Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 10:07 am GMT

PDB ID	:	5HL7
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus in complex with lefamulin
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on	:	2016-01-14
Resolution	:	3.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

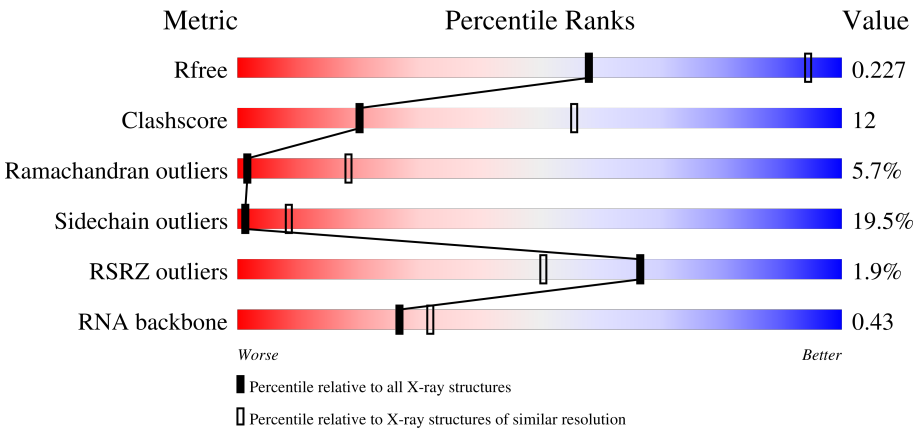
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

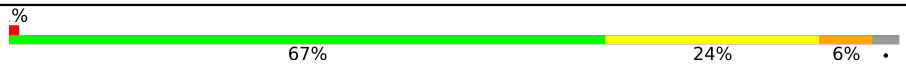
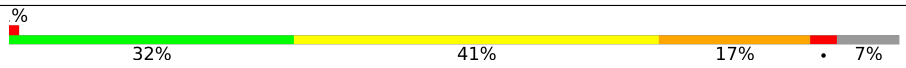
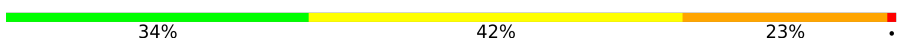
The reported resolution of this entry is 3.55 Å.

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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)
RNA backbone	3102	1008 (4.10-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	277	
2	X	2923	
3	Y	114	

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Mol	Chain	Length	Quality of chain
4	B	220	55% 34% 9%
5	C	207	53% 34% 9%
6	D	179	6% 78% 13% 8%
7	E	178	3% 65% 19% 5% 12%
8	G	145	% 54% 36% 10%
9	H	122	52% 38% 10%
10	I	140	4% 57% 24% 12% 6%
11	J	144	3% 60% 32%
12	K	122	51% 42%
13	L	119	67% 18% 6% 8%
14	M	116	2% 54% 28% 12% 5%
15	N	118	51% 41% 7%
16	O	102	62% 33% 5%
17	P	117	% 57% 33% 5%
18	Q	91	62% 32% 5%
19	R	105	6% 51% 29% 17%
20	S	217	47% 23% 6% 23%
21	T	94	% 48% 23% 9% 20%
22	U	62	39% 55% 11% 32%
23	V	69	49% 42% 6%
24	W	59	42% 39% 14%
25	Z	58	41% 28% 5% 26%
26	2	45	9% 56% 33% 7%
27	3	66	50% 30% 11% 9%
28	4	37	59% 78% 19%

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	3114	-	-	-	X
29	MN	X	3155	-	-	-	X
29	MN	X	3186	-	-	-	X
29	MN	X	3225	-	-	-	X
29	MN	X	3421	-	-	-	X
29	MN	X	3446	-	-	-	X
29	MN	X	3454	-	-	-	X
29	MN	X	3458	-	-	-	X
29	MN	X	3471	-	-	-	X
30	MG	A	302	-	-	-	X
30	MG	G	201	-	-	-	X
30	MG	P	201	-	-	-	X
30	MG	X	3087	-	-	-	X
30	MG	X	3180	-	-	-	X
30	MG	X	3196	-	-	-	X
30	MG	X	3230	-	-	-	X
30	MG	X	3236	-	-	-	X
30	MG	X	3244	-	-	-	X
30	MG	X	3248	-	-	-	X
30	MG	X	3250	-	-	-	X
30	MG	X	3252	-	-	-	X
30	MG	X	3253	-	-	-	X
30	MG	X	3254	-	-	-	X
30	MG	X	3255	-	-	-	X
30	MG	X	3265	-	-	-	X
30	MG	X	3286	-	-	-	X
30	MG	X	3293	-	-	-	X
30	MG	X	3294	-	-	-	X
30	MG	X	3306	-	-	-	X
30	MG	X	3308	-	-	-	X
30	MG	X	3327	-	-	-	X
30	MG	X	3332	-	-	-	X
30	MG	X	3335	-	-	-	X
30	MG	X	3336	-	-	-	X
30	MG	X	3337	-	-	-	X
30	MG	X	3339	-	-	-	X
30	MG	X	3340	-	-	-	X
30	MG	X	3341	-	-	-	X
30	MG	X	3342	-	-	-	X
30	MG	X	3344	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MG	X	3346	-	-	-	X
30	MG	X	3348	-	-	-	X
30	MG	X	3349	-	-	-	X
30	MG	X	3351	-	-	-	X
30	MG	X	3352	-	-	-	X
30	MG	X	3358	-	-	-	X
30	MG	X	3365	-	-	-	X
30	MG	X	3370	-	-	-	X
30	MG	X	3382	-	-	-	X
30	MG	X	3386	-	-	-	X
30	MG	X	3391	-	-	-	X
30	MG	X	3393	-	-	-	X
30	MG	X	3398	-	-	-	X
30	MG	X	3400	-	-	-	X
30	MG	X	3413	-	-	-	X
30	MG	X	3417	-	-	-	X
30	MG	X	3441	-	-	-	X
30	MG	X	3445	-	-	-	X
30	MG	X	3449	-	-	-	X
30	MG	X	3475	-	-	-	X
30	MG	X	3487	-	-	-	X
30	MG	X	3488	-	-	-	X
30	MG	Y	203	-	-	-	X
30	MG	Y	210	-	-	-	X
30	MG	Y	212	-	-	-	X
33	SPD	X	3498	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition (i)

There are 35 unique types of molecules in this entry. The entry contains 81462 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	1667	1007	331	324	5	0	0	0

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	2705	57983	25884	10620	18774	2705	0	0	0

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Y	114	2430	1086	436	794	114	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	1547	967	289	286	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	199	1324	823	250	249	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	165	853	512	165	174	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	157	915	559	172	182	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	G	145	1090	682	202	203	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	122	884	548	167	165	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	131	819	498	164	156	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	138	1001	641	187	170	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	119	906	556	175	174	1	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	L	109	673	411	134	128	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	M	110	807	510	162	135	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	N	116	922	581	183	154	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	O	102	751	477	138	135	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	P	112	853	531	161	158	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	Q	90	583	365	103	112	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	R	102	627	382	120	124	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	S	167	1087	682	191	212	2	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
21	T	75	559	349	110	100	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
22	U	42	242	149	48	45	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
23	V	65	486	299	89	98	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
24	W	57	437	271	82	84	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	Z	43	339	208	70	57	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	2	43	350	213	85	51	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	3	60	405	248	81	74	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	4	36	181	107	36	36	2	0	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
29	A	1	1	1	0	0
29	X	268	Total 268	Mn 268	0	0
29	Y	2	Total 2	Mn 2	0	0
29	R	1	Total 1	Mn 1	0	0
29	T	1	Total 1	Mn 1	0	0
29	Z	1	Total 1	Mn 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
30	A	3	3	3	0	0
30	X	218	Total 218	Mg 218	0	0
30	Y	10	Total 10	Mg 10	0	0
30	C	2	Total 2	Mg 2	0	0
30	G	2	Total 2	Mg 2	0	0
30	I	1	Total 1	Mg 1	0	0
30	J	1	Total 1	Mg 1	0	0

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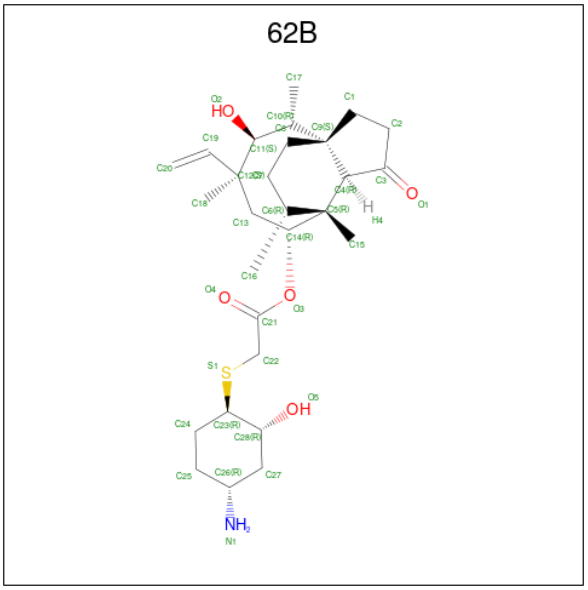
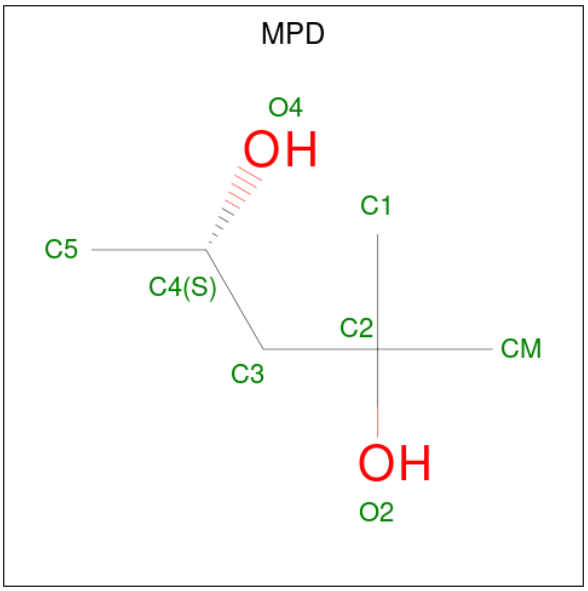
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
30	M	1	1	1	0	0
			Total	Mg		
30	O	1	1	1	0	0
			Total	Mg		
30	P	1	1	1	0	0

- Molecule 31 is Lefamulin (three-letter code: 62B) (formula: $C_{28}H_{45}NO_5S$).



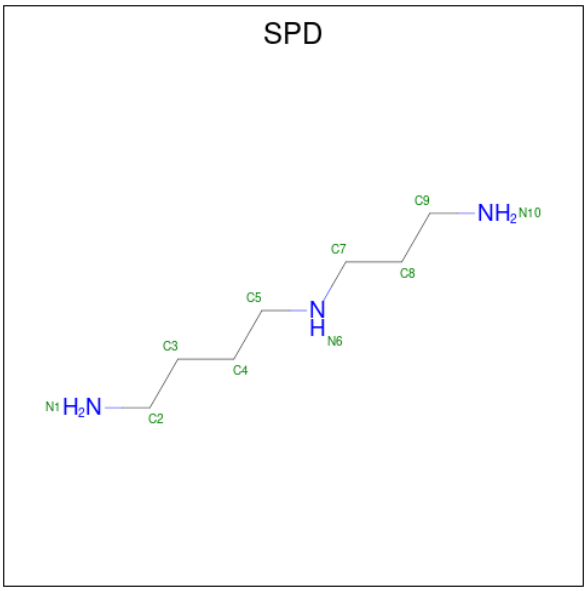
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
31	X	1	35	28	1	5	1	0	0

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



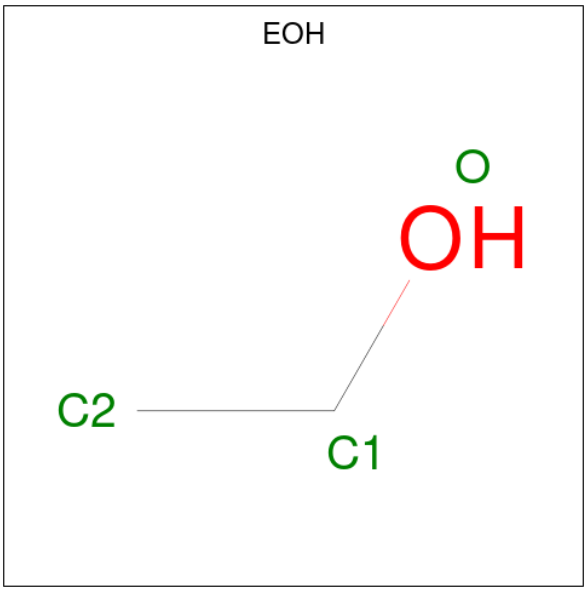
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	X	1	Total	C	O		0	0
			8	6	2			
32	J	1	Total	C	O		0	0
			8	6	2			
32	Q	1	Total	C	O		0	0
			8	6	2			
32	Z	1	Total	C	O		0	0
			8	6	2			

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



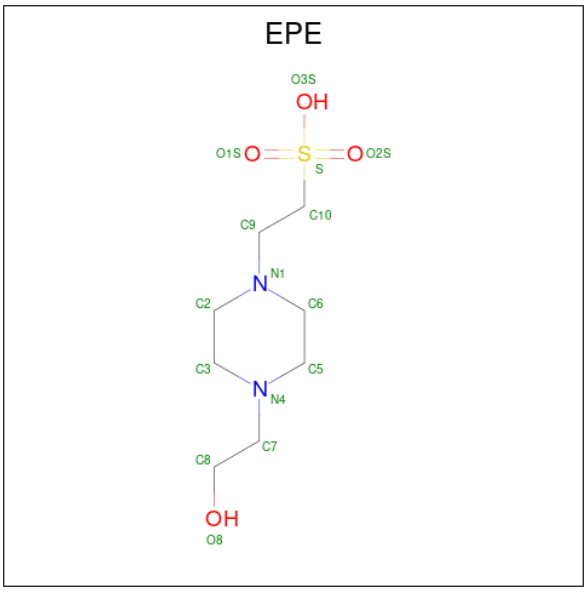
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	Y	1	Total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

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
34	X	1	3	2	1	0	0
			Total	C	O		
34	X	1	3	2	1	0	0
			Total	C	O		
34	S	1	3	2	1	0	0

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



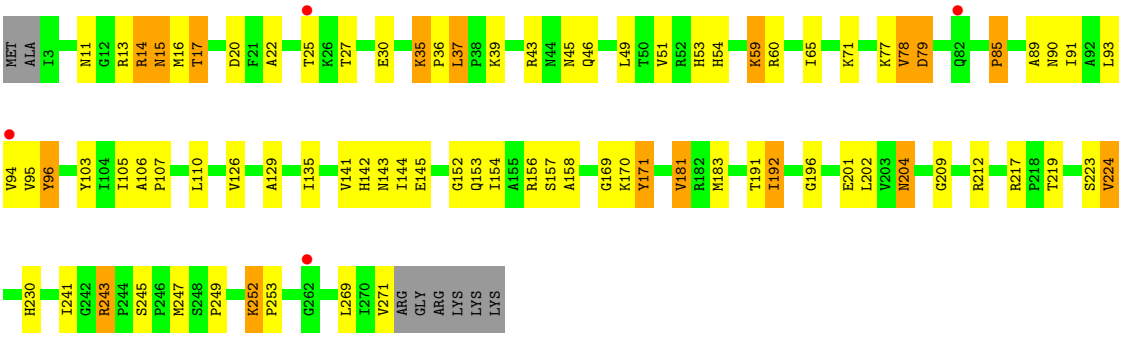
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
35	N	1	15	8	2	4	1	0	0

3 Residue-property plots (i)

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

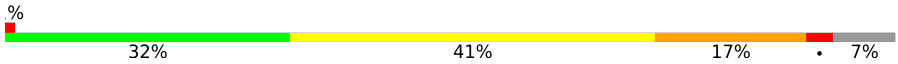
- Molecule 1: 50S ribosomal protein L2

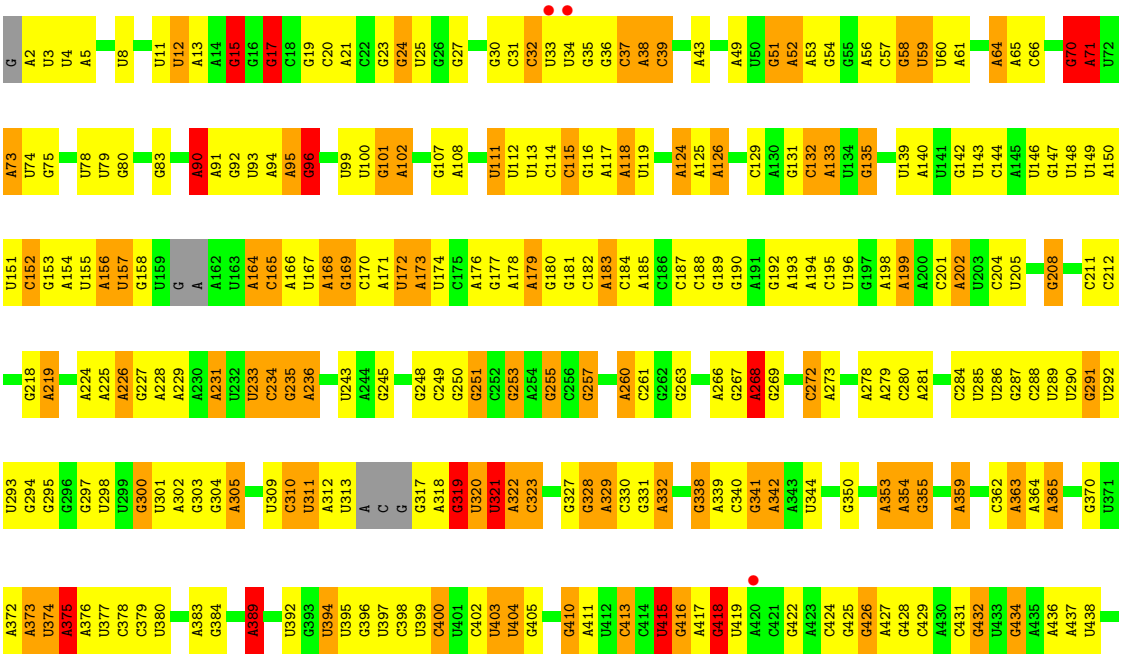
Chain A:

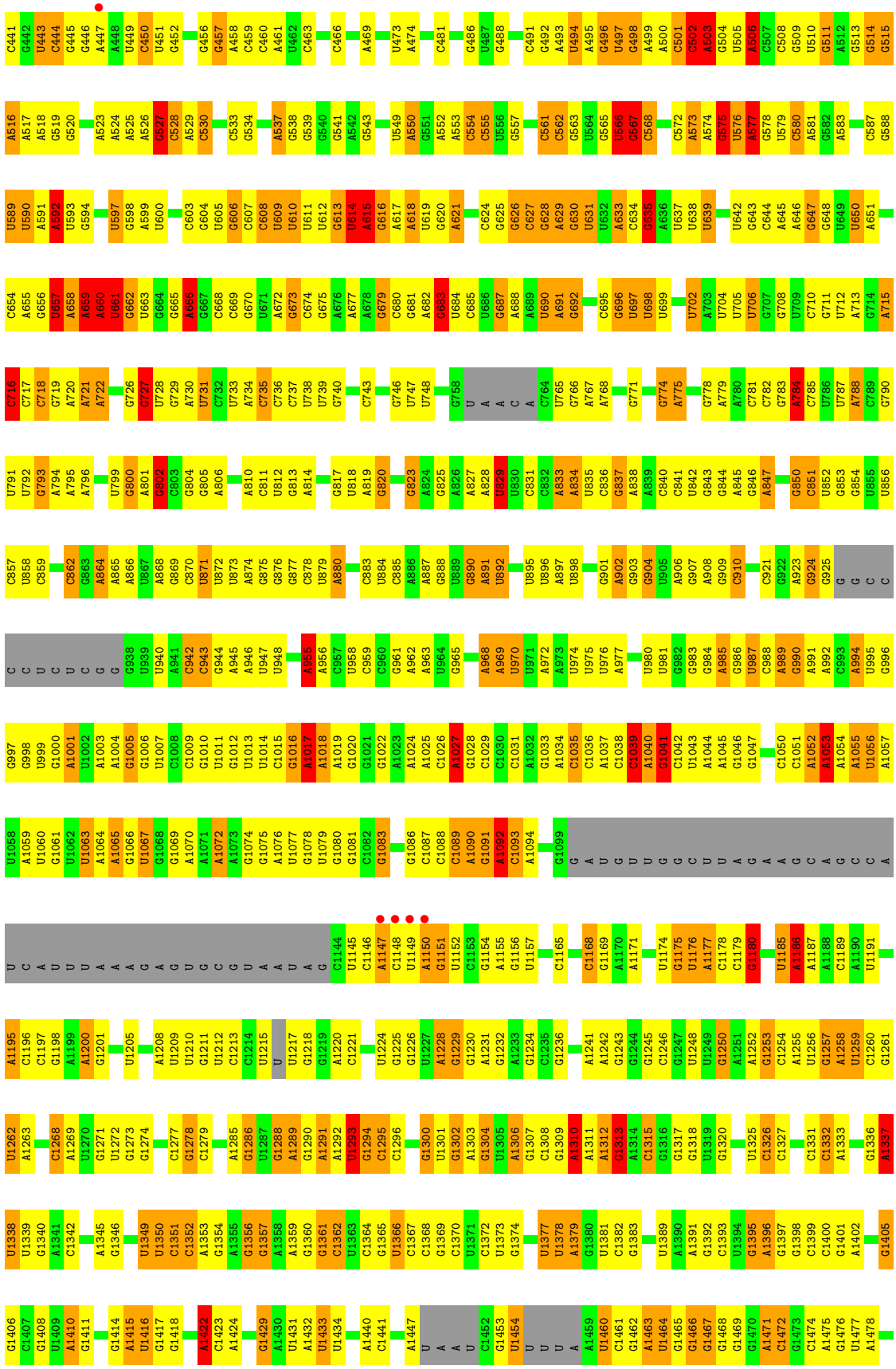


- Molecule 2: 23S ribosomal RNA

Chain X:



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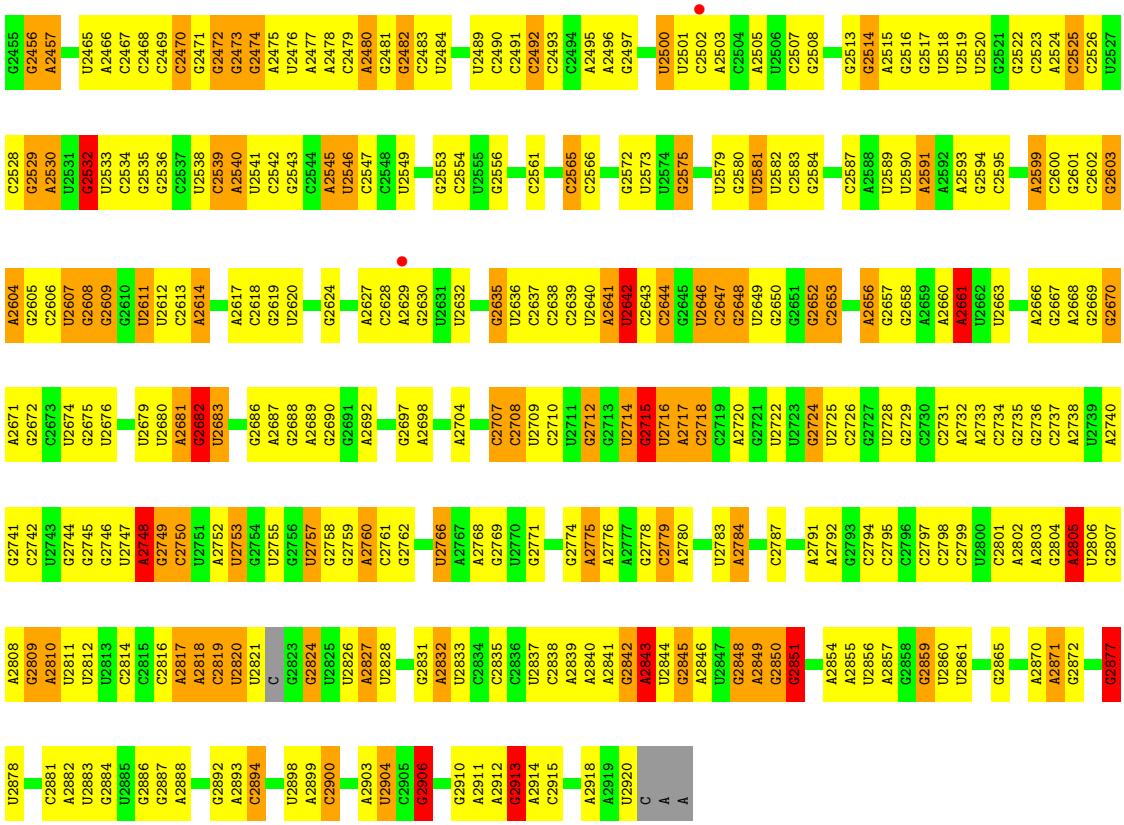

• Molecule 3: 5S ribosomal RNA

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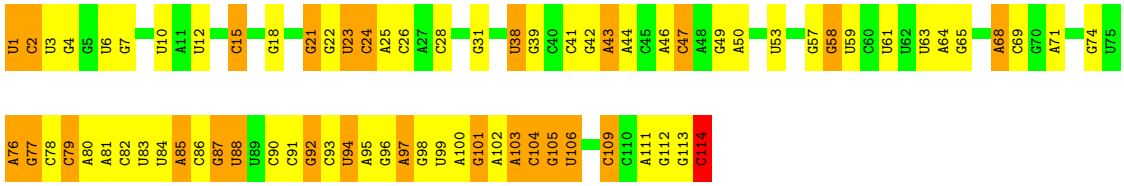
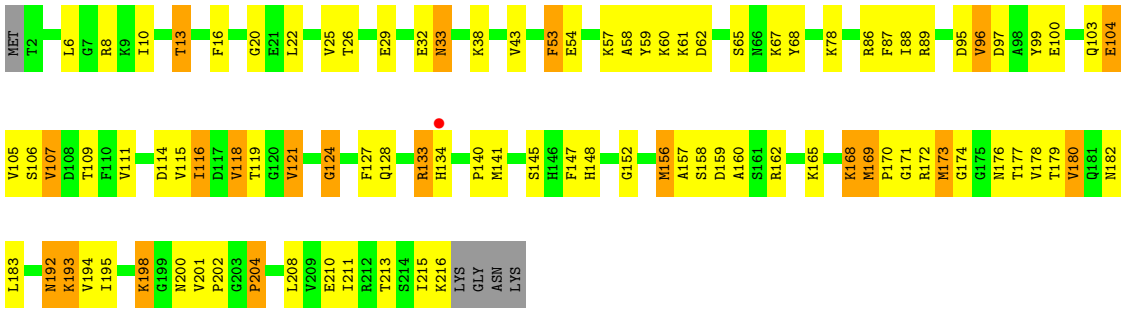


• Molecule 4: 50S ribosomal protein L3

Chain B:



• Molecule 5: 50S ribosomal protein L4

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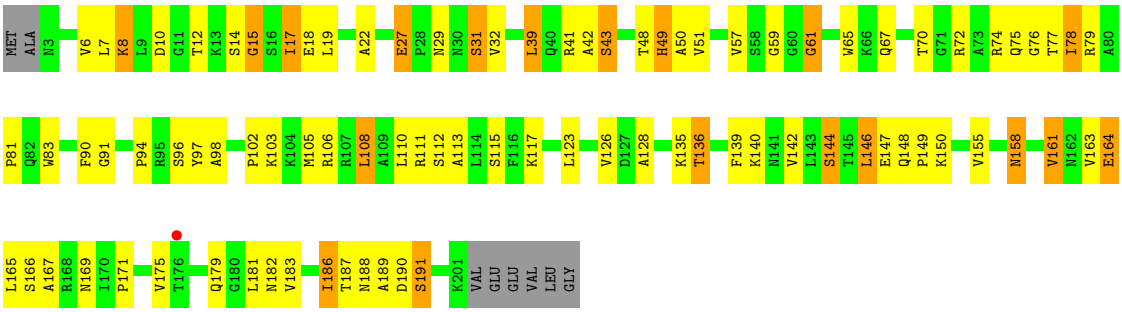

- Molecule 6: 50S ribosomal protein L5

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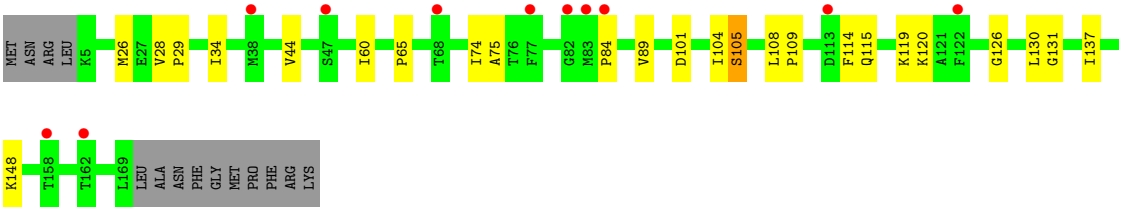

- Molecule 7: 50S ribosomal protein L6

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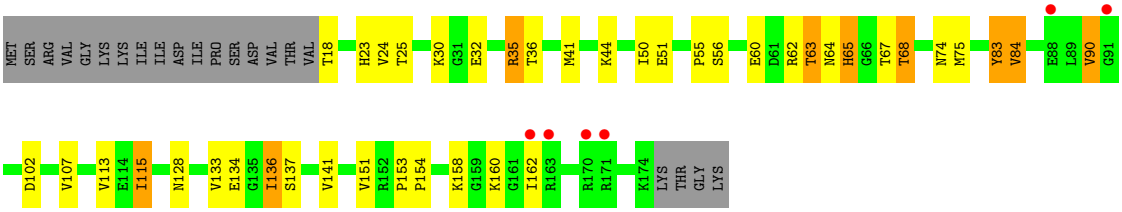

- Molecule 8: 50S ribosomal protein L13

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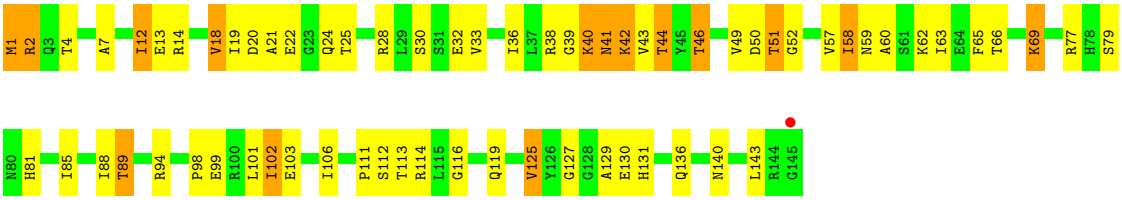

- Molecule 9: 50S ribosomal protein L14

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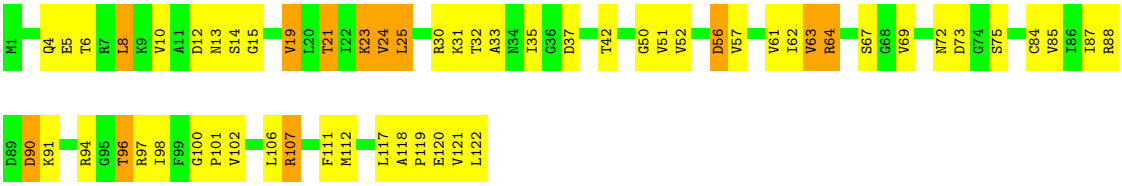

• Molecule 10: 50S ribosomal protein L15

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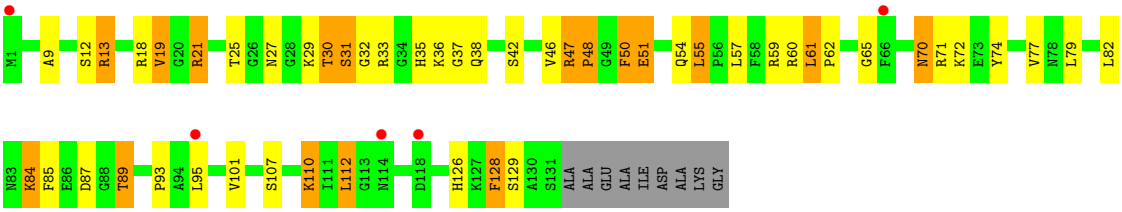

• Molecule 11: 50S ribosomal protein L16

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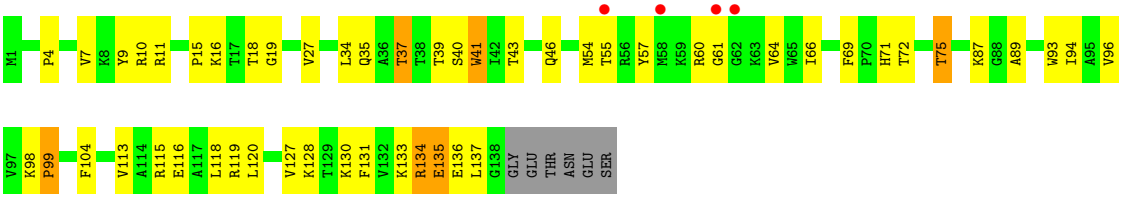

• Molecule 12: 50S ribosomal protein L17

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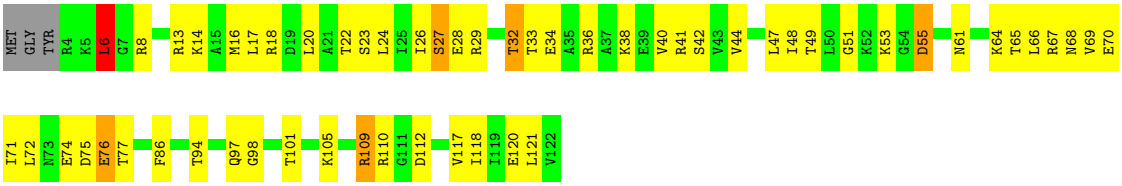
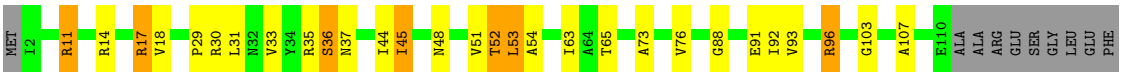


• Molecule 13: 50S ribosomal protein L18

Chain L:



• Molecule 14: 50S ribosomal protein L19

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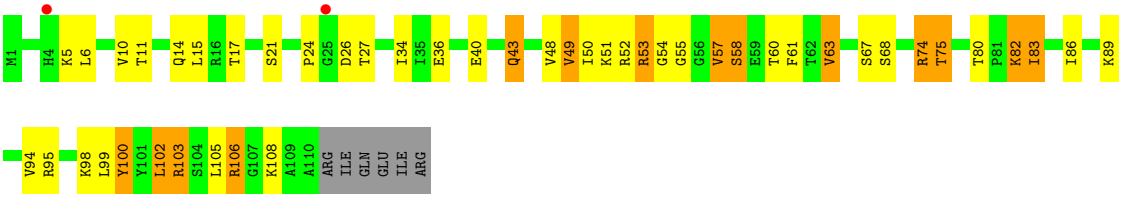

• Molecule 15: 50S ribosomal protein L20

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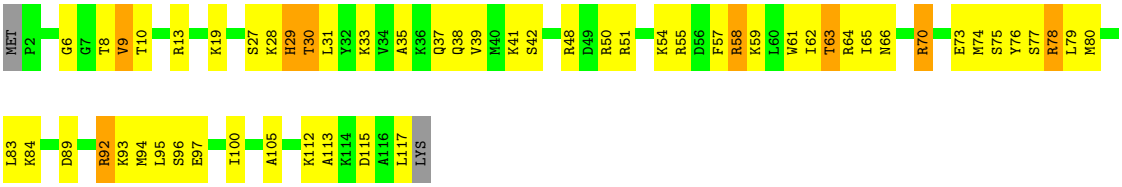

• Molecule 16: 50S ribosomal protein L21

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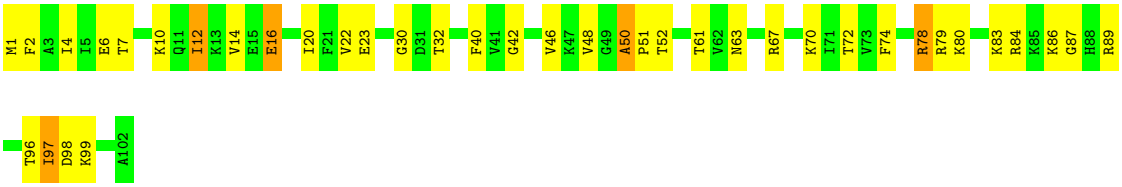

• Molecule 17: 50S ribosomal protein L22

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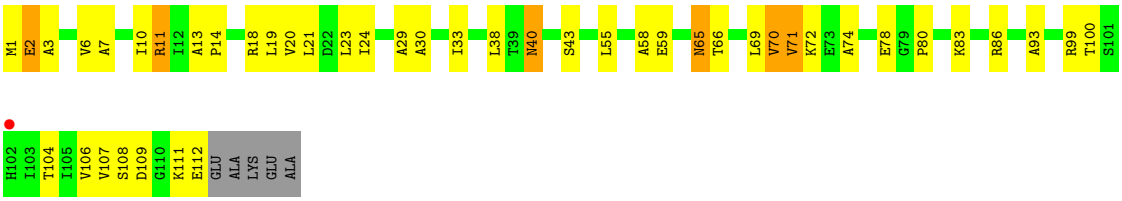
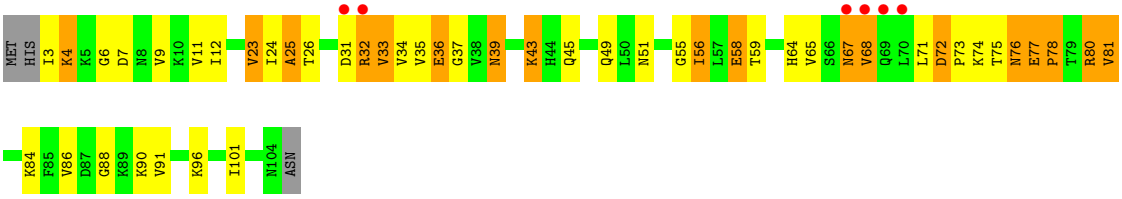


• Molecule 18: 50S ribosomal protein L23

Chain Q:

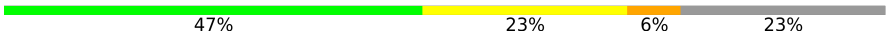
• Molecule 19: 50S ribosomal protein L24

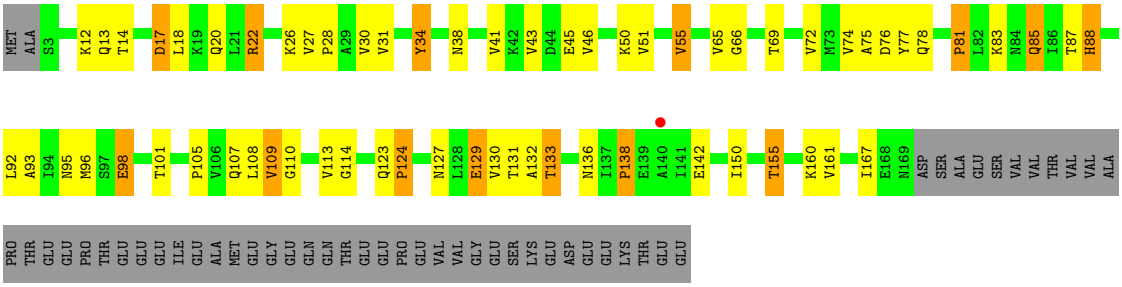
Chain R:



- Molecule 20: 50S ribosomal protein L25

Chain S:





- Molecule 21: 50S ribosomal protein L27

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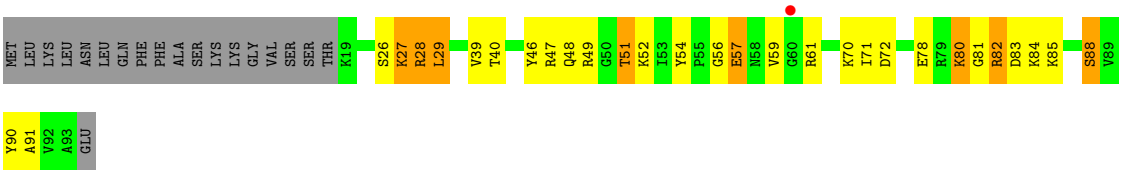

- Molecule 22: 50S ribosomal protein L28

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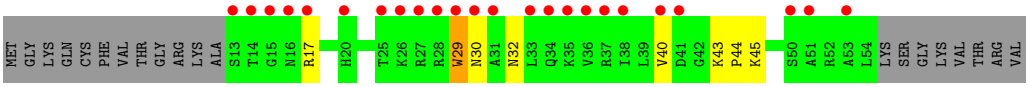
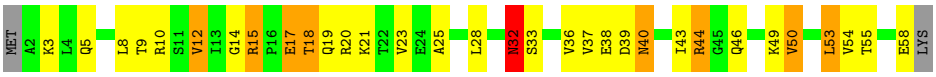


- Molecule 23: 50S ribosomal protein L29

Chain V:

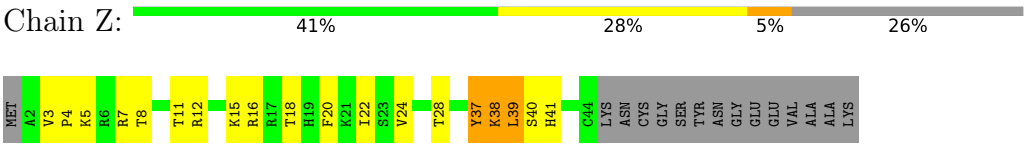
- Molecule 24: 50S ribosomal protein L30

Chain W:



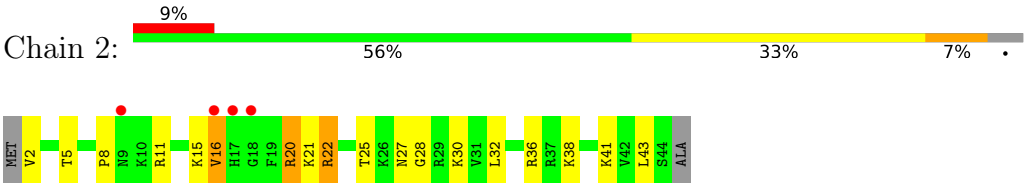
• Molecule 25: 50S ribosomal protein L32

Chain Z:



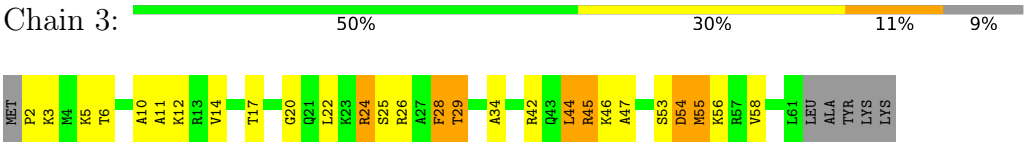
• Molecule 26: 50S ribosomal protein L34

Chain 2:



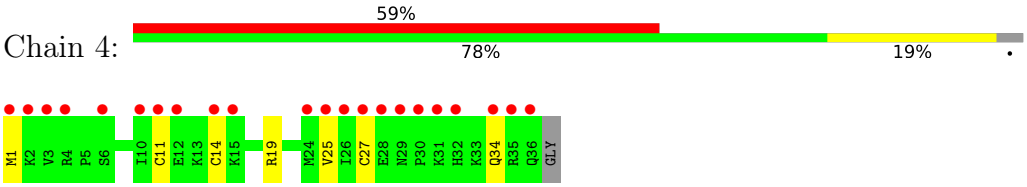
• Molecule 27: 50S ribosomal protein L35

Chain 3:



• Molecule 28: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.4 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	11847 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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: MG, EPE, MN, EOH, MPD, SPD, 62B

