Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 06:25 am GMT

PDB ID	:	5NRG
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with RB02
Authors	:	Yonath, A.; Matzov, D.; Eyal, Z.; Ben Hamou, R.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Fridman, M.
Deposited on	:	2017-04-23
Resolution	:	3.44 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

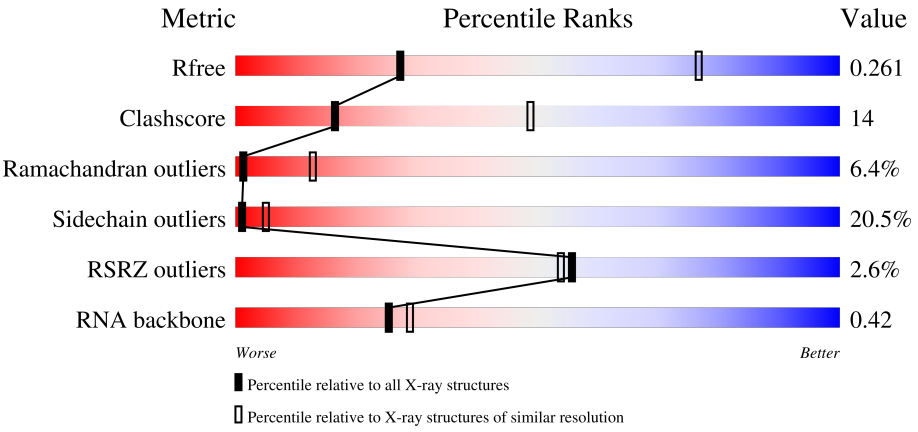
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.44 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	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (3.50-3.38)
RNA backbone	3102	1024 (3.92-2.96)

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	X	2923	34% 38% 18% 7%
2	Y	114	42% 39% 18%
3	A	277	4% 51% 33% 10% 6%

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Mol	Chain	Length	Quality of chain
4	B	220	57% 34% 7%
5	C	207	43% 37% 16%
6	D	179	18% 51% 18% 7% 23%
7	E	178	5% 54% 24% 5% 17%
8	G	145	55% 36% 7%
9	H	122	50% 40% 10%
10	I	140	5% 44% 35% 12% 9%
11	J	144	62% 28% 6%
12	K	122	52% 39% 7%
13	L	119	8% 67% 21% 8%
14	M	116	56% 31% 9%
15	N	118	57% 33% 8%
16	O	102	54% 32% 13%
17	P	117	53% 38%
18	Q	91	10% 49% 38% 11%
19	R	105	10% 58% 30% 9%
20	S	217	6% 45% 30% 6% 20%
21	T	94	56% 21% 19%
22	V	69	41% 38% 16% 6%
23	W	59	49% 41% 7%
24	Z	58	38% 31% 7% 24%
25	2	45	16% 56% 33% 9%
26	3	66	74% 21%

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
29	MN	X	3062	-	-	-	X
29	MN	X	3075	-	-	-	X
30	MG	3	104	-	-	-	X
30	MG	J	201	-	-	-	X
30	MG	X	3202	-	-	-	X
30	MG	X	3242	-	-	-	X
30	MG	X	3260	-	-	-	X
30	MG	X	3264	-	-	-	X
30	MG	X	3266	-	-	-	X
30	MG	X	3271	-	-	-	X
30	MG	X	3274	-	-	-	X
30	MG	X	3279	-	-	-	X
30	MG	X	3280	-	-	-	X
30	MG	X	3283	-	-	-	X

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 80800 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	X	2710	58141	25956	10658	18816	2711	0	1	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	260	1641	1008	314	315	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1534	961	287	281	5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	198	1365	852	256	255	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	137	926	580	165	177	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	E	147	Total	C	N	O	0	0	0
			793	481	154	158			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1062	664	194	201	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			902	561	173	166	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	127	Total	C	N	O	0	0	0
			780	467	162	151			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1011	651	184	172	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			883	539	176	167	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			672	410	126	136			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	111	Total 779	C 492	N 147	O 140	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total 937	C 590	N 186	O 157	S 4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	101	Total 700	C 445	N 128	O 127	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total 852	C 532	N 161	O 156	S 3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total 656	C 411	N 111	O 132	S 2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	102	Total 596	C 365	N 111	O 120	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	174	Total 1145	C 722	N 204	O 217	S 2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	76	Total	C	N	O	0	0	0
			561	349	107	105			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	0	0	0
			519	319	96	104			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	W	57	Total	C	N	O	0	0	0
			437	272	83	82			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Z	44	Total	C	N	O	S	0	0	0
			337	205	75	54	3			

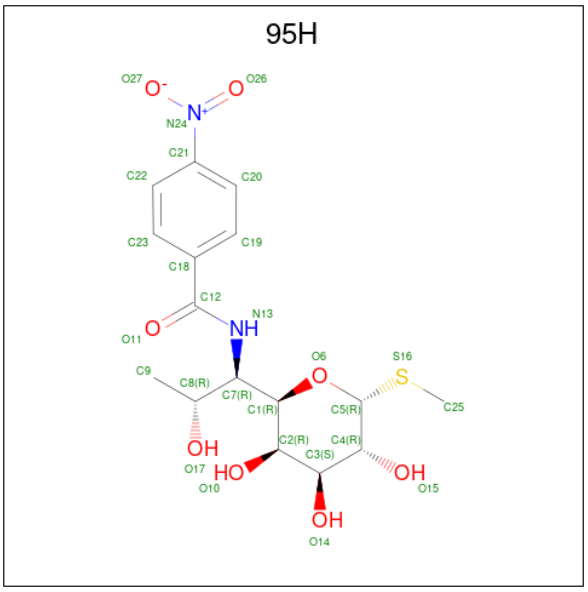
- Molecule 25 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	2	44	Total	C	N	O	S	0	0	0
			360	219	87	53	1			

- Molecule 26 is a protein called 50S ribosomal protein L35.

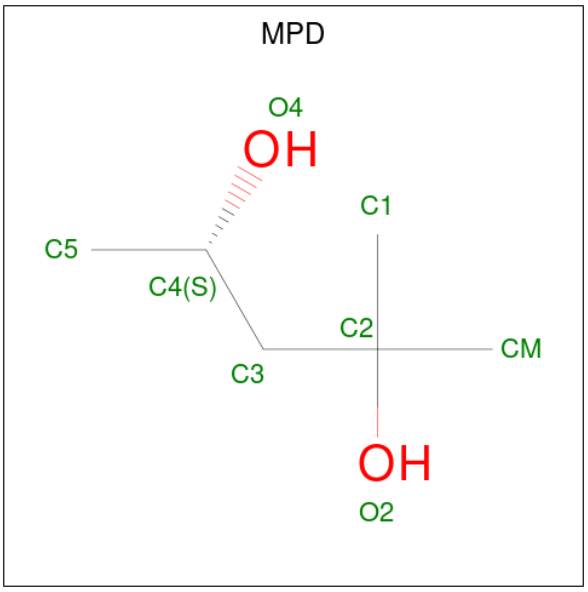
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	3	65	Total	C	N	O	S	0	0	0
			419	257	83	78	1			

- Molecule 27 is {N}-[(1 {R},2 {R})-1-[(2 {R},3 {R},4 {S},5 {R},6 {R})-6-methylsulfanyl-3, 4,5-tris(oxidanyl)oxan-2-yl]-2-oxidanyl-propy l]-4-nitro-benzamide (three-letter code: 95H) (formula: $C_{16}H_{22}N_2O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
27	X	1	Total	C	N	O	S	1	0
			27	16	2	8	1		

- Molecule 28 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	X	1	Total	C	O	0	0
			8	6	2		
28	X	1	Total	C	O	0	0
			8	6	2		

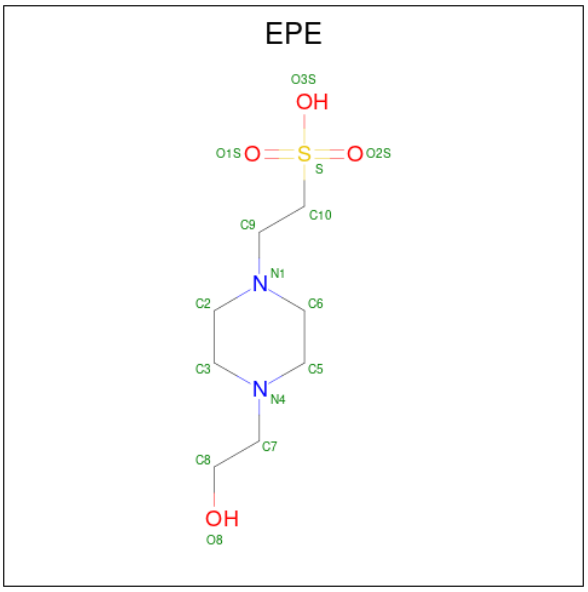
- Molecule 29 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	203	Total Mn 203 203	0	0
29	Y	1	Total Mn 1 1	0	0
29	E	1	Total Mn 1 1	0	0
29	I	1	Total Mn 1 1	0	0
29	Z	1	Total Mn 1 1	0	0
29	3	3	Total Mn 3 3	0	0

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

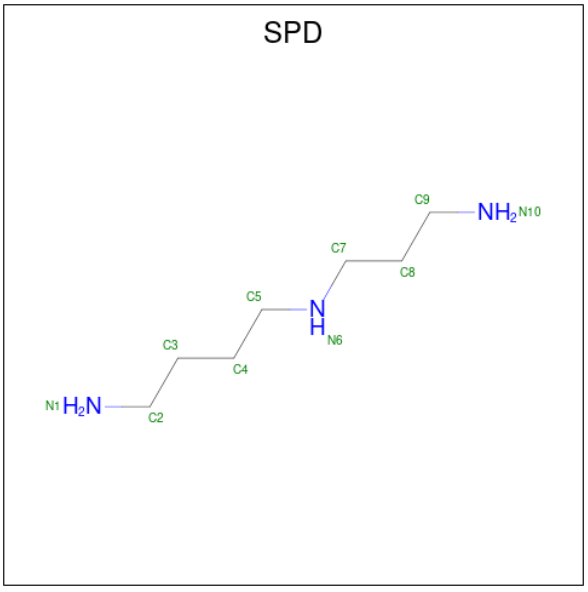
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	78	Total Mg 78 78	0	0
30	Y	2	Total Mg 2 2	0	0
30	C	1	Total Mg 1 1	0	0
30	G	1	Total Mg 1 1	0	0
30	J	1	Total Mg 1 1	0	0
30	3	1	Total Mg 1 1	0	0

- Molecule 31 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 32 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

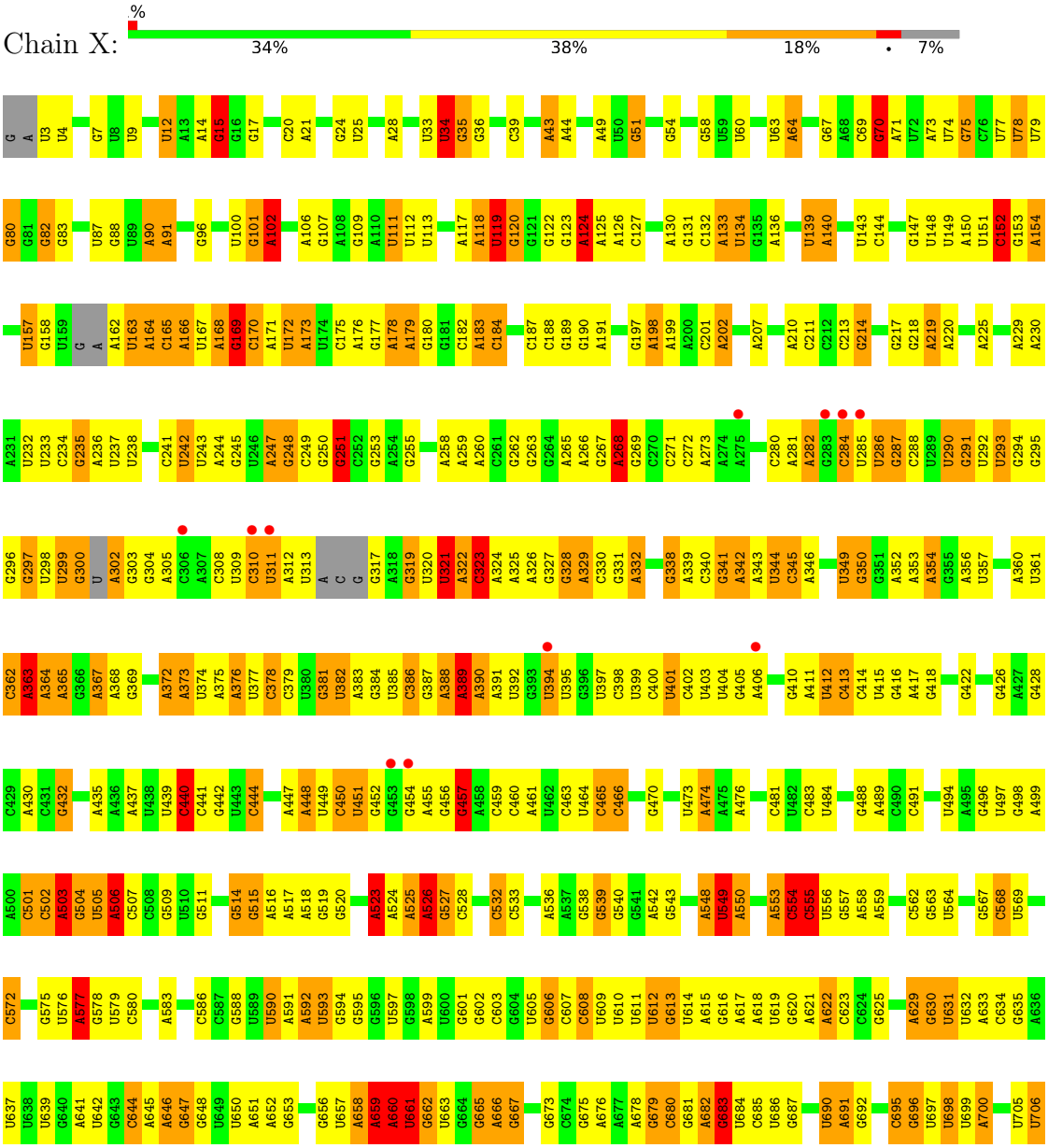


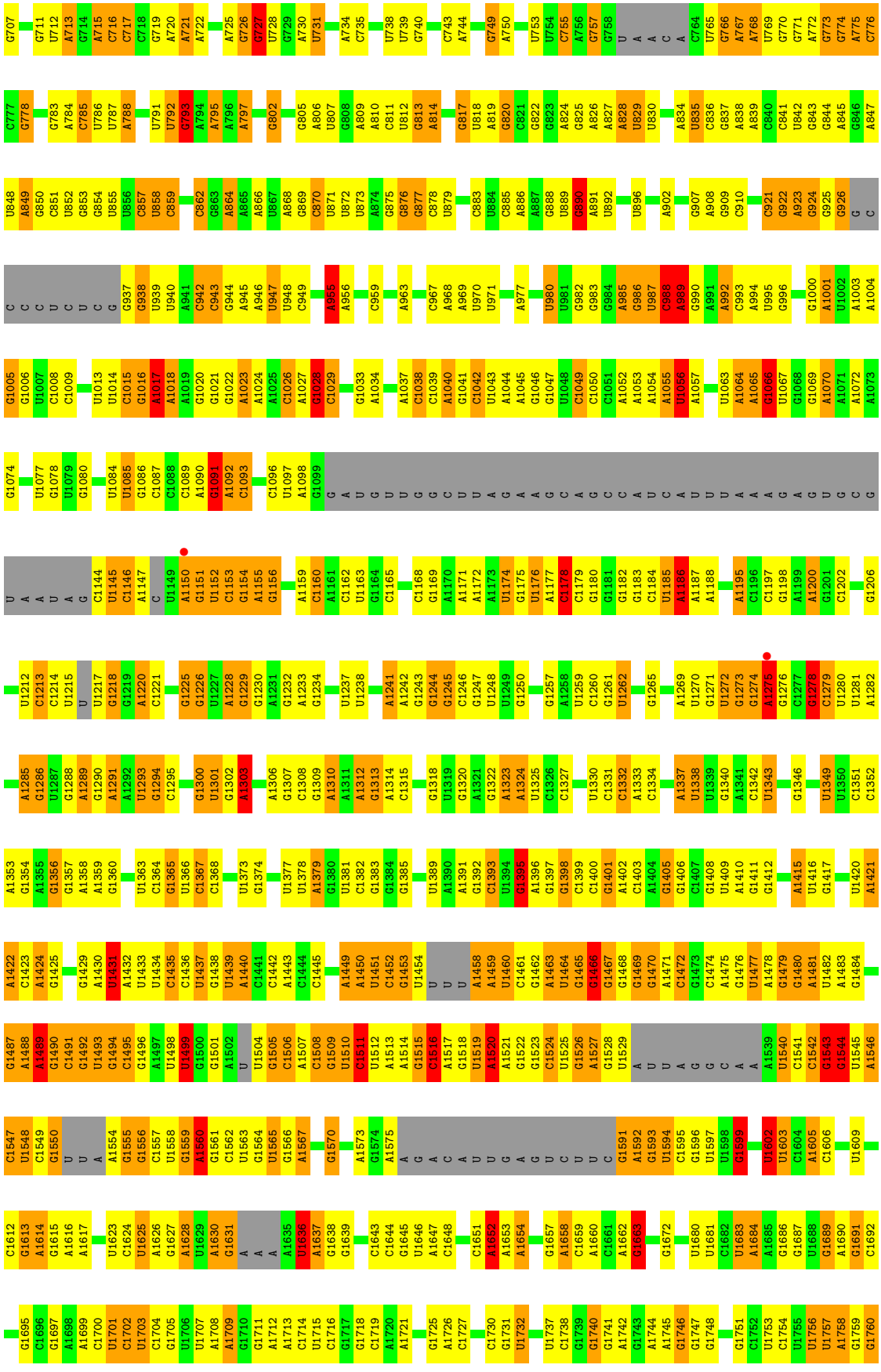
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N		0	0
			10	7	3			

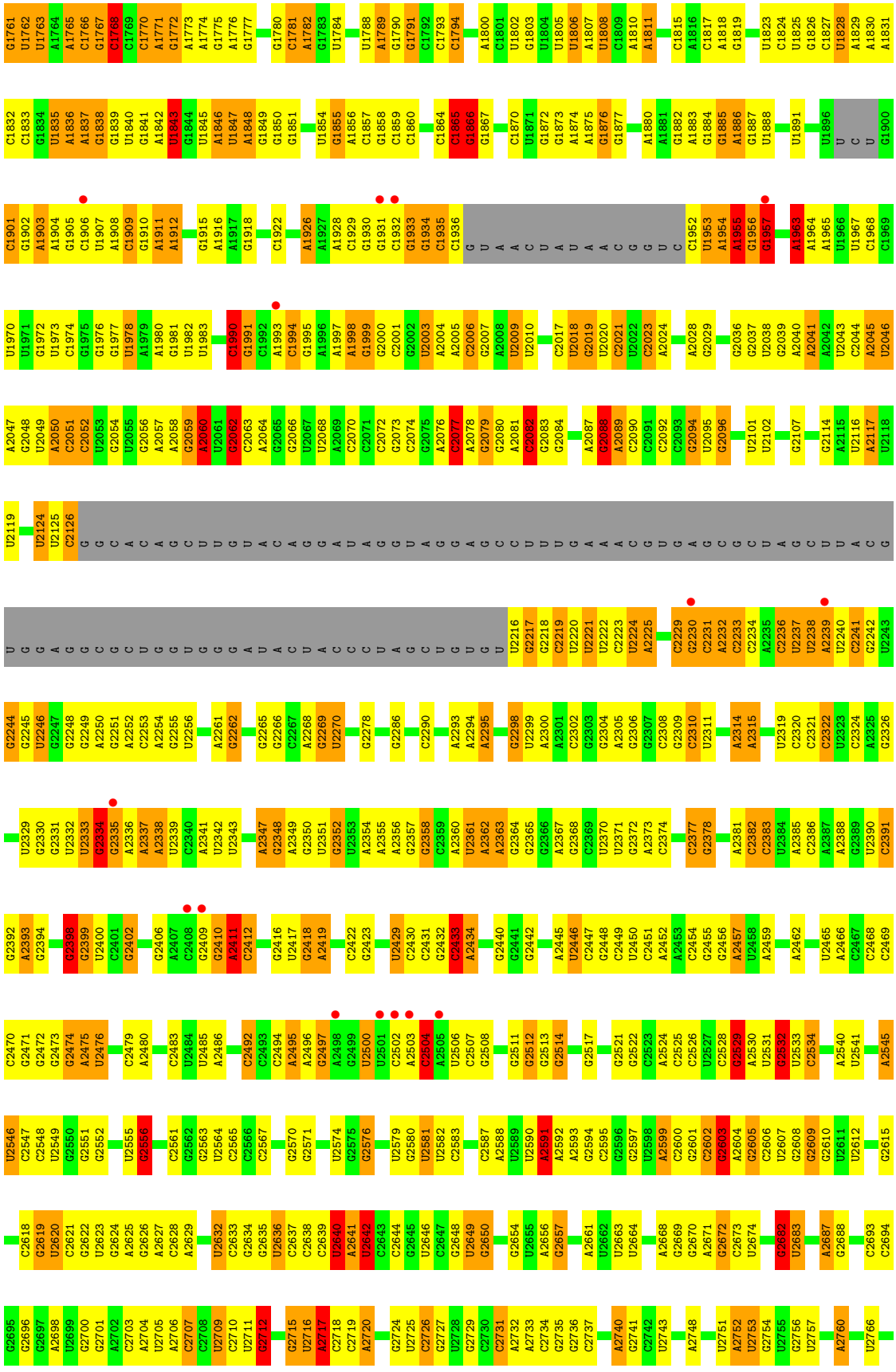
3 Residue-property plots (i)

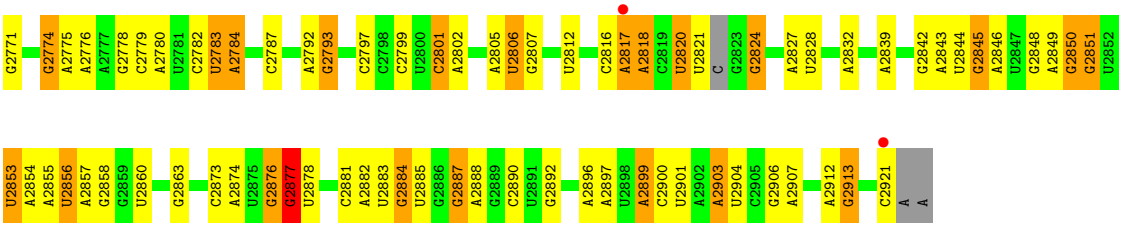
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 23S ribosomal RNA

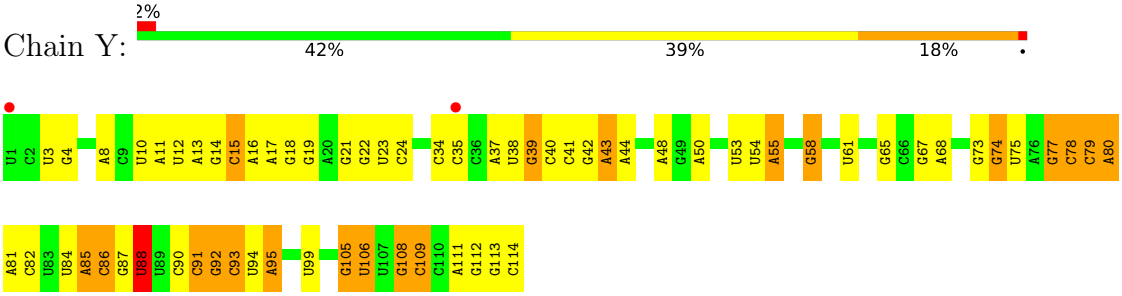




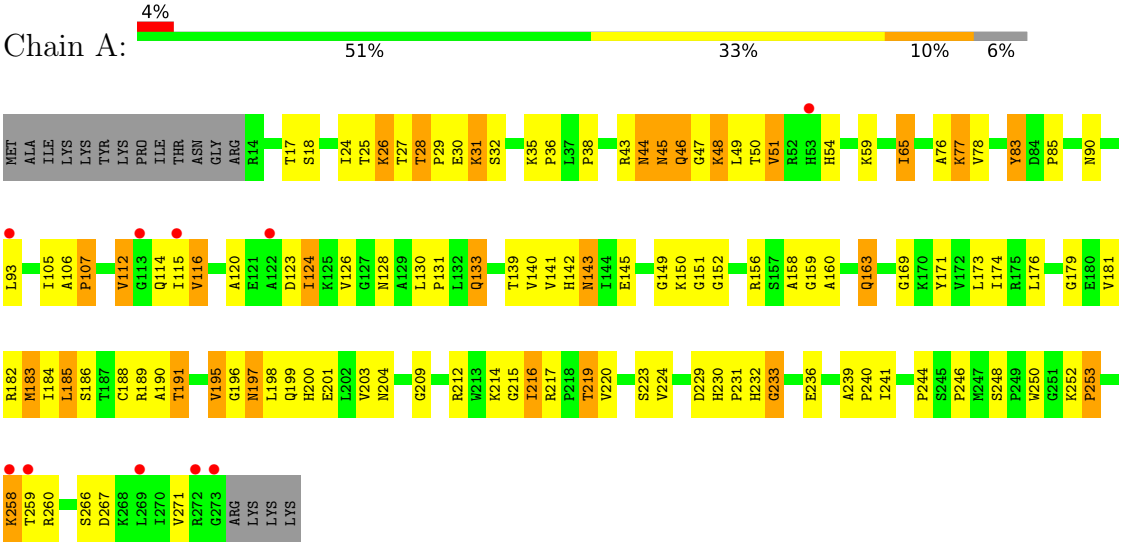




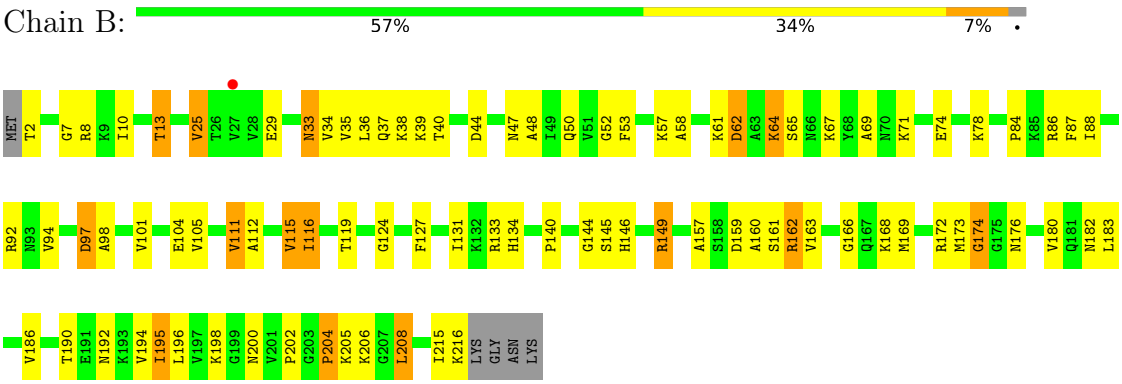
• Molecule 2: 5S ribosomal RNA



• Molecule 3: 50S ribosomal protein L2

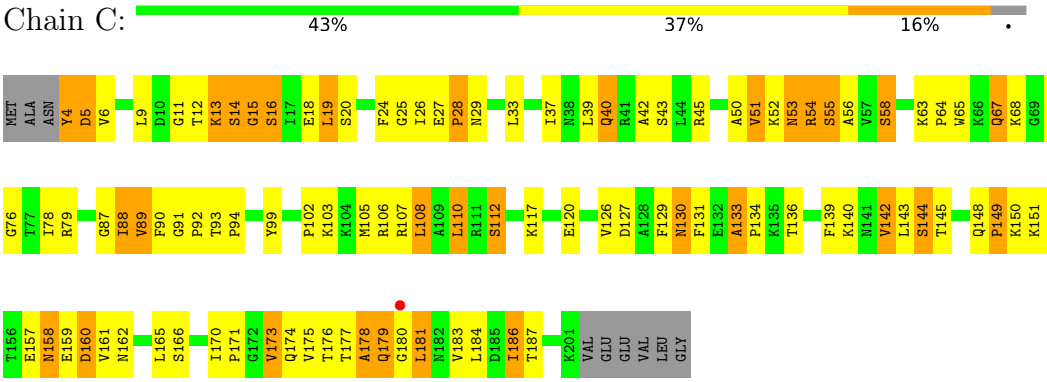


• Molecule 4: 50S ribosomal protein L3



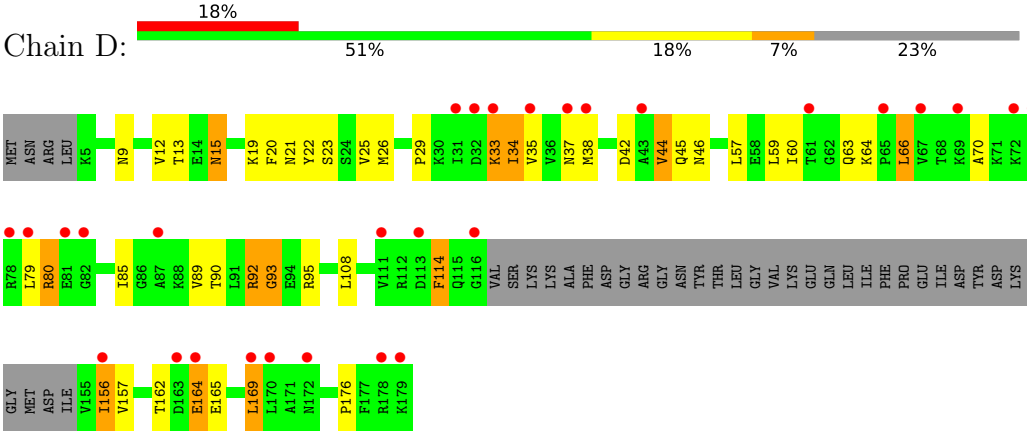
• Molecule 5: 50S ribosomal protein L4

Chain C:



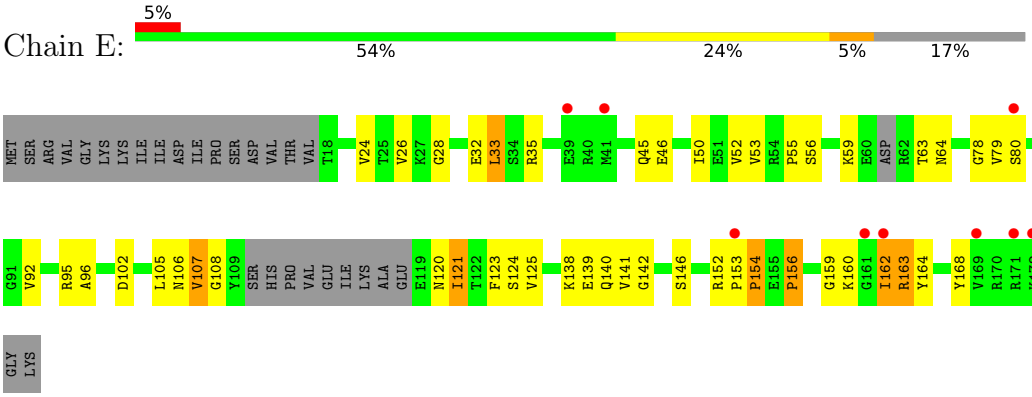
• Molecule 6: 50S ribosomal protein L5

Chain D:



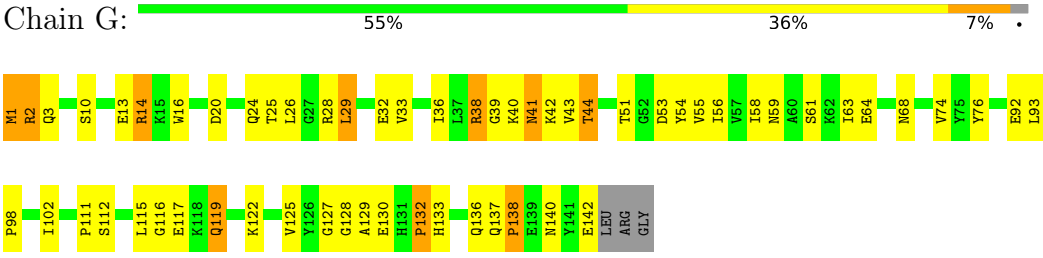
• Molecule 7: 50S ribosomal protein L6

Chain E:



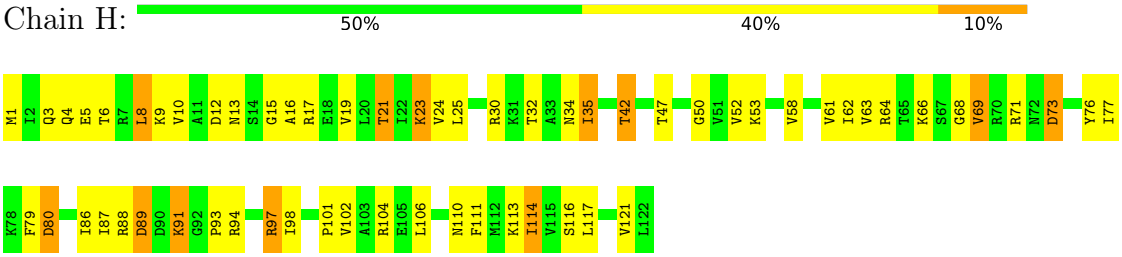
• Molecule 8: 50S ribosomal protein L13

Chain G:



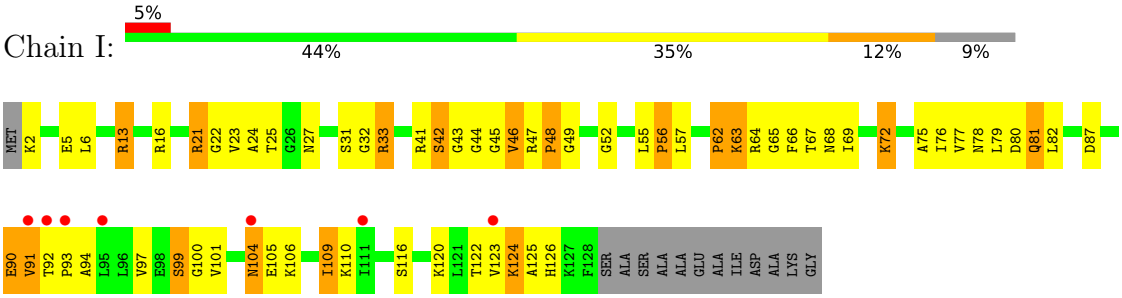
• Molecule 9: 50S ribosomal protein L14

Chain H:



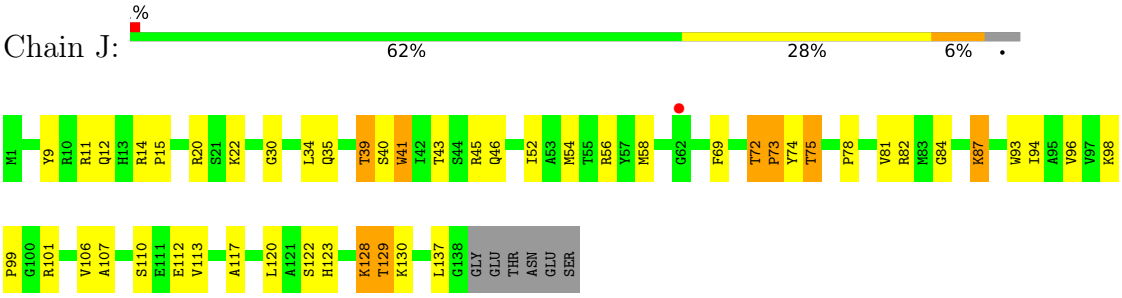
• Molecule 10: 50S ribosomal protein L15

Chain I:



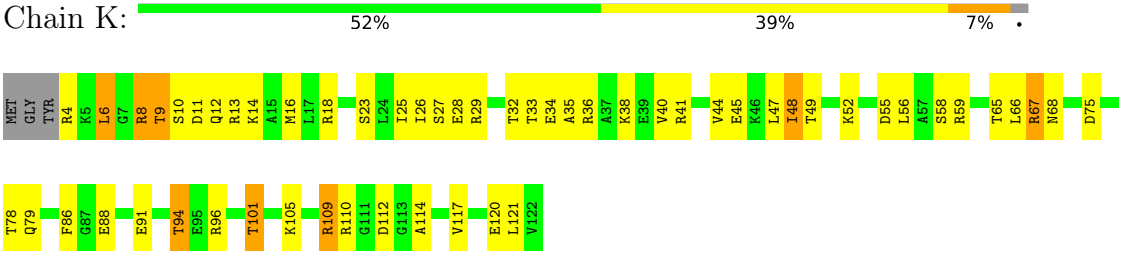
• Molecule 11: 50S ribosomal protein L16

Chain J:



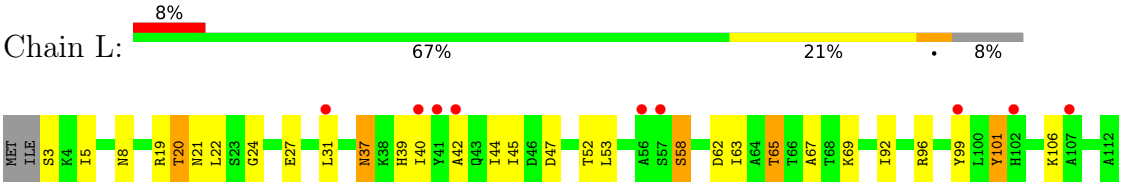
• Molecule 12: 50S ribosomal protein L17

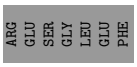
Chain K:



• Molecule 13: 50S ribosomal protein L18

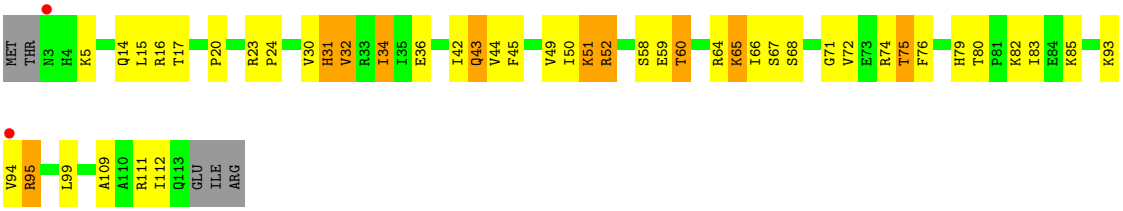
Chain L:





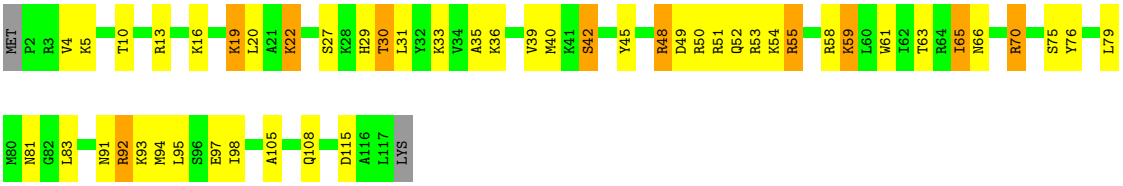
• Molecule 14: 50S ribosomal protein L19

Chain M:



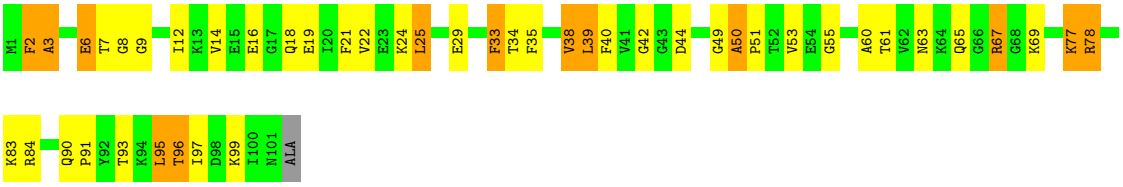
• Molecule 15: 50S ribosomal protein L20

Chain N:



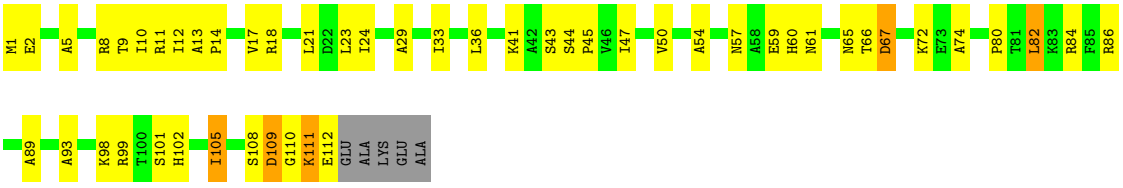
• Molecule 16: 50S ribosomal protein L21

Chain O:



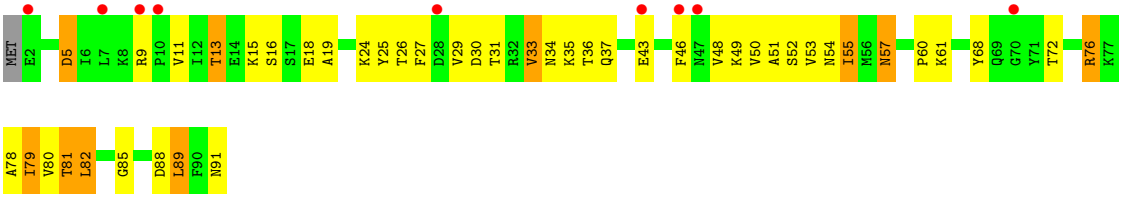
• Molecule 17: 50S ribosomal protein L22

Chain P:

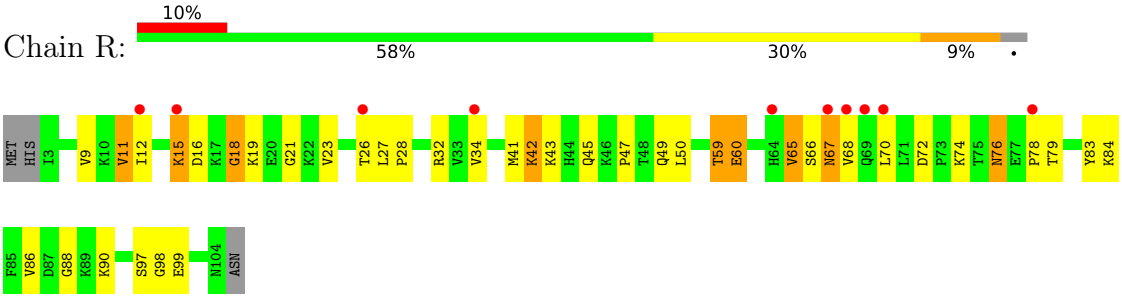


• Molecule 18: 50S ribosomal protein L23

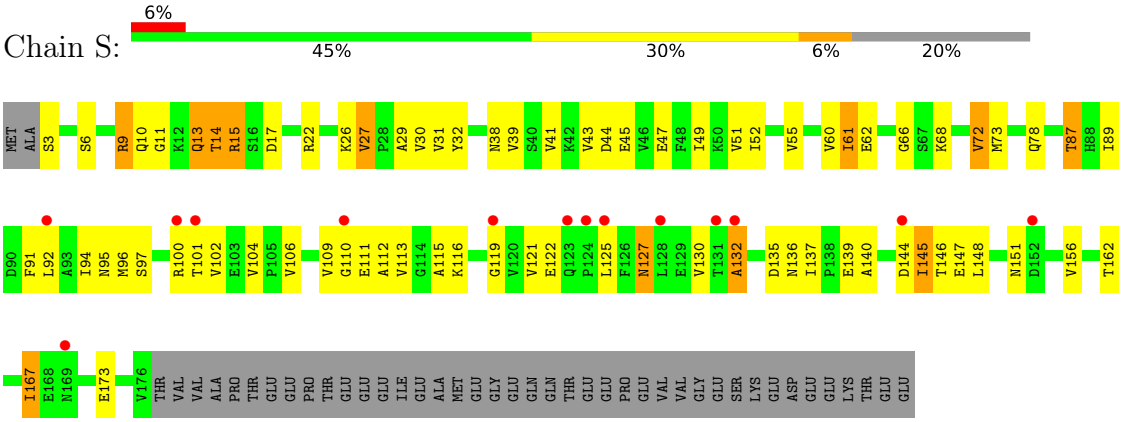
Chain Q:



