:C:N4	2.34	0.40
1:A:885:A:H2'	1:A:886:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1296:U:H2'	1:A:1297:G:O4'	2.21	0.40
4:D:9:CYS:HA	4:D:12:CYS:HB2	2.03	0.40
4:D:121:VAL:O	4:D:134:ASP:HA	2.22	0.40
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.83	0.40
8:H:127:LEU:HA	8:H:127:LEU:HD13	1.93	0.40
20:T:64:ASP:CG	20:T:81:LYS:HZ2	2.24	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:79:ARG:CB	10:J:79:ARG:NE[8_665]	1.89	0.31

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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
2	B	232/234 (99%)	179 (77%)	37 (16%)	16 (7%)	1 9
3	C	204/206 (99%)	150 (74%)	39 (19%)	15 (7%)	1 8
4	D	206/208 (99%)	179 (87%)	20 (10%)	7 (3%)	3 24
5	E	148/150 (99%)	133 (90%)	12 (8%)	3 (2%)	7 34
6	F	99/101 (98%)	94 (95%)	4 (4%)	1 (1%)	15 49
7	G	153/155 (99%)	129 (84%)	16 (10%)	8 (5%)	2 14
8	H	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	10 40
9	I	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	4 25
10	J	96/98 (98%)	66 (69%)	18 (19%)	12 (12%)	0 2
11	K	117/119 (98%)	98 (84%)	12 (10%)	7 (6%)	1 12
12	L	122/124 (98%)	94 (77%)	16 (13%)	12 (10%)	0 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	123/125 (98%)	98 (80%)	22 (18%)	3 (2%)	6 31
14	N	58/60 (97%)	45 (78%)	11 (19%)	2 (3%)	3 24
15	O	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13 45
16	P	81/83 (98%)	69 (85%)	10 (12%)	2 (2%)	5 30
17	Q	102/104 (98%)	87 (85%)	8 (8%)	7 (7%)	1 9
18	R	71/73 (97%)	59 (83%)	9 (13%)	3 (4%)	3 19
19	S	78/80 (98%)	62 (80%)	10 (13%)	6 (8%)	1 7
20	T	97/99 (98%)	70 (72%)	18 (19%)	9 (9%)	0 4
21	V	22/24 (92%)	18 (82%)	4 (18%)	0	100 100
All	All	2356/2396 (98%)	1935 (82%)	301 (13%)	120 (5%)	2 15

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	234	PRO
3	C	5	ILE
3	C	61	ALA
3	C	144	SER
3	C	179	ARG
4	D	36	ARG
4	D	71	SER
7	G	83	ALA
7	G	137	LYS
8	H	51	VAL
9	I	56	LEU
9	I	118	LYS
10	J	90	LEU
11	K	117	ASN
11	K	128	ALA
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
12	L	48	PRO
13	M	7	VAL
17	Q	81	ARG
17	Q	95	TYR
18	R	47	THR
19	S	5	LEU

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Mol	Chain	Res	Type
19	S	30	LEU
20	T	73	HIS
20	T	94	ALA
2	B	14	GLY
2	B	16	HIS
2	B	17	PHE
2	B	95	GLN
2	B	208	ILE
2	B	229	VAL
3	C	154	SER
3	C	168	ALA
3	C	181	ASN
7	G	41	ARG
9	I	127	LYS
10	J	33	GLN
10	J	34	VAL
10	J	50	ILE
10	J	72	VAL
11	K	13	GLN
12	L	79	GLU
12	L	109	GLY
16	P	52	ASP
17	Q	14	LYS
17	Q	80	GLY
19	S	52	TYR
19	S	53	ASN
19	S	69	HIS
2	B	36	ARG
2	B	123	ALA
2	B	232	PRO
3	C	83	ARG
5	E	22	GLY
6	F	38	GLU
7	G	7	ALA
7	G	35	LYS
10	J	32	ALA
10	J	55	LYS
10	J	73	ASP
10	J	83	GLU
11	K	101	SER
12	L	19	ARG
12	L	23	LYS

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Mol	Chain	Res	Type
14	N	23	ARG
17	Q	49	GLU
18	R	25	THR
18	R	54	ARG
20	T	9	ASN
20	T	11	SER
20	T	99	LEU
2	B	178	ARG
3	C	12	LEU
3	C	36	ASP
7	G	138	LYS
9	I	121	ARG
10	J	40	LEU
11	K	127	LYS
12	L	62	SER
13	M	23	TYR
13	M	124	PRO
17	Q	99	SER
19	S	9	VAL
20	T	74	LYS
2	B	20	GLU
2	B	87	ARG
3	C	60	ALA
3	C	146	ALA
4	D	5	ILE
4	D	29	PRO
4	D	208	SER
5	E	153	LYS
7	G	82	GLY
7	G	155	ARG
10	J	31	GLY
11	K	27	ASN
12	L	105	TYR
14	N	14	PRO
15	O	88	ARG
20	T	95	ALA
20	T	97	ALA
2	B	116	GLU
2	B	126	GLU
3	C	98	ASN
4	D	129	ASN
4	D	171	GLY