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.26	0/1697	0.56	0/2332
2	X	0.96	108/64923 (0.2%)	1.63	1547/101215 (1.5%)
3	Y	0.90	10/2717 (0.4%)	1.73	90/4232 (2.1%)
4	B	0.68	0/1570	0.90	2/2117 (0.1%)
5	C	0.72	0/1343	0.98	1/1838 (0.1%)
6	D	0.33	0/855	0.56	0/1185
7	E	0.44	0/925	0.61	0/1279
8	G	0.78	0/1112	0.87	0/1507
9	H	0.62	0/891	0.80	0/1203
10	I	0.75	0/827	1.02	2/1121 (0.2%)
11	J	0.61	0/1023	0.80	0/1388
12	K	0.35	0/909	0.62	1/1217 (0.1%)
13	L	0.50	0/678	0.69	0/927
14	M	0.72	0/819	0.94	2/1107 (0.2%)
15	N	0.83	0/934	0.99	0/1241
16	O	0.84	1/761 (0.1%)	0.97	3/1022 (0.3%)
17	P	0.41	0/861	0.64	0/1160
18	Q	0.57	0/589	0.78	0/808
19	R	0.67	1/631 (0.2%)	0.85	0/863
20	S	0.60	0/1099	0.84	0/1509
21	T	0.59	0/565	0.79	0/751
22	U	0.37	0/247	0.57	0/344
23	V	0.50	0/487	0.64	0/654
24	W	0.73	0/439	0.93	0/593
25	Z	0.80	0/345	0.90	0/460
26	2	0.72	0/353	0.94	0/463
27	3	0.75	0/409	1.07	1/550 (0.2%)
28	4	0.41	0/180	0.66	0/249
All	All	0.89	120/88189 (0.1%)	1.50	1649/133335 (1.2%)

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
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1186	A	N9-C4	-12.81	1.30	1.37
2	X	1289	A	N9-C4	-11.75	1.30	1.37
2	X	2845	G	N9-C4	-9.65	1.30	1.38
2	X	1065	A	N9-C4	-9.16	1.32	1.37
2	X	2740	A	N9-C4	-8.95	1.32	1.37
2	X	1295	C	N3-C4	-8.57	1.27	1.33
2	X	721	A	N9-C4	-8.40	1.32	1.37
2	X	1395	G	N9-C4	7.83	1.44	1.38
2	X	1289	A	C5-C4	7.67	1.44	1.38
2	X	2648	G	N1-C2	-7.57	1.31	1.37
3	Y	68	A	N9-C4	-7.52	1.33	1.37
2	X	1310	A	N9-C4	-7.48	1.33	1.37
2	X	2845	G	C2-N3	-7.47	1.26	1.32
2	X	1065	A	N7-C5	-7.40	1.34	1.39
2	X	574	A	N9-C4	-7.19	1.33	1.37
2	X	2738	A	N9-C4	-6.98	1.33	1.37
2	X	2087	A	N9-C4	-6.97	1.33	1.37
2	X	515	G	C5-C4	6.95	1.43	1.38
3	Y	58	G	N9-C4	-6.94	1.32	1.38
2	X	865	A	N9-C4	-6.92	1.33	1.37
2	X	2740	A	N7-C5	-6.84	1.35	1.39
2	X	621	A	C5-C4	-6.77	1.34	1.38
3	Y	93	C	N1-C2	6.75	1.47	1.40
2	X	2707	C	N1-C6	-6.72	1.33	1.37
2	X	660	A	O3'-P	6.70	1.69	1.61
2	X	2037	G	C5-C4	-6.68	1.33	1.38
2	X	1719	C	N1-C6	-6.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	373	A	C5-C4	6.63	1.43	1.38
2	X	2604	A	N3-C4	-6.62	1.30	1.34
2	X	720	A	N3-C4	-6.59	1.30	1.34
2	X	1302	G	C2-N3	-6.57	1.27	1.32
2	X	24	G	N7-C5	-6.48	1.35	1.39
2	X	2050	A	C6-N1	-6.45	1.31	1.35
2	X	2355	A	N9-C4	-6.44	1.33	1.37
2	X	1285	A	N9-C4	-6.42	1.33	1.37
19	R	68	VAL	CA-CB	6.37	1.68	1.54
2	X	1289	A	N3-C4	-6.32	1.31	1.34
2	X	2661	A	C5-C4	-6.29	1.34	1.38
2	X	721	A	N7-C5	-6.29	1.35	1.39
2	X	2845	G	C5-C6	-6.28	1.36	1.42
2	X	2648	G	C6-N1	-6.25	1.35	1.39
2	X	2661	A	C6-N1	-6.15	1.31	1.35
2	X	515	G	N9-C8	6.15	1.42	1.37
2	X	1040	A	N9-C4	-6.11	1.34	1.37
3	Y	92	G	N1-C2	6.10	1.42	1.37
2	X	721	A	N3-C4	-6.09	1.31	1.34
2	X	1395	G	N7-C5	6.09	1.43	1.39
2	X	2595	C	N1-C6	-6.08	1.33	1.37
2	X	1312	A	N9-C4	-6.06	1.34	1.37
2	X	721	A	C5-C6	-6.06	1.35	1.41
2	X	2066	G	N7-C5	-6.04	1.35	1.39
2	X	681	G	N7-C5	-6.03	1.35	1.39
2	X	955	A	N7-C5	-5.98	1.35	1.39
2	X	1051	C	N1-C6	-5.94	1.33	1.37
2	X	550	A	P-O5'	5.91	1.65	1.59
2	X	1046	G	N1-C2	5.90	1.42	1.37
2	X	2911	A	N9-C4	-5.81	1.34	1.37
2	X	603	C	N3-C4	-5.80	1.29	1.33
2	X	518	A	N9-C4	-5.79	1.34	1.37
2	X	1195	A	N9-C4	-5.75	1.34	1.37
2	X	659	A	N9-C4	5.71	1.41	1.37
2	X	663	U	C2-N3	-5.70	1.33	1.37
2	X	1395	G	N3-C4	5.66	1.39	1.35
2	X	2846	A	N9-C4	-5.66	1.34	1.37
2	X	1171	A	N3-C4	-5.65	1.31	1.34
2	X	617	A	N9-C4	-5.61	1.34	1.37
3	Y	86	C	N3-C4	-5.61	1.30	1.33
2	X	660	A	C3'-O3'	5.60	1.50	1.42
3	Y	99	U	N1-C2	5.59	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	88	U	N1-C2	5.58	1.43	1.38
2	X	2744	G	N1-C2	-5.57	1.33	1.37
2	X	890	G	N9-C4	-5.56	1.33	1.38
2	X	2599	A	N9-C4	-5.56	1.34	1.37
2	X	1065	A	N3-C4	-5.54	1.31	1.34
2	X	2749	G	C5-C4	-5.53	1.34	1.38
2	X	2845	G	N9-C8	5.51	1.41	1.37
2	X	666	A	N9-C4	-5.50	1.34	1.37
2	X	1786	A	N9-C4	5.47	1.41	1.37
2	X	1180	G	C6-N1	5.46	1.43	1.39
2	X	2893	A	N3-C4	-5.45	1.31	1.34
2	X	1782	A	N9-C4	-5.45	1.34	1.37
2	X	994	A	N3-C4	-5.44	1.31	1.34
2	X	2716	U	C2-N3	-5.43	1.33	1.37
2	X	2708	C	N1-C6	-5.43	1.33	1.37
2	X	833	A	N9-C4	-5.42	1.34	1.37
2	X	2536	G	N1-C2	-5.42	1.33	1.37
2	X	503	A	C5-C6	-5.41	1.36	1.41
3	Y	92	G	N9-C4	-5.38	1.33	1.38
3	Y	7	G	N9-C4	5.37	1.42	1.38
2	X	1186	A	C5-C6	-5.36	1.36	1.41
2	X	2047	A	C6-N1	-5.36	1.31	1.35
2	X	1065	A	C5-C6	-5.34	1.36	1.41
2	X	1027	A	C5-C4	-5.33	1.35	1.38
2	X	1174	U	C2-N3	-5.32	1.34	1.37
2	X	2604	A	N9-C4	-5.31	1.34	1.37
2	X	519	G	N7-C5	-5.31	1.36	1.39
2	X	1180	G	N9-C8	5.24	1.41	1.37
2	X	515	G	N1-C2	5.24	1.42	1.37
2	X	616	G	C5-C4	-5.21	1.34	1.38
2	X	2546	U	C2-N3	-5.20	1.34	1.37
2	X	1574	G	C5-C4	5.18	1.42	1.38
2	X	503	A	N7-C5	-5.18	1.36	1.39
16	O	6	GLU	CG-CD	5.18	1.59	1.51
2	X	994	A	C6-N1	-5.17	1.31	1.35
2	X	962	A	N9-C4	-5.17	1.34	1.37
2	X	1291	A	C6-N1	-5.17	1.31	1.35
3	Y	98	G	N3-C4	-5.14	1.31	1.35
2	X	1200	A	N7-C5	-5.13	1.36	1.39
2	X	1567	A	N9-C4	5.13	1.41	1.37
2	X	845	A	N9-C4	-5.11	1.34	1.37
2	X	2848	G	N3-C4	-5.09	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1379	A	N9-C4	-5.07	1.34	1.37
2	X	1701	U	N1-C6	-5.07	1.33	1.38
2	X	955	A	N3-C4	5.06	1.37	1.34
2	X	2522	G	N3-C4	-5.06	1.31	1.35
2	X	2080	G	C6-N1	-5.06	1.36	1.39
2	X	2894	C	N1-C6	-5.04	1.34	1.37
2	X	116	G	N9-C4	5.01	1.42	1.38
2	X	363	A	N7-C5	-5.01	1.36	1.39
2	X	1050	C	N3-C4	-5.00	1.30	1.33