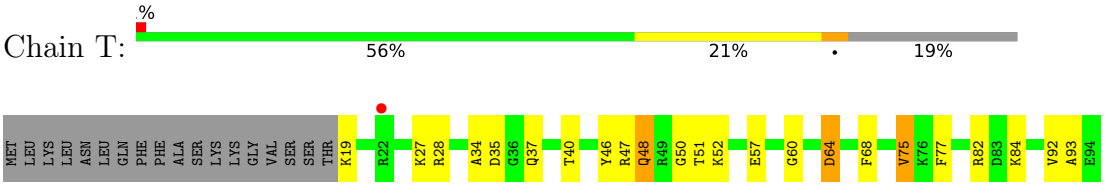
• Molecule 19: 50S ribosomal protein L24



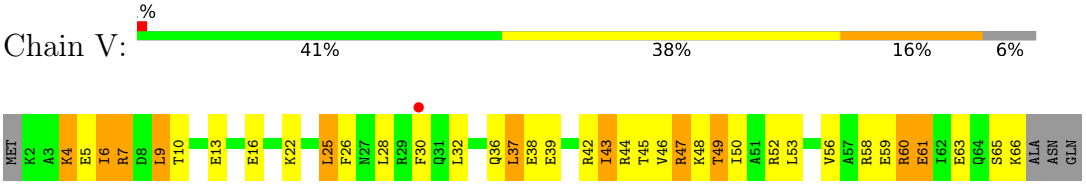
• Molecule 20: 50S ribosomal protein L25



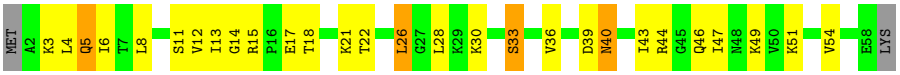
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L29

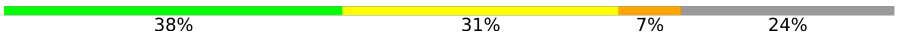


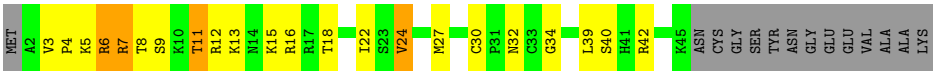
• Molecule 23: 50S ribosomal protein L30



• Molecule 24: 50S ribosomal protein L32

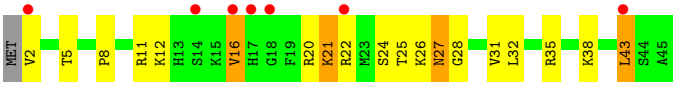
Chain Z:





• Molecule 25: 50S ribosomal protein L34

Chain 2:



• Molecule 26: 50S ribosomal protein L35

Chain 3:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	279.80Å 279.80Å 873.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.37 – 3.44 49.77 – 3.44	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.37-3.44) 96.1 (49.77-3.44)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.219 , 0.261 0.219 , 0.261	Depositor DCC
R_{free} test set	12721 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	99.6	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 72.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	80800	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SPD, EPE, MG, MN, MPD, 95H

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	X	0.86	66/65104 (0.1%)	1.53	1119/101503 (1.1%)
2	Y	0.76	1/2717 (0.0%)	1.41	46/4232 (1.1%)
3	A	0.49	0/1665	0.73	0/2275
4	B	0.58	0/1557	0.71	0/2102
5	C	0.60	0/1386	0.82	1/1890 (0.1%)
6	D	0.45	1/934 (0.1%)	0.53	0/1273
7	E	0.29	0/798	0.58	0/1102
8	G	0.47	0/1083	0.67	0/1466
9	H	0.49	0/908	0.71	0/1221
10	I	0.45	0/789	0.77	0/1073
11	J	0.57	1/1034 (0.1%)	0.65	1/1401 (0.1%)
12	K	0.40	0/885	0.62	0/1185
13	L	0.35	0/678	0.58	0/934
14	M	0.53	0/790	0.80	0/1071
15	N	0.62	0/949	0.79	0/1258
16	O	0.62	1/710 (0.1%)	0.84	1/962 (0.1%)
17	P	0.64	0/860	0.73	0/1159
18	Q	0.46	0/662	0.62	0/898
19	R	0.44	0/601	0.67	0/830
20	S	0.43	0/1158	0.58	0/1588
21	T	0.49	0/567	0.70	0/756
22	V	0.43	0/520	0.61	0/694
23	W	0.56	0/439	0.67	0/592
24	Z	0.59	0/342	0.73	0/456
25	2	0.66	0/363	0.73	0/475
26	3	0.41	0/424	0.70	0/578
All	All	0.79	70/87923 (0.1%)	1.39	1168/132974 (0.9%)

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	A	0	3
4	B	0	5
5	C	0	5
7	E	0	1
8	G	0	5
9	H	0	1
10	I	0	4
11	J	0	1
14	M	0	1
16	O	0	2
18	Q	0	1
19	R	0	2
All	All	0	31

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2088	G	C8-N7	15.26	1.40	1.30
1	X	2474	G	C8-N7	15.10	1.40	1.30
1	X	2059	G	C5-C4	12.16	1.46	1.38
1	X	1000	G	C5-C4	-11.92	1.30	1.38
1	X	1931	G	N3-C4	10.72	1.43	1.35
1	X	1715	U	C5-C6	10.55	1.43	1.34
1	X	2845	G	N9-C4	-10.19	1.29	1.38
1	X	1186	A	N9-C4	-10.07	1.31	1.37
1	X	828	A	N9-C4	-9.88	1.31	1.37
11	J	69	PHE	C-N	-9.63	1.16	1.34
1	X	2089[A]	A	N3-C4	9.41	1.40	1.34
1	X	2089[B]	A	N3-C4	9.41	1.40	1.34
1	X	1289	A	N9-C4	-9.22	1.32	1.37
1	X	2474	G	N9-C8	9.10	1.44	1.37
1	X	1931	G	N9-C4	8.76	1.45	1.38
1	X	2088	G	N7-C5	8.66	1.44	1.39
6	D	108	LEU	C-N	8.62	1.50	1.34
1	X	1715	U	N1-C6	7.62	1.44	1.38
1	X	1000	G	N7-C5	7.32	1.43	1.39
1	X	630	G	N9-C4	-7.18	1.32	1.38
1	X	2845	G	C2-N3	-6.86	1.27	1.32
16	O	77	LYS	CA-CB	6.69	1.68	1.53
1	X	2088	G	N9-C8	6.68	1.42	1.37
1	X	373	A	C6-N6	6.62	1.39	1.33
1	X	2740	A	N9-C4	-6.59	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1303	A	N9-C4	-6.57	1.33	1.37
1	X	550	A	P-O5'	6.54	1.66	1.59
1	X	992	A	N9-C4	-6.44	1.33	1.37
1	X	2797	C	C4-N4	6.39	1.39	1.33
1	X	1065	A	N9-C4	-6.38	1.34	1.37
1	X	1289	A	C5-C4	6.25	1.43	1.38
1	X	2059	G	C8-N7	6.24	1.34	1.30
1	X	1000	G	N9-C8	-5.94	1.33	1.37
2	Y	92	G	N9-C4	-5.93	1.33	1.38
1	X	1278	G	N9-C4	-5.84	1.33	1.38
1	X	428	G	N9-C4	5.80	1.42	1.38
1	X	2446	U	C5-C6	5.77	1.39	1.34
1	X	373	A	C5-C4	5.76	1.42	1.38
1	X	1178	C	N1-C6	5.74	1.40	1.37
1	X	2707	C	N1-C6	-5.74	1.33	1.37
1	X	350	G	N9-C4	5.70	1.42	1.38
1	X	1186	A	N3-C4	-5.66	1.31	1.34
1	X	1758	A	N9-C4	5.66	1.41	1.37
1	X	1303	A	C5-C6	-5.64	1.35	1.41
1	X	1751	G	N9-C8	5.64	1.41	1.37
1	X	428	G	N3-C4	5.60	1.39	1.35
1	X	518	A	N9-C4	-5.56	1.34	1.37
1	X	515	G	N9-C8	5.55	1.41	1.37
1	X	2059	G	C5-C6	5.52	1.47	1.42
1	X	2402	G	N7-C5	5.51	1.42	1.39
1	X	1289	A	N3-C4	-5.44	1.31	1.34
1	X	2545	A	N9-C4	5.44	1.41	1.37
1	X	1289	A	N9-C8	5.43	1.42	1.37
1	X	859	C	N1-C6	-5.39	1.33	1.37
1	X	1360	G	N9-C4	-5.36	1.33	1.38
1	X	955	A	N3-C4	5.34	1.38	1.34
1	X	2059	G	N9-C8	5.33	1.41	1.37
1	X	1065	A	N3-C4	-5.27	1.31	1.34
1	X	553	A	C5-C6	5.25	1.45	1.41
1	X	2661	A	C5-C4	-5.24	1.35	1.38
1	X	575	G	N9-C8	5.24	1.41	1.37
1	X	54	G	C8-N7	5.24	1.34	1.30
1	X	503	A	C5-C6	-5.23	1.36	1.41
1	X	1489	A	N9-C4	5.20	1.41	1.37
1	X	602	G	N9-C4	-5.18	1.33	1.38
1	X	1003	A	N9-C4	-5.13	1.34	1.37
1	X	2740	A	N3-C4	-5.10	1.31	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	2845	G	N3-C4	-5.07	1.31	1.35
1	X	1285	A	N9-C4	-5.04	1.34	1.37
1	X	515	G	C5-C4	5.02	1.41	1.38