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Mol	Chain	Res	Type
10	J	36	GLY
12	L	51	ALA
17	Q	98	LEU
20	T	102	GLY
12	L	18	VAL
16	P	10	GLY
3	C	205	GLY
8	H	83	ILE
11	K	48	ILE
3	C	81	GLY
5	E	77	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	B	202/202 (100%)	185 (92%)	17 (8%)	11	38
3	C	160/160 (100%)	152 (95%)	8 (5%)	24	57
4	D	180/180 (100%)	169 (94%)	11 (6%)	18	51
5	E	115/115 (100%)	106 (92%)	9 (8%)	12	41
6	F	90/90 (100%)	86 (96%)	4 (4%)	28	61
7	G	126/126 (100%)	118 (94%)	8 (6%)	18	49
8	H	119/119 (100%)	115 (97%)	4 (3%)	37	67
9	I	98/98 (100%)	91 (93%)	7 (7%)	14	45
10	J	88/88 (100%)	84 (96%)	4 (4%)	27	61
11	K	90/90 (100%)	88 (98%)	2 (2%)	52	76
12	L	104/104 (100%)	100 (96%)	4 (4%)	33	64
13	M	100/100 (100%)	94 (94%)	6 (6%)	19	51
14	N	49/49 (100%)	48 (98%)	1 (2%)	55	78
15	O	79/79 (100%)	76 (96%)	3 (4%)	33	64
16	P	72/72 (100%)	67 (93%)	5 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	Q	96/96 (100%)	92 (96%)	4 (4%)	30 62
18	R	64/64 (100%)	63 (98%)	1 (2%)	62 81
19	S	71/71 (100%)	66 (93%)	5 (7%)	15 46
20	T	76/76 (100%)	73 (96%)	3 (4%)	32 63
21	V	19/19 (100%)	18 (95%)	1 (5%)	22 56
All	All	1998/1998 (100%)	1891 (95%)	107 (5%)	22 55

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	17	PHE
2	B	23	ARG
2	B	24	TRP
2	B	33	TYR
2	B	96	ARG
2	B	110	GLN
2	B	111	ARG
2	B	117	GLU
2	B	153	ARG
2	B	163	PHE
2	B	178	ARG
2	B	204	ASN
2	B	205	ASP
2	B	209	ARG
2	B	226	ARG
2	B	236	TYR
2	B	240	GLN
3	C	21	ARG
3	C	38	ARG
3	C	93	LYS
3	C	105	GLU
3	C	107	GLN
3	C	108	ASN
3	C	131	ARG
3	C	167	TRP
4	D	10	ARG
4	D	49	ARG
4	D	57	ARG
4	D	76	ARG
4	D	83	SER

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Mol	Chain	Res	Type
4	D	122	ARG
4	D	134	ASP
4	D	151	LYS
4	D	168	ARG
4	D	176	LEU
4	D	191	ARG
5	E	10	MET
5	E	18	ARG
5	E	19	MET
5	E	27	ARG
5	E	43	LEU
5	E	64	ARG
5	E	79	GLU
5	E	125	SER
5	E	145	LYS
6	F	47	ARG
6	F	55	ASP
6	F	86	ARG
6	F	92	LYS
7	G	3	ARG
7	G	6	ARG
7	G	8	GLU
7	G	45	ASP
7	G	72	ARG
7	G	76	ARG
7	G	138	LYS
7	G	156	TRP
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	99	GLU
9	I	2	GLU
9	I	58	HIS
9	I	79	LEU
9	I	87	GLN
9	I	104	ARG
9	I	113	LYS
9	I	121	ARG
10	J	9	ARG
10	J	45	ARG
10	J	51	ARG
10	J	59	SER

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Mol	Chain	Res	Type
11	K	92	GLU
11	K	117	ASN
12	L	13	LYS
12	L	28	LYS
12	L	54	LYS
12	L	89	ARG
13	M	14	ARG
13	M	31	LYS
13	M	32	GLU
13	M	50	GLU
13	M	81	LEU
13	M	110	ARG
14	N	9	LYS
15	O	39	LEU
15	O	59	MET
15	O	64	ARG
16	P	1	MET
16	P	8	ARG
16	P	15	PRO
16	P	28	ARG
16	P	42	ARG
17	Q	13	ASP
17	Q	63	ARG
17	Q	70	ARG
17	Q	101	ARG
18	R	53	ARG
19	S	6	LYS
19	S	7	LYS
19	S	12	ASP
19	S	25	LYS
19	S	29	ARG
20	T	19	SER
20	T	42	GLN
20	T	83	ARG
21	V	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
3	C	6	HIS
4	D	161	ASN

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Mol	Chain	Res	Type
6	F	73	ASN
9	I	38	GLN
15	O	46	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1508 (99%)	303 (20%)	51 (3%)
22	W	3/4 (75%)	0	0
23	X	9/11 (81%)	3 (33%)	1 (11%)
All	All	1519/1523 (99%)	306 (20%)	52 (3%)

All (306) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	20	U
1	A	26	A
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	64	G
1	A	65	U
1	A	94	A
1	A	102	A
1	A	108	G
1	A	109	A
1	A	114	C
1	A	123	G
1	A	124	A
1	A	125	C
1	A	138	G
1	A	150	G
1	A	151	G
1	A	156	A
1	A	157	C