All (1649) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	93	C	N3-C2-O2	-20.18	107.77	121.90
2	X	2845	G	N3-C4-C5	18.48	137.84	128.60
3	Y	93	C	N1-C2-O2	16.73	128.94	118.90
2	X	1395	G	N1-C6-O6	-16.42	110.05	119.90
2	X	1289	A	C2-N3-C4	-16.32	102.44	110.60
2	X	2845	G	N3-C4-N9	-16.31	116.22	126.00
2	X	2529	G	N1-C6-O6	15.72	129.33	119.90
2	X	627	C	O5'-P-OP2	-15.70	91.57	105.70
3	Y	86	C	C6-N1-C2	-15.44	114.12	120.30
2	X	721	A	C2-N3-C4	-14.88	103.16	110.60
2	X	1065	A	C2-N3-C4	-14.64	103.28	110.60
2	X	1186	A	C2-N3-C4	-14.13	103.54	110.60
2	X	2845	G	C2-N3-C4	-13.53	105.14	111.90
2	X	1289	A	C5-N7-C8	-13.36	97.22	103.90
3	Y	88	U	N3-C2-O2	-13.30	112.89	122.20
3	Y	99	U	N3-C2-O2	-13.27	112.91	122.20
2	X	1361	G	N1-C6-O6	13.25	127.85	119.90
2	X	1368	C	C6-N1-C2	13.21	125.58	120.30
2	X	2740	A	N1-C6-N6	13.12	126.47	118.60
2	X	721	A	N1-C6-N6	13.07	126.44	118.60
2	X	515	G	C5-N7-C8	-13.06	97.77	104.30
2	X	2529	G	C6-C5-N7	-12.97	122.62	130.40
2	X	2089	A	N1-C6-N6	12.95	126.37	118.60
2	X	1361	G	C5-C6-O6	-12.81	120.92	128.60
2	X	515	G	N7-C8-N9	12.78	119.49	113.10
3	Y	86	C	N3-C2-O2	-12.43	113.20	121.90
2	X	1574	G	C8-N9-C4	-12.29	101.48	106.40
2	X	2716	U	N3-C4-O4	-12.24	110.83	119.40
2	X	2078	A	C2-N3-C4	-12.21	104.49	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1289	A	C5-C6-N1	-12.16	111.62	117.70
2	X	2845	G	C5-N7-C8	-12.09	98.26	104.30
2	X	1165	C	C6-N1-C2	-12.02	115.49	120.30
2	X	373	A	C2-N3-C4	-12.00	104.60	110.60
2	X	2035	C	C6-N1-C2	11.85	125.04	120.30
2	X	373	A	N1-C2-N3	11.71	135.16	129.30
3	Y	88	U	N1-C2-O2	11.69	130.98	122.80
2	X	2529	G	C4-C5-N7	11.67	115.47	110.80
2	X	2391	C	C6-N1-C2	11.60	124.94	120.30
2	X	1180	G	C5-C6-O6	-11.41	121.75	128.60
2	X	587	C	C6-N1-C2	11.39	124.86	120.30
2	X	716	C	C6-N1-C2	-11.34	115.77	120.30
2	X	1289	A	N1-C6-N6	11.28	125.37	118.60
2	X	2532	G	C5-C6-O6	11.27	135.36	128.60
2	X	2845	G	N3-C2-N2	-11.17	112.08	119.90
2	X	721	A	C5-C6-N1	-11.07	112.17	117.70
2	X	515	G	C4-C5-N7	10.96	115.18	110.80
2	X	1395	G	C5-C6-N1	10.93	116.96	111.50
2	X	2081	A	N1-C2-N3	10.93	134.76	129.30
2	X	1065	A	C5-N7-C8	-10.75	98.53	103.90
2	X	2845	G	C4-C5-N7	10.74	115.09	110.80
2	X	721	A	C5-N7-C8	-10.73	98.53	103.90
2	X	2481	G	C8-N9-C4	-10.73	102.11	106.40
2	X	955	A	N1-C6-N6	10.72	125.03	118.60
2	X	657	U	N1-C2-O2	10.72	130.30	122.80
2	X	2085	A	N1-C6-N6	10.72	125.03	118.60
2	X	2595	C	C6-N1-C2	10.69	124.58	120.30
2	X	515	G	C8-N9-C4	-10.67	102.13	106.40
2	X	2529	G	C5-C6-O6	-10.61	122.23	128.60
2	X	1065	A	C5-C6-N1	-10.57	112.42	117.70
2	X	211	C	C6-N1-C2	10.54	124.52	120.30
2	X	2086	A	N1-C6-N6	10.53	124.92	118.60
2	X	2740	A	C6-C5-N7	-10.53	124.93	132.30
2	X	1496	G	N9-C4-C5	10.52	109.61	105.40
2	X	2532	G	N1-C6-O6	-10.52	113.59	119.90
2	X	1065	A	N1-C6-N6	10.44	124.86	118.60
2	X	1229	G	N9-C4-C5	-10.41	101.24	105.40
2	X	1395	G	N3-C4-C5	-10.37	123.41	128.60
3	Y	99	U	N1-C2-O2	10.35	130.04	122.80
2	X	1289	A	N7-C8-N9	10.32	118.96	113.80
2	X	2083	G	N3-C2-N2	-10.27	112.71	119.90
3	Y	82	C	N3-C2-O2	-10.26	114.72	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2078	A	N1-C2-N3	10.24	134.42	129.30
2	X	1065	A	N7-C8-N9	10.21	118.90	113.80
2	X	2738	A	C2-N3-C4	-10.20	105.50	110.60
2	X	1186	A	N3-C4-C5	10.19	133.93	126.80
3	Y	58	G	N3-C4-C5	10.12	133.66	128.60
2	X	660	A	P-O3'-C3'	10.10	131.82	119.70
2	X	721	A	C6-C5-N7	-10.06	125.26	132.30
2	X	1180	G	C4-C5-N7	10.05	114.82	110.80
2	X	1496	G	C4-C5-N7	-10.05	106.78	110.80
2	X	1360	G	N1-C6-O6	10.03	125.92	119.90
2	X	1746	G	N1-C6-O6	9.93	125.86	119.90
2	X	2716	U	C5-C4-O4	9.93	131.86	125.90
2	X	2050	A	N1-C6-N6	-9.86	112.68	118.60
2	X	2844	U	N1-C2-N3	9.84	120.81	114.90
2	X	2845	G	N1-C6-O6	9.83	125.80	119.90
2	X	1360	G	C2-N3-C4	-9.83	106.99	111.90
2	X	2419	A	N1-C6-N6	9.80	124.48	118.60
2	X	2844	U	N3-C2-O2	-9.74	115.38	122.20
2	X	1011	U	N3-C4-O4	9.73	126.21	119.40
2	X	2079	G	C4-C5-N7	9.71	114.69	110.80
2	X	1229	G	N1-C6-O6	9.69	125.71	119.90
3	Y	7	G	N3-C4-C5	-9.67	123.76	128.60
2	X	1289	A	C6-C5-N7	-9.66	125.54	132.30
3	Y	93	C	C6-N1-C2	-9.62	116.45	120.30
2	X	1574	G	N7-C8-N9	9.61	117.90	113.10
2	X	2599	A	C8-N9-C4	9.60	109.64	105.80
2	X	323	C	C6-N1-C2	-9.58	116.47	120.30
2	X	617	A	C8-N9-C4	9.58	109.63	105.80
2	X	902	A	N1-C6-N6	-9.57	112.86	118.60
3	Y	98	G	N3-C4-N9	-9.56	120.26	126.00
2	X	2079	G	C6-C5-N7	-9.55	124.67	130.40
2	X	2881	C	C6-N1-C2	-9.54	116.48	120.30
2	X	696	G	N1-C6-O6	-9.48	114.21	119.90
2	X	2583	C	N1-C2-O2	9.43	124.56	118.90
2	X	2061	U	N3-C4-O4	9.34	125.94	119.40
27	3	44	LEU	CA-CB-CG	9.33	136.76	115.30
2	X	1230	G	N1-C6-O6	9.33	125.50	119.90
2	X	35	G	C8-N9-C4	9.31	110.12	106.40
2	X	2740	A	C5-N7-C8	-9.31	99.25	103.90
2	X	862	C	C6-N1-C2	9.30	124.02	120.30
2	X	2603	G	C2-N3-C4	-9.28	107.26	111.90
2	X	1175	G	O5'-P-OP2	-9.28	97.35	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1663	G	N1-C6-O6	9.21	125.42	119.90
2	X	503	A	C5-N7-C8	-9.20	99.30	103.90
2	X	1229	G	C5-C6-O6	-9.19	123.09	128.60
2	X	2474	G	C6-C5-N7	-9.17	124.90	130.40
2	X	1593	G	N3-C4-C5	-9.12	124.04	128.60
2	X	2391	C	N3-C4-C5	9.12	125.55	121.90
2	X	2740	A	C2-N3-C4	-9.12	106.04	110.60
2	X	515	G	N1-C6-O6	9.08	125.35	119.90
2	X	854	G	C8-N9-C4	-9.08	102.77	106.40
2	X	2523	C	C6-N1-C2	9.06	123.92	120.30
2	X	511	G	C5-C6-O6	9.04	134.03	128.60
2	X	1186	A	C5-N7-C8	-9.04	99.38	103.90
2	X	1200	A	C8-N9-C4	-9.04	102.19	105.80
2	X	566	U	O5'-P-OP2	-9.03	97.57	105.70
2	X	1361	G	C6-C5-N7	-9.00	125.00	130.40
2	X	2845	G	C8-N9-C1'	8.99	138.68	127.00
2	X	1065	A	C6-C5-N7	-8.98	126.02	132.30
2	X	511	G	N1-C6-O6	-8.96	114.53	119.90
2	X	1357	G	C5-C6-O6	8.94	133.96	128.60
2	X	1663	G	C5-C6-O6	-8.93	123.24	128.60
2	X	2474	G	N1-C6-O6	8.92	125.25	119.90
2	X	2079	G	C5-C6-O6	-8.89	123.26	128.60
2	X	666	A	N1-C6-N6	8.88	123.93	118.60
2	X	503	A	N7-C8-N9	8.87	118.23	113.80
2	X	2740	A	C5-C6-N1	-8.86	113.27	117.70
3	Y	68	A	C2-N3-C4	-8.85	106.17	110.60
2	X	373	A	C5-C6-N1	-8.84	113.28	117.70
2	X	2278	G	C6-C5-N7	-8.84	125.10	130.40
2	X	2064	A	C8-N9-C4	-8.84	102.27	105.80
2	X	2063	C	O5'-P-OP1	-8.81	97.77	105.70
2	X	1806	U	C5-C6-N1	-8.78	118.31	122.70
2	X	2042	A	O5'-P-OP1	-8.78	97.80	105.70
2	X	696	G	C2-N3-C4	8.73	116.27	111.90
2	X	2298	G	N3-C2-N2	8.73	126.01	119.90
2	X	2603	G	N3-C4-C5	8.73	132.96	128.60
2	X	527	G	N1-C6-O6	8.71	125.12	119.90
2	X	2085	A	C5-C6-N6	-8.69	116.75	123.70
2	X	555	C	O5'-P-OP2	-8.64	97.92	105.70
2	X	2642	U	C5-C4-O4	-8.64	120.71	125.90
2	X	2843	A	O5'-P-OP2	-8.64	97.93	105.70
3	Y	86	C	C2-N1-C1'	8.63	128.29	118.80
2	X	781	C	C6-N1-C2	8.62	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1289	A	N1-C2-N3	8.61	133.61	129.30
2	X	2089	A	C5-N7-C8	-8.60	99.60	103.90
2	X	1395	G	C2-N3-C4	8.58	116.19	111.90
2	X	660	A	OP1-P-OP2	-8.56	106.75	119.60
2	X	1230	G	C5-C6-O6	-8.56	123.46	128.60
2	X	515	G	C6-C5-N7	-8.55	125.27	130.40
2	X	2071	C	C5-C4-N4	-8.50	114.25	120.20
2	X	2720	A	N1-C6-N6	-8.50	113.50	118.60
2	X	666	A	C5-N7-C8	-8.49	99.65	103.90
2	X	2669	G	C2-N3-C4	-8.49	107.65	111.90
2	X	850	G	N3-C4-C5	-8.49	124.36	128.60
2	X	2648	G	C5-C6-N1	8.48	115.74	111.50
2	X	1491	C	C6-N1-C2	-8.46	116.91	120.30
2	X	743	C	C6-N1-C2	8.46	123.69	120.30
2	X	2047	A	N1-C6-N6	-8.46	113.53	118.60
2	X	2724	G	C2-N3-C4	-8.43	107.68	111.90
2	X	503	A	C2-N3-C4	-8.43	106.39	110.60
2	X	721	A	C4-C5-N7	8.41	114.90	110.70
2	X	1065	A	C8-N9-C4	-8.40	102.44	105.80
2	X	389	A	C8-N9-C4	-8.40	102.44	105.80
2	X	1017	A	C8-N9-C4	-8.35	102.46	105.80
2	X	955	A	N9-C4-C5	-8.33	102.47	105.80
2	X	617	A	O5'-P-OP1	-8.32	98.21	105.70
2	X	503	A	C8-N9-C4	-8.30	102.48	105.80
2	X	1180	G	C5-N7-C8	-8.29	100.16	104.30
2	X	1289	A	C4-C5-N7	8.27	114.83	110.70
2	X	2081	A	C2-N3-C4	-8.26	106.47	110.60
2	X	2632	U	C6-N1-C2	-8.24	116.06	121.00
2	X	2583	C	N3-C2-O2	-8.23	116.14	121.90
2	X	1180	G	O4'-C1'-N9	8.22	114.78	108.20
3	Y	82	C	C6-N1-C2	-8.21	117.02	120.30
2	X	910	C	C6-N1-C2	8.21	123.58	120.30
2	X	268	A	O4'-C1'-N9	8.20	114.76	108.20
2	X	2089	A	C6-C5-N7	-8.19	126.57	132.30
2	X	721	A	N7-C8-N9	8.19	117.89	113.80
2	X	1246	C	O5'-P-OP2	-8.17	98.35	105.70
2	X	353	A	O4'-C1'-N9	8.16	114.73	108.20
2	X	565	G	C8-N9-C4	8.15	109.66	106.40
2	X	1055	A	N1-C6-N6	8.15	123.49	118.60
2	X	1360	G	C6-C5-N7	-8.14	125.52	130.40
2	X	2089	A	C4-C5-N7	8.14	114.77	110.70
2	X	1306	A	C2-N3-C4	-8.12	106.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2529	G	N9-C4-C5	-8.12	102.15	105.40
2	X	2546	U	N3-C4-O4	-8.12	113.72	119.40
2	X	1370	C	N3-C4-C5	8.11	125.14	121.90
2	X	580	C	N1-C2-O2	-8.11	114.03	118.90
2	X	2639	C	N3-C4-C5	8.11	125.14	121.90
2	X	687	G	C5-C6-N1	-8.10	107.45	111.50
2	X	1360	G	N9-C4-C5	-8.10	102.16	105.40
2	X	1056	U	O4'-C1'-N1	8.08	114.67	108.20
2	X	1395	G	N3-C4-N9	8.08	130.85	126.00
2	X	2051	C	N1-C2-O2	8.06	123.74	118.90
2	X	1378	U	C2-N1-C1'	8.06	127.37	117.70
2	X	1229	G	C4-C5-N7	8.05	114.02	110.80
2	X	1029	C	O5'-P-OP2	-8.04	98.47	105.70
2	X	613	G	O5'-P-OP1	-8.01	98.49	105.70
2	X	1031	C	C6-N1-C2	8.01	123.50	120.30
2	X	1361	G	C4-C5-N7	8.01	114.00	110.80
2	X	2298	G	N3-C4-N9	8.01	130.80	126.00
2	X	1362	C	C2-N1-C1'	-8.00	110.01	118.80
2	X	1292	A	O5'-P-OP1	-7.98	98.52	105.70
2	X	2646	U	N3-C2-O2	-7.92	116.66	122.20
2	X	2816	C	C6-N1-C2	7.90	123.46	120.30
2	X	2086	A	N9-C4-C5	-7.89	102.64	105.80
2	X	1229	G	C8-N9-C4	7.88	109.55	106.40
2	X	2740	A	C4-C5-N7	7.88	114.64	110.70
2	X	2532	G	N9-C4-C5	7.88	108.55	105.40
3	Y	58	G	N3-C4-N9	-7.87	121.28	126.00
2	X	565	G	N9-C4-C5	-7.87	102.25	105.40
2	X	2538	U	C6-N1-C2	-7.87	116.28	121.00
2	X	1046	G	N3-C2-N2	-7.86	114.40	119.90
2	X	2637	C	N1-C2-O2	7.86	123.62	118.90
2	X	2484	U	C6-N1-C2	7.86	125.72	121.00
3	Y	86	C	N1-C2-O2	7.86	123.62	118.90
2	X	1659	C	N3-C4-N4	7.86	123.50	118.00
2	X	2529	G	C5-N7-C8	-7.85	100.37	104.30
2	X	706	U	N3-C2-O2	-7.84	116.71	122.20
2	X	580	C	N3-C4-N4	7.84	123.48	118.00
2	X	2667	G	N1-C6-O6	7.84	124.60	119.90
3	Y	106	U	N3-C2-O2	-7.84	116.71	122.20
2	X	12	U	N3-C2-O2	-7.83	116.72	122.20
2	X	567	G	N1-C6-O6	7.83	124.59	119.90
2	X	2608	G	N1-C6-O6	-7.82	115.21	119.90
2	X	515	G	C2-N3-C4	-7.82	107.99	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	88	U	C2-N1-C1'	7.82	127.08	117.70
3	Y	15	C	C5-C4-N4	-7.81	114.73	120.20
2	X	2601	G	C8-N9-C4	-7.81	103.28	106.40
2	X	1065	A	N1-C2-N3	7.80	133.20	129.30
3	Y	79	C	C5-C4-N4	-7.80	114.74	120.20
2	X	245	G	C8-N9-C4	7.79	109.52	106.40
3	Y	87	G	N3-C4-C5	7.79	132.50	128.60
2	X	1186	A	N1-C6-N6	7.79	123.27	118.60
2	X	363	A	N1-C6-N6	7.79	123.27	118.60
3	Y	95	A	C8-N9-C4	7.79	108.92	105.80
2	X	1232	G	C8-N9-C4	7.78	109.51	106.40
2	X	2910	G	C5-C6-O6	7.78	133.26	128.60
2	X	2062	G	N3-C4-N9	7.76	130.65	126.00
2	X	2546	U	C5-C6-N1	-7.76	118.82	122.70
2	X	1593	G	N3-C4-N9	7.74	130.65	126.00
2	X	1180	G	C5-C6-N1	7.74	115.37	111.50
2	X	615	A	N1-C6-N6	-7.74	113.96	118.60
2	X	1727	C	C6-N1-C2	7.73	123.39	120.30
2	X	341	G	C4-C5-N7	7.73	113.89	110.80
3	Y	79	C	N3-C4-N4	7.72	123.40	118.00
2	X	1519	U	C6-N1-C2	-7.71	116.37	121.00
2	X	373	A	C4-C5-C6	7.69	120.84	117.00
2	X	2845	G	C4-N9-C1'	-7.68	116.52	126.50
3	Y	7	G	N3-C4-N9	7.67	130.60	126.00
2	X	32	C	C6-N1-C2	7.66	123.36	120.30
2	X	519	G	N1-C6-O6	7.66	124.50	119.90
2	X	2842	G	O5'-P-OP2	-7.66	98.81	105.70
2	X	2278	G	C4-N9-C1'	7.65	136.45	126.50
2	X	828	A	C8-N9-C4	-7.65	102.74	105.80
2	X	2079	G	N3-C4-N9	7.65	130.59	126.00
2	X	706	U	N1-C2-O2	7.64	128.15	122.80
2	X	1702	C	C6-N1-C2	7.63	123.35	120.30
2	X	374	U	N3-C2-O2	-7.62	116.86	122.20
2	X	617	A	C2-N3-C4	-7.62	106.79	110.60
2	X	728	U	N3-C4-C5	-7.62	110.03	114.60
2	X	659	A	C2-N3-C4	7.62	114.41	110.60
2	X	13	A	C8-N9-C4	7.60	108.84	105.80
2	X	2478	A	N1-C6-N6	7.59	123.15	118.60
2	X	2755	U	O5'-P-OP2	-7.58	98.88	105.70
2	X	2839	A	C5-C6-N1	7.58	121.49	117.70
2	X	1561	G	C8-N9-C4	-7.58	103.37	106.40
2	X	2079	G	C5-N7-C8	-7.58	100.51	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1052	A	N1-C6-N6	7.58	123.14	118.60
2	X	1593	G	C4-N9-C1'	7.58	136.35	126.50
2	X	2708	C	C6-N1-C2	7.58	123.33	120.30
2	X	1512	U	N3-C2-O2	-7.54	116.92	122.20
2	X	2027	G	C8-N9-C4	7.54	109.42	106.40
2	X	627	C	OP1-P-OP2	7.54	130.91	119.60
3	Y	58	G	N1-C6-O6	7.54	124.42	119.90
2	X	1372	C	C6-N1-C2	7.53	123.31	120.30
3	Y	93	C	C2-N1-C1'	7.53	127.08	118.80
2	X	608	C	C6-N1-C2	-7.53	117.29	120.30
2	X	1418	G	C8-N9-C4	-7.53	103.39	106.40
2	X	2583	C	C2-N1-C1'	7.52	127.07	118.80
2	X	2392	G	N1-C6-O6	7.51	124.41	119.90
2	X	2589	U	N3-C2-O2	-7.51	116.95	122.20
2	X	1352	C	O5'-P-OP1	-7.50	98.95	105.70
3	Y	92	G	N3-C4-C5	7.50	132.35	128.60
2	X	2642	U	N3-C4-O4	7.50	124.65	119.40
2	X	2709	U	N3-C2-O2	-7.49	116.96	122.20
2	X	598	G	N9-C4-C5	-7.48	102.41	105.40
2	X	1499	U	N3-C2-O2	-7.48	116.96	122.20
2	X	2474	G	C2-N3-C4	-7.47	108.17	111.90
2	X	1186	A	C4-C5-N7	7.46	114.43	110.70
2	X	1307	G	N1-C6-O6	7.45	124.37	119.90
2	X	2084	G	N1-C2-N2	-7.45	109.49	116.20
2	X	853	G	O5'-P-OP2	-7.45	98.99	105.70
2	X	355	G	C4-N9-C1'	7.44	136.17	126.50
2	X	1337	A	N1-C6-N6	7.43	123.06	118.60
2	X	2419	A	C2-N3-C4	-7.43	106.88	110.60
2	X	2530	A	N1-C2-N3	-7.43	125.58	129.30
2	X	2529	G	C2-N3-C4	-7.42	108.19	111.90
2	X	2669	G	N1-C2-N3	7.42	128.35	123.90
2	X	2720	A	C5-C6-N1	7.42	121.41	117.70
2	X	2648	G	N1-C6-O6	-7.41	115.46	119.90
2	X	854	G	N9-C4-C5	7.40	108.36	105.40
2	X	24	G	N1-C6-O6	7.40	124.34	119.90
2	X	666	A	C4-C5-N7	7.39	114.40	110.70
2	X	251	G	N1-C6-O6	7.39	124.33	119.90
2	X	1289	A	N3-C4-C5	7.39	131.97	126.80
2	X	1357	G	N9-C4-C5	7.38	108.35	105.40
2	X	2298	G	N9-C4-C5	-7.38	102.45	105.40
2	X	1050	C	N3-C4-C5	7.38	124.85	121.90
2	X	728	U	N3-C4-O4	7.37	124.56	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	865	A	C5-C6-N6	7.37	129.60	123.70
2	X	1180	G	N7-C8-N9	7.37	116.79	113.10
2	X	696	G	C5-C6-N1	7.37	115.18	111.50
2	X	503	A	C4-C5-N7	7.36	114.38	110.70
2	X	263	G	C8-N9-C4	-7.36	103.46	106.40
2	X	575	G	C2-N3-C4	7.36	115.58	111.90
2	X	795	A	OP1-P-OP2	-7.36	108.57	119.60
2	X	1496	G	N3-C4-N9	-7.36	121.59	126.00
2	X	1663	G	C6-C5-N7	-7.36	125.99	130.40
2	X	2047	A	O5'-P-OP1	-7.35	99.08	105.70
2	X	2484	U	C5-C6-N1	-7.35	119.02	122.70
2	X	1200	A	N7-C8-N9	7.34	117.47	113.80
2	X	1827	C	C6-N1-C2	7.34	123.24	120.30
2	X	2298	G	C6-C5-N7	-7.34	126.00	130.40
2	X	1320	G	N3-C4-C5	-7.32	124.94	128.60
2	X	2809	G	N1-C6-O6	-7.32	115.51	119.90
2	X	604	G	N1-C6-O6	7.30	124.28	119.90
2	X	2278	G	C8-N9-C1'	-7.30	117.51	127.00
2	X	511	G	C4-C5-N7	-7.30	107.88	110.80
2	X	2050	A	N1-C2-N3	7.29	132.94	129.30
2	X	2540	A	C8-N9-C4	-7.29	102.88	105.80
2	X	1395	G	C5-C6-O6	7.28	132.97	128.60
2	X	1307	G	C2-N3-C4	-7.28	108.26	111.90
2	X	2392	G	C5-C6-O6	-7.28	124.23	128.60
2	X	2419	A	C5-N7-C8	-7.27	100.26	103.90
2	X	2278	G	N1-C6-O6	7.27	124.26	119.90
2	X	657	U	C2-N1-C1'	7.26	126.42	117.70
2	X	2528	C	C2-N1-C1'	-7.26	110.82	118.80
2	X	2762	G	N1-C6-O6	7.26	124.25	119.90
2	X	1180	G	C2-N3-C4	7.25	115.53	111.90
2	X	1496	G	C5-C6-O6	7.25	132.95	128.60
2	X	590	U	N3-C2-O2	-7.24	117.13	122.20
2	X	350	G	O4'-C1'-N9	7.24	113.99	108.20
2	X	987	U	N1-C2-N3	7.24	119.24	114.90
2	X	2086	A	C5-C6-N6	-7.24	117.91	123.70
2	X	2749	G	C2-N3-C4	7.23	115.52	111.90
2	X	1019	A	O5'-P-OP2	-7.22	99.20	105.70
2	X	20	C	C5-C4-N4	-7.22	115.14	120.20
2	X	2667	G	C6-C5-N7	-7.21	126.07	130.40
2	X	1568	U	P-O3'-C3'	7.21	128.35	119.70
2	X	633	A	C8-N9-C4	-7.20	102.92	105.80
2	X	1395	G	N3-C2-N2	7.20	124.94	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	199	A	N1-C6-N6	7.20	122.92	118.60
2	X	716	C	N3-C2-O2	-7.19	116.87	121.90
2	X	2904	U	N3-C2-O2	-7.19	117.17	122.20
2	X	2034	U	C5-C6-N1	-7.18	119.11	122.70
2	X	20	C	C6-N1-C2	7.18	123.17	120.30
2	X	2035	C	N3-C4-C5	7.17	124.77	121.90
2	X	1326	C	C2-N3-C4	-7.17	116.31	119.90
2	X	1512	U	N3-C4-O4	-7.17	114.38	119.40
2	X	1806	U	N3-C4-O4	-7.17	114.38	119.40
2	X	1010	G	N9-C4-C5	-7.17	102.53	105.40
2	X	503	A	N1-C6-N6	7.14	122.88	118.60
2	X	2472	G	C2-N3-C4	7.14	115.47	111.90
2	X	1046	G	N1-C2-N2	7.13	122.62	116.20
2	X	566	U	O4'-C1'-N1	7.12	113.90	108.20
2	X	2492	C	C6-N1-C2	-7.12	117.45	120.30
2	X	1357	G	N3-C4-N9	-7.12	121.73	126.00
2	X	1041	G	C8-N9-C4	7.12	109.25	106.40
2	X	1368	C	C5-C4-N4	-7.11	115.22	120.20
2	X	990	G	O5'-P-OP2	-7.11	99.30	105.70
2	X	2283	G	C5-C6-N1	7.11	115.05	111.50
2	X	17	G	N1-C6-O6	7.11	124.16	119.90
2	X	1433	U	C2-N1-C1'	7.10	126.22	117.70
2	X	1516	C	C6-N1-C2	-7.09	117.46	120.30
2	X	568	C	C6-N1-C2	7.09	123.14	120.30
2	X	2043	U	OP1-P-O3'	7.09	120.79	105.20
2	X	2906	G	C8-N9-C4	-7.08	103.57	106.40
2	X	1360	G	C4-C5-N7	7.08	113.63	110.80
2	X	2089	A	C5-C6-N6	-7.08	118.04	123.70
2	X	2418	G	O4'-C1'-N9	7.07	113.86	108.20
2	X	2540	A	N9-C4-C5	7.07	108.63	105.80
2	X	2391	C	C2-N1-C1'	-7.06	111.03	118.80
3	Y	15	C	C6-N1-C2	7.06	123.12	120.30
2	X	600	U	C6-N1-C2	-7.06	116.77	121.00
2	X	1200	A	C5-N7-C8	-7.06	100.37	103.90
2	X	2317	G	N1-C6-O6	7.06	124.14	119.90
2	X	565	G	C5-C6-O6	-7.05	124.37	128.60
2	X	2849	A	N1-C6-N6	-7.04	114.37	118.60
2	X	2055	U	N1-C2-N3	7.04	119.13	114.90
2	X	778	G	C4-C5-N7	7.04	113.61	110.80
2	X	1257	G	C8-N9-C4	-7.03	103.59	106.40
2	X	2844	U	C6-N1-C2	-7.03	116.78	121.00
2	X	1189	C	O5'-P-OP2	-7.03	99.38	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	851	C	OP1-P-O3'	7.02	120.64	105.20
2	X	1033	G	N3-C4-N9	7.01	130.21	126.00
2	X	604	G	C5-C6-N1	-7.00	108.00	111.50
2	X	1975	G	C5-C6-O6	-7.00	124.40	128.60
2	X	1040	A	C8-N9-C4	6.99	108.59	105.80
2	X	2061	U	C5-C4-O4	-6.98	121.71	125.90
2	X	983	G	C8-N9-C4	-6.97	103.61	106.40
2	X	850	G	N3-C4-N9	6.97	130.18	126.00
2	X	721	A	N3-C4-C5	6.97	131.68	126.80
2	X	323	C	N3-C2-O2	-6.96	117.03	121.90
2	X	696	G	N3-C4-C5	-6.96	125.12	128.60
2	X	657	U	C6-N1-C1'	-6.95	111.47	121.20
2	X	2062	G	O5'-P-OP2	-6.95	99.45	105.70
2	X	2046	U	N3-C4-C5	6.94	118.76	114.60
2	X	576	U	N3-C2-O2	-6.93	117.35	122.20
2	X	373	A	C6-C5-N7	-6.93	127.45	132.30
2	X	2473	G	C8-N9-C4	6.93	109.17	106.40
2	X	2419	A	C4-C5-N7	6.93	114.16	110.70
2	X	2062	G	N9-C4-C5	-6.92	102.63	105.40
2	X	1711	G	C5-C6-N1	6.92	114.96	111.50
2	X	2083	G	N1-C2-N2	6.91	122.42	116.20
2	X	2845	G	N1-C2-N2	6.91	122.42	116.20
2	X	2477	A	C8-N9-C4	-6.91	103.04	105.80
2	X	788	A	C2-N3-C4	-6.91	107.15	110.60
2	X	2653	C	O5'-P-OP1	-6.91	99.48	105.70
2	X	2541	U	C5-C6-N1	-6.90	119.25	122.70
2	X	1230	G	C6-C5-N7	-6.90	126.26	130.40
2	X	577	A	C6-N1-C2	-6.89	114.46	118.60
2	X	955	A	C5-C6-N6	-6.89	118.19	123.70
2	X	2333	U	N3-C2-O2	-6.89	117.38	122.20
3	Y	114	C	C2-N1-C1'	6.89	126.38	118.80
2	X	1758	A	C8-N9-C4	-6.88	103.05	105.80
2	X	1496	G	N1-C6-O6	-6.88	115.77	119.90
2	X	2085	A	N9-C4-C5	-6.88	103.05	105.80
2	X	2079	G	N1-C6-O6	6.88	124.03	119.90
2	X	2085	A	C4-C5-N7	6.88	114.14	110.70
2	X	2446	U	C5-C4-O4	6.88	130.03	125.90
2	X	1315	C	N3-C2-O2	-6.87	117.09	121.90
2	X	721	A	O4'-C1'-N9	6.87	113.70	108.20
2	X	1063	U	C5-C4-O4	6.87	130.02	125.90
2	X	1186	A	N3-C4-N9	-6.87	121.91	127.40
2	X	2740	A	C4-C5-C6	6.87	120.43	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2456	G	C6-C5-N7	-6.86	126.28	130.40
2	X	2470	C	N1-C2-O2	-6.86	114.78	118.90
2	X	1320	G	N3-C4-N9	6.86	130.12	126.00
2	X	2298	G	N1-C2-N2	-6.86	110.03	116.20
2	X	1072	A	C8-N9-C4	6.86	108.54	105.80
2	X	890	G	N3-C4-C5	6.86	132.03	128.60
2	X	505	U	O5'-P-OP2	-6.86	99.53	105.70
2	X	1318	G	N3-C4-C5	-6.86	125.17	128.60
2	X	2038	U	OP1-P-O3'	6.86	120.28	105.20
2	X	2054	G	O5'-P-OP1	-6.85	99.53	105.70
2	X	1746	G	C2-N3-C4	-6.85	108.47	111.90
2	X	2288	C	C2-N1-C1'	6.84	126.33	118.80
2	X	1361	G	N9-C4-C5	-6.84	102.67	105.40
3	Y	92	G	N3-C4-N9	-6.83	121.90	126.00
2	X	36	G	N3-C4-N9	6.83	130.10	126.00
2	X	2845	G	C5-C6-O6	-6.83	124.50	128.60
2	X	35	G	C2-N3-C4	-6.83	108.49	111.90
2	X	633	A	N7-C8-N9	6.83	117.21	113.80
2	X	651	A	O5'-P-OP1	-6.83	99.56	105.70
2	X	575	G	C8-N9-C4	-6.82	103.67	106.40
2	X	721	A	N1-C2-N3	6.82	132.71	129.30
2	X	1020	G	N1-C6-O6	-6.82	115.81	119.90
2	X	2910	G	C4-C5-N7	-6.82	108.07	110.80
16	O	50	ALA	C-N-CD	6.82	142.72	128.40
2	X	955	A	N3-C4-N9	6.82	132.85	127.40
2	X	2854	A	N1-C6-N6	6.82	122.69	118.60
3	Y	7	G	C4-N9-C1'	6.82	135.36	126.50
2	X	2870	A	C8-N9-C4	-6.81	103.08	105.80
2	X	24	G	C6-C5-N7	-6.81	126.32	130.40
2	X	846	G	N3-C4-C5	-6.80	125.20	128.60
2	X	1687	G	N1-C6-O6	6.80	123.98	119.90
2	X	355	G	C6-C5-N7	-6.80	126.32	130.40
2	X	1700	C	C6-N1-C2	-6.79	117.58	120.30
2	X	2433	C	N1-C2-O2	6.79	122.97	118.90
2	X	1805	U	C6-N1-C2	6.78	125.07	121.00
3	Y	98	G	N9-C4-C5	6.78	108.11	105.40
2	X	1661	C	N1-C2-O2	-6.78	114.83	118.90
2	X	2419	A	C6-C5-N7	-6.78	127.56	132.30
2	X	2602	C	C6-N1-C2	-6.78	117.59	120.30
2	X	519	G	C6-C5-N7	-6.77	126.34	130.40
2	X	617	A	N3-C4-C5	6.77	131.54	126.80
2	X	2047	A	C5-C6-N1	6.76	121.08	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2071	C	N3-C4-N4	6.76	122.73	118.00
2	X	2456	G	N3-C4-N9	6.75	130.05	126.00
2	X	2668	A	C6-N1-C2	-6.75	114.55	118.60
2	X	1499	U	N1-C2-N3	6.75	118.95	114.90
2	X	389	A	N7-C8-N9	6.75	117.17	113.80
2	X	341	G	C5-C6-O6	-6.74	124.56	128.60
2	X	494	U	N3-C4-O4	6.74	124.12	119.40
2	X	1065	A	C4-C5-N7	6.74	114.07	110.70
2	X	2065	G	N1-C2-N3	6.74	127.94	123.90
2	X	2048	G	C5-C6-N1	6.74	114.87	111.50
2	X	2480	A	C8-N9-C4	-6.74	103.11	105.80
2	X	1165	C	C5-C6-N1	6.72	124.36	121.00
2	X	590	U	N1-C2-N3	6.72	118.93	114.90
2	X	1263	A	N1-C6-N6	-6.71	114.57	118.60
2	X	2565	C	N3-C4-C5	6.71	124.59	121.90
2	X	696	G	O5'-P-OP2	-6.71	99.66	105.70
2	X	1262	U	C6-N1-C2	6.70	125.02	121.00
2	X	1248	U	N3-C2-O2	-6.70	117.51	122.20
2	X	2738	A	N3-C4-C5	6.69	131.48	126.80
2	X	1705	G	C8-N9-C4	6.69	109.08	106.40
3	Y	68	A	C5-C6-N1	-6.68	114.36	117.70
2	X	1662	A	C5-C6-N6	-6.68	118.36	123.70
2	X	1180	G	C8-N9-C4	-6.67	103.73	106.40
2	X	1810	A	N1-C6-N6	6.67	122.60	118.60
3	Y	95	A	N9-C4-C5	-6.67	103.13	105.80
2	X	492	G	N3-C4-N9	-6.67	122.00	126.00
2	X	666	A	C2-N3-C4	-6.66	107.27	110.60
2	X	533	C	N3-C4-C5	-6.66	119.24	121.90
2	X	1079	U	O5'-P-OP1	-6.66	99.70	105.70
3	Y	114	C	N1-C2-O2	6.66	122.90	118.90
2	X	716	C	N1-C2-N3	6.66	123.86	119.20
2	X	1362	C	N3-C4-N4	-6.66	113.34	118.00
2	X	1957	G	N3-C4-N9	6.66	129.99	126.00
2	X	2048	G	C2-N3-C4	6.66	115.23	111.90
3	Y	79	C	C2-N1-C1'	6.66	126.12	118.80
2	X	376	A	C8-N9-C4	-6.65	103.14	105.80
2	X	2716	U	C5-C6-N1	-6.65	119.37	122.70
2	X	2072	C	N1-C2-O2	-6.65	114.91	118.90
2	X	198	A	C8-N9-C4	6.65	108.46	105.80
2	X	71	A	O5'-P-OP1	-6.65	99.72	105.70
2	X	355	G	C4-C5-C6	6.64	122.79	118.80
2	X	687	G	N1-C6-O6	6.64	123.88	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2298	G	C4-C5-N7	6.64	113.46	110.80
2	X	2682	G	O4'-C1'-N9	6.64	113.51	108.20
2	X	506	A	C2-N3-C4	-6.63	107.28	110.60
2	X	1236	G	C5-C6-N1	-6.63	108.19	111.50
2	X	102	A	N1-C6-N6	6.62	122.57	118.60
2	X	2079	G	N9-C4-C5	-6.62	102.75	105.40
2	X	12	U	C2-N1-C1'	6.62	125.64	117.70
2	X	2861	U	C6-N1-C2	6.61	124.97	121.00
2	X	1368	C	N3-C2-O2	6.61	126.53	121.90
2	X	2074	C	C6-N1-C2	-6.61	117.66	120.30
2	X	373	A	N1-C6-N6	6.60	122.56	118.60
2	X	2044	C	O5'-P-OP2	6.60	118.62	110.70
2	X	2643	C	O5'-P-OP2	6.60	118.62	110.70
2	X	656	G	C8-N9-C4	-6.60	103.76	106.40
2	X	2068	U	C6-N1-C2	-6.60	117.04	121.00
2	X	2608	G	N3-C2-N2	6.60	124.52	119.90
2	X	359	A	C8-N9-C4	-6.59	103.16	105.80
2	X	2639	C	C6-N1-C2	6.59	122.94	120.30
2	X	2667	G	C8-N9-C4	6.59	109.03	106.40
2	X	70	G	P-O3'-C3'	6.59	127.61	119.70
2	X	1370	C	C2-N3-C4	-6.58	116.61	119.90
2	X	1651	C	C6-N1-C2	6.58	122.93	120.30
2	X	781	C	N3-C4-C5	6.58	124.53	121.90
2	X	833	A	C2-N3-C4	-6.57	107.31	110.60
3	Y	82	C	N3-C4-N4	-6.57	113.40	118.00
2	X	2388	A	N1-C6-N6	6.57	122.54	118.60
2	X	717	C	C6-N1-C2	-6.56	117.67	120.30
2	X	2731	C	N1-C2-O2	6.56	122.84	118.90
2	X	12	U	N1-C2-O2	6.56	127.39	122.80
2	X	530	C	C6-N1-C2	6.56	122.92	120.30
2	X	1368	C	N3-C4-C5	6.56	124.52	121.90
2	X	1180	G	N1-C2-N3	-6.56	119.97	123.90
2	X	2283	G	C5-C6-O6	-6.54	124.67	128.60
2	X	205	U	C5-C6-N1	-6.54	119.43	122.70
2	X	355	G	C8-N9-C1'	-6.54	118.50	127.00
2	X	1431	U	C6-N1-C2	-6.54	117.08	121.00
2	X	2045	A	C6-N1-C2	-6.53	114.68	118.60
2	X	2474	G	C4-C5-C6	6.53	122.72	118.80
2	X	648	G	C4-C5-N7	-6.53	108.19	110.80
2	X	181	G	N3-C4-C5	6.52	131.86	128.60
2	X	2839	A	C2-N3-C4	6.51	113.86	110.60
2	X	96	G	N1-C6-O6	6.51	123.81	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2900	C	N3-C2-O2	-6.50	117.35	121.90
2	X	782	C	C6-N1-C2	6.50	122.90	120.30
2	X	2710	C	O5'-P-OP2	-6.50	99.85	105.70
2	X	503	A	C6-C5-N7	-6.50	127.75	132.30
2	X	2545	A	C8-N9-C4	-6.50	103.20	105.80
2	X	1016	G	C8-N9-C4	-6.49	103.80	106.40
2	X	2541	U	C6-N1-C2	6.49	124.90	121.00
16	O	86	LYS	CD-CE-NZ	6.49	126.63	111.70
2	X	790	G	C5-C6-N1	6.49	114.75	111.50
2	X	1165	C	N1-C2-O2	-6.49	115.01	118.90
2	X	779	A	N1-C6-N6	6.49	122.49	118.60
3	Y	2	C	C6-N1-C2	6.48	122.89	120.30
2	X	902	A	N9-C4-C5	6.48	108.39	105.80
3	Y	58	G	C5-N7-C8	-6.48	101.06	104.30
2	X	853	G	N1-C6-O6	6.48	123.79	119.90
2	X	1855	G	C8-N9-C4	-6.48	103.81	106.40
2	X	129	C	C6-N1-C2	6.47	122.89	120.30
2	X	2530	A	C2-N3-C4	6.47	113.83	110.60
2	X	648	G	N1-C6-O6	-6.46	116.02	119.90
2	X	666	A	N3-C4-C5	6.46	131.32	126.80
2	X	2534	C	N1-C2-O2	6.46	122.78	118.90
2	X	955	A	C6-C5-N7	-6.46	127.78	132.30
2	X	871	U	N3-C4-O4	6.45	123.92	119.40
2	X	2035	C	C5-C6-N1	-6.45	117.77	121.00
2	X	706	U	C2-N1-C1'	6.45	125.44	117.70
2	X	1018	A	O5'-P-OP2	-6.45	99.90	105.70
2	X	565	G	C4-C5-N7	6.45	113.38	110.80
2	X	1703	U	C5-C6-N1	-6.45	119.48	122.70
2	X	2083	G	C5-C6-O6	-6.45	124.73	128.60
2	X	1310	A	C8-N9-C4	6.44	108.38	105.80
2	X	1339	U	C2-N1-C1'	-6.43	109.98	117.70
2	X	2064	A	N9-C4-C5	6.43	108.37	105.80
2	X	802	G	C5-C6-O6	-6.42	124.75	128.60
2	X	2481	G	N7-C8-N9	6.42	116.31	113.10
2	X	555	C	C6-N1-C2	-6.42	117.73	120.30
2	X	1025	A	N1-C2-N3	-6.41	126.10	129.30
2	X	2661	A	N7-C8-N9	-6.41	110.60	113.80
2	X	1315	C	C4-C5-C6	6.41	120.60	117.40
3	Y	1	U	N3-C2-O2	-6.40	117.72	122.20
2	X	2749	G	N1-C6-O6	-6.40	116.06	119.90
3	Y	92	G	C5-C6-N1	-6.40	108.30	111.50
2	X	374	U	N1-C2-O2	6.40	127.28	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	82	C	N1-C2-O2	6.40	122.74	118.90
2	X	2474	G	N9-C4-C5	-6.39	102.84	105.40
2	X	715	A	O4'-C1'-N9	-6.39	103.09	108.20
2	X	2066	G	C6-C5-N7	-6.39	126.57	130.40
2	X	2066	G	O5'-P-OP2	-6.39	99.95	105.70
2	X	2065	G	C2-N3-C4	-6.39	108.71	111.90
2	X	2532	G	C8-N9-C4	-6.39	103.84	106.40
2	X	1308	C	C6-N1-C2	6.38	122.85	120.30
3	Y	106	U	N1-C2-O2	6.38	127.26	122.80
2	X	850	G	OP2-P-O3'	6.37	119.22	105.20
2	X	1286	G	N3-C4-N9	6.37	129.82	126.00
2	X	1342	C	C6-N1-C2	6.37	122.85	120.30
2	X	2484	U	N3-C4-O4	-6.36	114.95	119.40
2	X	1285	A	C8-N9-C4	6.36	108.34	105.80
2	X	1296	C	C2-N3-C4	-6.36	116.72	119.90
2	X	846	G	N1-C2-N2	-6.35	110.48	116.20
2	X	1658	A	C2-N3-C4	-6.35	107.42	110.60
2	X	491	C	C6-N1-C2	-6.35	117.76	120.30
2	X	1781	C	N3-C4-N4	6.35	122.45	118.00
2	X	2050	A	C5-C6-N6	6.35	128.78	123.70
3	Y	58	G	C2-N3-C4	-6.34	108.73	111.90
2	X	1814	A	C2-N3-C4	6.34	113.77	110.60
2	X	365	A	N1-C6-N6	-6.34	114.80	118.60
2	X	1277	C	N3-C4-C5	6.34	124.44	121.90
2	X	1746	G	C5-N7-C8	-6.34	101.13	104.30
2	X	503	A	C5-C6-N1	-6.34	114.53	117.70
2	X	1016	G	N7-C8-N9	6.33	116.27	113.10
2	X	1055	A	C5-C6-N6	-6.33	118.63	123.70
2	X	2530	A	C5-C6-N6	-6.33	118.64	123.70
2	X	2757	U	N3-C4-O4	6.33	123.83	119.40
2	X	557	G	C8-N9-C4	6.33	108.93	106.40
2	X	1307	G	N3-C4-C5	6.33	131.76	128.60
2	X	2647	C	C6-N1-C2	-6.33	117.77	120.30
2	X	488	G	N3-C4-C5	-6.32	125.44	128.60
2	X	211	C	N3-C4-C5	6.32	124.43	121.90
2	X	373	A	N7-C8-N9	6.32	116.96	113.80
2	X	794	A	OP2-P-O3'	6.32	119.11	105.20
2	X	2795	C	C6-N1-C2	6.32	122.83	120.30
2	X	1040	A	O5'-P-OP2	-6.32	100.02	105.70
2	X	342	A	N1-C6-N6	6.31	122.39	118.60
2	X	2670	G	N1-C6-O6	-6.31	116.11	119.90
2	X	2492	C	N3-C2-O2	-6.31	117.48	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1401	G	C4-N9-C1'	6.31	134.70	126.50
2	X	1746	G	C6-C5-N7	-6.30	126.62	130.40
2	X	2283	G	C2-N3-C4	6.30	115.05	111.90
2	X	1063	U	N3-C2-O2	-6.30	117.79	122.20
2	X	784	A	C2-N3-C4	6.30	113.75	110.60
2	X	2838	C	C6-N1-C2	6.30	122.82	120.30
2	X	790	G	C2-N3-C4	6.29	115.05	111.90
2	X	2063	C	C5-C6-N1	6.29	124.14	121.00
2	X	2474	G	C5-C6-N1	-6.29	108.36	111.50
2	X	1855	G	C5-C6-O6	6.28	132.37	128.60
2	X	2088	G	N3-C4-N9	6.28	129.77	126.00
2	X	1661	C	C2-N3-C4	-6.28	116.76	119.90
2	X	2522	G	O5'-P-OP1	6.28	118.23	110.70
2	X	2810	A	N1-C6-N6	-6.28	114.83	118.60
2	X	2472	G	N1-C2-N3	-6.27	120.14	123.90
2	X	2762	G	N3-C2-N2	-6.27	115.51	119.90
2	X	243	U	C5-C6-N1	-6.26	119.57	122.70
2	X	1399	C	C6-N1-C2	-6.26	117.80	120.30
2	X	610	U	O5'-P-OP1	-6.26	100.07	105.70
2	X	1454	U	C5-C4-O4	-6.26	122.15	125.90
2	X	2666	A	C6-N1-C2	-6.25	114.85	118.60
2	X	2264	G	N3-C4-N9	6.25	129.75	126.00
2	X	520	G	N9-C4-C5	-6.25	102.90	105.40
2	X	834	A	C8-N9-C4	-6.25	103.30	105.80
2	X	2798	C	N1-C2-O2	-6.25	115.15	118.90
2	X	1378	U	N3-C4-O4	6.24	123.77	119.40
2	X	2084	G	C5-C6-O6	6.24	132.34	128.60
2	X	988	C	C6-N1-C2	6.24	122.80	120.30
2	X	1310	A	N3-C4-C5	6.24	131.17	126.80
2	X	2072	C	N3-C4-N4	6.23	122.36	118.00
2	X	1664	G	N1-C6-O6	6.23	123.64	119.90
2	X	263	G	N3-C4-C5	-6.23	125.49	128.60
2	X	113	U	C2-N1-C1'	6.22	125.17	117.70
2	X	1228	A	N1-C6-N6	6.22	122.33	118.60
2	X	1005	G	C5-C6-O6	6.22	132.33	128.60
2	X	1492	G	N3-C2-N2	-6.22	115.55	119.90
2	X	784	A	C8-N9-C4	6.22	108.29	105.80
2	X	362	C	C6-N1-C2	-6.21	117.81	120.30
2	X	2604	A	C5-C6-N1	-6.21	114.59	117.70
2	X	2589	U	N1-C2-O2	6.21	127.15	122.80
2	X	135	G	N1-C6-O6	6.21	123.62	119.90
2	X	976	U	C5-C6-N1	-6.21	119.60	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	105	G	N1-C2-N2	-6.21	110.61	116.20
2	X	58	G	N1-C6-O6	-6.20	116.18	119.90
2	X	590	U	C5-C4-O4	6.20	129.62	125.90
2	X	365	A	N9-C4-C5	6.19	108.28	105.80
2	X	198	A	N1-C6-N6	6.19	122.31	118.60
2	X	198	A	N9-C4-C5	-6.19	103.32	105.80
2	X	1359	A	O5'-P-OP1	6.18	118.12	110.70
2	X	2064	A	N7-C8-N9	6.18	116.89	113.80
2	X	607	C	C2-N3-C4	-6.18	116.81	119.90
2	X	2546	U	C2-N3-C4	-6.18	123.29	127.00
2	X	2805	A	C8-N9-C4	-6.18	103.33	105.80
2	X	1362	C	C6-N1-C1'	6.18	128.21	120.80
2	X	2085	A	C6-C5-N7	-6.17	127.98	132.30
2	X	621	A	C2-N3-C4	6.17	113.69	110.60
2	X	496	G	N3-C4-C5	-6.17	125.52	128.60
2	X	611	U	N3-C4-O4	6.17	123.72	119.40
2	X	698	U	N3-C2-O2	-6.17	117.88	122.20
2	X	1278	G	N1-C6-O6	-6.16	116.20	119.90
3	Y	105	G	N9-C4-C5	-6.16	102.94	105.40
2	X	2759	G	C8-N9-C4	6.16	108.86	106.40
2	X	2421	C	C6-N1-C2	6.16	122.76	120.30
2	X	354	A	O5'-P-OP2	-6.16	100.16	105.70
2	X	527	G	C5-C6-O6	-6.16	124.91	128.60
2	X	2735	G	C8-N9-C4	-6.16	103.94	106.40
2	X	1243	G	N1-C6-O6	6.15	123.59	119.90
2	X	1313	G	N3-C4-C5	-6.15	125.52	128.60
2	X	2529	G	C5-C6-N1	-6.15	108.42	111.50
2	X	1020	G	N3-C2-N2	6.15	124.21	119.90
2	X	1719	C	N1-C2-O2	-6.15	115.21	118.90
2	X	2877	G	C8-N9-C4	-6.15	103.94	106.40
2	X	1491	C	C5-C6-N1	6.15	124.08	121.00
2	X	2317	G	C5-C6-N1	-6.15	108.42	111.50
3	Y	92	G	N1-C6-O6	6.15	123.59	119.90
2	X	2841	A	C8-N9-C4	6.14	108.26	105.80
2	X	2045	A	C5-C6-N1	6.14	120.77	117.70
2	X	1377	U	C5-C6-N1	-6.14	119.63	122.70
2	X	2661	A	N1-C6-N6	-6.14	114.92	118.60
2	X	865	A	N3-C4-N9	-6.13	122.49	127.40
2	X	587	C	O5'-P-OP2	-6.13	100.18	105.70
2	X	1011	U	C5-C4-O4	-6.13	122.22	125.90
2	X	493	A	C8-N9-C4	-6.12	103.35	105.80
2	X	102	A	C5-N7-C8	-6.12	100.84	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2846	A	C8-N9-C4	6.12	108.25	105.80
2	X	2062	G	N3-C2-N2	6.12	124.18	119.90
2	X	2530	A	O4'-C1'-N9	-6.11	103.31	108.20
2	X	1308	C	C5-C6-N1	-6.11	117.94	121.00
2	X	635	G	O5'-P-OP2	-6.11	100.20	105.70
2	X	1746	G	C5-C6-N1	-6.11	108.45	111.50
2	X	2066	G	C4-C5-N7	6.10	113.24	110.80
2	X	24	G	C4-C5-C6	6.10	122.46	118.80
2	X	1395	G	N1-C2-N2	-6.10	110.71	116.20
2	X	880	A	N1-C6-N6	6.09	122.26	118.60
2	X	2417	U	C5-C6-N1	6.09	125.75	122.70
2	X	2667	G	N9-C4-C5	-6.09	102.96	105.40
2	X	892	U	C5-C6-N1	-6.09	119.65	122.70
2	X	2599	A	C2-N3-C4	-6.09	107.56	110.60
2	X	1377	U	C6-N1-C2	6.08	124.65	121.00
2	X	997	G	N1-C6-O6	-6.08	116.25	119.90
2	X	2841	A	O5'-P-OP1	-6.08	100.23	105.70
2	X	2740	A	N7-C8-N9	6.08	116.84	113.80
2	X	885	C	O5'-P-OP2	-6.08	100.23	105.70
2	X	1351	C	OP2-P-O3'	6.08	118.56	105.20
2	X	1065	A	N3-C4-C5	6.07	131.05	126.80
2	X	2854	A	C5-C6-N6	-6.07	118.84	123.70
2	X	2269	G	N1-C6-O6	6.07	123.54	119.90
2	X	726	G	C4-C5-N7	-6.06	108.38	110.80
2	X	621	A	C5-C6-N1	6.06	120.73	117.70
2	X	1339	U	C6-N1-C2	6.06	124.64	121.00
2	X	1399	C	C5-C6-N1	6.06	124.03	121.00
2	X	1695	G	N3-C2-N2	-6.06	115.66	119.90
2	X	1704	C	C6-N1-C2	6.06	122.72	120.30
3	Y	92	G	N1-C2-N2	6.05	121.65	116.20
2	X	515	G	C5-C6-O6	-6.05	124.97	128.60
2	X	2828	U	O5'-P-OP2	6.05	117.96	110.70
2	X	2470	C	C2-N3-C4	-6.05	116.88	119.90
2	X	2027	G	OP2-P-O3'	6.05	118.50	105.20
2	X	661	U	C5-C6-N1	6.04	125.72	122.70
2	X	865	A	C2-N3-C4	-6.04	107.58	110.60
2	X	1855	G	N9-C4-C5	6.04	107.82	105.40
2	X	1723	A	N1-C6-N6	6.04	122.22	118.60
2	X	891	A	C5-C6-N1	-6.04	114.68	117.70
2	X	1492	G	N1-C6-O6	6.04	123.52	119.90
2	X	2609	G	C6-C5-N7	-6.04	126.78	130.40
3	Y	98	G	N3-C4-C5	6.04	131.62	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	616	G	C5-C6-N1	6.04	114.52	111.50
2	X	637	U	C5-C4-O4	6.04	129.52	125.90
2	X	2456	G	N9-C4-C5	-6.04	102.99	105.40
2	X	255	G	O5'-P-OP2	-6.03	100.27	105.70
2	X	2046	U	N3-C2-O2	6.03	126.42	122.20
2	X	1805	U	N3-C2-O2	6.03	126.42	122.20
3	Y	76	A	C8-N9-C4	-6.03	103.39	105.80
3	Y	105	G	N3-C2-N2	6.03	124.12	119.90
2	X	1320	G	C6-C5-N7	-6.03	126.78	130.40
2	X	778	G	C5-C6-O6	-6.03	124.98	128.60
2	X	712	U	O5'-P-OP1	-6.02	100.28	105.70
2	X	2042	A	C8-N9-C4	-6.02	103.39	105.80
2	X	2048	G	O5'-P-OP2	6.02	117.92	110.70
2	X	496	G	N1-C6-O6	6.01	123.51	119.90
2	X	1175	G	N3-C2-N2	6.01	124.11	119.90
2	X	1410	A	N1-C6-N6	-6.01	114.99	118.60
2	X	1050	C	N3-C4-N4	-6.01	113.80	118.00
2	X	1704	C	N3-C4-C5	6.01	124.30	121.90
2	X	2039	G	C2-N3-C4	-6.00	108.90	111.90
2	X	598	G	C8-N9-C1'	-6.00	119.19	127.00
2	X	996	G	C6-C5-N7	-6.00	126.80	130.40
2	X	2030	A	N1-C6-N6	-6.00	115.00	118.60
2	X	2724	G	N1-C2-N3	6.00	127.50	123.90
2	X	650	U	C2-N1-C1'	-5.99	110.51	117.70
2	X	1024	A	N1-C6-N6	5.99	122.20	118.60
2	X	1496	G	C6-C5-N7	5.99	134.00	130.40
2	X	1646	U	N3-C4-C5	-5.99	111.01	114.60
2	X	2642	U	C2-N1-C1'	5.99	124.89	117.70
2	X	1360	G	C8-N9-C4	5.99	108.80	106.40
2	X	2088	G	C5-C6-O6	-5.99	125.01	128.60
2	X	2591	A	OP1-P-OP2	5.99	128.58	119.60
2	X	199	A	C6-C5-N7	-5.99	128.11	132.30
2	X	890	G	C2-N3-C4	-5.99	108.91	111.90
2	X	1004	A	C2-N3-C4	-5.98	107.61	110.60
2	X	1543	G	N3-C4-C5	-5.98	125.61	128.60
2	X	1593	G	C8-N9-C1'	-5.98	119.22	127.00
2	X	374	U	C2-N1-C1'	5.98	124.87	117.70
2	X	1307	G	N3-C2-N2	-5.98	115.72	119.90
2	X	1596	G	N3-C4-N9	5.97	129.59	126.00
2	X	600	U	N3-C2-O2	-5.97	118.02	122.20
2	X	36	G	N3-C4-C5	-5.97	125.62	128.60
2	X	515	G	O4'-C1'-N9	5.97	112.97	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	52	A	O5'-P-OP2	-5.97	100.33	105.70
2	X	825	G	N9-C4-C5	-5.97	103.01	105.40
2	X	2442	G	N1-C6-O6	5.97	123.48	119.90
2	X	533	C	C6-N1-C2	-5.96	117.91	120.30
2	X	598	G	N1-C6-O6	5.96	123.48	119.90
2	X	983	G	N9-C4-C5	5.96	107.79	105.40
2	X	1574	G	C4-N9-C1'	5.96	134.25	126.50
2	X	2591	A	O5'-P-OP2	-5.96	100.33	105.70
2	X	834	A	C6-N1-C2	-5.96	115.02	118.60
2	X	1699	A	N1-C6-N6	5.96	122.18	118.60
2	X	2086	A	C6-C5-N7	-5.96	128.13	132.30
2	X	11	U	C6-N1-C2	-5.96	117.42	121.00
2	X	608	C	C5-C6-N1	5.96	123.98	121.00
2	X	253	G	OP1-P-OP2	-5.96	110.67	119.60
2	X	2062	G	C4-C5-N7	5.96	113.18	110.80
2	X	19	G	N1-C6-O6	5.95	123.47	119.90
2	X	341	G	C6-C5-N7	-5.95	126.83	130.40
2	X	530	C	N3-C2-O2	5.95	126.07	121.90
2	X	1566	G	N3-C4-C5	5.95	131.57	128.60
2	X	655	A	N1-C6-N6	5.95	122.17	118.60
2	X	2046	U	C2-N1-C1'	-5.95	110.56	117.70
2	X	2304	G	C4-N9-C1'	5.95	134.23	126.50
3	Y	68	A	N3-C4-C5	5.94	130.96	126.80
2	X	90	A	P-O3'-C3'	5.94	126.83	119.70
2	X	496	G	N3-C4-N9	5.94	129.57	126.00
2	X	1245	G	N1-C6-O6	5.94	123.46	119.90
2	X	610	U	C5-C4-O4	5.93	129.46	125.90
2	X	1351	C	C6-N1-C2	-5.93	117.93	120.30
2	X	825	G	C4-C5-N7	5.93	113.17	110.80
2	X	2394	G	C8-N9-C4	-5.93	104.03	106.40
2	X	2482	G	N3-C2-N2	-5.93	115.75	119.90
2	X	2543	G	C5-C6-N1	5.93	114.46	111.50
2	X	70	G	N3-C4-C5	-5.93	125.64	128.60
2	X	350	G	C2-N3-C4	5.93	114.86	111.90
2	X	633	A	C5-N7-C8	-5.93	100.94	103.90
3	Y	104	C	N3-C2-O2	-5.93	117.75	121.90
2	X	1205	U	N1-C2-N3	5.92	118.45	114.90
2	X	959	C	N3-C4-C5	-5.92	119.53	121.90
2	X	1295	C	C6-N1-C2	-5.92	117.93	120.30
2	X	2321	C	C6-N1-C2	5.92	122.67	120.30
2	X	687	G	C6-C5-N7	-5.91	126.85	130.40
2	X	2624	G	C5-C6-O6	5.91	132.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	93	C	O4'-C1'-N1	5.91	112.93	108.20
2	X	831	C	C6-N1-C2	5.91	122.66	120.30
2	X	2013	G	C8-N9-C4	-5.91	104.04	106.40
2	X	520	G	C8-N9-C4	5.91	108.76	106.40
2	X	537	A	C2-N3-C4	-5.90	107.65	110.60
2	X	614	U	O5'-P-OP1	-5.90	100.39	105.70
2	X	1006	G	OP2-P-O3'	5.90	118.17	105.20
2	X	834	A	N3-C4-C5	-5.90	122.67	126.80
2	X	2910	G	N1-C6-O6	-5.90	116.36	119.90
2	X	592	A	C2-N3-C4	5.89	113.55	110.60
2	X	2637	C	N3-C2-O2	-5.89	117.77	121.90
2	X	2661	A	C5-C6-N1	5.89	120.65	117.70
2	X	1229	G	N3-C4-C5	5.89	131.55	128.60
3	Y	79	C	C6-N1-C1'	-5.89	113.73	120.80
2	X	793	G	O5'-P-OP2	-5.89	100.40	105.70
2	X	846	G	N3-C4-N9	5.89	129.53	126.00
2	X	199	A	C5-N7-C8	-5.89	100.96	103.90
2	X	687	G	C4-C5-C6	5.89	122.33	118.80
2	X	12	U	OP2-P-O3'	5.88	118.14	105.20
2	X	2851	G	C8-N9-C4	-5.88	104.05	106.40
2	X	305	A	N1-C6-N6	-5.87	115.08	118.60
2	X	626	G	C8-N9-C4	5.87	108.75	106.40
2	X	2028	A	C5-C6-N6	-5.87	119.00	123.70
2	X	2279	G	C6-C5-N7	-5.87	126.88	130.40
2	X	696	G	O5'-P-OP1	5.87	117.74	110.70
2	X	1310	A	C2-N3-C4	-5.86	107.67	110.60
2	X	2545	A	C2-N3-C4	5.86	113.53	110.60
2	X	2415	A	C8-N9-C4	-5.86	103.46	105.80
2	X	660	A	O5'-P-OP2	5.86	117.73	110.70
2	X	2062	G	OP1-P-OP2	5.86	128.38	119.60
2	X	2068	U	N1-C2-N3	5.86	118.41	114.90
2	X	687	G	C8-N9-C4	-5.85	104.06	106.40
2	X	1746	G	C4-C5-N7	5.85	113.14	110.80
2	X	1975	G	N1-C6-O6	5.85	123.41	119.90
3	Y	71	A	N1-C6-N6	5.85	122.11	118.60
2	X	2480	A	N7-C8-N9	5.85	116.73	113.80
2	X	1352	C	O5'-P-OP2	5.84	117.71	110.70
2	X	561	C	O5'-P-OP1	5.84	117.71	110.70
3	Y	101	G	C2-N3-C4	-5.84	108.98	111.90
2	X	631	U	N1-C2-N3	5.84	118.41	114.90
2	X	1017	A	N7-C8-N9	5.84	116.72	113.80
3	Y	93	C	N1-C2-N3	5.84	123.29	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2718	C	C6-N1-C2	-5.84	117.97	120.30
2	X	1201	G	C6-C5-N7	-5.83	126.90	130.40
2	X	2709	U	N1-C2-N3	5.83	118.40	114.90
2	X	573	A	O5'-P-OP1	5.82	117.68	110.70
2	X	1065	A	C4-C5-C6	5.82	119.91	117.00
2	X	1418	G	N7-C8-N9	5.82	116.01	113.10
2	X	613	G	N3-C4-C5	-5.82	125.69	128.60
2	X	1231	A	C8-N9-C4	5.82	108.13	105.80
2	X	1356	G	C6-N1-C2	-5.82	121.61	125.10
2	X	2033	C	N3-C4-N4	-5.82	113.93	118.00
2	X	890	G	N3-C4-N9	-5.82	122.51	126.00
2	X	1855	G	C4-C5-N7	-5.82	108.47	110.80
2	X	2642	U	C5-C6-N1	5.81	125.61	122.70
2	X	2304	G	C8-N9-C1'	-5.81	119.45	127.00
3	Y	103	A	C6-N1-C2	5.81	122.09	118.60
2	X	1288	G	C8-N9-C4	5.81	108.72	106.40
2	X	2611	U	C5-C6-N1	5.81	125.60	122.70
2	X	657	U	N1-C2-N3	-5.81	111.42	114.90
2	X	1092	A	N1-C6-N6	-5.80	115.12	118.60
3	Y	109	C	N1-C2-O2	5.80	122.38	118.90
2	X	2448	G	C2-N3-C4	5.80	114.80	111.90
2	X	681	G	C6-C5-N7	-5.80	126.92	130.40
2	X	2565	C	C6-N1-C2	5.80	122.62	120.30
2	X	2850	G	N3-C4-N9	5.80	129.48	126.00
2	X	965	G	N1-C6-O6	-5.80	116.42	119.90
2	X	1286	G	C6-C5-N7	-5.79	126.92	130.40
2	X	494	U	N1-C2-O2	-5.79	118.75	122.80
2	X	1017	A	N9-C4-C5	5.79	108.12	105.80
2	X	1342	C	N3-C4-C5	5.79	124.22	121.90
2	X	1381	U	N3-C4-O4	5.79	123.45	119.40
2	X	598	G	C8-N9-C4	5.79	108.72	106.40
2	X	2063	C	N1-C2-O2	-5.79	115.43	118.90
2	X	2648	G	C4-C5-C6	-5.78	115.33	118.80
2	X	1005	G	C4-C5-N7	-5.78	108.49	110.80
2	X	1257	G	N3-C2-N2	-5.78	115.86	119.90
2	X	2715	G	C5-C6-N1	-5.77	108.61	111.50
2	X	828	A	N7-C8-N9	5.77	116.69	113.80
2	X	70	G	C8-N9-C4	-5.77	104.09	106.40
2	X	2344	C	C6-N1-C2	-5.77	117.99	120.30
2	X	2391	C	C5-C6-N1	-5.77	118.12	121.00
2	X	992	A	C2-N3-C4	-5.77	107.72	110.60
2	X	829	U	N1-C2-O2	-5.76	118.77	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	35	G	N7-C8-N9	-5.76	110.22	113.10
2	X	1422	A	C8-N9-C4	5.76	108.11	105.80
2	X	1566	G	N3-C2-N2	-5.76	115.87	119.90
2	X	2079	G	C8-N9-C1'	-5.76	119.51	127.00
2	X	1746	G	N7-C8-N9	5.75	115.98	113.10
2	X	2017	C	N1-C2-O2	-5.75	115.45	118.90
2	X	496	G	C6-C5-N7	-5.75	126.95	130.40
2	X	1234	G	O5'-P-OP2	-5.75	100.52	105.70
2	X	1357	G	C5-C6-N1	-5.75	108.62	111.50
2	X	1662	A	C8-N9-C4	-5.75	103.50	105.80
2	X	1490	G	O5'-P-OP2	-5.75	100.53	105.70
2	X	32	C	N3-C4-C5	5.75	124.20	121.90
2	X	604	G	C4-C5-C6	5.75	122.25	118.80
2	X	721	A	C8-N9-C4	-5.75	103.50	105.80
2	X	1659	C	N3-C4-C5	-5.75	119.60	121.90
2	X	1566	G	N3-C4-N9	-5.75	122.55	126.00
2	X	21	A	N1-C6-N6	5.74	122.05	118.60
2	X	726	G	N1-C6-O6	-5.74	116.45	119.90
2	X	955	A	C4-C5-C6	5.74	119.87	117.00
2	X	2013	G	C6-C5-N7	-5.74	126.95	130.40
2	X	2278	G	C4-C5-C6	5.74	122.25	118.80
2	X	2845	G	N7-C8-N9	5.74	115.97	113.10
2	X	2911	A	C8-N9-C4	5.74	108.10	105.80
2	X	1258	A	O5'-P-OP2	-5.74	100.53	105.70
2	X	1805	U	N1-C2-N3	-5.74	111.45	114.90
2	X	1318	G	N3-C4-N9	5.74	129.44	126.00
2	X	27	G	C8-N9-C4	5.74	108.69	106.40
2	X	610	U	C6-N1-C1'	5.74	129.23	121.20
3	Y	105	G	C8-N9-C1'	-5.74	119.54	127.00
2	X	611	U	C4-C5-C6	5.73	123.14	119.70
2	X	2861	U	C5-C6-N1	-5.73	119.83	122.70
2	X	587	C	C5-C6-N1	-5.73	118.14	121.00
2	X	1432	A	N1-C6-N6	-5.72	115.17	118.60
2	X	2716	U	C2-N1-C1'	-5.72	110.83	117.70
2	X	2728	U	C6-N1-C2	-5.72	117.57	121.00
2	X	17	G	C5-C6-O6	-5.72	125.17	128.60
2	X	363	A	C6-C5-N7	-5.72	128.30	132.30
2	X	2077	C	N3-C2-O2	-5.72	117.90	121.90
2	X	661	U	P-O3'-C3'	5.72	126.56	119.70
2	X	492	G	N3-C4-C5	5.72	131.46	128.60
2	X	697	U	C6-N1-C2	-5.72	117.57	121.00
2	X	1288	G	N7-C8-N9	-5.72	110.24	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1360	G	C5-C6-N1	-5.72	108.64	111.50
2	X	2683	U	C5-C4-O4	-5.72	122.47	125.90
2	X	1574	G	N9-C4-C5	5.71	107.69	105.40
2	X	2044	C	C6-N1-C2	-5.71	118.02	120.30
2	X	2632	U	C5-C6-N1	5.71	125.56	122.70
2	X	73	A	C8-N9-C4	-5.71	103.52	105.80
2	X	1689	G	C6-C5-N7	5.71	133.83	130.40
2	X	992	A	C5-C6-N1	-5.71	114.85	117.70
2	X	1700	C	C5-C6-N1	5.71	123.85	121.00
2	X	2539	C	O5'-P-OP1	-5.71	100.56	105.70
2	X	181	G	N1-C6-O6	5.71	123.32	119.90
2	X	662	G	O5'-P-OP1	-5.70	100.57	105.70
2	X	1171	A	C5-C6-N6	5.70	128.26	123.70
2	X	2086	A	C4-C5-N7	5.70	113.55	110.70
2	X	2708	C	N3-C4-C5	5.70	124.18	121.90
2	X	2740	A	O4'-C1'-N9	-5.70	103.64	108.20
2	X	794	A	N1-C6-N6	5.70	122.02	118.60
2	X	1033	G	OP1-P-O3'	5.70	117.74	105.20
2	X	708	G	O5'-P-OP2	-5.70	100.57	105.70
2	X	592	A	N1-C6-N6	-5.69	115.18	118.60
2	X	875	G	C5-C6-O6	5.69	132.02	128.60
2	X	1506	C	N3-C2-O2	-5.69	117.92	121.90
2	X	253	G	C8-N9-C4	-5.69	104.12	106.40
2	X	820	G	O5'-P-OP2	-5.69	100.58	105.70
3	Y	86	C	N1-C2-N3	5.69	123.18	119.20
2	X	1643	C	C6-N1-C2	5.68	122.57	120.30
2	X	2072	C	C5-C4-N4	-5.68	116.22	120.20
2	X	854	G	C5-C6-N1	-5.68	108.66	111.50
2	X	2535	G	C5-C6-O6	-5.68	125.19	128.60
2	X	1711	G	C2-N3-C4	5.68	114.74	111.90
2	X	19	G	OP1-P-OP2	-5.67	111.09	119.60
2	X	580	C	N3-C2-O2	5.67	125.87	121.90
4	B	204	PRO	N-CA-C	-5.67	97.35	112.10
2	X	721	A	C4-C5-C6	5.67	119.84	117.00
2	X	1827	C	N3-C4-C5	5.67	124.17	121.90
2	X	1201	G	C5-C6-O6	-5.67	125.20	128.60
2	X	1704	C	N1-C2-O2	5.67	122.30	118.90
2	X	2039	G	N1-C2-N3	5.67	127.30	123.90
2	X	2050	A	N9-C4-C5	5.67	108.07	105.80
2	X	2278	G	N3-C4-N9	5.67	129.40	126.00
2	X	350	G	C5-C6-N1	5.67	114.33	111.50
2	X	959	C	C6-N1-C2	-5.67	118.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1320	G	C5-C6-O6	-5.67	125.20	128.60
2	X	871	U	C4-C5-C6	5.66	123.10	119.70
2	X	687	G	N7-C8-N9	5.66	115.93	113.10
2	X	2432	G	C8-N9-C4	5.66	108.66	106.40
2	X	1357	G	C8-N9-C4	-5.66	104.14	106.40
2	X	2449	C	C5-C6-N1	5.66	123.83	121.00
2	X	880	A	C5-C6-N6	-5.65	119.18	123.70
2	X	1012	G	C5-C6-N1	-5.65	108.68	111.50
2	X	988	C	OP1-P-OP2	-5.65	111.13	119.60
3	Y	103	A	N1-C2-N3	-5.65	126.48	129.30
2	X	1817	C	O5'-P-OP2	5.64	117.47	110.70
2	X	2054	G	C5-C6-O6	-5.64	125.22	128.60
2	X	577	A	C5-C6-N1	5.64	120.52	117.70
2	X	2333	U	N1-C2-O2	5.63	126.75	122.80
2	X	1065	A	N3-C4-N9	-5.63	122.89	127.40
2	X	1506	C	N1-C2-O2	5.63	122.28	118.90
2	X	1512	U	N1-C2-O2	5.63	126.74	122.80
2	X	1719	C	N3-C4-C5	-5.63	119.65	121.90
2	X	1721	A	C2-N3-C4	-5.63	107.78	110.60
2	X	2473	G	O5'-P-OP2	-5.63	100.63	105.70
2	X	1225	G	N1-C2-N3	5.63	127.28	123.90
2	X	588	G	C5-C6-O6	-5.62	125.23	128.60
2	X	644	C	C5-C6-N1	5.62	123.81	121.00
2	X	113	U	N1-C2-O2	5.62	126.73	122.80
2	X	2064	A	N1-C2-N3	5.62	132.11	129.30
2	X	657	U	N3-C2-O2	-5.62	118.27	122.20
2	X	1171	A	N9-C4-C5	5.62	108.05	105.80
2	X	1175	G	N3-C4-C5	-5.62	125.79	128.60
2	X	2755	U	N1-C2-O2	-5.62	118.87	122.80
3	Y	109	C	N3-C2-O2	-5.61	117.97	121.90
2	X	718	C	N3-C4-N4	5.61	121.93	118.00
2	X	735	C	C6-N1-C2	-5.61	118.06	120.30
2	X	1011	U	C5-C6-N1	5.61	125.50	122.70
2	X	2034	U	C4-C5-C6	5.61	123.06	119.70
2	X	2848	G	N1-C6-O6	5.61	123.26	119.90
2	X	257	G	N1-C2-N2	-5.60	111.16	116.20
2	X	2241	C	C6-N1-C2	5.60	122.54	120.30
2	X	576	U	N1-C2-O2	5.60	126.72	122.80
2	X	1701	U	O5'-P-OP1	-5.60	100.66	105.70
3	Y	85	A	C8-N9-C4	5.59	108.04	105.80
2	X	1318	G	C6-C5-N7	-5.59	127.05	130.40
2	X	696	G	C6-C5-N7	5.59	133.75	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1279	C	N3-C4-N4	5.59	121.91	118.00
2	X	1357	G	C4-C5-N7	-5.59	108.56	110.80
2	X	2477	A	N9-C4-C5	5.59	108.04	105.80
2	X	2851	G	N9-C4-C5	5.59	107.64	105.40
2	X	1484	G	C4-C5-N7	5.59	113.03	110.80
2	X	1318	G	C4-N9-C1'	5.58	133.76	126.50
2	X	2904	U	N1-C2-O2	5.58	126.71	122.80
2	X	698	U	N1-C2-O2	5.58	126.71	122.80
3	Y	104	C	N1-C2-O2	5.58	122.25	118.90
2	X	1076	A	N1-C6-N6	5.58	121.95	118.60
2	X	2027	G	N1-C2-N2	-5.58	111.18	116.20
2	X	2841	A	OP1-P-OP2	5.58	127.97	119.60
3	Y	58	G	C4-C5-N7	5.58	113.03	110.80
3	Y	76	A	N7-C8-N9	5.58	116.59	113.80