All (1168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2474	G	C5-N7-C8	-23.23	92.68	104.30
1	X	2088	G	C5-N7-C8	-21.74	93.43	104.30
1	X	2059	G	C6-C5-N7	20.68	142.81	130.40
1	X	2059	G	C4-C5-C6	-20.37	106.58	118.80
1	X	2845	G	N3-C4-C5	18.55	137.88	128.60
1	X	2088	G	N7-C8-N9	18.50	122.35	113.10
1	X	2059	G	N3-C4-N9	-18.40	114.96	126.00
1	X	2474	G	N7-C8-N9	18.30	122.25	113.10
1	X	1303	A	C2-N3-C4	-17.05	102.07	110.60
1	X	2845	G	N3-C4-N9	-16.89	115.87	126.00
1	X	2474	G	C8-N9-C4	-16.52	99.79	106.40
1	X	2088	G	C8-N9-C4	-16.52	99.79	106.40
1	X	2474	G	C4-C5-N7	16.41	117.36	110.80
1	X	1186	A	C2-N3-C4	-16.05	102.58	110.60
1	X	1560	A	N1-C6-N6	-15.97	109.02	118.60
1	X	1065	A	C2-N3-C4	-15.77	102.71	110.60
1	X	2059	G	N3-C4-C5	14.91	136.06	128.60
1	X	1931	G	N3-C4-N9	13.53	134.12	126.00
1	X	1289	A	C2-N3-C4	-13.50	103.85	110.60
1	X	1000	G	C5-C6-O6	13.43	136.66	128.60
1	X	2059	G	C8-N9-C4	-12.99	101.20	106.40
1	X	630	G	N3-C4-C5	12.92	135.06	128.60
1	X	2845	G	C2-N3-C4	-12.92	105.44	111.90
1	X	2059	G	N7-C8-N9	12.89	119.55	113.10
1	X	2797	C	N3-C4-C5	-12.73	116.81	121.90
1	X	1715	U	C5-C6-N1	12.63	129.01	122.70
1	X	2079	G	C5-C6-O6	-12.50	121.10	128.60
1	X	2797	C	C5-C4-N4	12.47	128.93	120.20
1	X	721	A	C2-N3-C4	-12.43	104.39	110.60
1	X	373	A	C5-C6-N1	-12.16	111.62	117.70
2	Y	93	C	N3-C2-O2	-12.10	113.43	121.90
1	X	1278	G	N3-C4-N9	-12.08	118.75	126.00
1	X	1000	G	N1-C6-O6	-11.98	112.71	119.90
1	X	1843	U	C5-C6-N1	11.78	128.59	122.70
1	X	2845	G	N3-C2-N2	-11.65	111.75	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2716	U	C5-C4-O4	11.61	132.87	125.90
1	X	515	G	C4-C5-N7	11.56	115.42	110.80
1	X	1186	A	C5-C6-N1	-11.46	111.97	117.70
1	X	2845	G	C5-N7-C8	-11.44	98.58	104.30
1	X	1244	G	N9-C4-C5	11.32	109.93	105.40
1	X	575	G	C5-N7-C8	-11.30	98.65	104.30
1	X	515	G	N7-C8-N9	11.30	118.75	113.10
1	X	1229	G	O5'-P-OP2	-11.27	95.56	105.70
1	X	1702	C	OP1-P-OP2	11.22	136.42	119.60
1	X	630	G	N3-C4-N9	-11.18	119.29	126.00
1	X	630	G	C2-N3-C4	-10.88	106.46	111.90
1	X	1278	G	N3-C4-C5	10.80	134.00	128.60
1	X	1520	A	C2-N3-C4	-10.80	105.20	110.60
1	X	797	A	N1-C6-N6	10.79	125.08	118.60
1	X	2433	C	N1-C2-O2	10.79	125.37	118.90
1	X	515	G	C5-N7-C8	-10.72	98.94	104.30
1	X	1289	A	C5-N7-C8	-10.72	98.54	103.90
1	X	2059	G	N1-C6-O6	-10.70	113.48	119.90
1	X	1715	U	C6-N1-C1'	10.64	136.09	121.20
1	X	350	G	N3-C4-C5	-10.63	123.28	128.60
2	Y	92	G	N3-C4-C5	10.63	133.92	128.60
1	X	2474	G	C6-C5-N7	-10.57	124.06	130.40
1	X	1065	A	N1-C2-N3	10.38	134.49	129.30
1	X	1702	C	O5'-P-OP2	-10.37	96.37	105.70
1	X	1000	G	N9-C4-C5	10.34	109.54	105.40
1	X	1560	A	C5-C6-N1	10.25	122.83	117.70
1	X	2088	G	N9-C4-C5	10.20	109.48	105.40
1	X	955	A	N9-C4-C5	-10.17	101.73	105.80
1	X	350	G	N3-C4-N9	10.12	132.07	126.00
1	X	2845	G	N1-C6-O6	10.10	125.96	119.90
2	Y	93	C	N1-C2-O2	10.10	124.96	118.90
1	X	695	C	N3-C4-C5	-10.07	117.87	121.90
1	X	2088	G	C4-C5-N7	10.05	114.82	110.80
1	X	828	A	C2-N3-C4	-10.02	105.59	110.60
1	X	858	U	O5'-P-OP2	-10.00	96.70	105.70
1	X	1065	A	C5-C6-N1	-9.99	112.70	117.70
1	X	323	C	C6-N1-C2	-9.99	116.31	120.30
1	X	1931	G	N9-C4-C5	-9.97	101.41	105.40
1	X	2081	A	N1-C2-N3	9.91	134.25	129.30
2	Y	88	U	C2-N1-C1'	9.91	129.59	117.70
1	X	2411	A	O4'-C1'-N9	9.90	116.12	108.20
1	X	1715	U	C4-C5-C6	-9.88	113.77	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	503	A	C5-N7-C8	-9.87	98.97	103.90
1	X	2716	U	N3-C4-O4	-9.87	112.49	119.40
1	X	1303	A	N3-C4-C5	9.81	133.67	126.80
1	X	2474	G	N1-C6-O6	9.79	125.77	119.90
1	X	2474	G	C8-N9-C1'	9.71	139.62	127.00
1	X	1957	G	C6-C5-N7	9.66	136.19	130.40
1	X	1024	A	N1-C6-N6	9.63	124.38	118.60
1	X	1065	A	N1-C6-N6	9.62	124.37	118.60
1	X	2740	A	C5-C6-N1	-9.55	112.92	117.70
1	X	2088	G	C8-N9-C1'	9.54	139.40	127.00
1	X	1165	C	C6-N1-C2	-9.53	116.49	120.30
1	X	2089[A]	A	C6-C5-N7	-9.50	125.65	132.30
1	X	2089[B]	A	C6-C5-N7	-9.50	125.65	132.30
1	X	515	G	C8-N9-C4	-9.48	102.61	106.40
1	X	2059	G	C5-C6-N1	9.41	116.21	111.50
1	X	575	G	N7-C8-N9	9.41	117.80	113.10
1	X	575	G	C4-C5-N7	9.37	114.55	110.80
1	X	515	G	C6-C5-N7	-9.36	124.78	130.40
1	X	2740	A	C2-N3-C4	-9.35	105.92	110.60
1	X	828	A	C5-N7-C8	-9.35	99.22	103.90
1	X	797	A	C6-C5-N7	-9.32	125.78	132.30
1	X	373	A	C2-N3-C4	-9.30	105.95	110.60
1	X	373	A	N1-C2-N3	9.30	133.95	129.30
1	X	1179	C	N1-C2-O2	9.27	124.46	118.90
1	X	1065	A	C5-N7-C8	-9.19	99.30	103.90
1	X	2740	A	N1-C6-N6	9.16	124.10	118.60
1	X	2720	A	C5-C6-N1	9.16	122.28	117.70
1	X	1257	G	C8-N9-C4	-9.15	102.74	106.40
1	X	2088	G	N3-C4-N9	-9.14	120.52	126.00
1	X	2079	G	N1-C6-O6	9.13	125.38	119.90
1	X	797	A	C5-N7-C8	-9.06	99.37	103.90
1	X	2081	A	C2-N3-C4	-9.06	106.07	110.60
1	X	1179	C	N3-C2-O2	-9.06	115.56	121.90
1	X	1303	A	C5-C6-N1	-9.05	113.18	117.70
1	X	630	G	C5-N7-C8	-9.02	99.79	104.30
1	X	955	A	N1-C6-N6	9.01	124.00	118.60
1	X	791	U	N3-C4-C5	-8.96	109.23	114.60
1	X	1360	G	N1-C6-O6	8.96	125.27	119.90
1	X	2844	U	N1-C2-N3	8.92	120.25	114.90
1	X	2526	C	N1-C2-O2	8.90	124.24	118.90
1	X	721	A	C5-C6-N1	-8.89	113.25	117.70
1	X	1963	A	C2-N3-C4	-8.89	106.16	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	88	U	N1-C2-O2	8.89	129.02	122.80
2	Y	88	U	N3-C2-O2	-8.88	115.99	122.20
1	X	1186	A	N1-C6-N6	8.86	123.92	118.60
1	X	1715	U	C6-N1-C2	-8.84	115.70	121.00
1	X	2059	G	N9-C4-C5	8.82	108.93	105.40
1	X	350	G	C5-C6-N1	8.82	115.91	111.50
1	X	1303	A	C5-N7-C8	-8.79	99.50	103.90
1	X	2877	G	N3-C4-C5	-8.75	124.22	128.60
1	X	1828	U	C2-N1-C1'	8.72	128.16	117.70
1	X	268	A	O4'-C1'-N9	8.69	115.15	108.20
1	X	791	U	C6-N1-C2	-8.67	115.80	121.00
1	X	1806	U	C5-C6-N1	-8.67	118.37	122.70
1	X	2047	A	N1-C6-N6	-8.67	113.40	118.60
1	X	2021	C	C6-N1-C2	-8.66	116.83	120.30
1	X	2079	G	N9-C4-C5	-8.63	101.95	105.40
1	X	2089[A]	A	C8-N9-C1'	-8.61	112.21	127.70
1	X	2089[B]	A	C8-N9-C1'	-8.61	112.21	127.70
1	X	1065	A	N7-C8-N9	8.60	118.10	113.80
1	X	2066	G	N1-C6-O6	8.59	125.05	119.90
1	X	1516	C	C6-N1-C2	-8.58	116.87	120.30
1	X	828	A	N3-C4-C5	8.54	132.78	126.80
1	X	198	A	N1-C6-N6	8.53	123.72	118.60
1	X	2261	A	N1-C6-N6	8.50	123.70	118.60
1	X	2079	G	C4-C5-N7	8.50	114.20	110.80
1	X	2391	C	C6-N1-C2	8.50	123.70	120.30
1	X	877	G	O5'-P-OP2	8.49	120.89	110.70
1	X	1303	A	C4-C5-N7	8.47	114.94	110.70
1	X	373	A	C4-C5-C6	8.46	121.23	117.00
1	X	1560	A	C6-N1-C2	-8.45	113.53	118.60
1	X	428	G	C2-N3-C4	8.44	116.12	111.90
2	Y	86	C	N3-C2-O2	-8.43	116.00	121.90
1	X	1931	G	N3-C4-C5	-8.43	124.39	128.60
1	X	1244	G	C8-N9-C4	-8.41	103.04	106.40
1	X	568	C	C6-N1-C2	8.38	123.65	120.30
1	X	323	C	C2-N1-C1'	8.37	128.01	118.80
1	X	1957	G	N3-C4-N9	-8.37	120.98	126.00
1	X	428	G	N3-C4-C5	-8.36	124.42	128.60
1	X	2059	G	C5-N7-C8	-8.35	100.12	104.30
1	X	2712	G	N1-C6-O6	8.35	124.91	119.90
1	X	2740	A	C6-C5-N7	-8.32	126.47	132.30
1	X	1957	G	C4-C5-C6	-8.32	113.81	118.80
1	X	588	G	C8-N9-C4	8.31	109.73	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2877	G	C2-N3-C4	8.31	116.06	111.90
1	X	1953	U	O4'-C1'-N1	8.30	114.84	108.20
2	Y	92	G	N3-C4-N9	-8.27	121.04	126.00
1	X	2845	G	N1-C2-N2	8.26	123.63	116.20
1	X	362	C	C6-N1-C2	-8.25	117.00	120.30
1	X	1050	C	C6-N1-C2	8.25	123.60	120.30
1	X	1520	A	C8-N9-C4	8.24	109.10	105.80
1	X	323	C	C5-C6-N1	8.23	125.12	121.00
1	X	828	A	N1-C6-N6	8.23	123.54	118.60
1	X	1000	G	N3-C4-N9	-8.21	121.07	126.00
1	X	797	A	N7-C8-N9	8.20	117.90	113.80
1	X	2080	G	C5-C6-O6	-8.19	123.69	128.60
1	X	797	A	C4-C5-N7	8.18	114.79	110.70
2	Y	93	C	C6-N1-C2	-8.16	117.03	120.30
1	X	503	A	C2-N3-C4	-8.15	106.53	110.60
1	X	1065	A	C6-C5-N7	-8.15	126.60	132.30
1	X	1186	A	N3-C4-C5	8.12	132.48	126.80
1	X	2599	A	N1-C6-N6	8.12	123.47	118.60
1	X	2565	C	C6-N1-C2	8.11	123.55	120.30
1	X	2529	G	N1-C6-O6	8.11	124.76	119.90
1	X	1289	A	N7-C8-N9	8.09	117.85	113.80
1	X	428	G	N3-C4-N9	8.08	130.85	126.00
1	X	1230	G	C8-N9-C4	8.08	109.63	106.40
1	X	1990	C	C5-C6-N1	8.08	125.04	121.00
1	X	1178	C	C6-N1-C2	-8.07	117.07	120.30
1	X	834	A	C8-N9-C4	-8.06	102.57	105.80
1	X	2529	G	C6-C5-N7	-8.02	125.59	130.40
1	X	2716	U	C2-N1-C1'	-8.01	108.08	117.70
1	X	503	A	N7-C8-N9	8.01	117.80	113.80
1	X	996	G	C6-C5-N7	-8.00	125.60	130.40
1	X	2591	A	C8-N9-C4	-8.00	102.60	105.80
1	X	1520	A	N1-C2-N3	7.99	133.29	129.30
1	X	503	A	C4-C5-N7	7.97	114.68	110.70
1	X	2089[A]	A	C4-N9-C1'	7.96	140.63	126.30
1	X	2089[B]	A	C4-N9-C1'	7.96	140.63	126.30
1	X	1715	U	C2-N1-C1'	-7.94	108.17	117.70
1	X	350	G	C2-N3-C4	7.94	115.87	111.90
1	X	996	G	N1-C6-O6	7.94	124.66	119.90
1	X	2748	A	N1-C6-N6	7.94	123.36	118.60
1	X	12	U	N3-C2-O2	-7.93	116.65	122.20
1	X	1244	G	C4-C5-N7	-7.92	107.63	110.80
1	X	721	A	N1-C6-N6	7.91	123.35	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2021	C	N3-C4-C5	-7.91	118.74	121.90
1	X	834	A	N9-C4-C5	7.91	108.96	105.80
1	X	955	A	C8-N9-C4	7.91	108.96	105.80
1	X	1715	U	C2-N3-C4	7.91	131.74	127.00
1	X	2472	G	C2-N3-C4	7.89	115.85	111.90
1	X	2474	G	C5-C6-O6	-7.88	123.87	128.60
1	X	575	G	N3-C4-C5	7.87	132.54	128.60
1	X	617	A	C8-N9-C4	7.87	108.95	105.80
1	X	853	G	C4-C5-N7	-7.87	107.65	110.80
1	X	2446	U	C5-C6-N1	7.86	126.63	122.70
1	X	828	A	C4-C5-N7	7.86	114.63	110.70
1	X	1499	U	N3-C2-O2	-7.83	116.72	122.20
2	Y	99	U	N3-C2-O2	-7.83	116.72	122.20
1	X	2845	G	C4-C5-N7	7.82	113.93	110.80
1	X	955	A	N1-C2-N3	-7.82	125.39	129.30
1	X	1229	G	C5-C6-O6	-7.81	123.92	128.60
2	Y	86	C	N1-C2-O2	7.78	123.57	118.90
1	X	2797	C	C6-N1-C2	-7.77	117.19	120.30
1	X	122	G	N1-C6-O6	-7.75	115.25	119.90
1	X	1065	A	C8-N9-C4	-7.74	102.70	105.80
1	X	2238	U	C2-N1-C1'	7.70	126.94	117.70
1	X	2670	G	N1-C6-O6	-7.70	115.28	119.90
1	X	2845	G	C5-C6-N1	-7.69	107.66	111.50
1	X	1289	A	N3-C4-C5	7.68	132.18	126.80
2	Y	86	C	C2-N1-C1'	7.65	127.21	118.80
1	X	1021	G	C8-N9-C4	7.65	109.46	106.40
1	X	2440	G	N1-C6-O6	7.65	124.49	119.90
1	X	1360	G	C2-N3-C4	-7.63	108.09	111.90
1	X	1186	A	N1-C2-N3	7.62	133.11	129.30
1	X	2640	U	C5-C6-N1	-7.62	118.89	122.70
1	X	955	A	C5-C6-N6	-7.60	117.62	123.70
1	X	1272	U	N3-C4-C5	-7.60	110.04	114.60
1	X	1978	U	C6-N1-C2	-7.60	116.44	121.00
1	X	2391	C	C5-C6-N1	-7.59	117.20	121.00
1	X	1732	U	N1-C2-N3	7.57	119.44	114.90
1	X	695	C	C2-N3-C4	7.53	123.67	119.90
1	X	588	G	N9-C4-C5	-7.53	102.39	105.40
1	X	2541	U	C5-C6-N1	-7.53	118.94	122.70
1	X	1843	U	C4-C5-C6	-7.51	115.19	119.70
1	X	2709	U	C5-C6-N1	-7.51	118.95	122.70
1	X	2797	C	C6-N1-C1'	7.50	129.80	120.80
2	Y	99	U	N1-C2-O2	7.50	128.05	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2446	U	C6-N1-C1'	7.49	131.69	121.20
1	X	2474	G	N3-C4-N9	-7.48	121.51	126.00
2	Y	79	C	C2-N1-C1'	7.47	127.02	118.80
1	X	2716	U	C5-C6-N1	-7.47	118.97	122.70
1	X	2006	C	C6-N1-C2	-7.47	117.31	120.30
1	X	661	U	N3-C4-O4	7.44	124.61	119.40
1	X	2845	G	C8-N9-C1'	7.44	136.67	127.00
1	X	2066	G	C5-C6-N1	-7.43	107.79	111.50
1	X	1289	A	N3-C4-N9	-7.42	121.46	127.40
1	X	2887	G	N3-C4-N9	7.42	130.45	126.00
1	X	2044	C	C4-C5-C6	7.42	121.11	117.40
1	X	695	C	N3-C4-N4	7.38	123.16	118.00
1	X	1230	G	N7-C8-N9	-7.38	109.41	113.10
1	X	1544	G	C2-N3-C4	7.36	115.58	111.90
1	X	1308	C	C2-N3-C4	-7.34	116.23	119.90
1	X	1226	G	N1-C6-O6	7.34	124.30	119.90
1	X	2064	A	C8-N9-C4	-7.34	102.86	105.80
1	X	557	G	O4'-C1'-N9	7.33	114.07	108.20
1	X	2541	U	C6-N1-C2	7.32	125.39	121.00
1	X	2717	A	C2-N3-C4	7.31	114.25	110.60
1	X	1229	G	N1-C6-O6	7.30	124.28	119.90
1	X	892	U	C5-C6-N1	-7.29	119.05	122.70
2	Y	79	C	C6-N1-C1'	-7.29	112.05	120.80
1	X	2302	C	N3-C4-C5	-7.28	118.99	121.90
1	X	635	G	C8-N9-C4	-7.27	103.49	106.40
1	X	1543	G	N3-C4-N9	7.26	130.35	126.00
1	X	2576	G	N3-C4-C5	-7.25	124.97	128.60
1	X	1064	A	C8-N9-C4	7.22	108.69	105.80
1	X	2576	G	N3-C4-N9	7.22	130.33	126.00
1	X	2576	G	C4-N9-C1'	7.21	135.88	126.50
1	X	2608	G	C5-C6-O6	7.21	132.93	128.60
1	X	2851	G	C8-N9-C4	-7.20	103.52	106.40
1	X	1968	C	C6-N1-C2	-7.19	117.42	120.30
1	X	2799	C	N1-C2-O2	-7.19	114.59	118.90
1	X	321	U	O4'-C1'-N1	7.18	113.94	108.20
1	X	797	A	O4'-C1'-N9	7.17	113.94	108.20
1	X	211	C	C6-N1-C2	7.17	123.17	120.30
1	X	2608	G	N1-C6-O6	-7.16	115.60	119.90
1	X	491	C	C6-N1-C2	-7.14	117.44	120.30
1	X	496	G	C8-N9-C4	-7.14	103.54	106.40
1	X	1257	G	N7-C8-N9	7.13	116.66	113.10
1	X	54	G	C5-N7-C8	-7.12	100.74	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	795	A	C5-C6-N6	-7.12	118.00	123.70
1	X	15	G	C8-N9-C4	7.12	109.25	106.40
1	X	2877	G	N3-C4-N9	7.11	130.27	126.00
1	X	1175	G	C6-N1-C2	-7.11	120.83	125.10
1	X	666	A	N1-C6-N6	7.10	122.86	118.60
1	X	698	U	N1-C2-O2	7.09	127.77	122.80
1	X	2045	A	N1-C2-N3	7.08	132.84	129.30
1	X	503	A	N1-C6-N6	7.06	122.83	118.60
1	X	1367	C	C2-N1-C1'	7.04	126.55	118.80
1	X	122	G	C6-C5-N7	7.04	134.62	130.40
1	X	1303	A	N1-C6-N6	7.02	122.81	118.60
1	X	1765	A	O4'-C1'-N9	7.01	113.81	108.20
1	X	1520	A	N9-C4-C5	-7.00	103.00	105.80
1	X	625	G	N3-C4-N9	6.99	130.20	126.00
1	X	890	G	P-O3'-C3'	6.99	128.09	119.70
1	X	2877	G	C5-C6-N1	6.99	114.99	111.50
1	X	2044	C	N1-C2-N3	6.99	124.09	119.20
1	X	184	C	C5-C6-N1	6.97	124.49	121.00
1	X	728	U	N3-C4-O4	6.97	124.28	119.40
1	X	1289	A	N1-C2-N3	6.96	132.78	129.30
1	X	721	A	C5-N7-C8	-6.96	100.42	103.90
1	X	1229	G	C4-C5-N7	6.96	113.58	110.80
1	X	373	A	C8-N9-C4	-6.95	103.02	105.80
1	X	728	U	C6-N1-C2	-6.95	116.83	121.00
1	X	996	G	C5-C6-O6	-6.93	124.44	128.60
1	X	54	G	C8-N9-C4	-6.92	103.63	106.40
1	X	1658	A	N1-C6-N6	6.91	122.75	118.60
1	X	2602	C	C6-N1-C2	-6.91	117.54	120.30
1	X	1244	G	N3-C4-N9	-6.90	121.86	126.00
1	X	496	G	N7-C8-N9	6.90	116.55	113.10
1	X	373	A	N7-C8-N9	6.90	117.25	113.80
1	X	2740	A	C4-C5-C6	6.90	120.45	117.00
1	X	2512	G	N1-C6-O6	6.90	124.04	119.90
1	X	1560	A	N9-C4-C5	6.89	108.56	105.80
1	X	2756	G	C5-C6-O6	6.88	132.73	128.60
1	X	852	U	C4-C5-C6	6.87	123.82	119.70
1	X	721	A	C6-C5-N7	-6.86	127.50	132.30
1	X	1828	U	C5-C6-N1	6.85	126.13	122.70
1	X	666	A	N7-C8-N9	6.85	117.22	113.80
1	X	2644	C	C6-N1-C2	6.84	123.04	120.30
1	X	428	G	C4-N9-C1'	6.84	135.39	126.50
1	X	2433	C	N3-C2-O2	-6.83	117.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2740	A	C5-N7-C8	-6.83	100.49	103.90
1	X	1015	C	C6-N1-C2	-6.81	117.58	120.30
1	X	1453	G	N3-C4-C5	-6.81	125.20	128.60
1	X	1028	G	C5-C6-N1	6.80	114.90	111.50
1	X	2565	C	N3-C4-C5	6.80	124.62	121.90
1	X	637	U	N3-C2-O2	-6.79	117.44	122.20
1	X	992	A	C5-C6-N1	-6.79	114.30	117.70
1	X	350	G	O4'-C1'-N9	6.79	113.63	108.20
1	X	54	G	N7-C8-N9	6.79	116.49	113.10
1	X	698	U	N3-C2-O2	-6.79	117.45	122.20
1	X	992	A	C2-N3-C4	-6.78	107.21	110.60
1	X	661	U	C5-C6-N1	6.78	126.09	122.70
1	X	2606	C	N3-C4-C5	-6.77	119.19	121.90
1	X	210	A	C8-N9-C4	6.77	108.51	105.80
1	X	2844	U	N1-C2-O2	-6.76	118.06	122.80
1	X	2876	G	C8-N9-C4	-6.76	103.69	106.40
1	X	1026	C	N3-C4-C5	6.76	124.60	121.90
1	X	849	A	N1-C6-N6	6.76	122.65	118.60
1	X	2398	G	C5-C6-N1	-6.75	108.12	111.50
1	X	575	G	C2-N3-C4	-6.75	108.53	111.90
1	X	2512	G	N3-C4-C5	6.75	131.97	128.60
1	X	367	A	N1-C6-N6	-6.71	114.57	118.60
1	X	2089[A]	A	C4-C5-C6	6.71	120.36	117.00
1	X	2089[B]	A	C4-C5-C6	6.71	120.36	117.00
1	X	1241	A	C8-N9-C4	6.70	108.48	105.80
1	X	2682	G	OP2-P-O3'	6.69	119.92	105.20
2	Y	82	C	N3-C2-O2	-6.68	117.22	121.90
2	Y	15	C	C5-C4-N4	-6.67	115.53	120.20
1	X	2064	A	N7-C8-N9	6.66	117.13	113.80
1	X	630	G	C4-C5-N7	6.66	113.46	110.80
1	X	985	A	C2-N3-C4	-6.66	107.27	110.60
2	Y	88	U	C6-N1-C1'	-6.66	111.88	121.20
1	X	2298	G	N1-C2-N2	-6.65	110.22	116.20
1	X	376	A	C8-N9-C4	-6.64	103.14	105.80
1	X	1229	G	N9-C4-C5	-6.64	102.74	105.40
1	X	1732	U	O4'-C1'-N1	6.64	113.51	108.20
1	X	2774	G	C6-C5-N7	-6.64	126.42	130.40
1	X	983	G	C8-N9-C4	-6.63	103.75	106.40
2	Y	92	G	N1-C6-O6	6.63	123.88	119.90
1	X	2657	G	N7-C8-N9	6.62	116.41	113.10
1	X	1293	U	N1-C2-N3	6.62	118.87	114.90
1	X	1732	U	C6-N1-C1'	6.62	130.46	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2529	G	C4-C5-N7	6.62	113.45	110.80
1	X	2657	G	C5-N7-C8	-6.61	100.99	104.30
1	X	124	A	C8-N9-C4	6.61	108.44	105.80
1	X	2576	G	C8-N9-C1'	-6.61	118.41	127.00
1	X	1866	G	C8-N9-C4	-6.60	103.76	106.40
1	X	152	C	N3-C2-O2	-6.58	117.30	121.90
1	X	644	C	C5-C6-N1	6.57	124.28	121.00
1	X	852	U	N1-C2-N3	6.57	118.84	114.90
1	X	2845	G	C4-N9-C1'	-6.56	117.97	126.50
2	Y	91	C	C6-N1-C2	-6.56	117.67	120.30
1	X	389	A	C8-N9-C4	-6.56	103.18	105.80
1	X	2517	G	C8-N9-C4	6.56	109.02	106.40
1	X	1560	A	C8-N9-C4	-6.55	103.18	105.80
1	X	728	U	N3-C4-C5	-6.54	110.68	114.60
1	X	2591	A	N7-C8-N9	6.54	117.07	113.80
1	X	377	U	O5'-P-OP2	-6.54	99.81	105.70
1	X	528	C	C6-N1-C2	-6.53	117.69	120.30
1	X	1751	G	N1-C6-O6	6.53	123.82	119.90
1	X	2044	C	C6-N1-C2	-6.53	117.69	120.30
1	X	680	C	C6-N1-C2	-6.53	117.69	120.30
1	X	369	G	C8-N9-C4	-6.52	103.79	106.40
1	X	666	A	C5-N7-C8	-6.52	100.64	103.90
1	X	711	G	C8-N9-C4	6.51	109.00	106.40
1	X	2603	G	N9-C4-C5	-6.50	102.80	105.40
1	X	350	G	C4-N9-C1'	6.50	134.95	126.50
1	X	853	G	N3-C2-N2	-6.49	115.36	119.90
2	Y	79	C	N3-C4-N4	6.47	122.53	118.00
1	X	743	C	C6-N1-C2	6.46	122.89	120.30
1	X	2063	C	C5-C6-N1	6.46	124.23	121.00
1	X	660	A	O4'-C1'-N9	6.46	113.36	108.20
2	Y	105	G	N9-C4-C5	-6.45	102.82	105.40
1	X	2078	A	N1-C2-N3	6.45	132.52	129.30
1	X	12	U	C2-N1-C1'	6.45	125.44	117.70
1	X	662	G	N3-C4-N9	6.45	129.87	126.00
1	X	2709	U	C2-N3-C4	-6.44	123.14	127.00
1	X	1715	U	O4'-C1'-N1	6.43	113.35	108.20
1	X	2066	G	C6-C5-N7	-6.43	126.54	130.40
1	X	2039	G	N1-C6-O6	6.42	123.75	119.90
1	X	2546	U	C5-C6-N1	-6.42	119.49	122.70
1	X	1953	U	C2-N1-C1'	-6.41	110.01	117.70
1	X	1931	G	C8-N9-C1'	-6.41	118.67	127.00
2	Y	105	G	C8-N9-C4	6.40	108.96	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	122	G	C4-N9-C1'	-6.40	118.18	126.50
1	X	2532	G	O5'-P-OP2	-6.40	99.94	105.70
1	X	1275	A	O4'-C1'-N9	6.40	113.32	108.20
1	X	64	A	C8-N9-C4	-6.39	103.24	105.80
1	X	2522	G	N1-C6-O6	6.39	123.74	119.90
1	X	2724	G	C2-N3-C4	-6.39	108.71	111.90
1	X	1652	A	N1-C6-N6	-6.38	114.77	118.60
1	X	1091	G	P-O3'-C3'	6.37	127.35	119.70
2	Y	91	C	N3-C4-C5	-6.37	119.35	121.90
1	X	1931	G	C6-C5-N7	-6.37	126.58	130.40
1	X	1560	A	C2-N3-C4	6.37	113.78	110.60
1	X	505	U	O5'-P-OP2	-6.36	99.97	105.70
1	X	853	G	C5-C6-N1	-6.36	108.32	111.50
1	X	1168	C	N1-C2-O2	6.35	122.71	118.90
2	Y	78	C	N3-C2-O2	-6.35	117.46	121.90
1	X	2711	U	O5'-P-OP2	6.35	118.32	110.70
1	X	2595	C	C6-N1-C2	6.34	122.84	120.30
1	X	2556	G	N3-C4-N9	-6.34	122.20	126.00
1	X	2657	G	N1-C6-O6	6.33	123.70	119.90
1	X	1017	A	C8-N9-C4	-6.33	103.27	105.80
1	X	12	U	N1-C2-O2	6.33	127.23	122.80
1	X	2446	U	O4'-C1'-N1	6.32	113.26	108.20
1	X	2709	U	N3-C2-O2	-6.32	117.77	122.20
1	X	1179	C	O5'-P-OP2	-6.32	100.01	105.70
1	X	1279	C	C5-C4-N4	-6.32	115.78	120.20
1	X	834	A	N1-C2-N3	6.31	132.46	129.30
1	X	828	A	C5-C6-N1	-6.31	114.55	117.70
1	X	2858	G	C8-N9-C4	6.31	108.92	106.40
2	Y	95	A	N1-C6-N6	6.30	122.38	118.60
1	X	1977	G	C5-C6-N1	-6.30	108.35	111.50
1	X	721	A	N1-C2-N3	6.29	132.44	129.30
1	X	1028	G	C5-C6-O6	-6.29	124.83	128.60
1	X	1978	U	C5-C6-N1	6.28	125.84	122.70
2	Y	95	A	C8-N9-C4	6.28	108.31	105.80
1	X	515	G	O4'-C1'-N9	6.28	113.22	108.20
1	X	611	U	N1-C2-N3	6.28	118.67	114.90
1	X	2079	G	N3-C4-N9	6.27	129.76	126.00
1	X	1543	G	N3-C4-C5	-6.27	125.46	128.60
1	X	2381	A	C5-C6-N1	6.27	120.83	117.70
1	X	1791	G	N3-C4-N9	-6.27	122.24	126.00
1	X	1758	A	C2-N3-C4	6.26	113.73	110.60
1	X	378	C	C6-N1-C2	-6.25	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2334	G	N3-C4-N9	-6.25	122.25	126.00
1	X	1811	A	C4-C5-C6	6.25	120.13	117.00
1	X	251	G	C5-C6-O6	-6.25	124.85	128.60
1	X	2076	A	N1-C2-N3	6.25	132.43	129.30
1	X	603	C	N3-C2-O2	-6.25	117.53	121.90
1	X	2720	A	N1-C6-N6	-6.25	114.85	118.60
1	X	1303	A	C6-N1-C2	6.25	122.35	118.60
1	X	1955	A	C2-N3-C4	6.25	113.72	110.60
2	Y	79	C	C5-C4-N4	-6.24	115.83	120.20
1	X	683	G	N9-C4-C5	6.24	107.90	105.40
1	X	1957	G	N3-C4-C5	6.24	131.72	128.60
1	X	608	C	C6-N1-C2	-6.22	117.81	120.30
1	X	1050	C	N3-C4-C5	6.21	124.38	121.90
1	X	1303	A	C6-C5-N7	-6.20	127.96	132.30
1	X	2556	G	C5-C6-N1	-6.20	108.40	111.50
1	X	834	A	N1-C6-N6	-6.19	114.89	118.60
1	X	2649	U	O4'-C1'-N1	6.19	113.16	108.20
1	X	2720	A	C2-N3-C4	6.19	113.70	110.60
1	X	2797	C	C2-N3-C4	6.19	123.00	119.90
1	X	2712	G	C2-N3-C4	-6.19	108.81	111.90
1	X	2642	U	C5-C4-O4	-6.19	122.19	125.90
1	X	2322	C	C6-N1-C2	-6.18	117.83	120.30
1	X	1707	U	N1-C2-N3	6.18	118.61	114.90
1	X	575	G	C8-N9-C4	-6.17	103.93	106.40
1	X	2583	C	C2-N1-C1'	6.17	125.58	118.80
1	X	2718	C	C6-N1-C2	-6.17	117.83	120.30
1	X	617	A	C2-N3-C4	-6.17	107.52	110.60
1	X	2080	G	C5-C6-N1	6.16	114.58	111.50
1	X	302	A	C8-N9-C4	6.16	108.26	105.80
1	X	1435	C	C5-C6-N1	6.16	124.08	121.00
1	X	1024	A	N9-C4-C5	-6.15	103.34	105.80
1	X	1175	G	N3-C4-C5	-6.15	125.53	128.60
2	Y	93	C	C2-N1-C1'	6.15	125.57	118.80
1	X	1990	C	C2-N3-C4	6.15	122.97	119.90
1	X	2361	U	C5-C6-N1	6.14	125.77	122.70
1	X	9	U	C2-N1-C1'	6.14	125.07	117.70
1	X	1360	G	C6-C5-N7	-6.14	126.72	130.40
1	X	1855	G	C8-N9-C4	-6.13	103.95	106.40
1	X	2089[A]	A	C4-C5-N7	6.13	113.77	110.70
1	X	2089[B]	A	C4-C5-N7	6.13	113.77	110.70
1	X	548	A	O4'-C1'-N9	6.13	113.10	108.20
1	X	2712	G	C5-C6-N1	-6.11	108.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2238	U	C6-N1-C1'	-6.11	112.64	121.20
1	X	1806	U	C2-N1-C1'	-6.11	110.37	117.70
1	X	1182	G	N1-C6-O6	6.11	123.56	119.90
1	X	488	G	N3-C4-C5	-6.10	125.55	128.60
1	X	1865	C	O4'-C1'-N1	6.09	113.08	108.20
1	X	503	A	C6-C5-N7	-6.09	128.04	132.30
1	X	1042	C	C4-C5-C6	6.08	120.44	117.40
1	X	1360	G	N3-C4-C5	6.08	131.64	128.60
1	X	683	G	C8-N9-C4	-6.08	103.97	106.40
1	X	985	A	N1-C2-N3	6.08	132.34	129.30
1	X	102	A	C2-N3-C4	-6.08	107.56	110.60
1	X	376	A	N7-C8-N9	6.08	116.84	113.80
1	X	2583	C	C6-N1-C2	-6.08	117.87	120.30
1	X	854	G	N3-C4-C5	-6.07	125.56	128.60
1	X	2446	U	C6-N1-C2	-6.06	117.36	121.00
1	X	2888	A	N1-C6-N6	-6.06	114.96	118.60
1	X	630	G	C8-N9-C1'	6.06	134.87	127.00
1	X	2546	U	C2-N3-C4	-6.05	123.37	127.00
1	X	612	U	N3-C4-C5	-6.05	110.97	114.60
1	X	660	A	C8-N9-C4	-6.05	103.38	105.80
1	X	1278	G	C8-N9-C4	-6.05	103.98	106.40
1	X	2337	A	C2-N3-C4	6.04	113.62	110.60
1	X	588	G	C5-C6-O6	-6.04	124.98	128.60
1	X	1499	U	N1-C2-O2	6.04	127.03	122.80
1	X	797	A	C2-N3-C4	-6.04	107.58	110.60
1	X	2637	C	C6-N1-C2	6.04	122.71	120.30
1	X	2006	C	N3-C4-C5	-6.03	119.49	121.90
2	Y	85	A	C8-N9-C4	6.02	108.21	105.80
1	X	656	G	C8-N9-C4	-6.02	103.99	106.40
1	X	2076	A	C6-N1-C2	-6.02	114.99	118.60
1	X	2419	A	N7-C8-N9	6.01	116.81	113.80
1	X	2682	G	N3-C4-N9	-6.01	122.39	126.00
1	X	2391	C	N3-C4-C5	6.01	124.30	121.90
2	Y	92	G	C6-N1-C2	6.01	128.71	125.10
1	X	675	G	N1-C6-O6	6.01	123.50	119.90
1	X	428	G	O4'-C1'-N9	6.01	113.00	108.20
1	X	1065	A	C4-C5-N7	6.01	113.70	110.70
1	X	2469	C	C6-N1-C2	6.01	122.70	120.30
1	X	2716	U	C6-N1-C1'	6.01	129.61	121.20
1	X	575	G	N3-C4-N9	-6.00	122.40	126.00
1	X	1320	G	C8-N9-C4	-6.00	104.00	106.40
1	X	2062	G	O4'-C1'-N9	6.00	113.00	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1453	G	N3-C4-N9	5.99	129.60	126.00
1	X	2640	U	C2-N3-C4	-5.99	123.40	127.00
5	C	181	LEU	CA-CB-CG	-5.99	101.51	115.30
11	J	84	GLY	N-CA-C	5.99	128.08	113.10
1	X	1559	G	N1-C2-N3	-5.99	120.31	123.90
1	X	2545	A	C2-N3-C4	5.99	113.59	110.60
1	X	2743	U	C5-C6-N1	-5.99	119.71	122.70
1	X	51	G	N3-C4-N9	5.98	129.59	126.00
1	X	1931	G	C4-N9-C1'	5.98	134.28	126.50
1	X	985	A	C5-C6-N1	-5.98	114.71	117.70
1	X	2017	C	N1-C2-O2	-5.98	115.31	118.90
1	X	2095	U	C5-C4-O4	-5.98	122.31	125.90
1	X	2877	G	N1-C6-O6	-5.98	116.31	119.90
1	X	1186	A	N3-C4-N9	-5.97	122.62	127.40
1	X	2472	G	C8-N9-C4	-5.97	104.01	106.40
1	X	2583	C	N1-C2-O2	5.97	122.48	118.90
1	X	2812	U	N1-C2-N3	5.97	118.48	114.90
1	X	122	G	C8-N9-C1'	5.96	134.75	127.00
1	X	2682	G	N3-C4-C5	5.96	131.58	128.60
1	X	2757	U	N1-C2-N3	5.96	118.48	114.90
1	X	2672	G	C5-C6-N1	-5.96	108.52	111.50
1	X	2887	G	C8-N9-C1'	-5.96	119.25	127.00
1	X	1709	A	N1-C6-N6	5.96	122.17	118.60
1	X	2657	G	C4-C5-N7	5.96	113.18	110.80
1	X	1028	G	C4-C5-N7	5.95	113.18	110.80
1	X	1229	G	C8-N9-C4	5.95	108.78	106.40
1	X	198	A	N9-C4-C5	-5.95	103.42	105.80
1	X	1308	C	N3-C4-C5	5.95	124.28	121.90
1	X	1245	G	C8-N9-C4	-5.94	104.02	106.40
1	X	1229	G	O5'-P-OP1	5.94	117.83	110.70
1	X	659	A	OP1-P-O3'	5.94	118.26	105.20
1	X	34	U	C5-C6-N1	5.93	125.67	122.70
1	X	1466	G	C4-N9-C1'	5.92	134.20	126.50
1	X	2419	A	C6-C5-N7	-5.92	128.15	132.30
1	X	1714	C	N3-C4-N4	5.91	122.14	118.00
1	X	834	A	C6-N1-C2	-5.91	115.05	118.60
1	X	198	A	C8-N9-C4	5.91	108.16	105.80
1	X	2609	G	C4-C5-N7	5.91	113.16	110.80
2	Y	65	G	N1-C6-O6	-5.91	116.36	119.90
1	X	555	C	O5'-P-OP2	-5.91	100.38	105.70
1	X	2474	G	N9-C4-C5	5.90	107.76	105.40
1	X	1466	G	C8-N9-C4	-5.90	104.04	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2703	C	C5-C6-N1	-5.90	118.05	121.00
1	X	20	C	C5-C6-N1	5.89	123.95	121.00
1	X	73	A	C8-N9-C4	-5.89	103.44	105.80
1	X	389	A	N7-C8-N9	5.89	116.75	113.80
1	X	835	U	C5-C6-N1	5.89	125.65	122.70
1	X	2881	C	C6-N1-C2	-5.89	117.94	120.30
1	X	533	C	N1-C2-O2	-5.89	115.37	118.90
1	X	1659	C	N3-C4-N4	5.88	122.12	118.00
1	X	2419	A	C5-C6-N1	-5.88	114.76	117.70
2	Y	77	G	C8-N9-C4	-5.88	104.05	106.40
1	X	1038	C	C6-N1-C2	-5.87	117.95	120.30
1	X	1186	A	C6-C5-N7	-5.87	128.19	132.30
1	X	2626	G	N1-C6-O6	-5.87	116.38	119.90
1	X	1186	A	C5-N7-C8	-5.87	100.97	103.90
1	X	835	U	C5-C4-O4	-5.87	122.38	125.90
1	X	1273	G	N9-C4-C5	5.87	107.75	105.40
1	X	36	G	N3-C4-C5	-5.86	125.67	128.60
1	X	1439	U	C6-N1-C2	-5.86	117.49	121.00
1	X	1648	C	C6-N1-C2	-5.86	117.96	120.30
1	X	1360	G	C4-C5-N7	5.86	113.14	110.80
1	X	51	G	N3-C4-C5	-5.85	125.67	128.60
1	X	1180	G	N1-C6-O6	5.85	123.41	119.90
1	X	695	C	C5-C6-N1	5.85	123.93	121.00
1	X	1866	G	C4-N9-C1'	5.85	134.10	126.50
1	X	1953	U	N1-C1'-C2'	5.85	121.60	114.00
1	X	2039	G	N3-C2-N2	-5.85	115.81	119.90
1	X	78	U	C2-N1-C1'	5.85	124.72	117.70
1	X	870	C	C6-N1-C2	-5.84	117.96	120.30
1	X	1746	G	N3-C4-N9	-5.84	122.49	126.00
1	X	1716	C	C5-C6-N1	5.84	123.92	121.00
1	X	263	G	C8-N9-C4	-5.83	104.07	106.40
1	X	666	A	C8-N9-C4	-5.83	103.47	105.80
1	X	1288	G	C5-C6-N1	5.83	114.42	111.50
1	X	2073	G	C8-N9-C4	-5.83	104.07	106.40
1	X	214	G	N1-C6-O6	5.83	123.40	119.90
1	X	662	G	N3-C4-C5	-5.83	125.69	128.60
1	X	2740	A	N7-C8-N9	5.83	116.72	113.80
1	X	728	U	C5-C6-N1	5.83	125.61	122.70
1	X	1024	A	C6-C5-N7	-5.83	128.22	132.30
1	X	2657	G	C5-C6-O6	-5.83	125.10	128.60
1	X	70	G	N3-C4-C5	-5.83	125.69	128.60
1	X	251	G	N1-C6-O6	5.82	123.39	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	509	G	C6-C5-N7	-5.82	126.91	130.40
1	X	788	A	C2-N3-C4	-5.82	107.69	110.60
1	X	1244	G	N3-C2-N2	-5.82	115.83	119.90
1	X	2080	G	C6-N1-C2	-5.82	121.61	125.10
1	X	1065	A	N3-C4-C5	5.82	130.87	126.80
1	X	1701	U	N1-C2-N3	5.81	118.39	114.90
1	X	1716	C	C2-N1-C1'	5.81	125.19	118.80
1	X	2419	A	C2-N3-C4	-5.81	107.69	110.60
1	X	2525	C	N3-C2-O2	5.81	125.97	121.90
1	X	577	A	N1-C6-N6	-5.81	115.11	118.60
1	X	1303	A	N3-C4-N9	-5.81	122.75	127.40
1	X	1026	C	C5-C4-N4	-5.80	116.14	120.20
1	X	514	G	N3-C4-C5	-5.80	125.70	128.60
1	X	695	C	C6-N1-C2	-5.80	117.98	120.30
1	X	1663	G	C4-C5-N7	5.79	113.12	110.80
1	X	853	G	N9-C4-C5	5.79	107.72	105.40
1	X	1716	C	N1-C2-O2	5.79	122.37	118.90
1	X	1978	U	C6-N1-C1'	5.78	129.29	121.20
1	X	1751	G	C5-C6-N1	-5.78	108.61	111.50
1	X	1811	A	N1-C6-N6	5.78	122.07	118.60
1	X	862	C	C6-N1-C2	5.78	122.61	120.30
1	X	2261	A	C5-N7-C8	-5.78	101.01	103.90
1	X	2521	G	N1-C6-O6	5.78	123.37	119.90
1	X	102	A	N1-C2-N3	5.77	132.19	129.30
1	X	2038	U	OP1-P-O3'	5.77	117.90	105.20
1	X	1016	G	N1-C6-O6	-5.77	116.44	119.90
1	X	1301	U	N1-C2-N3	5.77	118.36	114.90
1	X	1278	G	C5-N7-C8	-5.77	101.42	104.30
1	X	35	G	C2-N3-C4	-5.76	109.02	111.90
1	X	1257	G	N3-C4-C5	-5.76	125.72	128.60
1	X	660	A	OP1-P-OP2	-5.76	110.96	119.60
1	X	1828	U	C6-N1-C1'	-5.76	113.13	121.20
1	X	2726	C	N1-C2-O2	-5.76	115.44	118.90
1	X	985	A	N7-C8-N9	5.75	116.68	113.80
1	X	1855	G	C5-C6-O6	5.75	132.05	128.60
1	X	2457	A	C2-N3-C4	-5.75	107.72	110.60
2	Y	92	G	C5-C6-N1	-5.75	108.62	111.50
1	X	1243	G	N1-C6-O6	5.75	123.35	119.90
1	X	1687	G	N1-C6-O6	5.75	123.35	119.90
1	X	1968	C	C2-N1-C1'	5.75	125.12	118.80
1	X	2062	G	O5'-P-OP2	-5.75	100.53	105.70
1	X	102	A	C5-C6-N1	-5.75	114.83	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	440	C	N1-C2-O2	5.75	122.35	118.90
1	X	902	A	N9-C4-C5	5.75	108.10	105.80
1	X	78	U	N3-C2-O2	-5.74	118.18	122.20
1	X	605	U	C5-C4-O4	5.74	129.35	125.90
1	X	2419	A	C8-N9-C4	-5.74	103.50	105.80
1	X	2063	C	C6-N1-C2	-5.74	118.00	120.30
1	X	778	G	C5-C6-O6	-5.74	125.16	128.60
1	X	855	U	C2-N3-C4	-5.74	123.56	127.00
1	X	1228	A	C2-N3-C4	-5.74	107.73	110.60
1	X	554	C	C5-C6-N1	5.74	123.87	121.00
1	X	2844	U	C2-N3-C4	-5.74	123.56	127.00
1	X	2084	G	N3-C4-C5	-5.73	125.73	128.60
1	X	2599	A	C8-N9-C4	5.73	108.09	105.80
1	X	20	C	N3-C4-N4	5.73	122.01	118.00
1	X	2051	C	OP2-P-O3'	5.73	117.81	105.20
1	X	1351	C	N1-C2-O2	5.73	122.34	118.90
1	X	1175	G	N3-C4-N9	5.72	129.44	126.00
1	X	2757	U	C6-N1-C2	-5.72	117.57	121.00
1	X	2622	G	C5-C6-O6	-5.72	125.17	128.60
1	X	2845	G	N7-C8-N9	5.72	115.96	113.10
1	X	1466	G	N7-C8-N9	5.71	115.96	113.10
1	X	1977	G	O5'-P-OP1	-5.71	100.56	105.70
1	X	989	A	C5-C6-N6	-5.71	119.13	123.70
1	X	2887	G	N9-C4-C5	-5.71	103.12	105.40
1	X	1300	G	N1-C2-N3	5.71	127.33	123.90
1	X	506	A	N1-C6-N6	5.71	122.02	118.60
1	X	642	U	N3-C4-O4	-5.71	115.41	119.40
1	X	876	G	N3-C4-C5	-5.71	125.75	128.60
1	X	2576	G	C6-C5-N7	-5.70	126.98	130.40
1	X	1646	U	N3-C4-O4	5.70	123.39	119.40
1	X	1794	C	C6-N1-C2	-5.70	118.02	120.30
1	X	1686	G	N1-C6-O6	5.70	123.32	119.90
1	X	2545	A	C8-N9-C4	-5.70	103.52	105.80
1	X	214	G	C5-C6-N1	-5.69	108.65	111.50
1	X	428	G	C8-N9-C1'	-5.69	119.60	127.00
1	X	1180	G	C2-N3-C4	-5.69	109.05	111.90
1	X	1915	G	C2-N3-C4	5.69	114.75	111.90
1	X	622	A	OP1-P-O3'	5.69	117.71	105.20
1	X	1244	G	C5-C6-O6	5.69	132.01	128.60
1	X	428	G	C5-C6-N1	5.68	114.34	111.50
1	X	608	C	N3-C4-N4	5.68	121.98	118.00
1	X	1876	G	C8-N9-C4	-5.68	104.13	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	791	U	N1-C2-N3	5.68	118.31	114.90
1	X	2548	C	C6-N1-C2	-5.68	118.03	120.30
2	Y	86	C	C6-N1-C1'	-5.68	113.98	120.80
1	X	2089[A]	A	N3-C4-N9	5.68	131.94	127.40
1	X	2089[B]	A	N3-C4-N9	5.68	131.94	127.40
1	X	2797	C	C4-C5-C6	5.68	120.24	117.40
1	X	1171	A	N1-C6-N6	-5.67	115.19	118.60
1	X	1791	G	N3-C4-C5	5.67	131.44	128.60
1	X	625	G	N9-C4-C5	-5.67	103.13	105.40
1	X	2469	C	O5'-P-OP2	-5.67	100.59	105.70
1	X	70	G	C2-N3-C4	5.67	114.73	111.90
1	X	1806	U	N1-C2-O2	-5.67	118.83	122.80
1	X	1953	U	C6-N1-C1'	5.67	129.13	121.20
1	X	2361	U	C2-N1-C1'	5.66	124.50	117.70
1	X	985	A	C8-N9-C4	-5.66	103.53	105.80
1	X	2756	G	C2-N3-C4	-5.65	109.07	111.90
1	X	1186	A	O4'-C1'-N9	-5.65	103.68	108.20
1	X	2650	G	N1-C6-O6	5.65	123.29	119.90
1	X	532	C	N1-C2-O2	-5.65	115.51	118.90
1	X	1399	C	C6-N1-C2	-5.65	118.04	120.30
1	X	2062	G	OP1-P-OP2	5.65	128.07	119.60
2	Y	58	G	N3-C4-C5	5.65	131.42	128.60
2	Y	79	C	N1-C2-O2	5.65	122.29	118.90
1	X	1289	A	C5-C6-N1	-5.64	114.88	117.70
1	X	2078	A	C4-C5-C6	5.64	119.82	117.00
1	X	877	G	C2-N3-C4	5.64	114.72	111.90
1	X	2754	G	N1-C6-O6	-5.64	116.52	119.90
1	X	707	G	N1-C6-O6	5.63	123.28	119.90
1	X	2043	U	OP1-P-O3'	5.63	117.58	105.20
1	X	2446	U	C2-N1-C1'	-5.63	110.95	117.70
1	X	2710	C	O5'-P-OP2	-5.63	100.63	105.70
1	X	1047	G	N1-C6-O6	5.63	123.28	119.90
1	X	365	A	C8-N9-C4	-5.62	103.55	105.80
1	X	1732	U	C6-N1-C2	-5.62	117.63	121.00
1	X	1565	U	C6-N1-C2	-5.62	117.63	121.00
1	X	2703	C	C2-N3-C4	-5.62	117.09	119.90
1	X	980	U	O5'-P-OP2	-5.62	100.65	105.70
1	X	1367	C	C6-N1-C1'	-5.61	114.07	120.80
1	X	1237	U	C5-C4-O4	5.61	129.26	125.90
1	X	1401	G	C4-N9-C1'	5.61	133.79	126.50
1	X	993	C	C6-N1-C2	5.61	122.54	120.30
1	X	2495	A	O4'-C1'-N9	5.61	112.69	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	341	G	C5-C6-O6	-5.60	125.24	128.60
1	X	2853	U	C6-N1-C2	5.60	124.36	121.00
1	X	797	A	C4-N9-C1'	5.60	136.38	126.30
1	X	532	C	N3-C4-C5	-5.60	119.66	121.90
1	X	2731	C	N1-C2-O2	5.59	122.25	118.90
1	X	1001	A	C8-N9-C4	5.59	108.03	105.80
1	X	2059	G	O5'-P-OP2	-5.59	100.67	105.70
1	X	1599	G	N3-C4-C5	5.58	131.39	128.60
1	X	2743	U	C2-N3-C4	-5.58	123.65	127.00
1	X	1516	C	N3-C2-O2	-5.58	117.99	121.90
1	X	1599	G	N3-C4-N9	-5.58	122.65	126.00
1	X	1544	G	C5-C6-N1	5.58	114.29	111.50
1	X	2801	C	N3-C4-C5	5.58	124.13	121.90
1	X	706	U	N3-C2-O2	-5.58	118.30	122.20
1	X	2552	G	C5-C6-O6	-5.58	125.25	128.60
1	X	1308	C	C5-C6-N1	-5.57	118.21	121.00
1	X	2411	A	N1-C2-N3	5.57	132.09	129.30
1	X	1175	G	C5-C6-N1	5.57	114.28	111.50
1	X	1303	A	N9-C4-C5	-5.57	103.57	105.80
1	X	2603	G	C4-C5-N7	5.57	113.03	110.80
1	X	2018	U	N3-C2-O2	-5.57	118.30	122.20
1	X	2050	A	O5'-P-OP1	-5.57	100.69	105.70
1	X	795	A	C5-C6-N1	5.57	120.48	117.70
1	X	1806	U	C2-N3-C4	-5.57	123.66	127.00
1	X	2066	G	C4-C5-C6	5.57	122.14	118.80
1	X	639	U	N1-C2-O2	5.56	126.69	122.80
1	X	119	U	OP1-P-OP2	-5.56	111.26	119.60
1	X	1703	U	N3-C4-O4	-5.56	115.51	119.40
1	X	1065	A	N3-C4-N9	-5.56	122.95	127.40
1	X	528	C	N3-C4-C5	-5.56	119.68	121.90
1	X	1570	G	N3-C4-C5	-5.56	125.82	128.60
1	X	656	G	N7-C8-N9	5.55	115.88	113.10
1	X	2797	C	O4'-C1'-N1	5.55	112.64	108.20
1	X	955	A	N3-C4-N9	5.55	131.84	127.40
1	X	1990	C	C6-N1-C2	-5.55	118.08	120.30
1	X	2077	C	N3-C2-O2	-5.55	118.01	121.90
1	X	2673	C	N3-C4-N4	5.55	121.88	118.00
1	X	1560	A	C5-C6-N6	5.55	128.14	123.70
1	X	902	A	N1-C6-N6	-5.55	115.27	118.60
1	X	1360	G	C5-N7-C8	-5.55	101.53	104.30
1	X	2358	G	C5-C6-N1	-5.55	108.73	111.50
1	X	35	G	N1-C2-N3	5.54	127.22	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1672	G	N1-C6-O6	5.54	123.22	119.90
1	X	511	G	C8-N9-C4	-5.53	104.19	106.40
1	X	963	A	C2-N3-C4	-5.53	107.83	110.60
1	X	610	U	N1-C2-N3	5.53	118.22	114.90
1	X	721	A	N3-C4-C5	5.53	130.67	126.80
1	X	21	A	C2-N3-C4	-5.53	107.84	110.60
1	X	1972	G	N1-C2-N3	-5.53	120.58	123.90
1	X	2044	C	N3-C4-C5	-5.52	119.69	121.90
1	X	1356	G	N1-C6-O6	5.52	123.21	119.90
1	X	2748	A	C5-C6-N6	-5.52	119.28	123.70
1	X	721	A	C4-C5-N7	5.52	113.46	110.70
1	X	2512	G	C2-N3-C4	-5.52	109.14	111.90
1	X	511	G	N3-C4-C5	-5.52	125.84	128.60
1	X	793	G	O4'-C1'-N9	5.52	112.61	108.20
1	X	1184	C	C6-N1-C2	5.52	122.51	120.30
1	X	1303	A	N7-C8-N9	5.52	116.56	113.80
1	X	1691	G	N3-C4-N9	-5.51	122.69	126.00
1	X	1609	U	N3-C4-O4	5.51	123.26	119.40
2	Y	77	G	N7-C8-N9	5.51	115.86	113.10
1	X	511	G	C5-C6-O6	5.51	131.91	128.60
1	X	1506	C	N1-C2-O2	5.51	122.20	118.90
1	X	1452	C	C6-N1-C2	-5.50	118.10	120.30
1	X	1703	U	C5-C6-N1	-5.50	119.95	122.70
1	X	2632	U	C6-N1-C2	-5.50	117.70	121.00
1	X	2842	G	C2-N3-C4	-5.49	109.15	111.90
1	X	2390	U	C5-C6-N1	-5.49	119.96	122.70
1	X	1332	C	C6-N1-C2	-5.49	118.11	120.30
1	X	2474	G	C2-N3-C4	-5.48	109.16	111.90
1	X	2887	G	C4-N9-C1'	5.48	133.63	126.50
1	X	1420	U	C6-N1-C2	-5.48	117.71	121.00
1	X	2298	G	C4-C5-N7	5.47	112.99	110.80
1	X	503	A	C8-N9-C4	-5.47	103.61	105.80
1	X	617	A	N7-C8-N9	-5.47	111.06	113.80
1	X	2429	U	C5-C6-N1	5.47	125.44	122.70
1	X	717	C	C6-N1-C2	-5.47	118.11	120.30
1	X	1591	G	C4-N9-C1'	5.47	133.61	126.50
1	X	1225	G	C8-N9-C4	-5.47	104.21	106.40
1	X	2378	G	N1-C6-O6	-5.47	116.62	119.90
1	X	996	G	C4-C5-N7	5.46	112.99	110.80
1	X	2074	C	N1-C2-O2	-5.46	115.62	118.90
1	X	835	U	C2-N1-C1'	5.46	124.25	117.70
1	X	1029	C	O5'-P-OP2	-5.46	100.79	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1976	G	C4-N9-C1'	5.46	133.59	126.50
1	X	715	A	O4'-C1'-N9	-5.45	103.84	108.20
1	X	824	A	C8-N9-C4	-5.45	103.62	105.80
1	X	2056	G	N3-C4-C5	5.45	131.32	128.60
1	X	2278	G	N3-C4-N9	5.44	129.27	126.00
1	X	1707	U	C6-N1-C2	-5.44	117.74	121.00
1	X	2394	G	C8-N9-C4	-5.44	104.22	106.40
1	X	1781	C	O5'-P-OP2	-5.44	100.81	105.70
1	X	2419	A	N1-C6-N6	5.43	121.86	118.60
1	X	610	U	C5-C6-N1	-5.43	119.98	122.70
1	X	611	U	N3-C2-O2	-5.43	118.40	122.20
1	X	727	G	C6-C5-N7	-5.43	127.14	130.40
1	X	2567	C	C5-C6-N1	-5.43	118.28	121.00
1	X	2079	G	C8-N9-C4	5.43	108.57	106.40
2	Y	105	G	C8-N9-C1'	-5.42	119.95	127.00
1	X	523	A	C4-C5-C6	5.42	119.71	117.00
1	X	1602	U	O4'-C1'-N1	5.42	112.53	108.20
1	X	2474	G	N9-C1'-C2'	5.42	121.04	114.00
1	X	70	G	P-O3'-C3'	5.41	126.19	119.70
1	X	501	C	C6-N1-C2	5.41	122.47	120.30
1	X	440	C	N3-C2-O2	-5.41	118.11	121.90
1	X	607	C	C2-N3-C4	-5.41	117.19	119.90
1	X	1042	C	C5-C6-N1	-5.41	118.29	121.00
1	X	1931	G	C4-C5-N7	5.41	112.96	110.80
1	X	2640	U	OP1-P-OP2	5.41	127.71	119.60
1	X	721	A	N7-C8-N9	5.41	116.50	113.80
1	X	1065	A	C4-C5-C6	5.40	119.70	117.00
1	X	378	C	C5-C6-N1	5.40	123.70	121.00
1	X	1705	G	C2-N3-C4	-5.40	109.20	111.90
1	X	2552	G	C5-C6-N1	5.39	114.20	111.50
1	X	791	U	C6-N1-C1'	5.39	128.74	121.20
1	X	2018	U	C2-N3-C4	-5.38	123.77	127.00
1	X	2045	A	C6-N1-C2	-5.38	115.37	118.60
1	X	511	G	N1-C6-O6	-5.38	116.67	119.90
1	X	1746	G	N1-C6-O6	5.38	123.13	119.90
1	X	78	U	N1-C2-O2	5.38	126.57	122.80
1	X	21	A	C4-C5-C6	5.38	119.69	117.00
1	X	457	G	C8-N9-C4	-5.38	104.25	106.40
1	X	1278	G	N7-C8-N9	5.37	115.78	113.10
1	X	1320	G	N3-C4-C5	-5.37	125.92	128.60
1	X	2603	G	C8-N9-C4	5.37	108.55	106.40
1	X	1660	A	C4-C5-C6	5.37	119.68	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2433	C	C2-N1-C1'	5.37	124.70	118.80
1	X	242	U	C4-C5-C6	5.36	122.92	119.70
1	X	1294	G	N3-C4-C5	-5.36	125.92	128.60
1	X	817	G	N3-C4-C5	-5.36	125.92	128.60
1	X	2278	G	C4-N9-C1'	5.36	133.46	126.50
1	X	1591	G	C8-N9-C4	-5.36	104.26	106.40
1	X	1702	C	C6-N1-C2	5.36	122.44	120.30
1	X	2483	C	C6-N1-C2	5.36	122.44	120.30
1	X	1232	G	N3-C4-N9	-5.35	122.79	126.00
1	X	1312	A	OP1-P-O3'	5.35	116.97	105.20
1	X	595	G	N1-C2-N3	5.35	127.11	123.90
1	X	2524	A	N1-C6-N6	-5.35	115.39	118.60
1	X	2599	A	N9-C4-C5	-5.35	103.66	105.80
1	X	532	C	N3-C4-N4	5.35	121.74	118.00
1	X	698	U	C2-N1-C1'	5.35	124.12	117.70
1	X	1300	G	C2-N3-C4	-5.35	109.23	111.90
1	X	791	U	C4-C5-C6	5.34	122.91	119.70
1	X	1768	C	C6-N1-C2	-5.34	118.16	120.30
1	X	2752	A	C8-N9-C4	-5.34	103.66	105.80
1	X	2797	C	N3-C4-N4	-5.34	114.26	118.00
1	X	2551	G	C5-N7-C8	-5.34	101.63	104.30
1	X	588	G	N3-C4-N9	5.33	129.20	126.00
1	X	661	U	C6-N1-C2	-5.33	117.80	121.00
1	X	43	A	O4'-C1'-N9	5.33	112.47	108.20
1	X	374	U	N3-C2-O2	-5.33	118.47	122.20
1	X	2302	C	C4-C5-C6	5.33	120.07	117.40
1	X	2476	U	C6-N1-C2	5.33	124.20	121.00
1	X	1570	G	N3-C4-N9	5.33	129.20	126.00
1	X	1658	A	C5-N7-C8	-5.33	101.24	103.90
1	X	2657	G	C6-C5-N7	-5.33	127.20	130.40
1	X	1838	G	C6-C5-N7	-5.32	127.21	130.40
1	X	526	A	N1-C6-N6	5.32	121.79	118.60
1	X	365	A	N9-C4-C5	5.31	107.93	105.80
1	X	1232	G	N3-C4-C5	5.31	131.25	128.60
1	X	509	G	N1-C6-O6	5.31	123.09	119.90
1	X	828	A	N3-C4-N9	-5.31	123.15	127.40
1	X	198	A	C5-C6-N6	-5.30	119.46	123.70
1	X	1021	G	N7-C8-N9	-5.30	110.45	113.10
1	X	1368	C	C6-N1-C2	5.30	122.42	120.30
1	X	1294	G	C6-N1-C2	-5.30	121.92	125.10
1	X	1689	G	C4-C5-N7	-5.30	108.68	110.80
1	X	2047	A	C6-N1-C2	-5.30	115.42	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1479	G	N3-C4-N9	-5.30	122.82	126.00
1	X	2089[A]	A	N3-C4-C5	-5.30	123.09	126.80
1	X	2089[B]	A	N3-C4-C5	-5.30	123.09	126.80
1	X	696	G	C2-N3-C4	5.29	114.55	111.90
1	X	1566	G	C8-N9-C4	-5.29	104.28	106.40
1	X	2381	A	C6-N1-C2	-5.29	115.43	118.60
1	X	1395	G	N1-C6-O6	5.29	123.07	119.90
1	X	34	U	C2-N1-C1'	5.29	124.04	117.70
1	X	630	G	N7-C8-N9	5.29	115.74	113.10
1	X	797	A	C5-C6-N6	-5.29	119.47	123.70
2	Y	92	G	N1-C2-N2	5.29	120.96	116.20
1	X	373	A	C5-C6-N6	5.28	127.93	123.70
1	X	1278	G	C6-N1-C2	5.28	128.27	125.10
1	X	549	U	P-O3'-C3'	5.28	126.04	119.70
1	X	262	G	C5-C6-O6	5.28	131.77	128.60
1	X	637	U	C5-C4-O4	5.28	129.07	125.90
1	X	1686	G	C5-N7-C8	-5.28	101.66	104.30
1	X	1981	G	N1-C2-N3	5.28	127.06	123.90
1	X	122	G	C4-C5-C6	-5.27	115.64	118.80
1	X	1659	C	N1-C2-O2	-5.27	115.74	118.90
1	X	2797	C	C2-N1-C1'	-5.27	113.00	118.80
1	X	1758	A	N3-C4-C5	-5.27	123.11	126.80
1	X	2082	C	C6-N1-C2	5.27	122.41	120.30
1	X	197	G	C2-N3-C4	-5.27	109.27	111.90
1	X	553	A	N1-C6-N6	-5.27	115.44	118.60
1	X	2068	U	C6-N1-C2	-5.27	117.84	121.00
1	X	1054	A	N1-C6-N6	-5.26	115.44	118.60
2	Y	78	C	C5-C4-N4	5.26	123.89	120.20
1	X	374	U	N1-C2-O2	5.26	126.48	122.80
1	X	1963	A	N1-C2-N3	5.26	131.93	129.30
1	X	1005	G	O5'-P-OP2	-5.26	100.97	105.70
1	X	2060	A	N1-C6-N6	-5.26	115.44	118.60
1	X	376	A	C4-N9-C1'	5.26	135.76	126.30
1	X	82	G	C5-C6-N1	-5.26	108.87	111.50
1	X	515	G	N3-C2-N2	5.26	123.58	119.90
1	X	73	A	C2-N3-C4	5.25	113.23	110.60
1	X	1278	G	C5-C6-N1	-5.25	108.87	111.50
1	X	2073	G	C6-C5-N7	-5.25	127.25	130.40
1	X	2529	G	C5-C6-O6	-5.25	125.45	128.60
1	X	2876	G	N9-C4-C5	5.25	107.50	105.40
1	X	1360	G	C5-C6-O6	-5.25	125.45	128.60
1	X	1004	A	C4-C5-C6	-5.25	114.38	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1289	A	C4-C5-N7	5.25	113.32	110.70
1	X	1343	U	C5-C6-N1	5.25	125.32	122.70
1	X	1602	U	C5-C4-O4	5.25	129.05	125.90
1	X	2661	A	N7-C8-N9	-5.25	111.18	113.80
1	X	1180	G	C4-C5-N7	5.25	112.90	110.80
1	X	1479	G	C5-C6-N1	-5.25	108.88	111.50
1	X	2641	A	C6-N1-C2	-5.25	115.45	118.60
1	X	102	A	C4-C5-C6	5.24	119.62	117.00
1	X	2094	G	N3-C4-N9	5.24	129.15	126.00
1	X	350	G	C8-N9-C1'	-5.24	120.19	127.00
1	X	605	U	N1-C2-N3	5.24	118.04	114.90
1	X	599	A	C6-N1-C2	-5.24	115.46	118.60
1	X	2052	C	OP1-P-OP2	-5.24	111.75	119.60
1	X	2565	C	C5-C6-N1	-5.24	118.38	121.00
1	X	350	G	C6-N1-C2	-5.23	121.96	125.10
1	X	1807	A	N1-C6-N6	5.23	121.74	118.60
1	X	2472	G	N9-C4-C5	5.23	107.49	105.40
2	Y	80	A	N1-C6-N6	5.23	121.74	118.60
1	X	1843	U	C5-C4-O4	-5.23	122.76	125.90
1	X	2682	G	C4-N9-C1'	-5.23	119.70	126.50
1	X	28	A	OP2-P-O3'	5.22	116.69	105.20
1	X	1511	C	C6-N1-C2	-5.22	118.21	120.30
1	X	2597	G	N1-C6-O6	-5.22	116.77	119.90
1	X	1291	A	OP1-P-OP2	5.22	127.43	119.60
1	X	465	C	C5-C6-N1	-5.22	118.39	121.00
1	X	586	C	C2-N1-C1'	-5.22	113.06	118.80
1	X	1245	G	C4-C5-C6	5.22	121.93	118.80
1	X	1291	A	O5'-P-OP2	-5.22	101.00	105.70
1	X	1691	G	N3-C4-C5	5.21	131.21	128.60
1	X	1056	U	O4'-C1'-N1	5.21	112.37	108.20
1	X	1180	G	C6-C5-N7	-5.21	127.27	130.40
1	X	1703	U	C5-C4-O4	5.21	129.03	125.90
1	X	2619	G	N3-C4-N9	5.21	129.13	126.00
1	X	494	U	N1-C2-O2	-5.21	119.15	122.80
1	X	1006	G	C5-C6-N1	-5.21	108.89	111.50
1	X	2278	G	C8-N9-C1'	-5.21	120.23	127.00
1	X	2609	G	C6-C5-N7	-5.21	127.28	130.40
16	O	25	LEU	CA-CB-CG	-5.21	103.32	115.30
2	Y	88	U	C5-C6-N1	5.21	125.30	122.70
1	X	1017	A	N7-C8-N9	5.21	116.40	113.80
1	X	2534	C	N3-C2-O2	-5.21	118.26	121.90
1	X	1636	U	P-O3'-C3'	5.20	125.94	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	648	G	C4-C5-N7	-5.20	108.72	110.80
1	X	2261	A	C6-C5-N7	-5.20	128.66	132.30
1	X	297	G	N3-C4-N9	-5.20	122.88	126.00
1	X	630	G	C4-N9-C1'	-5.20	119.74	126.50
1	X	2620	U	C5-C6-N1	5.20	125.30	122.70
1	X	635	G	N7-C8-N9	5.20	115.70	113.10
1	X	1050	C	C5-C6-N1	-5.20	118.40	121.00
1	X	2043	U	N1-C2-N3	5.19	118.02	114.90
1	X	2044	C	OP2-P-O3'	5.19	116.62	105.20
1	X	885	C	C4-C5-C6	5.19	119.99	117.40
1	X	1955	A	C5-C6-N1	5.18	120.29	117.70
1	X	1978	U	O4'-C1'-N1	5.18	112.35	108.20
1	X	559	A	C8-N9-C4	5.18	107.87	105.80
1	X	1047	G	C6-C5-N7	-5.18	127.29	130.40
1	X	2654	G	C8-N9-C4	-5.18	104.33	106.40
1	X	2793	G	C8-N9-C4	-5.18	104.33	106.40
1	X	2064	A	C5-N7-C8	-5.18	101.31	103.90
1	X	2727	G	C8-N9-C4	5.18	108.47	106.40
1	X	778	G	N1-C6-O6	5.17	123.00	119.90
1	X	1712	A	OP2-P-O3'	5.17	116.58	105.20
1	X	2740	A	N1-C2-N3	5.17	131.89	129.30
1	X	1291	A	C8-N9-C4	5.17	107.87	105.80
1	X	34	U	N1-C2-O2	5.17	126.42	122.80
1	X	1295	C	OP1-P-OP2	5.17	127.35	119.60
1	X	1732	U	C5-C4-O4	5.17	129.00	125.90
1	X	2576	G	C4-C5-C6	5.17	121.90	118.80
1	X	1721	A	C8-N9-C4	-5.16	103.73	105.80
1	X	2724	G	N1-C6-O6	5.16	123.00	119.90
1	X	1968	C	N1-C2-O2	5.16	122.00	118.90
1	X	1686	G	C4-C5-N7	5.16	112.86	110.80
1	X	263	G	C6-C5-N7	-5.16	127.31	130.40
1	X	568	C	C5-C6-N1	-5.16	118.42	121.00
1	X	1953	U	C3'-C2'-C1'	-5.16	97.38	101.50
1	X	70	G	O4'-C1'-N9	5.16	112.33	108.20
1	X	2066	G	C8-N9-C4	-5.16	104.34	106.40
1	X	2839	A	C2-N3-C4	5.16	113.18	110.60
1	X	1160	C	C6-N1-C2	5.15	122.36	120.30
1	X	12	U	C6-N1-C2	-5.15	117.91	121.00
1	X	2504	C	C5-C6-N1	5.15	123.57	121.00
1	X	1245	G	N3-C4-C5	-5.15	126.03	128.60
1	X	152	C	N1-C2-O2	5.14	121.99	118.90
1	X	1153	C	N1-C2-O2	5.14	121.99	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1232	G	C2-N3-C4	-5.14	109.33	111.90
1	X	1412	G	C2-N3-C4	5.14	114.47	111.90
1	X	892	U	C2-N1-C1'	-5.14	111.53	117.70
1	X	985	A	O5'-P-OP1	-5.14	101.07	105.70
1	X	1356	G	C5-C6-O6	-5.14	125.52	128.60
1	X	2433	C	P-O3'-C3'	5.14	125.87	119.70
1	X	1023	A	C2-N3-C4	-5.14	108.03	110.60
1	X	381	G	C6-C5-N7	-5.14	127.32	130.40
1	X	1566	G	N3-C4-C5	-5.14	126.03	128.60
1	X	2446	U	C4-C5-C6	-5.14	116.62	119.70
1	X	569	U	N3-C2-O2	5.13	125.79	122.20
1	X	1168	C	N3-C2-O2	-5.13	118.31	121.90
1	X	1182	G	C5-C6-O6	-5.13	125.52	128.60
1	X	1244	G	C6-C5-N7	5.13	133.48	130.40
1	X	2393	A	C8-N9-C4	5.13	107.85	105.80
1	X	2724	G	N3-C4-C5	5.13	131.16	128.60
1	X	2851	G	N7-C8-N9	5.13	115.66	113.10
1	X	1080	G	N1-C6-O6	5.13	122.97	119.90
1	X	1746	G	C8-N9-C4	-5.13	104.35	106.40
1	X	536	A	C2-N3-C4	-5.12	108.04	110.60
1	X	2063	C	C4-C5-C6	-5.12	114.84	117.40
2	Y	73	G	C4-C5-N7	-5.12	108.75	110.80
1	X	577	A	C2-N3-C4	5.12	113.16	110.60
2	Y	95	A	N9-C4-C5	-5.12	103.75	105.80
1	X	169	G	O4'-C1'-N9	5.12	112.29	108.20
1	X	2583	C	C5-C6-N1	5.12	123.56	121.00
1	X	435	A	C8-N9-C4	5.12	107.85	105.80
1	X	613	G	OP2-P-O3'	5.11	116.45	105.20
1	X	1244	G	C8-N9-C1'	5.11	133.64	127.00
1	X	1855	G	N3-C4-C5	-5.11	126.05	128.60
1	X	1262	U	C6-N1-C2	5.11	124.06	121.00
1	X	2269	G	N1-C6-O6	5.10	122.96	119.90
1	X	2383	C	C6-N1-C2	-5.10	118.26	120.30
1	X	590	U	C5-C4-O4	5.10	128.96	125.90
1	X	1963	A	C5-C6-N1	-5.10	115.15	117.70
1	X	1802	U	C5-C6-N1	-5.10	120.15	122.70
1	X	601	G	N1-C6-O6	-5.10	116.84	119.90
1	X	1867	G	C4-N9-C1'	5.10	133.13	126.50
1	X	2567	C	C6-N1-C2	5.10	122.34	120.30
1	X	323	C	C2-N3-C4	5.10	122.45	119.90
1	X	675	G	C6-C5-N7	-5.10	127.34	130.40
1	X	852	U	C6-N1-C2	-5.10	117.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1200	A	C8-N9-C4	-5.10	103.76	105.80
1	X	1273	G	C8-N9-C4	-5.10	104.36	106.40
1	X	1784	U	N3-C4-O4	5.10	122.97	119.40
1	X	1838	G	C8-N9-C4	-5.10	104.36	106.40
1	X	2023	C	OP1-P-O3'	5.09	116.41	105.20
1	X	1711	G	O5'-P-OP1	-5.09	101.12	105.70
1	X	2406	G	N1-C6-O6	5.09	122.95	119.90
1	X	1712	A	N1-C6-N6	5.09	121.65	118.60
1	X	2334	G	N3-C4-C5	5.09	131.14	128.60
1	X	558	A	OP2-P-O3'	5.09	116.39	105.20
1	X	1022	G	C5-C6-O6	-5.08	125.55	128.60
1	X	36	G	N3-C4-N9	5.08	129.05	126.00
1	X	797	A	C8-N9-C4	-5.08	103.77	105.80
1	X	2615	G	N1-C6-O6	-5.08	116.85	119.90
2	Y	109	C	N1-C2-O2	5.08	121.95	118.90
1	X	1020	G	N1-C6-O6	-5.08	116.85	119.90
1	X	2700	G	N1-C6-O6	5.08	122.95	119.90
1	X	14	A	C5-C6-N1	-5.08	115.16	117.70
1	X	2706	A	N3-C4-C5	5.07	130.35	126.80
1	X	556	U	C6-N1-C2	5.07	124.04	121.00
1	X	1293	U	C4-C5-C6	5.07	122.74	119.70
1	X	263	G	N1-C6-O6	5.07	122.94	119.90
1	X	1041	G	C8-N9-C4	5.07	108.43	106.40
1	X	1169	G	N9-C4-C5	5.07	107.43	105.40
1	X	1393	C	C5-C6-N1	5.07	123.53	121.00
1	X	1972	G	C4-C5-N7	5.07	112.83	110.80
1	X	21	A	N1-C2-N3	5.07	131.83	129.30
1	X	1458	A	O4'-C1'-N9	5.06	112.25	108.20
1	X	2885	U	N3-C4-O4	5.06	122.94	119.40
1	X	1686	G	C5-C6-O6	-5.06	125.56	128.60
1	X	381	G	C4-N9-C1'	5.06	133.08	126.50
1	X	988	C	OP1-P-OP2	-5.06	112.02	119.60
1	X	2529	G	C5-N7-C8	-5.06	101.77	104.30
1	X	367	A	C5-C6-N1	5.06	120.23	117.70
1	X	1972	G	C5-C6-O6	-5.06	125.57	128.60
1	X	2670	G	N9-C4-C5	5.06	107.42	105.40
1	X	69	C	N3-C2-O2	-5.05	118.36	121.90
1	X	666	A	C2-N3-C4	-5.05	108.07	110.60
1	X	1972	G	C2-N3-C4	5.05	114.43	111.90
1	X	2602	C	C5-C6-N1	5.05	123.53	121.00
1	X	363	A	N1-C6-N6	5.05	121.63	118.60
1	X	705	U	C5-C6-N1	-5.05	120.17	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2601	G	C8-N9-C4	-5.05	104.38	106.40
1	X	2619	G	C6-C5-N7	-5.05	127.37	130.40
1	X	514	G	N1-C2-N2	-5.05	111.66	116.20
1	X	1431	U	C5-C6-N1	5.05	125.22	122.70
1	X	1460	U	C6-N1-C2	-5.04	117.97	121.00
1	X	2627	A	C2-N3-C4	-5.04	108.08	110.60
1	X	1009	C	O5'-P-OP2	-5.04	101.16	105.70
1	X	20	C	C5-C4-N4	-5.04	116.67	120.20
1	X	795	A	C4-C5-N7	5.04	113.22	110.70
1	X	2599	A	C4-C5-C6	5.04	119.52	117.00
1	X	2682	G	O4'-C1'-N9	5.04	112.23	108.20
1	X	2839	A	C5-C6-N1	5.04	120.22	117.70
1	X	2887	G	C4-C5-N7	5.04	112.81	110.80
1	X	516	A	C4-C5-C6	5.04	119.52	117.00
1	X	1279	C	C2-N1-C1'	5.04	124.34	118.80
1	X	1968	C	N3-C2-O2	-5.03	118.38	121.90
1	X	542	A	C8-N9-C4	5.03	107.81	105.80
1	X	1066	G	O5'-P-OP2	-5.03	101.17	105.70
1	X	1226	G	C5-C6-N1	-5.03	108.99	111.50
1	X	349	U	O5'-P-OP2	-5.03	101.18	105.70
1	X	1901	C	P-O3'-C3'	5.03	125.73	119.70
1	X	2601	G	N1-C6-O6	-5.03	116.88	119.90
1	X	1310	A	C8-N9-C4	5.02	107.81	105.80
1	X	2648	G	C8-N9-C4	-5.02	104.39	106.40
1	X	2793	G	N7-C8-N9	5.02	115.61	113.10
1	X	2735	G	C5-C6-N1	-5.02	108.99	111.50
1	X	70	G	C5-C6-N1	5.02	114.01	111.50
1	X	297	G	N9-C4-C5	5.02	107.41	105.40
1	X	631	U	N1-C2-N3	5.02	117.91	114.90
1	X	1704	C	O5'-P-OP1	5.02	116.72	110.70
1	X	1782	A	C2-N3-C4	-5.01	108.09	110.60
1	X	1183	G	N1-C6-O6	-5.01	116.89	119.90
1	X	74	U	C6-N1-C2	-5.01	117.99	121.00
1	X	102	A	C6-C5-N7	-5.01	128.79	132.30
1	X	607	C	OP1-P-O3'	5.01	116.22	105.20
1	X	883	C	N3-C2-O2	5.01	125.41	121.90
1	X	2446	U	C2-N3-C4	5.01	130.01	127.00
1	X	2715	G	C5-C6-N1	-5.01	108.99	111.50
1	X	2021	C	C2-N3-C4	5.00	122.40	119.90
1	X	1915	G	N3-C4-C5	-5.00	126.10	128.60
1	X	2382	C	N3-C4-C5	5.00	123.90	121.90