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Mol	Chain	Res	Type
1	A	176	U
1	A	189	U
1	A	190	G
1	A	201	A
1	A	203	A
1	A	208	U
1	A	209	U
1	A	211	G
1	A	212	C
1	A	221	G
1	A	226	G
1	A	242	G
1	A	245	A
1	A	246	G
1	A	253	G
1	A	260	G
1	A	261	G
1	A	262	C
1	A	274	A
1	A	276	G
1	A	277	A
1	A	284	G
1	A	288	G
1	A	296	G
1	A	316	A
1	A	323	C
1	A	324	A
1	A	327	G
1	A	339	A
1	A	340	C
1	A	341	G
1	A	342	G
1	A	345	G
1	A	347	C
1	A	349	G
1	A	357	G
1	A	362	U
1	A	364	C
1	A	367	C
1	A	368	A
1	A	379	G
1	A	401	G

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Mol	Chain	Res	Type
1	A	407	A
1	A	408	G
1	A	409	A
1	A	414	C
1	A	417	C
1	A	418	G
1	A	424	U
1	A	434	A
1	A	442	A
1	A	445	A
1	A	446	A
1	A	447	A
1	A	454	A
1	A	455	C
1	A	456	G
1	A	469	G
1	A	479	A
1	A	480	A
1	A	481	U
1	A	483	G
1	A	494	C
1	A	495	U
1	A	501	C
1	A	507	G
1	A	513	G
1	A	515	A
1	A	516	A
1	A	522	A
1	A	528	C
1	A	530	A
1	A	531	G
1	A	542	A
1	A	544	U
1	A	552	C
1	A	553	G
1	A	555	A
1	A	556	A
1	A	559	G
1	A	562	G
1	A	565	U
1	A	566	A
1	A	590	A

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Mol	Chain	Res	Type
1	A	599	G
1	A	616	G
1	A	621	G
1	A	632	G
1	A	636	A
1	A	648	A
1	A	649	G
1	A	655	U
1	A	670	A
1	A	671	G
1	A	684	C
1	A	685	A
1	A	686	G
1	A	688	U
1	A	700	C
1	A	704	G
1	A	705	A
1	A	706	U
1	A	707	G
1	A	733	G
1	A	738	G
1	A	756	G
1	A	760	A
1	A	776	U
1	A	777	A
1	A	778	C
1	A	796	U
1	A	800	C
1	A	811	A
1	A	822	U
1	A	823	C
1	A	824	U
1	A	825	C
1	A	844	G
1	A	846	G
1	A	847	U
1	A	848	U
1	A	849	A
1	A	867	G
1	A	868	U
1	A	879	G
1	A	891	A

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Mol	Chain	Res	Type
1	A	896	A
1	A	899	G
1	A	903	G
1	A	904	G
1	A	911	C
1	A	912	A
1	A	919	G
1	A	920	U
1	A	937	U
1	A	938	U
1	A	943	G
1	A	945	A
1	A	946	A
1	A	948	G
1	A	952	A
1	A	953	G
1	A	954	A
1	A	960	A
1	A	966	C
1	A	968	U
1	A	969	U
1	A	970	G
1	A	975	G
1	A	976	C
1	A	978	A
1	A	979	G
1	A	981	G
1	A	982	A
1	A	983	A
1	A	984	C
1	A	987	G
1	A	994	A
1	A	999	G
1	A	1001	G
1	A	1002	G
1	A	1004	G
1	A	1013	G
1	A	1020	C
1	A	1022	U
1	A	1025	C
1	A	1035	G
1	A	1036	C

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Mol	Chain	Res	Type
1	A	1037	A
1	A	1043	G
1	A	1047	U
1	A	1071	G
1	A	1076	G
1	A	1077	U
1	A	1083	A
1	A	1106	G
1	A	1107	U
1	A	1108	U
1	A	1109	G
1	A	1111	C
1	A	1112	A
1	A	1119	C
1	A	1120	G
1	A	1121	G
1	A	1122	C
1	A	1128	A
1	A	1139	A
1	A	1141	U
1	A	1152	G
1	A	1162	G
1	A	1163	G
1	A	1164	A
1	A	1168	G
1	A	1172	A
1	A	1174	G
1	A	1177	U
1	A	1178	G
1	A	1180	U
1	A	1181	C
1	A	1182	A
1	A	1183	G
1	A	1185	A
1	A	1193	U
1	A	1194	A
1	A	1195	C
1	A	1205	G
1	A	1206	A
1	A	1207	C
1	A	1219	A
1	A	1221	U

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Mol	Chain	Res	Type
1	A	1230	C
1	A	1231	A
1	A	1234	G
1	A	1237	A
1	A	1238	U
1	A	1239	G
1	A	1251	C
1	A	1256	A
1	A	1259	U
1	A	1261	A
1	A	1262	U
1	A	1266	A
1	A	1268	A
1	A	1279	C
1	A	1280	A
1	A	1281	G
1	A	1282	U
1	A	1283	U
1	A	1293	G
1	A	1296	U
1	A	1298	C
1	A	1299	A
1	A	1300	A
1	A	1301	C
1	A	1304	G
1	A	1319	G
1	A	1321	A
1	A	1327	A
1	A	1328	G
1	A	1329	U
1	A	1330	A
1	A	1334	G
1	A	1341	A
1	A	1343	C
1	A	1344	C
1	A	1345	A
1	A	1346	U
1	A	1350	G
1	A	1352	G
1	A	1361	G
1	A	1363	U
1	A	1376	A