2	X	70	G	C4-N9-C1'	5.58	133.75	126.50
2	X	463	C	C6-N1-C2	-5.58	118.07	120.30
2	X	1035	C	C6-N1-C2	5.58	122.53	120.30
2	X	1574	G	N3-C4-C5	-5.57	125.81	128.60
2	X	2738	A	N3-C4-N9	-5.57	122.94	127.40
2	X	1454	U	N3-C4-O4	5.57	123.30	119.40
2	X	1490	G	N3-C4-N9	5.57	129.34	126.00
2	X	496	G	C5-C6-O6	-5.57	125.26	128.60
2	X	2036	G	N1-C6-O6	-5.57	116.56	119.90
2	X	683	G	N1-C2-N3	5.56	127.24	123.90
2	X	1497	A	N1-C6-N6	-5.56	115.26	118.60
2	X	2024	A	N1-C2-N3	5.56	132.08	129.30
2	X	2084	G	N1-C2-N3	5.56	127.24	123.90
2	X	852	U	N1-C2-N3	5.56	118.23	114.90
2	X	1245	G	C5-C6-O6	-5.56	125.27	128.60
2	X	2089	A	N9-C4-C5	-5.56	103.58	105.80
2	X	2608	G	C5-C6-O6	5.56	131.93	128.60
2	X	718	C	C5-C6-N1	5.56	123.78	121.00
2	X	1320	G	C8-N9-C4	-5.56	104.18	106.40
2	X	656	G	N9-C4-C5	5.55	107.62	105.40
2	X	1039	C	C2-N1-C1'	-5.55	112.70	118.80
2	X	865	A	N9-C4-C5	5.55	108.02	105.80
2	X	1022	G	N1-C2-N2	-5.54	111.21	116.20
2	X	1025	A	C5-C6-N1	5.54	120.47	117.70
2	X	1803	G	OP2-P-O3'	5.54	117.39	105.20
2	X	2595	C	C5-C4-N4	-5.54	116.32	120.20
5	C	189	ALA	N-CA-C	-5.54	96.04	111.00
2	X	2093	C	O5'-P-OP1	5.54	117.35	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	666	A	C5-C6-N1	-5.53	114.93	117.70
2	X	1306	A	N1-C2-N3	5.53	132.07	129.30
2	X	2717	A	O5'-P-OP1	-5.53	100.72	105.70
2	X	1254	C	C6-N1-C2	-5.53	118.09	120.30
2	X	2039	G	N1-C6-O6	5.53	123.22	119.90
2	X	2661	A	C5-N7-C8	5.53	106.67	103.90
2	X	2089	A	N7-C8-N9	5.53	116.56	113.80
2	X	2470	C	N1-C2-N3	5.53	123.07	119.20
2	X	611	U	N3-C4-C5	-5.52	111.29	114.60
2	X	1838	G	N3-C4-C5	-5.52	125.84	128.60
2	X	527	G	C6-C5-N7	-5.52	127.09	130.40
2	X	541	G	C5-C6-O6	-5.52	125.29	128.60
2	X	575	G	N7-C8-N9	5.52	115.86	113.10
2	X	983	G	C4-C5-N7	-5.52	108.59	110.80
2	X	1593	G	C2-N3-C4	5.52	114.66	111.90
2	X	2388	A	C5-N7-C8	-5.52	101.14	103.90
2	X	519	G	C4-C5-C6	5.52	122.11	118.80
2	X	627	C	N3-C4-N4	5.52	121.86	118.00
2	X	637	U	N3-C4-O4	-5.52	115.54	119.40
2	X	1814	A	N3-C4-C5	-5.52	122.94	126.80
2	X	557	G	O4'-C1'-N9	5.52	112.61	108.20
2	X	497	U	O4'-C1'-N1	5.51	112.61	108.20
2	X	1268	C	C5-C4-N4	-5.51	116.34	120.20
2	X	30	G	N1-C6-O6	5.51	123.21	119.90
2	X	2079	G	C4-N9-C1'	5.51	133.67	126.50
3	Y	84	U	N3-C2-O2	-5.51	118.34	122.20
2	X	659	A	N1-C2-N3	-5.51	126.54	129.30
2	X	1414	G	C5-C6-O6	5.51	131.91	128.60
2	X	1360	G	N3-C4-C5	5.51	131.35	128.60
2	X	1332	C	OP2-P-O3'	5.51	117.32	105.20
2	X	865	A	C5-C6-N1	-5.51	114.95	117.70
2	X	688	A	C8-N9-C4	-5.50	103.60	105.80
2	X	199	A	N7-C8-N9	5.50	116.55	113.80
2	X	263	G	C4-N9-C1'	5.50	133.65	126.50
2	X	988	C	N3-C4-N4	-5.50	114.15	118.00
2	X	2280	G	OP2-P-O3'	5.50	117.30	105.20
2	X	2668	A	C5-C6-N1	5.50	120.45	117.70
2	X	1967	U	C6-N1-C2	-5.50	117.70	121.00
2	X	516	A	C4-C5-C6	5.50	119.75	117.00
2	X	1291	A	C5-N7-C8	5.50	106.65	103.90
2	X	2859	G	N3-C4-N9	5.50	129.30	126.00
2	X	1312	A	OP1-P-O3'	5.49	117.29	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	515	G	N3-C4-C5	5.49	131.35	128.60
2	X	1168	C	C6-N1-C2	5.49	122.50	120.30
2	X	1304	G	C8-N9-C4	5.49	108.59	106.40
2	X	1044	A	O5'-P-OP1	-5.49	100.76	105.70
2	X	2709	U	C2-N3-C4	-5.49	123.71	127.00
2	X	791	U	N1-C2-N3	5.48	118.19	114.90
2	X	1262	U	C5-C4-O4	-5.48	122.61	125.90
2	X	2298	G	C8-N9-C1'	-5.48	119.87	127.00
10	I	37	GLY	N-CA-C	-5.48	99.39	113.10
2	X	639	U	N1-C2-O2	5.48	126.64	122.80
2	X	1596	G	C2-N3-C4	5.48	114.64	111.90
2	X	2292	U	N1-C2-O2	5.48	126.64	122.80
2	X	1806	U	C2-N3-C4	-5.48	123.71	127.00
2	X	2641	A	N1-C2-N3	5.48	132.04	129.30
2	X	375	A	C2-N3-C4	5.48	113.34	110.60
2	X	1362	C	C5-C4-N4	5.48	124.03	120.20
2	X	1519	U	N3-C2-O2	-5.48	118.37	122.20
2	X	1719	C	N1-C2-N3	5.48	123.03	119.20
2	X	2045	A	N1-C6-N6	-5.48	115.31	118.60
2	X	2540	A	N1-C6-N6	-5.48	115.31	118.60
3	Y	77	G	C5-C6-O6	-5.48	125.31	128.60
2	X	722	A	C4-C5-C6	-5.47	114.26	117.00
2	X	260	A	C8-N9-C4	-5.47	103.61	105.80
2	X	503	A	O4'-C1'-N9	5.47	112.58	108.20
2	X	2742	C	O5'-P-OP2	-5.47	100.77	105.70
2	X	2766	U	N3-C2-O2	-5.47	118.37	122.20
2	X	2068	U	N3-C4-O4	5.47	123.23	119.40
2	X	1660	A	N1-C6-N6	-5.47	115.32	118.60
2	X	15	G	C2-N3-C4	-5.47	109.17	111.90
2	X	599	A	C5-C6-N1	5.47	120.43	117.70
2	X	2658	G	C8-N9-C4	-5.47	104.21	106.40
2	X	1977	G	O5'-P-OP1	-5.46	100.78	105.70
2	X	2599	A	N9-C4-C5	-5.46	103.61	105.80
2	X	2048	G	O5'-P-OP1	-5.46	100.78	105.70
2	X	834	A	N9-C4-C5	5.46	107.98	105.80
2	X	782	C	N3-C4-C5	5.46	124.08	121.90
2	X	825	G	N1-C6-O6	5.46	123.17	119.90
2	X	2277	G	C8-N9-C4	-5.46	104.22	106.40
2	X	2575	G	N1-C2-N2	5.46	121.11	116.20
2	X	508	C	OP2-P-O3'	5.45	117.20	105.20
2	X	1195	A	C2-N3-C4	-5.45	107.87	110.60
2	X	1075	G	N3-C4-N9	-5.45	122.73	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	778	G	N9-C4-C5	-5.45	103.22	105.40
3	Y	82	C	C5-C4-N4	5.45	124.02	120.20
2	X	59	U	N1-C2-N3	5.45	118.17	114.90
2	X	727	G	C4-N9-C1'	5.45	133.58	126.50
2	X	1304	G	N7-C8-N9	-5.45	110.38	113.10
2	X	2094	G	O5'-P-OP1	-5.45	100.80	105.70
2	X	43	A	O4'-C1'-N9	5.44	112.55	108.20
2	X	617	A	N7-C8-N9	-5.44	111.08	113.80
2	X	2530	A	N1-C6-N6	5.44	121.87	118.60
2	X	702	U	N3-C4-C5	-5.44	111.34	114.60
2	X	1318	G	C6-N1-C2	-5.44	121.84	125.10
2	X	226	A	N1-C6-N6	-5.44	115.34	118.60
2	X	2686	G	N3-C4-C5	5.44	131.32	128.60
2	X	698	U	C2-N1-C1'	5.44	124.22	117.70
2	X	1466	G	C8-N9-C4	-5.44	104.22	106.40
2	X	850	G	N3-C2-N2	5.44	123.70	119.90
2	X	1010	G	N1-C2-N2	-5.43	111.31	116.20
2	X	1016	G	C4-N9-C1'	5.43	133.56	126.50
2	X	2728	U	C5-C6-N1	5.43	125.42	122.70
2	X	2068	U	N1-C2-O2	-5.43	119.00	122.80
2	X	443	U	C6-N1-C2	-5.43	117.74	121.00
2	X	779	A	C2-N3-C4	-5.43	107.89	110.60
2	X	2027	G	N9-C4-C5	-5.43	103.23	105.40
2	X	561	C	C5-C4-N4	-5.42	116.40	120.20
2	X	1339	U	C5-C6-N1	-5.42	119.99	122.70
2	X	2590	U	C5-C4-O4	5.42	129.15	125.90
2	X	400	C	C6-N1-C2	-5.42	118.13	120.30
2	X	1007	U	C6-N1-C2	-5.42	117.75	121.00
2	X	1231	A	C2-N3-C4	-5.42	107.89	110.60
2	X	70	G	C2-N3-C4	5.42	114.61	111.90
2	X	2752	A	C4-C5-C6	5.42	119.71	117.00
3	Y	97	A	N1-C6-N6	-5.42	115.35	118.60
2	X	806	A	C8-N9-C4	-5.41	103.64	105.80
3	Y	86	C	C5-C4-N4	5.41	123.99	120.20
2	X	1026	C	C6-N1-C2	5.41	122.46	120.30
3	Y	106	U	N3-C4-O4	-5.41	115.61	119.40
2	X	597	U	C2-N1-C1'	-5.41	111.21	117.70
2	X	983	G	C5-C6-O6	5.41	131.85	128.60
2	X	1045	A	O5'-P-OP1	5.41	117.19	110.70
2	X	2063	C	C5-C4-N4	-5.41	116.42	120.20
2	X	1865	C	N3-C2-O2	-5.41	118.12	121.90
2	X	628	G	N7-C8-N9	5.40	115.80	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	6	LEU	CA-CB-CG	5.40	127.73	115.30
2	X	370	G	N1-C6-O6	5.40	123.14	119.90
2	X	702	U	N1-C2-N3	5.40	118.14	114.90
2	X	268	A	C8-N9-C4	5.40	107.96	105.80
2	X	1865	C	N1-C2-O2	5.40	122.14	118.90
2	X	2650	G	C4-C5-N7	-5.39	108.64	110.80
2	X	1429	G	N9-C4-C5	-5.39	103.25	105.40
2	X	1488	A	C2-N3-C4	5.39	113.29	110.60
2	X	615	A	C5-C6-N6	5.38	128.01	123.70
2	X	2635	G	N9-C4-C5	5.38	107.55	105.40
2	X	2056	G	N3-C2-N2	5.38	123.67	119.90
2	X	847	A	C5-C6-N6	-5.38	119.40	123.70
2	X	1981	G	N9-C4-C5	-5.38	103.25	105.40
2	X	12	U	C6-N1-C2	-5.38	117.77	121.00
2	X	2467	C	C6-N1-C2	-5.38	118.15	120.30
2	X	958	U	N1-C2-N3	5.38	118.12	114.90
2	X	2913	G	C6-C5-N7	-5.38	127.17	130.40
2	X	415	U	OP1-P-O3'	5.37	117.02	105.20
2	X	2456	G	C4-C5-N7	5.37	112.95	110.80
2	X	102	A	C4-C5-N7	5.37	113.38	110.70
2	X	1752	C	C6-N1-C2	-5.37	118.15	120.30
2	X	438	U	N1-C2-O2	5.37	126.56	122.80
2	X	1185	U	O4'-C1'-N1	-5.36	103.91	108.20
2	X	1705	G	C2-N3-C4	-5.36	109.22	111.90
2	X	502	C	C5-C6-N1	-5.36	118.32	121.00
2	X	1236	G	C2-N3-C4	-5.36	109.22	111.90
2	X	1255	A	N1-C6-N6	5.36	121.82	118.60
2	X	132	C	C6-N1-C2	-5.36	118.16	120.30
2	X	515	G	C5'-C4'-O4'	5.36	115.53	109.10
2	X	2543	G	C5-C6-O6	-5.36	125.39	128.60
2	X	1225	G	C2-N3-C4	-5.36	109.22	111.90
2	X	2587	C	C6-N1-C2	5.36	122.44	120.30
2	X	610	U	C2-N1-C1'	-5.35	111.28	117.70
2	X	1307	G	OP2-P-O3'	5.35	116.97	105.20
2	X	1806	U	C6-N1-C2	5.35	124.21	121.00
2	X	1981	G	N1-C2-N3	5.35	127.11	123.90
2	X	1723	A	C2-N3-C4	-5.34	107.93	110.60
2	X	2714	U	OP2-P-O3'	5.34	116.96	105.20
2	X	2304	G	C4-C5-C6	5.34	122.00	118.80
2	X	182	C	N1-C2-O2	5.34	122.10	118.90
2	X	2532	G	N3-C4-N9	-5.34	122.80	126.00
2	X	2607	U	C5-C6-N1	-5.34	120.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1727	C	C2-N1-C1'	-5.34	112.93	118.80
2	X	989	A	N1-C6-N6	-5.33	115.40	118.60
2	X	2038	U	N3-C4-O4	-5.33	115.67	119.40
2	X	1972	G	C6-C5-N7	-5.33	127.20	130.40
2	X	2417	U	C2-N1-C1'	5.33	124.10	117.70
2	X	820	G	C8-N9-C4	5.33	108.53	106.40
2	X	2094	G	N3-C4-C5	-5.33	125.94	128.60
2	X	2481	G	N9-C4-C5	5.32	107.53	105.40
2	X	193	A	C8-N9-C4	-5.32	103.67	105.80
3	Y	105	G	C8-N9-C4	5.32	108.53	106.40
2	X	1053	A	OP1-P-O3'	5.32	116.90	105.20
2	X	1295	C	C5-C4-N4	5.32	123.92	120.20
2	X	1562	C	C6-N1-C2	-5.32	118.17	120.30
2	X	1699	A	OP1-P-OP2	-5.32	111.62	119.60
2	X	196	U	N3-C4-C5	-5.32	111.41	114.60
2	X	1701	U	C4-C5-C6	5.32	122.89	119.70
2	X	1784	U	N3-C4-O4	-5.32	115.68	119.40
2	X	2517	G	N3-C4-N9	5.32	129.19	126.00
2	X	2303	G	C2-N3-C4	-5.32	109.24	111.90
2	X	1333	A	C5-C6-N6	-5.32	119.45	123.70
2	X	2523	C	C5-C6-N1	-5.32	118.34	121.00
2	X	2833	U	C5-C6-N1	-5.32	120.04	122.70
2	X	488	G	C5-C6-N1	5.31	114.16	111.50
2	X	2538	U	N1-C2-N3	5.31	118.08	114.90
2	X	2740	A	N9-C4-C5	-5.31	103.68	105.80
2	X	1175	G	N3-C4-N9	5.30	129.18	126.00
2	X	1326	C	C5-C6-N1	-5.30	118.35	121.00
2	X	2081	A	C6-N1-C2	-5.30	115.42	118.60
3	Y	7	G	C8-N9-C1'	-5.30	120.11	127.00
2	X	721	A	N3-C4-N9	-5.30	123.16	127.40
2	X	1250	G	O5'-P-OP2	-5.30	100.93	105.70
3	Y	114	C	C6-N1-C2	-5.30	118.18	120.30
2	X	102	A	C6-C5-N7	-5.30	128.59	132.30
2	X	1191	U	C5-C6-N1	-5.30	120.05	122.70
3	Y	87	G	N3-C4-N9	-5.30	122.82	126.00
2	X	1175	G	N1-C2-N2	-5.30	111.43	116.20
2	X	1998	A	C8-N9-C4	-5.30	103.68	105.80
2	X	2044	C	N3-C4-N4	5.29	121.71	118.00
2	X	1372	C	N3-C4-C5	5.29	124.02	121.90
2	X	1690	A	N1-C6-N6	5.29	121.78	118.60
2	X	2000	G	C2-N3-C4	-5.29	109.25	111.90
2	X	226	A	N9-C4-C5	5.29	107.92	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1293	U	C4-C5-C6	5.29	122.87	119.70
2	X	2528	C	C6-N1-C2	5.29	122.42	120.30
2	X	1490	G	N3-C4-C5	-5.29	125.96	128.60
2	X	2845	G	C4-C5-C6	-5.29	115.63	118.80
2	X	1025	A	C2-N3-C4	5.28	113.24	110.60
2	X	2264	G	N3-C4-C5	-5.28	125.96	128.60
2	X	1278	G	C2-N3-C4	5.28	114.54	111.90
2	X	2844	U	C2-N3-C4	-5.28	123.83	127.00
2	X	1663	G	C4-C5-N7	5.28	112.91	110.80
2	X	27	G	N3-C4-C5	5.28	131.24	128.60
2	X	1033	G	N3-C4-C5	-5.28	125.96	128.60
2	X	2456	G	N3-C2-N2	5.28	123.59	119.90
2	X	1360	G	C5-C6-O6	-5.28	125.44	128.60
2	X	2292	U	N3-C4-O4	-5.28	115.71	119.40
2	X	2644	C	N1-C2-O2	-5.28	115.73	118.90
2	X	2810	A	C5-C6-N1	5.27	120.34	117.70
2	X	679	G	O5'-P-OP2	-5.27	100.96	105.70
2	X	1695	G	C8-N9-C4	-5.27	104.29	106.40
2	X	2033	C	N3-C2-O2	-5.27	118.21	121.90
2	X	679	G	N1-C6-O6	5.26	123.06	119.90
2	X	825	G	C5-C6-O6	-5.26	125.44	128.60
2	X	1296	C	C5-C6-N1	-5.26	118.37	121.00
2	X	2304	G	N1-C2-N2	-5.26	111.47	116.20
2	X	648	G	N9-C4-C5	5.26	107.50	105.40
2	X	2281	C	C6-N1-C2	5.26	122.40	120.30
2	X	1289	A	C4-C5-C6	5.25	119.63	117.00
2	X	2062	G	C5-C6-O6	-5.25	125.45	128.60
2	X	102	A	N7-C8-N9	5.25	116.43	113.80
2	X	2542	C	C6-N1-C2	5.25	122.40	120.30
2	X	2583	C	C6-N1-C2	-5.25	118.20	120.30
2	X	496	G	C4-N9-C1'	5.25	133.33	126.50
2	X	1273	G	N3-C2-N2	-5.25	116.22	119.90
2	X	1289	A	N3-C4-N9	-5.25	123.20	127.40
2	X	1593	G	C5-C6-N1	5.25	114.12	111.50
2	X	355	G	N1-C6-O6	5.25	123.05	119.90
2	X	2603	G	C8-N9-C4	5.25	108.50	106.40
2	X	2060	A	N1-C2-N3	5.25	131.92	129.30
2	X	2041	A	C2-N3-C4	-5.25	107.98	110.60
2	X	1180	G	C4-C5-C6	-5.24	115.65	118.80
2	X	2469	C	C5-C6-N1	-5.24	118.38	121.00
2	X	2516	G	C8-N9-C4	5.24	108.50	106.40
2	X	2748	A	C2-N3-C4	-5.24	107.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	865	A	N1-C6-N6	-5.24	115.45	118.60
2	X	520	G	C4-C5-N7	5.24	112.90	110.80
2	X	1031	C	N3-C4-C5	5.24	124.00	121.90
2	X	2643	C	C6-N1-C2	-5.24	118.20	120.30
2	X	1017	A	C5-C6-N6	5.24	127.89	123.70
2	X	1258	A	C8-N9-C4	5.24	107.90	105.80
2	X	2062	G	C6-C5-N7	-5.24	127.26	130.40
2	X	627	C	N3-C2-O2	5.24	125.56	121.90
3	Y	76	A	C5-N7-C8	-5.24	101.28	103.90
2	X	1377	U	C2-N1-C1'	-5.23	111.42	117.70
2	X	1695	G	N1-C6-O6	5.23	123.04	119.90
2	X	23	G	OP1-P-OP2	5.23	127.45	119.60
2	X	1429	G	C4-C5-N7	5.23	112.89	110.80
2	X	2088	G	N1-C6-O6	5.23	123.04	119.90
2	X	2481	G	N3-C4-C5	-5.23	125.99	128.60
2	X	1278	G	C6-C5-N7	5.23	133.54	130.40
2	X	17	G	N9-C4-C5	-5.23	103.31	105.40
2	X	968	A	O4'-C1'-N9	5.22	112.38	108.20
2	X	1024	A	C5-N7-C8	-5.22	101.29	103.90
2	X	1253	G	C4-C5-N7	5.22	112.89	110.80
2	X	1662	A	N1-C6-N6	5.22	121.73	118.60
2	X	2669	G	C6-C5-N7	-5.22	127.27	130.40
2	X	168	A	C8-N9-C4	-5.22	103.71	105.80
2	X	607	C	N1-C2-O2	-5.22	115.77	118.90
2	X	1782	A	N3-C4-C5	5.22	130.45	126.80
2	X	102	A	C2-N3-C4	-5.21	107.99	110.60
2	X	208	G	N1-C6-O6	-5.21	116.77	119.90
2	X	1304	G	OP2-P-O3'	5.21	116.67	105.20
2	X	1378	U	C6-N1-C1'	-5.21	113.90	121.20
2	X	1253	G	C5-C6-O6	-5.21	125.47	128.60
2	X	1981	G	N1-C2-N2	-5.21	111.51	116.20
2	X	1378	U	N3-C2-O2	-5.21	118.55	122.20
2	X	2384	U	C6-N1-C2	-5.21	117.87	121.00
2	X	113	U	N3-C2-O2	-5.21	118.55	122.20
2	X	991	A	O5'-P-OP2	5.21	116.95	110.70
2	X	457	G	C8-N9-C4	-5.21	104.32	106.40
2	X	661	U	C2-N1-C1'	5.21	123.95	117.70
2	X	1080	G	C4-C5-N7	5.20	112.88	110.80
2	X	1259	U	C6-N1-C2	5.20	124.12	121.00
2	X	2063	C	N3-C2-O2	5.20	125.54	121.90
2	X	1701	U	C5-C6-N1	-5.20	120.10	122.70
2	X	212	C	C6-N1-C2	5.20	122.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	498	G	C8-N9-C4	-5.20	104.32	106.40
2	X	1561	G	N9-C4-C5	5.20	107.48	105.40
2	X	1636	U	P-O3'-C3'	5.20	125.94	119.70
2	X	2517	G	C8-N9-C1'	-5.20	120.24	127.00
2	X	37	C	C2-N3-C4	-5.20	117.30	119.90
2	X	2094	G	N1-C2-N3	5.20	127.02	123.90
2	X	2534	C	N3-C2-O2	-5.20	118.26	121.90
2	X	1056	U	O5'-P-OP2	-5.20	101.02	105.70
2	X	2317	G	N3-C2-N2	-5.20	116.26	119.90
3	Y	1	U	N1-C2-O2	5.20	126.44	122.80
2	X	1051	C	C4-C5-C6	5.19	120.00	117.40
2	X	1295	C	N3-C2-O2	-5.19	118.26	121.90
2	X	1201	G	C4-C5-N7	5.19	112.88	110.80
2	X	981	U	OP2-P-O3'	5.19	116.62	105.20
2	X	2757	U	C2-N1-C1'	5.19	123.93	117.70
2	X	1700	C	N1-C2-O2	5.19	122.01	118.90
2	X	2290	C	C6-N1-C2	-5.19	118.22	120.30
2	X	2757	U	O5'-P-OP2	-5.19	101.03	105.70
2	X	1337	A	N9-C4-C5	-5.19	103.72	105.80
2	X	2529	G	C4-C5-C6	5.19	121.91	118.80
2	X	592	A	C4-C5-C6	-5.18	114.41	117.00
2	X	853	G	C5-C6-O6	-5.18	125.49	128.60
2	X	1370	C	C5-C4-N4	-5.18	116.57	120.20
14	M	54	GLY	N-CA-C	5.18	126.05	113.10
2	X	562	C	O5'-P-OP1	-5.18	101.04	105.70
2	X	2841	A	N9-C4-C5	-5.18	103.73	105.80
2	X	2288	C	C6-N1-C1'	-5.18	114.59	120.80
2	X	831	C	C2-N3-C4	-5.18	117.31	119.90
2	X	2643	C	O5'-P-OP1	-5.18	101.04	105.70
2	X	500	A	C2-N3-C4	-5.17	108.01	110.60
2	X	1700	C	N3-C2-O2	-5.17	118.28	121.90
2	X	2394	G	N3-C4-C5	-5.17	126.01	128.60
2	X	2614	A	OP1-P-OP2	-5.17	111.84	119.60
2	X	1055	A	C4-C5-N7	5.17	113.28	110.70
3	Y	98	G	C2-N3-C4	-5.17	109.31	111.90
2	X	1045	A	C8-N9-C4	5.17	107.87	105.80
2	X	1302	G	N3-C2-N2	-5.17	116.28	119.90
2	X	1401	G	N3-C4-C5	-5.17	126.02	128.60
2	X	2697	G	OP2-P-O3'	5.17	116.57	105.20
2	X	1081	G	N1-C6-O6	5.17	123.00	119.90
2	X	1981	G	N3-C4-N9	5.16	129.10	126.00
2	X	1003	A	N1-C6-N6	-5.16	115.50	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1047	G	C4-N9-C1'	5.16	133.21	126.50
2	X	1196	C	C5-C4-N4	5.16	123.81	120.20
2	X	1661	C	OP2-P-O3'	5.16	116.55	105.20
2	X	2059	G	C4-C5-N7	5.16	112.86	110.80
2	X	2456	G	N1-C2-N2	-5.16	111.56	116.20
2	X	2683	U	C2-N1-C1'	5.16	123.89	117.70
4	B	133	ARG	NE-CZ-NH2	5.16	122.88	120.30
2	X	116	G	N3-C4-C5	-5.16	126.02	128.60
2	X	670	G	O5'-P-OP2	-5.16	101.06	105.70
2	X	779	A	N1-C2-N3	5.16	131.88	129.30
2	X	30	G	C8-N9-C4	-5.16	104.34	106.40
2	X	743	C	N3-C4-C5	5.16	123.96	121.90
2	X	2493	C	C6-N1-C2	5.15	122.36	120.30
2	X	1818	A	C2-N3-C4	5.15	113.18	110.60
2	X	2088	G	O4'-C1'-N9	5.15	112.32	108.20
16	O	50	ALA	C-N-CA	-5.15	100.36	122.00
2	X	987	U	C4-C5-C6	5.15	122.79	119.70
2	X	1566	G	N1-C6-O6	5.15	122.99	119.90
2	X	2722	U	N3-C2-O2	5.15	125.81	122.20
2	X	418	G	O4'-C1'-N9	5.15	112.32	108.20
2	X	1664	G	C2-N3-C4	-5.15	109.33	111.90
2	X	2686	G	N3-C4-N9	-5.15	122.91	126.00
2	X	617	A	C4-C5-C6	-5.14	114.43	117.00
2	X	1177	A	N9-C4-C5	5.14	107.86	105.80
2	X	802	G	C4-C5-N7	5.14	112.86	110.80
2	X	24	G	C5-C6-O6	-5.14	125.52	128.60
2	X	1351	C	C5-C6-N1	5.14	123.57	121.00
3	Y	82	C	O4'-C1'-N1	5.14	112.31	108.20
10	I	51	GLU	N-CA-C	5.14	124.87	111.00
2	X	1041	G	N9-C4-C5	-5.14	103.34	105.40
2	X	1368	C	OP1-P-O3'	5.13	116.49	105.20
2	X	2306	G	C4-C5-N7	5.13	112.85	110.80
2	X	126	A	C2-N3-C4	5.13	113.17	110.60
2	X	319	G	C5-C6-O6	-5.13	125.52	128.60
3	Y	21	G	N3-C4-N9	-5.13	122.92	126.00
2	X	1186	A	C5-C6-N1	-5.13	115.14	117.70
2	X	2667	G	C5-C6-N1	-5.13	108.94	111.50
2	X	2838	C	C5-C6-N1	-5.13	118.44	121.00
2	X	1232	G	N9-C4-C5	-5.12	103.35	105.40
2	X	1695	G	N3-C4-N9	-5.12	122.93	126.00
2	X	2027	G	N3-C2-N2	5.12	123.49	119.90
2	X	2704	A	OP2-P-O3'	5.12	116.47	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	875	G	C4-C5-N7	-5.12	108.75	110.80
2	X	1273	G	OP2-P-O3'	5.12	116.46	105.20
2	X	2036	G	C4-C5-N7	-5.12	108.75	110.80
2	X	1291	A	OP2-P-O3'	5.12	116.46	105.20
2	X	1972	G	C5-C6-O6	-5.12	125.53	128.60
2	X	806	A	N7-C8-N9	5.12	116.36	113.80
2	X	1262	U	N3-C4-C5	5.12	117.67	114.60
3	Y	105	G	C2-N3-C4	-5.11	109.34	111.90
2	X	1315	C	C5-C6-N1	-5.11	118.44	121.00
2	X	1495	C	C6-N1-C2	-5.11	118.25	120.30
2	X	2041	A	C5-C6-N1	-5.11	115.14	117.70
2	X	2898	U	C5-C4-O4	-5.11	122.83	125.90
3	Y	94	U	C5-C6-N1	-5.11	120.14	122.70
2	X	2062	G	OP1-P-O3'	5.11	116.44	105.20
2	X	2081	A	N7-C8-N9	5.11	116.35	113.80
2	X	2270	U	N3-C4-C5	5.11	117.66	114.60
2	X	2606	C	C6-N1-C2	-5.11	118.26	120.30
2	X	1596	G	N3-C4-C5	-5.11	126.05	128.60
2	X	2097	G	C2-N3-C4	-5.11	109.35	111.90
2	X	890	G	C5-N7-C8	-5.10	101.75	104.30
2	X	17	G	C6-C5-N7	-5.10	127.34	130.40
2	X	115	C	C6-N1-C2	-5.10	118.26	120.30
2	X	835	U	C2-N1-C1'	5.10	123.82	117.70
2	X	1224	U	C5-C6-N1	-5.10	120.15	122.70
2	X	488	G	N3-C4-N9	5.10	129.06	126.00
2	X	2583	C	C6-N1-C1'	-5.10	114.68	120.80
2	X	661	U	OP2-P-O3'	5.09	116.41	105.20
2	X	2073	G	C4-C5-N7	5.09	112.84	110.80
2	X	2525	C	O5'-P-OP1	-5.09	101.11	105.70
2	X	1984	C	N3-C4-C5	5.09	123.94	121.90
2	X	845	A	OP1-P-O3'	5.09	116.40	105.20
2	X	1061	G	C8-N9-C4	-5.09	104.36	106.40
3	Y	78	C	C6-N1-C2	-5.09	118.26	120.30
2	X	2027	G	N1-C6-O6	-5.09	116.85	119.90
2	X	2524	A	N1-C6-N6	-5.09	115.55	118.60
2	X	2871	A	N1-C2-N3	5.09	131.84	129.30
2	X	376	A	N7-C8-N9	5.09	116.34	113.80
2	X	1055	A	C6-C5-N7	-5.09	128.74	132.30
2	X	733	U	O5'-P-OP1	-5.08	101.12	105.70
2	X	562	C	N3-C4-C5	-5.08	119.87	121.90
2	X	605	U	N1-C2-N3	5.08	117.95	114.90
2	X	1020	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2046	U	N1-C2-O2	-5.08	119.24	122.80
2	X	2906	G	C4-C5-C6	5.08	121.85	118.80
2	X	580	C	C5-C4-N4	-5.08	116.64	120.20
2	X	1576	A	C2-N3-C4	5.08	113.14	110.60
2	X	1786	A	O5'-P-OP1	-5.08	101.13	105.70
2	X	1782	A	C2-N3-C4	-5.08	108.06	110.60
2	X	514	G	C5-C6-O6	-5.08	125.56	128.60
2	X	1010	G	C8-N9-C4	5.08	108.43	106.40
2	X	1686	G	C5-C6-O6	-5.08	125.56	128.60
2	X	1046	G	N3-C4-N9	-5.07	122.96	126.00
2	X	1286	G	N3-C4-C5	-5.07	126.06	128.60
2	X	2538	U	N3-C4-C5	-5.07	111.56	114.60
2	X	580	C	N3-C4-C5	-5.07	119.87	121.90
2	X	1665	U	N1-C2-N3	5.07	117.94	114.90
2	X	2082	C	C6-N1-C2	5.07	122.33	120.30
2	X	2599	A	N1-C2-N3	5.07	131.84	129.30
2	X	2814	C	C6-N1-C2	-5.07	118.27	120.30
2	X	835	U	C5-C4-O4	-5.07	122.86	125.90
2	X	997	G	OP1-P-O3'	5.07	116.35	105.20
2	X	1396	A	N1-C6-N6	5.07	121.64	118.60
2	X	2298	G	C4-N9-C1'	5.07	133.09	126.50
2	X	2787	C	C6-N1-C2	-5.07	118.27	120.30
2	X	625	G	C5-C6-O6	-5.07	125.56	128.60
2	X	1604	C	N1-C2-O2	5.06	121.94	118.90
2	X	2682	G	OP2-P-O3'	5.06	116.34	105.20
2	X	1011	U	N3-C4-C5	-5.06	111.56	114.60
2	X	2449	C	C2-N1-C1'	5.06	124.37	118.80
2	X	2838	C	C2-N1-C1'	-5.06	113.23	118.80
2	X	2753	U	N3-C2-O2	-5.06	118.66	122.20
2	X	997	G	C8-N9-C4	-5.06	104.38	106.40
2	X	1593	G	C8-N9-C4	-5.06	104.38	106.40
2	X	1980	A	O5'-P-OP2	5.06	116.77	110.70
2	X	272	C	N1-C2-O2	5.06	121.94	118.90
2	X	552	A	N1-C6-N6	5.06	121.64	118.60
2	X	829	U	N3-C2-O2	5.06	125.74	122.20
2	X	1701	U	OP1-P-OP2	5.06	127.19	119.60
2	X	2089	A	C2-N3-C4	-5.06	108.07	110.60
2	X	567	G	N3-C2-N2	-5.05	116.36	119.90
2	X	589	U	C6-N1-C2	5.05	124.03	121.00
2	X	1004	A	N3-C4-C5	5.05	130.34	126.80
2	X	1083	G	N1-C6-O6	5.05	122.93	119.90
2	X	1243	G	C6-C5-N7	-5.05	127.37	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2750	C	OP1-P-O3'	5.05	116.31	105.20
2	X	2554	C	C6-N1-C2	5.05	122.32	120.30
2	X	245	G	N7-C8-N9	-5.05	110.58	113.10
2	X	853	G	N3-C2-N2	-5.05	116.37	119.90
2	X	1025	A	C4-C5-C6	-5.05	114.48	117.00
2	X	1230	G	C4-C5-N7	5.05	112.82	110.80
2	X	1301	U	N1-C2-O2	-5.04	119.27	122.80
2	X	2036	G	N9-C1'-C2'	-5.04	106.45	112.00
2	X	2491	C	O5'-P-OP2	-5.04	101.16	105.70
2	X	554	C	OP2-P-O3'	5.04	116.30	105.20
2	X	1957	G	N3-C4-C5	-5.04	126.08	128.60
2	X	2047	A	C4-C5-C6	-5.04	114.48	117.00
2	X	2604	A	C2-N3-C4	-5.04	108.08	110.60
2	X	2808	A	O5'-P-OP2	5.04	116.75	110.70
2	X	793	G	O4'-C1'-N9	5.04	112.23	108.20
2	X	2097	G	C4-C5-C6	5.04	121.83	118.80
2	X	2304	G	N1-C2-N3	5.04	126.92	123.90
2	X	234	C	N1-C2-O2	-5.04	115.88	118.90
2	X	1932	C	C2-N1-C1'	-5.04	113.26	118.80
2	X	2047	A	C6-C5-N7	5.04	135.83	132.30
2	X	862	C	N3-C4-C5	5.04	123.92	121.90
2	X	996	G	C5-C6-O6	-5.04	125.58	128.60
2	X	814	A	N1-C6-N6	-5.04	115.58	118.60
2	X	1288	G	O5'-P-OP2	-5.04	101.17	105.70
2	X	1395	G	C6-C5-N7	5.04	133.42	130.40
2	X	1781	C	N1-C2-O2	-5.04	115.88	118.90
2	X	2009	U	N1-C2-O2	5.04	126.33	122.80
2	X	2287	C	O5'-P-OP1	-5.04	101.17	105.70
14	M	53	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	X	231	A	N1-C6-N6	5.03	121.62	118.60
2	X	612	U	C4-C5-C6	5.03	122.72	119.70
2	X	656	G	N7-C8-N9	5.03	115.61	113.10
2	X	2833	U	C6-N1-C2	5.03	124.02	121.00
2	X	2668	A	N1-C2-N3	5.03	131.81	129.30
2	X	2855	A	O4'-C1'-N9	-5.03	104.18	108.20
2	X	1566	G	N1-C2-N2	5.03	120.72	116.20
2	X	2566	C	C5-C6-N1	-5.03	118.49	121.00
2	X	263	G	C4-C5-C6	5.02	121.81	118.80
2	X	598	G	O5'-P-OP2	-5.02	101.18	105.70
2	X	2850	G	N3-C4-C5	-5.02	126.09	128.60
2	X	609	U	C6-N1-C2	-5.02	117.99	121.00
2	X	1257	G	N7-C8-N9	5.02	115.61	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	2546	U	N3-C4-C5	5.02	117.61	114.60
2	X	2738	A	N1-C2-N3	5.02	131.81	129.30
2	X	211	C	N1-C2-N3	-5.02	115.69	119.20
2	X	902	A	C5-C6-N6	5.01	127.71	123.70
2	X	2321	C	C2-N1-C1'	-5.01	113.28	118.80
2	X	1016	G	C6-C5-N7	-5.01	127.39	130.40
2	X	1488	A	C8-N9-C4	-5.01	103.80	105.80
2	X	2043	U	OP2-P-O3'	-5.01	94.17	105.20
2	X	2522	G	N1-C6-O6	5.01	122.91	119.90
3	Y	98	G	N3-C2-N2	-5.01	116.39	119.90
2	X	199	A	C4-C5-N7	5.01	113.20	110.70
2	X	321	U	O5'-P-OP2	-5.01	101.19	105.70
2	X	2762	G	C5-C6-N1	-5.01	109.00	111.50
2	X	728	U	C6-N1-C2	-5.01	118.00	121.00
2	X	985	A	C2-N3-C4	-5.01	108.10	110.60
2	X	1370	C	C6-N1-C2	5.01	122.30	120.30
2	X	800	G	C5-C6-O6	-5.00	125.60	128.60
2	X	1009	C	N1-C2-O2	5.00	121.90	118.90
3	Y	88	U	C6-N1-C1'	-5.00	114.19	121.20
2	X	1981	G	C6-C5-N7	-5.00	127.40	130.40
2	X	2058	A	C2-N3-C4	5.00	113.10	110.60
2	X	2607	U	C6-N1-C2	5.00	124.00	121.00
2	X	1649	C	N3-C4-C5	-5.00	119.90	121.90
2	X	2474	G	OP1-P-O3'	5.00	116.20	105.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	10	ALA	Peptide
27	3	17	THR	Peptide
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	Peptide
10	I	35	HIS	Peptide
16	O	80	LYS	Peptide
17	P	70	VAL	Peptide
20	S	17	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1667	0	1292	51	0
2	X	57983	0	29161	923	0
3	Y	2430	0	1229	58	0
4	B	1547	0	1514	66	0
5	C	1324	0	1175	57	0
6	D	853	0	444	6	0
7	E	915	0	648	22	0
8	G	1090	0	1034	48	0
9	H	884	0	902	45	0
10	I	819	0	687	43	0
11	J	1001	0	971	37	0
12	K	906	0	930	36	0
13	L	673	0	538	19	0
14	M	807	0	803	32	0
15	N	922	0	973	61	0
16	O	751	0	743	22	0
17	P	853	0	900	30	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	4	0
23	V	486	0	469	10	0
24	W	437	0	467	26	0
25	Z	339	0	350	23	0
26	2	350	0	383	12	0
27	3	405	0	363	19	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1574	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1574) 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91
2:X:498:G:H21	2:X:503:A:H8	1.19	0.90
23:V:10:THR:O	23:V:12:SER:N	2.05	0.89
8:G:65:PHE:HB3	8:G:69:LYS:HD3	1.55	0.89
10:I:57:LEU:HD11	27:3:12:LYS:CB	2.03	0.88
2:X:304:G:H1	2:X:413:C:H42	1.18	0.87
2:X:2775:A:H1'	7:E:67:THR:HG22	1.54	0.87
13:L:45:ILE:HG23	13:L:52:THR:HB	1.55	0.87
9:H:31:LYS:HG3	9:H:32:THR:HG22	1.54	0.87
3:Y:15:C:H42	3:Y:105:G:H21	1.17	0.87
2:X:1290:G:OP2	15:N:13:ARG:NH2	2.07	0.86
15:N:10:THR:HG21	35:N:201:EPE:H32	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1063:U:H3	2:X:1186:A:H62	1.24	0.85
2:X:657:U:O4	2:X:659:A:N6	2.10	0.85
2:X:501:C:H3'	2:X:502:C:H5"	1.59	0.84
5:C:113:ALA:HB1	5:C:181:LEU:HD22	1.61	0.83
2:X:591:A:H4'	2:X:592:A:H5'	1.59	0.82
2:X:79:U:HO2'	2:X:389:A:H8	1.27	0.82
2:X:2649:U:O2'	2:X:2845:G:N2	2.13	0.82
2:X:1460:U:H3	2:X:1628:A:H61	1.24	0.82
9:H:101:PRO:HD3	14:M:68:SER:HB2	1.62	0.81
9:H:63:VAL:HG21	9:H:102:VAL:HG22	1.62	0.81
11:J:116:GLU:OE1	11:J:119:ARG:NH1	2.13	0.81
1:A:89:ALA:HB2	1:A:158:ALA:HA	1.63	0.81
15:N:61:TRP:CE2	15:N:93:LYS:HB2	2.16	0.80
2:X:627:C:OP2	35:N:201:EPE:H61	1.82	0.80
6:D:101:ASP:HA	6:D:130:LEU:HD11	1.62	0.80
2:X:1605:A:H1'	32:X:3004:MPD:HM1	1.64	0.80
2:X:1487:G:H1	2:X:1597:U:H3	1.27	0.79
2:X:2419:A:H2	2:X:2451:C:H42	1.28	0.79
3:Y:15:C:N4	3:Y:105:G:H21	1.81	0.79
5:C:147:GLU:HA	5:C:167:ALA:HB1	1.64	0.79
3:Y:77:G:H1	3:Y:94:U:H3	1.28	0.79
14:M:24:PRO:HA	14:M:49:VAL:HB	1.63	0.79
20:S:81:PRO:O	20:S:83:LYS:N	2.16	0.79
25:Z:15:LYS:O	25:Z:18:THR:HG23	1.83	0.78
2:X:2382:C:O2	2:X:2389:G:N2	2.16	0.78
2:X:1302:G:OP1	25:Z:16:ARG:NH2	2.15	0.78
2:X:1467:G:O2'	2:X:1543:G:O2'	2.02	0.78
14:M:106:ARG:CZ	14:M:106:ARG:HA	2.13	0.78
2:X:1952:C:N3	2:X:1956:G:N2	2.30	0.77
12:K:105:LYS:HA	12:K:117:VAL:HG12	1.66	0.77
2:X:2850:G:H5'	4:B:67:LYS:HE3	1.63	0.77
8:G:57:VAL:HB	8:G:125:VAL:HG13	1.65	0.77
11:J:135:GLU:OE2	32:J:201:MPD:O4	2.01	0.77
2:X:1876:G:N2	2:X:1920:C:O2	2.18	0.77
2:X:2470:C:H2'	2:X:2471:G:H8	1.50	0.77
8:G:14:ARG:NH1	8:G:50:ASP:O	2.17	0.77
5:C:108:LEU:O	5:C:112:SER:OG	2.02	0.77
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.66	0.77
2:X:1894:G:O6	2:X:1902:G:N2	2.17	0.77
17:P:21:LEU:HD22	17:P:74:ALA:HB1	1.67	0.77
15:N:10:THR:HG23	35:N:201:EPE:H71	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1726:A:H61	2:X:1750:U:H3	1.33	0.76
8:G:44:THR:O	8:G:44:THR:OG1	2.01	0.76
1:A:243:ARG:HD3	1:A:247:MET:HE1	1.66	0.76
15:N:27:SER:HA	15:N:30:THR:HG23	1.67	0.76
2:X:1289:A:OP1	15:N:13:ARG:NH1	2.19	0.76
2:X:1796:A:O2'	2:X:1985:C:OP1	2.03	0.76
3:Y:15:C:H42	3:Y:105:G:N2	1.83	0.75
3:Y:79:C:H42	3:Y:92:G:H1	1.33	0.75
8:G:7:ALA:H	8:G:46:THR:HG21	1.48	0.75
5:C:31:SER:HB3	10:I:9:ALA:HB2	1.67	0.75
2:X:272:C:N3	2:X:416:G:N2	2.33	0.75
2:X:1346:G:H4'	26:2:8:PRO:HG2	1.69	0.75
9:H:4:GLN:HG2	9:H:5:GLU:HG2	1.66	0.75
24:W:40:ASN:HB3	24:W:43:ILE:H	1.52	0.75
1:A:78:VAL:HG12	1:A:79:ASP:H	1.52	0.74
5:C:61:GLY:HA2	5:C:77:THR:HG23	1.68	0.74
2:X:589:U:O4	2:X:592:A:N6	2.19	0.74
2:X:1472:C:N4	2:X:1617:A:OP2	2.19	0.74
2:X:2860:U:H5"	12:K:49:THR:HG21	1.70	0.74
2:X:2331:G:H22	2:X:2339:U:H3	1.36	0.74
14:M:102:LEU:O	14:M:103:ARG:NH2	2.21	0.74
2:X:2761:C:H41	2:X:2797:C:H6	1.32	0.74
1:A:171:TYR:OH	2:X:2250:A:OP1	2.05	0.73
2:X:629:A:H62	2:X:1289:A:H2	1.33	0.73
2:X:1501:G:H2'	2:X:1502:A:H8	1.52	0.73
3:Y:18:G:H1	3:Y:61:U:H3	1.35	0.73
2:X:864:A:OP2	2:X:1226:G:N2	2.17	0.73
2:X:1501:G:H22	2:X:2729:G:H22	1.36	0.73
2:X:903:G:OP2	21:T:85:LYS:NZ	2.22	0.73
2:X:683:G:C6	2:X:696:G:C6	2.77	0.73
2:X:995:U:OP1	33:Y:213:SPD:N1	2.22	0.72
2:X:1490:G:O2'	2:X:1491:C:O5'	2.07	0.72
2:X:1400:C:O2'	2:X:1836:A:H1'	1.90	0.72
2:X:1013:U:O3'	24:W:14:GLY:HA2	1.88	0.72
4:B:53:PHE:HB3	4:B:87:PHE:HB2	1.72	0.72
2:X:1711:G:N2	2:X:2020:U:O4	2.18	0.71
2:X:2495:A:HO2'	2:X:2496:A:H8	1.37	0.71
2:X:229:A:O2'	2:X:231:A:N1	2.22	0.71
2:X:1881:A:H62	2:X:1915:G:H8	1.38	0.71
2:X:1810:A:H5'	2:X:2635:G:H4'	1.73	0.71
4:B:10:ILE:HD12	14:M:6:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2007:G:O2'	2:X:2009:U:OP2	2.05	0.70
7:E:133:VAL:HG11	7:E:141:VAL:HG13	1.71	0.70
2:X:1293:U:H5"	2:X:1294:G:H5"	1.73	0.70
2:X:659:A:H1'	2:X:660:A:H5'	1.73	0.70
2:X:1487:G:N2	2:X:1597:U:O2	2.24	0.70
18:Q:57:ASN:O	18:Q:58:TYR:HD1	1.74	0.70
2:X:460:C:O2	2:X:1891:U:O2'	2.09	0.70
2:X:1185:U:OP2	8:G:66:THR:OG1	2.05	0.70
2:X:1663:G:HO2'	26:2:2:VAL:N	1.88	0.70
3:Y:38:U:O2'	3:Y:43:A:N6	2.25	0.70
2:X:956:A:C6	11:J:11:ARG:HD2	2.27	0.70
13:L:36:SER:OG	13:L:37:ASN:N	2.24	0.69
4:B:38:LYS:NZ	4:B:96:VAL:O	2.19	0.69
2:X:788:A:O2'	2:X:1703:U:OP1	2.09	0.69
2:X:2604:A:H5"	2:X:2605:G:H5'	1.75	0.69
5:C:158:ASN:HA	5:C:161:VAL:HG22	1.75	0.69
2:X:164:A:H1'	2:X:165:C:H5'	1.74	0.68
2:X:634:C:HO2'	27:3:2:PRO:N	1.91	0.68
11:J:69:PHE:HB3	11:J:71:HIS:CE1	2.27	0.68
2:X:1261:G:OP1	16:O:67:ARG:NH2	2.26	0.68
5:C:14:SER:OG	5:C:15:GLY:N	2.22	0.68
13:L:73:ALA:HB1	13:L:107:ALA:HB2	1.72	0.68
5:C:43:SER:HA	5:C:98:ALA:HB2	1.75	0.68
1:A:224:VAL:HG11	2:X:1815:C:H5"	1.76	0.68
2:X:1063:U:H3	2:X:1186:A:N6	1.90	0.68
2:X:1494:G:C8	2:X:1495:C:H5	2.11	0.68
2:X:878:C:H2'	2:X:879:U:C6	2.28	0.68
2:X:2290:C:OP2	21:T:27:LYS:NZ	2.25	0.68
9:H:51:VAL:HG12	9:H:94:ARG:HH21	1.58	0.68
2:X:1460:U:H3	2:X:1628:A:N6	1.92	0.68
3:Y:31:G:H1	3:Y:47:C:H42	1.38	0.68
18:Q:55:ILE:HG13	18:Q:78:ALA:HB2	1.76	0.68
2:X:2314:A:O2'	2:X:2315:A:H2'	1.93	0.68
4:B:156:MET:HB2	4:B:160:ALA:HB3	1.75	0.68
2:X:715:A:H4'	2:X:716:C:H5'	1.74	0.67
2:X:2906:G:C2	25:Z:39:LEU:HD21	2.29	0.67
2:X:878:C:H1'	10:I:48:PRO:HB3	1.76	0.67
2:X:2101:U:H2'	2:X:2102:U:C6	2.28	0.67
2:X:2707:C:H5'	4:B:202:PRO:HA	1.76	0.67
1:A:78:VAL:HA	1:A:94:VAL:HA	1.76	0.67
3:Y:46:A:OP1	13:L:35:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:136:THR:HG22	5:C:140:LYS:NZ	2.10	0.67
2:X:321:U:O2'	2:X:322:A:OP2	2.13	0.67
2:X:2334:G:O2'	2:X:2337:A:N6	2.21	0.67
11:J:40:SER:OG	11:J:41:TRP:N	2.27	0.67
12:K:105:LYS:HB2	25:Z:41:HIS:HA	1.75	0.67
2:X:1826:G:N2	2:X:1845:U:O2'	2.27	0.66
2:X:1467:G:HO2'	2:X:1543:G:HO2'	1.44	0.66
2:X:2672:G:O6	33:X:3493:SPD:H81	1.95	0.66
2:X:1518:G:H1	2:X:1562:C:H42	1.42	0.66
19:R:72:ASP:OD1	19:R:72:ASP:N	2.29	0.66
2:X:2805:A:O2'	2:X:2807:G:O2'	2.13	0.66
5:C:8:LYS:HZ2	5:C:8:LYS:HB2	1.61	0.66
1:A:35:LYS:O	1:A:37:LEU:N	2.27	0.66
4:B:192:ASN:HB2	4:B:194:VAL:HG23	1.77	0.66
18:Q:49:LYS:HD3	18:Q:50:VAL:HG12	1.78	0.66
2:X:183:A:H5'	2:X:481:C:H1'	1.77	0.66
2:X:1683:U:H2'	2:X:1684:A:H5"	1.76	0.65
9:H:75:SER:OG	14:M:74:ARG:NH2	2.27	0.65
2:X:1835:U:H2'	2:X:1836:A:H5"	1.79	0.65
1:A:217:ARG:NH1	2:X:736:C:OP1	2.29	0.65
2:X:1501:G:H2'	2:X:1502:A:C8	2.32	0.65
18:Q:50:VAL:HG13	18:Q:51:ALA:H	1.61	0.65
2:X:280:C:H2'	2:X:281:A:H8	1.62	0.65
3:Y:80:A:H61	3:Y:91:C:H42	1.45	0.65
19:R:80:ARG:NH2	19:R:96:LYS:HA	2.12	0.65
14:M:102:LEU:O	14:M:103:ARG:CZ	2.45	0.65
26:2:16:VAL:H	26:2:21:LYS:HG2	1.62	0.65
8:G:18:VAL:HG23	8:G:140:ASN:HA	1.78	0.65
2:X:718:C:H5"	5:C:81:PRO:HD2	1.79	0.65
2:X:1710:G:O3'	9:H:6:THR:HG23	1.96	0.64
2:X:2817:A:O2'	2:X:2818:A:OP2	2.14	0.64
15:N:93:LYS:O	15:N:97:GLU:N	2.22	0.64
15:N:29:HIS:CD2	15:N:30:THR:HG22	2.33	0.64
2:X:1313:G:OP2	2:X:1689:G:O2'	2.16	0.64
3:Y:21:G:H22	3:Y:58:G:N2	1.95	0.64
1:A:78:VAL:O	1:A:95:VAL:HG12	1.98	0.64
3:Y:4:G:H1	3:Y:111:A:H62	1.46	0.64
2:X:503:A:H2	2:X:517:A:H62	1.44	0.64
2:X:1041:G:H5"	15:N:92:ARG:HH12	1.63	0.64
2:X:1723:A:H2	2:X:1791:G:C8	2.16	0.64
12:K:8:ARG:O	12:K:13:ARG:NH1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HD3	1:A:85:PRO:HB2	1.80	0.64
2:X:630:G:C6	10:I:30:THR:HG21	2.33	0.64
17:P:20:VAL:HA	17:P:23:LEU:HD12	1.79	0.64
21:T:54:TYR:HD2	21:T:80:LYS:HE3	1.63	0.64
1:A:107:PRO:HA	1:A:196:GLY:H	1.63	0.63
11:J:18:THR:OG1	11:J:19:GLY:N	2.32	0.63
1:A:15:ASN:O	1:A:204:ASN:ND2	2.31	0.63
2:X:876:G:O2'	10:I:36:LYS:HD2	1.97	0.63
2:X:78:U:H2'	2:X:79:U:C6	2.32	0.63
2:X:679:G:H2'	2:X:680:C:C6	2.34	0.63
20:S:75:ALA:HB2	20:S:92:LEU:HB2	1.80	0.63
1:A:209:GLY:HA2	1:A:212:ARG:HB2	1.80	0.63
3:Y:46:A:P	13:L:35:ARG:HH12	2.22	0.63
2:X:1805:U:H2'	2:X:1811:A:H62	1.64	0.63
2:X:418:G:O2'	2:X:419:U:OP2	2.17	0.63
2:X:1089:C:O2	2:X:1091:G:N1	2.31	0.63
25:Z:38:LYS:H	25:Z:38:LYS:HZ2	1.46	0.63
2:X:1037:A:OP1	15:N:50:ARG:NH1	2.32	0.62
2:X:1526:G:N2	2:X:1550:G:H1	1.96	0.62
7:E:136:ILE:HD12	7:E:137:SER:H	1.63	0.62
8:G:14:ARG:HG2	8:G:52:GLY:O	1.99	0.62
20:S:28:PRO:O	20:S:88:HIS:HA	2.00	0.62
2:X:268:A:N6	2:X:473:U:O2'	2.32	0.62
5:C:103:LYS:HA	5:C:106:ARG:NE	2.15	0.62
24:W:5:GLN:HG3	24:W:36:VAL:HG22	1.81	0.62
2:X:956:A:H2'	11:J:11:ARG:NH1	2.10	0.62
2:X:1887:G:H22	2:X:1910:G:H1'	1.63	0.62
2:X:2553:G:O2'	28:4:1:MET:N	2.32	0.62
5:C:149:PRO:HD2	5:C:187:THR:HA	1.82	0.62
18:Q:28:ASP:HA	18:Q:77:LYS:HA	1.80	0.62
2:X:1875:A:H2'	2:X:1876:G:C8	2.34	0.62
3:Y:6:U:OP1	13:L:11:ARG:NH2	2.32	0.62
11:J:69:PHE:HB3	11:J:71:HIS:HE1	1.64	0.62
9:H:88:ARG:O	9:H:90:ASP:N	2.33	0.62
2:X:817:G:H2'	2:X:818:U:H6	1.64	0.62
2:X:1836:A:O2'	2:X:1837:A:O4'	2.17	0.62
2:X:1492:G:O2'	2:X:1574:G:N2	2.32	0.62
1:A:59:LYS:HG2	2:X:1615:G:H4'	1.81	0.61
2:X:501:C:H3'	2:X:502:C:C5'	2.29	0.61
1:A:145:GLU:HA	1:A:152:GLY:HA2	1.82	0.61
2:X:2848:G:H2'	2:X:2849:A:H8	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1515:G:O2'	2:X:1516:C:O5'	2.16	0.61
10:I:128:PHE:HD1	10:I:129:SER:H	1.48	0.61
5:C:50:ALA:HB2	5:C:94:PRO:HD3	1.83	0.61
2:X:1332:C:H4'	12:K:67:ARG:NH2	2.16	0.61
2:X:1599:G:OP1	2:X:1761:G:N2	2.28	0.61
2:X:2050:A:H5'	2:X:2644:C:H4'	1.83	0.61
4:B:26:THR:HG21	4:B:201:VAL:HG12	1.82	0.61
15:N:92:ARG:O	15:N:93:LYS:HB3	1.98	0.61
2:X:2470:C:H2'	2:X:2471:G:C8	2.33	0.61
15:N:9:VAL:HG23	15:N:10:THR:HG23	1.82	0.61
4:B:140:PRO:HG2	4:B:145:SER:HB2	1.83	0.61
15:N:59:LYS:O	15:N:63:THR:HG23	2.01	0.61
2:X:1515:G:H22	2:X:1565:U:H3	1.48	0.61
28:4:14:CYS:HA	28:4:27:CYS:HA	1.82	0.61
4:B:8:ARG:NH2	4:B:54:GLU:OE2	2.33	0.60
2:X:124:A:OP2	26:2:20:ARG:HD3	2.01	0.60
7:E:18:THR:N	7:E:32:GLU:OE2	2.34	0.60
2:X:609:U:O4	16:O:79:ARG:HD3	2.01	0.60
2:X:1041:G:OP1	15:N:92:ARG:HG2	2.01	0.60
2:X:661:U:H1'	2:X:662:G:C8	2.37	0.60
3:Y:79:C:N4	3:Y:92:G:H1	1.99	0.60
8:G:4:THR:HG23	15:N:61:TRP:CZ3	2.36	0.60
9:H:15:GLY:HA3	9:H:50:GLY:HA3	1.84	0.60
2:X:1065:A:H2'	2:X:1067:U:H5'	1.82	0.60
25:Z:28:THR:HG23	25:Z:37:TYR:CE1	2.37	0.60
4:B:95:ASP:O	4:B:97:ASP:N	2.31	0.60
8:G:113:THR:O	8:G:116:GLY:N	2.33	0.60
16:O:22:VAL:HG22	16:O:23:GLU:H	1.66	0.60
20:S:72:VAL:HG12	20:S:93:ALA:HA	1.83	0.60
3:Y:74:G:H22	3:Y:97:A:H61	1.47	0.60
14:M:105:LEU:O	14:M:106:ARG:NH1	2.35	0.60
2:X:528:C:H5"	2:X:529:A:OP1	2.01	0.60
2:X:1773:A:H2'	2:X:1774:A:H8	1.66	0.60
2:X:329:A:N6	2:X:398:C:H42	1.99	0.59
2:X:665:G:H4'	2:X:666:A:H5"	1.82	0.59
2:X:1512:U:H2'	2:X:1513:A:C8	2.37	0.59
2:X:1886:A:N6	2:X:1910:G:O2'	2.35	0.59
2:X:460:C:H2'	2:X:461:A:C8	2.38	0.59
2:X:125:A:N7	2:X:126:A:C6	2.71	0.59
2:X:107:G:H2'	2:X:108:A:H8	1.67	0.59
2:X:630:G:P	10:I:21:ARG:HH22	2.24	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1147:A:H2'	2:X:1148:C:O4'	2.02	0.59
2:X:1836:A:H2'	2:X:1837:A:C8	2.37	0.59
2:X:2549:U:O2'	2:X:2674:U:OP1	2.20	0.59
2:X:424:C:H2'	2:X:425:G:C8	2.37	0.59
2:X:1487:G:N2	2:X:1597:U:C2	2.71	0.59
2:X:1793:C:H2'	2:X:1794:C:H6	1.67	0.59
2:X:338:G:H2'	2:X:339:A:H8	1.67	0.59
2:X:999:U:H5"	11:J:87:LYS:HD2	1.85	0.59
2:X:1362:C:OP1	2:X:1691:G:O2'	2.18	0.59
2:X:1488:A:N6	2:X:1595:C:H42	2.00	0.59
2:X:1916:A:H1'	2:X:2114:G:H5'	1.85	0.59
3:Y:113:G:H2'	3:Y:114:C:H5'	1.85	0.59
2:X:1440:A:HO2'	2:X:1514:A:HO2'	1.34	0.59
4:B:100:GLU:O	4:B:103:GLN:HG2	2.02	0.59
2:X:1150:A:H4'	2:X:1150:A:OP1	2.01	0.59
2:X:1513:A:H3'	2:X:1514:A:H8	1.67	0.59
5:C:102:PRO:HB2	5:C:105:MET:HG3	1.83	0.59
15:N:10:THR:CG2	35:N:201:EPE:H71	2.32	0.59
16:O:42:GLY:HA2	16:O:46:VAL:HG12	1.85	0.59
2:X:1415:A:O2'	2:X:1417:G:N7	2.30	0.59
5:C:150:LYS:HA	5:C:188:ASN:OD1	2.02	0.59
8:G:136:GLN:N	8:G:136:GLN:OE1	2.35	0.59
16:O:2:PHE:CE1	16:O:42:GLY:HA3	2.38	0.58
2:X:2120:G:H21	2:X:2225:A:N6	2.00	0.58
2:X:1422:A:O2'	2:X:1423:C:O5'	2.21	0.58
9:H:87:ILE:HG12	9:H:88:ARG:H	1.69	0.58
24:W:50:VAL:HB	24:W:53:LEU:HD11	1.85	0.58
1:A:183:MET:HE2	1:A:269:LEU:HA	1.84	0.58
2:X:3:U:H2'	2:X:4:U:C6	2.38	0.58
4:B:111:VAL:O	4:B:114:ASP:HB2	2.02	0.58
11:J:34:LEU:HB2	11:J:118:LEU:HD13	1.85	0.58
22:U:43:LYS:O	22:U:45:LYS:N	2.36	0.58
25:Z:38:LYS:H	25:Z:38:LYS:NZ	2.00	0.58
2:X:268:A:O2'	2:X:269:G:H4'	2.04	0.58
2:X:1507:A:H2'	2:X:1508:C:H5'	1.85	0.58
2:X:90:A:H8	2:X:90:A:OP1	1.86	0.58
2:X:355:G:O2'	33:X:3498:SPD:H72	2.04	0.58
2:X:1180:G:H1'	2:X:2065:G:H4'	1.86	0.58
2:X:994:A:H5"	3:Y:85:A:N6	2.19	0.58
2:X:1875:A:H2'	2:X:1876:G:H8	1.68	0.58
2:X:2465:U:O2'	2:X:2466:A:H5"	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:83:ILE:HD13	14:M:86:ILE:HD11	1.84	0.58
2:X:870:C:HO2'	10:I:50:PHE:HD2	1.50	0.58
2:X:904:G:O2'	2:X:961:G:O6	2.15	0.58
12:K:27:SER:O	12:K:29:ARG:N	2.37	0.58
2:X:95:A:H5'	2:X:96:G:OP2	2.04	0.58
2:X:1508:C:HO2'	2:X:1509:G:C5'	2.16	0.58
4:B:59:TYR:O	4:B:61:LYS:N	2.37	0.58
7:E:74:ASN:O	7:E:83:TYR:OH	2.21	0.58
10:I:57:LEU:HD21	27:3:11:ALA:HB3	1.86	0.58
17:P:7:ALA:HB1	17:P:10:ILE:HD11	1.85	0.58
2:X:187:C:H2'	2:X:188:C:H6	1.69	0.57
2:X:1492:G:N7	2:X:1493:U:H5	2.01	0.57
21:T:57:GLU:HB2	21:T:88:SER:HB3	1.86	0.57
2:X:1300:G:OP2	17:P:99:ARG:NH2	2.37	0.57
2:X:1628:A:H4'	2:X:1628:A:OP1	2.02	0.57
2:X:2331:G:N2	2:X:2339:U:H3	2.02	0.57
2:X:2682:G:O2'	2:X:2683:U:OP2	2.22	0.57
12:K:24:LEU:HG	12:K:121:LEU:HD23	1.86	0.57
2:X:133:A:H61	2:X:146:U:H3	1.52	0.57
2:X:1885:G:H1'	2:X:1911:A:H62	1.69	0.57
5:C:8:LYS:HB2	5:C:8:LYS:NZ	2.17	0.57
9:H:98:ILE:HB	9:H:118:ALA:HA	1.86	0.57
2:X:83:G:H1	2:X:101:G:HO2'	1.53	0.57
2:X:318:A:C6	2:X:319:G:H1'	2.38	0.57
2:X:418:G:O2'	2:X:446:G:N1	2.34	0.57
16:O:74:PHE:HE1	16:O:83:LYS:HB2	1.68	0.57
2:X:811:C:H2'	2:X:812:U:H5'	1.85	0.57
2:X:1821:U:H2'	2:X:1822:C:H6	1.70	0.57
2:X:1998:A:O2'	2:X:1999:G:OP1	2.22	0.57
2:X:2843:A:OP1	4:B:127:PHE:HB2	2.04	0.57
16:O:98:ASP:OD1	16:O:98:ASP:N	2.38	0.57
2:X:498:G:N2	2:X:503:A:H8	1.96	0.57
2:X:506:A:N1	2:X:515:G:H8	2.02	0.57
17:P:71:VAL:HA	17:P:107:VAL:HA	1.86	0.57
18:Q:6:ILE:HG23	18:Q:33:VAL:HG11	1.87	0.57
19:R:4:LYS:HB3	19:R:4:LYS:HZ2	1.69	0.57
2:X:302:A:N6	2:X:450:C:C2	2.72	0.57
2:X:1504:U:HO2'	2:X:1505:G:P	2.28	0.57
20:S:98:GLU:HA	20:S:129:GLU:O	2.05	0.57
20:S:155:THR:O	20:S:155:THR:OG1	2.23	0.57
23:V:39:GLU:HG2	23:V:42:ARG:HE	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:N	2:X:1846:A:OP1	2.38	0.57
2:X:15:G:H4'	25:Z:18:THR:HB	1.85	0.57
2:X:2904:U:C5	25:Z:40:SER:HA	2.40	0.57
2:X:645:A:O2'	2:X:647:G:O2'	2.18	0.57
2:X:1498:U:HO2'	2:X:1499:U:H5	1.53	0.57
2:X:319:G:N7	2:X:400:C:N4	2.53	0.57
2:X:1353:A:H2'	2:X:1354:G:C8	2.40	0.57
2:X:1780:G:OP1	14:M:95:ARG:HD2	2.05	0.57
8:G:4:THR:OG1	15:N:61:TRP:HH2	1.88	0.57
9:H:24:VAL:HB	9:H:30:ARG:HD2	1.87	0.57
24:W:39:ASP:OD2	24:W:44:ARG:NH2	2.37	0.57
2:X:529:A:H1'	19:R:55:GLY:HA2	1.87	0.56
2:X:2241:C:H2'	2:X:2242:G:O4'	2.05	0.56
2:X:2370:U:O2'	2:X:2400:U:O2'	2.22	0.56
14:M:26:ASP:O	14:M:49:VAL:HG23	2.05	0.56
15:N:6:GLY:O	35:N:201:EPE:H72	2.04	0.56
16:O:63:ASN:HD21	16:O:96:THR:HB	1.69	0.56
21:T:82:ARG:HH12	21:T:84:LYS:HG3	1.69	0.56
2:X:300:G:N2	2:X:302:A:N7	2.52	0.56
2:X:579:U:H5'	15:N:42:SER:OG	2.04	0.56
2:X:1563:U:H2'	2:X:1564:G:C8	2.40	0.56
2:X:2807:G:N1	8:G:103:GLU:OE1	2.34	0.56
17:P:70:VAL:O	17:P:71:VAL:O	2.23	0.56
2:X:311:U:H3	2:X:404:U:H3	1.54	0.56
2:X:459:C:O2'	2:X:1907:U:O2'	2.23	0.56
2:X:1055:A:H5"	15:N:77:SER:HB2	1.87	0.56
2:X:2495:A:O2'	2:X:2496:A:H8	1.87	0.56
2:X:2784:A:N1	7:E:67:THR:HG21	2.19	0.56
4:B:67:LYS:HA	4:B:86:ARG:NH2	2.19	0.56
7:E:113:VAL:HG21	7:E:151:VAL:HG11	1.87	0.56
19:R:23:VAL:HA	19:R:35:VAL:HA	1.86	0.56
2:X:2290:C:H4'	2:X:2356:A:H4'	1.88	0.56
11:J:40:SER:HB3	11:J:127:VAL:HG12	1.87	0.56
15:N:10:THR:CG2	35:N:201:EPE:H32	2.33	0.56
24:W:10:ARG:HG3	24:W:10:ARG:HH11	1.70	0.56
2:X:107:G:H2'	2:X:108:A:C8	2.41	0.56
7:E:102:ASP:H	7:E:115:ILE:HD13	1.71	0.56
9:H:63:VAL:HB	9:H:106:LEU:HD11	1.86	0.56
10:I:57:LEU:CD1	27:3:12:LYS:CB	2.80	0.56
10:I:95:LEU:H	10:I:112:LEU:HD23	1.71	0.56
2:X:1518:G:H1	2:X:1562:C:N4	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:38:GLN:O	15:N:42:SER:HB2	2.06	0.56
2:X:99:U:O2	2:X:101:G:N1	2.37	0.56
2:X:955:A:C4	11:J:15:PRO:HG3	2.40	0.56
2:X:2835:C:H1'	25:Z:39:LEU:HD22	1.88	0.56
11:J:43:THR:N	11:J:46:GLN:OE1	2.33	0.56
2:X:322:A:O2'	2:X:323:C:H5'	2.05	0.56
2:X:2507:C:H2'	2:X:2508:G:H5'	1.87	0.56
8:G:22:GLU:HA	8:G:62:LYS:HB2	1.88	0.56
5:C:135:LYS:O	5:C:139:PHE:N	2.39	0.56
27:3:24:ARG:HD2	27:3:42:ARG:O	2.06	0.56
2:X:657:U:C4	2:X:659:A:N6	2.74	0.56
2:X:2358:G:O2'	2:X:2363:A:N1	2.31	0.56
5:C:7:LEU:HD23	5:C:8:LYS:N	2.20	0.56
2:X:575:G:N3	2:X:575:G:H2'	2.21	0.55
2:X:715:A:H4'	2:X:716:C:C5'	2.36	0.55
2:X:2807:G:C8	32:X:3006:MPD:H13	2.40	0.55
2:X:2877:G:H5'	2:X:2878:U:OP2	2.07	0.55
1:A:65:ILE:HA	1:A:103:TYR:HB2	1.88	0.55
2:X:273:A:OP2	2:X:297:G:N2	2.29	0.55
2:X:638:U:H2'	2:X:639:U:C6	2.40	0.55
2:X:1405:G:H2'	2:X:1406:G:C8	2.41	0.55
2:X:2403:A:C5	13:L:96:ARG:HD2	2.41	0.55
17:P:55:LEU:HD23	17:P:69:LEU:HD12	1.88	0.55
2:X:2026:C:O2	2:X:2714:U:O2'	2.24	0.55
8:G:60:ALA:HB3	8:G:127:GLY:HA2	1.88	0.55
21:T:71:ILE:HD13	21:T:91:ALA:HB2	1.89	0.55
2:X:1053:A:OP2	8:G:40:LYS:NZ	2.35	0.55
2:X:1758:A:N1	2:X:1759:G:N2	2.54	0.55
2:X:1845:U:HO2'	2:X:1846:A:P	2.29	0.55
4:B:128:GLN:HB2	4:B:173:MET:HG3	1.88	0.55
7:E:62:ARG:HA	7:E:65:HIS:HD2	1.72	0.55
2:X:135:G:H1	2:X:144:C:H42	1.53	0.55
2:X:383:A:H2'	2:X:384:G:O4'	2.06	0.55
2:X:1526:G:N2	2:X:1550:G:H22	2.05	0.55
2:X:2479:C:H2'	2:X:2480:A:C8	2.41	0.55
9:H:8:LEU:HD12	9:H:19:VAL:HG23	1.89	0.55
2:X:568:C:O2	2:X:597:U:O2'	2.21	0.55
2:X:955:A:N3	11:J:15:PRO:HG3	2.22	0.55
10:I:128:PHE:HD1	10:I:129:SER:N	2.03	0.55
2:X:613:G:H2'	2:X:2057:A:N7	2.22	0.55
2:X:2112:C:H42	2:X:2261:A:H61	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:73:ASP:HB3	14:M:82:LYS:HE3	1.88	0.55
2:X:627:C:C5	35:N:201:EPE:H102	2.42	0.55
8:G:4:THR:HG23	15:N:61:TRP:HZ3	1.70	0.55
14:M:98:LYS:HB3	14:M:100:TYR:HE1	1.72	0.55
2:X:2313:A:H4'	2:X:2314:A:O4'	2.07	0.55
24:W:8:LEU:HB2	24:W:28:LEU:HD13	1.89	0.55
2:X:955:A:N7	2:X:956:A:C5	2.74	0.54
8:G:43:VAL:HG23	15:N:100:ILE:HG12	1.88	0.54
16:O:32:THR:HG22	16:O:61:THR:HG23	1.88	0.54
2:X:1836:A:O2'	2:X:1837:A:O5'	2.24	0.54
8:G:2:ARG:NH2	8:G:2:ARG:HA	2.22	0.54
16:O:20:ILE:HG23	16:O:97:ILE:HD11	1.88	0.54
11:J:134:ARG:HH12	20:S:123:GLN:CD	2.11	0.54
2:X:870:C:H1'	10:I:50:PHE:CE2	2.42	0.54
2:X:1488:A:H61	2:X:1595:C:H42	1.54	0.54
2:X:1576:A:N3	2:X:1577:G:C8	2.76	0.54
16:O:16:GLU:HA	16:O:97:ILE:HB	1.88	0.54
10:I:60:ARG:O	10:I:61:LEU:HG	2.08	0.54
19:R:36:GLU:OE2	19:R:37:GLY:N	2.41	0.54
20:S:51:VAL:O	20:S:55:VAL:HG23	2.07	0.54
1:A:156:ARG:HB2	2:X:1845:U:H3'	1.89	0.54
2:X:111:U:H5'	2:X:112:U:OP2	2.08	0.54
2:X:1821:U:H2'	2:X:1822:C:C6	2.42	0.54
2:X:2725:U:H2'	2:X:2726:C:C6	2.43	0.54
26:2:32:LEU:HD22	26:2:43:LEU:HD23	1.89	0.54
2:X:37:C:H2'	2:X:38:A:C8	2.42	0.54
2:X:627:C:OP2	35:N:201:EPE:O2S	2.24	0.54
2:X:1885:G:HO2'	2:X:1886:A:P	2.30	0.54
4:B:16:PHE:CE1	4:B:22:LEU:HD13	2.43	0.54
22:U:17:ARG:O	22:U:29:TRP:HD1	1.90	0.54
2:X:267:G:H2'	2:X:268:A:H5"	1.89	0.54
2:X:2361:U:OP2	13:L:17:ARG:NH1	2.41	0.54
14:M:94:VAL:HG11	14:M:99:LEU:HD21	1.89	0.54
17:P:11:ARG:HA	17:P:100:THR:HG22	1.89	0.54
2:X:986:G:H5"	10:I:32:GLY:HA2	1.89	0.54
2:X:1658:A:N1	17:P:93:ALA:HB2	2.23	0.54
2:X:1813:A:H1'	2:X:1965:A:N6	2.23	0.54
27:3:22:LEU:CB	27:3:44:LEU:HB3	2.37	0.54
2:X:100:U:H3'	2:X:101:G:H5'	1.89	0.54
2:X:218:G:H4'	2:X:219:A:H4'	1.90	0.54
2:X:1576:A:H4'	2:X:1577:G:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1762:U:H5'	2:X:1763:U:OP2	2.08	0.54
10:I:85:PHE:HA	10:I:89:THR:HG23	1.89	0.54
2:X:618:A:O2'	2:X:619:U:H5'	2.08	0.53
2:X:1983:U:H1'	2:X:2579:U:OP1	2.07	0.53
2:X:342:A:N1	2:X:365:A:O2'	2.33	0.53
2:X:1366:U:H5"	2:X:1367:C:H5	1.73	0.53
2:X:1733:A:H2'	2:X:1734:A:C8	2.43	0.53
1:A:142:HIS:N	1:A:192:ILE:O	2.41	0.53
2:X:1065:A:H3'	2:X:1065:A:C8	2.44	0.53
2:X:1474:C:H2'	2:X:1475:A:H8	1.73	0.53
9:H:56:ASP:OD1	9:H:56:ASP:N	2.36	0.53
2:X:499:A:N3	2:X:503:A:O2'	2.41	0.53
2:X:2231:C:O2'	2:X:2232:A:H8	1.92	0.53
9:H:13:ASN:CG	9:H:96:THR:H	2.11	0.53
2:X:2232:A:H5'	2:X:2233:C:P	2.48	0.53
2:X:2457:A:N3	2:X:2457:A:H2'	2.24	0.53
2:X:687:G:N2	2:X:690:U:OP2	2.42	0.53
2:X:730:A:C8	2:X:819:A:C6	2.96	0.53
2:X:2732:A:H2'	2:X:2733:A:O4'	2.08	0.53
8:G:21:ALA:HB1	8:G:63:ILE:HD13	1.91	0.53
10:I:29:LYS:O	10:I:30:THR:HB	2.09	0.53
2:X:148:U:H2'	2:X:149:U:C6	2.44	0.53
2:X:1352:C:O2'	2:X:1429:G:O2'	2.25	0.53
27:3:22:LEU:CB	27:3:44:LEU:HD22	2.39	0.53
2:X:59:U:O2'	2:X:74:U:OP2	2.22	0.53
2:X:155:U:H5'	2:X:156:A:OP2	2.09	0.53
1:A:201:GLU:HG3	1:A:202:LEU:HD12	1.91	0.53
2:X:1306:A:C2	2:X:2040:A:C4	2.97	0.53
2:X:1523:G:H1	2:X:1557:C:H42	1.56	0.53
2:X:2058:A:C6	2:X:2525:C:H1'	2.44	0.53
4:B:134:HIS:CE1	4:B:168:LYS:HB2	2.44	0.53
19:R:26:THR:HA	19:R:33:VAL:HG12	1.91	0.53
23:V:25:LEU:HD11	23:V:29:ARG:NH1	2.24	0.53
2:X:309:U:O2'	2:X:310:C:OP2	2.19	0.53
2:X:415:U:H5'	2:X:416:G:OP1	2.09	0.52
2:X:620:G:C6	2:X:621:A:N6	2.77	0.52
2:X:1514:A:H3'	2:X:1515:G:H8	1.74	0.52
2:X:1518:G:N2	2:X:1562:C:N3	2.52	0.52
4:B:119:THR:CB	4:B:179:THR:HG22	2.38	0.52
4:B:182:ASN:O	4:B:183:LEU:HD23	2.09	0.52
8:G:39:GLY:C	8:G:41:ASN:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:16:SER:O	18:Q:20:MET:HG3	2.10	0.52
2:X:955:A:C6	11:J:15:PRO:HD3	2.44	0.52
2:X:1349:U:H4'	2:X:1350:U:O5'	2.08	0.52
2:X:1823:U:H2'	2:X:1824:C:C6	2.43	0.52
2:X:2271:U:O2'	2:X:2272:U:H5'	2.09	0.52
2:X:2507:C:C2'	2:X:2508:G:H5'	2.39	0.52
3:Y:69:C:H42	3:Y:102:A:H61	1.58	0.52