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	156	ARG	Peptide
3	A	195	VAL	Peptide
3	A	50	THR	Peptide
4	B	159	ASP	Peptide
4	B	166	GLY	Peptide
4	B	204	PRO	Peptide
4	B	58	ALA	Peptide
4	B	97	ASP	Peptide
5	C	133	ALA	Peptide
5	C	142	VAL	Peptide
5	C	165	LEU	Peptide
5	C	28	PRO	Peptide
5	C	53	ASN	Peptide
7	E	152	ARG	Peptide
8	G	132	PRO	Peptide
8	G	136	GLN	Peptide
8	G	137	GLN	Peptide
8	G	138	PRO	Peptide
8	G	68	ASN	Peptide
9	H	110	ASN	Peptide
10	I	23	VAL	Peptide
10	I	24	ALA	Peptide
10	I	49	GLY	Peptide
10	I	81	GLN	Peptide
11	J	99	PRO	Peptide
14	M	45	PHE	Peptide
16	O	55	GLY	Peptide
16	O	77	LYS	Peptide
18	Q	55	ILE	Peptide
19	R	74	LYS	Peptide
19	R	83	TYR	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	X	58141	0	29232	1120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Y	2430	0	1229	57	0
3	A	1641	0	1415	71	0
4	B	1534	0	1495	52	0
5	C	1365	0	1258	88	0
6	D	926	0	824	33	0
7	E	793	0	475	17	0
8	G	1062	0	1000	34	0
9	H	902	0	956	39	0
10	I	780	0	621	38	0
11	J	1011	0	988	30	0
12	K	883	0	890	41	0
13	L	672	0	515	13	0
14	M	779	0	726	28	0
15	N	937	0	1003	47	0
16	O	700	0	629	32	0
17	P	852	0	905	32	0
18	Q	656	0	615	33	0
19	R	596	0	450	23	0
20	S	1145	0	991	40	0
21	T	561	0	555	16	0
22	V	519	0	530	24	0
23	W	437	0	474	18	0
24	Z	337	0	343	19	0
25	2	360	0	402	16	0
26	3	419	0	323	10	0
27	X	27	0	0	2	0
28	X	16	0	28	2	0
29	3	3	0	0	0	0
29	E	1	0	0	0	0
29	I	1	0	0	0	0
29	X	203	0	0	0	0
29	Y	1	0	0	0	0
29	Z	1	0	0	0	0
30	3	1	0	0	0	0
30	C	1	0	0	0	0
30	G	1	0	0	0	0
30	J	1	0	0	0	0
30	X	78	0	0	0	0
30	Y	2	0	0	0	0
31	X	15	0	17	0	0
32	X	10	0	19	3	0
All	All	80800	0	48908	1794	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (1794) 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)
5:C:40:GLN:HE22	5:C:178:ALA:HB2	1.24	1.00
1:X:1835:U:H2'	1:X:1836:A:H5"	1.45	0.98
1:X:1515:G:H1	1:X:1564:G:H1	1.11	0.96
1:X:2850:G:OP2	4:B:86:ARG:NH2	2.00	0.93
1:X:630:G:OP2	10:I:21:ARG:NH2	2.03	0.92
1:X:922:G:O6	1:X:943:C:N4	2.03	0.92
1:X:1352:C:H42	1:X:1374:G:H1	1.17	0.92
1:X:152:C:H41	1:X:177:G:H1	1.10	0.92
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.50	0.92
1:X:273:A:OP2	1:X:297:G:N2	2.02	0.92
18:Q:61:LYS:H	18:Q:72:THR:HG22	1.33	0.91
1:X:83:G:H21	1:X:102:A:H2	1.18	0.91
1:X:1487:G:N2	1:X:1597:U:O2	2.03	0.90
1:X:1815:C:H5"	3:A:224:VAL:HG11	1.49	0.90
1:X:2707:C:H5'	4:B:202:PRO:HA	1.53	0.90
1:X:1303:A:H2	1:X:2041:A:H62	1.17	0.90
2:Y:21:G:H1	2:Y:58:G:H1	1.17	0.89
18:Q:82:LEU:HD12	18:Q:85:GLY:HA3	1.52	0.88
1:X:1683:U:H2'	1:X:1684:A:H5"	1.56	0.88
5:C:54:ARG:O	5:C:56:ALA:N	2.06	0.88
2:Y:48:A:OP1	13:L:67:ALA:N	2.06	0.87
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.56	0.87
23:W:40:ASN:HB3	23:W:43:ILE:H	1.39	0.86
1:X:124:A:H5'	25:2:20:ARG:HD3	1.55	0.86
1:X:1247:G:O2'	1:X:1275:A:N6	2.09	0.86
1:X:2088:G:OP1	5:C:68:LYS:NZ	2.08	0.85
22:V:7:ARG:O	22:V:60:ARG:NH2	2.09	0.85
1:X:1542:C:H3'	1:X:1543:G:H5"	1.56	0.85
1:X:198:A:N6	1:X:201:C:OP2	2.10	0.85
5:C:25:GLY:O	5:C:27:GLU:N	2.10	0.84
1:X:2496:A:O2'	11:J:56:ARG:NH1	2.09	0.84
1:X:131:G:N1	1:X:148:U:O2	2.12	0.83
1:X:1501:G:H22	1:X:2729:G:H22	1.26	0.83
1:X:2649:U:O2'	1:X:2845:G:N2	2.12	0.82
4:B:8:ARG:NH1	4:B:206:LYS:O	2.13	0.82
1:X:658:A:H3'	1:X:659:A:H5"	1.62	0.82
9:H:76:TYR:HB2	14:M:75:THR:HG23	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:33:LEU:HD11	5:C:181:LEU:HD11	1.62	0.81
17:P:2:GLU:HG3	17:P:109:ASP:H	1.45	0.81
7:E:78:GLY:O	7:E:80:SER:N	2.13	0.81
1:X:503:A:H2	1:X:517:A:H62	1.26	0.81
1:X:1290:G:OP2	15:N:13:ARG:NH2	2.14	0.80
3:A:46:GLN:OE1	3:A:48:LYS:N	2.15	0.80
20:S:49:ILE:HA	20:S:52:ILE:HG22	1.63	0.80
2:Y:15:C:H42	2:Y:105:G:H21	1.27	0.80
1:X:1832:C:H1'	3:A:51:VAL:HG21	1.64	0.79
9:H:93:PRO:HD3	9:H:114:ILE:HG22	1.63	0.79
13:L:19:ARG:NH1	13:L:47:ASP:OD2	2.16	0.79
1:X:151:U:H2'	1:X:152:C:O2	1.83	0.79
9:H:88:ARG:HB3	9:H:94:ARG:HD3	1.64	0.78
1:X:498:G:H21	1:X:503:A:H8	1.28	0.78
1:X:778:G:O6	1:X:806:A:C8	2.36	0.78
3:A:212:ARG:HG2	3:A:216:ILE:HA	1.65	0.78
1:X:1472:C:N4	1:X:1617:A:OP2	2.15	0.78
25:2:16:VAL:H	25:2:21:LYS:HG3	1.49	0.78
1:X:504:G:C8	25:2:38:LYS:HG2	2.19	0.77
12:K:105:LYS:HB2	24:Z:42:ARG:HG2	1.66	0.77
1:X:1037:A:OP1	15:N:50:ARG:NH1	2.17	0.77
20:S:113:VAL:HB	20:S:147:GLU:HA	1.65	0.77
1:X:1065:A:H62	1:X:1185:U:H3	1.33	0.77
1:X:1465:G:H2'	1:X:1466:G:C8	2.19	0.77
24:Z:15:LYS:O	24:Z:18:THR:HG23	1.85	0.77
5:C:108:LEU:O	5:C:112:SER:OG	2.02	0.77
1:X:1512:U:H2'	1:X:1513:A:C8	2.20	0.77
1:X:778:G:O6	1:X:806:A:N7	2.18	0.77
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.67	0.77
3:A:107:PRO:HA	3:A:195:VAL:HA	1.66	0.76
5:C:176:THR:OG1	5:C:179:GLN:OE1	2.02	0.76
1:X:787:U:H2'	1:X:788:A:C8	2.20	0.76
1:X:243:U:O2	1:X:260:A:N6	2.17	0.76
20:S:109:VAL:HG11	20:S:145:ILE:H	1.50	0.76
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.67	0.76
10:I:106:LYS:H	10:I:125:ALA:HB1	1.51	0.76
1:X:1514:A:H3'	1:X:1515:G:H8	1.50	0.75
5:C:177:THR:O	5:C:181:LEU:HD12	1.86	0.75
12:K:109:ARG:NH1	12:K:112:ASP:OD2	2.20	0.75
1:X:1212:U:H3	1:X:1220:A:H61	1.32	0.75
1:X:1866:G:C6	1:X:1954:A:H5"	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:721:A:H8	1:X:2096:G:H21	1.33	0.75
5:C:14:SER:O	5:C:14:SER:OG	2.03	0.75
1:X:2717:A:OP1	12:K:4:ARG:NH2	2.18	0.75
18:Q:34:ASN:ND2	18:Q:37:GLN:OE1	2.19	0.74
3:A:179:GLY:H	3:A:271:VAL:HG13	1.50	0.74
20:S:109:VAL:HB	20:S:144:ASP:HA	1.69	0.74
1:X:1886:A:N6	1:X:1910:G:O2'	2.20	0.74
3:A:131:PRO:HA	3:A:189:ARG:HA	1.69	0.74
1:X:788:A:O2'	1:X:1703:U:OP1	2.06	0.74
18:Q:26:THR:HB	18:Q:79:ILE:HG22	1.68	0.74
3:A:45:ASN:OD1	3:A:45:ASN:N	2.21	0.73
1:X:1593:G:H5'	1:X:1593:G:H8	1.54	0.73
18:Q:5:ASP:OD1	18:Q:5:ASP:N	2.21	0.73
1:X:2883:U:H2'	1:X:2884:G:H8	1.52	0.73
2:Y:15:C:N4	2:Y:105:G:H21	1.86	0.73
1:X:1492:G:N7	1:X:1493:U:H5	1.87	0.73
21:T:48:GLN:NE2	21:T:50:GLY:O	2.21	0.73
1:X:719:G:H1'	5:C:74:ARG:HE	1.54	0.73
1:X:319:G:H22	1:X:326:A:H61	1.37	0.72
1:X:460:C:O2	1:X:1891:U:O2'	2.06	0.72
14:M:16:ARG:H	14:M:79:HIS:HD2	1.36	0.72
5:C:103:LYS:HA	5:C:106:ARG:HD2	1.71	0.72
1:X:323:C:H5'	1:X:324:A:C8	2.24	0.72
1:X:2232:A:N6	1:X:2246:U:O4	2.17	0.72
1:X:422:G:H1	1:X:444:C:H42	1.38	0.72
16:O:25:LEU:HD22	16:O:33:PHE:HE2	1.55	0.72
5:C:117:LYS:NZ	5:C:183:VAL:O	2.18	0.72
1:X:1323:A:O2'	1:X:1325:U:OP2	2.07	0.72
1:X:717:C:H5"	5:C:89:VAL:HG11	1.71	0.72
1:X:2883:U:H2'	1:X:2884:G:C8	2.24	0.72
5:C:40:GLN:NE2	5:C:178:ALA:HB2	2.01	0.72
1:X:2358:G:O2'	1:X:2363:A:N1	2.23	0.71
4:B:38:LYS:NZ	4:B:97:ASP:HA	2.05	0.71
15:N:91:ASN:O	15:N:93:LYS:N	2.23	0.71
16:O:63:ASN:H	16:O:95:LEU:HA	1.54	0.71
1:X:1440:A:O2'	1:X:1514:A:O2'	2.08	0.71
1:X:715:A:H4'	1:X:716:C:H5"	1.72	0.71
1:X:1415:A:O2'	1:X:1417:G:N7	2.21	0.71
21:T:35:ASP:HA	21:T:75:VAL:HG12	1.73	0.71
1:X:755:C:H42	1:X:766:G:H1	1.39	0.70
1:X:1383:G:N2	1:X:1644:C:O2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:142:HIS:N	3:A:191:THR:O	2.25	0.70
6:D:162:THR:HG22	6:D:164:GLU:H	1.55	0.70
1:X:682:A:H4'	1:X:683:G:H5'	1.74	0.70
1:X:1563:U:H2'	1:X:1564:G:H8	1.57	0.70
4:B:192:ASN:HB3	4:B:194:VAL:HG23	1.74	0.70
1:X:2351:U:H3	1:X:2358:G:H1	1.37	0.70
1:X:2712:G:OP2	14:M:51:LYS:NZ	2.19	0.70
10:I:120:LYS:HA	10:I:124:LYS:HA	1.74	0.70
6:D:38:MET:HG2	6:D:57:LEU:HD22	1.73	0.69
18:Q:91:ASN:ND2	22:V:36:GLN:OE1	2.25	0.69
1:X:1302:G:OP1	24:Z:16:ARG:NH2	2.25	0.69
12:K:8:ARG:HD2	12:K:16:MET:HE2	1.73	0.69
14:M:52:ARG:HH11	14:M:52:ARG:HG3	1.55	0.69
1:X:1063:U:H3	1:X:1186:A:H62	1.41	0.69
4:B:97:ASP:OD1	4:B:98:ALA:N	2.25	0.69
1:X:83:G:H1	1:X:101:G:HO2'	1.39	0.69
1:X:2355:A:H2'	1:X:2356:A:C8	2.27	0.69
5:C:78:ILE:HD12	5:C:79:ARG:HG2	1.74	0.69
22:V:59:GLU:O	22:V:63:GLU:N	2.23	0.69
4:B:7:GLY:HA2	4:B:53:PHE:CZ	2.29	0.68
1:X:1563:U:H2'	1:X:1564:G:C8	2.28	0.68
10:I:78:ASN:ND2	10:I:105:GLU:O	2.26	0.68
18:Q:50:VAL:HA	18:Q:82:LEU:HA	1.74	0.68
1:X:659:A:O2'	1:X:660:A:O5'	2.12	0.68
1:X:2126:C:O4'	1:X:2218:G:N2	2.26	0.68
9:H:79:PHE:HD1	14:M:72:VAL:HG22	1.59	0.68
1:X:735:C:O2'	1:X:825:G:OP1	2.12	0.68
1:X:1289:A:OP1	15:N:13:ARG:NH1	2.27	0.67
3:A:54:HIS:HB2	3:A:215:GLY:HA2	1.77	0.67
1:X:2311:U:H3	1:X:2411:A:N6	1.92	0.67
1:X:841:C:H2'	1:X:842:U:C6	2.28	0.67
1:X:1174:U:O2	4:B:162:ARG:NH2	2.27	0.67
1:X:1934:G:O2'	1:X:1935:C:O4'	2.11	0.67
1:X:539:G:OP1	17:P:8:ARG:NH1	2.28	0.67
12:K:6:LEU:HB3	12:K:13:ARG:NH1	2.10	0.67
18:Q:16:SER:HB2	18:Q:26:THR:HG21	1.76	0.67
21:T:92:VAL:HG22	21:T:93:ALA:H	1.60	0.67
1:X:2843:A:OP1	4:B:127:PHE:HB2	1.95	0.67
1:X:2419:A:H2	1:X:2451:C:H42	1.41	0.66
2:Y:15:C:H42	2:Y:105:G:N2	1.92	0.66
1:X:498:G:OP1	5:C:58:SER:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:579:U:H5'	15:N:42:SER:OG	1.95	0.66
2:Y:79:C:H42	2:Y:92:G:H1	1.42	0.66
1:X:2101:U:H2'	1:X:2102:U:C6	2.31	0.66
1:X:2571:G:OP1	32:X:3286:SPD:N1	2.29	0.66
2:Y:18:G:H1	2:Y:61:U:H3	1.42	0.66
10:I:80:ASP:O	10:I:82:LEU:N	2.27	0.66
15:N:59:LYS:O	15:N:63:THR:HG23	1.96	0.66
1:X:658:A:H3'	1:X:659:A:C5'	2.26	0.66
1:X:132:C:N3	1:X:147:G:N2	2.42	0.66
1:X:235:G:N2	1:X:466:C:OP1	2.28	0.66
4:B:87:PHE:CD2	4:B:208:LEU:HD13	2.31	0.66
18:Q:25:TYR:HD2	18:Q:82:LEU:HD21	1.60	0.66
1:X:793:G:H5"	17:P:89:ALA:HB2	1.78	0.66
1:X:2329:U:H2'	1:X:2330:G:H8	1.59	0.66
16:O:19:GLU:HA	16:O:96:THR:HA	1.77	0.66
1:X:457:G:OP1	1:X:2434:A:P	2.53	0.66
3:A:24:ILE:HG22	3:A:25:THR:H	1.59	0.66
6:D:22:TYR:OH	6:D:165:GLU:OE2	2.14	0.66
23:W:40:ASN:HB2	23:W:43:ILE:HB	1.78	0.66
1:X:1275:A:OP1	1:X:1275:A:H4'	1.94	0.66
1:X:1449:A:H61	1:X:1459:A:H5'	1.61	0.66
1:X:1405:G:H2'	1:X:1406:G:H8	1.60	0.66
5:C:37:ILE:HD11	5:C:181:LEU:HD13	1.76	0.66
21:T:46:TYR:HD2	21:T:48:GLN:HG2	1.61	0.66
1:X:1244:G:H1	1:X:1278:G:H1	1.44	0.65
1:X:1663:G:HO2'	25:2:2:VAL:N	1.94	0.65
1:X:1756:U:H2'	1:X:1757:U:H5'	1.77	0.65
1:X:299:U:O2'	1:X:300:G:N7	2.29	0.65
1:X:1465:G:H2'	1:X:1466:G:H8	1.60	0.65
1:X:1846:A:H4'	1:X:1847:U:H5"	1.78	0.65
1:X:1872:G:H1	1:X:1922:C:H42	1.43	0.65
1:X:415:U:H3	1:X:450:C:N4	1.94	0.65
1:X:1092:A:N6	1:X:1156:G:O2'	2.30	0.65
28:X:3002:MPD:O4	28:X:3002:MPD:O2	2.14	0.65
15:N:45:TYR:O	15:N:48:ARG:HG3	1.97	0.65
1:X:162:A:H3'	1:X:163:U:H2'	1.77	0.65
1:X:258:A:H1'	1:X:430:A:C8	2.32	0.65
1:X:650:U:H3	1:X:666:A:H2	1.42	0.65
1:X:1092:A:H61	1:X:1156:G:H1'	1.60	0.65
1:X:1933:G:N2	1:X:1934:G:O4'	2.30	0.65
16:O:7:THR:OG1	16:O:8:GLY:N	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:862:C:H42	1:X:1229:G:H1	1.44	0.65
1:X:1422:A:O2'	1:X:1423:C:O4'	2.13	0.65
1:X:1823:U:H2'	1:X:1824:C:C6	2.32	0.65
6:D:12:VAL:O	6:D:15:ASN:ND2	2.26	0.65
1:X:1461:C:N4	1:X:1462:G:N7	2.45	0.64
1:X:1550:G:HO2'	1:X:1554:A:H2	1.43	0.64
1:X:1560:A:H3'	1:X:1561:G:H8	1.62	0.64
2:Y:74:G:H21	20:S:78:GLN:HE22	1.44	0.64
15:N:52:GLN:O	15:N:55:ARG:HG3	1.96	0.64
1:X:2339:U:O2	6:D:37:ASN:ND2	2.30	0.64
5:C:12:THR:HG22	5:C:13:LYS:H	1.62	0.64
1:X:1540:U:O2	1:X:1625:U:O2'	2.16	0.64
1:X:2007:G:O2'	1:X:2009:U:OP2	2.14	0.64
1:X:2876:G:H2'	1:X:2877:G:O4'	1.97	0.64
3:A:244:PRO:HA	3:A:250:TRP:HA	1.77	0.64
11:J:43:THR:N	11:J:46:GLN:OE1	2.27	0.64
1:X:683:G:C6	1:X:696:G:C6	2.86	0.64
1:X:1261:G:OP1	16:O:67:ARG:NH1	2.30	0.64
2:Y:39:G:C8	6:D:66:LEU:HD21	2.32	0.64
11:J:30:GLY:HA2	11:J:107:ALA:HB2	1.79	0.64
2:Y:39:G:H8	6:D:66:LEU:HD21	1.63	0.64
1:X:118:A:O2'	1:X:119:U:O2	2.15	0.64
10:I:90:GLU:HG3	10:I:91:VAL:HG23	1.79	0.64
1:X:152:C:N4	1:X:177:G:H1	1.90	0.64
1:X:361:U:H2'	1:X:362:C:H6	1.63	0.64
7:E:156:PRO:HG2	7:E:159:GLY:O	1.98	0.64
1:X:1063:U:H3	1:X:1186:A:N6	1.96	0.64
1:X:1528:G:H22	1:X:1545:U:H3	1.46	0.64
3:A:160:ALA:CB	3:A:195:VAL:H	2.10	0.64
1:X:2314:A:O2'	1:X:2315:A:O5'	2.16	0.63
2:Y:113:G:C2	2:Y:114:C:H1'	2.33	0.63
5:C:64:PRO:HD3	5:C:76:GLY:O	1.98	0.63
13:L:37:ASN:OD1	13:L:37:ASN:N	2.29	0.63
21:T:48:GLN:HE22	21:T:51:THR:HA	1.63	0.63
1:X:1815:C:C5'	3:A:224:VAL:HG11	2.25	0.63
5:C:158:ASN:O	5:C:158:ASN:ND2	2.30	0.63
5:C:180:GLY:H	5:C:183:VAL:CG2	2.12	0.63
16:O:25:LEU:HD22	16:O:33:PHE:CE2	2.34	0.63
20:S:109:VAL:HG13	20:S:110:GLY:H	1.62	0.63
1:X:78:U:H2'	1:X:79:U:C6	2.33	0.63
1:X:321:U:O2'	1:X:322:A:OP2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:828:A:H2'	1:X:829:U:H4'	1.79	0.63
7:E:24:VAL:HA	7:E:28:GLY:HA3	1.79	0.63
1:X:810:A:H2'	1:X:811:C:C6	2.34	0.63
1:X:1953:U:N3	1:X:1954:A:N7	2.43	0.63
2:Y:74:G:H21	20:S:78:GLN:NE2	1.97	0.63
23:W:30:LYS:O	23:W:33:SER:OG	2.15	0.63
1:X:858:U:H2'	1:X:859:C:C6	2.34	0.63
1:X:878:C:H2'	1:X:879:U:C6	2.34	0.63
17:P:2:GLU:OE1	17:P:109:ASP:HB2	1.99	0.63
5:C:4:TYR:HD2	5:C:20:SER:H	1.45	0.63
1:X:1217:U:H3'	1:X:1218:G:C8	2.34	0.62
1:X:1377:U:OP1	18:Q:15:LYS:NZ	2.26	0.62
1:X:2370:U:O2'	1:X:2400:U:O2'	2.16	0.62
1:X:1963:A:H2	1:X:1970:U:H3	1.48	0.62
16:O:16:GLU:OE2	16:O:99:LYS:HA	1.99	0.62
22:V:25:LEU:HA	22:V:28:LEU:HD12	1.80	0.62
1:X:514:G:H2'	1:X:515:G:H5'	1.81	0.62
1:X:942:C:H2'	1:X:943:C:C5	2.33	0.62
1:X:1592:A:O2'	1:X:1593:G:OP2	2.16	0.62
2:Y:92:G:OP1	20:S:14:THR:OG1	2.14	0.62
1:X:684:U:H2'	1:X:685:C:C6	2.34	0.62
1:X:2856:U:H2'	1:X:2857:A:C8	2.34	0.62
1:X:1479:G:N2	1:X:1605:A:N1	2.46	0.62
23:W:18:THR:HB	23:W:49:LYS:HZ3	1.64	0.62
22:V:61:GLU:O	22:V:65:SER:OG	2.18	0.62
23:W:18:THR:HB	23:W:49:LYS:NZ	2.14	0.62
1:X:706:U:O2'	10:I:13:ARG:HA	2.00	0.62
1:X:1756:U:C2'	1:X:1757:U:H5'	2.30	0.62
1:X:2618:C:H2'	1:X:2619:G:H8	1.64	0.62
22:V:4:LYS:NZ	22:V:5:GLU:O	2.23	0.62
1:X:353:A:O2'	1:X:354:A:OP2	2.17	0.62
1:X:1091:G:O2'	1:X:1092:A:OP2	2.15	0.62
1:X:2532:G:OP1	27:X:3001:95H:O14	2.18	0.62
1:X:218:G:H4'	1:X:219:A:H4'	1.81	0.62
1:X:2333:U:OP2	1:X:2334:G:N2	2.33	0.62
8:G:58:ILE:HD11	8:G:129:ALA:HA	1.82	0.62
19:R:97:SER:O	19:R:99:GLU:HG2	1.99	0.62
1:X:2492:C:N4	1:X:2512:G:O6	2.17	0.61
22:V:60:ARG:HA	22:V:63:GLU:HB3	1.81	0.61
20:S:11:GLY:O	20:S:13:GLN:NE2	2.33	0.61
1:X:363:A:OP2	5:C:134:PRO:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:460:C:H2'	1:X:461:A:C8	2.35	0.61
1:X:679:G:H2'	1:X:680:C:C6	2.34	0.61
1:X:921:C:H42	1:X:944:G:H1	1.49	0.61
1:X:1708:A:H61	1:X:2023:C:H42	1.48	0.61
2:Y:3:U:H3	2:Y:112:G:H22	1.46	0.61
1:X:2329:U:H2'	1:X:2330:G:C8	2.35	0.61
1:X:2051:C:H2'	1:X:2052:C:H6	1.65	0.61
21:T:46:TYR:CD2	21:T:48:GLN:HG2	2.36	0.61
1:X:162:A:OP1	1:X:166:A:N6	2.33	0.61
1:X:319:G:H2'	1:X:319:G:N3	2.16	0.61
1:X:1488:A:O2'	1:X:1489:A:OP1	2.18	0.61
1:X:2060:A:O2'	1:X:2062:G:OP2	2.18	0.61
5:C:133:ALA:HB1	5:C:136:THR:OG1	2.01	0.61
1:X:2116:U:H2'	1:X:2117:A:C8	2.35	0.61
1:X:75:G:N2	1:X:111:U:O2	2.33	0.61
1:X:119:U:O2'	1:X:120:G:O5'	2.12	0.61
1:X:613:G:H2'	1:X:2057:A:N7	2.14	0.61
1:X:1039:C:C5	8:G:1:MET:HG2	2.36	0.61
1:X:1819:G:O2'	1:X:1857:C:OP1	2.17	0.61
1:X:2101:U:HO2'	1:X:2624:G:HO2'	1.46	0.61
10:I:43:GLY:O	10:I:45:GLY:N	2.33	0.61
1:X:498:G:N2	1:X:503:A:H8	1.98	0.61
1:X:1097:U:O4	1:X:1151:G:N1	2.34	0.61
1:X:1593:G:H5'	1:X:1593:G:C8	2.36	0.61
1:X:1596:G:H2'	1:X:1597:U:H6	1.64	0.61
1:X:2618:C:H2'	1:X:2619:G:C8	2.35	0.61
2:Y:40:C:C2'	6:D:63:GLN:HE21	2.14	0.61
3:A:18:SER:O	3:A:18:SER:OG	2.17	0.61
1:X:378:C:H2'	1:X:379:C:H6	1.66	0.60
1:X:459:C:O2'	1:X:1907:U:O2'	2.09	0.60
1:X:460:C:H2'	1:X:461:A:H8	1.66	0.60
5:C:129:PHE:CD1	5:C:157:GLU:HG3	2.36	0.60
6:D:162:THR:HB	6:D:165:GLU:HB3	1.83	0.60
1:X:1847:U:O2	3:A:201:GLU:N	2.27	0.60
4:B:48:ALA:HB2	4:B:92:ARG:HB3	1.82	0.60
1:X:365:A:OP1	5:C:161:VAL:CG2	2.50	0.60
2:Y:38:U:O2'	2:Y:43:A:N6	2.33	0.60
1:X:811:C:N4	1:X:812:U:O4	2.34	0.60
1:X:1152:U:H2'	1:X:1153:C:H6	1.67	0.60
1:X:1487:G:H2'	1:X:1488:A:C8	2.36	0.60
1:X:90:A:O2'	1:X:91:A:H8	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:527:G:OP2	19:R:45:GLN:NE2	2.30	0.60
1:X:152:C:OP1	1:X:1396:A:O2'	2.18	0.60
1:X:921:C:H41	1:X:942:C:N4	1.99	0.60
1:X:1498:U:HO2'	1:X:1499:U:H5	1.50	0.60
1:X:1522:G:N2	1:X:1558:U:O2	2.21	0.60
1:X:2382:C:H1'	21:T:47:ARG:NH1	2.16	0.60
1:X:2445:A:H2'	1:X:2446:U:O4'	2.00	0.60
1:X:268:A:N6	1:X:473:U:O2'	2.34	0.60
1:X:606:G:OP2	16:O:78:ARG:NH2	2.35	0.60
1:X:634:C:HO2'	26:3:2:PRO:N	1.99	0.60
1:X:2500:U:OP1	1:X:2502:C:N4	2.34	0.60
16:O:39:LEU:O	16:O:49:GLY:HA3	2.01	0.60
20:S:109:VAL:HG11	20:S:145:ILE:N	2.16	0.60
4:B:10:ILE:HD11	4:B:29:GLU:HB2	1.84	0.60
12:K:59:ARG:HA	12:K:86:PHE:CZ	2.37	0.60
5:C:148:GLN:H	5:C:166:SER:HA	1.67	0.60
1:X:450:C:H4'	1:X:451:U:H5'	1.83	0.59
5:C:6:VAL:HG13	5:C:15:GLY:HA2	1.84	0.59
5:C:53:ASN:C	5:C:55:SER:H	2.05	0.59
5:C:179:GLN:CD	5:C:179:GLN:H	2.05	0.59
23:W:8:LEU:HB2	23:W:28:LEU:HD22	1.83	0.59
1:X:2077:C:H1'	4:B:169:MET:HE1	1.82	0.59
10:I:106:LYS:N	10:I:125:ALA:HB1	2.17	0.59
19:R:28:PRO:HD2	19:R:34:VAL:HA	1.82	0.59
26:3:24:ARG:CB	26:3:47:ALA:HB1	2.33	0.59
1:X:1614:A:O4'	1:X:1615:G:N2	2.35	0.59
22:V:25:LEU:HB2	22:V:46:VAL:HG11	1.85	0.59
1:X:591:A:H4'	1:X:592:A:H5'	1.84	0.59
1:X:629:A:H62	1:X:1289:A:H2	1.50	0.59
3:A:160:ALA:HB3	3:A:195:VAL:H	1.66	0.59
1:X:2357:G:O3'	21:T:52:LYS:HE2	2.03	0.59
9:H:80:ASP:OD2	14:M:64:ARG:NH2	2.36	0.59
14:M:16:ARG:N	14:M:79:HIS:HD2	2.01	0.59
18:Q:60:PRO:HB3	18:Q:72:THR:O	2.02	0.59
19:R:11:VAL:HA	19:R:21:GLY:HA2	1.83	0.59
1:X:342:A:N1	1:X:365:A:O2'	2.30	0.59
7:E:123:PHE:O	7:E:125:VAL:N	2.32	0.59
1:X:1597:U:O3'	1:X:1767:G:N2	2.36	0.59
2:Y:78:C:H42	20:S:15:ARG:HH22	1.51	0.59
3:A:145:GLU:HA	3:A:152:GLY:HA2	1.84	0.59
11:J:75:THR:HG21	11:J:87:LYS:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:16:ARG:H	14:M:79:HIS:CD2	2.20	0.59
18:Q:89:LEU:HB2	22:V:30:PHE:HE1	1.68	0.59
1:X:1280:U:H2'	1:X:1281:U:C6	2.37	0.59
1:X:1281:U:H2'	1:X:1282:A:C8	2.38	0.59
1:X:1300:G:P	17:P:99:ARG:HH22	2.26	0.59
1:X:1636:U:O2'	1:X:1637:A:OP1	2.19	0.59
1:X:1866:G:H2'	1:X:1954:A:N3	2.18	0.59
1:X:2216:U:H2'	1:X:2217:G:N1	2.17	0.59
3:A:46:GLN:HE22	3:A:48:LYS:NZ	2.01	0.59
9:H:73:ASP:N	9:H:73:ASP:OD1	2.32	0.59
1:X:90:A:O2'	1:X:91:A:O5'	2.21	0.58
1:X:630:G:P	10:I:21:ARG:HH22	2.26	0.58
1:X:1091:G:O2'	1:X:1154:G:N1	2.36	0.58
1:X:1359:A:OP1	17:P:11:ARG:HD3	2.02	0.58
1:X:2687:A:H8	1:X:2687:A:OP1	1.85	0.58
1:X:1353:A:H2'	1:X:1354:G:C8	2.38	0.58
1:X:1365:G:H2'	1:X:1367:C:C5	2.38	0.58
10:I:99:SER:O	10:I:101:VAL:N	2.36	0.58
1:X:1013:U:O3'	23:W:14:GLY:HA2	2.03	0.58
1:X:1269:A:H2'	1:X:1270:U:H6	1.67	0.58
1:X:2370:U:H2'	1:X:2371:U:C6	2.38	0.58
6:D:93:GLY:O	6:D:95:ARG:N	2.37	0.58
12:K:36:ARG:O	12:K:40:VAL:HG12	2.03	0.58
1:X:1018:A:O5'	1:X:1225:G:N2	2.36	0.58
1:X:2383:C:H4'	21:T:28:ARG:HD3	1.85	0.58
10:I:63:LYS:HG3	10:I:91:VAL:HB	1.85	0.58
20:S:51:VAL:HG11	20:S:61:ILE:HD12	1.85	0.58
23:W:5:GLN:HB2	23:W:36:VAL:HG12	1.86	0.58
1:X:188:C:H42	1:X:214:G:H1	1.51	0.58
1:X:339:A:H2'	1:X:340:C:H6	1.69	0.58
1:X:2092:C:H1'	1:X:2476:U:H3	1.68	0.58
1:X:168:A:H3'	1:X:169:G:H5'	1.85	0.58
1:X:126:A:H5"	1:X:127:C:O4'	2.04	0.58
1:X:132:C:N4	1:X:134:U:O4	2.37	0.58
1:X:1514:A:N6	1:X:1565:U:H3	2.01	0.58
8:G:20:ASP:HA	8:G:58:ILE:HG22	1.85	0.58
8:G:39:GLY:HA3	8:G:51:THR:HG23	1.85	0.58
14:M:32:VAL:HA	14:M:42:ILE:HD13	1.86	0.58
19:R:59:THR:OG1	19:R:60:GLU:N	2.37	0.58
1:X:2322:C:H1'	1:X:2365:G:N2	2.18	0.58
12:K:27:SER:O	12:K:29:ARG:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:515:G:H22	25:2:38:LYS:HD2	1.69	0.58
1:X:2431:C:H2'	1:X:2432:G:O4'	2.04	0.58
3:A:149:GLY:O	3:A:151:GLY:N	2.33	0.58
9:H:6:THR:O	9:H:21:THR:HG22	2.03	0.58
1:X:234:C:O2'	1:X:235:G:O4'	2.22	0.57
1:X:365:A:OP1	5:C:161:VAL:HG21	2.04	0.57
1:X:695:C:N3	1:X:696:G:C5	2.72	0.57
1:X:1442:C:H2'	1:X:1443:A:C8	2.39	0.57
1:X:1887:G:H22	1:X:1910:G:H1'	1.69	0.57
1:X:2314:A:HO2'	1:X:2315:A:P	2.26	0.57
1:X:2360:A:H5'	1:X:2362:A:H1'	1.86	0.57
20:S:44:ASP:OD2	20:S:47:GLU:HG3	2.04	0.57
1:X:1206:G:N2	16:O:90:GLN:OE1	2.27	0.57
1:X:2446:U:H2'	1:X:2447:C:C6	2.38	0.57
3:A:163:GLN:O	3:A:174:ILE:HG23	2.04	0.57
5:C:5:ASP:OD1	5:C:5:ASP:N	2.37	0.57
1:X:1410:A:H2'	1:X:1411:G:O4'	2.04	0.57
1:X:1957:G:O2'	1:X:1995:G:O6	2.17	0.57
1:X:2906:G:H2'	1:X:2907:A:C8	2.40	0.57
8:G:2:ARG:HA	8:G:2:ARG:HH11	1.70	0.57
9:H:23:LYS:HA	9:H:23:LYS:HE3	1.86	0.57
25:2:16:VAL:N	25:2:21:LYS:HG3	2.17	0.57
18:Q:89:LEU:HB2	22:V:30:PHE:CE1	2.38	0.57
1:X:140:A:N3	1:X:1445:C:O2'	2.30	0.57
1:X:1488:A:H3'	1:X:1489:A:C2	2.39	0.57
1:X:1758:A:N7	1:X:1772:G:N1	2.51	0.57
2:Y:37:A:O2'	2:Y:44:A:N1	2.37	0.57
11:J:78:PRO:HB2	11:J:81:VAL:HG21	1.86	0.57
1:X:259:A:H2'	1:X:260:A:C8	2.39	0.57
1:X:1373:U:H2'	1:X:1374:G:C8	2.40	0.57
1:X:1452:C:HO2'	1:X:1631:G:N2	2.02	0.57
1:X:1828:U:H4'	1:X:1828:U:OP2	2.02	0.57
5:C:11:GLY:HA2	5:C:142:VAL:HG12	1.87	0.57
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.31	0.57
1:X:1238:U:H1'	15:N:4:VAL:HG22	1.86	0.57
10:I:32:GLY:O	10:I:33:ARG:HD3	2.04	0.57
11:J:39:THR:HG23	11:J:98:LYS:HA	1.87	0.57
1:X:187:C:H2'	1:X:188:C:H6	1.69	0.57
1:X:271:C:H5'	1:X:324:A:O2'	2.05	0.57
1:X:328:G:N2	1:X:329:A:N7	2.53	0.57
1:X:1314:A:H5"	12:K:36:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2906:G:H2'	1:X:2907:A:H8	1.70	0.57
3:A:209:GLY:HA2	3:A:212:ARG:HB2	1.87	0.57
15:N:29:HIS:CD2	15:N:30:THR:HG22	2.40	0.57
20:S:31:VAL:HG12	20:S:91:PHE:HB2	1.87	0.57
20:S:112:ALA:H	20:S:116:LYS:HE3	1.70	0.57
1:X:1625:U:O4	1:X:1626:A:N6	2.38	0.56
1:X:90:A:H4'	1:X:91:A:H5'	1.86	0.56
1:X:169:G:HO2'	1:X:170:C:H6	1.52	0.56
1:X:661:U:H2'	1:X:662:G:H8	1.69	0.56
1:X:1244:G:H22	1:X:1278:G:N2	2.03	0.56
1:X:1558:U:N3	1:X:1559:G:N7	2.53	0.56
1:X:1864:C:H1'	1:X:1955:A:N3	2.20	0.56
17:P:23:LEU:HD23	24:Z:24:VAL:HG13	1.87	0.56
20:S:106:VAL:HG23	20:S:127:ASN:HA	1.86	0.56
1:X:683:G:H2'	1:X:684:U:H6	1.70	0.56
1:X:1197:C:H2'	1:X:1198:G:O4'	2.05	0.56
1:X:1514:A:H61	1:X:1565:U:H3	1.52	0.56
16:O:33:PHE:HD1	16:O:34:THR:N	2.02	0.56
19:R:97:SER:O	19:R:99:GLU:N	2.38	0.56
1:X:501:C:H3'	1:X:502:C:H5"	1.87	0.56
1:X:554:C:H5'	1:X:555:C:OP2	2.06	0.56
1:X:2370:U:H2'	1:X:2371:U:H6	1.70	0.56
1:X:1523:G:H1'	1:X:1556:G:H1	1.71	0.56
1:X:1542:C:H3'	1:X:1543:G:C5'	2.33	0.56
1:X:2334:G:O3'	1:X:2337:A:N6	2.39	0.56
17:P:111:LYS:HE2	17:P:112:GLU:N	2.20	0.56
1:X:681:G:O2'	1:X:683:G:H4'	2.05	0.56
1:X:785:C:H5'	1:X:1811:A:H3'	1.88	0.56
1:X:1382:C:N4	1:X:1383:G:O6	2.39	0.56
1:X:2354:A:H2'	1:X:2355:A:C8	2.40	0.56
1:X:2687:A:H2'	1:X:2688:G:C8	2.41	0.56
8:G:2:ARG:HA	8:G:2:ARG:NH1	2.21	0.56
15:N:76:TYR:OH	15:N:92:ARG:NH1	2.39	0.56
20:S:61:ILE:HG23	20:S:72:VAL:HG12	1.87	0.56
1:X:532:C:H4'	17:P:60:HIS:CD2	2.41	0.56
1:X:1963:A:H2	1:X:1970:U:N3	2.03	0.56
11:J:34:LEU:HD11	11:J:129:THR:HB	1.88	0.56
1:X:946:A:H2'	1:X:947:U:H5'	1.88	0.56
1:X:2333:U:OP1	1:X:2334:G:N1	2.39	0.56
1:X:2411:A:HO2'	1:X:2412:C:P	2.29	0.56
21:T:60:GLY:HA3	21:T:68:PHE:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:678:A:N3	1:X:2430:C:H4'	2.21	0.56
1:X:2860:U:H5"	12:K:49:THR:HG21	1.87	0.56
3:A:44:ASN:OD1	3:A:44:ASN:N	2.38	0.56
1:X:139:U:O2'	1:X:140:A:O5'	2.25	0.55
1:X:606:G:H22	1:X:621:A:H2	1.52	0.55
1:X:1481:A:H61	1:X:1603:U:H3	1.53	0.55
1:X:1835:U:H2'	1:X:1836:A:C5'	2.27	0.55
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.86	0.55
1:X:268:A:O2'	1:X:269:G:H4'	2.06	0.55
8:G:26:LEU:HA	8:G:63:ILE:HD11	1.88	0.55
1:X:157:U:H2'	1:X:158:G:H8	1.70	0.55
1:X:797:A:H62	1:X:2636:U:H3	1.55	0.55
1:X:1096:C:N4	1:X:1152:U:O4	2.39	0.55
6:D:57:LEU:HD12	6:D:60:ILE:HD12	1.87	0.55
1:X:1449:A:N6	1:X:1459:A:H5'	2.22	0.55
1:X:1515:G:N2	1:X:1564:G:N2	2.55	0.55
1:X:1658:A:P	1:X:1658:A:H8	2.30	0.55
1:X:1953:U:H1'	1:X:1954:A:H5'	1.88	0.55
9:H:114:ILE:HA	9:H:117:LEU:HD13	1.87	0.55
12:K:67:ARG:O	12:K:68:ASN:HB2	2.07	0.55
1:X:1505:G:H8	1:X:1506:C:C5	2.25	0.55
1:X:1523:G:H1'	1:X:1556:G:N1	2.22	0.55
1:X:1870:C:O2'	3:A:253:PRO:HB2	2.06	0.55
5:C:51:VAL:HG11	5:C:91:GLY:HA3	1.89	0.55
7:E:154:PRO:HA	7:E:162:ILE:HG22	1.88	0.55
12:K:23:SER:HA	12:K:26:ILE:HD12	1.89	0.55
12:K:40:VAL:O	12:K:44:VAL:HG12	2.07	0.55
1:X:293:U:H2'	1:X:294:G:C8	2.42	0.55
1:X:1065:A:C8	1:X:1065:A:H3'	2.42	0.55
1:X:1510:U:H2'	1:X:1511:C:O4'	2.06	0.55
1:X:2324:C:H42	1:X:2348:G:H1	1.53	0.55
17:P:9:THR:HG22	17:P:80:PRO:HD2	1.89	0.55
1:X:1933:G:N3	1:X:1934:G:H5'	2.22	0.55
2:Y:78:C:H2'	2:Y:79:C:C5	2.42	0.55
8:G:44:THR:O	8:G:44:THR:OG1	2.24	0.55
12:K:55:ASP:N	12:K:55:ASP:OD1	2.40	0.55
13:L:39:HIS:HB2	13:L:58:SER:OG	2.07	0.55
19:R:76:ASN:OD1	19:R:76:ASN:N	2.35	0.55
1:X:280:C:H2'	1:X:281:A:C8	2.42	0.55
1:X:1476:G:H2'	1:X:1477:U:C6	2.42	0.55
1:X:1918:G:O2'	1:X:2262:G:O2'	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:91:C:H2'	2:Y:92:G:C8	2.42	0.55
10:I:106:LYS:H	10:I:125:ALA:CB	2.18	0.55
14:M:30:VAL:HB	14:M:85:LYS:HG2	1.88	0.55
1:X:140:A:H61	1:X:1639:G:HO2'	1.54	0.55
1:X:1493:U:H1'	1:X:1494:G:H5'	1.89	0.55
5:C:4:TYR:HB2	5:C:19:LEU:HA	1.88	0.55
5:C:154:VAL:HG12	5:C:155:VAL:H	1.72	0.55
1:X:319:G:H22	1:X:326:A:N6	2.03	0.54
1:X:877:G:H2'	1:X:878:C:C6	2.41	0.54
1:X:1683:U:C2'	1:X:1684:A:H5"	2.34	0.54
10:I:62:PRO:O	10:I:90:GLU:HG2	2.07	0.54
1:X:17:G:OP1	24:Z:11:THR:HB	2.06	0.54
3:A:182:ARG:HA	3:A:266:SER:HA	1.89	0.54
13:L:20:THR:HG23	13:L:21:ASN:H	1.71	0.54
18:Q:46:PHE:HB2	18:Q:48:VAL:HG22	1.89	0.54
1:X:1766:C:H2'	1:X:1767:G:H5'	1.89	0.54
6:D:9:ASN:O	6:D:13:THR:OG1	2.16	0.54
16:O:60:ALA:HB1	16:O:96:THR:O	2.07	0.54
1:X:1810:A:H5'	1:X:2635:G:H4'	1.89	0.54
2:Y:40:C:H2'	6:D:63:GLN:HE21	1.72	0.54
3:A:45:ASN:HB3	3:A:49:LEU:O	2.07	0.54
1:X:1177:A:H4'	1:X:1178:C:H5'	1.88	0.54
1:X:1695:G:OP1	12:K:33:THR:HG21	2.06	0.54
2:Y:77:G:H1	2:Y:94:U:H3	1.56	0.54
4:B:162:ARG:HG2	4:B:163:VAL:N	2.22	0.54
19:R:72:ASP:CB	19:R:99:GLU:HG3	2.37	0.54
1:X:1400:C:H42	1:X:1405:G:H1	1.55	0.54
1:X:1527:A:H61	1:X:1546:A:H62	1.56	0.54
1:X:2010:U:H4'	1:X:2633:C:H4'	1.89	0.54
5:C:136:THR:O	5:C:140:LYS:N	2.33	0.54
5:C:139:PHE:O	5:C:142:VAL:HG13	2.07	0.54
5:C:160:ASP:N	5:C:160:ASP:OD1	2.38	0.54
8:G:54:TYR:CD2	8:G:122:LYS:HB3	2.43	0.54
1:X:1038:C:OP2	15:N:54:LYS:NZ	2.39	0.54
7:E:160:LYS:CB	7:E:163:ARG:HE	2.21	0.54
19:R:42:LYS:HG2	19:R:43:LYS:N	2.23	0.54
1:X:179:A:H8	1:X:179:A:OP2	1.91	0.54
1:X:907:G:H2'	1:X:908:A:O4'	2.08	0.54
1:X:1847:U:C5	3:A:159:GLY:HA3	2.42	0.54
1:X:2335:G:P	1:X:2337:A:H62	2.30	0.54
2:Y:79:C:N3	2:Y:92:G:N2	2.52	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:83:TYR:CD2	3:A:85:PRO:HD2	2.43	0.54
4:B:215:ILE:O	4:B:216:LYS:HG2	2.08	0.54
1:X:687:G:N2	1:X:690:U:OP2	2.41	0.54
1:X:1492:G:N2	1:X:1508:C:N3	2.52	0.54
1:X:633:A:H2'	1:X:634:C:O4'	2.08	0.54
1:X:739:U:OP1	3:A:59:LYS:NZ	2.35	0.54
1:X:1876:G:H2'	1:X:1877:G:C8	2.43	0.54
1:X:2470:C:H2'	1:X:2471:G:C8	2.42	0.54
5:C:107:ARG:HA	5:C:110:LEU:HD12	1.90	0.54
1:X:660:A:O2'	1:X:661:U:O5'	2.25	0.53
5:C:13:LYS:O	5:C:15:GLY:N	2.40	0.53
9:H:35:ILE:HA	9:H:62:ILE:HG22	1.90	0.53
1:X:1700:C:H2'	1:X:1701:U:C6	2.44	0.53
1:X:676:A:N3	1:X:2442:G:O2'	2.39	0.53
1:X:778:G:C6	1:X:806:A:N7	2.76	0.53
1:X:1973:U:H2'	1:X:1974:C:C6	2.43	0.53
1:X:100:U:H3'	1:X:101:G:H5'	1.91	0.53
1:X:2410:G:C5	1:X:2411:A:H2	2.25	0.53
4:B:33:ASN:HB3	4:B:105:VAL:HG12	1.91	0.53
21:T:35:ASP:HB2	21:T:77:PHE:HD1	1.74	0.53
1:X:292:U:H2'	1:X:293:U:C6	2.43	0.53
1:X:641:A:H62	28:X:3003:MPD:H52	1.72	0.53
1:X:661:U:O2'	1:X:662:G:H5'	2.08	0.53
1:X:665:G:H4'	1:X:666:A:H5"	1.90	0.53
1:X:967:C:O2'	21:T:34:ALA:HB2	2.08	0.53
1:X:1395:G:C8	1:X:1408:G:O6	2.61	0.53
1:X:2625:A:OP1	3:A:233:GLY:HA3	2.09	0.53
20:S:112:ALA:HB1	20:S:115:ALA:HB3	1.89	0.53
1:X:2642:U:H1'	24:Z:4:PRO:HB3	1.91	0.53
5:C:33:LEU:HD21	5:C:181:LEU:HD21	1.91	0.53
17:P:29:ALA:O	17:P:33:ILE:HG12	2.08	0.53
1:X:189:G:H2'	1:X:190:G:H8	1.73	0.53
1:X:343:A:H1'	1:X:362:C:H1'	1.90	0.53
1:X:1767:G:HO2'	1:X:1768:C:H6	1.55	0.53
5:C:53:ASN:C	5:C:55:SER:N	2.63	0.53
1:X:340:C:H2'	1:X:341:G:O4'	2.09	0.53
1:X:1352:C:H2'	1:X:1353:A:H8	1.74	0.53
1:X:2391:C:H2'	1:X:2392:G:O4'	2.08	0.53
1:X:328:G:HO2'	1:X:329:A:H8	1.56	0.53
1:X:1373:U:H2'	1:X:1374:G:H8	1.73	0.53
18:Q:54:ASN:HB2	18:Q:79:ILE:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:153:G:O2'	1:X:154:A:P	2.67	0.53
1:X:259:A:H2'	1:X:260:A:H8	1.74	0.53
1:X:311:U:H2'	1:X:312:A:H8	1.74	0.53
1:X:1526:G:N1	1:X:1548:U:O4	2.37	0.53
1:X:1680:U:H2'	1:X:1681:U:H6	1.73	0.53
1:X:1866:G:H2'	1:X:1954:A:C2	2.44	0.53
1:X:2625:A:OP1	3:A:239:ALA:HB1	2.09	0.53
14:M:66:ILE:HA	14:M:71:GLY:HA2	1.90	0.53
16:O:38:VAL:O	16:O:53:VAL:HG12	2.09	0.53
25:2:28:GLY:O	25:2:32:LEU:HG	2.09	0.53
1:X:683:G:H2'	1:X:684:U:C6	2.44	0.52
1:X:864:A:OP2	1:X:1226:G:N2	2.27	0.52
1:X:1281:U:H2'	1:X:1282:A:H8	1.73	0.52
1:X:1469:G:O2'	1:X:1470:G:C8	2.62	0.52
1:X:1482:U:H2'	1:X:1483:A:H8	1.74	0.52
1:X:1746:G:H2'	1:X:1747:G:H8	1.74	0.52
1:X:2650:G:O5'	1:X:2845:G:N2	2.42	0.52
12:K:14:LYS:O	12:K:18:ARG:HG3	2.08	0.52
12:K:32:THR:HG22	12:K:33:THR:N	2.23	0.52
12:K:91:GLU:OE2	12:K:91:GLU:N	2.41	0.52
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.08	0.52
18:Q:15:LYS:HA	18:Q:18:GLU:HG2	1.91	0.52
1:X:2089[B]:A:O2'	1:X:2090:C:H6	1.91	0.52
17:P:5:ALA:HB3	17:P:54:ALA:HB2	1.90	0.52
1:X:1241:A:H2'	1:X:1242:A:C8	2.44	0.52
1:X:1478:A:H2'	1:X:1479:G:O4'	2.10	0.52
1:X:1494:G:O2'	1:X:1495:C:H5'	2.09	0.52
3:A:196:GLY:O	3:A:198:LEU:N	2.43	0.52
18:Q:51:ALA:N	18:Q:81:THR:O	2.37	0.52
1:X:178:A:H8	1:X:178:A:OP2	1.93	0.52
1:X:645:A:O2'	1:X:647:G:O2'	2.24	0.52
1:X:665:G:H4'	1:X:666:A:C5'	2.39	0.52
1:X:1836:A:O2'	1:X:1837:A:O5'	2.28	0.52
9:H:61:VAL:HB	9:H:87:ILE:HD11	1.91	0.52
1:X:1244:G:N2	1:X:1278:G:N2	2.58	0.52
1:X:1520:A:H2	1:X:1560:A:C6	2.26	0.52
14:M:93:LYS:H	14:M:111:ARG:CB	2.23	0.52
1:X:661:U:H2'	1:X:662:G:C8	2.45	0.52
1:X:695:C:O5'	1:X:695:C:H6	1.93	0.52
1:X:1074:G:OP2	11:J:128:LYS:NZ	2.40	0.52
15:N:27:SER:HA	15:N:30:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:6:GLU:HB2	16:O:39:LEU:HD23	1.91	0.52
1:X:1322:G:N2	1:X:1365:G:H5"	2.25	0.52
1:X:1573:A:N1	1:X:1591:G:O2'	2.42	0.52
11:J:81:VAL:HG12	11:J:82:ARG:O	2.10	0.52
5:C:42:ALA:O	5:C:45:ARG:HG2	2.09	0.52
1:X:1492:G:N2	1:X:1508:C:C4	2.78	0.52
1:X:2250:A:H2'	1:X:2251:G:O4'	2.10	0.52
2:Y:4:G:H1	2:Y:111:A:H62	1.57	0.52
3:A:105:ILE:O	3:A:107:PRO:HD3	2.10	0.52
19:R:27:LEU:HA	19:R:34:VAL:HG22	1.92	0.52
1:X:214:G:OP1	25:2:26:LYS:NZ	2.42	0.51
1:X:387:G:N2	1:X:388:A:N7	2.57	0.51
1:X:572:C:N4	1:X:2806:U:OP2	2.43	0.51
1:X:580:C:O3'	15:N:53:ARG:NH1	2.42	0.51
1:X:1469:G:H8	1:X:1469:G:OP2	1.93	0.51
1:X:1627:G:H2'	1:X:1628:A:H5"	1.91	0.51
1:X:1760:G:N1	1:X:1761:G:O6	2.42	0.51
1:X:339:A:H2'	1:X:340:C:C6	2.44	0.51
1:X:956:A:H2'	11:J:9:TYR:OH	2.10	0.51
1:X:1053:A:O4'	15:N:59:LYS:HG2	2.10	0.51
1:X:1269:A:H2'	1:X:1270:U:C6	2.46	0.51
1:X:1400:C:O2'	1:X:1836:A:H1'	2.09	0.51
1:X:1636:U:H2'	1:X:1637:A:C8	2.45	0.51
1:X:1848:A:H2'	1:X:1849:G:C8	2.44	0.51
1:X:2446:U:H2'	1:X:2447:C:H6	1.74	0.51
12:K:8:ARG:O	12:K:13:ARG:NH1	2.43	0.51
16:O:2:PHE:HB3	16:O:42:GLY:H	1.76	0.51
17:P:57:ASN:O	17:P:61:ASN:HB2	2.11	0.51
1:X:321:U:H1'	1:X:322:A:H5"	1.93	0.51
1:X:785:C:H42	1:X:802:G:H1	1.57	0.51
1:X:1916:A:H1'	1:X:2114:G:H5'	1.92	0.51
1:X:169:G:O2'	1:X:170:C:H6	1.93	0.51
1:X:344:U:O2'	1:X:345:C:H5"	2.10	0.51
1:X:577:A:H2'	1:X:577:A:N3	2.25	0.51
1:X:921:C:N4	1:X:922:G:N7	2.58	0.51
1:X:2774:G:O6	1:X:2782:C:H5"	2.11	0.51
3:A:169:GLY:C	3:A:171:TYR:H	2.13	0.51
12:K:27:SER:C	12:K:29:ARG:H	2.14	0.51
1:X:659:A:O2'	1:X:660:A:P	2.68	0.51
1:X:1391:A:C8	1:X:1392:G:C8	2.99	0.51
1:X:2465:U:O2'	1:X:2466:A:H5"	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2620:U:H2'	1:X:2621:C:C6	2.45	0.51
8:G:59:ASN:H	8:G:128:GLY:H	1.59	0.51
20:S:60:VAL:HG23	20:S:94:ILE:HD11	1.91	0.51
1:X:111:U:H5'	1:X:112:U:OP2	2.10	0.51
1:X:540:G:N3	17:P:61:ASN:ND2	2.52	0.51
1:X:1933:G:N3	1:X:1933:G:H2'	2.25	0.51
1:X:2668:A:H2'	1:X:2669:G:C8	2.46	0.51
1:X:2903:A:H5'	1:X:2904:U:H5'	1.91	0.51
8:G:116:GLY:HA2	8:G:119:GLN:HG3	1.90	0.51
10:I:104:ASN:OD1	10:I:104:ASN:N	2.43	0.51
20:S:132:ALA:HB3	20:S:137:ILE:CB	2.40	0.51
1:X:83:G:N2	1:X:102:A:H2	1.97	0.51
1:X:1063:U:O2'	1:X:1065:A:H2	1.93	0.51
1:X:1482:U:H2'	1:X:1483:A:C8	2.45	0.51
1:X:2892:G:H21	12:K:4:ARG:HH12	1.59	0.51
2:Y:78:C:H2'	2:Y:79:C:H5	1.75	0.51
10:I:64:ARG:O	10:I:93:PRO:HD2	2.11	0.51
11:J:73:PRO:HB3	11:J:93:TRP:CZ3	2.45	0.51
1:X:82:G:N1	1:X:102:A:OP2	2.35	0.51
1:X:665:G:H4'	1:X:666:A:O5'	2.10	0.51
1:X:1313:G:OP2	1:X:1689:G:O2'	2.20	0.51
22:V:46:VAL:O	22:V:50:ILE:HG13	2.10	0.51
1:X:90:A:O2'	1:X:91:A:P	2.68	0.51
1:X:148:U:H2'	1:X:149:U:C6	2.46	0.51
1:X:514:G:C2'	1:X:515:G:H5'	2.40	0.51
1:X:1096:C:H42	1:X:1151:G:N2	2.09	0.51
23:W:40:ASN:CB	23:W:43:ILE:H	2.18	0.51
24:Z:30:CYS:HB3	24:Z:34:GLY:HA3	1.93	0.51
1:X:87:U:H5"	1:X:88:G:H5'	1.93	0.51
1:X:2470:C:H2'	1:X:2471:G:H8	1.77	0.51
5:C:171:PRO:HB2	5:C:173:VAL:HG12	1.92	0.51
1:X:43:A:H2'	1:X:44:A:O4'	2.11	0.50
1:X:296:G:H5'	1:X:297:G:OP2	2.10	0.50
1:X:304:G:N2	1:X:414:C:C2	2.79	0.50
1:X:1843:U:H3'	1:X:1843:U:H6	1.76	0.50
1:X:1909:C:H2'	1:X:1910:G:O4'	2.11	0.50
1:X:2051:C:H2'	1:X:2052:C:C6	2.45	0.50
1:X:2253:C:H2'	1:X:2254:A:O4'	2.11	0.50
5:C:6:VAL:HG13	5:C:15:GLY:CA	2.41	0.50
23:W:11:SER:OG	23:W:13:ILE:HG13	2.09	0.50
1:X:183:A:H5'	1:X:481:C:H1'	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:24:GLN:O	8:G:63:ILE:HG13	2.11	0.50
9:H:117:LEU:H	9:H:117:LEU:HD12	1.75	0.50
1:X:1303:A:H2	1:X:2041:A:N6	1.99	0.50
1:X:1830:A:H3'	1:X:1831:A:H8	1.76	0.50
1:X:2511:G:OP1	11:J:45:ARG:HD3	2.12	0.50
3:A:77:LYS:HA	3:A:93:LEU:HA	1.94	0.50
3:A:107:PRO:CA	3:A:195:VAL:HA	2.40	0.50
10:I:125:ALA:O	10:I:126:HIS:ND1	2.44	0.50
11:J:110:SER:HB3	11:J:113:VAL:HG23	1.94	0.50
17:P:9:THR:HG23	17:P:102:HIS:HE1	1.77	0.50
18:Q:43:GLU:OE2	18:Q:49:LYS:HA	2.11	0.50
1:X:281:A:H2'	1:X:282:A:O4'	2.10	0.50
1:X:1356:G:C5	1:X:1357:G:C6	2.99	0.50
1:X:1463:A:H3'	1:X:1464:U:H5"	1.92	0.50
1:X:1508:C:O2'	1:X:1509:G:O5'	2.29	0.50
1:X:1708:A:H61	1:X:2023:C:N4	2.09	0.50
1:X:1770:C:H1'	1:X:1771:A:H5'	1.92	0.50
4:B:33:ASN:HB3	4:B:105:VAL:CG1	2.41	0.50
7:E:120:ASN:OD1	7:E:121:ILE:N	2.42	0.50
17:P:1:MET:HG2	17:P:2:GLU:OE2	2.11	0.50
1:X:322:A:H2'	1:X:323:C:O4'	2.12	0.50
1:X:731:U:O5'	25:2:12:LYS:NZ	2.45	0.50
1:X:793:G:H2'	1:X:795:A:N7	2.26	0.50
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.92	0.50
24:Z:39:LEU:HB2	24:Z:42:ARG:HD2	1.92	0.50
1:X:563:G:H2'	1:X:564:U:C6	2.46	0.50
1:X:813:G:H2'	1:X:814:A:C8	2.47	0.50
1:X:1245:G:C2	1:X:1278:G:C2	3.00	0.50
1:X:1550:G:O2'	1:X:1554:A:H2	1.92	0.50
1:X:2338:A:H3'	1:X:2339:U:C6	2.47	0.50
5:C:64:PRO:HG3	5:C:78:ILE:HG23	1.93	0.50
12:K:55:ASP:OD1	12:K:58:SER:OG	2.22	0.50
15:N:61:TRP:O	15:N:65:ILE:HG12	2.10	0.50
1:X:1144:C:H5"	1:X:1145:U:OP2	2.12	0.50
1:X:1346:G:H4'	25:2:8:PRO:HG2	1.93	0.50
1:X:2244:G:C2	1:X:2245:G:C8	3.00	0.50
13:L:39:HIS:CD2	13:L:58:SER:HB2	2.47	0.50
1:X:623:C:O3'	15:N:31:LEU:HD13	2.12	0.50
1:X:1049:C:H1'	1:X:1056:U:C4	2.46	0.50
1:X:1513:A:H2'	1:X:1514:A:O4'	2.12	0.50
1:X:1761:G:H21	1:X:1762:U:H1'	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2341:A:H2'	1:X:2342:U:C6	2.47	0.50
3:A:212:ARG:HH11	3:A:216:ILE:HB	1.77	0.50
4:B:39:LYS:O	4:B:47:ASN:HA	2.11	0.50
15:N:19:LYS:HA	15:N:19:LYS:HE3	1.94	0.50
16:O:24:LYS:HA	16:O:93:THR:OG1	2.11	0.50
1:X:344:U:HO2'	1:X:345:C:H6	1.59	0.50
1:X:1244:G:N2	1:X:1278:G:H22	2.10	0.50
1:X:1543:G:N7	1:X:1544:G:C2	2.80	0.50
1:X:2220:U:H2'	1:X:2221:U:C6	2.47	0.50
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.94	0.50
6:D:44:VAL:HB	6:D:46:ASN:H	1.76	0.50
9:H:71:ARG:NH2	9:H:104:ARG:HG3	2.26	0.50
20:S:73:MET:HG3	20:S:94:ILE:HD13	1.94	0.50
1:X:345:C:H2'	1:X:346:A:C8	2.46	0.49
6:D:114:PHE:CB	6:D:176:PRO:HB2	2.41	0.49
17:P:67:ASP:N	17:P:67:ASP:OD1	2.45	0.49
20:S:45:GLU:HG2	20:S:49:ILE:HD11	1.94	0.49
1:X:1275:A:H2'	1:X:1276:G:O4'	2.11	0.49
1:X:2817:A:O2'	1:X:2818:A:OP2	2.28	0.49
3:A:239:ALA:N	3:A:240:PRO:HD3	2.27	0.49
19:R:70:LEU:HA	19:R:76:ASN:HA	1.94	0.49
1:X:305:A:H61	1:X:411:A:H62	1.60	0.49
1:X:389:A:H2'	1:X:390:A:O4'	2.12	0.49
1:X:646:A:C8	1:X:700:A:C6	3.00	0.49
1:X:989:A:C4	1:X:2475:A:C2	3.00	0.49
1:X:1250:G:O2'	1:X:1274:G:N2	2.35	0.49
1:X:1732:U:H2'	1:X:1742:A:N6	2.27	0.49
1:X:2642:U:C2	24:Z:4:PRO:HA	2.47	0.49
15:N:27:SER:HB2	15:N:31:LEU:HG	1.94	0.49
19:R:12:ILE:CG2	19:R:18:GLY:HA2	2.42	0.49
23:W:40:ASN:O	23:W:44:ARG:HB2	2.13	0.49
1:X:153:G:O2'	1:X:154:A:OP2	2.28	0.49
1:X:338:G:H1	1:X:386:C:H42	1.60	0.49
1:X:811:C:H2'	1:X:812:U:H5'	1.94	0.49
1:X:1303:A:N6	1:X:2040:A:H5"	2.26	0.49
1:X:1491:C:O2	1:X:1492:G:N2	2.45	0.49
1:X:2352:G:H8	1:X:2352:G:O5'	1.95	0.49
2:Y:55:A:H5'	6:D:23:SER:OG	2.12	0.49
4:B:115:VAL:HG23	4:B:182:ASN:HA	1.93	0.49
1:X:955:A:N7	1:X:956:A:C6	2.81	0.49
1:X:1306:A:H2'	1:X:1307:G:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1700:C:H2'	1:X:1701:U:H6	1.77	0.49
1:X:1762:U:H5'	1:X:1763:U:OP2	2.12	0.49
1:X:2299:U:H5"	1:X:2300:A:OP1	2.13	0.49
1:X:2342:U:O3'	13:L:3:SER:N	2.46	0.49
5:C:158:ASN:C	5:C:160:ASP:H	2.14	0.49
8:G:115:LEU:O	8:G:119:GLN:HG2	2.12	0.49
9:H:88:ARG:O	9:H:89:ASP:HB2	2.13	0.49
10:I:116:SER:HB2	10:I:126:HIS:NE2	2.28	0.49
15:N:36:LYS:HG2	15:N:40:MET:HE2	1.95	0.49
1:X:119:U:HO2'	1:X:120:G:P	2.35	0.49
1:X:170:C:H2'	1:X:171:A:C8	2.47	0.49
1:X:591:A:H4'	1:X:592:A:C5'	2.43	0.49
1:X:786:U:H2'	1:X:787:U:O4'	2.13	0.49
1:X:1072:A:H1'	1:X:2514:G:H5'	1.94	0.49
1:X:1423:C:O2'	1:X:1512:U:H1'	2.13	0.49
1:X:1505:G:C8	1:X:1506:C:C5	3.00	0.49
1:X:1680:U:H2'	1:X:1681:U:C6	2.48	0.49
20:S:27:VAL:HG13	20:S:43:VAL:HG23	1.93	0.49
1:X:189:G:H2'	1:X:190:G:C8	2.48	0.49
1:X:506:A:H5'	1:X:507:C:H5	1.77	0.49
1:X:1424:A:H2'	1:X:1425:G:C8	2.47	0.49
1:X:2848:G:C2	1:X:2849:A:N7	2.81	0.49
3:A:223:SER:HA	3:A:232:HIS:HB2	1.95	0.49
4:B:104:GLU:CD	4:B:104:GLU:H	2.16	0.49
1:X:372:A:H62	19:R:15:LYS:HG2	1.77	0.49
1:X:753:U:H3	1:X:768:A:H61	1.60	0.49
1:X:1151:G:H2'	1:X:1151:G:N3	2.27	0.49
1:X:1543:G:N7	1:X:1544:G:N1	2.61	0.49
1:X:2314:A:O2'	1:X:2315:A:H3'	2.12	0.49
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.94	0.49
20:S:135:ASP:O	20:S:137:ILE:N	2.46	0.49
23:W:44:ARG:HA	23:W:47:ILE:HD12	1.93	0.49
1:X:463:C:H2'	1:X:464:U:C6	2.48	0.49
1:X:876:G:H22	10:I:46:VAL:HG11	1.76	0.49
1:X:1245:G:C2	1:X:1246:C:C5	3.00	0.49
1:X:2241:C:H2'	1:X:2242:G:O4'	2.12	0.49
4:B:38:LYS:HZ1	4:B:97:ASP:HA	1.76	0.49
6:D:162:THR:HB	6:D:165:GLU:H	1.78	0.49
1:X:1781:C:H2'	1:X:1782:A:C8	2.47	0.49
1:X:2912:A:H4'	1:X:2913:G:O4'	2.13	0.49
5:C:53:ASN:CB	5:C:87:GLY:HA2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:93:THR:HB	5:C:94:PRO:HD2	1.95	0.49
15:N:94:MET:HE3	16:O:12:ILE:HA	1.94	0.49
1:X:323:C:O2	1:X:323:C:H2'	2.13	0.48
1:X:631:U:H2'	1:X:632:U:C6	2.48	0.48
1:X:685:C:H2'	1:X:686:U:C6	2.48	0.48
1:X:2231:C:O2'	1:X:2232:A:H8	1.96	0.48
2:Y:14:G:C6	2:Y:67:G:C2	3.01	0.48
22:V:44:ARG:O	22:V:48:LYS:HG3	2.12	0.48
1:X:683:G:N2	1:X:697:U:C6	2.77	0.48
1:X:1352:C:H2'	1:X:1353:A:C8	2.48	0.48
1:X:1746:G:C2'	1:X:1747:G:H8	2.27	0.48
1:X:2232:A:H5'	1:X:2233:C:P	2.53	0.48
1:X:2901:U:O2'	12:K:101:THR:O	2.29	0.48
3:A:26:LYS:HB2	3:A:26:LYS:HE3	1.60	0.48
3:A:123:ASP:OD2	3:A:124:ILE:HG13	2.13	0.48
9:H:68:GLY:O	9:H:69:VAL:HG23	2.12	0.48
15:N:48:ARG:HD2	15:N:49:ASP:OD1	2.12	0.48
22:V:49:THR:O	22:V:53:LEU:HG	2.13	0.48
1:X:896:U:H4'	23:W:46:GLN:HA	1.95	0.48
1:X:1452:C:N4	1:X:1458:A:OP1	2.44	0.48
1:X:1754:C:HO2'	1:X:2878:U:H3	1.60	0.48
1:X:1887:G:H2'	1:X:1888:U:C6	2.48	0.48
1:X:2581:U:H2'	1:X:2582:U:C6	2.48	0.48
6:D:29:PRO:HB2	6:D:169:LEU:HD12	1.95	0.48
20:S:6:SER:HB3	20:S:43:VAL:HG12	1.95	0.48
1:X:280:C:H2'	1:X:281:A:H8	1.77	0.48
1:X:1015:C:H2'	1:X:1016:G:O4'	2.13	0.48
1:X:1016:G:H3'	1:X:1017:A:H5"	1.95	0.48
1:X:1039:C:C6	8:G:1:MET:HG2	2.48	0.48
1:X:1494:G:N7	1:X:1495:C:H5	2.11	0.48
5:C:12:THR:O	5:C:13:LYS:HD2	2.12	0.48