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Mol	Chain	Res	Type
1	A	1379	C
1	A	1380	A
1	A	1382	C
1	A	1400	A
1	A	1425	G
1	A	1426	A
1	A	1452	G
1	A	1458	U
1	A	1460	A
1	A	1461	C
1	A	1464	G
1	A	1469	A
1	A	1471	G
1	A	1474	G
1	A	1480	A
1	A	1481	G
1	A	1483	U
1	A	1494	G
1	A	1496	A
1	A	1497	G
1	A	1506	G
1	A	1507	G
1	A	1510	C
1	A	1511	A
1	A	1516	C
23	X	33	U
23	X	34	I
23	X	35	C

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	50	A
1	A	64	G
1	A	101	G
1	A	123	G
1	A	155	A
1	A	175	G
1	A	189	U
1	A	210	U
1	A	211	G

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Mol	Chain	Res	Type
1	A	276	G
1	A	340	C
1	A	407	A
1	A	408	G
1	A	417	C
1	A	445	A
1	A	468	G
1	A	494	C
1	A	500	G
1	A	558	G
1	A	670	A
1	A	684	C
1	A	776	U
1	A	795	C
1	A	847	U
1	A	866	A
1	A	867	G
1	A	959	U
1	A	968	U
1	A	969	U
1	A	1035	G
1	A	1036	C
1	A	1046	G
1	A	1076	G
1	A	1127	C
1	A	1163	G
1	A	1171	G
1	A	1182	A
1	A	1192	U
1	A	1205	G
1	A	1206	A
1	A	1220	A
1	A	1279	C
1	A	1281	G
1	A	1316	C
1	A	1328	G
1	A	1345	A
1	A	1362	U
1	A	1378	A
1	A	1379	C
1	A	1481	G
23	X	34	I

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	RSP	X	32	23	17,21,22	0.97	1 (5%)	22,30,33	1.10	2 (9%)

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
23	RSP	X	32	23	-	7/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	X	32	RSP	C2-N3	2.58	1.38	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	32	RSP	S2-C2-N3	-2.75	116.72	121.49
23	X	32	RSP	C1'-N1-C2	2.38	123.71	118.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	X	32	RSP	C3'-C4'-C5'-O5'
23	X	32	RSP	O4'-C4'-C5'-O5'
23	X	32	RSP	C2'-C1'-N1-C6
23	X	32	RSP	O4'-C1'-N1-C6
23	X	32	RSP	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
23	X	32	RSP	O4'-C1'-N1-C2
23	X	32	RSP	C2'-C1'-N1-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 106 ligands modelled in this entry, 105 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
24	PAR	A	1601	-	45,45,45	1.42	7 (15%)	64,67,67	1.70	15 (23%)

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
24	PAR	A	1601	-	-	2/18/94/94	1/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C52-C42	4.32	1.61	1.52
24	A	1601	PAR	O54-C14	2.96	1.49	1.41
24	A	1601	PAR	C64-C54	2.91	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	PAR	C11-C21	2.55	1.57	1.52
24	A	1601	PAR	C22-C12	-2.52	1.48	1.53
24	A	1601	PAR	C14-C24	2.36	1.57	1.52
24	A	1601	PAR	C62-C52	2.03	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1601	PAR	O33-C14-C24	6.31	119.08	108.22
24	A	1601	PAR	O52-C13-C23	3.86	115.95	107.96
24	A	1601	PAR	O34-C34-C44	-3.48	102.31	110.35
24	A	1601	PAR	C34-C24-N24	-3.13	104.63	111.05
24	A	1601	PAR	O43-C13-C23	-2.97	101.15	104.98
24	A	1601	PAR	O11-C11-O51	2.83	118.57	110.67
24	A	1601	PAR	O34-C34-C24	-2.61	105.53	110.22
24	A	1601	PAR	C13-O52-C52	-2.40	112.02	117.96
24	A	1601	PAR	O52-C13-O43	-2.33	108.91	111.43
24	A	1601	PAR	O54-C54-C44	2.32	113.90	109.69
24	A	1601	PAR	C23-C33-C43	-2.23	99.28	103.22
24	A	1601	PAR	C14-O33-C33	-2.21	112.49	117.96
24	A	1601	PAR	C22-C32-C42	2.19	115.06	109.53
24	A	1601	PAR	O51-C51-C61	2.15	111.78	106.44
24	A	1601	PAR	C34-C44-C54	-2.03	106.61	110.24

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C41-C51-C61-O61
24	A	1601	PAR	O51-C11-O11-C42

All (1) ring outliers are listed below:

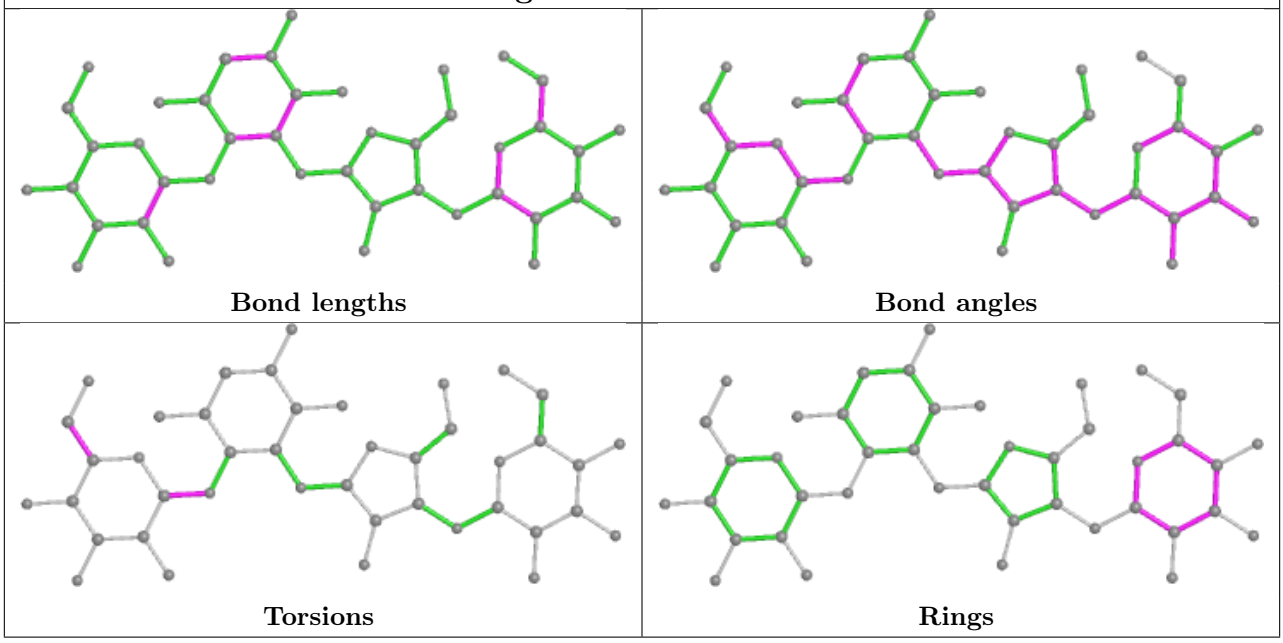
Mol	Chain	Res	Type	Atoms
24	A	1601	PAR	C14-C24-C34-C44-C54-O54