2:X:460:C:H2'	2:X:461:A:H8	1.72	0.52
2:X:1930:G:H2'	2:X:1931:G:H8	1.75	0.52
2:X:870:C:H1'	10:I:50:PHE:HE2	1.74	0.52
2:X:2268:A:H2'	2:X:2269:G:C8	2.44	0.52
2:X:858:U:H2'	2:X:859:C:C6	2.44	0.52
2:X:2760:A:C2	4:B:216:LYS:HB2	2.45	0.52
4:B:119:THR:HA	4:B:179:THR:HG22	1.90	0.52
17:P:30:ALA:HA	17:P:33:ILE:HD12	1.90	0.52
21:T:81:GLY:O	21:T:82:ARG:NE	2.42	0.52
2:X:38:A:H2'	2:X:39:C:O4'	2.10	0.52
2:X:416:G:OP2	2:X:469:A:N6	2.42	0.52
2:X:668:C:H2'	2:X:669:C:C6	2.45	0.52
2:X:1733:A:H2'	2:X:1734:A:H8	1.74	0.52
2:X:1862:G:H1	2:X:1957:G:H21	1.58	0.52
2:X:2819:C:H42	2:X:2824:G:H1	1.58	0.52
3:Y:74:G:H1	3:Y:97:A:H62	1.57	0.52
2:X:142:G:N2	2:X:1640:U:O3'	2.29	0.52
2:X:627:C:OP2	35:N:201:EPE:C6	2.57	0.52
2:X:719:G:H1'	5:C:74:ARG:HE	1.73	0.52
2:X:1516:C:H42	2:X:1564:G:H1	1.56	0.52
2:X:1211:G:H2'	2:X:1212:U:C6	2.44	0.52
2:X:1770:C:O2'	2:X:1771:A:H8	1.93	0.52
2:X:2018:U:O2'	2:X:2019:G:H5'	2.09	0.52
2:X:2581:U:H2'	2:X:2582:U:C6	2.45	0.52
6:D:105:SER:O	6:D:105:SER:OG	2.27	0.52
7:E:90:VAL:O	7:E:160:LYS:HA	2.10	0.52
11:J:55:THR:HG22	11:J:64:VAL:HG11	1.92	0.52
15:N:61:TRP:CD2	15:N:93:LYS:HB2	2.45	0.52
2:X:721:A:H8	2:X:2096:G:H21	1.57	0.52
18:Q:49:LYS:HE2	18:Q:50:VAL:H	1.74	0.52
2:X:17:G:H5"	25:Z:11:THR:HG21	1.92	0.52
2:X:1013:U:H2'	2:X:1014:U:C6	2.45	0.52
2:X:2286:G:H1'	2:X:2454:C:C2	2.44	0.52
4:B:20:GLY:O	9:H:73:ASP:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:O	1:A:171:TYR:N	2.43	0.51
2:X:955:A:N7	2:X:956:A:C6	2.79	0.51
13:L:30:ARG:HD2	13:L:45:ILE:HD12	1.92	0.51
15:N:6:GLY:HA3	35:N:201:EPE:H52	1.92	0.51
2:X:1315:C:OP1	12:K:32:THR:HG23	2.10	0.51
3:Y:3:U:H3	3:Y:112:G:H1	1.58	0.51
14:M:48:VAL:O	14:M:63:VAL:HA	2.10	0.51
2:X:1492:G:C8	2:X:1493:U:H5	2.29	0.51
4:B:215:ILE:O	4:B:216:LYS:HG2	2.10	0.51
5:C:8:LYS:NZ	5:C:12:THR:O	2.43	0.51
5:C:190:ASP:OD1	5:C:191:SER:N	2.39	0.51
17:P:14:PRO:O	17:P:18:ARG:HG3	2.10	0.51
1:A:43:ARG:HG3	1:A:49:LEU:HA	1.93	0.51
2:X:1336:G:N1	2:X:1684:A:OP2	2.36	0.51
2:X:1471:A:H1'	2:X:1472:C:C4	2.45	0.51
2:X:1508:C:O2'	2:X:1509:G:O5'	2.28	0.51
2:X:2109:A:H2'	2:X:2110:G:O4'	2.10	0.51
4:B:67:LYS:HA	4:B:86:ARG:HH22	1.76	0.51
4:B:169:MET:HB2	4:B:170:PRO:CD	2.41	0.51
9:H:100:GLY:H	9:H:119:PRO:HG2	1.76	0.51
1:A:156:ARG:NH1	2:X:1844:G:OP2	2.43	0.51
2:X:804:G:O2'	2:X:805:G:H5'	2.10	0.51
4:B:107:VAL:HG21	4:B:193:LYS:HA	1.93	0.51
2:X:234:C:O2'	2:X:235:G:C8	2.59	0.51
2:X:280:C:H2'	2:X:281:A:C8	2.44	0.51
2:X:1383:G:N2	2:X:1644:C:O2	2.26	0.51
2:X:1526:G:C8	2:X:1527:A:C6	2.98	0.51
2:X:2126:C:H2'	2:X:2127:G:H8	1.75	0.51
2:X:2736:G:H2'	2:X:2737:C:C6	2.46	0.51
2:X:179:A:OP2	2:X:179:A:H8	1.94	0.51
2:X:1353:A:H2'	2:X:1354:G:H8	1.75	0.51
2:X:2052:C:H5'	4:B:162:ARG:HH21	1.75	0.51
2:X:2687:A:H2'	2:X:2688:G:O4'	2.11	0.51
5:C:65:TRP:CZ2	5:C:75:GLN:HG3	2.45	0.51
12:K:29:ARG:HB3	12:K:120:GLU:HB3	1.93	0.51
15:N:10:THR:HA	15:N:13:ARG:HB2	1.93	0.51
2:X:895:U:O2	24:W:46:GLN:NE2	2.43	0.51
2:X:1000:G:H2'	2:X:1001:A:H2'	1.93	0.51
2:X:1017:A:H8	2:X:1017:A:OP1	1.93	0.51
2:X:1526:G:H21	2:X:1550:G:H22	1.58	0.51
2:X:2646:U:O2	4:B:169:MET:HE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:4:G:N3	3:Y:112:G:N2	2.59	0.51
2:X:51:G:O2'	2:X:118:A:N1	2.31	0.51
2:X:774:G:H2'	2:X:1802:U:H1'	1.92	0.51
2:X:1185:U:H4'	2:X:1186:A:O4'	2.10	0.51
2:X:1490:G:O2'	2:X:1491:C:O4'	2.29	0.51
2:X:1507:A:C2'	2:X:1508:C:H5'	2.40	0.51
2:X:2442:G:H4'	10:I:59:ARG:O	2.11	0.51
2:X:173:A:H2'	2:X:174:U:C6	2.46	0.51
2:X:363:A:H4'	2:X:365:A:C8	2.46	0.51
2:X:1378:U:H3'	2:X:1434:U:O2	2.11	0.51
2:X:2059:G:N2	2:X:2599:A:OP2	2.43	0.51
3:Y:38:U:HO2'	3:Y:43:A:N6	2.08	0.51
15:N:10:THR:OG1	35:N:201:EPE:H31	2.11	0.51
2:X:657:U:O2	2:X:657:U:H2'	2.10	0.50
2:X:1072:A:N3	2:X:2513:G:O2'	2.36	0.50
3:Y:22:G:N2	3:Y:26:C:N3	2.59	0.50
9:H:4:GLN:OE1	9:H:23:LYS:NZ	2.45	0.50
12:K:61:ASN:HA	12:K:64:LYS:HE3	1.93	0.50
17:P:65:ASN:HD22	17:P:65:ASN:H	1.59	0.50
1:A:43:ARG:HE	1:A:49:LEU:HD12	1.77	0.50
2:X:658:A:H3'	2:X:659:A:C5'	2.41	0.50
2:X:1176:U:H6	2:X:1176:U:H5'	1.77	0.50
2:X:1887:G:O6	2:X:1910:G:N2	2.45	0.50
2:X:2289:U:H2'	2:X:2290:C:H6	1.76	0.50
2:X:2479:C:C4	2:X:2480:A:C6	2.99	0.50
10:I:19:VAL:CG2	10:I:30:THR:HG23	2.42	0.50
2:X:1542:C:H3'	2:X:1543:G:H5"	1.94	0.50
2:X:2257:G:H2'	2:X:2258:U:H6	1.76	0.50
2:X:2811:U:H2'	2:X:2812:U:C6	2.46	0.50
3:Y:91:C:H2'	3:Y:92:G:C8	2.46	0.50
4:B:88:ILE:O	4:B:89:ARG:NH2	2.43	0.50
4:B:119:THR:CA	4:B:179:THR:HG22	2.41	0.50
14:M:82:LYS:NZ	14:M:82:LYS:HB3	2.26	0.50
14:M:98:LYS:HB3	14:M:100:TYR:CE1	2.46	0.50
2:X:201:C:H5'	2:X:2271:U:OP1	2.12	0.50
5:C:29:ASN:OD1	5:C:32:VAL:HG23	2.12	0.50
8:G:112:SER:O	8:G:112:SER:OG	2.25	0.50
12:K:70:GLU:O	12:K:72:LEU:N	2.45	0.50
15:N:76:TYR:CZ	15:N:80:MET:HG3	2.46	0.50
20:S:105:PRO:HD2	20:S:124:PRO:HA	1.93	0.50
2:X:17:G:OP1	25:Z:11:THR:HG22	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:422:G:H1	2:X:444:C:H42	1.58	0.50
2:X:1041:G:H5"	15:N:92:ARG:NH1	2.26	0.50
2:X:1746:G:H2'	2:X:1747:G:H8	1.76	0.50
19:R:39:ASN:O	19:R:39:ASN:ND2	2.41	0.50
27:3:53:SER:O	27:3:56:LYS:HG2	2.12	0.50
2:X:2043:U:H2'	2:X:2044:C:C6	2.47	0.50
2:X:2539:C:H2'	2:X:2540:A:O4'	2.12	0.50
9:H:120:GLU:OE1	14:M:67:SER:OG	2.28	0.50
15:N:27:SER:HB2	15:N:31:LEU:HG	1.94	0.50
27:3:24:ARG:HG2	27:3:24:ARG:HH11	1.77	0.50
2:X:581:A:H4'	15:N:57:PHE:HE1	1.76	0.50
2:X:704:U:H2'	2:X:705:U:O4'	2.12	0.50
2:X:1337:A:H4'	2:X:1338:U:H5"	1.94	0.50
2:X:1405:G:H2'	2:X:1406:G:H8	1.75	0.50
2:X:1922:C:H2'	2:X:1923:A:H8	1.76	0.50
21:T:56:GLY:H	21:T:59:VAL:HB	1.76	0.50
1:A:241:ILE:HG13	2:X:1929:C:H5"	1.94	0.50
2:X:132:C:H2'	2:X:133:A:O4'	2.12	0.50
2:X:1392:G:C6	2:X:1393:C:C4	3.00	0.50
2:X:1873:G:O2'	2:X:1874:A:O4'	2.20	0.50
19:R:49:GLN:O	19:R:51:ASN:N	2.42	0.50
2:X:64:A:H2	18:Q:68:TYR:CD2	2.30	0.50
2:X:683:G:C2	2:X:696:G:C4	3.00	0.50
2:X:897:A:H2'	2:X:898:U:H6	1.75	0.50
2:X:90:A:OP1	2:X:90:A:C8	2.65	0.49
2:X:194:A:H2'	2:X:195:C:C6	2.47	0.49
2:X:1336:G:O2'	2:X:1684:A:N6	2.45	0.49
2:X:1378:U:OP1	2:X:1434:U:N3	2.41	0.49
2:X:2904:U:H5	25:Z:40:SER:HA	1.75	0.49
5:C:8:LYS:HA	5:C:14:SER:H	1.77	0.49
9:H:64:ARG:NH1	9:H:101:PRO:O	2.41	0.49
14:M:51:LYS:HD3	14:M:100:TYR:OH	2.12	0.49
26:2:22:ARG:O	26:2:28:GLY:HA3	2.12	0.49
2:X:896:U:H2'	2:X:897:A:H8	1.77	0.49
2:X:1514:A:H3'	2:X:1515:G:C8	2.47	0.49
2:X:2803:A:C2	2:X:2805:A:C4	3.01	0.49
11:J:75:THR:HG21	11:J:87:LYS:HB2	1.94	0.49
12:K:23:SER:O	12:K:24:LEU:HB3	2.11	0.49
24:W:8:LEU:HD12	24:W:53:LEU:O	2.11	0.49
2:X:2:A:H4'	2:X:3:U:O4'	2.13	0.49
4:B:16:PHE:HB2	14:M:14:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:88:ILE:O	8:G:89:THR:HB	2.12	0.49
11:J:66:ILE:HG12	11:J:104:PHE:HE1	1.75	0.49
2:X:204:C:H1'	2:X:253:G:O6	2.12	0.49
2:X:683:G:N1	2:X:696:G:C5	2.80	0.49
2:X:799:U:H2'	2:X:800:G:H8	1.76	0.49
2:X:1197:C:H2'	2:X:1198:G:O4'	2.12	0.49
2:X:1261:G:OP2	16:O:89:ARG:NH1	2.45	0.49
2:X:1635:A:H2'	2:X:1635:A:N3	2.26	0.49
2:X:1986:G:H2'	2:X:1987:A:O4'	2.13	0.49
8:G:77:ARG:O	8:G:85:ILE:HD12	2.12	0.49
14:M:106:ARG:HA	14:M:106:ARG:NH1	2.27	0.49
15:N:8:THR:H	35:N:201:EPE:H81	1.78	0.49
1:A:181:VAL:HG23	1:A:271:VAL:HB	1.95	0.49
2:X:379:C:H2'	2:X:380:U:H6	1.77	0.49
2:X:787:U:H2'	2:X:788:A:C8	2.48	0.49
2:X:955:A:C2	11:J:15:PRO:HB3	2.47	0.49
2:X:2299:U:H5"	2:X:2300:A:OP1	2.11	0.49
10:I:65:GLY:O	10:I:93:PRO:HB2	2.11	0.49
12:K:53:LYS:HB3	12:K:55:ASP:OD1	2.13	0.49
17:P:71:VAL:C	17:P:108:SER:H	2.16	0.49
19:R:56:ILE:HB	19:R:58:GLU:HG2	1.94	0.49
21:T:88:SER:HB2	21:T:90:TYR:HE1	1.76	0.49
24:W:18:THR:HB	24:W:49:LYS:NZ	2.28	0.49
2:X:633:A:H2'	2:X:634:C:O4'	2.13	0.49
11:J:93:TRP:O	11:J:94:ILE:HD13	2.12	0.49
1:A:230:HIS:CD2	1:A:249:PRO:HG3	2.48	0.49
2:X:609:U:H2'	2:X:610:U:O4'	2.13	0.49
2:X:635:G:O2'	27:3:3:LYS:HA	2.13	0.49
2:X:747:U:H2'	2:X:748:U:C6	2.47	0.49
2:X:1259:U:H2'	2:X:1260:C:H6	1.78	0.49
2:X:1527:A:H2	2:X:1549:C:C4	2.31	0.49
5:C:181:LEU:HD23	5:C:181:LEU:O	2.13	0.49
7:E:44:LYS:HE3	7:E:56:SER:CB	2.43	0.49
8:G:39:GLY:O	8:G:41:ASN:N	2.42	0.49
13:L:44:ILE:O	13:L:53:LEU:HD12	2.12	0.49
18:Q:34:ASN:O	18:Q:38:VAL:HG23	2.12	0.49
19:R:80:ARG:CZ	19:R:96:LYS:HA	2.43	0.49
19:R:84:LYS:HA	19:R:90:LYS:O	2.13	0.49
25:Z:28:THR:HG23	25:Z:37:TYR:HE1	1.77	0.49
2:X:157:U:H2'	2:X:158:G:H8	1.76	0.49
2:X:94:A:H2'	2:X:95:A:O4'	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:425:G:H1	2:X:441:C:H42	1.59	0.49
2:X:1498:U:O2'	2:X:1499:U:H5	1.94	0.49
2:X:2362:A:OP2	13:L:17:ARG:HG2	2.12	0.49
2:X:2446:U:H2'	2:X:2447:C:C6	2.47	0.49
3:Y:12:U:OP2	3:Y:68:A:O2'	2.28	0.49
2:X:12:U:H2'	2:X:12:U:O2	2.12	0.49
2:X:266:A:H2'	2:X:267:G:O4'	2.13	0.49
2:X:2627:A:O2'	2:X:2628:C:H5'	2.13	0.49
3:Y:76:A:C2	3:Y:96:G:C4	3.01	0.49
10:I:57:LEU:HD11	27:3:12:LYS:CA	2.43	0.49
13:L:29:PRO:HD2	13:L:88:GLY:HA2	1.95	0.49
2:X:267:G:C2'	2:X:268:A:H5"	2.42	0.48
2:X:945:A:O2'	2:X:946:A:H5'	2.13	0.48
2:X:1487:G:C2	2:X:1597:U:O2	2.65	0.48
2:X:1597:U:O3'	2:X:1767:G:N2	2.46	0.48
9:H:30:ARG:HD3	9:H:32:THR:O	2.13	0.48
2:X:654:C:H42	2:X:662:G:H1	1.60	0.48
2:X:1304:G:H5"	25:Z:20:PHE:CE2	2.48	0.48
2:X:1973:U:H2'	2:X:1974:C:C6	2.48	0.48
8:G:79:SER:OG	8:G:81:HIS:HB2	2.12	0.48
12:K:14:LYS:O	12:K:18:ARG:HG3	2.12	0.48
12:K:74:GLU:O	12:K:76:GLU:N	2.46	0.48
2:X:767:A:H2'	2:X:768:A:H8	1.78	0.48
2:X:1815:C:H2'	2:X:1816:A:O4'	2.13	0.48
2:X:1932:C:O2'	2:X:1956:G:N7	2.44	0.48
10:I:19:VAL:HG21	10:I:30:THR:HG23	1.95	0.48
18:Q:50:VAL:O	18:Q:82:LEU:HD23	2.13	0.48
2:X:514:G:C2'	2:X:515:G:H5'	2.43	0.48
2:X:538:G:OP2	33:X:3494:SPD:H91	2.14	0.48
2:X:719:G:OP1	5:C:76:GLY:HA3	2.13	0.48
2:X:2842:G:H2'	2:X:2843:A:H5"	1.95	0.48
2:X:278:A:H2'	2:X:279:A:C8	2.47	0.48
2:X:810:A:H2'	2:X:811:C:C6	2.49	0.48
2:X:1560:A:H4'	32:X:3004:MPD:H12	1.95	0.48
2:X:1770:C:O2'	2:X:1771:A:OP2	2.30	0.48
2:X:1806:U:C5	2:X:1811:A:N7	2.81	0.48
2:X:2257:G:O3'	22:U:32:ASN:HB3	2.13	0.48
4:B:53:PHE:CG	4:B:54:GLU:N	2.81	0.48
4:B:118:VAL:HG23	4:B:180:VAL:HG23	1.94	0.48
5:C:148:GLN:HB2	5:C:186:ILE:O	2.13	0.48
15:N:66:ASN:O	15:N:70:ARG:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:U:29:TRP:CG	22:U:30:ASN:N	2.81	0.48
1:A:79:ASP:HB3	1:A:93:LEU:O	2.13	0.48
2:X:994:A:H5"	3:Y:85:A:H61	1.76	0.48
2:X:1540:U:H1'	2:X:1625:U:H4'	1.94	0.48
2:X:1699:A:H1'	4:B:127:PHE:CE1	2.48	0.48
2:X:2646:U:H5"	4:B:165:LYS:HA	1.95	0.48
4:B:67:LYS:HD2	4:B:68:TYR:CE1	2.48	0.48
9:H:102:VAL:O	9:H:121:VAL:HA	2.13	0.48
10:I:70:ASN:O	10:I:72:LYS:N	2.45	0.48
2:X:683:G:N2	2:X:697:U:C6	2.81	0.48
2:X:719:G:H1'	5:C:74:ARG:NE	2.28	0.48
2:X:998:G:C5	2:X:999:U:C5	3.02	0.48
2:X:2082:C:OP1	25:Z:5:LYS:NZ	2.38	0.48
2:X:2357:G:O3'	21:T:52:LYS:HE3	2.13	0.48
2:X:317:G:H2'	2:X:318:A:O4'	2.13	0.48
2:X:514:G:H2'	2:X:515:G:H5'	1.94	0.48
2:X:1494:G:C8	2:X:1495:C:C5	2.99	0.48
2:X:187:C:H2'	2:X:188:C:C6	2.49	0.48
2:X:888:G:N2	2:X:980:U:C2	2.82	0.48
2:X:1522:G:H2'	2:X:1523:G:H8	1.78	0.48
3:Y:65:G:O6	3:Y:105:G:N2	2.44	0.48
3:Y:90:C:H2'	3:Y:91:C:C6	2.49	0.48
3:Y:103:A:H2'	3:Y:104:C:O4'	2.13	0.48
5:C:140:LYS:HA	5:C:142:VAL:HG12	1.95	0.48
19:R:75:THR:HB	19:R:76:ASN:ND2	2.29	0.48
21:T:29:LEU:H	21:T:29:LEU:HD12	1.79	0.48
24:W:12:VAL:HG12	24:W:20:ARG:HG2	1.96	0.48
2:X:226:A:O2'	2:X:466:C:O2	2.32	0.48
2:X:731:U:H5	2:X:833:A:H61	1.58	0.48
2:X:987:U:OP1	10:I:33:ARG:HB3	2.14	0.48
2:X:1088:C:H5'	2:X:1089:C:OP1	2.13	0.48
12:K:6:LEU:HA	12:K:13:ARG:HD3	1.96	0.48
12:K:51:GLY:HA2	12:K:86:PHE:CE2	2.49	0.48
20:S:22:ARG:NE	20:S:87:THR:HG23	2.29	0.48
2:X:606:G:H22	2:X:621:A:H2	1.61	0.47
3:Y:1:U:O2'	3:Y:2:C:OP2	2.29	0.47
7:E:84:VAL:HG23	7:E:134:GLU:H	1.78	0.47
23:V:63:GLU:HA	23:V:66:LYS:NZ	2.28	0.47
25:Z:8:THR:HG22	25:Z:12:ARG:HB3	1.96	0.47
2:X:24:G:H2'	2:X:25:U:H6	1.79	0.47
2:X:660:A:N3	2:X:660:A:O4'	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:665:G:H4'	2:X:666:A:C5'	2.44	0.47
2:X:1700:C:H2'	2:X:1701:U:C6	2.49	0.47
2:X:1700:C:H2'	2:X:1701:U:H6	1.78	0.47
15:N:58:ARG:HA	15:N:61:TRP:CD1	2.48	0.47
20:S:76:ASP:CG	20:S:77:TYR:H	2.18	0.47
1:A:223:SER:OG	2:X:1853:C:H5"	2.15	0.47
2:X:3:U:H2'	2:X:4:U:H6	1.78	0.47
2:X:2856:U:H2'	2:X:2857:A:H8	1.79	0.47
9:H:13:ASN:OD1	9:H:96:THR:N	2.42	0.47
15:N:66:ASN:OD1	15:N:70:ARG:NH1	2.47	0.47
18:Q:55:ILE:HD11	18:Q:76:ARG:NE	2.29	0.47
2:X:294:G:C2	2:X:295:G:C8	3.02	0.47
2:X:437:A:O2'	2:X:456:G:OP1	2.25	0.47
2:X:706:U:O2'	10:I:13:ARG:HA	2.14	0.47
2:X:841:C:H2'	2:X:842:U:C6	2.49	0.47
2:X:1259:U:H2'	2:X:1260:C:C6	2.49	0.47
2:X:2712:G:OP1	14:M:51:LYS:NZ	2.48	0.47
20:S:136:ASN:O	20:S:138:PRO:HD3	2.14	0.47
2:X:1488:A:H61	2:X:1595:C:N4	2.11	0.47
2:X:1963:A:OP2	2:X:1988:C:N4	2.48	0.47
2:X:2675:G:H2'	2:X:2676:U:C6	2.50	0.47
8:G:94:ARG:HA	8:G:98:PRO:HB3	1.96	0.47
2:X:331:G:O2'	2:X:332:A:O5'	2.31	0.47
2:X:566:U:H2'	2:X:567:G:N7	2.28	0.47
2:X:829:U:C5	2:X:837:G:C5	3.03	0.47
2:X:1515:G:HO2'	2:X:1516:C:P	2.37	0.47
2:X:1575:A:N3	2:X:1576:A:H5'	2.30	0.47
2:X:2856:U:H2'	2:X:2857:A:C8	2.50	0.47
3:Y:21:G:H22	3:Y:58:G:H22	1.62	0.47
2:X:627:C:H5	35:N:201:EPE:H102	1.77	0.47
2:X:1336:G:H5"	2:X:1337:A:OP1	2.15	0.47
2:X:1474:C:H2'	2:X:1475:A:C8	2.48	0.47
2:X:1478:A:H61	2:X:1605:A:H62	1.61	0.47
2:X:1511:C:H5'	2:X:1512:U:OP1	2.14	0.47
2:X:1575:A:H2'	2:X:1576:A:C5'	2.45	0.47
2:X:2289:U:H2'	2:X:2290:C:C6	2.50	0.47
2:X:2642:U:C2	25:Z:4:PRO:HA	2.49	0.47
3:Y:6:U:H3	3:Y:109:C:H42	1.63	0.47
10:I:70:ASN:C	10:I:72:LYS:H	2.17	0.47
13:L:30:ARG:HD2	13:L:45:ILE:CD1	2.44	0.47
17:P:6:VAL:HG22	17:P:104:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Q:51:ALA:HB3	18:Q:81:THR:O	2.15	0.47
19:R:72:ASP:N	19:R:73:PRO:HD2	2.29	0.47
20:S:26:LYS:HE3	20:S:26:LYS:HB2	1.68	0.47
21:T:83:ASP:OD1	21:T:84:LYS:N	2.42	0.47
24:W:15:ARG:HD3	24:W:53:LEU:HD23	1.97	0.47
2:X:1885:G:O2'	2:X:1886:A:O5'	2.28	0.47
2:X:2519:U:H2'	2:X:2520:U:C6	2.49	0.47
2:X:2882:A:C6	2:X:2883:U:C4	3.02	0.47
12:K:22:THR:OG1	12:K:67:ARG:HB2	2.15	0.47
2:X:909:G:C6	2:X:910:C:N4	2.82	0.47
8:G:25:THR:HB	8:G:28:ARG:HG3	1.95	0.47
10:I:12:SER:OG	10:I:13:ARG:HG3	2.15	0.47
15:N:78:ARG:CB	15:N:78:ARG:HH11	2.28	0.47
15:N:93:LYS:CA	15:N:96:SER:HB3	2.45	0.47
2:X:58:G:N2	2:X:70:G:C4	2.83	0.47
2:X:523:A:H2'	2:X:524:A:C8	2.50	0.47
2:X:1331:C:H5"	12:K:69:VAL:HG13	1.96	0.47
2:X:1379:A:C6	2:X:1382:C:N3	2.83	0.47
2:X:1820:G:O2'	2:X:1927:A:N1	2.43	0.47
2:X:2688:G:H2'	2:X:2689:A:C8	2.49	0.47
2:X:2783:U:H3'	28:4:19:ARG:O	2.15	0.47
20:S:95:ASN:OD1	20:S:96:MET:N	2.48	0.47
2:X:233:U:O2'	2:X:234:C:H5'	2.15	0.46
2:X:379:C:C2	2:X:380:U:C5	3.03	0.46
2:X:1015:C:O2'	2:X:1027:A:N3	2.44	0.46
2:X:1211:G:H2'	2:X:1212:U:H6	1.80	0.46
2:X:1357:G:C2	2:X:1366:U:H5'	2.51	0.46
2:X:1510:U:H3	2:X:1571:G:H22	1.62	0.46
2:X:1514:A:H61	2:X:1567:A:H1'	1.80	0.46
2:X:2903:A:H5"	2:X:2904:U:H5'	1.97	0.46
3:Y:68:A:C2	3:Y:103:A:N1	2.83	0.46
13:L:45:ILE:HG22	13:L:51:VAL:O	2.15	0.46
19:R:32:ARG:HB3	19:R:64:HIS:HA	1.98	0.46
2:X:1528:G:H1	2:X:1547:C:H42	1.62	0.46
2:X:1876:G:H2'	2:X:1877:G:C8	2.51	0.46
2:X:2026:C:H5"	2:X:2750:C:O2'	2.16	0.46
4:B:33:ASN:HB2	4:B:105:VAL:CG2	2.45	0.46
20:S:27:VAL:HG12	20:S:28:PRO:O	2.14	0.46
1:A:11:ASN:OD1	1:A:14:ARG:NH1	2.48	0.46
2:X:868:A:H2'	2:X:869:G:C8	2.50	0.46
2:X:1036:C:H2'	2:X:1037:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1651:C:H4'	2:X:1652:A:O5'	2.15	0.46
2:X:1869:G:C2	2:X:1928:A:C2	3.04	0.46
2:X:2011:U:H2'	2:X:2012:G:C8	2.51	0.46
2:X:2338:A:H3'	2:X:2339:U:H5	1.81	0.46
3:Y:63:U:O2'	3:Y:64:A:H5'	2.15	0.46
5:C:110:LEU:HA	5:C:110:LEU:HD23	1.51	0.46
8:G:49:VAL:O	8:G:51:THR:HG22	2.15	0.46
35:N:201:EPE:H82	35:N:201:EPE:H51	1.61	0.46
19:R:86:VAL:CB	19:R:90:LYS:HG3	2.46	0.46
2:X:2:A:H4'	2:X:3:U:H5'	1.98	0.46
2:X:659:A:O2'	2:X:660:A:H4'	2.15	0.46
2:X:1151:G:H2'	2:X:1152:U:H6	1.81	0.46
2:X:1395:G:C6	2:X:1408:G:N7	2.84	0.46
2:X:2912:A:H4'	2:X:2913:G:O4'	2.16	0.46
3:Y:21:G:N2	3:Y:58:G:H22	2.13	0.46
4:B:106:SER:O	4:B:109:THR:HG23	2.15	0.46
17:P:24:ILE:HD12	17:P:24:ILE:HA	1.80	0.46
24:W:37:VAL:HG11	24:W:43:ILE:HG12	1.96	0.46
25:Z:39:LEU:O	25:Z:41:HIS:ND1	2.48	0.46
2:X:38:A:H1'	5:C:48:THR:O	2.16	0.46
2:X:257:G:N7	27:3:5:LYS:HE3	2.31	0.46
2:X:515:G:H1	26:2:38:LYS:NZ	2.14	0.46
2:X:579:U:H2'	2:X:580:C:C6	2.50	0.46
2:X:955:A:C2	11:J:15:PRO:HG3	2.51	0.46
2:X:1848:A:H2'	2:X:1849:G:C8	2.50	0.46
2:X:2078:A:C2	2:X:2079:G:O6	2.69	0.46
10:I:47:ARG:HE	10:I:47:ARG:HB2	1.55	0.46
14:M:34:ILE:CD1	14:M:43:GLN:HG3	2.45	0.46
17:P:80:PRO:O	17:P:100:THR:OG1	2.28	0.46
1:A:153:GLN:HB3	2:X:1845:U:C4	2.51	0.46
2:X:39:C:O2'	2:X:658:A:N1	2.42	0.46
2:X:291:G:H2'	2:X:292:U:C6	2.51	0.46
2:X:1016:G:O5'	2:X:1016:G:H8	1.99	0.46
2:X:2670:G:OP2	33:X:3493:SPD:H72	2.15	0.46
5:C:103:LYS:HA	5:C:106:ARG:HE	1.80	0.46
24:W:10:ARG:HG3	24:W:10:ARG:NH1	2.30	0.46
2:X:684:U:H2'	2:X:685:C:H6	1.80	0.46
2:X:1093:C:H3'	2:X:1094:A:H8	1.80	0.46
2:X:1539:A:H2'	2:X:1540:U:C5	2.51	0.46
2:X:1609:U:H2'	2:X:1610:G:C8	2.50	0.46
4:B:133:ARG:HH11	4:B:171:GLY:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:51:VAL:CG1	5:C:91:GLY:HA3	2.44	0.46
9:H:6:THR:O	9:H:21:THR:HG23	2.15	0.46
18:Q:16:SER:HB2	18:Q:26:THR:OG1	2.16	0.46
2:X:195:C:O2'	2:X:847:A:N3	2.46	0.46
2:X:305:A:H62	2:X:410:G:N2	2.14	0.46
2:X:402:C:H2'	2:X:403:U:O4'	2.16	0.46
2:X:527:G:OP2	19:R:43:LYS:N	2.37	0.46
2:X:1065:A:H62	2:X:1185:U:H3	1.63	0.46
2:X:1494:G:N7	2:X:1495:C:H5	2.13	0.46
2:X:2126:C:H2'	2:X:2127:G:C8	2.50	0.46
2:X:2670:G:H2'	2:X:2671:A:C8	2.51	0.46
2:X:2749:G:H2'	2:X:2750:C:C6	2.50	0.46
5:C:17:ILE:HG13	5:C:18:GLU:N	2.31	0.46
5:C:179:GLN:O	5:C:182:ASN:N	2.43	0.46
10:I:21:ARG:HD3	10:I:21:ARG:HA	1.56	0.46
15:N:61:TRP:O	15:N:65:ILE:HD12	2.14	0.46
15:N:89:ASP:OD2	16:O:51:PRO:HG3	2.15	0.46
24:W:17:GLU:O	24:W:20:ARG:HB2	2.16	0.46
24:W:40:ASN:HB2	24:W:43:ILE:HB	1.98	0.46
2:X:32:C:O2'	2:X:33:U:H5'	2.16	0.46
2:X:811:C:C2'	2:X:812:U:H5'	2.46	0.46
2:X:1810:A:C2	2:X:2614:A:C4	3.03	0.46
2:X:1848:A:H2'	2:X:1849:G:H8	1.79	0.46
2:X:2287:C:H2'	2:X:2288:C:H6	1.81	0.46
2:X:2807:G:N7	32:X:3006:MPD:H13	2.31	0.46
9:H:90:ASP:O	9:H:91:LYS:HB2	2.16	0.46
11:J:40:SER:HB3	11:J:127:VAL:CG1	2.45	0.46
15:N:83:LEU:CD2	15:N:113:ALA:HB2	2.46	0.46
24:W:50:VAL:HB	24:W:53:LEU:CD1	2.46	0.46
2:X:496:G:P	2:X:1286:G:H22	2.38	0.45
2:X:1490:G:N3	2:X:1490:G:H2'	2.31	0.45
2:X:1518:G:C4	2:X:1519:U:C5	3.04	0.45
2:X:1700:C:C2	2:X:1701:U:C5	3.03	0.45
2:X:2338:A:H3'	2:X:2339:U:C5	2.51	0.45
2:X:2619:G:C6	2:X:2620:U:C4	3.04	0.45
1:A:78:VAL:HG12	1:A:79:ASP:N	2.26	0.45
2:X:340:C:H2'	2:X:341:G:O4'	2.16	0.45
2:X:1506:C:C4	2:X:1507:A:C6	3.05	0.45
2:X:1609:U:H2'	2:X:1610:G:H8	1.81	0.45
7:E:133:VAL:HG21	7:E:141:VAL:HA	1.98	0.45
15:N:105:ALA:HB1	16:O:40:PHE:HZ	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:14:VAL:HG12	16:O:20:ILE:HG21	1.98	0.45
23:V:18:ILE:O	23:V:22:LYS:HG3	2.17	0.45
2:X:434:G:C8	2:X:436:A:C8	3.05	0.45
2:X:1074:G:OP2	11:J:128:LYS:NZ	2.41	0.45
2:X:1150:A:C8	2:X:1151:G:C8	3.03	0.45
2:X:1410:A:H2'	2:X:1411:G:O4'	2.15	0.45
2:X:1793:C:H2'	2:X:1794:C:C6	2.49	0.45
2:X:2776:A:O2'	7:E:63:THR:HG22	2.16	0.45
3:Y:21:G:N1	3:Y:22:G:O6	2.50	0.45
11:J:137:LEU:CB	20:S:77:TYR:OH	2.63	0.45
2:X:59:U:H2'	2:X:74:U:H5	1.82	0.45
2:X:502:C:HO2'	2:X:503:A:P	2.39	0.45
2:X:650:U:N3	2:X:666:A:C2	2.79	0.45
2:X:801:A:H2'	2:X:802:G:O4'	2.16	0.45
2:X:840:C:H2'	2:X:841:C:H6	1.81	0.45
2:X:1505:G:C8	2:X:1506:C:C5	3.05	0.45
2:X:2319:U:H2'	2:X:2320:C:H6	1.80	0.45
2:X:2361:U:O2'	2:X:2362:A:OP1	2.34	0.45
3:Y:4:G:C2	3:Y:112:G:C2	3.04	0.45
1:A:71:LYS:O	1:A:96:TYR:OH	2.30	0.45
1:A:91:ILE:HG22	1:A:105:ILE:HA	1.99	0.45
2:X:734:A:H2'	2:X:735:C:C6	2.51	0.45
2:X:2804:G:H5"	2:X:2805:A:H5'	1.97	0.45
4:B:33:ASN:N	4:B:33:ASN:OD1	2.49	0.45
9:H:13:ASN:ND2	9:H:96:THR:H	2.15	0.45
17:P:72:LYS:HD3	17:P:108:SER:HB2	1.98	0.45
21:T:46:TYR:HD1	21:T:48:GLN:HE21	1.64	0.45
24:W:19:GLN:O	24:W:23:VAL:HG23	2.16	0.45
2:X:65:A:H1'	2:X:502:C:N4	2.32	0.45
2:X:683:G:C4	2:X:696:G:C2	3.05	0.45
2:X:784:A:H1'	2:X:785:C:H5	1.81	0.45
2:X:1575:A:H2'	2:X:1576:A:H5'	1.99	0.45
2:X:2831:G:H2'	2:X:2832:A:O4'	2.17	0.45
5:C:39:LEU:O	5:C:39:LEU:HD12	2.16	0.45
6:D:28:VAL:HA	6:D:29:PRO:HD3	1.82	0.45
12:K:23:SER:HA	12:K:26:ILE:HB	1.99	0.45
1:A:129:ALA:HA	1:A:191:THR:HA	1.98	0.45
2:X:319:G:N2	2:X:320:U:O3'	2.49	0.45
2:X:1992:C:H5"	2:X:1993:A:H2'	1.99	0.45
2:X:2718:C:C4	2:X:2746:G:N2	2.85	0.45
3:Y:57:G:H3'	3:Y:58:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:147:PHE:O	4:B:148:HIS:ND1	2.50	0.45
9:H:87:ILE:HD11	9:H:91:LYS:HA	1.99	0.45
2:X:201:C:H2'	2:X:202:A:H5"	1.98	0.45
2:X:1268:C:H2'	2:X:1269:A:C8	2.52	0.45
2:X:2318:U:O2'	2:X:2401:C:O2	2.35	0.45
2:X:2774:G:H2'	2:X:2775:A:C8	2.52	0.45
5:C:70:THR:HG22	5:C:72:ARG:HG3	1.99	0.45
15:N:92:ARG:O	15:N:94:MET:N	2.50	0.45
16:O:2:PHE:HE2	16:O:4:ILE:HD11	1.81	0.45
23:V:31:GLN:HB3	23:V:37:LEU:HG	1.99	0.45
2:X:327:G:O2'	2:X:328:G:H8	1.98	0.45
2:X:511:G:N2	2:X:729:G:H1'	2.32	0.45
2:X:529:A:H5"	19:R:45:GLN:CB	2.47	0.45
2:X:1065:A:C8	2:X:1065:A:C3'	3.00	0.45
2:X:2779:C:H3'	2:X:2780:A:H8	1.81	0.45
33:X:3495:SPD:H52	33:X:3495:SPD:H81	1.83	0.45
9:H:51:VAL:HG12	9:H:94:ARG:NH2	2.29	0.45
10:I:84:LYS:HG2	10:I:89:THR:HG22	1.99	0.45
11:J:115:ARG:CZ	11:J:131:PHE:HD2	2.30	0.45
16:O:20:ILE:CG2	16:O:97:ILE:HD11	2.47	0.45
21:T:71:ILE:HG12	21:T:72:ASP:N	2.32	0.45
2:X:901:G:H2'	2:X:902:A:C8	2.52	0.45
2:X:2811:U:H2'	2:X:2812:U:H6	1.81	0.45
2:X:2818:A:H2'	2:X:2819:C:O4'	2.17	0.45
4:B:116:ILE:HD12	4:B:211:ILE:CG2	2.47	0.45
5:C:149:PRO:HA	5:C:169:ASN:O	2.16	0.45
1:A:91:ILE:HA	1:A:106:ALA:H	1.81	0.44
2:X:1854:U:H2'	2:X:1855:G:O4'	2.16	0.44
5:C:39:LEU:O	5:C:42:ALA:HB3	2.17	0.44
10:I:82:LEU:H	10:I:84:LYS:HE3	1.83	0.44
24:W:9:THR:HG21	24:W:55:THR:HG23	1.99	0.44
27:3:24:ARG:HG2	27:3:24:ARG:NH1	2.31	0.44
2:X:523:A:H2'	2:X:524:A:O4'	2.16	0.44
2:X:1257:G:OP1	15:N:19:LYS:HE2	2.17	0.44
2:X:1651:C:H5"	2:X:1652:A:H5'	1.99	0.44
2:X:1765:A:O2'	2:X:1766:C:O4'	2.31	0.44
2:X:1979:A:C6	2:X:1980:A:N1	2.86	0.44
2:X:2004:A:N6	2:X:2005:A:C6	2.85	0.44
2:X:2572:G:H2'	2:X:2573:U:O4'	2.17	0.44
2:X:2903:A:C5'	2:X:2904:U:H5'	2.47	0.44
5:C:7:LEU:HD21	5:C:126:VAL:H	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:63:ILE:HD12	8:G:63:ILE:HA	1.77	0.44
2:X:59:U:O2'	2:X:73:A:H2'	2.18	0.44
2:X:249:C:H4'	2:X:431:C:O2'	2.18	0.44
2:X:624:C:OP1	15:N:33:LYS:HG3	2.18	0.44
2:X:1038:C:H1'	16:O:10:LYS:HE3	1.99	0.44
2:X:1208:A:H2'	2:X:1209:U:C6	2.53	0.44
2:X:1212:U:H2'	2:X:1213:C:O4'	2.18	0.44
2:X:1295:C:H1'	5:C:83:TRP:HA	1.99	0.44
2:X:1365:G:H2'	2:X:1367:C:C5	2.52	0.44
2:X:1377:U:H4'	2:X:1378:U:OP2	2.17	0.44
2:X:1986:G:C6	2:X:1987:A:C5	3.06	0.44
2:X:2125:U:H2'	2:X:2126:C:O4'	2.17	0.44
3:Y:3:U:H2'	3:Y:4:G:C8	2.53	0.44
7:E:30:LYS:H	7:E:35:ARG:CB	2.30	0.44
17:P:40:ASN:HD22	17:P:40:ASN:H	1.64	0.44
18:Q:3:ALA:HB1	18:Q:41:ALA:HB2	1.97	0.44
2:X:51:G:O2'	2:X:118:A:N6	2.50	0.44
2:X:591:A:H4'	2:X:592:A:C5'	2.40	0.44
2:X:614:U:C4	2:X:618:A:C4	3.06	0.44
2:X:963:A:H4'	3:Y:94:U:O2	2.18	0.44
2:X:2642:U:N1	25:Z:4:PRO:HA	2.33	0.44
2:X:2817:A:C2	2:X:2827:A:C2	3.06	0.44
4:B:22:LEU:N	9:H:72:ASN:O	2.45	0.44
5:C:148:GLN:N	5:C:148:GLN:OE1	2.49	0.44
12:K:109:ARG:HD3	12:K:112:ASP:OD1	2.17	0.44
13:L:54:ALA:HB1	13:L:76:VAL:HG23	1.99	0.44
15:N:6:GLY:C	35:N:201:EPE:H72	2.38	0.44
2:X:15:G:O2'	25:Z:18:THR:HG21	2.17	0.44
2:X:810:A:H2'	2:X:811:C:H6	1.82	0.44
2:X:1424:A:H5'	2:X:1512:U:H1'	1.99	0.44
2:X:1463:A:H3'	2:X:1464:U:H5"	1.98	0.44
2:X:1478:A:H61	2:X:1605:A:N6	2.16	0.44
2:X:1561:G:C8	2:X:1562:C:C6	3.06	0.44
2:X:1701:U:H2'	2:X:1702:C:H6	1.83	0.44
2:X:2449:C:H6	2:X:2449:C:H2'	1.52	0.44
2:X:2871:A:H2'	2:X:2872:G:C8	2.52	0.44
7:E:63:THR:OG1	7:E:64:ASN:N	2.50	0.44
11:J:39:THR:CG2	11:J:99:PRO:HD2	2.47	0.44
11:J:43:THR:HG22	11:J:46:GLN:CD	2.38	0.44
11:J:43:THR:HG22	11:J:46:GLN:OE1	2.18	0.44
19:R:77:GLU:HA	19:R:78:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:218:G:C4'	2:X:219:A:H4'	2.48	0.44
2:X:906:A:H2'	2:X:907:G:O4'	2.17	0.44
2:X:1091:G:H2'	2:X:1154:G:N1	2.32	0.44
2:X:1515:G:N2	2:X:1516:C:C2	2.86	0.44
2:X:2670:G:C2	2:X:2799:C:C2	3.06	0.44
2:X:2724:G:H2'	2:X:2725:U:O4'	2.17	0.44
8:G:38:ARG:HA	8:G:119:GLN:NE2	2.32	0.44
9:H:102:VAL:HG13	9:H:106:LEU:HD12	1.99	0.44
17:P:10:ILE:HD13	17:P:10:ILE:HA	1.78	0.44
20:S:78:GLN:HB2	20:S:87:THR:O	2.17	0.44
26:2:15:LYS:O	26:2:16:VAL:HB	2.17	0.44
2:X:424:C:N4	2:X:425:G:O6	2.50	0.44
2:X:658:A:H3'	2:X:659:A:H5"	1.99	0.44
2:X:675:G:N2	2:X:677:A:H3'	2.33	0.44
2:X:840:C:H2'	2:X:841:C:C6	2.52	0.44
2:X:868:A:C6	2:X:869:G:C6	3.06	0.44
2:X:908:A:O4'	3:Y:96:G:N2	2.43	0.44
2:X:994:A:H2'	2:X:995:U:O4'	2.17	0.44
2:X:2734:C:O3'	12:K:64:LYS:HG3	2.17	0.44
2:X:2859:G:H21	12:K:98:GLY:HA3	1.83	0.44
5:C:146:LEU:HD22	5:C:146:LEU:HA	1.82	0.44
1:A:144:ILE:HB	1:A:154:ILE:HB	2.00	0.44
2:X:31:C:C4	2:X:32:C:C5	3.06	0.44
2:X:799:U:H4'	2:X:1310:A:H61	1.81	0.44
2:X:1468:G:H2'	2:X:1469:G:O4'	2.17	0.44
2:X:1677:G:C6	2:X:1679:A:C4	3.06	0.44
2:X:1767:G:HO2'	2:X:1768:C:H6	1.66	0.44
2:X:2757:U:H2'	2:X:2758:G:C8	2.53	0.44
2:X:2768:A:H2'	2:X:2769:G:O4'	2.18	0.44
5:C:96:SER:O	5:C:98:ALA:N	2.50	0.44
14:M:94:VAL:CG1	14:M:99:LEU:HD21	2.48	0.44
20:S:127:ASN:HA	20:S:160:LYS:O	2.16	0.44
2:X:168:A:H3'	2:X:169:G:H5'	1.99	0.44
2:X:534:G:OP2	33:X:3497:SPD:H22	2.18	0.44
2:X:660:A:H1'	2:X:661:U:O5'	2.17	0.44
2:X:1492:G:O2'	2:X:1574:G:N3	2.51	0.44
2:X:2848:G:C2	2:X:2849:A:N7	2.86	0.44
5:C:22:ALA:O	5:C:111:ARG:HD3	2.18	0.44
8:G:58:ILE:HD12	8:G:58:ILE:HA	1.67	0.44
9:H:10:VAL:HA	9:H:84:CYS:O	2.18	0.44
13:L:73:ALA:HB2	13:L:103:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:50:ILE:HD12	14:M:50:ILE:HG23	1.63	0.44
20:S:46:VAL:O	20:S:50:LYS:HG3	2.17	0.44
24:W:3:LYS:HG2	24:W:38:GLU:HA	1.99	0.44
24:W:15:ARG:NH1	24:W:15:ARG:HB3	2.33	0.44
2:X:396:G:H2'	2:X:397:U:H5'	1.99	0.43
2:X:615:A:H2'	2:X:615:A:N3	2.33	0.43
2:X:1751:G:N7	32:X:3010:MPD:H11	2.33	0.43
2:X:2079:G:H4'	4:B:156:MET:O	2.18	0.43
2:X:2089:A:H8	31:X:3003:62B:N1	2.15	0.43
2:X:2218:G:H2'	2:X:2219:C:C6	2.53	0.43
2:X:2269:G:H2'	2:X:2270:U:O4'	2.18	0.43
5:C:57:VAL:O	5:C:59:GLY:N	2.44	0.43
15:N:33:LYS:O	15:N:37:GLN:HG3	2.18	0.43
2:X:17:G:P	25:Z:11:THR:HG22	2.58	0.43
2:X:328:G:N2	2:X:399:U:O2	2.45	0.43
2:X:410:G:H21	2:X:411:A:H62	1.65	0.43
2:X:1351:C:OP1	2:X:1352:C:OP2	2.35	0.43
2:X:1629:U:H2'	2:X:1630:A:H5"	2.00	0.43
2:X:2298:G:H5'	21:T:28:ARG:HD3	2.00	0.43
2:X:2360:A:H5'	2:X:2362:A:H1'	2.00	0.43
4:B:8:ARG:HH21	4:B:54:GLU:CD	2.21	0.43
16:O:12:ILE:HD13	16:O:12:ILE:HA	1.54	0.43
17:P:19:LEU:HD23	17:P:19:LEU:HA	1.87	0.43
2:X:767:A:H2'	2:X:768:A:C8	2.52	0.43
2:X:2617:A:H2'	2:X:2618:C:C6	2.54	0.43
4:B:198:LYS:HE3	4:B:198:LYS:HB2	1.89	0.43
5:C:49:HIS:O	5:C:49:HIS:ND1	2.46	0.43
12:K:38:LYS:HB3	12:K:41:ARG:NH2	2.34	0.43
14:M:57:VAL:HG12	14:M:58:SER:N	2.33	0.43
21:T:80:LYS:HB2	21:T:84:LYS:C	2.38	0.43
2:X:32:C:N4	2:X:33:U:O4	2.52	0.43
2:X:327:G:H2'	2:X:327:G:N3	2.33	0.43
2:X:509:G:N2	2:X:513:G:C5	2.86	0.43
2:X:1054:A:N3	2:X:1197:C:H1'	2.33	0.43
2:X:1072:A:N6	2:X:1169:G:H2'	2.33	0.43
2:X:1527:A:H2	2:X:1549:C:N3	2.16	0.43
2:X:2098:A:H2'	2:X:2099:G:C8	2.53	0.43
2:X:2344:C:H2'	2:X:2345:A:O4'	2.18	0.43
2:X:2660:A:H2'	2:X:2661:A:O4'	2.18	0.43
3:Y:81:A:H61	3:Y:90:C:H42	1.66	0.43
9:H:117:LEU:O	9:H:117:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:72:LYS:HB2	17:P:108:SER:HB2	1.99	0.43
19:R:12:ILE:H	19:R:67:ASN:HA	1.83	0.43
1:A:13:ARG:HA	1:A:16:MET:HG3	2.00	0.43
2:X:79:U:O2'	2:X:389:A:H8	1.97	0.43
2:X:291:G:H2'	2:X:292:U:H6	1.84	0.43
2:X:327:G:O2'	2:X:328:G:O5'	2.33	0.43
2:X:896:U:H2'	2:X:897:A:C8	2.54	0.43
2:X:1035:C:H2'	2:X:1036:C:H6	1.84	0.43
2:X:1042:C:P	15:N:92:ARG:HH22	2.42	0.43
2:X:1185:U:H2'	8:G:66:THR:HG22	2.00	0.43
2:X:1304:G:OP2	25:Z:16:ARG:NH1	2.52	0.43
2:X:1885:G:H1'	2:X:1911:A:N6	2.32	0.43
2:X:2883:U:H2'	2:X:2884:G:C8	2.54	0.43
3:Y:74:G:H1	3:Y:97:A:N6	2.15	0.43
4:B:140:PRO:HG2	4:B:145:SER:CB	2.47	0.43
12:K:8:ARG:NH1	12:K:16:MET:SD	2.91	0.43
13:L:14:ARG:O	13:L:18:VAL:HG23	2.19	0.43
1:A:106:ALA:HA	1:A:107:PRO:HD3	1.77	0.43
2:X:142:G:H5'	2:X:143:U:OP2	2.18	0.43
2:X:150:A:C6	2:X:151:U:C4	3.06	0.43
2:X:642:U:O2'	2:X:643:G:H5'	2.19	0.43
2:X:691:A:H2	2:X:2376:G:H21	1.66	0.43
2:X:1229:G:OP1	10:I:31:SER:HA	2.18	0.43
2:X:1526:G:N7	2:X:1527:A:N1	2.67	0.43
2:X:1565:U:H2'	2:X:1566:G:O4'	2.18	0.43
3:Y:3:U:O2'	3:Y:25:A:N3	2.50	0.43
3:Y:49:G:C6	3:Y:50:A:C6	3.07	0.43
4:B:95:ASP:C	4:B:97:ASP:H	2.22	0.43
8:G:40:LYS:HB3	8:G:40:LYS:HE2	1.82	0.43
11:J:98:LYS:HA	11:J:99:PRO:HD2	1.70	0.43
19:R:25:ALA:HB3	19:R:34:VAL:HG23	1.99	0.43
2:X:114:C:H2'	2:X:115:C:H6	1.82	0.43
2:X:224:A:O4'	2:X:236:A:H1'	2.18	0.43
2:X:683:G:C5	2:X:696:G:N1	2.87	0.43
2:X:1356:G:C5	2:X:1357:G:C6	3.07	0.43
2:X:1397:G:C6	2:X:1398:G:H1'	2.54	0.43
2:X:1683:U:C2'	2:X:1684:A:H5"	2.47	0.43
2:X:2283:G:H2'	2:X:2284:U:O4'	2.18	0.43
2:X:2514:G:H2'	2:X:2515:A:C8	2.54	0.43
2:X:2652:G:H2'	2:X:2653:C:C6	2.53	0.43
2:X:2712:G:O6	32:X:3005:MPD:O4	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:117:LYS:HD3	5:C:117:LYS:HA	1.80	0.43
6:D:130:LEU:HD13	6:D:130:LEU:HA	1.68	0.43
9:H:12:ASP:CG	9:H:85:VAL:HG13	2.39	0.43
10:I:19:VAL:HG22	10:I:27:ASN:HB3	2.01	0.43
15:N:65:ILE:HG21	15:N:80:MET:HE2	2.01	0.43
18:Q:14:GLU:OE1	18:Q:14:GLU:N	2.39	0.43
2:X:974:U:H2'	2:X:975:U:O4'	2.19	0.43
2:X:1361:G:H1'	2:X:1660:A:N6	2.34	0.43
2:X:1975:G:H1	2:X:1985:C:H42	1.65	0.43
2:X:2820:U:H1'	2:X:2824:G:N2	2.34	0.43
7:E:65:HIS:HA	7:E:68:THR:OG1	2.18	0.43
10:I:19:VAL:CG1	10:I:30:THR:HG23	2.49	0.43
11:J:37:THR:HG21	11:J:130:LYS:HE3	2.01	0.43
12:K:44:VAL:O	12:K:48:ILE:HG23	2.18	0.43
15:N:70:ARG:HD2	15:N:70:ARG:HA	1.81	0.43
15:N:92:ARG:HG2	15:N:92:ARG:H	1.72	0.43
2:X:312:A:N3	2:X:312:A:H2'	2.33	0.43
2:X:691:A:H3'	2:X:692:G:H8	1.84	0.43
2:X:903:G:N3	2:X:2295:A:H2'	2.34	0.43
2:X:1723:A:O5'	2:X:1723:A:H8	2.02	0.43
2:X:2801:C:H2'	2:X:2802:A:O4'	2.19	0.43
10:I:110:LYS:HA	10:I:129:SER:CB	2.49	0.43
15:N:31:LEU:HD23	15:N:31:LEU:N	2.34	0.43
21:T:80:LYS:HB2	21:T:84:LYS:O	2.19	0.43
2:X:53:A:H2'	2:X:54:G:O4'	2.19	0.43
2:X:192:G:O6	2:X:208:G:O2'	2.28	0.43
2:X:784:A:H8	2:X:784:A:H5"	1.84	0.43
2:X:1373:U:H2'	2:X:1374:G:O4'	2.17	0.43
2:X:1561:G:H8	2:X:1562:C:C6	2.36	0.43
2:X:2000:G:H2'	2:X:2001:C:C6	2.54	0.43
2:X:2314:A:C6	2:X:2316:G:C5	3.07	0.43
2:X:2446:U:O4	27:3:28:PHE:CD1	2.72	0.43
2:X:2775:A:H1'	7:E:67:THR:CG2	2.38	0.43
7:E:60:GLU:O	7:E:63:THR:HG23	2.18	0.43
8:G:30:SER:HA	8:G:106:ILE:HG12	2.01	0.43
9:H:25:LEU:HA	9:H:25:LEU:HD23	1.67	0.43
2:X:514:G:OP2	26:2:38:LYS:HE3	2.19	0.42
2:X:631:U:H1'	5:C:90:PHE:CD1	2.53	0.42
2:X:862:C:O2'	2:X:884:U:H5"	2.19	0.42
2:X:1599:G:H2'	2:X:1599:G:N3	2.34	0.42
2:X:2783:U:H5"	28:4:19:ARG:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2794:C:H41	32:X:3008:MPD:C1	2.32	0.42
33:X:3497:SPD:HN11	33:X:3497:SPD:H51	1.84	0.42
3:Y:68:A:N1	3:Y:103:A:N1	2.66	0.42
14:M:106:ARG:HA	14:M:106:ARG:NE	2.34	0.42
19:R:71:LEU:CB	19:R:73:PRO:HD2	2.49	0.42
24:W:8:LEU:O	24:W:32:ASN:N	2.42	0.42
28:4:25:VAL:N	28:4:34:GLN:O	2.52	0.42
1:A:20:ASP:O	1:A:22:ALA:N	2.47	0.42
2:X:183:A:OP2	2:X:183:A:H3'	2.20	0.42
2:X:428:G:N2	2:X:429:C:H1'	2.34	0.42
2:X:818:U:O2	2:X:823:G:O2'	2.31	0.42
2:X:1490:G:C5	2:X:1509:G:N2	2.87	0.42
2:X:1521:A:N7	2:X:1561:G:N1	2.68	0.42
2:X:1528:G:C8	2:X:1529:U:C4	3.07	0.42
2:X:1732:U:O2	2:X:1744:A:H5'	2.19	0.42
2:X:2848:G:N3	2:X:2849:A:C8	2.87	0.42
3:Y:111:A:H2'	3:Y:112:G:O4'	2.18	0.42
8:G:99:GLU:O	8:G:103:GLU:HB2	2.18	0.42
15:N:95:LEU:HD12	15:N:95:LEU:HA	1.75	0.42
20:S:108:LEU:HB3	20:S:109:VAL:H	1.57	0.42
2:X:774:G:H5"	2:X:775:A:H5"	2.02	0.42
2:X:868:A:H2'	2:X:869:G:H8	1.84	0.42
2:X:1039:C:C4	8:G:1:MET:HA	2.54	0.42
2:X:1512:U:H2'	2:X:1513:A:H8	1.84	0.42
2:X:1735:C:O2	2:X:1740:G:N2	2.48	0.42
2:X:2092:C:H1'	2:X:2476:U:H3	1.83	0.42
2:X:2518:U:O2	2:X:2518:U:H2'	2.19	0.42
3:Y:21:G:N2	3:Y:58:G:N2	2.66	0.42
9:H:63:VAL:HB	9:H:106:LEU:CD1	2.50	0.42
11:J:54:MET:HE1	11:J:104:PHE:CG	2.55	0.42
16:O:74:PHE:CE1	16:O:83:LYS:HB2	2.52	0.42
20:S:105:PRO:CD	20:S:124:PRO:HA	2.50	0.42
24:W:15:ARG:HB3	24:W:15:ARG:HH11	1.84	0.42
2:X:563:G:H4'	17:P:18:ARG:NE	2.34	0.42
2:X:684:U:H2'	2:X:685:C:C6	2.54	0.42
2:X:874:A:N7	2:X:2274:A:O2'	2.52	0.42
2:X:1491:C:H4'	2:X:1593:G:H5"	2.02	0.42
2:X:1962:G:H1'	2:X:1991:G:N2	2.35	0.42
2:X:2482:G:H2'	2:X:2483:C:C6	2.55	0.42
8:G:59:ASN:OD1	8:G:129:ALA:HB2	2.18	0.42
23:V:46:VAL:O	23:V:50:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:92:G:H2'	2:X:93:U:C6	2.55	0.42
2:X:537:A:H2'	2:X:538:G:O4'	2.20	0.42
2:X:738:U:H1'	2:X:1391:A:H1'	2.00	0.42
2:X:2000:G:H2'	2:X:2001:C:H6	1.85	0.42
9:H:14:SER:O	9:H:52:VAL:HG22	2.19	0.42
9:H:24:VAL:HG12	9:H:33:ALA:HB2	2.01	0.42
9:H:87:ILE:HG12	9:H:88:ARG:N	2.32	0.42
10:I:19:VAL:CG2	10:I:27:ASN:HB3	2.49	0.42
21:T:82:ARG:HG2	21:T:83:ASP:N	2.34	0.42
2:X:924:G:N2	2:X:925:G:N7	2.67	0.42
2:X:2747:U:H2'	2:X:2748:A:H8	1.83	0.42
3:Y:46:A:H2'	3:Y:47:C:O4'	2.19	0.42
5:C:123:LEU:O	5:C:188:ASN:HA	2.19	0.42
12:K:27:SER:C	12:K:29:ARG:H	2.22	0.42
17:P:72:LYS:N	17:P:106:VAL:O	2.46	0.42
19:R:7:ASP:N	19:R:23:VAL:HG13	2.35	0.42
2:X:152:C:C2'	2:X:153:G:H5'	2.50	0.42
2:X:443:U:H2'	2:X:444:C:C6	2.54	0.42
2:X:672:A:H4'	2:X:673:G:H5'	2.02	0.42
2:X:690:U:H5"	2:X:691:A:OP2	2.20	0.42
2:X:879:U:C2	2:X:880:A:C8	3.08	0.42
2:X:1595:C:C2	2:X:1596:G:C8	3.07	0.42
2:X:1881:A:C8	2:X:1882:G:C8	3.07	0.42
2:X:1905:G:H2'	2:X:1906:C:O4'	2.18	0.42
2:X:2398:G:H2'	2:X:2399:G:O4'	2.20	0.42
2:X:2580:G:H5"	2:X:2581:U:OP2	2.20	0.42
3:Y:92:G:O5'	3:Y:92:G:H8	2.02	0.42
4:B:26:THR:HG21	4:B:201:VAL:CG1	2.46	0.42
7:E:158:LYS:O	7:E:160:LYS:N	2.52	0.42
8:G:39:GLY:C	8:G:41:ASN:N	2.72	0.42
9:H:33:ALA:HB1	9:H:37:ASP:HB3	2.00	0.42
10:I:33:ARG:O	10:I:33:ARG:HG3	2.16	0.42
18:Q:63:LYS:N	18:Q:70:GLY:O	2.52	0.42
21:T:46:TYR:CD1	21:T:48:GLN:NE2	2.88	0.42
27:3:44:LEU:HD23	27:3:45:ARG:H	1.85	0.42
1:A:157:SER:HB3	2:X:1846:A:H5'	2.01	0.42
2:X:727:G:H5'	26:2:27:ASN:ND2	2.35	0.42
2:X:1059:A:O2'	2:X:1060:U:H5'	2.20	0.42
2:X:1168:C:H2'	2:X:1169:G:O4'	2.18	0.42
2:X:1217:U:H6	2:X:1217:U:H2'	1.63	0.42
2:X:1612:C:O2'	2:X:1613:G:H5"	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2466:A:O2'	2:X:2627:A:OP1	2.32	0.42
2:X:2679:U:H2'	2:X:2680:U:O4'	2.19	0.42
2:X:2681:A:N1	2:X:2692:A:H5"	2.34	0.42
3:Y:4:G:N2	3:Y:111:A:N7	2.60	0.42
5:C:163:VAL:HG13	5:C:164:GLU:N	2.35	0.42
6:D:34:ILE:HA	6:D:148:LYS:HA	2.02	0.42
8:G:42:LYS:HB2	8:G:44:THR:HG23	2.00	0.42
8:G:46:THR:HB	15:N:64:ARG:HH21	1.85	0.42
12:K:47:LEU:HD23	12:K:47:LEU:HA	1.89	0.42
13:L:44:ILE:HB	13:L:54:ALA:HB2	2.02	0.42
15:N:65:ILE:HG21	15:N:80:MET:CE	2.50	0.42
23:V:28:LEU:HD11	23:V:42:ARG:HG2	2.01	0.42
23:V:38:GLU:H	23:V:38:GLU:HG3	1.52	0.42
2:X:1064:A:C2	2:X:1185:U:C2	3.08	0.42
2:X:1682:C:H4'	2:X:2737:C:O2	2.20	0.42
2:X:1734:A:H62	2:X:1741:G:H21	1.67	0.42
2:X:1805:U:H3'	2:X:1811:A:N6	2.35	0.42
2:X:2065:G:H2'	2:X:2066:G:O4'	2.20	0.42
6:D:114:PHE:CB	6:D:120:LYS:HA	2.49	0.42
21:T:88:SER:HB2	21:T:90:TYR:CE1	2.54	0.42
27:3:54:ASP:HB3	27:3:55:MET:H	1.48	0.42
1:A:17:THR:HG23	1:A:204:ASN:HD22	1.84	0.42
1:A:30:GLU:OE1	1:A:103:TYR:OH	2.24	0.42
2:X:674:C:H4'	2:X:695:C:O2	2.20	0.42
2:X:956:A:C5	11:J:11:ARG:HD2	2.55	0.42
2:X:1724:U:N3	2:X:1791:G:OP2	2.52	0.42
2:X:1770:C:O2'	2:X:1771:A:H5'	2.20	0.42
2:X:1770:C:H1'	2:X:1771:A:H5'	2.02	0.42
2:X:1805:U:N3	2:X:1811:A:C8	2.88	0.42
2:X:1857:C:O5'	2:X:1857:C:H6	2.03	0.42
2:X:2343:U:H2'	2:X:2344:C:C6	2.55	0.42
2:X:2757:U:H2'	2:X:2758:G:H8	1.84	0.42
33:X:3497:SPD:H52	33:X:3497:SPD:H81	1.82	0.42
4:B:16:PHE:H	14:M:14:GLN:NE2	2.17	0.42
5:C:19:LEU:HA	5:C:19:LEU:HD23	1.85	0.42
2:X:329:A:N3	2:X:329:A:H2'	2.35	0.41
2:X:629:A:N6	2:X:1289:A:H2	2.08	0.41
2:X:817:G:O2'	2:X:818:U:H5'	2.20	0.41
2:X:877:G:H2'	2:X:878:C:C6	2.55	0.41
2:X:1731:G:N3	2:X:1746:G:N2	2.68	0.41
2:X:2649:U:H5'	4:B:172:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2758:G:OP1	4:B:182:ASN:ND2	2.34	0.41
24:W:17:GLU:O	24:W:21:LYS:HG3	2.19	0.41
2:X:169:G:H2'	2:X:169:G:N3	2.34	0.41
2:X:332:A:H61	2:X:394:U:H3	1.68	0.41
2:X:1573:A:C2	2:X:1592:A:C8	3.08	0.41
2:X:1967:U:C4	2:X:1991:G:H4'	2.55	0.41
2:X:2257:G:H2'	2:X:2258:U:C6	2.55	0.41
2:X:2424:G:C6	2:X:2425:U:C4	3.08	0.41
4:B:118:VAL:HB	4:B:201:VAL:HG23	2.00	0.41
8:G:36:ILE:HD13	8:G:36:ILE:N	2.35	0.41
10:I:36:LYS:NZ	10:I:42:SER:O	2.53	0.41
18:Q:67:ARG:HD2	18:Q:68:TYR:CE1	2.55	0.41
2:X:70:G:N2	2:X:71:A:N1	2.68	0.41
2:X:510:U:C2	2:X:833:A:C6	3.08	0.41
2:X:1288:G:N7	10:I:18:ARG:NH2	2.64	0.41
2:X:1423:C:H2'	2:X:1424:A:C8	2.56	0.41
2:X:2431:C:H2'	2:X:2432:G:O4'	2.19	0.41
5:C:136:THR:O	5:C:140:LYS:HD2	2.21	0.41
8:G:38:ARG:NH1	8:G:111:PRO:HG3	2.35	0.41
14:M:61:PHE:O	14:M:75:THR:HA	2.20	0.41
15:N:83:LEU:HD23	15:N:83:LEU:HA	1.90	0.41
20:S:107:GLN:HA	20:S:138:PRO:HG2	2.01	0.41
23:V:45:THR:HA	23:V:48:LYS:HD2	2.01	0.41
2:X:59:U:H1'	2:X:73:A:C4	2.55	0.41
2:X:187:C:C2	2:X:188:C:C5	3.07	0.41
2:X:375:A:C5	2:X:378:C:C4	3.08	0.41
2:X:984:G:O6	33:X:3495:SPD:H32	2.21	0.41
2:X:1091:G:H4'	2:X:1092:A:O5'	2.20	0.41
2:X:1835:U:H2'	2:X:1836:A:C5'	2.50	0.41
2:X:2333:U:OP2	2:X:2334:G:N1	2.53	0.41
2:X:2489:U:H2'	2:X:2490:C:O4'	2.21	0.41
2:X:2714:U:H2'	2:X:2715:G:O4'	2.21	0.41
2:X:2774:G:N2	2:X:2775:A:N6	2.68	0.41
2:X:2851:G:OP2	4:B:65:SER:HB2	2.21	0.41
2:X:2886:G:C2	2:X:2888:A:H1'	2.56	0.41
4:B:13:THR:O	4:B:25:VAL:HG12	2.20	0.41
4:B:178:VAL:HG12	4:B:202:PRO:HG3	2.01	0.41
5:C:78:ILE:HD13	5:C:78:ILE:H	1.85	0.41
5:C:103:LYS:HA	5:C:106:ARG:CD	2.50	0.41
9:H:91:LYS:HD2	9:H:111:PHE:CE1	2.55	0.41
12:K:17:LEU:HD23	12:K:17:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:9:VAL:H	15:N:9:VAL:HG22	1.57	0.41
2:X:152:C:H2'	2:X:153:G:H5'	2.02	0.41
2:X:426:G:C6	2:X:427:A:C5	3.08	0.41
2:X:529:A:H3'	2:X:530:C:C6	2.56	0.41
2:X:627:C:H5	35:N:201:EPE:C10	2.33	0.41
2:X:1151:G:H2'	2:X:1152:U:C6	2.54	0.41
2:X:1508:C:O2'	2:X:1509:G:P	2.78	0.41
2:X:1550:G:H8	2:X:1550:G:H3'	1.85	0.41
2:X:1979:A:OP1	9:H:42:THR:OG1	2.29	0.41
2:X:2803:A:C6	2:X:2809:G:H1'	2.55	0.41
2:X:2856:U:C2	2:X:2857:A:N7	2.89	0.41
3:Y:90:C:H2'	3:Y:91:C:H6	1.84	0.41
8:G:102:ILE:HB	8:G:125:VAL:HG11	2.02	0.41
12:K:20:LEU:HB3	12:K:40:VAL:HG21	2.02	0.41
1:A:85:PRO:HB3	2:X:1614:A:H2'	2.03	0.41
2:X:626:G:P	35:N:201:EPE:H62	2.61	0.41
2:X:796:A:C6	2:X:834:A:C5	3.09	0.41
2:X:1241:A:C6	2:X:1242:A:C6	3.08	0.41
2:X:1271:G:H2'	2:X:1272:U:H6	1.86	0.41
2:X:1325:U:C2	2:X:1364:C:O2	2.74	0.41
2:X:1326:C:H2'	2:X:1327:C:H6	1.86	0.41
2:X:1441:C:H5'	2:X:1514:A:O2'	2.21	0.41
11:J:39:THR:HG22	11:J:98:LYS:HA	2.02	0.41
11:J:57:TYR:HE1	11:J:113:VAL:HG13	1.85	0.41
17:P:1:MET:HB3	17:P:2:GLU:H	1.59	0.41
1:A:252:LYS:HA	1:A:253:PRO:HD3	1.84	0.41
2:X:24:G:H2'	2:X:25:U:C6	2.56	0.41
2:X:156:A:H61	2:X:172:U:H3	1.69	0.41
2:X:228:A:C6	2:X:229:A:H1'	2.56	0.41
2:X:968:A:C2'	2:X:969:A:H5'	2.51	0.41
2:X:974:U:O2'	24:W:25:ALA:O	2.23	0.41
2:X:1065:A:H3'	2:X:1065:A:H8	1.83	0.41
2:X:1089:C:H4'	2:X:1090:A:H5"	2.03	0.41
2:X:1526:G:N7	2:X:1527:A:C6	2.88	0.41
2:X:1548:U:H5"	2:X:1549:C:OP2	2.20	0.41
2:X:1982:U:H5	2:X:2584:G:N2	2.18	0.41
2:X:2097:G:C6	2:X:2098:A:C5	3.08	0.41
2:X:2342:U:H2'	2:X:2343:U:C6	2.56	0.41
2:X:2607:U:C5	2:X:2608:G:C6	3.09	0.41
4:B:133:ARG:NH1	4:B:171:GLY:N	2.69	0.41
13:L:73:ALA:HB1	13:L:107:ALA:CB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:34:ILE:O	14:M:40:GLU:HA	2.20	0.41
16:O:78:ARG:HD3	16:O:79:ARG:NH2	2.36	0.41
18:Q:5:ASP:N	18:Q:5:ASP:OD1	2.53	0.41
2:X:608:C:H2'	2:X:609:U:O4'	2.21	0.41
2:X:970:U:H6	2:X:970:U:H2'	1.75	0.41
2:X:1352:C:H42	2:X:1374:G:H1	1.69	0.41
2:X:1550:G:H3'	2:X:1550:G:C8	2.56	0.41
2:X:2000:G:C6	2:X:2001:C:C4	3.08	0.41
2:X:2819:C:N4	2:X:2824:G:H1	2.17	0.41
2:X:2837:U:O2	2:X:2856:U:H1'	2.21	0.41
15:N:35:ALA:O	15:N:39:VAL:HG23	2.21	0.41
17:P:13:ALA:HA	17:P:14:PRO:HD3	1.87	0.41
17:P:29:ALA:O	17:P:33:ILE:HG13	2.20	0.41
17:P:69:LEU:HD23	17:P:69:LEU:HA	1.82	0.41
2:X:56:A:C6	2:X:57:C:C4	3.09	0.41
2:X:124:A:C6	26:2:11:ARG:HD3	2.56	0.41
2:X:394:U:H2'	2:X:395:U:H6	1.86	0.41
2:X:1392:G:C5	2:X:1393:C:C5	3.09	0.41
2:X:1476:G:H2'	2:X:1477:U:C6	2.55	0.41
2:X:1699:A:C8	2:X:1700:C:C5	3.09	0.41
2:X:1871:U:C2	2:X:1872:G:C8	3.09	0.41
2:X:1994:C:C4	2:X:1995:G:C5	3.09	0.41
2:X:2075:G:O4'	2:X:2843:A:C6	2.74	0.41
2:X:2532:G:O2'	2:X:2533:U:H5'	2.21	0.41
3:Y:57:G:H3'	3:Y:58:G:H8	1.86	0.41
4:B:141:MET:HG3	4:B:148:HIS:CE1	2.55	0.41
8:G:12:ILE:HG12	8:G:13:GLU:N	2.33	0.41
11:J:55:THR:CG2	11:J:64:VAL:HG11	2.50	0.41
12:K:18:ARG:HB2	12:K:67:ARG:HD3	2.03	0.41
16:O:70:LYS:HD2	16:O:87:GLY:HA3	2.03	0.41
20:S:34:TYR:CD1	20:S:95:ASN:HB2	2.56	0.41
21:T:70:LYS:HE3	21:T:70:LYS:HB2	1.75	0.41
27:3:25:SER:C	27:3:26:ARG:HD3	2.41	0.41
2:X:666:A:N3	2:X:666:A:O4'	2.53	0.41
2:X:1252:A:H2'	2:X:1253:G:O4'	2.21	0.41
2:X:1482:U:H2'	2:X:1483:A:H8	1.86	0.41
2:X:2306:G:C6	2:X:2307:G:C5	3.08	0.41
2:X:2437:G:H2'	2:X:2438:A:O4'	2.21	0.41
3:Y:100:A:O2'	3:Y:101:G:H5'	2.20	0.41
8:G:33:VAL:HG11	8:G:106:ILE:HD13	2.03	0.41
17:P:3:ALA:HB3	17:P:58:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:S:17:ASP:O	20:S:20:GLN:HB2	2.20	0.41
21:T:51:THR:HB	21:T:54:TYR:CE1	2.56	0.41
27:3:20:GLY:O	27:3:45:ARG:HA	2.21	0.41
2:X:5:A:C2	2:X:2918:A:C2	3.09	0.40
2:X:250:G:H4'	2:X:432:G:C5	2.56	0.40
2:X:804:G:C2'	2:X:805:G:H5'	2.51	0.40
2:X:1228:A:H2'	2:X:1229:G:O4'	2.21	0.40
2:X:1486:C:N3	2:X:1487:G:C6	2.89	0.40
2:X:1515:G:O2'	2:X:1516:C:P	2.78	0.40
2:X:2500:U:OP1	2:X:2502:C:N4	2.55	0.40
2:X:2850:G:OP2	4:B:86:ARG:NH2	2.51	0.40
2:X:2914:A:H2'	2:X:2915:C:O4'	2.21	0.40
4:B:121:VAL:H	4:B:121:VAL:HG12	1.52	0.40
10:I:84:LYS:HD3	10:I:89:THR:HG21	2.03	0.40
12:K:29:ARG:HH12	12:K:118:ILE:HG21	1.86	0.40
12:K:38:LYS:HB3	12:K:41:ARG:HH21	1.86	0.40
15:N:80:MET:HE1	15:N:95:LEU:HD23	2.03	0.40
17:P:20:VAL:HG21	17:P:43:SER:HB2	2.03	0.40
20:S:45:GLU:OE1	20:S:85:GLN:NE2	2.54	0.40
24:W:18:THR:HB	24:W:49:LYS:HZ1	1.85	0.40
1:A:43:ARG:NH1	2:X:736:C:H1'	2.36	0.40
1:A:142:HIS:CE1	1:A:143:ASN:HB2	2.56	0.40
2:X:49:A:C8	2:X:51:G:N2	2.89	0.40
2:X:260:A:C2'	2:X:261:C:H5'	2.51	0.40
2:X:320:U:H6	2:X:320:U:O5'	2.03	0.40
2:X:630:G:OP1	10:I:21:ARG:NH2	2.54	0.40
2:X:710:C:H2'	2:X:711:G:H8	1.86	0.40
2:X:843:G:H2'	2:X:844:G:C8	2.57	0.40
2:X:942:C:H2'	2:X:943:C:H5'	2.03	0.40
2:X:1771:A:O2'	2:X:1772:G:O5'	2.36	0.40
2:X:2382:C:H1'	21:T:47:ARG:NH1	2.37	0.40
2:X:2402:G:N2	2:X:2405:A:OP2	2.45	0.40
7:E:136:ILE:H	7:E:136:ILE:HG13	1.62	0.40
7:E:154:PRO:HG3	7:E:162:ILE:O	2.20	0.40
8:G:33:VAL:HA	8:G:36:ILE:HG12	2.04	0.40
9:H:35:ILE:HD13	9:H:62:ILE:HG22	2.02	0.40
9:H:107:ARG:HB2	9:H:107:ARG:HH11	1.86	0.40
1:A:11:ASN:O	1:A:14:ARG:HB3	2.21	0.40
2:X:24:G:O2'	17:P:78:GLU:O	2.40	0.40
2:X:51:G:O2'	2:X:118:A:C6	2.73	0.40
2:X:659:A:C2	2:X:661:U:OP1	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:897:A:H2'	2:X:898:U:C6	2.56	0.40
2:X:1875:A:C8	2:X:1875:A:H3'	2.57	0.40
2:X:2338:A:H2'	2:X:2338:A:N3	2.36	0.40
2:X:2406:G:H2'	2:X:2407:A:C8	2.56	0.40
2:X:2419:A:H5"	27:3:26:ARG:NH1	2.37	0.40
10:I:72:LYS:C	10:I:74:TYR:H	2.23	0.40
14:M:99:LEU:O	14:M:102:LEU:HD22	2.21	0.40
20:S:65:VAL:HG12	20:S:66:GLY:N	2.36	0.40
2:X:516:A:C2	2:X:517:A:C4	3.09	0.40
2:X:561:C:C2'	2:X:562:C:H5'	2.52	0.40
2:X:577:A:H2'	15:N:28:LYS:HE3	2.03	0.40
2:X:1209:U:H2'	2:X:1210:U:C6	2.57	0.40
2:X:1332:C:H4'	12:K:67:ARG:CZ	2.51	0.40
2:X:1484:G:O2'	2:X:1485:G:H5'	2.21	0.40
2:X:1599:G:C5	2:X:1600:A:C5	3.10	0.40
2:X:1841:G:C6	2:X:1842:A:C6	3.09	0.40
2:X:1876:G:H2'	2:X:1877:G:H8	1.87	0.40
2:X:2413:U:O2	21:T:49:ARG:HD3	2.22	0.40
2:X:2446:U:H2'	2:X:2447:C:H6	1.86	0.40
2:X:2647:C:O4'	4:B:169:MET:HE2	2.22	0.40
2:X:2656:A:C2	2:X:2914:A:C8	3.10	0.40
2:X:2810:A:H2'	2:X:2811:U:C6	2.56	0.40
4:B:6:LEU:HD23	4:B:6:LEU:HA	1.86	0.40
8:G:20:ASP:HA	8:G:58:ILE:HG22	2.03	0.40
12:K:34:GLU:HA	12:K:117:VAL:HG21	2.02	0.40
14:M:15:LEU:HD23	14:M:15:LEU:HA	1.89	0.40
18:Q:3:ALA:HB1	18:Q:41:ALA:CB	2.51	0.40
1:A:54:HIS:NE2	2:X:1850:G:OP1	2.55	0.40
1:A:247:MET:HE3	1:A:247:MET:HB2	1.94	0.40
2:X:64:A:O3'	18:Q:70:GLY:HA3	2.21	0.40
2:X:146:U:H2'	2:X:147:G:O4'	2.22	0.40
2:X:189:G:H2'	2:X:190:G:H8	1.86	0.40
2:X:494:U:H4'	2:X:495:A:OP2	2.20	0.40
2:X:739:U:H1'	2:X:1416:U:O2	2.21	0.40
2:X:870:C:H2'	2:X:871:U:O4'	2.20	0.40
2:X:2255:G:H2'	2:X:2256:U:C6	2.57	0.40
3:Y:23:U:O2'	3:Y:24:C:OP2	2.35	0.40
4:B:156:MET:HB3	4:B:157:ALA:H	1.63	0.40
5:C:51:VAL:HG11	5:C:91:GLY:HA3	2.04	0.40
12:K:51:GLY:HA2	12:K:86:PHE:CZ	2.56	0.40
15:N:62:ILE:HG23	15:N:76:TYR:CE2	2.57	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	
1	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	15
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	3	25
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	2	19
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	1	9
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	1	18
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	5	34
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	9	45
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	0	7
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1	11
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	1	17
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	2	22
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	2	23
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	2	21
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	17	57
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	1	18
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0	5
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0	5
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100	100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	2	21
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	2	22
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	8	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	6 37
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	6 37
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0 5
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100 100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	1 18