15:N:66:ASN:HA	15:N:76:TYR:HB2	1.95	0.48
18:Q:25:TYR:CE2	18:Q:82:LEU:HD11	2.48	0.48
1:X:1498:U:O2'	1:X:1499:U:H5	1.95	0.48
1:X:1805:U:H2'	1:X:1811:A:N6	2.27	0.48
1:X:2731:C:H2'	1:X:2732:A:O4'	2.13	0.48
1:X:525:A:N3	1:X:527:G:H5"	2.28	0.48
1:X:1337:A:H4'	1:X:1338:U:H5"	1.95	0.48
1:X:1955:A:C8	1:X:1956:G:H1'	2.49	0.48
11:J:35:GLN:HB3	11:J:130:LYS:HB3	1.96	0.48
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:235:G:H4'	1:X:236:A:OP1	2.12	0.48
1:X:502:C:O2'	1:X:503:A:O5'	2.30	0.48
1:X:810:A:H2'	1:X:811:C:H6	1.78	0.48
1:X:888:G:N2	1:X:980:U:C2	2.82	0.48
1:X:923:A:N6	1:X:946:A:N7	2.61	0.48
1:X:1023:A:H2'	1:X:1026:C:H42	1.79	0.48
1:X:2268:A:H2'	1:X:2269:G:C8	2.49	0.48
2:Y:3:U:H3	2:Y:112:G:H1	1.60	0.48
5:C:9:LEU:CB	5:C:12:THR:HB	2.44	0.48
10:I:41:ARG:O	10:I:42:SER:OG	2.30	0.48
25:2:27:ASN:O	25:2:31:VAL:N	2.44	0.48
1:X:3:U:H2'	1:X:4:U:C6	2.48	0.48
1:X:323:C:H5'	1:X:324:A:N7	2.28	0.48
1:X:1151:G:N2	1:X:1152:U:O4	2.47	0.48
1:X:2308:C:O2'	1:X:2309:G:H5'	2.13	0.48
1:X:2331:G:N2	1:X:2339:U:H3	2.12	0.48
1:X:2391:C:H5'	21:T:64:ASP:HB2	1.94	0.48
4:B:133:ARG:HA	4:B:173:MET:SD	2.53	0.48
18:Q:31:THR:C	18:Q:33:VAL:H	2.17	0.48
1:X:187:C:H2'	1:X:188:C:C6	2.49	0.48
1:X:323:C:H5'	1:X:324:A:H8	1.77	0.48
1:X:1070:A:H1'	1:X:1178:C:H41	1.79	0.48
1:X:1289:A:H5"	15:N:13:ARG:HH12	1.79	0.48
1:X:1313:G:H2'	1:X:1314:A:H8	1.79	0.48
1:X:1436:C:O2'	1:X:1437:U:P	2.72	0.48
1:X:1978:U:H2'	1:X:1980:A:OP2	2.14	0.48
1:X:2331:G:H22	1:X:2339:U:H3	1.62	0.48
1:X:2342:U:H2'	1:X:2343:U:C6	2.49	0.48
1:X:2801:C:H2'	1:X:2802:A:O4'	2.14	0.48
3:A:46:GLN:OE1	3:A:47:GLY:N	2.47	0.48
11:J:15:PRO:HG3	11:J:72:THR:HG21	1.95	0.48
17:P:50:VAL:HB	17:P:105:ILE:HD11	1.96	0.48
20:S:156:VAL:N	20:S:173:GLU:O	2.47	0.48
1:X:118:A:H4'	1:X:119:U:H5'	1.95	0.47
1:X:945:A:H2'	1:X:946:A:H5'	1.96	0.47
1:X:1504:U:O2	1:X:1505:G:N2	2.46	0.47
1:X:2320:C:H2'	1:X:2321:C:O4'	2.13	0.47
7:E:90:VAL:O	7:E:92:VAL:N	2.46	0.47
9:H:25:LEU:HA	9:H:25:LEU:HD23	1.76	0.47
14:M:65:LYS:HD2	14:M:66:ILE:H	1.79	0.47
14:M:74:ARG:HG2	14:M:76:PHE:CE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:16:LYS:O	15:N:20:LEU:HG	2.14	0.47
18:Q:57:ASN:HB3	18:Q:76:ARG:HD3	1.96	0.47
1:X:483:C:H2'	1:X:484:U:C6	2.49	0.47
1:X:525:A:H4'	1:X:526:A:OP1	2.14	0.47
1:X:889:U:C2'	1:X:890:G:H5'	2.44	0.47
1:X:938:G:H5'	1:X:939:U:OP2	2.13	0.47
1:X:1055:A:OP1	15:N:75:SER:HB2	2.13	0.47
1:X:1270:U:H2'	1:X:1271:G:C8	2.49	0.47
1:X:1511:C:H5'	1:X:1512:U:OP1	2.15	0.47
1:X:2820:U:H1'	1:X:2824:G:N2	2.29	0.47
9:H:63:VAL:HG13	9:H:102:VAL:HG13	1.95	0.47
24:Z:30:CYS:CB	24:Z:34:GLY:HA3	2.44	0.47
1:X:1323:A:HO2'	1:X:1325:U:P	2.31	0.47
1:X:1466:G:C6	1:X:1467:G:C8	3.02	0.47
1:X:1508:C:H1'	1:X:1593:G:H22	1.79	0.47
1:X:1775:G:H2'	1:X:1776:A:C8	2.49	0.47
1:X:2873:C:H42	1:X:2884:G:H1	1.63	0.47
6:D:33:LYS:HE2	6:D:92:ARG:HH12	1.79	0.47
14:M:52:ARG:HA	14:M:60:THR:O	2.14	0.47
19:R:9:VAL:HG22	19:R:23:VAL:HG22	1.95	0.47
20:S:111:GLU:O	20:S:146:THR:HA	2.15	0.47
1:X:77:U:H2'	1:X:78:U:C6	2.49	0.47
1:X:378:C:H2'	1:X:379:C:C6	2.45	0.47
1:X:381:G:N2	1:X:382:U:H1'	2.29	0.47
1:X:499:A:N3	1:X:503:A:O2'	2.42	0.47
1:X:725:A:H2'	1:X:726:G:C8	2.49	0.47
1:X:1353:A:H2'	1:X:1354:G:H8	1.79	0.47
1:X:1990:C:H4'	1:X:1991:G:OP1	2.13	0.47
1:X:2736:G:H2'	1:X:2737:C:C6	2.49	0.47
5:C:184:LEU:HD23	5:C:184:LEU:HA	1.81	0.47
6:D:33:LYS:HG3	6:D:157:VAL:HG21	1.96	0.47
15:N:19:LYS:HE3	15:N:22:LYS:HE3	1.96	0.47
1:X:770:G:C6	1:X:771:G:N1	2.82	0.47
1:X:1490:G:O2'	1:X:1491:C:O4'	2.24	0.47
1:X:1554:A:H2'	1:X:1555:G:C5	2.50	0.47
1:X:1874:A:O2'	1:X:1875:A:N7	2.47	0.47
1:X:2221:U:H2'	1:X:2222:U:O4'	2.14	0.47
1:X:2672:G:O6	32:X:3286:SPD:H32	2.14	0.47
2:Y:12:U:OP2	2:Y:68:A:O2'	2.21	0.47
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.95	0.47
10:I:66:PHE:O	10:I:94:ALA:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:58:ARG:HA	22:V:61:GLU:HB3	1.96	0.47
1:X:619:U:H2'	1:X:620:G:C8	2.50	0.47
1:X:1562:C:H2'	1:X:1563:U:C6	2.50	0.47
8:G:25:THR:HB	8:G:28:ARG:HG3	1.95	0.47
14:M:94:VAL:HG21	14:M:99:LEU:HD21	1.96	0.47
1:X:124:A:C5'	25:2:20:ARG:HD3	2.37	0.47
1:X:329:A:H2'	1:X:329:A:N3	2.29	0.47
1:X:778:G:C6	1:X:806:A:C5	3.03	0.47
1:X:1398:G:H2'	1:X:1398:G:N3	2.30	0.47
1:X:2732:A:H2'	1:X:2733:A:O4'	2.13	0.47
1:X:2874:A:H8	1:X:2874:A:O5'	1.98	0.47
4:B:134:HIS:ND1	4:B:168:LYS:HB3	2.30	0.47
5:C:150:LYS:HA	5:C:187:THR:O	2.14	0.47
16:O:50:ALA:HB1	16:O:51:PRO:HD2	1.97	0.47
22:V:22:LYS:HB3	22:V:22:LYS:HE2	1.60	0.47
1:X:24:G:H2'	1:X:25:U:C6	2.50	0.47
1:X:1186:A:C4	1:X:1188:A:C8	3.03	0.47
1:X:1379:A:C6	1:X:1382:C:N3	2.82	0.47
1:X:1514:A:H3'	1:X:1515:G:C8	2.39	0.47
2:Y:53:U:O2'	6:D:26:MET:HG2	2.14	0.47
4:B:62:ASP:N	4:B:62:ASP:OD1	2.48	0.47
1:X:33:U:O2'	1:X:34:U:H5"	2.15	0.47
1:X:1381:U:O2'	1:X:1421:A:H2'	2.14	0.47
1:X:1760:G:C2	1:X:1761:G:N7	2.83	0.47
1:X:2775:A:H2'	1:X:2776:A:C8	2.50	0.47
1:X:168:A:C3'	1:X:169:G:H5'	2.45	0.47
1:X:250:G:H4'	1:X:432:G:C5	2.50	0.47
1:X:1145:U:O2'	1:X:1146:C:H5"	2.15	0.47
1:X:1286:G:N2	5:C:88:ILE:HG21	2.30	0.47
1:X:1528:G:H1	1:X:1545:U:H3	1.62	0.47
1:X:1740:G:C6	1:X:1741:G:C4	3.03	0.47
1:X:2021:C:O2	1:X:2021:C:H2'	2.14	0.47
1:X:2347:A:N3	1:X:2347:A:H2'	2.29	0.47
1:X:2367:A:H2'	1:X:2368:G:H8	1.80	0.47
1:X:2603:G:H5"	1:X:2604:A:OP1	2.15	0.47
1:X:2671:A:H62	32:X:3286:SPD:H52	1.80	0.47
5:C:11:GLY:HA2	5:C:142:VAL:CG1	2.45	0.47
12:K:45:GLU:O	12:K:49:THR:HG23	2.15	0.47
15:N:50:ARG:HG2	15:N:53:ARG:NH2	2.30	0.47
1:X:364:A:H5"	5:C:159:GLU:HB3	1.98	0.46
1:X:365:A:H5'	1:X:383:A:H1'	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:384:G:C6	1:X:385:U:C4	3.02	0.46
1:X:474:A:OP2	1:X:474:A:H8	1.98	0.46
1:X:506:A:H5'	1:X:507:C:C5	2.50	0.46
1:X:1385:G:C2	1:X:1643:C:C2	3.03	0.46
1:X:1392:G:H2'	1:X:1393:C:C6	2.50	0.46
1:X:2623:U:H2'	1:X:2624:G:O4'	2.15	0.46
1:X:119:U:O2'	1:X:120:G:P	2.74	0.46
1:X:562:C:O2'	17:P:18:ARG:NH2	2.47	0.46
1:X:757:G:N3	1:X:757:G:H2'	2.29	0.46
1:X:1528:G:N2	1:X:1545:U:H3	2.11	0.46
14:M:24:PRO:HA	14:M:49:VAL:HB	1.96	0.46
16:O:33:PHE:CD1	16:O:34:THR:N	2.83	0.46
18:Q:89:LEU:HB3	18:Q:91:ASN:H	1.79	0.46
1:X:247:A:H5"	1:X:248:G:OP2	2.15	0.46
1:X:666:A:H3'	1:X:667:G:H8	1.80	0.46
1:X:1040:A:H4'	15:N:91:ASN:ND2	2.31	0.46
1:X:1699:A:H1'	4:B:127:PHE:CE1	2.50	0.46
1:X:2229:C:H5'	1:X:2230:G:OP1	2.15	0.46
1:X:2349:A:H2'	1:X:2350:G:O4'	2.16	0.46
1:X:2591:A:C6	1:X:2592:A:N1	2.83	0.46
3:A:90:ASN:HA	3:A:106:ALA:H	1.81	0.46
5:C:149:PRO:HD2	5:C:186:ILE:HA	1.97	0.46
10:I:91:VAL:HG12	10:I:92:THR:H	1.79	0.46
14:M:31:HIS:HB3	14:M:83:ILE:HD12	1.95	0.46
16:O:67:ARG:HA	16:O:91:PRO:HA	1.96	0.46
17:P:36:LEU:HD23	17:P:36:LEU:HA	1.66	0.46
1:X:164:A:H1'	1:X:165:C:H5'	1.97	0.46
1:X:177:G:O2'	1:X:178:A:H5'	2.15	0.46
1:X:506:A:H3'	1:X:507:C:H6	1.81	0.46
1:X:1501:G:N2	1:X:2729:G:H22	2.03	0.46
4:B:194:VAL:HG12	4:B:195:ILE:N	2.31	0.46
15:N:58:ARG:HA	15:N:61:TRP:CE3	2.50	0.46
16:O:3:ALA:HA	16:O:40:PHE:O	2.16	0.46
1:X:437:A:O2'	1:X:456:G:OP1	2.23	0.46
1:X:922:G:N2	1:X:924:G:H5"	2.31	0.46
1:X:1084:U:H2'	1:X:1085:U:O4'	2.15	0.46
1:X:1159:A:H2'	1:X:1160:C:O4'	2.15	0.46
1:X:1318:G:N2	1:X:1327:C:C2	2.84	0.46
1:X:1333:A:H2'	1:X:1334:C:C6	2.50	0.46
1:X:1364:C:H2'	1:X:1365:G:O4'	2.15	0.46
1:X:1423:C:H2'	1:X:1424:A:H8	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1658:A:C2	17:P:93:ALA:HB2	2.51	0.46
1:X:909:G:OP2	11:J:22:LYS:HE2	2.15	0.46
1:X:1072:A:N3	1:X:2513:G:O2'	2.42	0.46
1:X:1092:A:O2'	1:X:1093:C:O4'	2.33	0.46
1:X:1400:C:HO2'	1:X:1836:A:H1'	1.79	0.46
2:Y:22:G:H8	2:Y:22:G:O5'	1.99	0.46
2:Y:58:G:H8	2:Y:58:G:O5'	1.99	0.46
5:C:4:TYR:HD2	5:C:19:LEU:HA	1.79	0.46
7:E:89:LEU:HD13	7:E:89:LEU:HA	1.77	0.46
13:L:31:LEU:HA	13:L:44:ILE:HD13	1.96	0.46
22:V:6:ILE:O	22:V:9:LEU:HD22	2.15	0.46
1:X:568:C:O2	1:X:597:U:O2'	2.30	0.46
1:X:1484:G:C2	1:X:1599:G:N2	2.84	0.46
1:X:1563:U:C2'	1:X:1564:G:H8	2.28	0.46
1:X:1697:G:C6	12:K:6:LEU:HD12	2.51	0.46
1:X:2005:A:H2'	1:X:2006:C:O4'	2.15	0.46
1:X:2124:U:H3	1:X:2219:C:H42	1.64	0.46
1:X:2314:A:O2'	1:X:2315:A:P	2.73	0.46
17:P:36:LEU:HD11	17:P:47:ILE:HG22	1.98	0.46
1:X:592:A:O2'	1:X:593:U:O5'	2.34	0.46
1:X:1044:A:H2'	1:X:1045:A:C8	2.51	0.46
1:X:1233:A:H2'	1:X:1234:G:O4'	2.16	0.46
1:X:1644:C:N4	1:X:1645:G:O6	2.49	0.46
1:X:1847:U:C4	3:A:159:GLY:HA3	2.50	0.46
1:X:2072:C:H5"	24:Z:15:LYS:HD2	1.97	0.46
1:X:2776:A:H1'	7:E:64:ASN:CB	2.45	0.46
3:A:116:VAL:HA	3:A:128:ASN:HA	1.98	0.46
3:A:174:ILE:O	3:A:181:VAL:HG13	2.16	0.46
4:B:116:ILE:HG12	4:B:183:LEU:O	2.15	0.46
5:C:171:PRO:O	5:C:173:VAL:N	2.45	0.46
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.81	0.46
15:N:94:MET:O	15:N:98:ILE:HG13	2.16	0.46
1:X:15:G:O2'	24:Z:18:THR:HG21	2.15	0.46
1:X:139:U:O2'	1:X:140:A:H8	1.98	0.46
1:X:631:U:H1'	5:C:90:PHE:CD1	2.51	0.46
1:X:695:C:N3	1:X:696:G:C6	2.83	0.46
1:X:921:C:H5	1:X:942:C:H41	1.63	0.46
1:X:1508:C:N3	1:X:1509:G:N1	2.63	0.46
1:X:2876:G:N1	1:X:2877:G:C8	2.84	0.46
3:A:31:LYS:NZ	3:A:32:SER:HA	2.31	0.46
5:C:12:THR:HG22	5:C:13:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:33:LYS:NZ	6:D:92:ARG:HH22	2.14	0.46
12:K:52:LYS:HE3	12:K:94:THR:HA	1.97	0.46
1:X:1400:C:N4	1:X:1405:G:H1	2.14	0.46
1:X:1644:C:P	18:Q:76:ARG:HH12	2.39	0.46
1:X:2377:C:H2'	1:X:2378:G:O4'	2.16	0.46
1:X:2725:U:H2'	1:X:2726:C:C6	2.51	0.46
2:Y:21:G:H2'	2:Y:22:G:C8	2.51	0.46
2:Y:40:C:H6	6:D:66:LEU:HD12	1.81	0.46
3:A:76:ALA:HB1	3:A:112:VAL:O	2.16	0.46
5:C:39:LEU:HD11	5:C:99:TYR:O	2.15	0.46
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.80	0.46
1:X:242:U:H2'	1:X:243:U:C6	2.51	0.45
1:X:769:U:H2'	1:X:770:G:O4'	2.16	0.45
1:X:1708:A:N6	1:X:2023:C:H42	2.13	0.45
1:X:1884:G:O2'	1:X:1912:A:N6	2.50	0.45
1:X:1994:C:H2'	1:X:1995:G:H5'	1.97	0.45
8:G:56:ILE:HG21	8:G:130:GLU:HG2	1.98	0.45
14:M:65:LYS:CD	14:M:66:ILE:H	2.28	0.45
15:N:22:LYS:CE	15:N:22:LYS:HA	2.46	0.45
22:V:10:THR:OG1	22:V:13:GLU:HG3	2.16	0.45
1:X:460:C:H5"	1:X:1906:C:O2'	2.15	0.45
1:X:489:A:OP1	5:C:45:ARG:HB2	2.16	0.45
1:X:755:C:N4	1:X:766:G:H1	2.11	0.45
1:X:948:U:H2'	1:X:949:C:C6	2.50	0.45
1:X:1008:C:O2'	1:X:2300:A:N3	2.42	0.45
1:X:1515:G:HO2'	1:X:1516:C:P	2.39	0.45
1:X:1612:C:C4	1:X:1614:A:C2	3.04	0.45
1:X:2507:C:H2'	1:X:2508:G:H5'	1.98	0.45
3:A:65:ILE:HD12	3:A:65:ILE:HA	1.71	0.45
5:C:129:PHE:CG	5:C:130:ASN:N	2.84	0.45
11:J:41:TRP:CE3	11:J:94:ILE:HG21	2.50	0.45
19:R:41:MET:HA	19:R:60:GLU:HB2	1.98	0.45
1:X:300:G:N2	1:X:302:A:N6	2.65	0.45
1:X:519:G:O2'	1:X:520:G:H5'	2.17	0.45
1:X:554:C:H6	1:X:554:C:H5"	1.82	0.45
1:X:797:A:N6	1:X:2636:U:H3	2.14	0.45
1:X:1488:A:N1	1:X:1596:G:C2	2.84	0.45
1:X:1643:C:P	18:Q:35:LYS:HG3	2.56	0.45
1:X:2082:C:H2'	1:X:2531:U:H4'	1.99	0.45
9:H:16:ALA:HB3	9:H:86:ILE:HD11	1.99	0.45
12:K:48:ILE:O	12:K:52:LYS:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:14:VAL:HG13	16:O:97:ILE:HG13	1.99	0.45
1:X:619:U:H4'	1:X:2529:G:C8	2.52	0.45
1:X:650:U:N3	1:X:666:A:C2	2.79	0.45
1:X:657:U:C4	1:X:659:A:N6	2.84	0.45
1:X:720:A:O2'	1:X:721:A:H5'	2.17	0.45
1:X:1452:C:O2'	1:X:1631:G:N2	2.49	0.45
1:X:1876:G:H2'	1:X:1877:G:H8	1.81	0.45
4:B:131:ILE:HD11	4:B:149:ARG:NH2	2.31	0.45
13:L:19:ARG:CZ	13:L:45:ILE:HD11	2.46	0.45
1:X:106:A:H2'	1:X:107:G:H8	1.82	0.45
1:X:305:A:C2	1:X:413:C:C2	3.04	0.45
1:X:683:G:C2	1:X:696:G:C4	3.05	0.45
1:X:805:G:H2'	1:X:806:A:O4'	2.15	0.45
1:X:946:A:C2'	1:X:947:U:H5'	2.46	0.45
1:X:1378:U:OP2	1:X:1431:U:O2'	2.32	0.45
1:X:1494:G:N2	1:X:1505:G:C8	2.82	0.45
1:X:1838:G:O5'	1:X:1838:G:H8	1.98	0.45
1:X:1933:G:C2	1:X:1952:C:C4	3.05	0.45
1:X:1983:U:H1'	1:X:2579:U:OP1	2.16	0.45
2:Y:40:C:C6	6:D:66:LEU:HD12	2.52	0.45
3:A:141:VAL:HG13	3:A:190:ALA:HB1	1.99	0.45
1:X:267:G:H2'	1:X:268:A:H5"	1.99	0.45
1:X:361:U:H2'	1:X:362:C:C6	2.47	0.45
1:X:937:G:C2	1:X:938:G:H4'	2.52	0.45
1:X:1449:A:H4'	1:X:1450:A:OP1	2.15	0.45
1:X:1998:A:O2'	1:X:1999:G:OP1	2.33	0.45
1:X:2048:G:H2'	1:X:2048:G:N3	2.32	0.45
1:X:2319:U:H2'	1:X:2320:C:C6	2.52	0.45
1:X:2367:A:H2'	1:X:2368:G:C8	2.51	0.45
2:Y:94:U:C5	2:Y:95:A:C5	3.05	0.45
9:H:50:GLY:O	9:H:53:LYS:NZ	2.37	0.45
1:X:139:U:O2'	1:X:140:A:C8	2.68	0.45
1:X:442:G:H8	1:X:442:G:O5'	1.99	0.45
1:X:1272:U:H2'	1:X:1273:G:O4'	2.17	0.45
1:X:1290:G:N3	15:N:33:LYS:HG2	2.32	0.45
1:X:2231:C:O2'	1:X:2232:A:O4'	2.34	0.45
1:X:2385:A:H61	10:I:47:ARG:NH2	2.15	0.45
8:G:142:GLU:OE1	8:G:142:GLU:N	2.50	0.45
14:M:31:HIS:ND1	14:M:43:GLN:O	2.49	0.45
19:R:15:LYS:HG2	19:R:16:ASP:H	1.82	0.45
20:S:101:THR:HA	20:S:130:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:22:ARG:O	25:2:28:GLY:HA3	2.17	0.45
1:X:295:G:H2'	1:X:296:G:O4'	2.17	0.45
1:X:309:U:O2'	1:X:310:C:OP2	2.31	0.45
1:X:749:G:HO2'	1:X:750:A:P	2.38	0.45
1:X:1176:U:H3'	1:X:1176:U:OP2	2.17	0.45
1:X:2003:U:H2'	1:X:2004:A:N7	2.32	0.45
1:X:2701:G:H5"	9:H:30:ARG:HE	1.81	0.45
5:C:117:LYS:HE2	5:C:180:GLY:O	2.17	0.45
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.99	0.45
9:H:64:ARG:NH1	9:H:101:PRO:O	2.47	0.45
23:W:40:ASN:HB3	23:W:43:ILE:N	2.20	0.45
24:Z:9:SER:OG	24:Z:12:ARG:N	2.42	0.45
1:X:251:G:N7	1:X:253:G:H1'	2.32	0.45
1:X:1516:C:H2'	1:X:1517:A:H8	1.82	0.45
7:E:156:PRO:CD	7:E:160:LYS:HA	2.47	0.45
12:K:109:ARG:HD2	12:K:114:ALA:HB3	1.98	0.45
17:P:10:ILE:O	17:P:12:ILE:N	2.50	0.45
19:R:84:LYS:HA	19:R:90:LYS:HA	1.99	0.45
26:3:60:GLN:OE1	26:3:60:GLN:HA	2.17	0.45
1:X:397:U:HO2'	1:X:398:C:H6	1.65	0.45
1:X:986:G:H8	1:X:986:G:O5'	2.00	0.45
1:X:2845:G:C5	1:X:2846:A:C8	3.05	0.45
1:X:2896:A:H2'	1:X:2897:A:C8	2.51	0.45
2:Y:90:C:H2'	2:Y:91:C:C6	2.52	0.45
12:K:29:ARG:HB3	12:K:120:GLU:CB	2.47	0.45
12:K:38:LYS:O	12:K:41:ARG:HB3	2.16	0.45
14:M:31:HIS:HD1	14:M:31:HIS:H	1.64	0.45
18:Q:57:ASN:H	18:Q:57:ASN:ND2	2.14	0.45
18:Q:61:LYS:N	18:Q:72:THR:HG22	2.16	0.45
23:W:47:ILE:HG23	23:W:54:VAL:HG11	1.98	0.45
1:X:49:A:C5	1:X:179:A:C6	3.05	0.44
1:X:123:G:N7	25:2:20:ARG:NH2	2.65	0.44
1:X:498:G:C6	1:X:499:A:C6	3.04	0.44
1:X:1056:U:OP2	15:N:70:ARG:NH2	2.44	0.44
1:X:1356:G:O2'	1:X:1357:G:H5'	2.16	0.44
1:X:1474:C:H2'	1:X:1475:A:C8	2.52	0.44
1:X:1793:C:H2'	1:X:1794:C:H6	1.82	0.44
1:X:2418:G:C6	1:X:2454:C:H1'	2.53	0.44
4:B:134:HIS:CD2	4:B:168:LYS:HE2	2.51	0.44
10:I:63:LYS:HG3	10:I:91:VAL:CB	2.47	0.44
22:V:37:LEU:HD22	22:V:39:GLU:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:24:G:H2'	1:X:25:U:H6	1.82	0.44
1:X:338:G:H1	1:X:386:C:N4	2.15	0.44
1:X:360:A:C6	1:X:361:U:C4	3.05	0.44
1:X:411:A:C2'	1:X:412:U:H5'	2.47	0.44
1:X:813:G:H2'	1:X:814:A:H8	1.81	0.44
1:X:1438:G:H2'	1:X:1439:U:O4'	2.17	0.44
1:X:1612:C:O2'	1:X:1613:G:H5"	2.18	0.44
1:X:2218:G:H2'	1:X:2219:C:C6	2.52	0.44
1:X:2234:C:H42	1:X:2244:G:H22	1.64	0.44
3:A:141:VAL:CG1	3:A:190:ALA:HB1	2.47	0.44
1:X:236:A:C8	1:X:236:A:O5'	2.71	0.44
1:X:237:U:H2'	1:X:238:U:O4'	2.16	0.44
1:X:448:A:H8	1:X:448:A:OP2	2.00	0.44
1:X:968:A:H4'	21:T:37:GLN:HG3	2.00	0.44
1:X:1265:G:N7	15:N:16:LYS:HE3	2.33	0.44
1:X:1806:U:C5	1:X:1811:A:N7	2.86	0.44
1:X:1839:G:H2'	1:X:1840:U:H6	1.83	0.44
1:X:2422:C:H2'	1:X:2423:G:C8	2.53	0.44
1:X:2775:A:H2'	1:X:2776:A:H8	1.81	0.44
20:S:29:ALA:N	20:S:41:VAL:O	2.49	0.44
1:X:1442:C:H2'	1:X:1443:A:H8	1.80	0.44
1:X:1507:A:H2'	1:X:1508:C:H5'	1.99	0.44
1:X:1612:C:H5"	3:A:26:LYS:HD3	1.99	0.44
1:X:1842:A:H4'	1:X:1843:U:OP1	2.17	0.44
1:X:2249:G:C6	1:X:2250:A:C6	3.06	0.44
2:Y:86:C:C5	2:Y:88:U:C2	3.05	0.44
4:B:13:THR:O	4:B:25:VAL:HG12	2.18	0.44
4:B:38:LYS:HZ3	4:B:97:ASP:HA	1.78	0.44
5:C:54:ARG:C	5:C:56:ALA:N	2.71	0.44
8:G:59:ASN:HA	8:G:127:GLY:HA2	2.00	0.44
9:H:98:ILE:HG12	9:H:117:LEU:HB2	2.00	0.44
1:X:321:U:HO2'	1:X:322:A:P	2.36	0.44
1:X:937:G:N3	1:X:937:G:H2'	2.32	0.44
1:X:1302:G:H5'	24:Z:8:THR:OG1	2.18	0.44
1:X:1872:G:H1	1:X:1922:C:N4	2.13	0.44
1:X:2305:A:OP1	11:J:11:ARG:HG3	2.18	0.44
9:H:61:VAL:O	9:H:63:VAL:HG23	2.17	0.44
19:R:41:MET:HA	19:R:60:GLU:CB	2.48	0.44
20:S:95:ASN:O	20:S:96:MET:HB2	2.17	0.44
1:X:7:G:H4'	8:G:16:TRP:CH2	2.52	0.44
1:X:356:A:H2'	1:X:357:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:889:U:H2'	1:X:890:G:H5'	1.99	0.44
1:X:995:U:OP1	2:Y:85:A:N1	2.50	0.44
1:X:1259:U:H2'	1:X:1260:C:C6	2.53	0.44
1:X:1314:A:H2'	1:X:1315:C:C6	2.52	0.44
1:X:2496:A:H2'	1:X:2497:G:O4'	2.17	0.44
1:X:2607:U:OP1	4:B:146:HIS:ND1	2.50	0.44
1:X:2632:U:H2'	1:X:2633:C:C6	2.53	0.44
5:C:4:TYR:CD2	5:C:19:LEU:HA	2.53	0.44
8:G:13:GLU:O	8:G:42:LYS:NZ	2.50	0.44
9:H:17:ARG:NH2	9:H:47:THR:HA	2.32	0.44
1:X:120:G:H4'	1:X:150:A:H5'	2.00	0.44
1:X:463:C:H2'	1:X:464:U:H6	1.83	0.44
1:X:502:C:HO2'	1:X:503:A:P	2.41	0.44
1:X:730:A:C8	1:X:819:A:C6	3.06	0.44
1:X:1245:G:C2	1:X:1246:C:C6	3.06	0.44
1:X:1542:C:H1'	1:X:1624:C:O2'	2.17	0.44
1:X:1761:G:O2'	1:X:1762:U:O5'	2.35	0.44
1:X:1848:A:H2'	1:X:1849:G:H8	1.83	0.44
1:X:1882:G:H2'	1:X:1883:A:O4'	2.18	0.44
1:X:2293:A:C2	1:X:2299:U:C5	3.06	0.44
2:Y:75:U:P	20:S:22:ARG:HH22	2.40	0.44
9:H:12:ASP:HA	9:H:97:ARG:O	2.18	0.44
1:X:1153:C:N3	1:X:1154:G:N2	2.65	0.44
1:X:1332:C:H4'	12:K:67:ARG:NH1	2.33	0.44
1:X:2620:U:H2'	1:X:2621:C:H6	1.82	0.44
19:R:32:ARG:O	19:R:65:VAL:HG23	2.18	0.44
24:Z:39:LEU:HA	24:Z:39:LEU:HD23	1.80	0.44
25:2:21:LYS:O	25:2:24:SER:OG	2.36	0.44
26:3:54:ASP:O	26:3:57:ARG:N	2.49	0.44
1:X:143:U:O2'	18:Q:36:THR:OG1	2.28	0.44
1:X:265:A:C2	1:X:476:A:N3	2.86	0.44
1:X:1065:A:C8	1:X:1065:A:C3'	3.00	0.44
1:X:1880:A:C6	1:X:1916:A:C6	3.06	0.44
1:X:2671:A:N6	1:X:2672:G:C6	2.85	0.44
1:X:2752:A:H1'	1:X:2753:U:H2'	2.00	0.44
2:Y:111:A:H2'	2:Y:112:G:C8	2.53	0.44
4:B:53:PHE:HB3	4:B:87:PHE:HB2	2.00	0.44
10:I:62:PRO:HD2	10:I:90:GLU:OE2	2.18	0.44
14:M:52:ARG:HG3	14:M:52:ARG:NH1	2.25	0.44
18:Q:19:ALA:HB1	18:Q:24:LYS:HB2	2.00	0.44
22:V:7:ARG:C	22:V:9:LEU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:622:A:O2'	1:X:2046:U:OP1	2.35	0.43
1:X:817:G:H2'	1:X:818:U:C6	2.53	0.43
1:X:1515:G:N2	1:X:1516:C:C2	2.86	0.43
1:X:1773:A:H2'	1:X:1774:A:H8	1.83	0.43
1:X:2411:A:O2'	1:X:2412:C:OP1	2.34	0.43
1:X:2479:C:N4	1:X:2480:A:N6	2.66	0.43
1:X:2587:C:H2'	1:X:2588:A:O4'	2.18	0.43
1:X:2668:A:H2'	1:X:2669:G:H8	1.82	0.43
7:E:105:LEU:O	7:E:107:VAL:N	2.51	0.43
8:G:38:ARG:HH11	8:G:111:PRO:HG3	1.83	0.43
1:X:172:U:H3'	1:X:173:A:H8	1.84	0.43
1:X:249:C:H2'	1:X:250:G:O4'	2.17	0.43
1:X:411:A:H2'	1:X:412:U:H5'	1.98	0.43
1:X:441:C:H2'	1:X:442:G:C8	2.52	0.43
1:X:712:U:H2'	1:X:713:A:O4'	2.17	0.43
1:X:1342:C:H2'	1:X:1343:U:O4'	2.17	0.43
1:X:1771:A:O2'	1:X:1772:G:O5'	2.32	0.43
3:A:171:TYR:HA	3:A:185:LEU:HA	2.01	0.43
3:A:258:LYS:HD2	3:A:260:ARG:HG2	2.00	0.43
8:G:40:LYS:O	8:G:41:ASN:HB2	2.18	0.43
18:Q:11:VAL:HG12	18:Q:13:THR:HG23	1.99	0.43
1:X:305:A:N6	1:X:411:A:H62	2.16	0.43
1:X:321:U:C4	1:X:326:A:C6	3.05	0.43
1:X:329:A:N6	1:X:398:C:N4	2.66	0.43
1:X:871:U:O2'	10:I:46:VAL:HG12	2.17	0.43
1:X:923:A:C6	1:X:945:A:N6	2.87	0.43
1:X:1150:A:H8	1:X:1151:G:H8	1.66	0.43
1:X:1501:G:H1	1:X:2729:G:H1	1.66	0.43
1:X:1726:A:C2	1:X:1727:C:C2	3.07	0.43
1:X:1843:U:H3'	1:X:1843:U:C6	2.53	0.43
1:X:2319:U:H4'	1:X:2402:G:H4'	2.00	0.43
1:X:2605:G:OP2	1:X:2605:G:H4'	2.17	0.43
2:Y:11:A:H4'	2:Y:13:A:C8	2.53	0.43
3:A:158:ALA:HB1	3:A:197:ASN:C	2.38	0.43
5:C:9:LEU:CB	5:C:14:SER:HB3	2.47	0.43
5:C:143:LEU:HD23	5:C:143:LEU:HA	1.72	0.43
10:I:109:ILE:H	10:I:109:ILE:HD12	1.82	0.43
26:3:49:LEU:N	26:3:49:LEU:HD23	2.33	0.43
1:X:666:A:H2'	1:X:667:G:H5'	2.00	0.43
1:X:870:C:H1'	10:I:47:ARG:HH21	1.82	0.43
1:X:1013:U:H2'	1:X:1014:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1382:C:H42	1:X:1645:G:H1	1.66	0.43
1:X:1516:C:C4	1:X:1517:A:N7	2.87	0.43
1:X:1760:G:C6	1:X:1761:G:N7	2.87	0.43
1:X:1840:U:H2'	1:X:1841:G:O4'	2.19	0.43
1:X:2036:G:OP1	17:P:41:LYS:HE2	2.18	0.43
1:X:2224:U:O2'	1:X:2225:A:H5"	2.18	0.43
1:X:2255:G:H2'	1:X:2256:U:O4'	2.17	0.43
1:X:2348:G:H5"	1:X:2349:A:OP2	2.17	0.43
4:B:64:LYS:H	4:B:64:LYS:HG2	1.52	0.43
5:C:170:ILE:HD12	5:C:174:GLN:O	2.18	0.43
10:I:45:GLY:C	10:I:46:VAL:HG23	2.38	0.43
17:P:82:LEU:O	17:P:84:ARG:HG2	2.19	0.43
23:W:39:ASP:OD1	23:W:44:ARG:NH2	2.52	0.43
1:X:1312:A:H4'	1:X:1313:G:OP1	2.19	0.43
1:X:2018:U:O2'	1:X:2019:G:H5'	2.18	0.43
1:X:2126:C:N3	1:X:2217:G:N1	2.66	0.43
1:X:2362:A:C8	1:X:2364:G:C6	3.06	0.43
1:X:2719:C:H4'	1:X:2890:C:O2	2.18	0.43
1:X:2783:U:H4'	1:X:2784:A:OP1	2.18	0.43
2:Y:11:A:H4'	2:Y:13:A:N7	2.33	0.43
3:A:258:LYS:HZ1	3:A:260:ARG:HB3	1.82	0.43
5:C:102:PRO:HD2	5:C:105:MET:HE3	2.00	0.43
12:K:9:THR:HG22	12:K:12:GLN:H	1.83	0.43
14:M:52:ARG:HH11	14:M:52:ARG:CG	2.26	0.43
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.82	0.43
20:S:32:TYR:O	20:S:92:LEU:HD12	2.18	0.43
1:X:338:G:H2'	1:X:339:A:H8	1.84	0.43
1:X:1155:A:H1'	1:X:1156:G:O4'	2.18	0.43
1:X:1773:A:H2'	1:X:1774:A:C8	2.54	0.43
1:X:1836:A:H2'	1:X:1837:A:C8	2.53	0.43
1:X:1953:U:N3	1:X:1955:A:N1	2.66	0.43
1:X:1963:A:H1'	1:X:1967:U:C2	2.53	0.43
1:X:2229:C:H42	1:X:2248:G:H1	1.65	0.43
1:X:2324:C:N4	1:X:2348:G:H1	2.15	0.43
3:A:143:ASN:OD1	3:A:152:GLY:HA3	2.17	0.43
10:I:65:GLY:HA2	10:I:93:PRO:HG2	2.00	0.43
1:X:147:G:H2'	1:X:148:U:O4'	2.19	0.43
1:X:266:A:H2'	1:X:267:G:O4'	2.17	0.43
1:X:909:G:C6	1:X:910:C:N4	2.87	0.43
1:X:1286:G:C6	5:C:51:VAL:HG23	2.53	0.43
1:X:1512:U:H2'	1:X:1513:A:H8	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1560:A:H5'	1:X:1561:G:OP2	2.19	0.43
1:X:1788:U:C3'	1:X:1789:A:H5"	2.48	0.43
1:X:2419:A:H2	1:X:2451:C:N4	2.14	0.43
1:X:2587:C:C2	1:X:2588:A:C8	3.06	0.43
2:Y:13:A:N3	2:Y:106:U:N3	2.66	0.43
2:Y:80:A:C6	2:Y:92:G:N1	2.86	0.43
2:Y:108:G:O2'	2:Y:109:C:H5'	2.19	0.43
4:B:34:VAL:HG12	4:B:35:VAL:O	2.19	0.43
4:B:182:ASN:C	4:B:183:LEU:HD12	2.39	0.43
9:H:91:LYS:HB3	9:H:111:PHE:CB	2.49	0.43
10:I:105:GLU:HA	10:I:125:ALA:HB2	2.00	0.43
12:K:67:ARG:HA	12:K:67:ARG:HD3	1.72	0.43
1:X:538:G:H2'	1:X:539:G:O4'	2.18	0.43
1:X:548:A:H4'	1:X:549:U:H5"	2.00	0.43
1:X:683:G:C8	1:X:684:U:C5	3.07	0.43
1:X:792:U:C4	1:X:2640:U:C5	3.07	0.43
1:X:1423:C:H2'	1:X:1424:A:C8	2.54	0.43
1:X:1841:G:H3'	1:X:1842:A:H2'	2.00	0.43
1:X:2646:U:H4'	4:B:163:VAL:HG12	2.01	0.43
3:A:173:LEU:HG	3:A:183:MET:HB2	1.99	0.43
8:G:33:VAL:HG13	8:G:55:VAL:HG11	2.01	0.43
9:H:87:ILE:HG22	9:H:88:ARG:N	2.33	0.43
1:X:401:U:H2'	1:X:402:C:O4'	2.18	0.43
1:X:629:A:H5'	5:C:89:VAL:CG2	2.49	0.43
1:X:773:G:O2'	1:X:774:G:H5'	2.18	0.43
1:X:1511:C:H2'	1:X:1567:A:N6	2.34	0.43
1:X:1753:U:C2	1:X:1777:G:N2	2.87	0.43
1:X:1885:G:O2'	1:X:1886:A:P	2.77	0.43
1:X:2448:G:H5"	1:X:2449:C:OP2	2.18	0.43
3:A:25:THR:HG22	3:A:203:VAL:HA	2.00	0.43
8:G:40:LYS:O	8:G:41:ASN:CB	2.67	0.43
8:G:97:ASN:N	8:G:97:ASN:OD1	2.51	0.43
10:I:91:VAL:O	10:I:92:THR:OG1	2.32	0.43
1:X:1595:C:H2'	1:X:1596:G:O4'	2.19	0.43
1:X:1725:G:H21	1:X:1789:A:H3'	1.84	0.43
1:X:1730:C:H2'	1:X:1731:G:O4'	2.19	0.43
1:X:2433:C:O2	1:X:2433:C:H2'	2.18	0.43
3:A:28:THR:HA	3:A:29:PRO:HD3	1.86	0.43
3:A:231:PRO:HD3	3:A:246:PRO:HA	1.99	0.43
8:G:95:ARG:HE	8:G:95:ARG:HB3	1.63	0.43
11:J:113:VAL:O	11:J:117:ALA:N	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:39:LEU:HA	16:O:39:LEU:HD13	1.72	0.43
1:X:162:A:H2'	1:X:162:A:N3	2.34	0.42
1:X:327:G:H2'	1:X:327:G:N3	2.34	0.42
1:X:328:G:O2'	1:X:329:A:H8	2.02	0.42
1:X:673:G:C5	1:X:681:G:N2	2.87	0.42
1:X:691:A:H5'	1:X:692:G:OP2	2.19	0.42
1:X:1162:C:H2'	1:X:1163:U:O4'	2.19	0.42
1:X:1195:A:H4'	15:N:81:ASN:CG	2.39	0.42
1:X:1270:U:H2'	1:X:1271:G:H8	1.83	0.42
1:X:1363:U:HO2'	1:X:2037:G:HO2'	1.63	0.42
1:X:1395:G:N2	1:X:1409:U:OP2	2.45	0.42
1:X:1511:C:H2'	1:X:1567:A:H61	1.84	0.42
1:X:2314:A:H2	1:X:2373:A:H62	1.66	0.42
1:X:2649:U:C2'	1:X:2845:G:H22	2.31	0.42
1:X:2719:C:H2'	1:X:2720:A:O4'	2.19	0.42
5:C:14:SER:O	5:C:16:SER:N	2.49	0.42
20:S:29:ALA:HB2	20:S:89:ILE:HB	2.01	0.42
1:X:7:G:H4'	8:G:16:TRP:HH2	1.83	0.42
1:X:302:A:N1	1:X:450:C:C4	2.87	0.42
1:X:341:G:H5"	1:X:342:A:OP1	2.19	0.42
1:X:1066:G:N2	1:X:1186:A:C2	2.88	0.42
1:X:1312:A:N6	1:X:1333:A:H4'	2.34	0.42
1:X:1323:A:O2'	1:X:1324:A:H5"	2.19	0.42
1:X:2089[B]:A:H61	27:X:3001:95H:C8	2.32	0.42
5:C:178:ALA:O	5:C:181:LEU:HB2	2.19	0.42
11:J:35:GLN:O	11:J:129:THR:HA	2.18	0.42
25:2:35:ARG:HD3	25:2:43:LEU:O	2.18	0.42
1:X:83:G:N1	1:X:101:G:O2'	2.41	0.42
1:X:460:C:H1'	1:X:1891:U:O2'	2.19	0.42
1:X:843:G:H2'	1:X:844:G:C8	2.54	0.42
1:X:994:A:H2'	1:X:995:U:O4'	2.18	0.42
1:X:1349:U:C2	1:X:1647:A:C2	3.07	0.42
1:X:1429:G:C2	1:X:1430:A:C6	3.08	0.42
1:X:2358:G:H4'	21:T:51:THR:H	1.85	0.42
1:X:2682:G:O2'	1:X:2683:U:P	2.77	0.42
1:X:2760:A:N1	4:B:216:LYS:HB2	2.34	0.42
1:X:2877:G:H5'	1:X:2878:U:OP2	2.20	0.42
5:C:4:TYR:CB	5:C:19:LEU:HA	2.49	0.42
20:S:167:ILE:H	20:S:167:ILE:HD12	1.85	0.42
22:V:28:LEU:HD21	22:V:42:ARG:HD2	2.00	0.42
26:3:23:LYS:O	26:3:49:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:190:G:H2'	1:X:191:A:O4'	2.20	0.42
1:X:201:C:H2'	1:X:202:A:H5"	2.02	0.42
1:X:290:U:H1'	1:X:291:G:N7	2.34	0.42
1:X:332:A:H61	1:X:394:U:H3	1.68	0.42
1:X:1053:A:H5"	15:N:63:THR:HG22	2.02	0.42
1:X:1280:U:H2'	1:X:1281:U:H6	1.82	0.42
2:Y:16:A:C2	2:Y:17:A:C5	3.08	0.42
2:Y:79:C:N4	2:Y:92:G:H1	2.12	0.42
9:H:106:LEU:H	9:H:106:LEU:HD12	1.83	0.42
11:J:40:SER:OG	11:J:41:TRP:N	2.52	0.42
16:O:67:ARG:H	16:O:67:ARG:HG3	1.40	0.42
18:Q:26:THR:CB	18:Q:79:ILE:HG22	2.42	0.42
24:Z:7:ARG:HH11	24:Z:7:ARG:HD3	1.73	0.42
1:X:683:G:N1	1:X:696:G:C5	2.88	0.42
1:X:767:A:H2'	1:X:768:A:C8	2.54	0.42
1:X:1330:U:H2'	1:X:1331:C:O4'	2.19	0.42
1:X:1458:A:H5"	1:X:1630:A:C2	2.55	0.42
1:X:1518:G:N2	1:X:1519:U:C2	2.88	0.42
1:X:2693:C:H5"	1:X:2694:C:OP2	2.20	0.42
22:V:63:GLU:HA	22:V:66:LYS:HG3	2.01	0.42
1:X:49:A:H5"	1:X:51:G:O4'	2.20	0.42
1:X:245:G:H5"	26:3:64:TYR:CE2	2.55	0.42
1:X:323:C:O5'	1:X:324:A:OP2	2.37	0.42
1:X:868:A:H2'	1:X:869:G:C8	2.54	0.42
1:X:956:A:H2	1:X:2304:G:N3	2.17	0.42
1:X:1065:A:H3'	1:X:1065:A:H8	1.82	0.42
1:X:1275:A:C8	1:X:1276:G:H1'	2.54	0.42
1:X:1637:A:N3	1:X:1637:A:H2'	2.35	0.42
1:X:1953:U:N3	1:X:1954:A:C8	2.86	0.42
2:Y:105:G:H8	2:Y:105:G:H2'	1.59	0.42
3:A:173:LEU:HA	3:A:183:MET:HA	2.02	0.42
3:A:212:ARG:NH1	3:A:216:ILE:HB	2.34	0.42
3:A:258:LYS:HZ2	3:A:260:ARG:HA	1.85	0.42
4:B:36:LEU:HD12	4:B:52:GLY:HA3	2.02	0.42
9:H:19:VAL:HG23	9:H:42:THR:O	2.20	0.42
20:S:22:ARG:NE	20:S:87:THR:HG22	2.35	0.42
1:X:665:G:N3	1:X:665:G:H2'	2.34	0.42
1:X:1602:U:O2'	1:X:1603:U:OP1	2.28	0.42
1:X:1701:U:H2'	1:X:1702:C:C6	2.55	0.42
1:X:2217:G:C8	1:X:2218:G:C6	3.07	0.42
1:X:2290:C:H4'	1:X:2356:A:H4'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2854:A:H2'	1:X:2899:A:H61	1.84	0.42
3:A:145:GLU:OE1	3:A:188:CYS:HA	2.19	0.42
5:C:179:GLN:OE1	5:C:179:GLN:N	2.43	0.42
13:L:19:ARG:NH2	13:L:45:ILE:HD11	2.34	0.42
16:O:7:THR:O	16:O:9:GLY:N	2.49	0.42
20:S:14:THR:HG23	20:S:17:ASP:OD2	2.19	0.42
1:X:177:G:O5'	1:X:177:G:H8	2.03	0.42
1:X:349:U:C5	1:X:350:G:C5	3.07	0.42
1:X:352:A:H1'	1:X:372:A:N3	2.35	0.42
1:X:720:A:C8	1:X:849:A:C6	3.07	0.42
1:X:1817:C:OP1	3:A:219:THR:HG23	2.19	0.42
1:X:1858:G:H2'	1:X:1859:C:C6	2.55	0.42
1:X:1865:C:N4	1:X:1926:A:C4	2.87	0.42
1:X:2222:U:C2	1:X:2223:C:H5	2.38	0.42
1:X:2417:U:H5'	26:3:35:ASN:HB3	2.01	0.42
1:X:2850:G:H5'	4:B:67:LYS:HB2	2.01	0.42
2:Y:93:C:H41	20:S:15:ARG:NH2	2.18	0.42
1:X:367:A:H2'	1:X:368:A:O4'	2.19	0.42
1:X:368:A:O5'	1:X:368:A:H8	2.03	0.42
1:X:523:A:H2'	1:X:524:A:O4'	2.20	0.42
1:X:847:A:C6	1:X:848:U:N3	2.87	0.42
1:X:1092:A:H2	1:X:1156:G:H21	1.62	0.42
1:X:1542:C:C5	1:X:1543:G:C8	3.08	0.42
1:X:2338:A:H5"	1:X:2339:U:OP2	2.19	0.42
1:X:2707:C:H1'	4:B:200:ASN:OD1	2.20	0.42
3:A:133:GLN:N	3:A:186:SER:O	2.52	0.42
8:G:29:LEU:O	8:G:33:VAL:HG23	2.20	0.42
8:G:42:LYS:HD2	8:G:51:THR:O	2.20	0.42
11:J:78:PRO:HB2	11:J:81:VAL:CG2	2.50	0.42
15:N:35:ALA:O	15:N:39:VAL:HG23	2.20	0.42
1:X:90:A:OP1	1:X:90:A:C8	2.72	0.42
1:X:190:G:C2	1:X:213:C:O2	2.72	0.42
1:X:812:U:H6	1:X:812:U:H2'	1.69	0.42
1:X:826:A:O5'	1:X:826:A:H8	2.03	0.42
1:X:923:A:N6	1:X:945:A:N7	2.68	0.42
1:X:926:G:H22	1:X:939:U:C2'	2.32	0.42
1:X:1042:C:P	15:N:92:ARG:HH21	2.43	0.42
1:X:1185:U:H4'	1:X:1186:A:O4'	2.19	0.42
1:X:1759:G:N2	1:X:1760:G:C2	2.88	0.42
1:X:2760:A:C2	4:B:216:LYS:HB2	2.55	0.42
5:C:153:LEU:O	5:C:153:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:117:LEU:HD12	9:H:117:LEU:N	2.35	0.42
10:I:6:LEU:HD23	10:I:6:LEU:HA	1.84	0.42
17:P:72:LYS:HD3	17:P:108:SER:HB2	2.02	0.42
20:S:9:ARG:HD2	20:S:13:GLN:OE1	2.19	0.42
1:X:79:U:C4	1:X:80:G:N7	2.88	0.41
1:X:1508:C:N3	1:X:1509:G:C2	2.87	0.41
1:X:1885:G:H1'	1:X:1911:A:H62	1.84	0.41
1:X:2388:A:OP1	26:3:26:ARG:HG2	2.20	0.41
1:X:2851:G:C8	4:B:64:LYS:HG3	2.55	0.41
3:A:120:ALA:HA	3:A:130:LEU:HD21	2.01	0.41
4:B:111:VAL:HG23	4:B:112:ALA:O	2.20	0.41
6:D:35:VAL:HA	6:D:89:VAL:O	2.20	0.41
11:J:73:PRO:HB3	11:J:93:TRP:CE3	2.54	0.41
11:J:74:TYR:CE1	11:J:94:ILE:HD11	2.54	0.41
22:V:44:ARG:O	22:V:47:ARG:HG3	2.20	0.41
1:X:77:U:H2'	1:X:78:U:H6	1.85	0.41
1:X:455:A:H8	1:X:455:A:O5'	2.03	0.41
1:X:1092:A:H61	1:X:1156:G:C1'	2.29	0.41
1:X:1364:C:O3'	12:K:110:ARG:NH2	2.54	0.41
1:X:1562:C:C2	1:X:1563:U:C5	3.08	0.41
1:X:1847:U:O2	3:A:200:HIS:HB3	2.20	0.41
1:X:1854:U:H2'	1:X:1855:G:O4'	2.20	0.41
1:X:1903:A:H2'	1:X:1904:A:O4'	2.20	0.41
1:X:2028:A:H2'	1:X:2029:G:O4'	2.20	0.41
1:X:2245:G:C6	1:X:2246:U:N3	2.88	0.41
1:X:2555:U:O3'	1:X:2556:G:H8	2.02	0.41
1:X:2580:G:C2	1:X:2610:G:H1'	2.56	0.41
3:A:46:GLN:HE22	3:A:48:LYS:HZ2	1.67	0.41
5:C:63:LYS:NZ	5:C:75:GLN:O	2.53	0.41
7:E:89:LEU:HD12	7:E:90:VAL:H	1.85	0.41
9:H:13:ASN:OD1	9:H:13:ASN:N	2.52	0.41
16:O:35:PHE:HZ	16:O:95:LEU:HD11	1.85	0.41
17:P:111:LYS:HD2	17:P:111:LYS:HA	1.66	0.41
1:X:660:A:H5"	5:C:43:SER:HB2	2.02	0.41
1:X:1244:G:N2	1:X:1279:C:C2	2.88	0.41
1:X:2591:A:C2	1:X:2674:U:H4'	2.55	0.41
6:D:64:LYS:HA	6:D:64:LYS:HD3	1.91	0.41
7:E:140:GLN:C	7:E:142:GLY:H	2.24	0.41
1:X:244:A:H61	1:X:258:A:H5"	1.85	0.41
1:X:325:A:C2	1:X:326:A:C4	3.08	0.41
1:X:797:A:C2	1:X:1808:U:C2	3.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1522:G:N2	1:X:1558:U:H1'	2.36	0.41
1:X:2049:U:OP2	24:Z:12:ARG:NH2	2.47	0.41
1:X:2286:G:C8	1:X:2454:C:C4	3.08	0.41
5:C:51:VAL:HB	5:C:92:PRO:HD2	2.02	0.41
6:D:60:ILE:H	6:D:60:ILE:HG13	1.63	0.41
9:H:102:VAL:O	9:H:121:VAL:HA	2.20	0.41
10:I:55:LEU:HA	10:I:56:PRO:HD3	1.73	0.41
15:N:4:VAL:HG12	15:N:5:LYS:O	2.20	0.41
19:R:42:LYS:HD2	19:R:59:THR:HG23	2.02	0.41
1:X:218:G:C4'	1:X:219:A:H4'	2.50	0.41
1:X:706:U:H1'	10:I:13:ARG:H	1.86	0.41
1:X:778:G:H8	1:X:778:G:O5'	2.03	0.41
1:X:1245:G:N2	1:X:1246:C:C2	2.88	0.41
1:X:1378:U:H2'	1:X:1434:U:O2	2.20	0.41
1:X:1480:G:H2'	1:X:1481:A:O4'	2.21	0.41
1:X:1491:C:C2	1:X:1492:G:N2	2.88	0.41
1:X:1933:G:C2	1:X:1934:G:H5'	2.55	0.41
1:X:2239:A:H62	1:X:2241:C:H42	1.68	0.41
1:X:2249:G:C2	1:X:2250:A:C4	3.08	0.41
1:X:2294:A:H5"	1:X:2295:A:H5'	2.02	0.41
1:X:2309:G:H4'	1:X:2416:G:O2'	2.20	0.41
1:X:2310:C:H2'	1:X:2311:U:O4'	2.21	0.41
1:X:2570:G:H2'	1:X:2571:G:C8	2.55	0.41
12:K:47:LEU:HD13	12:K:66:LEU:CD1	2.50	0.41
15:N:91:ASN:O	15:N:91:ASN:CG	2.58	0.41
18:Q:11:VAL:HG23	18:Q:27:PHE:HA	2.03	0.41
20:S:31:VAL:HG22	20:S:39:VAL:O	2.21	0.41
22:V:43:ILE:H	22:V:43:ILE:HG13	1.39	0.41
22:V:63:GLU:HA	22:V:66:LYS:NZ	2.35	0.41
1:X:153:G:C2	1:X:177:G:C2	3.09	0.41
1:X:157:U:C2	1:X:158:G:C8	3.08	0.41
1:X:383:A:N6	1:X:384:G:C2	2.89	0.41
1:X:390:A:H2'	1:X:391:A:C8	2.55	0.41
1:X:820:G:C4	1:X:839:A:C8	3.09	0.41
1:X:1281:U:C2	1:X:1282:A:C8	3.09	0.41
1:X:1492:G:C8	1:X:1493:U:H5	2.38	0.41
1:X:1963:A:H2	1:X:1970:U:C4	2.37	0.41
1:X:2088:G:C8	1:X:2528:C:H1'	2.55	0.41
1:X:2234:C:N4	1:X:2244:G:H22	2.19	0.41
1:X:2398:G:C6	1:X:2399:G:N7	2.89	0.41
1:X:2474:G:C8	1:X:2528:C:O4'	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2512:G:H5"	11:J:46:GLN:HE21	1.84	0.41
1:X:2530:A:H4'	1:X:2531:U:OP1	2.20	0.41
1:X:2599:A:O2'	1:X:2602:C:OP1	2.38	0.41
6:D:157:VAL:O	6:D:157:VAL:HG12	2.20	0.41
7:E:153:PRO:HA	7:E:154:PRO:HD3	1.52	0.41
11:J:87:LYS:HB2	11:J:87:LYS:HE2	1.70	0.41
16:O:21:PHE:N	16:O:21:PHE:CD1	2.89	0.41
1:X:1379:A:O2'	1:X:1381:U:OP2	2.31	0.41
1:X:1526:G:H22	1:X:1547:C:N4	2.18	0.41
1:X:1872:G:H2'	1:X:1873:G:O4'	2.21	0.41
1:X:2239:A:H62	1:X:2241:C:N4	2.18	0.41
1:X:2634:G:H2'	1:X:2635:G:O4'	2.20	0.41
1:X:2704:A:H2'	1:X:2705:U:C6	2.55	0.41
1:X:2876:G:C4	1:X:2882:A:C2	3.08	0.41
2:Y:18:G:H2'	2:Y:19:G:H8	1.86	0.41
2:Y:81:A:H61	2:Y:90:C:H42	1.69	0.41
4:B:37:GLN:OE1	4:B:39:LYS:HE3	2.20	0.41
5:C:4:TYR:HB3	5:C:5:ASP:H	1.50	0.41
6:D:57:LEU:HD12	6:D:57:LEU:HA	1.93	0.41
9:H:17:ARG:NH2	9:H:47:THR:HG22	2.35	0.41
9:H:24:VAL:HG11	9:H:30:ARG:HG2	2.03	0.41
16:O:25:LEU:HA	16:O:25:LEU:HD23	1.72	0.41
16:O:65:GLN:HG3	16:O:93:THR:HG23	2.01	0.41
23:W:17:GLU:O	23:W:21:LYS:HG3	2.21	0.41
1:X:400:C:H2'	1:X:401:U:O4'	2.21	0.41
1:X:422:G:H1	1:X:444:C:N4	2.12	0.41
1:X:454:G:H1	1:X:465:C:H42	1.68	0.41
1:X:726:G:H5"	1:X:727:G:OP2	2.21	0.41
1:X:788:A:OP1	4:B:144:GLY:HA2	2.21	0.41
1:X:862:C:N4	1:X:1229:G:H1	2.16	0.41
1:X:870:C:H4'	1:X:2455:G:C5	2.56	0.41
1:X:987:U:C2'	1:X:988:C:H5'	2.51	0.41
1:X:1695:G:H5"	12:K:35:ALA:CB	2.51	0.41
1:X:1850:G:H2'	1:X:1851:G:O4'	2.20	0.41
1:X:1903:A:H2'	1:X:1904:A:C8	2.56	0.41
1:X:1928:A:H2'	1:X:1929:C:H6	1.86	0.41
4:B:69:ALA:HB2	4:B:84:PRO:HB3	2.01	0.41
5:C:151:LYS:HA	5:C:170:ILE:O	2.20	0.41
8:G:32:GLU:O	8:G:36:ILE:HG12	2.20	0.41
11:J:54:MET:HE1	11:J:106:VAL:HG11	2.03	0.41
13:L:40:ILE:HD11	13:L:101:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:65:ILE:CD1	15:N:95:LEU:HB3	2.50	0.41
15:N:93:LYS:O	15:N:97:GLU:HB2	2.21	0.41
17:P:14:PRO:O	17:P:18:ARG:HG3	2.21	0.41
1:X:49:A:C6	1:X:179:A:C5	3.09	0.41
1:X:125:A:H8	1:X:126:A:C5	2.39	0.41
1:X:187:C:H4'	1:X:220:A:C2	2.56	0.41
1:X:241:C:O2'	1:X:651:A:N3	2.48	0.41
1:X:272:C:H5'	1:X:297:G:C6	2.56	0.41
1:X:608:C:H2'	1:X:609:U:O4'	2.21	0.41
1:X:864:A:C4	1:X:1228:A:C2	3.08	0.41
1:X:947:U:H2'	1:X:948:U:C6	2.56	0.41
1:X:1045:A:H2'	1:X:1046:G:O4'	2.21	0.41
1:X:1301:U:OP1	24:Z:13:LYS:NZ	2.29	0.41
1:X:1352:C:N3	1:X:1374:G:N2	2.48	0.41
1:X:1746:G:HO2'	1:X:1747:G:H8	1.69	0.41
1:X:1770:C:O2'	1:X:1771:A:H5'	2.20	0.41
1:X:1780:G:OP1	14:M:95:ARG:HD2	2.21	0.41
1:X:1788:U:H3	1:X:1789:A:N6	2.19	0.41
1:X:1825:U:O2'	1:X:1829:A:N3	2.48	0.41
1:X:1953:U:N3	1:X:1955:A:C6	2.89	0.41
1:X:2269:G:H2'	1:X:2270:U:O4'	2.21	0.41
1:X:2563:G:C6	1:X:2564:U:C4	3.08	0.41
1:X:2876:G:C6	1:X:2877:G:C5	3.09	0.41
6:D:34:ILE:HD11	6:D:156:ILE:HA	2.03	0.41
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.03	0.41
9:H:8:LEU:HD12	9:H:8:LEU:N	2.36	0.41
14:M:15:LEU:HA	14:M:79:HIS:CD2	2.55	0.41
14:M:34:ILE:HG13	14:M:82:LYS:HE3	2.02	0.41
1:X:439:U:H2'	1:X:440:C:H6	1.85	0.41
1:X:503:A:N1	1:X:517:A:N7	2.69	0.41
1:X:660:A:N7	5:C:176:THR:HG22	2.36	0.41
1:X:716:C:H2'	1:X:717:C:H6	1.86	0.41
1:X:775:A:O2'	1:X:776:C:H5'	2.21	0.41
1:X:857:C:H5'	10:I:22:GLY:HA3	2.01	0.41
1:X:886:A:C2	1:X:982:G:C2	3.09	0.41
1:X:992:A:H1'	1:X:1028:G:C8	2.56	0.41
1:X:1212:U:H2'	1:X:1213:C:O4'	2.21	0.41
1:X:1490:G:H2'	1:X:1491:C:C6	2.56	0.41
1:X:1832:C:H2'	1:X:1833:C:H6	1.86	0.41
3:A:139:THR:HG22	3:A:140:VAL:O	2.21	0.41
8:G:74:VAL:HB	8:G:76:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:105:ALA:HB1	16:O:40:PHE:CZ	2.56	0.41
19:R:15:LYS:HB3	19:R:18:GLY:H	1.86	0.41
26:3:33:PHE:C	26:3:35:ASN:H	2.24	0.41
1:X:58:G:N2	1:X:70:G:C4	2.89	0.40
1:X:284:C:H2'	1:X:286:U:OP1	2.21	0.40
1:X:317:G:H3'	1:X:317:G:N3	2.35	0.40
1:X:327:G:C2	1:X:328:G:N7	2.89	0.40
1:X:505:U:H2'	1:X:506:A:H5"	2.02	0.40
1:X:811:C:N4	1:X:812:U:C4	2.89	0.40
1:X:1155:A:H1'	1:X:1156:G:C4'	2.50	0.40
1:X:1652:A:H1'	1:X:1654:A:OP2	2.20	0.40
1:X:2223:C:H2'	1:X:2224:U:C6	2.57	0.40
1:X:2231:C:HO2'	1:X:2232:A:H8	1.69	0.40
1:X:2248:G:C2	1:X:2249:G:C8	3.09	0.40
10:I:63:LYS:HA	10:I:91:VAL:HG23	2.03	0.40
14:M:49:VAL:O	14:M:50:ILE:HD13	2.21	0.40
16:O:2:PHE:HB3	16:O:42:GLY:N	2.36	0.40
20:S:95:ASN:C	20:S:97:SER:H	2.24	0.40
24:Z:5:LYS:O	24:Z:6:ARG:HG2	2.21	0.40
1:X:133:A:C8	1:X:134:U:C6	3.09	0.40
1:X:457:G:OP1	1:X:2434:A:OP1	2.39	0.40
1:X:652:A:H2'	1:X:653:G:H5'	2.01	0.40
1:X:662:G:H2'	1:X:663:U:O4'	2.21	0.40
1:X:1760:G:N1	1:X:1761:G:N7	2.69	0.40
1:X:1904:A:H2'	1:X:1905:G:O4'	2.21	0.40
1:X:2000:G:C5	1:X:2001:C:C5	3.09	0.40
1:X:2638:C:H2'	1:X:2639:C:C6	2.55	0.40
2:Y:21:G:H22	2:Y:58:G:N2	2.19	0.40
11:J:43:THR:HG22	11:J:45:ARG:H	1.85	0.40
11:J:52:ILE:CG2	11:J:56:ARG:HH21	2.34	0.40
18:Q:57:ASN:OD1	18:Q:76:ARG:NH1	2.54	0.40
21:T:52:LYS:HE3	21:T:52:LYS:HB2	1.78	0.40
1:X:1701:U:H2'	1:X:1702:C:H6	1.87	0.40
1:X:2410:G:C6	1:X:2411:A:C2	3.09	0.40
1:X:2494:C:H4'	11:J:123:HIS:CE1	2.57	0.40
1:X:2504:C:H5"	1:X:2506:U:O4	2.21	0.40
1:X:2549:U:O2'	1:X:2674:U:OP1	2.22	0.40
1:X:2646:U:H5'	4:B:163:VAL:O	2.21	0.40
2:Y:21:G:N2	2:Y:58:G:N2	2.69	0.40
2:Y:39:G:H5'	2:Y:40:C:H5"	2.02	0.40
8:G:14:ARG:HB2	8:G:53:ASP:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:1:MET:HB3	9:H:1:MET:HE2	1.39	0.40
12:K:52:LYS:NZ	12:K:96:ARG:O	2.52	0.40
15:N:83:LEU:HA	15:N:83:LEU:HD23	1.71	0.40
17:P:13:ALA:O	17:P:17:VAL:HG23	2.20	0.40
18:Q:55:ILE:CD1	18:Q:78:ALA:HB2	2.52	0.40
23:W:22:THR:O	23:W:26:LEU:HD12	2.21	0.40
1:X:350:G:H2'	1:X:352:A:OP2	2.22	0.40
1:X:410:G:H8	1:X:410:G:OP2	2.05	0.40
1:X:1379:A:N1	1:X:1382:C:N3	2.70	0.40
1:X:1449:A:O2'	1:X:1451:U:O4	2.19	0.40
1:X:2126:C:N3	1:X:2217:G:C6	2.89	0.40
1:X:2694:C:O2	7:E:108:GLY:HA2	2.21	0.40
2:Y:41:C:O4'	6:D:63:GLN:NE2	2.55	0.40
4:B:36:LEU:N	4:B:50:GLN:O	2.48	0.40
7:E:33:LEU:C	7:E:35:ARG:H	2.24	0.40
17:P:44:SER:N	17:P:45:PRO:HD2	2.36	0.40
1:X:268:A:H2'	1:X:269:G:O4'	2.21	0.40
1:X:286:U:H5"	1:X:287:G:OP1	2.22	0.40
1:X:502:C:O2'	1:X:503:A:P	2.80	0.40
1:X:660:A:C8	5:C:176:THR:HG22	2.56	0.40
1:X:922:G:N1	1:X:924:G:N7	2.69	0.40
1:X:1524:C:H42	1:X:1550:G:H1	1.69	0.40
1:X:1594:U:H3'	1:X:1595:C:H5'	2.03	0.40
1:X:1933:G:H2'	1:X:1934:G:C5'	2.52	0.40
1:X:2236:C:H5"	1:X:2237:U:O5'	2.21	0.40
1:X:2779:C:H2'	1:X:2780:A:O4'	2.21	0.40
1:X:2848:G:H2'	1:X:2849:A:H8	1.86	0.40
2:Y:8:A:C2	2:Y:108:G:H8	2.39	0.40
4:B:182:ASN:O	4:B:183:LEU:HD12	2.22	0.40
5:C:64:PRO:HB2	5:C:65:TRP:CE3	2.56	0.40
6:D:70:ALA:HB2	6:D:85:ILE:HD12	2.03	0.40
13:L:39:HIS:C	13:L:40:ILE:HD12	2.42	0.40
13:L:65:THR:O	13:L:69:LYS:N	2.49	0.40
19:R:66:SER:N	19:R:67:ASN:OD1	2.55	0.40
19:R:86:VAL:O	19:R:88:GLY:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
3	A	258/277 (93%)	189 (73%)	47 (18%)	22 (8%)	1 8
4	B	213/220 (97%)	180 (84%)	22 (10%)	11 (5%)	2 17
5	C	196/207 (95%)	147 (75%)	30 (15%)	19 (10%)	0 6
6	D	133/179 (74%)	115 (86%)	14 (10%)	4 (3%)	4 29
7	E	141/178 (79%)	79 (56%)	35 (25%)	27 (19%)	0 1
8	G	140/145 (97%)	127 (91%)	9 (6%)	4 (3%)	4 30
9	H	120/122 (98%)	110 (92%)	8 (7%)	2 (2%)	9 41
10	I	125/140 (89%)	65 (52%)	34 (27%)	26 (21%)	0 1
11	J	136/144 (94%)	121 (89%)	11 (8%)	4 (3%)	4 30
12	K	117/122 (96%)	105 (90%)	7 (6%)	5 (4%)	2 21
13	L	108/119 (91%)	83 (77%)	15 (14%)	10 (9%)	0 7
14	M	109/116 (94%)	88 (81%)	14 (13%)	7 (6%)	1 13
15	N	114/118 (97%)	111 (97%)	2 (2%)	1 (1%)	17 54
16	O	99/102 (97%)	81 (82%)	14 (14%)	4 (4%)	3 23
17	P	110/117 (94%)	103 (94%)	6 (6%)	1 (1%)	17 54
18	Q	88/91 (97%)	75 (85%)	12 (14%)	1 (1%)	14 50
19	R	100/105 (95%)	71 (71%)	19 (19%)	10 (10%)	0 6
20	S	172/217 (79%)	133 (77%)	25 (14%)	14 (8%)	1 9
21	T	74/94 (79%)	61 (82%)	11 (15%)	2 (3%)	5 32
22	V	63/69 (91%)	59 (94%)	3 (5%)	1 (2%)	9 42
23	W	55/59 (93%)	52 (94%)	3 (6%)	0	100 100
24	Z	42/58 (72%)	37 (88%)	4 (10%)	1 (2%)	6 34
25	2	42/45 (93%)	39 (93%)	2 (5%)	1 (2%)	6 34
26	3	63/66 (96%)	49 (78%)	11 (18%)	3 (5%)	2 19
All	All	2818/3110 (91%)	2280 (81%)	358 (13%)	180 (6%)	1 13