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	PAR	1	0

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

Ligand PAR A 1601



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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1507/1508 (99%)	-0.11	4 (0%) 94 95	66, 105, 180, 256	0
2	B	234/234 (100%)	0.31	12 (5%) 28 28	105, 149, 202, 218	0
3	C	206/206 (100%)	-0.06	6 (2%) 51 51	103, 141, 182, 195	0
4	D	208/208 (100%)	0.08	7 (3%) 45 44	91, 122, 158, 177	0
5	E	150/150 (100%)	-0.15	1 (0%) 87 90	75, 99, 125, 148	0
6	F	101/101 (100%)	-0.18	1 (0%) 82 83	100, 135, 158, 171	0
7	G	155/155 (100%)	-0.20	2 (1%) 77 78	102, 130, 176, 199	0
8	H	138/138 (100%)	-0.14	1 (0%) 87 90	74, 94, 124, 151	0
9	I	127/127 (100%)	0.30	6 (4%) 31 32	91, 146, 179, 196	0
10	J	98/98 (100%)	1.00	23 (23%) 0 0	100, 170, 236, 255	0
11	K	119/119 (100%)	0.04	4 (3%) 45 44	77, 108, 141, 171	0
12	L	124/124 (100%)	0.05	5 (4%) 38 37	66, 104, 143, 174	0
13	M	125/125 (100%)	0.70	17 (13%) 3 2	99, 139, 170, 217	0
14	N	60/60 (100%)	0.23	1 (1%) 70 69	110, 128, 163, 199	0
15	O	88/88 (100%)	0.03	1 (1%) 80 81	83, 108, 146, 186	0
16	P	83/83 (100%)	0.20	1 (1%) 79 79	78, 95, 120, 165	0
17	Q	104/104 (100%)	0.35	5 (4%) 30 31	71, 97, 141, 210	0
18	R	73/73 (100%)	0.29	3 (4%) 37 36	98, 118, 179, 216	0
19	S	80/80 (100%)	0.06	1 (1%) 77 78	123, 163, 195, 205	0
20	T	99/99 (100%)	0.15	1 (1%) 82 83	67, 101, 141, 148	0
21	V	24/24 (100%)	0.28	0 100 100	109, 129, 151, 173	0
22	W	4/4 (100%)	1.21	0 100 100	107, 109, 110, 138	0
23	X	9/11 (81%)	0.23	0 100 100	117, 131, 190, 193	0
All	All	3916/3919 (99%)	0.04	102 (2%) 56 54	66, 116, 183, 256	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	124	PRO	8.5
17	Q	105	ALA	7.3
11	K	128	ALA	7.1
13	M	126	LYS	7.1
10	J	28	ARG	6.4
10	J	34	VAL	6.4
17	Q	104	LYS	6.2
1	A	1516	C	5.9
1	A	1111	C	5.6
13	M	123	ALA	5.6
14	N	12	ARG	5.4
13	M	122	LYS	5.3
15	O	89	GLY	5.3
4	D	35	ARG	5.3
13	M	125	ARG	5.1
13	M	120	LYS	4.8
10	J	74	ILE	4.6
4	D	37	PRO	4.6
11	K	129	SER	4.5
2	B	132	LYS	4.4
10	J	22	LYS	4.4
10	J	30	SER	4.3
11	K	11	LYS	4.2
3	C	206	GLU	4.2
9	I	128	ARG	4.2
19	S	3	ARG	4.1
13	M	41	PRO	4.1
10	J	4	ILE	4.1
10	J	87	THR	4.0
10	J	29	ARG	4.0
2	B	237	ALA	4.0
10	J	72	VAL	4.0
2	B	207	ALA	3.8
10	J	33	GLN	3.8
17	Q	103	GLY	3.7
4	D	47	ARG	3.6
2	B	11	LEU	3.6
10	J	73	ASP	3.5
13	M	43	THR	3.4
18	R	16	PRO	3.3
18	R	18	ARG	3.3
13	M	119	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
10	J	10	GLY	3.3
18	R	17	SER	3.2
10	J	6	ILE	3.1
4	D	38	TYR	3.1
13	M	121	LYS	3.1
17	Q	100	LYS	3.1
4	D	33	MET	3.1
20	T	9	ASN	3.0
10	J	31	GLY	3.0
1	A	1510	C	2.9
13	M	4	ILE	2.8
12	L	112	ASP	2.8
5	E	17	ALA	2.8
3	C	193	TYR	2.8
13	M	39	ILE	2.7
10	J	32	ALA	2.6
4	D	36	ARG	2.6
2	B	136	VAL	2.6
12	L	128	ALA	2.5
7	G	84	ASN	2.5
2	B	131	PRO	2.5
2	B	165	VAL	2.5
9	I	14	VAL	2.5
13	M	40	ASN	2.4
3	C	155	GLY	2.4
10	J	5	ARG	2.4
10	J	37	PRO	2.4
4	D	23	GLY	2.3
10	J	36	GLY	2.3
2	B	192	SER	2.3
10	J	35	SER	2.3
13	M	118	ALA	2.3
17	Q	73	VAL	2.3
12	L	27	LEU	2.3
3	C	196	LEU	2.3
6	F	14	LEU	2.3
10	J	47	PHE	2.3
1	A	1508	A	2.3
9	I	65	VAL	2.2
12	L	19	ARG	2.2
8	H	54	ASP	2.2
13	M	117	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
10	J	99	LYS	2.2
3	C	189	ALA	2.2
9	I	15	ALA	2.2
9	I	101	PHE	2.2
2	B	35	GLU	2.2
13	M	16	ASP	2.2
16	P	83	GLU	2.1
11	K	127	LYS	2.1
10	J	96	ILE	2.1
2	B	10	LEU	2.1
9	I	66	ARG	2.1
10	J	70	ARG	2.1
12	L	33	ARG	2.1
3	C	194	GLY	2.1
13	M	15	VAL	2.0
2	B	163	PHE	2.0
7	G	156	TRP	2.0
2	B	208	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	RSP	X	32	20/21	0.73	0.25	191,199,203,206	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1613	1/1	0.38	0.72	103,103,103,103	0