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL
1	A	192	ILE
4	B	53	PHE
4	B	96	VAL
4	B	99	TYR
4	B	204	PRO
5	C	15	GLY
5	C	128	ALA
5	C	158	ASN
5	C	166	SER
5	C	175	VAL
6	D	44	VAL
6	D	84	PRO
6	D	104	ILE
6	D	108	LEU
6	D	137	ILE
7	E	50	ILE
7	E	55	PRO
8	G	2	ARG
10	I	30	THR
10	I	46	VAL
10	I	48	PRO
10	I	77	VAL
11	J	4	PRO
11	J	61	GLY
11	J	135	GLU
12	K	75	ASP
12	K	77	THR

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Mol	Chain	Res	Type
13	L	63	ILE
13	L	92	ILE
14	M	36	GLU
16	O	50	ALA
17	P	71	VAL
19	R	25	ALA
19	R	101	ILE
20	S	34	TYR
20	S	109	VAL
20	S	150	ILE
22	U	40	VAL
23	V	3	ALA
23	V	11	THR
27	3	54	ASP
1	A	25	THR
1	A	79	ASP
1	A	126	VAL
1	A	170	LYS
1	A	224	VAL
5	C	97	TYR
5	C	144	SER
5	C	191	SER
6	D	74	ILE
6	D	131	GLY
7	E	35	ARG
9	H	25	LEU
10	I	71	ARG
10	I	101	VAL
10	I	110	LYS
10	I	126	HIS
11	J	10	ARG
11	J	99	PRO
12	K	28	GLU
12	K	76	GLU
13	L	91	GLU
14	M	55	GLY
18	Q	50	VAL
18	Q	66	GLY
18	Q	83	LYS
18	Q	90	PHE
19	R	74	LYS
20	S	81	PRO