All (180) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	35	LYS
3	A	36	PRO
3	A	38	PRO
3	A	51	VAL
3	A	77	LYS
3	A	78	VAL
3	A	124	ILE
3	A	248	SER
3	A	253	PRO
4	B	61	LYS
4	B	101	VAL
4	B	176	ASN
5	C	29	ASN
5	C	52	LYS
5	C	55	SER
5	C	67	GLN
5	C	127	ASP
6	D	19	LYS
7	E	33	LEU
7	E	52	VAL
7	E	53	VAL
7	E	79	VAL
7	E	90	VAL
7	E	106	ASN
7	E	107	VAL
7	E	141	VAL
7	E	156	PRO
8	G	10	SER
8	G	138	PRO
9	H	89	ASP
9	H	113	LYS
10	I	27	ASN
10	I	44	GLY
10	I	46	VAL
10	I	48	PRO
10	I	56	PRO
10	I	57	LEU
10	I	62	PRO
10	I	76	ILE
10	I	99	SER
14	M	34	ILE
14	M	109	ALA

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Mol	Chain	Res	Type
16	O	50	ALA
19	R	47	PRO
19	R	67	ASN
20	S	140	ALA
3	A	126	VAL
3	A	197	ASN
3	A	233	GLY
4	B	94	VAL
4	B	160	ALA
4	B	204	PRO
5	C	24	PHE
5	C	26	ILE
5	C	28	PRO
5	C	126	VAL
5	C	173	VAL
7	E	50	ILE
7	E	55	PRO
7	E	56	SER
7	E	59	LYS
7	E	95	ARG
7	E	124	SER
7	E	154	PRO
8	G	41	ASN
10	I	25	THR
10	I	63	LYS
10	I	81	GLN
10	I	100	GLY
10	I	123	VAL
11	J	20	ARG
13	L	5	ILE
13	L	20	THR
13	L	22	LEU
14	M	36	GLU
15	N	92	ARG
16	O	3	ALA
16	O	69	LYS
19	R	18	GLY
19	R	19	LYS
19	R	98	GLY
20	S	38	ASN
20	S	55	VAL
20	S	66	GLY