25	MG	A	1611	1/1	0.51	0.49	101,101,101,101	0
25	MG	A	1686	1/1	0.56	0.81	93,93,93,93	0
25	MG	A	1606	1/1	0.60	1.37	79,79,79,79	0
25	MG	A	1643	1/1	0.62	0.28	113,113,113,113	0
25	MG	A	1612	1/1	0.62	0.94	97,97,97,97	0
25	MG	A	1674	1/1	0.63	0.38	82,82,82,82	0
25	MG	A	1617	1/1	0.63	1.49	101,101,101,101	0
25	MG	A	1676	1/1	0.64	0.50	133,133,133,133	0
25	MG	A	1648	1/1	0.64	0.61	81,81,81,81	0
25	MG	A	1698	1/1	0.65	1.26	100,100,100,100	0
25	MG	A	1609	1/1	0.66	0.31	119,119,119,119	0
25	MG	A	1691	1/1	0.68	0.50	93,93,93,93	0
25	MG	A	1687	1/1	0.68	0.70	105,105,105,105	0
25	MG	A	1664	1/1	0.69	0.47	98,98,98,98	0
25	MG	A	1634	1/1	0.70	1.29	97,97,97,97	0
25	MG	A	1699	1/1	0.70	1.02	94,94,94,94	0
25	MG	A	1675	1/1	0.71	0.69	97,97,97,97	0
25	MG	A	1683	1/1	0.72	1.04	121,121,121,121	0
25	MG	A	1602	1/1	0.75	0.75	92,92,92,92	0
25	MG	A	1679	1/1	0.75	0.52	85,85,85,85	0
25	MG	A	1692	1/1	0.77	1.31	86,86,86,86	0
25	MG	A	1628	1/1	0.79	0.69	84,84,84,84	0
25	MG	A	1697	1/1	0.79	0.38	94,94,94,94	0
25	MG	A	1607	1/1	0.79	0.34	104,104,104,104	0
25	MG	A	1685	1/1	0.79	0.69	86,86,86,86	0
25	MG	A	1605	1/1	0.80	0.13	94,94,94,94	0
25	MG	A	1653	1/1	0.80	0.60	88,88,88,88	0
25	MG	X	101	1/1	0.81	0.47	137,137,137,137	0
25	MG	A	1614	1/1	0.82	0.50	111,111,111,111	0
25	MG	A	1633	1/1	0.82	0.62	99,99,99,99	0
25	MG	A	1662	1/1	0.82	1.03	115,115,115,115	0
25	MG	A	1677	1/1	0.83	0.37	91,91,91,91	0
25	MG	A	1671	1/1	0.83	1.22	74,74,74,74	0
25	MG	W	101	1/1	0.84	0.70	84,84,84,84	0
25	MG	A	1681	1/1	0.85	0.78	91,91,91,91	0
25	MG	A	1610	1/1	0.85	0.37	88,88,88,88	0
25	MG	A	1663	1/1	0.85	0.59	98,98,98,98	0
25	MG	A	1608	1/1	0.85	0.21	108,108,108,108	0
25	MG	A	1646	1/1	0.86	0.31	88,88,88,88	0
25	MG	J	202	1/1	0.86	0.39	95,95,95,95	0
25	MG	A	1632	1/1	0.87	0.61	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1678	1/1	0.87	0.35	92,92,92,92	0
25	MG	A	1668	1/1	0.87	0.13	112,112,112,112	0
25	MG	A	1635	1/1	0.87	0.88	79,79,79,79	0
25	MG	E	201	1/1	0.88	0.94	66,66,66,66	0
25	MG	A	1618	1/1	0.88	0.96	70,70,70,70	0
25	MG	A	1649	1/1	0.89	0.85	78,78,78,78	0
25	MG	A	1665	1/1	0.89	0.12	61,61,61,61	0
25	MG	A	1623	1/1	0.90	0.46	81,81,81,81	0
25	MG	A	1673	1/1	0.90	0.24	115,115,115,115	0
25	MG	A	1680	1/1	0.91	0.46	95,95,95,95	0
25	MG	A	1654	1/1	0.91	0.33	82,82,82,82	0
25	MG	A	1604	1/1	0.91	0.39	86,86,86,86	0
25	MG	A	1696	1/1	0.92	0.40	96,96,96,96	0
25	MG	A	1619	1/1	0.92	0.29	94,94,94,94	0
25	MG	A	1636	1/1	0.92	0.63	86,86,86,86	0
25	MG	A	1672	1/1	0.92	0.99	89,89,89,89	0
25	MG	A	1684	1/1	0.93	0.10	82,82,82,82	0
25	MG	A	1657	1/1	0.93	0.76	60,60,60,60	0
25	MG	A	1647	1/1	0.93	0.42	88,88,88,88	0
25	MG	A	1637	1/1	0.93	1.01	107,107,107,107	0
25	MG	A	1640	1/1	0.93	0.29	90,90,90,90	0
25	MG	A	1615	1/1	0.93	0.32	84,84,84,84	0
25	MG	A	1627	1/1	0.93	0.63	66,66,66,66	0
25	MG	A	1682	1/1	0.94	0.45	121,121,121,121	0
25	MG	A	1645	1/1	0.94	0.14	67,67,67,67	0
25	MG	A	1638	1/1	0.94	0.39	84,84,84,84	0
25	MG	A	1694	1/1	0.94	0.58	72,72,72,72	0
25	MG	A	1625	1/1	0.94	0.35	65,65,65,65	0
25	MG	A	1630	1/1	0.94	0.10	81,81,81,81	0
25	MG	A	1655	1/1	0.95	0.27	71,71,71,71	0
25	MG	A	1670	1/1	0.95	0.67	85,85,85,85	0
25	MG	A	1666	1/1	0.95	0.41	84,84,84,84	0
25	MG	A	1693	1/1	0.96	0.60	83,83,83,83	0
25	MG	A	1629	1/1	0.96	0.51	59,59,59,59	0
25	MG	A	1603	1/1	0.96	0.51	76,76,76,76	0
24	PAR	A	1601	42/42	0.96	0.19	76,88,98,105	0
25	MG	A	1620	1/1	0.96	0.47	56,56,56,56	0
25	MG	A	1656	1/1	0.96	0.54	71,71,71,71	0
25	MG	A	1622	1/1	0.96	0.33	65,65,65,65	0
25	MG	A	1669	1/1	0.96	0.29	90,90,90,90	0
25	MG	A	1659	1/1	0.96	0.59	100,100,100,100	0
25	MG	A	1660	1/1	0.96	0.24	68,68,68,68	0