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Mol	Chain	Res	Type
20	S	98	GLU
20	S	110	GLY
20	S	130	VAL
20	S	131	THR
20	S	167	ILE
1	A	245	SER
4	B	58	ALA
6	D	75	ALA
6	D	109	PRO
7	E	51	GLU
7	E	107	VAL
7	E	128	ASN
7	E	153	PRO
8	G	40	LYS
8	G	89	THR
10	I	13	ARG
10	I	62	PRO
10	I	87	ASP
11	J	133	LYS
11	J	136	GLU
12	K	6	LEU
14	M	5	LYS
14	M	89	LYS
16	O	52	THR
20	S	12	LYS
20	S	88	HIS
20	S	132	ALA
20	S	142	GLU
22	U	44	PRO
24	W	32	ASN
25	Z	22	ILE
26	2	16	VAL
27	3	28	PHE
27	3	34	ALA
27	3	46	LYS
1	A	39	LYS
1	A	110	LEU
1	A	135	ILE
4	B	60	LYS
4	B	176	ASN
6	D	60	ILE
6	D	89	VAL

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Mol	Chain	Res	Type
6	D	119	LYS
6	D	126	GLY
8	G	130	GLU
9	H	64	ARG
10	I	79	LEU
11	J	9	TYR
11	J	60	ARG
12	K	68	ASN
12	K	71	ILE
14	M	108	LYS
16	O	7	THR
19	R	58	GLU
19	R	67	ASN
19	R	76	ASN
19	R	88	GLY
20	S	13	GLN
20	S	129	GLU
20	S	138	PRO
27	3	47	ALA
1	A	37	LEU
1	A	252	LYS
11	J	89	ALA
13	L	65	THR
16	O	99	LYS
18	Q	86	SER
20	S	38	ASN
27	3	29	THR
27	3	45	ARG
5	C	27	GLU
5	C	171	PRO
6	D	115	GLN
7	E	36	THR
11	J	7	VAL
19	R	6	GLY
19	R	65	VAL
19	R	77	GLU
20	S	124	PRO
1	A	85	PRO
6	D	65	PRO
13	L	93	VAL
20	S	114	GLY
4	B	152	GLY

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Mol	Chain	Res	Type
20	S	133	THR
23	V	6	ILE
10	I	55	LEU
16	O	30	GLY
19	R	78	PRO
19	R	81	VAL
4	B	124	GLY
5	C	61	GLY
7	E	90	VAL
20	S	74	VAL

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
1	A	112/224 (50%)	97 (87%)	15 (13%)	4 23
4	B	150/177 (85%)	121 (81%)	29 (19%)	1 8
5	C	106/169 (63%)	84 (79%)	22 (21%)	1 7
6	D	15/158 (10%)	13 (87%)	2 (13%)	4 23
7	E	51/156 (33%)	39 (76%)	12 (24%)	1 5
8	G	106/123 (86%)	87 (82%)	19 (18%)	2 11
9	H	91/100 (91%)	74 (81%)	17 (19%)	1 9
10	I	56/108 (52%)	39 (70%)	17 (30%)	0 3
11	J	90/119 (76%)	80 (89%)	10 (11%)	6 31
12	K	91/102 (89%)	77 (85%)	14 (15%)	2 18
13	L	40/95 (42%)	30 (75%)	10 (25%)	0 4
14	M	75/102 (74%)	53 (71%)	22 (29%)	0 3
15	N	91/98 (93%)	70 (77%)	21 (23%)	1 5
16	O	71/86 (83%)	63 (89%)	8 (11%)	6 30
17	P	89/94 (95%)	77 (86%)	12 (14%)	4 22
18	Q	41/82 (50%)	34 (83%)	7 (17%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	R	44/90 (49%)	26 (59%)	18 (41%)	0 1
20	S	88/190 (46%)	73 (83%)	15 (17%)	2 13
21	T	53/75 (71%)	40 (76%)	13 (24%)	0 4
22	U	8/52 (15%)	7 (88%)	1 (12%)	4 25
23	V	47/62 (76%)	35 (74%)	12 (26%)	0 4
24	W	50/53 (94%)	38 (76%)	12 (24%)	0 4
25	Z	38/51 (74%)	32 (84%)	6 (16%)	2 17
26	2	35/40 (88%)	29 (83%)	6 (17%)	2 13
27	3	33/57 (58%)	27 (82%)	6 (18%)	1 10
28	4	2/35 (6%)	1 (50%)	1 (50%)	0 0
All	All	1673/2698 (62%)	1346 (80%)	327 (20%)	1 8

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	15	ASN
1	A	17	THR
1	A	45	ASN
1	A	46	GLN
1	A	53	HIS
1	A	59	LYS
1	A	90	ASN
1	A	96	TYR
1	A	141	VAL
1	A	171	TYR
1	A	181	VAL
1	A	204	ASN
1	A	219	THR
1	A	243	ARG
4	B	13	THR
4	B	29	GLU
4	B	32	GLU
4	B	33	ASN
4	B	43	VAL
4	B	62	ASP
4	B	78	LYS
4	B	104	GLU

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Mol	Chain	Res	Type
4	B	107	VAL
4	B	115	VAL
4	B	116	ILE
4	B	118	VAL
4	B	121	VAL
4	B	156	MET
4	B	158	SER
4	B	159	ASP
4	B	168	LYS
4	B	169	MET
4	B	173	MET
4	B	177	THR
4	B	180	VAL
4	B	192	ASN
4	B	193	LYS
4	B	195	ILE
4	B	198	LYS
4	B	200	ASN
4	B	208	LEU
4	B	210	GLU
4	B	213	THR
5	C	6	VAL
5	C	8	LYS
5	C	10	ASP
5	C	17	ILE
5	C	31	SER
5	C	39	LEU
5	C	41	ARG
5	C	43	SER
5	C	49	HIS
5	C	67	GLN
5	C	78	ILE
5	C	79	ARG
5	C	108	LEU
5	C	115	SER
5	C	136	THR
5	C	144	SER
5	C	146	LEU
5	C	155	VAL
5	C	164	GLU
5	C	165	LEU
5	C	183	VAL

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Mol	Chain	Res	Type
5	C	186	ILE
6	D	26	MET
6	D	105	SER
7	E	23	HIS
7	E	24	VAL
7	E	25	THR
7	E	41	MET
7	E	63	THR
7	E	65	HIS
7	E	68	THR
7	E	75	MET
7	E	83	TYR
7	E	84	VAL
7	E	115	ILE
7	E	136	ILE
8	G	1	MET
8	G	12	ILE
8	G	18	VAL
8	G	19	ILE
8	G	24	GLN
8	G	32	GLU
8	G	41	ASN
8	G	42	LYS
8	G	44	THR
8	G	46	THR
8	G	51	THR
8	G	58	ILE
8	G	69	LYS
8	G	101	LEU
8	G	102	ILE
8	G	114	ARG
8	G	125	VAL
8	G	131	HIS
8	G	143	LEU
9	H	8	LEU
9	H	19	VAL
9	H	21	THR
9	H	23	LYS
9	H	24	VAL
9	H	56	ASP
9	H	57	VAL
9	H	61	VAL