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Mol	Chain	Res	Type
20	S	148	LEU
22	V	6	ILE
26	3	23	LYS
3	A	107	PRO
3	A	236	GLU
3	A	252	LYS
4	B	157	ALA
4	B	161	SER
4	B	205	LYS
5	C	54	ARG
5	C	144	SER
5	C	149	PRO
5	C	178	ALA
6	D	80	ARG
6	D	114	PHE
7	E	32	GLU
7	E	45	GLN
7	E	102	ASP
7	E	121	ILE
10	I	13	ARG
10	I	68	ASN
10	I	75	ALA
12	K	75	ASP
12	K	78	THR
12	K	79	GLN
13	L	42	ALA
13	L	99	TYR
14	M	59	GLU
19	R	49	GLN
19	R	50	LEU
20	S	10	GLN
20	S	68	LYS
20	S	104	VAL
20	S	139	GLU
21	T	82	ARG
21	T	84	LYS
26	3	15	LYS
3	A	44	ASN
5	C	120	GLU
5	C	130	ASN
7	E	46	GLU
7	E	96	ALA

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Mol	Chain	Res	Type
7	E	139	GLU
7	E	164	TYR
8	G	132	PRO
10	I	42	SER
10	I	72	LYS
10	I	124	LYS
11	J	14	ARG
11	J	73	PRO
11	J	101	ARG
13	L	92	ILE
16	O	44	ASP
18	Q	30	ASP
20	S	132	ALA
20	S	136	ASN
24	Z	32	ASN
3	A	191	THR
3	A	217	ARG
5	C	131	PHE
6	D	93	GLY
7	E	138	LYS
7	E	168	TYR
10	I	97	VAL
10	I	110	LYS
12	K	28	GLU
12	K	88	GLU
13	L	27	GLU
13	L	62	ASP
13	L	106	LYS
19	R	15	LYS
26	3	16	ARG
3	A	150	LYS
3	A	241	ILE
4	B	186	VAL
5	C	58	SER
10	I	91	VAL
13	L	24	GLY
14	M	23	ARG
14	M	112	ILE
17	P	110	GLY
20	S	119	GLY
20	S	151	ASN
4	B	174	GLY

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Mol	Chain	Res	Type
7	E	26	VAL
19	R	78	PRO
10	I	52	GLY
3	A	220	VAL
19	R	65	VAL
20	S	145	ILE
25	2	16	VAL
3	A	112	VAL
5	C	15	GLY
10	I	69	ILE
10	I	77	VAL
14	M	20	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
3	A	125/224 (56%)	93 (74%)	32 (26%)	0 2
4	B	146/177 (82%)	119 (82%)	27 (18%)	1 7
5	C	118/169 (70%)	92 (78%)	26 (22%)	1 4
6	D	78/158 (49%)	61 (78%)	17 (22%)	1 4
7	E	26/155 (17%)	20 (77%)	6 (23%)	1 3
8	G	103/123 (84%)	86 (84%)	17 (16%)	2 11
9	H	95/100 (95%)	74 (78%)	21 (22%)	1 4
10	I	51/108 (47%)	36 (71%)	15 (29%)	0 2
11	J	92/119 (77%)	78 (85%)	14 (15%)	3 15
12	K	84/102 (82%)	69 (82%)	15 (18%)	2 8
13	L	40/95 (42%)	31 (78%)	9 (22%)	1 3
14	M	68/102 (67%)	52 (76%)	16 (24%)	1 3
15	N	95/98 (97%)	81 (85%)	14 (15%)	3 16
16	O	56/86 (65%)	41 (73%)	15 (27%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	P	89/94 (95%)	77 (86%)	12 (14%)	4 19
18	Q	64/82 (78%)	48 (75%)	16 (25%)	0 3
19	R	36/90 (40%)	28 (78%)	8 (22%)	1 4
20	S	91/190 (48%)	71 (78%)	20 (22%)	1 4
21	T	53/75 (71%)	46 (87%)	7 (13%)	4 20
22	V	55/62 (89%)	38 (69%)	17 (31%)	0 2
23	W	50/53 (94%)	40 (80%)	10 (20%)	1 5
24	Z	35/51 (69%)	27 (77%)	8 (23%)	1 3
25	2	37/40 (92%)	31 (84%)	6 (16%)	2 12
26	3	26/57 (46%)	23 (88%)	3 (12%)	5 25
All	All	1713/2610 (66%)	1362 (80%)	351 (20%)	1 5

All (351) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	17	THR
3	A	26	LYS
3	A	27	THR
3	A	28	THR
3	A	30	GLU
3	A	31	LYS
3	A	43	ARG
3	A	45	ASN
3	A	46	GLN
3	A	48	LYS
3	A	65	ILE
3	A	83	TYR
3	A	114	GLN
3	A	115	ILE
3	A	116	VAL
3	A	133	GLN
3	A	143	ASN
3	A	163	GLN
3	A	176	LEU
3	A	183	MET
3	A	184	ILE
3	A	185	LEU
3	A	199	GLN

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Mol	Chain	Res	Type
3	A	204	ASN
3	A	214	LYS
3	A	216	ILE
3	A	219	THR
3	A	229	ASP
3	A	230	HIS
3	A	258	LYS
3	A	259	THR
3	A	267	ASP
4	B	2	THR
4	B	13	THR
4	B	25	VAL
4	B	33	ASN
4	B	40	THR
4	B	44	ASP
4	B	57	LYS
4	B	62	ASP
4	B	64	LYS
4	B	65	SER
4	B	71	LYS
4	B	74	GLU
4	B	78	LYS
4	B	88	ILE
4	B	111	VAL
4	B	115	VAL
4	B	116	ILE
4	B	119	THR
4	B	149	ARG
4	B	162	ARG
4	B	172	ARG
4	B	180	VAL
4	B	190	THR
4	B	195	ILE
4	B	196	LEU
4	B	198	LYS
4	B	208	LEU
5	C	4	TYR
5	C	5	ASP
5	C	13	LYS
5	C	14	SER
5	C	16	SER
5	C	18	GLU

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Mol	Chain	Res	Type
5	C	19	LEU
5	C	40	GLN
5	C	51	VAL
5	C	67	GLN
5	C	70	THR
5	C	88	ILE
5	C	89	VAL
5	C	108	LEU
5	C	110	LEU
5	C	112	SER
5	C	144	SER
5	C	145	THR
5	C	152	VAL
5	C	153	LEU
5	C	158	ASN
5	C	160	ASP
5	C	162	ASN
5	C	175	VAL
5	C	179	GLN
5	C	186	ILE
6	D	15	ASN
6	D	20	PHE
6	D	21	ASN
6	D	25	VAL
6	D	33	LYS
6	D	34	ILE
6	D	42	ASP
6	D	44	VAL
6	D	45	GLN
6	D	59	LEU
6	D	66	LEU
6	D	79	LEU
6	D	80	ARG
6	D	92	ARG
6	D	156	ILE
6	D	164	GLU
6	D	169	LEU
7	E	63	THR
7	E	84	VAL
7	E	89	LEU
7	E	146	SER
7	E	162	ILE

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Mol	Chain	Res	Type
7	E	163	ARG
8	G	1	MET
8	G	2	ARG
8	G	3	GLN
8	G	14	ARG
8	G	29	LEU
8	G	38	ARG
8	G	43	VAL
8	G	44	THR
8	G	61	SER
8	G	64	GLU
8	G	92	GLU
8	G	93	LEU
8	G	112	SER
8	G	117	GLU
8	G	119	GLN
8	G	133	HIS
8	G	140	ASN
9	H	3	GLN
9	H	8	LEU
9	H	9	LYS
9	H	10	VAL
9	H	21	THR
9	H	23	LYS
9	H	32	THR
9	H	34	ASN
9	H	35	ILE
9	H	42	THR
9	H	52	VAL
9	H	58	VAL
9	H	66	LYS
9	H	69	VAL
9	H	73	ASP
9	H	77	ILE
9	H	80	ASP
9	H	91	LYS
9	H	97	ARG
9	H	114	ILE
9	H	116	SER
10	I	2	LYS
10	I	5	GLU
10	I	16	ARG

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Mol	Chain	Res	Type
10	I	21	ARG
10	I	31	SER
10	I	33	ARG
10	I	48	PRO
10	I	67	THR
10	I	72	LYS
10	I	79	LEU
10	I	87	ASP
10	I	90	GLU
10	I	104	ASN
10	I	109	ILE
10	I	122	THR
11	J	12	GLN
11	J	39	THR
11	J	41	TRP
11	J	58	MET
11	J	72	THR
11	J	75	THR
11	J	87	LYS
11	J	96	VAL
11	J	112	GLU
11	J	120	LEU
11	J	122	SER
11	J	128	LYS
11	J	129	THR
11	J	137	LEU
12	K	6	LEU
12	K	8	ARG
12	K	9	THR
12	K	10	SER
12	K	11	ASP
12	K	25	ILE
12	K	34	GLU
12	K	48	ILE
12	K	56	LEU
12	K	65	THR
12	K	67	ARG
12	K	94	THR
12	K	101	THR
12	K	109	ARG
12	K	121	LEU
13	L	8	ASN

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Mol	Chain	Res	Type
13	L	37	ASN
13	L	52	THR
13	L	53	LEU
13	L	58	SER
13	L	63	ILE
13	L	65	THR
13	L	96	ARG
13	L	101	TYR
14	M	5	LYS
14	M	14	GLN
14	M	17	THR
14	M	31	HIS
14	M	32	VAL
14	M	43	GLN
14	M	44	VAL
14	M	51	LYS
14	M	52	ARG
14	M	58	SER
14	M	60	THR
14	M	65	LYS
14	M	67	SER
14	M	75	THR
14	M	80	THR
14	M	95	ARG
15	N	10	THR
15	N	19	LYS
15	N	22	LYS
15	N	30	THR
15	N	42	SER
15	N	48	ARG
15	N	51	ARG
15	N	55	ARG
15	N	59	LYS
15	N	65	ILE
15	N	70	ARG
15	N	79	LEU
15	N	108	GLN
15	N	115	ASP
16	O	2	PHE
16	O	6	GLU
16	O	18	GLN
16	O	22	VAL

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Mol	Chain	Res	Type
16	O	29	GLU
16	O	33	PHE
16	O	38	VAL
16	O	39	LEU
16	O	61	THR
16	O	67	ARG
16	O	78	ARG
16	O	83	LYS
16	O	84	ARG
16	O	95	LEU
16	O	96	THR
17	P	43	SER
17	P	59	GLU
17	P	65	ASN
17	P	66	THR
17	P	67	ASP
17	P	82	LEU
17	P	86	ARG
17	P	98	LYS
17	P	101	SER
17	P	105	ILE
17	P	109	ASP
17	P	111	LYS
18	Q	5	ASP
18	Q	9	ARG
18	Q	13	THR
18	Q	29	VAL
18	Q	33	VAL
18	Q	52	SER
18	Q	53	VAL
18	Q	57	ASN
18	Q	68	TYR
18	Q	76	ARG
18	Q	79	ILE
18	Q	80	VAL
18	Q	81	THR
18	Q	82	LEU
18	Q	88	ASP
18	Q	89	LEU
19	R	11	VAL
19	R	26	THR
19	R	42	LYS

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Mol	Chain	Res	Type
19	R	59	THR
19	R	60	GLU
19	R	68	VAL
19	R	76	ASN
19	R	79	THR
20	S	3	SER
20	S	9	ARG
20	S	13	GLN
20	S	14	THR
20	S	15	ARG
20	S	26	LYS
20	S	27	VAL
20	S	30	VAL
20	S	61	ILE
20	S	62	GLU
20	S	72	VAL
20	S	87	THR
20	S	100	ARG
20	S	102	VAL
20	S	121	VAL
20	S	122	GLU
20	S	125	LEU
20	S	127	ASN
20	S	162	THR
20	S	167	ILE
21	T	19	LYS
21	T	27	LYS
21	T	40	THR
21	T	48	GLN
21	T	57	GLU
21	T	64	ASP
21	T	75	VAL
22	V	4	LYS
22	V	7	ARG
22	V	9	LEU
22	V	16	GLU
22	V	25	LEU
22	V	26	PHE
22	V	32	LEU
22	V	37	LEU
22	V	38	GLU
22	V	43	ILE

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Mol	Chain	Res	Type
22	V	45	THR
22	V	47	ARG
22	V	49	THR
22	V	52	ARG
22	V	56	VAL
22	V	60	ARG
22	V	61	GLU
23	W	3	LYS
23	W	4	LEU
23	W	5	GLN
23	W	6	ILE
23	W	12	VAL
23	W	15	ARG
23	W	26	LEU
23	W	33	SER
23	W	40	ASN
23	W	51	LYS
24	Z	3	VAL
24	Z	6	ARG
24	Z	7	ARG
24	Z	11	THR
24	Z	22	ILE
24	Z	24	VAL
24	Z	27	MET
24	Z	40	SER
25	2	5	THR
25	2	11	ARG
25	2	21	LYS
25	2	25	THR
25	2	27	ASN
25	2	43	LEU
26	3	32	LEU
26	3	49	LEU
26	3	53	SER

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

Mol	Chain	Res	Type
8	G	3	GLN
10	I	78	ASN
14	M	79	HIS
18	Q	91	ASN

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Mol	Chain	Res	Type
20	S	38	ASN
20	S	78	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2690/2923 (92%)	711 (26%)	31 (1%)
2	Y	113/114 (99%)	17 (15%)	0
All	All	2803/3037 (92%)	728 (25%)	31 (1%)

All (728) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	12	U
1	X	15	G
1	X	34	U
1	X	35	G
1	X	39	C
1	X	60	U
1	X	63	U
1	X	64	A
1	X	67	G
1	X	70	G
1	X	71	A
1	X	75	G
1	X	80	G
1	X	90	A
1	X	91	A
1	X	96	G
1	X	101	G
1	X	102	A
1	X	109	G
1	X	111	U
1	X	113	U
1	X	117	A
1	X	118	A
1	X	119	U
1	X	120	G
1	X	124	A
1	X	130	A
1	X	133	A

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Mol	Chain	Res	Type
1	X	134	U
1	X	136	A
1	X	139	U
1	X	140	A
1	X	144	C
1	X	152	C
1	X	154	A
1	X	157	U
1	X	163	U
1	X	164	A
1	X	165	C
1	X	166	A
1	X	167	U
1	X	168	A
1	X	169	G
1	X	170	C
1	X	172	U
1	X	173	A
1	X	175	C
1	X	176	A
1	X	178	A
1	X	179	A
1	X	180	G
1	X	182	C
1	X	183	A
1	X	184	C
1	X	199	A
1	X	202	A
1	X	207	A
1	X	217	G
1	X	219	A
1	X	225	A
1	X	229	A
1	X	230	A
1	X	232	U
1	X	233	U
1	X	235	G
1	X	247	A
1	X	248	G
1	X	251	G
1	X	255	G
1	X	268	A

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Mol	Chain	Res	Type
1	X	282	A
1	X	284	C
1	X	285	U
1	X	286	U
1	X	287	G
1	X	288	C
1	X	290	U
1	X	291	G
1	X	293	U
1	X	298	U
1	X	299	U
1	X	300	G
1	X	303	G
1	X	308	C
1	X	310	C
1	X	311	U
1	X	313	U
1	X	319	G
1	X	320	U
1	X	321	U
1	X	322	A
1	X	323	C
1	X	328	G
1	X	329	A
1	X	330	C
1	X	331	G
1	X	332	A
1	X	338	G
1	X	342	A
1	X	344	U
1	X	345	C
1	X	354	A
1	X	363	A
1	X	364	A
1	X	372	A
1	X	373	A
1	X	375	A
1	X	376	A
1	X	382	U
1	X	386	C
1	X	388	A
1	X	389	A

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Mol	Chain	Res	Type
1	X	390	A
1	X	392	U
1	X	394	U
1	X	395	U
1	X	399	U
1	X	401	U
1	X	403	U
1	X	404	U
1	X	405	G
1	X	406	A
1	X	412	U
1	X	413	C
1	X	416	G
1	X	417	A
1	X	418	G
1	X	426	G
1	X	432	G
1	X	440	C
1	X	444	C
1	X	447	A
1	X	448	A
1	X	449	U
1	X	450	C
1	X	451	U
1	X	452	G
1	X	457	G
1	X	466	C
1	X	470	G
1	X	474	A
1	X	497	U
1	X	503	A
1	X	504	G
1	X	506	A
1	X	523	A
1	X	525	A
1	X	526	A
1	X	527	G
1	X	539	G
1	X	543	G
1	X	549	U
1	X	550	A
1	X	553	A

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Mol	Chain	Res	Type
1	X	554	C
1	X	555	C
1	X	567	G
1	X	572	C
1	X	576	U
1	X	577	A
1	X	578	G
1	X	583	A
1	X	590	U
1	X	592	A
1	X	593	U
1	X	594	G
1	X	606	G
1	X	612	U
1	X	615	A
1	X	616	G
1	X	618	A
1	X	629	A
1	X	644	C
1	X	646	A
1	X	647	G
1	X	658	A
1	X	659	A
1	X	660	A
1	X	661	U
1	X	665	G
1	X	667	G
1	X	679	G
1	X	682	A
1	X	683	G
1	X	690	U
1	X	691	A
1	X	698	U
1	X	699	U
1	X	700	A
1	X	713	A
1	X	716	C
1	X	722	A
1	X	726	G
1	X	727	G
1	X	731	U
1	X	734	A

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Mol	Chain	Res	Type
1	X	738	U
1	X	740	G
1	X	744	A
1	X	749	G
1	X	755	C
1	X	757	G
1	X	765	U
1	X	766	G
1	X	767	A
1	X	768	A
1	X	772	A
1	X	773	G
1	X	774	G
1	X	775	A
1	X	776	C
1	X	783	G
1	X	784	A
1	X	785	C
1	X	792	U
1	X	793	G
1	X	802	G
1	X	807	U
1	X	809	A
1	X	813	G
1	X	814	A
1	X	820	G
1	X	822	G
1	X	827	A
1	X	829	U
1	X	830	U
1	X	835	U
1	X	836	C
1	X	837	G
1	X	838	A
1	X	845	A
1	X	850	G
1	X	851	C
1	X	857	C
1	X	864	A
1	X	866	A
1	X	872	U
1	X	873	U

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Mol	Chain	Res	Type
1	X	875	G
1	X	890	G
1	X	891	A
1	X	921	C
1	X	922	G
1	X	923	A
1	X	924	G
1	X	925	G
1	X	926	G
1	X	938	G
1	X	940	U
1	X	942	C
1	X	943	C
1	X	947	U
1	X	955	A
1	X	959	C
1	X	969	A
1	X	970	U
1	X	971	U
1	X	977	A
1	X	985	A
1	X	986	G
1	X	987	U
1	X	988	C
1	X	989	A
1	X	990	G
1	X	1001	A
1	X	1005	G
1	X	1017	A
1	X	1018	A
1	X	1027	A
1	X	1029	C
1	X	1033	G
1	X	1034	A
1	X	1040	A
1	X	1043	U
1	X	1049	C
1	X	1052	A
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1064	A

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Mol	Chain	Res	Type
1	X	1066	G
1	X	1067	U
1	X	1069	G
1	X	1070	A
1	X	1077	U
1	X	1078	G
1	X	1085	U
1	X	1086	G
1	X	1087	C
1	X	1089	C
1	X	1090	A
1	X	1091	G
1	X	1092	A
1	X	1093	C
1	X	1098	A
1	X	1145	U
1	X	1146	C
1	X	1147	A
1	X	1150	A
1	X	1151	G
1	X	1152	U
1	X	1154	G
1	X	1155	A
1	X	1156	G
1	X	1172	A
1	X	1174	U
1	X	1176	U
1	X	1178	C
1	X	1185	U
1	X	1186	A
1	X	1187	A
1	X	1195	A
1	X	1200	A
1	X	1202	C
1	X	1213	C
1	X	1214	C
1	X	1215	U
1	X	1218	G
1	X	1220	A
1	X	1221	C
1	X	1248	U
1	X	1262	U

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Mol	Chain	Res	Type
1	X	1274	G
1	X	1275	A
1	X	1278	G
1	X	1285	A
1	X	1286	G
1	X	1291	A
1	X	1293	U
1	X	1294	G
1	X	1303	A
1	X	1309	G
1	X	1310	A
1	X	1313	G
1	X	1323	A
1	X	1324	A
1	X	1337	A
1	X	1338	U
1	X	1340	G
1	X	1349	U
1	X	1358	A
1	X	1365	G
1	X	1366	U
1	X	1379	A
1	X	1389	U
1	X	1395	G
1	X	1397	G
1	X	1398	G
1	X	1401	G
1	X	1402	A
1	X	1403	C
1	X	1405	G
1	X	1415	A
1	X	1416	U
1	X	1421	A
1	X	1422	A
1	X	1424	A
1	X	1431	U
1	X	1432	A
1	X	1433	U
1	X	1435	C
1	X	1437	U
1	X	1440	A
1	X	1449	A

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Mol	Chain	Res	Type
1	X	1450	A
1	X	1451	U
1	X	1453	G
1	X	1454	U
1	X	1459	A
1	X	1460	U
1	X	1463	A
1	X	1464	U
1	X	1465	G
1	X	1466	G
1	X	1467	G
1	X	1468	G
1	X	1469	G
1	X	1470	G
1	X	1471	A
1	X	1472	C
1	X	1477	U
1	X	1480	G
1	X	1481	A
1	X	1487	G
1	X	1488	A
1	X	1489	A
1	X	1490	G
1	X	1491	C
1	X	1492	G
1	X	1493	U
1	X	1494	G
1	X	1495	C
1	X	1496	G
1	X	1499	U
1	X	1505	G
1	X	1508	C
1	X	1509	G
1	X	1510	U
1	X	1511	C
1	X	1515	G
1	X	1516	C
1	X	1519	U
1	X	1520	A
1	X	1521	A
1	X	1524	C
1	X	1525	U

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Mol	Chain	Res	Type
1	X	1526	G
1	X	1527	A
1	X	1529	U
1	X	1540	U
1	X	1541	C
1	X	1542	C
1	X	1543	G
1	X	1544	G
1	X	1546	A
1	X	1547	C
1	X	1548	U
1	X	1549	C
1	X	1550	G
1	X	1555	G
1	X	1556	G
1	X	1557	C
1	X	1560	A
1	X	1567	A
1	X	1570	G
1	X	1575	A
1	X	1592	A
1	X	1593	G
1	X	1594	U
1	X	1599	G
1	X	1602	U
1	X	1603	U
1	X	1605	A
1	X	1606	C
1	X	1613	G
1	X	1614	A
1	X	1616	A
1	X	1623	U
1	X	1625	U
1	X	1628	A
1	X	1630	A
1	X	1631	G
1	X	1636	U
1	X	1637	A
1	X	1638	G
1	X	1651	C
1	X	1652	A
1	X	1653	A

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Mol	Chain	Res	Type
1	X	1654	A
1	X	1657	G
1	X	1662	A
1	X	1663	G
1	X	1683	U
1	X	1684	A
1	X	1690	A
1	X	1691	G
1	X	1692	C
1	X	1709	A
1	X	1713	A
1	X	1718	G
1	X	1719	C
1	X	1737	U
1	X	1738	C
1	X	1740	G
1	X	1744	A
1	X	1745	A
1	X	1748	G
1	X	1756	U
1	X	1757	U
1	X	1760	G
1	X	1761	G
1	X	1762	U
1	X	1763	U
1	X	1765	A
1	X	1766	C
1	X	1767	G
1	X	1768	C
1	X	1770	C
1	X	1771	A
1	X	1772	G
1	X	1789	A
1	X	1790	G
1	X	1791	G
1	X	1800	A
1	X	1803	G
1	X	1808	U
1	X	1818	A
1	X	1826	G
1	X	1827	C
1	X	1835	U

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Mol	Chain	Res	Type
1	X	1836	A
1	X	1837	A
1	X	1843	U
1	X	1845	U
1	X	1846	A
1	X	1847	U
1	X	1848	A
1	X	1856	A
1	X	1860	C
1	X	1865	C
1	X	1866	G
1	X	1886	A
1	X	1901	C
1	X	1902	G
1	X	1903	A
1	X	1908	A
1	X	1909	C
1	X	1911	A
1	X	1912	A
1	X	1926	A
1	X	1930	G
1	X	1932	C
1	X	1933	G
1	X	1934	G
1	X	1935	C
1	X	1936	C
1	X	1954	A
1	X	1955	A
1	X	1956	G
1	X	1957	G
1	X	1964	A
1	X	1965	A
1	X	1982	U
1	X	1990	C
1	X	1991	G
1	X	1993	A
1	X	1994	C
1	X	1997	A
1	X	1998	A
1	X	1999	G
1	X	2003	U
1	X	2009	U