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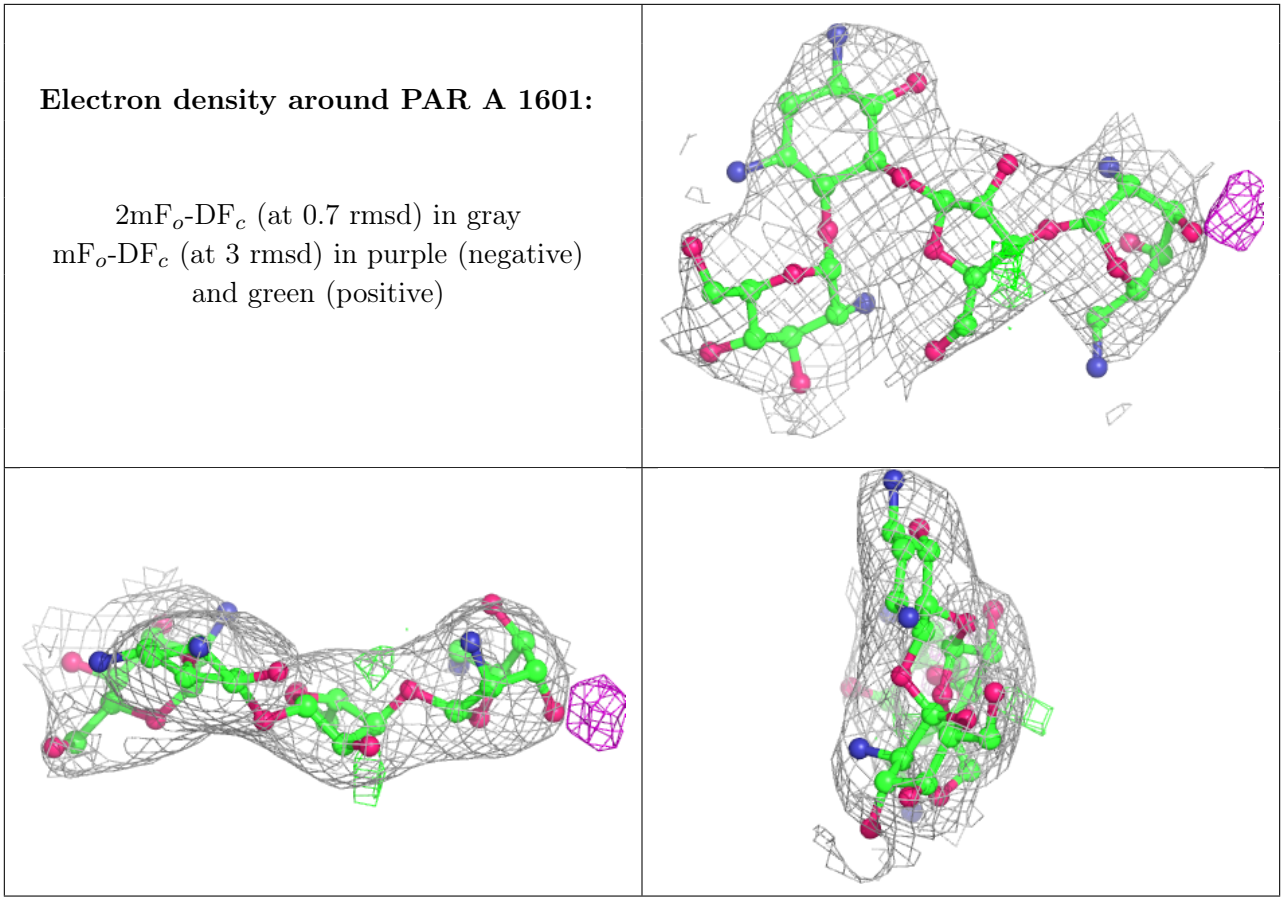
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	MG	A	1642	1/1	0.97	0.27	63,63,63,63	0
25	MG	A	1658	1/1	0.97	0.24	76,76,76,76	0
25	MG	A	1624	1/1	0.97	0.67	56,56,56,56	0
25	MG	A	1644	1/1	0.97	0.51	86,86,86,86	0
25	MG	A	1661	1/1	0.97	1.00	83,83,83,83	0
25	MG	A	1639	1/1	0.97	0.30	81,81,81,81	0
25	MG	A	1689	1/1	0.97	0.34	83,83,83,83	0
25	MG	J	201	1/1	0.97	0.54	90,90,90,90	0
25	MG	A	1690	1/1	0.97	0.28	87,87,87,87	0
25	MG	A	1631	1/1	0.97	0.45	64,64,64,64	0
25	MG	A	1641	1/1	0.97	0.86	63,63,63,63	0
25	MG	A	1688	1/1	0.98	0.44	65,65,65,65	0
25	MG	A	1650	1/1	0.98	0.20	67,67,67,67	0
25	MG	A	1695	1/1	0.98	0.06	105,105,105,105	0
25	MG	A	1621	1/1	0.98	0.56	62,62,62,62	0
25	MG	A	1616	1/1	0.98	0.64	91,91,91,91	0
25	MG	A	1667	1/1	0.98	0.63	101,101,101,101	0
25	MG	A	1651	1/1	0.99	0.14	67,67,67,67	0
25	MG	A	1652	1/1	0.99	0.19	70,70,70,70	0
25	MG	A	1626	1/1	0.99	0.41	76,76,76,76	0
26	ZN	N	101	1/1	0.99	0.18	125,125,125,125	0
26	ZN	D	301	1/1	1.00	0.31	131,131,131,131	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PAR A 1601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.