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Mol	Chain	Res	Type
1	X	2019	G
1	X	2020	U
1	X	2024	A
1	X	2041	A
1	X	2045	A
1	X	2046	U
1	X	2050	A
1	X	2054	G
1	X	2058	A
1	X	2059	G
1	X	2060	A
1	X	2070	C
1	X	2077	C
1	X	2079	G
1	X	2082	C
1	X	2083	G
1	X	2087	A
1	X	2088	G
1	X	2094	G
1	X	2096	G
1	X	2107	G
1	X	2117	A
1	X	2119	U
1	X	2124	U
1	X	2125	U
1	X	2126	C
1	X	2217	G
1	X	2219	C
1	X	2221	U
1	X	2224	U
1	X	2225	A
1	X	2229	C
1	X	2230	G
1	X	2231	C
1	X	2232	A
1	X	2233	C
1	X	2236	C
1	X	2237	U
1	X	2238	U
1	X	2239	A
1	X	2240	U
1	X	2241	C

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Mol	Chain	Res	Type
1	X	2244	G
1	X	2246	U
1	X	2252	A
1	X	2262	G
1	X	2265	G
1	X	2266	G
1	X	2270	U
1	X	2295	A
1	X	2298	G
1	X	2306	G
1	X	2310	C
1	X	2315	A
1	X	2326	G
1	X	2332	U
1	X	2333	U
1	X	2334	G
1	X	2335	G
1	X	2336	A
1	X	2338	A
1	X	2347	A
1	X	2348	G
1	X	2352	G
1	X	2361	U
1	X	2362	A
1	X	2363	A
1	X	2372	G
1	X	2374	C
1	X	2377	C
1	X	2386	C
1	X	2393	A
1	X	2398	G
1	X	2399	G
1	X	2409	G
1	X	2410	G
1	X	2411	A
1	X	2412	C
1	X	2418	G
1	X	2429	U
1	X	2433	C
1	X	2434	A
1	X	2450	U
1	X	2452	A

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Mol	Chain	Res	Type
1	X	2456	G
1	X	2457	A
1	X	2459	A
1	X	2462	A
1	X	2468	C
1	X	2473	G
1	X	2475	A
1	X	2485	U
1	X	2486	A
1	X	2492	C
1	X	2495	A
1	X	2497	G
1	X	2500	U
1	X	2503	A
1	X	2504	C
1	X	2514	G
1	X	2529	G
1	X	2532	G
1	X	2533	U
1	X	2534	C
1	X	2540	A
1	X	2545	A
1	X	2546	U
1	X	2547	C
1	X	2556	G
1	X	2561	C
1	X	2574	U
1	X	2576	G
1	X	2581	U
1	X	2590	U
1	X	2591	A
1	X	2593	A
1	X	2594	G
1	X	2600	C
1	X	2603	G
1	X	2605	G
1	X	2609	G
1	X	2612	U
1	X	2628	C
1	X	2629	A
1	X	2636	U
1	X	2640	U

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Mol	Chain	Res	Type
1	X	2641	A
1	X	2642	U
1	X	2656	A
1	X	2657	G
1	X	2663	U
1	X	2664	U
1	X	2682	G
1	X	2683	U
1	X	2687	A
1	X	2696	G
1	X	2698	A
1	X	2709	U
1	X	2712	G
1	X	2715	G
1	X	2716	U
1	X	2717	A
1	X	2734	C
1	X	2740	A
1	X	2741	G
1	X	2751	U
1	X	2753	U
1	X	2760	A
1	X	2766	U
1	X	2771	G
1	X	2778	G
1	X	2784	A
1	X	2787	C
1	X	2792	A
1	X	2793	G
1	X	2805	A
1	X	2806	U
1	X	2807	G
1	X	2817	A
1	X	2818	A
1	X	2820	U
1	X	2821	U
1	X	2824	G
1	X	2827	A
1	X	2828	U
1	X	2832	A
1	X	2850	G
1	X	2853	U

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Mol	Chain	Res	Type
1	X	2855	A
1	X	2856	U
1	X	2863	G
1	X	2877	G
1	X	2884	G
1	X	2887	G
1	X	2899	A
1	X	2900	C
1	X	2903	A
1	X	2913	G
1	X	2921	C
2	Y	10	U
2	Y	23	U
2	Y	24	C
2	Y	34	C
2	Y	35	C
2	Y	39	G
2	Y	42	G
2	Y	43	A
2	Y	50	A
2	Y	54	U
2	Y	55	A
2	Y	74	G
2	Y	84	U
2	Y	87	G
2	Y	88	U
2	Y	106	U
2	Y	108	G

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	90	A
1	X	165	C
1	X	285	U
1	X	373	A
1	X	502	C
1	X	525	A
1	X	614	U
1	X	616	G
1	X	836	C
1	X	890	G

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Mol	Chain	Res	Type
1	X	1028	G
1	X	1091	G
1	X	1176	U
1	X	1310	A
1	X	1323	A
1	X	1488	A
1	X	1510	U
1	X	1520	A
1	X	1556	G
1	X	1636	U
1	X	1653	A
1	X	1885	G
1	X	1901	C
1	X	1963	A
1	X	2062	G
1	X	2087	A
1	X	2314	A
1	X	2433	C
1	X	2682	G
1	X	2783	U
1	X	2816	C

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 299 ligands modelled in this entry, 294 are monoatomic - leaving 5 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	$\#\|Z\|>2$
32	SPD	X	3286	-	9,9,9	0.34	0	8,8,8	0.30	0
27	95H	X	3001	-	25,28,28	1.86	5 (20%)	32,40,40	2.67	9 (28%)
28	MPD	X	3002	-	7,7,7	0.34	0	9,10,10	0.15	0
28	MPD	X	3003	-	7,7,7	1.65	1 (14%)	9,10,10	0.68	0
31	EPE	X	3285	-	15,15,15	0.54	0	18,20,20	0.74	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SPD	X	3286	-	-	0/7/7/7	-
27	95H	X	3001	-	-	5/20/42/42	0/2/2/2
28	MPD	X	3002	-	-	2/5/5/5	-
28	MPD	X	3003	-	-	1/5/5/5	-
31	EPE	X	3285	-	-	5/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	X	3001	95H	C12-N13	6.46	1.48	1.34
28	X	3003	MPD	C3-C2	3.80	1.64	1.53
27	X	3001	95H	C18-C12	-3.27	1.43	1.50
27	X	3001	95H	C21-N24	2.94	1.52	1.45
27	X	3001	95H	O10-C2	-2.55	1.37	1.43
27	X	3001	95H	C20-C21	2.53	1.43	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	X	3001	95H	C22-C21-N24	-9.15	112.49	119.38
27	X	3001	95H	C20-C21-N24	7.11	124.73	119.38
27	X	3001	95H	C20-C19-C18	-4.25	115.83	120.78
27	X	3001	95H	C23-C18-C19	4.03	124.32	118.59
27	X	3001	95H	C18-C12-N13	-3.05	111.21	117.06
27	X	3001	95H	O10-C2-C1	2.74	117.21	109.94
27	X	3001	95H	C23-C18-C12	-2.71	111.85	120.62
31	X	3285	EPE	O2S-S-C10	2.35	109.75	106.92
27	X	3001	95H	O10-C2-C3	-2.21	105.23	110.35
27	X	3001	95H	C23-C22-C21	-2.18	117.05	120.08

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	X	3001	95H	O6-C5-S16-C25
31	X	3285	EPE	C10-C9-N1-C6
31	X	3285	EPE	C9-C10-S-O2S
27	X	3001	95H	C18-C12-N13-C7
27	X	3001	95H	O11-C12-N13-C7
31	X	3285	EPE	C9-C10-S-O3S
31	X	3285	EPE	C10-C9-N1-C2
27	X	3001	95H	C20-C21-N24-O26
27	X	3001	95H	C22-C21-N24-O26
28	X	3003	MPD	C2-C3-C4-C5
31	X	3285	EPE	C9-C10-S-O1S
28	X	3002	MPD	C1-C2-C3-C4
28	X	3002	MPD	C2-C3-C4-O4

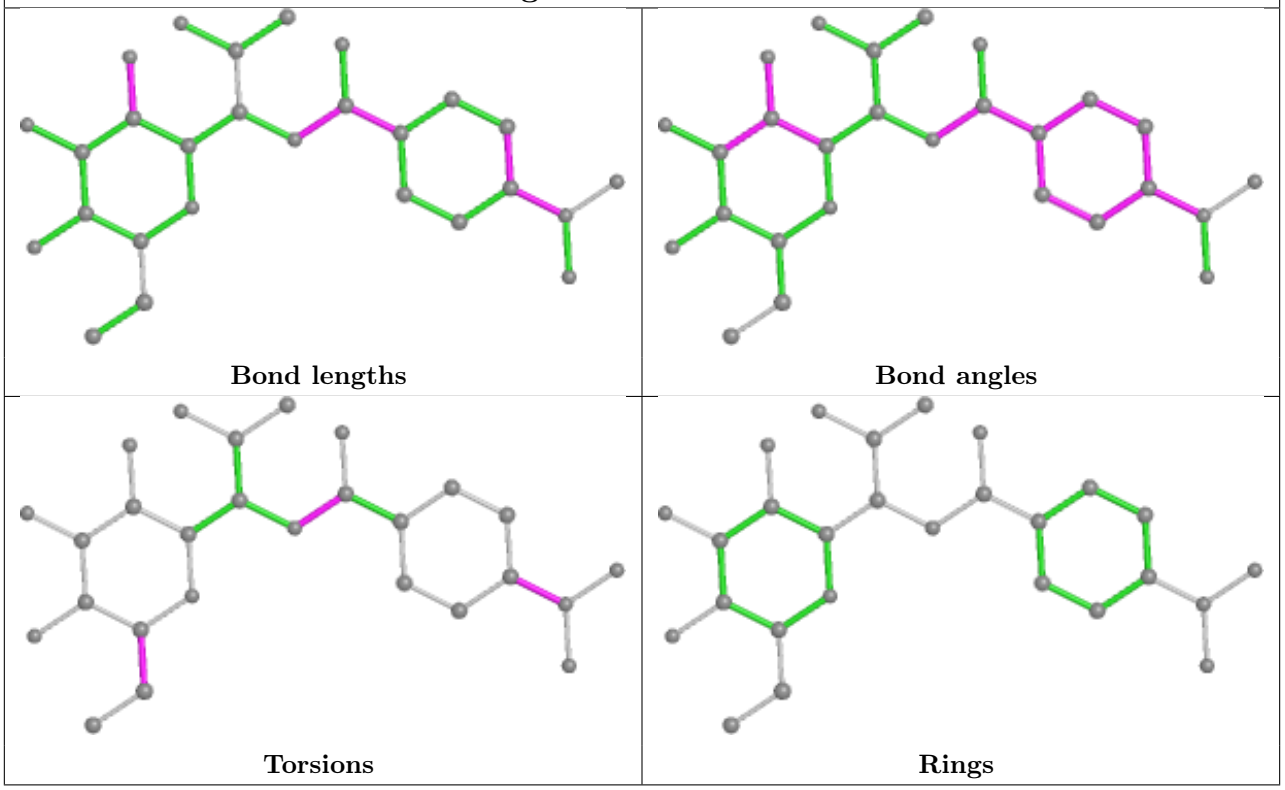
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3286	SPD	3	0
27	X	3001	95H	2	0
28	X	3002	MPD	1	0
28	X	3003	MPD	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 95H X 3001



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	J	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	69:PHE	C	70:PRO	N	1.16

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	X	2710/2923 (92%)	-0.12	30 (1%) 80 77	46, 97, 197, 300	0
2	Y	114/114 (100%)	0.10	2 (1%) 68 66	68, 128, 188, 250	0
3	A	260/277 (93%)	0.18	10 (3%) 40 39	87, 134, 168, 183	0
4	B	215/220 (97%)	-0.22	1 (0%) 91 89	50, 74, 96, 119	0
5	C	198/207 (95%)	-0.15	1 (0%) 91 89	63, 92, 113, 140	0
6	D	137/179 (76%)	1.23	33 (24%) 0 1	162, 186, 212, 219	0
7	E	147/178 (82%)	0.00	9 (6%) 21 23	122, 156, 181, 185	0
8	G	142/145 (97%)	-0.22	0 100 100	58, 70, 87, 95	0
9	H	122/122 (100%)	-0.03	0 100 100	75, 93, 118, 125	0
10	I	127/140 (90%)	0.25	7 (5%) 25 26	49, 108, 135, 139	0
11	J	138/144 (95%)	-0.05	1 (0%) 87 85	69, 89, 116, 141	0
12	K	119/122 (97%)	-0.15	0 100 100	63, 81, 115, 135	0
13	L	110/119 (92%)	0.26	9 (8%) 11 14	106, 120, 143, 152	0
14	M	111/116 (95%)	-0.02	2 (1%) 68 66	77, 91, 127, 151	0
15	N	116/118 (98%)	-0.18	0 100 100	49, 65, 90, 102	0
16	O	101/102 (99%)	-0.40	0 100 100	47, 79, 98, 115	0
17	P	112/117 (95%)	-0.00	0 100 100	59, 70, 103, 129	0
18	Q	90/91 (98%)	0.44	9 (10%) 7 9	100, 123, 152, 170	0
19	R	102/105 (97%)	0.30	10 (9%) 7 10	95, 115, 171, 180	0
20	S	174/217 (80%)	0.17	14 (8%) 12 15	75, 102, 184, 192	0
21	T	76/94 (80%)	0.00	1 (1%) 77 74	76, 88, 113, 155	0
22	V	65/69 (94%)	0.04	1 (1%) 73 71	119, 136, 160, 164	0
23	W	57/59 (96%)	0.22	0 100 100	59, 71, 95, 103	0
24	Z	44/58 (75%)	0.02	0 100 100	55, 86, 144, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	2	44/45 (97%)	1.09	7 (15%) 1 3	80, 89, 96, 104	0
26	3	65/66 (98%)	-0.02	1 (1%) 73 71	70, 81, 95, 100	0
All	All	5696/6147 (92%)	-0.01	148 (2%) 56 54	46, 96, 186, 300	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	D	73	SER	12.7
6	D	74	ILE	11.5
6	D	75	ALA	9.1
6	D	179	LYS	7.7
6	D	32	ASP	5.6
6	D	77	PHE	5.5
13	L	42	ALA	5.2
13	L	40	ILE	5.2
3	A	269	LEU	4.9
25	2	17	HIS	4.8
6	D	72	LYS	4.6
6	D	76	THR	4.6
6	D	170	LEU	4.5
6	D	69	LYS	4.5
19	R	68	VAL	4.4
6	D	163	ASP	4.4
13	L	56	ALA	4.3
20	S	100	ARG	4.3
6	D	178	ARG	4.3
6	D	116	GLY	4.2
3	A	259	THR	4.1
1	X	1150	A	3.8
6	D	31	ILE	3.8
20	S	124	PRO	3.6
19	R	70	LEU	3.6
3	A	273	GLY	3.6
18	Q	2	GLU	3.6
20	S	123	GLN	3.6
6	D	113	ASP	3.5
14	M	3	ASN	3.5
18	Q	70	GLY	3.4
6	D	87	ALA	3.4
18	Q	43	GLU	3.4
19	R	34	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	X	2505	A	3.3
7	E	171	ARG	3.2
20	S	125	LEU	3.2
25	2	22	ARG	3.2
1	X	1906	C	3.1
3	A	272	ARG	3.1
13	L	41	TYR	3.1
10	I	104	ASN	3.1
18	Q	9	ARG	3.1
19	R	67	ASN	3.0
1	X	1931	G	3.0
6	D	81	GLU	2.9
6	D	43	ALA	2.9
6	D	38	MET	2.9
1	X	311	U	2.9
6	D	67	VAL	2.9
19	R	69	GLN	2.9
20	S	119	GLY	2.9
18	Q	46	PHE	2.8
10	I	92	THR	2.8
10	I	91	VAL	2.8
1	X	2921	C	2.8
1	X	306	C	2.8
6	D	33	LYS	2.7
1	X	1993	A	2.7
18	Q	10	PRO	2.7
1	X	2503	A	2.7
1	X	1932	C	2.7
2	Y	1	U	2.7
20	S	128	LEU	2.7
25	2	2	VAL	2.7
3	A	93	LEU	2.7
20	S	169	ASN	2.7
20	S	101	THR	2.7
1	X	1957	G	2.7
1	X	275	A	2.6
19	R	78	PRO	2.6
7	E	153	PRO	2.6
6	D	79	LEU	2.6
18	Q	7	LEU	2.6
6	D	164	GLU	2.6
1	X	2408	C	2.6

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Mol	Chain	Res	Type	RSRZ
18	Q	28	ASP	2.6
20	S	144	ASP	2.6
25	2	18	GLY	2.6
1	X	1275	A	2.5
7	E	39	GLU	2.5
20	S	110	GLY	2.5
6	D	169	LEU	2.5
3	A	258	LYS	2.5
6	D	37	ASN	2.5
19	R	64	HIS	2.5
6	D	111	VAL	2.5
4	B	27	VAL	2.4
6	D	65	PRO	2.4
1	X	285	U	2.4
6	D	156	ILE	2.4
19	R	26	THR	2.4
19	R	15	LYS	2.4
7	E	80	SER	2.4
7	E	169	VAL	2.4
11	J	62	GLY	2.4
3	A	53	HIS	2.4
3	A	115	ILE	2.4
13	L	57	SER	2.4
25	2	14	SER	2.4
20	S	132	ALA	2.4
1	X	394	U	2.4
25	2	43	LEU	2.3
10	I	123	VAL	2.3
6	D	82	GLY	2.3
1	X	2501	U	2.3
3	A	113	GLY	2.3
2	Y	35	C	2.3
6	D	172	ASN	2.3
1	X	2502	C	2.3
10	I	95	LEU	2.3
7	E	162	ILE	2.3
13	L	107	ALA	2.3
1	X	2817	A	2.3
6	D	35	VAL	2.3
22	V	30	PHE	2.3
1	X	2335	G	2.2
21	T	22	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
10	I	93	PRO	2.2
10	I	111	ILE	2.2
1	X	2230	G	2.2
3	A	122	ALA	2.2
5	C	180	GLY	2.2
20	S	152	ASP	2.2
1	X	2498	A	2.2
1	X	453	G	2.2
20	S	131	THR	2.2
14	M	94	VAL	2.2
6	D	78	ARG	2.2
13	L	99	TYR	2.2
1	X	283	G	2.2
7	E	41	MET	2.1
25	2	16	VAL	2.1
13	L	31	LEU	2.1
1	X	2239	A	2.1
1	X	2409	G	2.1
1	X	454	G	2.1
13	L	102	HIS	2.1
7	E	161	GLY	2.1
6	D	61	THR	2.1
18	Q	47	ASN	2.1
1	X	310	C	2.1
1	X	284	C	2.1
19	R	12	ILE	2.0
7	E	172	LYS	2.0
20	S	92	LEU	2.0
26	3	2	PRO	2.0
1	X	406	A	2.0

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

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

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
30	MG	X	3255	1/1	-0.21	0.34	112,112,112,112	0
30	MG	J	201	1/1	0.17	2.12	107,107,107,107	0
30	MG	X	3268	1/1	0.21	0.31	134,134,134,134	0
30	MG	X	3240	1/1	0.28	0.30	87,87,87,87	0
29	MN	X	3145	1/1	0.37	0.32	144,144,144,144	0
30	MG	X	3224	1/1	0.38	0.28	97,97,97,97	0
30	MG	X	3271	1/1	0.42	0.67	90,90,90,90	0
30	MG	X	3246	1/1	0.43	0.27	131,131,131,131	0
30	MG	X	3261	1/1	0.46	0.36	163,163,163,163	0
30	MG	C	301	1/1	0.50	0.37	74,74,74,74	0
29	MN	X	3222	1/1	0.52	0.27	142,142,142,142	0
29	MN	X	3214	1/1	0.54	0.35	125,125,125,125	0
30	MG	X	3260	1/1	0.55	0.89	73,73,73,73	0
30	MG	X	3227	1/1	0.57	0.19	93,93,93,93	0
29	MN	X	3062	1/1	0.62	0.41	135,135,135,135	0
30	MG	X	3202	1/1	0.64	0.44	64,64,64,64	0
29	MN	X	3172	1/1	0.67	0.10	126,126,126,126	0
29	MN	X	3203	1/1	0.67	0.18	141,141,141,141	0
29	MN	X	3156	1/1	0.67	0.34	104,104,104,104	0
30	MG	X	3266	1/1	0.67	0.41	119,119,119,119	0
29	MN	X	3169	1/1	0.68	0.40	98,98,98,98	0
29	MN	X	3179	1/1	0.70	0.19	110,110,110,110	0
30	MG	X	3267	1/1	0.70	0.19	91,91,91,91	0
30	MG	X	3247	1/1	0.70	0.33	69,69,69,69	0
29	MN	X	3191	1/1	0.70	0.11	126,126,126,126	0
30	MG	X	3280	1/1	0.70	0.53	66,66,66,66	0
29	MN	X	3194	1/1	0.70	0.25	140,140,140,140	0
29	MN	X	3229	1/1	0.70	0.14	144,144,144,144	0
30	MG	3	104	1/1	0.70	0.47	56,56,56,56	0
29	MN	X	3234	1/1	0.71	0.22	137,137,137,137	0
29	MN	X	3075	1/1	0.73	0.45	102,102,102,102	0
29	MN	X	3142	1/1	0.73	0.11	111,111,111,111	0
30	MG	X	3283	1/1	0.73	0.42	59,59,59,59	0
29	MN	X	3187	1/1	0.74	0.15	112,112,112,112	0
30	MG	X	3242	1/1	0.74	0.41	60,60,60,60	0
29	MN	X	3141	1/1	0.74	0.29	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	3	101	1/1	0.74	0.21	96,96,96,96	0
29	MN	X	3205	1/1	0.75	0.13	143,143,143,143	0
29	MN	X	3231	1/1	0.75	0.17	125,125,125,125	0
30	MG	X	3265	1/1	0.75	0.24	73,73,73,73	0
30	MG	X	3274	1/1	0.76	0.86	69,69,69,69	0
30	MG	X	3181	1/1	0.76	0.36	89,89,89,89	0
30	MG	X	3279	1/1	0.77	0.54	66,66,66,66	0
29	MN	X	3131	1/1	0.77	0.35	114,114,114,114	0
30	MG	X	3257	1/1	0.77	0.04	156,156,156,156	0
30	MG	X	3112	1/1	0.78	0.38	84,84,84,84	0
30	MG	X	3228	1/1	0.78	0.24	65,65,65,65	0
30	MG	X	3264	1/1	0.78	0.47	102,102,102,102	0
29	MN	X	3198	1/1	0.80	0.34	100,100,100,100	0
29	MN	X	3171	1/1	0.80	0.18	117,117,117,117	0
29	MN	X	3092	1/1	0.81	0.24	87,87,87,87	0
30	MG	X	3276	1/1	0.81	0.82	67,67,67,67	0
30	MG	X	3196	1/1	0.81	0.50	78,78,78,78	0
29	MN	X	3096	1/1	0.81	0.46	98,98,98,98	0
30	MG	X	3204	1/1	0.81	0.28	67,67,67,67	0
29	MN	X	3189	1/1	0.81	0.14	123,123,123,123	0
29	MN	X	3051	1/1	0.81	0.22	100,100,100,100	0
29	MN	X	3150	1/1	0.81	0.22	98,98,98,98	0
29	MN	3	102	1/1	0.82	0.31	101,101,101,101	0
29	MN	X	3165	1/1	0.82	0.12	109,109,109,109	0
29	MN	X	3192	1/1	0.82	0.10	106,106,106,106	0
30	MG	X	3182	1/1	0.82	0.81	53,53,53,53	0
29	MN	X	3199	1/1	0.83	0.23	131,131,131,131	0
28	MPD	X	3003	8/8	0.83	0.30	80,80,80,80	0
29	MN	3	103	1/1	0.83	0.48	129,129,129,129	0
30	MG	X	3217	1/1	0.83	0.66	64,64,64,64	0
30	MG	X	3223	1/1	0.83	0.79	71,71,71,71	0
29	MN	X	3176	1/1	0.84	0.13	128,128,128,128	0
30	MG	X	3277	1/1	0.84	0.51	59,59,59,59	0
29	MN	X	3162	1/1	0.84	0.10	110,110,110,110	0
29	MN	X	3170	1/1	0.84	0.22	103,103,103,103	0
30	MG	X	3258	1/1	0.85	0.23	64,64,64,64	0
29	MN	X	3147	1/1	0.85	0.10	113,113,113,113	0
29	MN	X	3074	1/1	0.86	0.16	129,129,129,129	0
29	MN	Z	101	1/1	0.86	0.32	109,109,109,109	0
30	MG	X	3158	1/1	0.86	0.33	48,48,48,48	0
30	MG	X	3256	1/1	0.86	0.39	91,91,91,91	0
30	MG	X	3263	1/1	0.86	0.46	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3235	1/1	0.87	0.10	118,118,118,118	0
29	MN	X	3225	1/1	0.87	0.23	101,101,101,101	0
30	MG	X	3168	1/1	0.87	0.18	73,73,73,73	0
29	MN	X	3212	1/1	0.87	0.19	117,117,117,117	0
29	MN	X	3157	1/1	0.87	0.18	87,87,87,87	0
30	MG	X	3251	1/1	0.87	0.16	65,65,65,65	0
29	MN	X	3006	1/1	0.87	0.14	49,49,49,49	0
30	MG	X	3259	1/1	0.88	0.57	61,61,61,61	0
29	MN	X	3029	1/1	0.88	0.17	82,82,82,82	0
29	MN	X	3178	1/1	0.88	0.27	108,108,108,108	0
29	MN	X	3151	1/1	0.88	0.10	97,97,97,97	0
29	MN	E	201	1/1	0.88	0.17	125,125,125,125	0
29	MN	X	3185	1/1	0.88	0.14	100,100,100,100	0
30	MG	X	3281	1/1	0.88	0.46	69,69,69,69	0
29	MN	X	3164	1/1	0.88	0.24	110,110,110,110	0
30	MG	X	3195	1/1	0.88	0.47	57,57,57,57	0
29	MN	X	3135	1/1	0.88	0.17	108,108,108,108	0
30	MG	X	3269	1/1	0.88	0.61	104,104,104,104	0
30	MG	X	3239	1/1	0.89	0.33	46,46,46,46	0
29	MN	X	3123	1/1	0.89	0.19	109,109,109,109	0
29	MN	X	3155	1/1	0.89	0.19	105,105,105,105	0
29	MN	X	3018	1/1	0.89	0.30	86,86,86,86	0
29	MN	X	3016	1/1	0.89	0.17	87,87,87,87	0
30	MG	X	3197	1/1	0.89	0.35	54,54,54,54	0
30	MG	X	3253	1/1	0.89	0.27	90,90,90,90	0
29	MN	X	3037	1/1	0.89	0.20	78,78,78,78	0
32	SPD	X	3286	10/10	0.89	0.25	65,65,65,65	0
30	MG	X	3218	1/1	0.90	0.29	74,74,74,74	0
29	MN	X	3052	1/1	0.90	0.14	121,121,121,121	0
29	MN	X	3154	1/1	0.90	0.25	114,114,114,114	0
29	MN	X	3206	1/1	0.90	0.21	127,127,127,127	0
29	MN	X	3073	1/1	0.90	0.17	120,120,120,120	0
30	MG	X	3232	1/1	0.90	0.10	67,67,67,67	0
30	MG	Y	203	1/1	0.90	0.07	122,122,122,122	0
30	MG	X	3238	1/1	0.90	0.76	58,58,58,58	0
29	MN	X	3163	1/1	0.90	0.14	99,99,99,99	0
29	MN	X	3215	1/1	0.90	0.18	119,119,119,119	0
29	MN	X	3190	1/1	0.90	0.21	117,117,117,117	0
30	MG	X	3254	1/1	0.91	0.38	67,67,67,67	0
30	MG	X	3152	1/1	0.91	0.33	57,57,57,57	0
29	MN	X	3184	1/1	0.91	0.09	126,126,126,126	0
29	MN	X	3082	1/1	0.91	0.19	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3233	1/1	0.91	0.13	59,59,59,59	0
29	MN	X	3008	1/1	0.91	0.13	50,50,50,50	0
30	MG	X	3193	1/1	0.91	0.51	78,78,78,78	0
29	MN	X	3071	1/1	0.91	0.23	83,83,83,83	0
29	MN	X	3208	1/1	0.91	0.15	77,77,77,77	0
29	MN	X	3026	1/1	0.91	0.21	94,94,94,94	0
29	MN	X	3174	1/1	0.91	0.16	115,115,115,115	0
29	MN	X	3130	1/1	0.91	0.17	94,94,94,94	0
29	MN	X	3053	1/1	0.91	0.13	96,96,96,96	0
29	MN	X	3061	1/1	0.91	0.07	119,119,119,119	0
30	MG	X	3250	1/1	0.92	0.63	66,66,66,66	0
29	MN	X	3033	1/1	0.92	0.34	90,90,90,90	0
29	MN	X	3139	1/1	0.92	0.07	102,102,102,102	0
30	MG	X	3160	1/1	0.92	0.15	69,69,69,69	0
29	MN	X	3219	1/1	0.92	0.07	118,118,118,118	0
30	MG	X	3241	1/1	0.92	0.07	91,91,91,91	0
30	MG	X	3226	1/1	0.92	0.30	74,74,74,74	0
30	MG	X	3243	1/1	0.92	0.29	54,54,54,54	0
30	MG	X	3072	1/1	0.92	0.35	41,41,41,41	0
30	MG	X	3273	1/1	0.92	0.07	57,57,57,57	0
29	MN	X	3125	1/1	0.92	0.10	86,86,86,86	0
30	MG	X	3036	1/1	0.93	0.16	55,55,55,55	0
29	MN	X	3031	1/1	0.93	0.18	80,80,80,80	0
29	MN	X	3013	1/1	0.93	0.41	67,67,67,67	0
30	MG	X	3201	1/1	0.93	0.38	66,66,66,66	0
30	MG	X	3126	1/1	0.93	0.44	58,58,58,58	0
28	MPD	X	3002	8/8	0.93	0.32	96,96,96,96	0
29	MN	X	3047	1/1	0.93	0.10	87,87,87,87	0
29	MN	X	3132	1/1	0.93	0.22	101,101,101,101	0
29	MN	X	3067	1/1	0.93	0.18	103,103,103,103	0
29	MN	X	3017	1/1	0.93	0.04	90,90,90,90	0
29	MN	X	3109	1/1	0.93	0.21	87,87,87,87	0
30	MG	X	3252	1/1	0.93	0.39	60,60,60,60	0
30	MG	X	3183	1/1	0.93	0.34	72,72,72,72	0
29	MN	X	3188	1/1	0.93	0.29	117,117,117,117	0
29	MN	X	3133	1/1	0.94	0.18	85,85,85,85	0
27	95H	X	3001	27/27	0.94	0.24	52,52,52,52	19
29	MN	X	3138	1/1	0.94	0.18	102,102,102,102	0
29	MN	I	201	1/1	0.94	0.31	95,95,95,95	0
29	MN	X	3039	1/1	0.94	0.16	94,94,94,94	0
30	MG	X	3270	1/1	0.94	0.26	68,68,68,68	0
29	MN	X	3159	1/1	0.94	0.18	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3161	1/1	0.94	0.07	130,130,130,130	0
29	MN	X	3209	1/1	0.94	0.13	105,105,105,105	0
29	MN	X	3120	1/1	0.94	0.14	72,72,72,72	0
30	MG	X	3058	1/1	0.94	0.49	63,63,63,63	0
29	MN	X	3186	1/1	0.94	0.17	104,104,104,104	0
29	MN	X	3055	1/1	0.94	0.11	129,129,129,129	0
29	MN	X	3144	1/1	0.94	0.13	80,80,80,80	0
30	MG	X	3282	1/1	0.94	0.20	63,63,63,63	0
29	MN	X	3221	1/1	0.94	0.07	141,141,141,141	0
30	MG	Y	202	1/1	0.94	0.16	54,54,54,54	0
29	MN	X	3076	1/1	0.94	0.14	93,93,93,93	0
29	MN	X	3167	1/1	0.94	0.08	110,110,110,110	0
29	MN	X	3081	1/1	0.94	0.17	57,57,57,57	0
29	MN	X	3068	1/1	0.94	0.17	84,84,84,84	0
29	MN	X	3059	1/1	0.94	0.15	92,92,92,92	0
29	MN	X	3065	1/1	0.95	0.12	85,85,85,85	0
29	MN	X	3007	1/1	0.95	0.30	61,61,61,61	0
29	MN	X	3102	1/1	0.95	0.32	77,77,77,77	0
29	MN	X	3021	1/1	0.95	0.11	68,68,68,68	0
29	MN	X	3230	1/1	0.95	0.10	126,126,126,126	0
29	MN	X	3111	1/1	0.95	0.13	80,80,80,80	0
29	MN	X	3117	1/1	0.95	0.09	66,66,66,66	0
29	MN	X	3005	1/1	0.95	0.30	53,53,53,53	0
29	MN	X	3038	1/1	0.95	0.18	73,73,73,73	0
30	MG	X	3245	1/1	0.95	0.23	63,63,63,63	0
29	MN	X	3056	1/1	0.95	0.19	94,94,94,94	0
29	MN	X	3057	1/1	0.95	0.16	93,93,93,93	0
30	MG	X	3248	1/1	0.95	0.42	66,66,66,66	0
30	MG	X	3249	1/1	0.95	0.16	89,89,89,89	0
29	MN	X	3207	1/1	0.95	0.09	92,92,92,92	0
29	MN	X	3028	1/1	0.95	0.23	90,90,90,90	0
29	MN	X	3045	1/1	0.95	0.13	88,88,88,88	0
29	MN	X	3210	1/1	0.95	0.23	107,107,107,107	0
30	MG	X	3213	1/1	0.95	0.26	47,47,47,47	0
30	MG	X	3216	1/1	0.95	0.20	43,43,43,43	0
29	MN	X	3012	1/1	0.95	0.29	72,72,72,72	0
29	MN	X	3088	1/1	0.95	0.22	68,68,68,68	0
30	MG	G	201	1/1	0.95	0.24	25,25,25,25	0
30	MG	X	3069	1/1	0.95	0.42	52,52,52,52	0
29	MN	X	3136	1/1	0.95	0.26	106,106,106,106	0
31	EPE	X	3285	15/15	0.95	0.20	72,72,72,72	0
29	MN	X	3090	1/1	0.95	0.18	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3066	1/1	0.96	0.12	91,91,91,91	0
29	MN	X	3103	1/1	0.96	0.47	81,81,81,81	0
29	MN	X	3105	1/1	0.96	0.17	71,71,71,71	0
29	MN	X	3106	1/1	0.96	0.21	99,99,99,99	0
29	MN	X	3140	1/1	0.96	0.07	100,100,100,100	0
29	MN	X	3107	1/1	0.96	0.24	68,68,68,68	0
29	MN	X	3046	1/1	0.96	0.12	94,94,94,94	0
29	MN	X	3023	1/1	0.96	0.21	70,70,70,70	0
29	MN	X	3173	1/1	0.96	0.44	112,112,112,112	0
29	MN	X	3084	1/1	0.96	0.28	71,71,71,71	0
30	MG	X	3032	1/1	0.96	0.59	31,31,31,31	0
29	MN	X	3175	1/1	0.96	0.11	103,103,103,103	0
29	MN	X	3119	1/1	0.96	0.08	77,77,77,77	0
29	MN	X	3054	1/1	0.96	0.34	82,82,82,82	0
29	MN	X	3048	1/1	0.96	0.07	117,117,117,117	0
29	MN	X	3091	1/1	0.96	0.13	61,61,61,61	0
29	MN	X	3127	1/1	0.96	0.15	79,79,79,79	0
29	MN	X	3064	1/1	0.96	0.37	124,124,124,124	0
29	MN	X	3035	1/1	0.96	0.43	104,104,104,104	0
30	MG	X	3237	1/1	0.96	0.17	93,93,93,93	0
29	MN	X	3098	1/1	0.96	0.41	70,70,70,70	0
29	MN	X	3100	1/1	0.96	0.18	59,59,59,59	0
29	MN	X	3134	1/1	0.96	0.11	84,84,84,84	0
29	MN	X	3093	1/1	0.97	0.14	61,61,61,61	0
29	MN	X	3236	1/1	0.97	0.06	104,104,104,104	0
29	MN	X	3278	1/1	0.97	0.14	99,99,99,99	0
30	MG	X	3244	1/1	0.97	0.23	57,57,57,57	0
29	MN	X	3094	1/1	0.97	0.12	83,83,83,83	0
29	MN	X	3110	1/1	0.97	0.20	65,65,65,65	0
29	MN	X	3027	1/1	0.97	0.15	89,89,89,89	0
29	MN	X	3113	1/1	0.97	0.09	75,75,75,75	0
29	MN	X	3114	1/1	0.97	0.20	65,65,65,65	0
30	MG	X	3275	1/1	0.97	0.25	57,57,57,57	0
29	MN	X	3137	1/1	0.97	0.18	72,72,72,72	0
29	MN	X	3116	1/1	0.97	0.31	78,78,78,78	0
29	MN	X	3097	1/1	0.97	0.15	79,79,79,79	0
29	MN	X	3087	1/1	0.97	0.18	63,63,63,63	0
29	MN	X	3020	1/1	0.97	0.15	78,78,78,78	0
29	MN	X	3220	1/1	0.97	0.06	112,112,112,112	0
29	MN	X	3089	1/1	0.97	0.14	69,69,69,69	0
29	MN	X	3166	1/1	0.97	0.11	95,95,95,95	0
29	MN	X	3063	1/1	0.97	0.17	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3015	1/1	0.97	0.38	63,63,63,63	0
29	MN	X	3146	1/1	0.97	0.09	101,101,101,101	0
29	MN	X	3060	1/1	0.97	0.10	84,84,84,84	0
30	MG	X	3262	1/1	0.97	0.28	82,82,82,82	0
29	MN	X	3148	1/1	0.97	0.39	91,91,91,91	0
29	MN	X	3200	1/1	0.97	0.11	136,136,136,136	0
29	MN	X	3101	1/1	0.98	0.19	60,60,60,60	0
29	MN	X	3034	1/1	0.98	0.11	94,94,94,94	0
29	MN	X	3049	1/1	0.98	0.23	81,81,81,81	0
29	MN	X	3070	1/1	0.98	0.27	97,97,97,97	0
29	MN	X	3050	1/1	0.98	0.19	98,98,98,98	0
29	MN	X	3040	1/1	0.98	0.16	79,79,79,79	0
29	MN	X	3108	1/1	0.98	0.21	70,70,70,70	0
29	MN	X	3041	1/1	0.98	0.09	75,75,75,75	0
29	MN	X	3177	1/1	0.98	0.43	110,110,110,110	0
29	MN	Y	201	1/1	0.98	0.07	95,95,95,95	0
29	MN	X	3044	1/1	0.98	0.18	93,93,93,93	0
29	MN	X	3030	1/1	0.98	0.06	89,89,89,89	0
29	MN	X	3079	1/1	0.98	0.12	70,70,70,70	0
29	MN	X	3095	1/1	0.98	0.12	69,69,69,69	0
29	MN	X	3115	1/1	0.98	0.19	63,63,63,63	0
29	MN	X	3080	1/1	0.98	0.21	59,59,59,59	0
29	MN	X	3024	1/1	0.98	0.23	74,74,74,74	0
29	MN	X	3025	1/1	0.98	0.12	79,79,79,79	0
29	MN	X	3143	1/1	0.98	0.22	44,44,44,44	0
29	MN	X	3083	1/1	0.98	0.19	56,56,56,56	0
29	MN	X	3077	1/1	0.99	0.18	88,88,88,88	0
29	MN	X	3104	1/1	0.99	0.26	86,86,86,86	0
29	MN	X	3121	1/1	0.99	0.07	67,67,67,67	0
29	MN	X	3122	1/1	0.99	0.19	82,82,82,82	0
29	MN	X	3022	1/1	0.99	0.14	74,74,74,74	0
29	MN	X	3124	1/1	0.99	0.22	76,76,76,76	0
30	MG	X	3272	1/1	0.99	0.10	60,60,60,60	0
29	MN	X	3011	1/1	0.99	0.28	40,40,40,40	0
29	MN	X	3004	1/1	0.99	0.29	60,60,60,60	0
29	MN	X	3128	1/1	0.99	0.14	62,62,62,62	0
29	MN	X	3149	1/1	0.99	0.12	102,102,102,102	0
29	MN	X	3129	1/1	0.99	0.25	74,74,74,74	0
29	MN	X	3009	1/1	0.99	0.28	59,59,59,59	0
29	MN	X	3211	1/1	0.99	0.12	100,100,100,100	0
29	MN	X	3153	1/1	0.99	0.17	99,99,99,99	0
29	MN	X	3042	1/1	0.99	0.14	80,80,80,80	0

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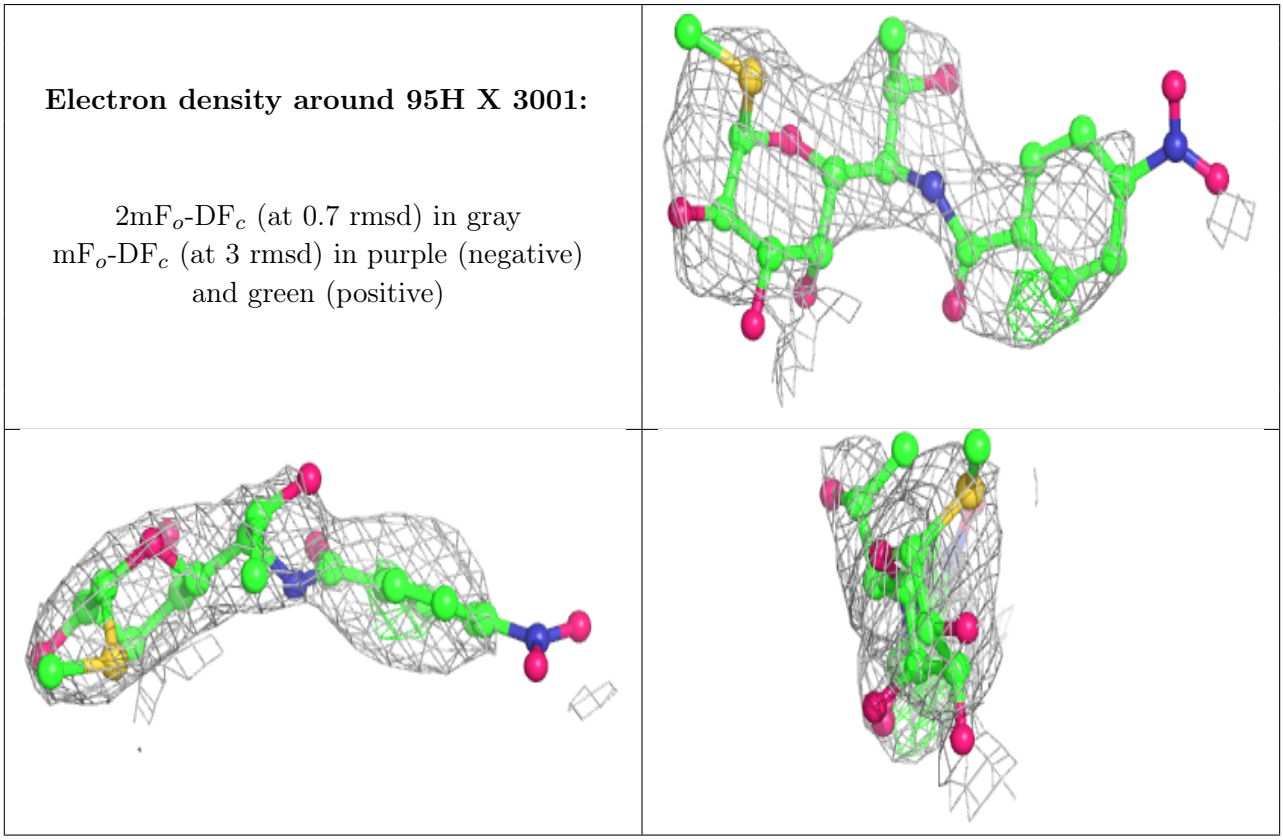
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3180	1/1	0.99	0.17	70,70,70,70	0
30	MG	X	3284	1/1	0.99	0.06	56,56,56,56	0
29	MN	X	3043	1/1	0.99	0.18	79,79,79,79	0
29	MN	X	3085	1/1	0.99	0.25	61,61,61,61	0
29	MN	X	3086	1/1	0.99	0.09	62,62,62,62	0
29	MN	X	3099	1/1	0.99	0.19	73,73,73,73	0
29	MN	X	3019	1/1	0.99	0.11	73,73,73,73	0
29	MN	X	3014	1/1	0.99	0.19	56,56,56,56	0
29	MN	X	3010	1/1	0.99	0.31	59,59,59,59	0
29	MN	X	3118	1/1	0.99	0.14	69,69,69,69	0
29	MN	X	3078	1/1	1.00	0.18	55,55,55,55	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.



6.5 Other polymers

There are no such residues in this entry.