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Mol	Chain	Res	Type
9	H	63	VAL
9	H	67	SER
9	H	69	VAL
9	H	90	ASP
9	H	96	THR
9	H	97	ARG
9	H	107	ARG
9	H	112	MET
9	H	122	LEU
10	I	19	VAL
10	I	21	ARG
10	I	25	THR
10	I	31	SER
10	I	38	GLN
10	I	47	ARG
10	I	50	PHE
10	I	51	GLU
10	I	54	GLN
10	I	55	LEU
10	I	61	LEU
10	I	70	ASN
10	I	84	LYS
10	I	89	THR
10	I	107	SER
10	I	112	LEU
10	I	128	PHE
11	J	16	LYS
11	J	27	VAL
11	J	35	GLN
11	J	37	THR
11	J	41	TRP
11	J	72	THR
11	J	75	THR
11	J	96	VAL
11	J	120	LEU
11	J	134	ARG
12	K	6	LEU
12	K	27	SER
12	K	32	THR
12	K	33	THR
12	K	36	ARG
12	K	42	SER

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Mol	Chain	Res	Type
12	K	55	ASP
12	K	65	THR
12	K	66	LEU
12	K	94	THR
12	K	97	GLN
12	K	101	THR
12	K	109	ARG
12	K	110	ARG
13	L	11	ARG
13	L	17	ARG
13	L	31	LEU
13	L	33	VAL
13	L	36	SER
13	L	45	ILE
13	L	48	ASN
13	L	52	THR
13	L	53	LEU
13	L	96	ARG
14	M	10	VAL
14	M	11	THR
14	M	17	THR
14	M	21	SER
14	M	27	THR
14	M	43	GLN
14	M	49	VAL
14	M	52	ARG
14	M	53	ARG
14	M	57	VAL
14	M	58	SER
14	M	60	THR
14	M	63	VAL
14	M	74	ARG
14	M	75	THR
14	M	80	THR
14	M	82	LYS
14	M	83	ILE
14	M	100	TYR
14	M	102	LEU
14	M	103	ARG
14	M	106	ARG
15	N	9	VAL
15	N	29	HIS

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Mol	Chain	Res	Type
15	N	30	THR
15	N	41	LYS
15	N	48	ARG
15	N	51	ARG
15	N	54	LYS
15	N	55	ARG
15	N	58	ARG
15	N	63	THR
15	N	70	ARG
15	N	73	GLU
15	N	74	MET
15	N	75	SER
15	N	78	ARG
15	N	79	LEU
15	N	84	LYS
15	N	92	ARG
15	N	112	LYS
15	N	115	ASP
15	N	117	LEU
16	O	1	MET
16	O	12	ILE
16	O	16	GLU
16	O	48	VAL
16	O	72	THR
16	O	78	ARG
16	O	84	ARG
16	O	97	ILE
17	P	2	GLU
17	P	11	ARG
17	P	38	LEU
17	P	40	ASN
17	P	59	GLU
17	P	65	ASN
17	P	66	THR
17	P	83	LYS
17	P	86	ARG
17	P	109	ASP
17	P	111	LYS
17	P	112	GLU
18	Q	5	ASP
18	Q	49	LYS
18	Q	58	TYR

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Mol	Chain	Res	Type
18	Q	72	THR
18	Q	76	ARG
18	Q	80	VAL
18	Q	87	ILE
19	R	3	ILE
19	R	4	LYS
19	R	9	VAL
19	R	23	VAL
19	R	24	ILE
19	R	31	ASP
19	R	32	ARG
19	R	33	VAL
19	R	36	GLU
19	R	39	ASN
19	R	43	LYS
19	R	56	ILE
19	R	59	THR
19	R	68	VAL
19	R	72	ASP
19	R	80	ARG
19	R	81	VAL
19	R	91	VAL
20	S	14	THR
20	S	18	LEU
20	S	22	ARG
20	S	30	VAL
20	S	31	VAL
20	S	41	VAL
20	S	43	VAL
20	S	55	VAL
20	S	69	THR
20	S	85	GLN
20	S	101	THR
20	S	113	VAL
20	S	133	THR
20	S	155	THR
20	S	161	VAL
21	T	26	SER
21	T	27	LYS
21	T	28	ARG
21	T	29	LEU
21	T	39	VAL

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Mol	Chain	Res	Type
21	T	40	THR
21	T	51	THR
21	T	57	GLU
21	T	61	ARG
21	T	78	GLU
21	T	80	LYS
21	T	82	ARG
21	T	88	SER
22	U	29	TRP
23	V	19	LYS
23	V	20	SER
23	V	23	GLU
23	V	29	ARG
23	V	30	PHE
23	V	34	THR
23	V	38	GLU
23	V	40	THR
23	V	43	ILE
23	V	52	ARG
23	V	56	VAL
23	V	62	ILE
24	W	12	VAL
24	W	15	ARG
24	W	17	GLU
24	W	18	THR
24	W	32	ASN
24	W	33	SER
24	W	40	ASN
24	W	44	ARG
24	W	50	VAL
24	W	53	LEU
24	W	54	VAL
24	W	58	GLU
25	Z	3	VAL
25	Z	7	ARG
25	Z	24	VAL
25	Z	37	TYR
25	Z	38	LYS
25	Z	39	LEU
26	2	5	THR
26	2	20	ARG
26	2	22	ARG

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Mol	Chain	Res	Type
26	2	25	THR
26	2	30	LYS
26	2	41	LYS
27	3	6	THR
27	3	14	VAL
27	3	24	ARG
27	3	29	THR
27	3	55	MET
27	3	58	VAL
28	4	11	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
14	M	14	GLN
16	O	63	ASN
17	P	40	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	645 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	663 (23%)	36 (1%)

All (663) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G
2	X	17	G
2	X	34	U
2	X	38	A
2	X	39	C
2	X	51	G
2	X	52	A
2	X	60	U
2	X	61	A
2	X	64	A
2	X	66	C

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Mol	Chain	Res	Type
2	X	70	G
2	X	71	A
2	X	75	G
2	X	80	G
2	X	90	A
2	X	91	A
2	X	95	A
2	X	96	G
2	X	101	G
2	X	111	U
2	X	117	A
2	X	118	A
2	X	119	U
2	X	124	A
2	X	131	G
2	X	133	A
2	X	139	U
2	X	140	A
2	X	152	C
2	X	154	A
2	X	156	A
2	X	157	U
2	X	164	A
2	X	165	C
2	X	166	A
2	X	167	U
2	X	169	G
2	X	170	C
2	X	171	A
2	X	172	U
2	X	173	A
2	X	176	A
2	X	177	G
2	X	178	A
2	X	179	A
2	X	180	G
2	X	183	A
2	X	184	C
2	X	185	A
2	X	199	A
2	X	202	A
2	X	219	A

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Mol	Chain	Res	Type
2	X	225	A
2	X	227	G
2	X	233	U
2	X	235	G
2	X	236	A
2	X	248	G
2	X	251	G
2	X	255	G
2	X	268	A
2	X	284	C
2	X	285	U
2	X	286	U
2	X	287	G
2	X	288	C
2	X	289	U
2	X	290	U
2	X	291	G
2	X	293	U
2	X	298	U
2	X	300	G
2	X	301	U
2	X	303	G
2	X	310	C
2	X	311	U
2	X	313	U
2	X	319	G
2	X	320	U
2	X	321	U
2	X	322	A
2	X	328	G
2	X	329	A
2	X	330	C
2	X	332	A
2	X	338	G
2	X	344	U
2	X	353	A
2	X	354	A
2	X	359	A
2	X	364	A
2	X	372	A
2	X	373	A
2	X	374	U

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Mol	Chain	Res	Type
2	X	375	A
2	X	377	U
2	X	389	A
2	X	392	U
2	X	394	U
2	X	403	U
2	X	404	U
2	X	405	G
2	X	410	G
2	X	413	C
2	X	415	U
2	X	416	G
2	X	417	A
2	X	418	G
2	X	426	G
2	X	432	G
2	X	434	G
2	X	444	C
2	X	445	G
2	X	447	A
2	X	449	U
2	X	450	C
2	X	451	U
2	X	452	G
2	X	457	G
2	X	458	A
2	X	474	A
2	X	486	G
2	X	497	U
2	X	501	C
2	X	502	C
2	X	503	A
2	X	504	G
2	X	506	A
2	X	526	A
2	X	527	G
2	X	528	C
2	X	539	G
2	X	543	G
2	X	549	U
2	X	550	A
2	X	553	A

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Mol	Chain	Res	Type
2	X	554	C
2	X	555	C
2	X	566	U
2	X	567	G
2	X	572	C
2	X	573	A
2	X	575	G
2	X	576	U
2	X	577	A
2	X	578	G
2	X	583	A
2	X	590	U
2	X	592	A
2	X	593	U
2	X	594	G
2	X	606	G
2	X	615	A
2	X	616	G
2	X	618	A
2	X	628	G
2	X	629	A
2	X	630	G
2	X	635	G
2	X	646	A
2	X	647	G
2	X	657	U
2	X	658	A
2	X	659	A
2	X	660	A
2	X	661	U
2	X	666	A
2	X	673	G
2	X	682	A
2	X	683	G
2	X	690	U
2	X	691	A
2	X	692	G
2	X	698	U
2	X	699	U
2	X	702	U
2	X	713	A
2	X	716	C

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Mol	Chain	Res	Type
2	X	722	A
2	X	727	G
2	X	731	U
2	X	737	C
2	X	740	G
2	X	746	G
2	X	765	U
2	X	766	G
2	X	771	G
2	X	774	G
2	X	775	A
2	X	783	G
2	X	784	A
2	X	792	U
2	X	793	G
2	X	802	G
2	X	813	G
2	X	820	G
2	X	823	G
2	X	827	A
2	X	829	U
2	X	836	C
2	X	837	G
2	X	838	A
2	X	850	G
2	X	851	C
2	X	856	U
2	X	857	C
2	X	864	A
2	X	866	A
2	X	872	U
2	X	873	U
2	X	883	C
2	X	887	A
2	X	890	G
2	X	891	A
2	X	892	U
2	X	904	G
2	X	921	C
2	X	923	A
2	X	924	G
2	X	940	U

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Mol	Chain	Res	Type
2	X	942	C
2	X	943	C
2	X	944	G
2	X	947	U
2	X	948	U
2	X	955	A
2	X	969	A
2	X	970	U
2	X	972	A
2	X	977	A
2	X	985	A
2	X	989	A
2	X	990	G
2	X	1001	A
2	X	1005	G
2	X	1017	A
2	X	1018	A
2	X	1027	A
2	X	1034	A
2	X	1039	C
2	X	1040	A
2	X	1041	G
2	X	1043	U
2	X	1052	A
2	X	1053	A
2	X	1056	U
2	X	1057	A
2	X	1066	G
2	X	1067	U
2	X	1069	G
2	X	1070	A
2	X	1077	U
2	X	1078	G
2	X	1083	G
2	X	1086	G
2	X	1087	C
2	X	1089	C
2	X	1090	A
2	X	1091	G
2	X	1092	A
2	X	1093	C
2	X	1145	U

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Mol	Chain	Res	Type
2	X	1146	C
2	X	1147	A
2	X	1150	A
2	X	1151	G
2	X	1155	A
2	X	1156	G
2	X	1157	U
2	X	1175	G
2	X	1176	U
2	X	1177	A
2	X	1178	C
2	X	1179	C
2	X	1180	G
2	X	1186	A
2	X	1187	A
2	X	1195	A
2	X	1200	A
2	X	1215	U
2	X	1218	G
2	X	1220	A
2	X	1221	C
2	X	1250	G
2	X	1256	U
2	X	1258	A
2	X	1262	U
2	X	1274	G
2	X	1278	G
2	X	1291	A
2	X	1293	U
2	X	1294	G
2	X	1300	G
2	X	1309	G
2	X	1310	A
2	X	1311	A
2	X	1312	A
2	X	1313	G
2	X	1317	G
2	X	1337	A
2	X	1338	U
2	X	1340	G
2	X	1345	A
2	X	1349	U

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Mol	Chain	Res	Type
2	X	1350	U
2	X	1366	U
2	X	1389	U
2	X	1396	A
2	X	1402	A
2	X	1405	G
2	X	1415	A
2	X	1416	U
2	X	1422	A
2	X	1433	U
2	X	1447	A
2	X	1453	G
2	X	1454	U
2	X	1460	U
2	X	1461	C
2	X	1462	G
2	X	1463	A
2	X	1464	U
2	X	1465	G
2	X	1466	G
2	X	1467	G
2	X	1471	A
2	X	1472	C
2	X	1481	A
2	X	1489	A
2	X	1490	G
2	X	1491	C
2	X	1492	G
2	X	1494	G
2	X	1495	C
2	X	1496	G
2	X	1497	A
2	X	1498	U
2	X	1499	U
2	X	1503	U
2	X	1504	U
2	X	1505	G
2	X	1508	C
2	X	1509	G
2	X	1510	U
2	X	1511	C
2	X	1512	U

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Mol	Chain	Res	Type
2	X	1513	A
2	X	1514	A
2	X	1515	G
2	X	1516	C
2	X	1519	U
2	X	1522	G
2	X	1527	A
2	X	1528	G
2	X	1529	U
2	X	1541	C
2	X	1542	C
2	X	1543	G
2	X	1544	G
2	X	1547	C
2	X	1548	U
2	X	1549	C
2	X	1550	G
2	X	1551	U
2	X	1556	G
2	X	1557	C
2	X	1559	G
2	X	1561	G
2	X	1568	U
2	X	1569	G
2	X	1573	A
2	X	1575	A
2	X	1576	A
2	X	1577	G
2	X	1592	A
2	X	1593	G
2	X	1594	U
2	X	1599	G
2	X	1605	A
2	X	1606	C
2	X	1607	A
2	X	1613	G
2	X	1616	A
2	X	1625	U
2	X	1628	A
2	X	1629	U
2	X	1630	A
2	X	1631	G

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Mol	Chain	Res	Type
2	X	1632	A
2	X	1636	U
2	X	1637	A
2	X	1638	G
2	X	1639	G
2	X	1652	A
2	X	1653	A
2	X	1654	A
2	X	1662	A
2	X	1678	A
2	X	1684	A
2	X	1690	A
2	X	1691	G
2	X	1692	C
2	X	1695	G
2	X	1718	G
2	X	1732	U
2	X	1740	G
2	X	1744	A
2	X	1746	G
2	X	1748	G
2	X	1756	U
2	X	1757	U
2	X	1758	A
2	X	1760	G
2	X	1761	G
2	X	1763	U
2	X	1764	A
2	X	1765	A
2	X	1766	C
2	X	1768	C
2	X	1770	C
2	X	1771	A
2	X	1772	G
2	X	1783	G
2	X	1785	G
2	X	1790	G
2	X	1791	G
2	X	1800	A
2	X	1824	C
2	X	1826	G
2	X	1827	C

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Mol	Chain	Res	Type
2	X	1835	U
2	X	1836	A
2	X	1837	A
2	X	1843	U
2	X	1846	A
2	X	1847	U
2	X	1856	A
2	X	1860	C
2	X	1865	C
2	X	1875	A
2	X	1876	G
2	X	1885	G
2	X	1886	A
2	X	1893	A
2	X	1902	G
2	X	1908	A
2	X	1911	A
2	X	1912	A
2	X	1918	G
2	X	1926	A
2	X	1929	C
2	X	1930	G
2	X	1932	C
2	X	1933	G
2	X	1953	U
2	X	1955	A
2	X	1956	G
2	X	1963	A
2	X	1964	A
2	X	1965	A
2	X	1967	U
2	X	1982	U
2	X	1991	G
2	X	1994	C
2	X	1997	A
2	X	1998	A
2	X	1999	G
2	X	2009	U
2	X	2019	G
2	X	2020	U
2	X	2024	A
2	X	2031	G

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Mol	Chain	Res	Type
2	X	2043	U
2	X	2045	A
2	X	2047	A
2	X	2048	G
2	X	2050	A
2	X	2057	A
2	X	2058	A
2	X	2059	G
2	X	2060	A
2	X	2068	U
2	X	2070	C
2	X	2078	A
2	X	2079	G
2	X	2081	A
2	X	2082	C
2	X	2083	G
2	X	2087	A
2	X	2088	G
2	X	2089	A
2	X	2096	G
2	X	2107	G
2	X	2118	U
2	X	2119	U
2	X	2125	U
2	X	2225	A
2	X	2228	C
2	X	2230	G
2	X	2231	C
2	X	2233	C
2	X	2234	C
2	X	2237	U
2	X	2238	U
2	X	2239	A
2	X	2240	U
2	X	2241	C
2	X	2244	G
2	X	2245	G
2	X	2246	U
2	X	2248	G
2	X	2252	A
2	X	2265	G
2	X	2266	G

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Mol	Chain	Res	Type
2	X	2270	U
2	X	2278	G
2	X	2293	A
2	X	2295	A
2	X	2300	A
2	X	2306	G
2	X	2310	C
2	X	2314	A
2	X	2332	U
2	X	2333	U
2	X	2334	G
2	X	2347	A
2	X	2348	G
2	X	2352	G
2	X	2354	A
2	X	2361	U
2	X	2362	A
2	X	2372	G
2	X	2374	C
2	X	2377	C
2	X	2379	A
2	X	2385	A
2	X	2388	A
2	X	2398	G
2	X	2399	G
2	X	2406	G
2	X	2409	G
2	X	2410	G
2	X	2412	C
2	X	2417	U
2	X	2429	U
2	X	2432	G
2	X	2433	C
2	X	2434	A
2	X	2441	G
2	X	2450	U
2	X	2452	A
2	X	2456	G
2	X	2457	A
2	X	2468	C
2	X	2472	G
2	X	2473	G

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Mol	Chain	Res	Type
2	X	2475	A
2	X	2492	C
2	X	2497	G
2	X	2500	U
2	X	2501	U
2	X	2503	A
2	X	2505	A
2	X	2514	G
2	X	2526	C
2	X	2529	G
2	X	2530	A
2	X	2532	G
2	X	2545	A
2	X	2546	U
2	X	2547	C
2	X	2556	G
2	X	2561	C
2	X	2565	C
2	X	2575	G
2	X	2581	U
2	X	2591	A
2	X	2593	A
2	X	2594	G
2	X	2600	C
2	X	2603	G
2	X	2609	G
2	X	2612	U
2	X	2613	C
2	X	2629	A
2	X	2630	G
2	X	2636	U
2	X	2638	C
2	X	2640	U
2	X	2641	A
2	X	2642	U
2	X	2648	G
2	X	2652	G
2	X	2656	A
2	X	2657	G
2	X	2661	A
2	X	2663	U
2	X	2681	A

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Mol	Chain	Res	Type
2	X	2682	G
2	X	2690	G
2	X	2698	A
2	X	2708	C
2	X	2712	G
2	X	2715	G
2	X	2716	U
2	X	2717	A
2	X	2741	G
2	X	2745	G
2	X	2748	A
2	X	2753	U
2	X	2760	A
2	X	2766	U
2	X	2771	G
2	X	2775	A
2	X	2778	G
2	X	2779	C
2	X	2784	A
2	X	2791	A
2	X	2792	A
2	X	2805	A
2	X	2806	U
2	X	2817	A
2	X	2818	A
2	X	2819	C
2	X	2820	U
2	X	2821	U
2	X	2824	G
2	X	2826	U
2	X	2827	A
2	X	2832	A
2	X	2840	A
2	X	2843	A
2	X	2851	G
2	X	2865	G
2	X	2877	G
2	X	2887	G
2	X	2892	G
2	X	2894	C
2	X	2899	A
2	X	2900	C

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Mol	Chain	Res	Type
2	X	2906	G
2	X	2913	G
2	X	2920	U
3	Y	10	U
3	Y	23	U
3	Y	24	C
3	Y	28	C
3	Y	38	U
3	Y	39	G
3	Y	41	C
3	Y	42	G
3	Y	43	A
3	Y	44	A
3	Y	47	C
3	Y	53	U
3	Y	59	U
3	Y	83	U
3	Y	87	G
3	Y	88	U
3	Y	106	U
3	Y	114	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	38	A
2	X	90	A
2	X	165	C
2	X	285	U
2	X	364	A
2	X	416	G
2	X	502	C
2	X	525	A
2	X	614	U
2	X	630	G
2	X	657	U
2	X	660	A
2	X	890	G
2	X	970	U
2	X	1028	G
2	X	1091	G
2	X	1149	U

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Mol	Chain	Res	Type
2	X	1177	A
2	X	1303	A
2	X	1310	A
2	X	1369	G
2	X	1490	G
2	X	1503	U
2	X	1510	U
2	X	1521	A
2	X	1568	U
2	X	1576	A
2	X	1636	U
2	X	1885	G
2	X	1901	C
2	X	2062	G
2	X	2239	A
2	X	2378	G
2	X	2457	A
2	X	2474	G
2	X	2611	U

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 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
33	SPD	X	3498	-	9,9,9	0.38	0	8,8,8	0.61	0
33	SPD	X	3496	-	9,9,9	0.27	0	8,8,8	0.19	0
34	EOH	X	3500	-	2,2,2	0.62	0	1,1,1	0.50	0
32	MPD	X	3006	-	7,7,7	1.00	1 (14%)	9,10,10	0.56	0
33	SPD	Y	213	-	9,9,9	0.20	0	8,8,8	0.13	0
33	SPD	X	3493	-	9,9,9	0.33	0	8,8,8	0.53	0
35	EPE	N	201	-	15,15,15	1.14	1 (6%)	18,20,20	1.39	2 (11%)
32	MPD	J	201	-	7,7,7	1.31	1 (14%)	9,10,10	0.69	0
32	MPD	X	3007	-	7,7,7	0.38	0	9,10,10	0.41	0
33	SPD	X	3497	-	9,9,9	0.12	0	8,8,8	0.34	0
31	62B	X	3003	-	37,38,38	1.03	2 (5%)	55,60,60	3.30	18 (32%)
32	MPD	X	3005	-	7,7,7	0.99	1 (14%)	9,10,10	0.66	0
32	MPD	X	3008	-	7,7,7	1.18	1 (14%)	9,10,10	0.68	0
33	SPD	X	3492	-	9,9,9	0.39	0	8,8,8	0.39	0
32	MPD	Z	101	-	7,7,7	0.62	0	9,10,10	0.22	0
32	MPD	X	3010	-	7,7,7	0.96	1 (14%)	9,10,10	0.42	0
32	MPD	Q	101	-	7,7,7	0.74	0	9,10,10	0.26	0
33	SPD	X	3495	-	9,9,9	0.24	0	8,8,8	0.36	0
34	EOH	X	3499	-	2,2,2	0.62	0	1,1,1	0.48	0
34	EOH	S	301	-	2,2,2	0.71	0	1,1,1	0.29	0
32	MPD	X	3004	-	7,7,7	1.16	1 (14%)	9,10,10	0.71	0
33	SPD	X	3494	-	9,9,9	0.21	0	8,8,8	0.31	0
32	MPD	X	3011	-	7,7,7	1.27	1 (14%)	9,10,10	0.46	0
32	MPD	X	3009	-	7,7,7	0.62	0	9,10,10	0.30	0

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
33	SPD	X	3498	-	-	3/7/7/7	-
33	SPD	X	3496	-	-	1/7/7/7	-
32	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	Y	213	-	-	2/7/7/7	-
33	SPD	X	3493	-	-	1/7/7/7	-
35	EPE	N	201	-	-	5/9/19/19	0/1/1/1
32	MPD	J	201	-	-	1/5/5/5	-
32	MPD	X	3007	-	-	0/5/5/5	-
33	SPD	X	3497	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	62B	X	3003	-	-	1/12/86/86	0/4/4/4
32	MPD	X	3005	-	-	2/5/5/5	-
32	MPD	X	3008	-	-	3/5/5/5	-
33	SPD	X	3492	-	-	4/7/7/7	-
32	MPD	Z	101	-	-	1/5/5/5	-
32	MPD	X	3010	-	-	1/5/5/5	-
32	MPD	Q	101	-	-	1/5/5/5	-
33	SPD	X	3495	-	-	5/7/7/7	-
32	MPD	X	3004	-	-	4/5/5/5	-
33	SPD	X	3494	-	-	3/7/7/7	-
32	MPD	X	3011	-	-	3/5/5/5	-
32	MPD	X	3009	-	-	2/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	3003	62B	C10-C11	4.35	1.60	1.56
35	N	201	EPE	C10-S	-3.77	1.72	1.77
31	X	3003	62B	C13-C12	-3.24	1.49	1.55
32	J	201	MPD	C3-C2	2.99	1.61	1.53
32	X	3011	MPD	C3-C2	2.81	1.61	1.53
32	X	3004	MPD	C3-C2	2.75	1.61	1.53
32	X	3008	MPD	C3-C2	2.73	1.61	1.53
32	X	3006	MPD	C3-C2	2.42	1.60	1.53
32	X	3010	MPD	C3-C2	2.10	1.59	1.53
32	X	3005	MPD	C3-C2	2.07	1.59	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	X	3003	62B	C18-C12-C11	12.98	115.64	108.06
31	X	3003	62B	C15-C5-C14	-8.58	100.50	108.95
31	X	3003	62B	C6-C5-C14	7.47	117.16	112.10
31	X	3003	62B	C24-C25-C26	-7.23	103.25	111.53
31	X	3003	62B	C13-C12-C19	-6.16	98.31	111.04
31	X	3003	62B	C13-C14-C5	-5.61	110.55	116.31
31	X	3003	62B	C1-C9-C8	-4.90	98.45	110.01
31	X	3003	62B	C13-C12-C11	4.64	117.24	112.70
31	X	3003	62B	C28-C23-S1	-4.52	103.18	111.10
31	X	3003	62B	C9-C10-C11	4.49	116.68	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	201	EPE	O3S-S-C10	-4.24	98.92	105.77
31	X	3003	62B	C12-C11-C10	4.19	118.69	114.58
31	X	3003	62B	C8-C9-C10	3.24	116.37	111.75
31	X	3003	62B	C2-C3-C4	-2.97	105.25	108.60
31	X	3003	62B	C17-C10-C11	-2.85	109.89	112.11
31	X	3003	62B	C7-C6-C5	-2.80	108.62	111.37
35	N	201	EPE	O2S-S-C10	2.63	110.08	106.92
31	X	3003	62B	C27-C26-C25	-2.33	107.86	110.24
31	X	3003	62B	C1-C9-C4	2.08	106.90	102.60
31	X	3003	62B	C8-C9-C4	2.06	109.42	106.56

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	3004	MPD	O2-C2-C3-C4
32	X	3004	MPD	C2-C3-C4-O4
35	N	201	EPE	N4-C7-C8-O8
33	X	3495	SPD	N6-C7-C8-C9
33	X	3498	SPD	C8-C7-N6-C5
33	X	3495	SPD	C7-C8-C9-N10
35	N	201	EPE	C8-C7-N4-C5
33	X	3495	SPD	C8-C7-N6-C5
33	X	3497	SPD	N1-C2-C3-C4
33	Y	213	SPD	C2-C3-C4-C5
35	N	201	EPE	S-C10-C9-N1
35	N	201	EPE	C10-C9-N1-C6
32	X	3008	MPD	O2-C2-C3-C4
33	X	3495	SPD	N1-C2-C3-C4
32	X	3006	MPD	C2-C3-C4-C5
32	X	3009	MPD	C2-C3-C4-C5
32	X	3011	MPD	C2-C3-C4-C5
32	J	201	MPD	C2-C3-C4-C5
32	Q	101	MPD	C2-C3-C4-C5
33	X	3492	SPD	N1-C2-C3-C4
33	X	3497	SPD	N6-C7-C8-C9
31	X	3003	62B	C21-C22-S1-C23
32	X	3004	MPD	C1-C2-C3-C4
32	X	3004	MPD	CM-C2-C3-C4
32	X	3008	MPD	C1-C2-C3-C4
32	X	3008	MPD	CM-C2-C3-C4
32	X	3011	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
32	X	3011	MPD	CM-C2-C3-C4
33	X	3492	SPD	C4-C5-N6-C7
33	X	3497	SPD	C2-C3-C4-C5
33	Y	213	SPD	C4-C5-N6-C7
33	X	3494	SPD	N1-C2-C3-C4
33	X	3496	SPD	N1-C2-C3-C4
33	X	3498	SPD	N1-C2-C3-C4
33	X	3495	SPD	C2-C3-C4-C5
35	N	201	EPE	C10-C9-N1-C2
33	X	3492	SPD	C3-C4-C5-N6
33	X	3497	SPD	C8-C7-N6-C5
33	X	3492	SPD	N6-C7-C8-C9
32	X	3005	MPD	O2-C2-C3-C4
33	X	3493	SPD	N1-C2-C3-C4
33	X	3494	SPD	C8-C7-N6-C5
33	X	3494	SPD	C2-C3-C4-C5
32	X	3010	MPD	C2-C3-C4-C5
32	Z	101	MPD	C2-C3-C4-C5
33	X	3498	SPD	C4-C5-N6-C7
32	X	3005	MPD	C2-C3-C4-O4
32	X	3009	MPD	C2-C3-C4-O4

There are no ring outliers.

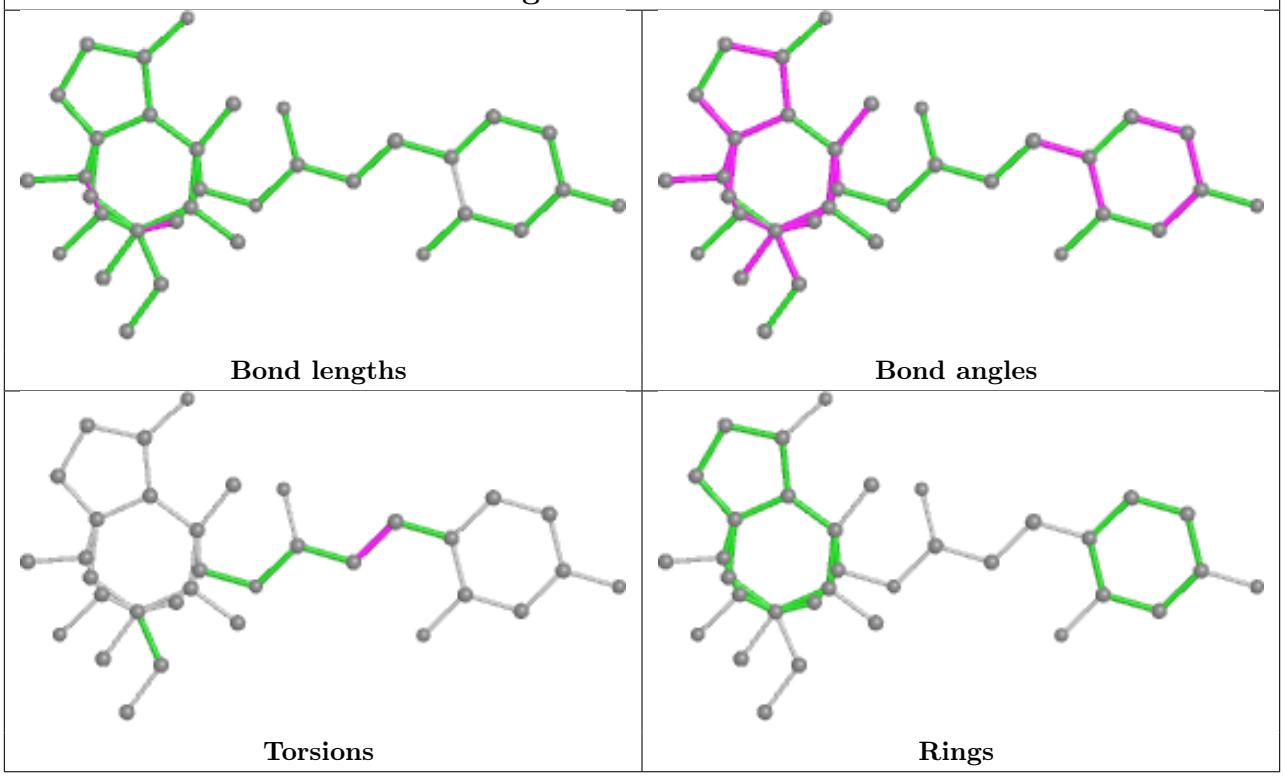
14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	X	3498	SPD	1	0
32	X	3006	MPD	2	0
33	Y	213	SPD	1	0
33	X	3493	SPD	2	0
35	N	201	EPE	17	0
32	J	201	MPD	1	0
33	X	3497	SPD	3	0
31	X	3003	62B	1	0
32	X	3005	MPD	1	0
32	X	3008	MPD	1	0
32	X	3010	MPD	1	0
33	X	3495	SPD	2	0
32	X	3004	MPD	2	0
33	X	3494	SPD	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 62B X 3003



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	269/277 (97%)	-0.31	4 (1%)	73	59	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.49	17 (0%)	89	80	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.63	0	100	100	76, 125, 175, 180	0
4	B	215/220 (97%)	-0.31	1 (0%)	91	83	62, 81, 99, 116	0
5	C	199/207 (96%)	-0.43	1 (0%)	91	83	64, 96, 113, 138	0
6	D	165/179 (92%)	0.02	11 (6%)	17	11	166, 193, 231, 239	0
7	E	157/178 (88%)	-0.26	6 (3%)	40	27	133, 172, 206, 212	0
8	G	145/145 (100%)	-0.20	1 (0%)	87	78	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.37	0	100	100	84, 102, 123, 128	0
10	I	131/140 (93%)	-0.02	5 (3%)	40	27	58, 116, 136, 142	0
11	J	138/144 (95%)	0.24	4 (2%)	51	35	77, 103, 135, 152	0
12	K	119/122 (97%)	-0.54	0	100	100	67, 84, 108, 141	0
13	L	109/119 (91%)	-0.83	0	100	100	121, 130, 157, 189	0
14	M	110/116 (94%)	-0.39	2 (1%)	68	52	85, 99, 132, 156	0
15	N	116/118 (98%)	-0.43	0	100	100	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.56	0	100	100	54, 88, 103, 109	0
17	P	112/117 (95%)	-0.01	1 (0%)	84	72	64, 75, 114, 139	0
18	Q	90/91 (98%)	-0.19	0	100	100	98, 122, 138, 170	0
19	R	102/105 (97%)	0.30	6 (5%)	22	13	98, 121, 189, 206	0
20	S	167/217 (76%)	-0.27	1 (0%)	89	80	87, 109, 199, 218	0
21	T	75/94 (79%)	-0.00	1 (1%)	77	63	85, 97, 115, 129	0
22	U	42/62 (67%)	2.37	24 (57%)	0	0	160, 172, 203, 213	0
23	V	65/69 (94%)	-0.07	0	100	100	134, 145, 159, 163	0
24	W	57/59 (96%)	0.21	0	100	100	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	43/58 (74%)	-0.26	0 100 100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.41	4 (9%) 8 5	83, 92, 102, 105	0
27	3	60/66 (90%)	-0.24	0 100 100	80, 89, 105, 109	0
28	4	36/37 (97%)	2.40	22 (61%) 0 0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	-0.32	111 (1%) 66 50	53, 103, 190, 280	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	16	ASN	5.7
22	U	30	ASN	5.4
28	4	32	HIS	5.2
22	U	27	ARG	5.1
28	4	30	PRO	5.0
22	U	17	ARG	4.9
28	4	29	ASN	4.7
28	4	31	LYS	4.6
22	U	15	GLY	4.5
19	R	70	LEU	4.3
7	E	88	GLU	4.2
28	4	24	MET	4.2
28	4	34	GLN	4.1
22	U	14	THR	4.1
19	R	69	GLN	3.9
22	U	29	TRP	3.9
6	D	83	MET	3.8
28	4	2	LYS	3.7
22	U	37	ARG	3.7
11	J	62	GLY	3.7
28	4	14	CYS	3.7
28	4	35	ARG	3.7
22	U	41	ASP	3.6
22	U	40	VAL	3.6
22	U	13	SER	3.6
22	U	26	LYS	3.6
28	4	12	GLU	3.5
28	4	27	CYS	3.5
2	X	2629	A	3.4
22	U	35	LYS	3.4
2	X	1150	A	3.4
22	U	20	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
20	S	140	ALA	3.3
22	U	31	ALA	3.3
10	I	95	LEU	3.2
1	A	94	VAL	3.1
22	U	38	ILE	3.1
6	D	162	THR	3.1
6	D	47	SER	3.0
10	I	114	ASN	3.0
22	U	36	VAL	3.0
2	X	2277	G	2.9
28	4	11	CYS	2.9
28	4	36	GLN	2.9
7	E	171	ARG	2.9
2	X	1876	G	2.8
6	D	84	PRO	2.8
22	U	34	GLN	2.8
28	4	10	ILE	2.8
19	R	67	ASN	2.8
11	J	58	MET	2.8
7	E	170	ARG	2.7
22	U	28	ARG	2.7
26	2	18	GLY	2.7
22	U	25	THR	2.7
14	M	25	GLY	2.7
28	4	6	SER	2.6
2	X	420	A	2.6
10	I	118	ASP	2.6
22	U	33	LEU	2.5
28	4	26	ILE	2.5
7	E	163	ARG	2.5
26	2	9	ASN	2.5
19	R	68	VAL	2.5
6	D	68	THR	2.5
28	4	25	VAL	2.5
6	D	158	THR	2.5
11	J	61	GLY	2.5
2	X	1148	C	2.5
2	X	1147	A	2.5
6	D	82	GLY	2.4
22	U	53	ALA	2.4
21	T	60	GLY	2.4
11	J	55	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	X	33	U	2.4
19	R	32	ARG	2.4
19	R	31	ASP	2.4
6	D	77	PHE	2.4
1	A	82	GLN	2.3
17	P	102	HIS	2.3
10	I	1	MET	2.3
6	D	113	ASP	2.3
14	M	4	HIS	2.3
2	X	447	A	2.3
5	C	176	THR	2.3
8	G	145	GLY	2.2
2	X	2345	A	2.2
2	X	34	U	2.2
6	D	38	MET	2.2
26	2	17	HIS	2.2
7	E	91	GLY	2.2
2	X	2238	U	2.2
22	U	50	SER	2.1
1	A	262	GLY	2.1
28	4	15	LYS	2.1
6	D	122	PHE	2.1
28	4	28	GLU	2.1
2	X	2502	C	2.1
4	B	134	HIS	2.1
26	2	16	VAL	2.1
28	4	1	MET	2.1
2	X	2239	A	2.0
1	A	25	THR	2.0
2	X	1877	G	2.0
2	X	1918	G	2.0
28	4	4	ARG	2.0
10	I	66	PHE	2.0
2	X	1149	U	2.0
28	4	3	VAL	2.0
7	E	162	ILE	2.0
22	U	51	ALA	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, 95th 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	Y	210	1/1	0.17	1.31	105,105,105,105	0
30	MG	X	3250	1/1	0.21	1.64	89,89,89,89	0
29	MN	X	3466	1/1	0.37	0.38	155,155,155,155	0
30	MG	X	3306	1/1	0.43	0.43	95,95,95,95	0
29	MN	X	3209	1/1	0.43	0.19	150,150,150,150	0
30	MG	X	3340	1/1	0.45	0.64	84,84,84,84	0
30	MG	X	3351	1/1	0.46	0.63	116,116,116,116	0
30	MG	X	3449	1/1	0.47	0.42	86,86,86,86	0
30	MG	X	3417	1/1	0.47	0.93	82,82,82,82	0
29	MN	X	3437	1/1	0.49	0.13	153,153,153,153	0
30	MG	X	3474	1/1	0.53	0.23	106,106,106,106	0
29	MN	X	3460	1/1	0.53	0.36	182,182,182,182	0
30	MG	X	3362	1/1	0.54	0.36	114,114,114,114	0
30	MG	X	3337	1/1	0.55	0.47	89,89,89,89	0
30	MG	Y	203	1/1	0.55	0.60	96,96,96,96	0
30	MG	X	3349	1/1	0.55	1.47	127,127,127,127	0
30	MG	X	3180	1/1	0.56	1.15	78,78,78,78	0
30	MG	X	3488	1/1	0.57	0.67	100,100,100,100	0
30	MG	X	3310	1/1	0.57	0.22	129,129,129,129	0
30	MG	X	3487	1/1	0.57	0.53	109,109,109,109	0
30	MG	X	3391	1/1	0.58	1.00	107,107,107,107	0
30	MG	X	3327	1/1	0.58	1.10	126,126,126,126	0
30	MG	X	3400	1/1	0.60	0.63	90,90,90,90	0
30	MG	X	3433	1/1	0.60	0.34	124,124,124,124	0
30	MG	X	3341	1/1	0.61	0.64	96,96,96,96	0
29	MN	X	3211	1/1	0.61	0.35	144,144,144,144	0
30	MG	A	303	1/1	0.62	0.31	94,94,94,94	0
29	MN	X	3324	1/1	0.62	0.16	164,164,164,164	0
30	MG	X	3308	1/1	0.63	0.44	77,77,77,77	0
30	MG	X	3335	1/1	0.63	0.70	61,61,61,61	0
30	MG	Y	212	1/1	0.64	0.63	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3471	1/1	0.66	1.22	130,130,130,130	0
29	MN	X	3446	1/1	0.66	0.45	142,142,142,142	0
30	MG	X	3087	1/1	0.66	0.66	55,55,55,55	0
30	MG	X	3344	1/1	0.66	0.85	91,91,91,91	0
29	MN	X	3202	1/1	0.66	0.22	173,173,173,173	0
29	MN	X	3263	1/1	0.66	0.35	166,166,166,166	0
29	MN	X	3421	1/1	0.67	0.45	111,111,111,111	0
30	MG	X	3393	1/1	0.67	1.22	104,104,104,104	0
30	MG	X	3248	1/1	0.68	0.55	69,69,69,69	0
30	MG	X	3294	1/1	0.68	0.45	108,108,108,108	0
30	MG	X	3445	1/1	0.69	1.41	104,104,104,104	0
30	MG	X	3386	1/1	0.69	0.40	88,88,88,88	0
30	MG	X	3253	1/1	0.69	1.55	112,112,112,112	0
30	MG	X	3435	1/1	0.69	0.28	153,153,153,153	0
33	SPD	X	3498	10/10	0.69	0.41	93,93,93,93	0
30	MG	X	3357	1/1	0.70	0.29	95,95,95,95	0
29	MN	X	3181	1/1	0.70	0.12	142,142,142,142	0
29	MN	X	3183	1/1	0.71	0.14	125,125,125,125	0
29	MN	X	3114	1/1	0.71	0.56	122,122,122,122	0
30	MG	X	3358	1/1	0.71	1.38	88,88,88,88	0
29	MN	X	3203	1/1	0.71	0.19	145,145,145,145	0
30	MG	X	3370	1/1	0.71	1.18	113,113,113,113	0
30	MG	X	3475	1/1	0.71	0.85	93,93,93,93	0
30	MG	X	3395	1/1	0.72	0.37	79,79,79,79	0
30	MG	X	3196	1/1	0.72	0.52	89,89,89,89	0
30	MG	G	202	1/1	0.72	0.37	77,77,77,77	0
30	MG	X	3222	1/1	0.72	0.21	80,80,80,80	0
29	MN	X	3425	1/1	0.73	0.30	101,101,101,101	0
29	MN	X	3225	1/1	0.73	0.53	157,157,157,157	0
30	MG	X	3428	1/1	0.73	0.12	105,105,105,105	0
30	MG	X	3254	1/1	0.73	0.77	66,66,66,66	0
30	MG	X	3293	1/1	0.73	0.47	117,117,117,117	0
30	MG	X	3236	1/1	0.73	0.71	88,88,88,88	0
29	MN	X	3210	1/1	0.73	0.22	201,201,201,201	0
30	MG	X	3398	1/1	0.73	0.59	99,99,99,99	0
30	MG	X	3361	1/1	0.74	0.37	86,86,86,86	0
30	MG	X	3255	1/1	0.74	0.62	94,94,94,94	0
30	MG	P	201	1/1	0.74	0.65	63,63,63,63	0
30	MG	X	3230	1/1	0.74	0.54	80,80,80,80	0
34	EOH	S	301	3/3	0.74	0.35	90,90,90,90	0
30	MG	X	3252	1/1	0.75	1.35	114,114,114,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3072	1/1	0.75	0.21	123,123,123,123	0
29	MN	X	3155	1/1	0.75	0.40	110,110,110,110	0
30	MG	X	3265	1/1	0.76	0.64	96,96,96,96	0
30	MG	X	3348	1/1	0.76	0.62	72,72,72,72	0
30	MG	X	3266	1/1	0.76	0.34	90,90,90,90	0
29	MN	X	3458	1/1	0.76	0.54	127,127,127,127	0
30	MG	X	3441	1/1	0.76	0.57	96,96,96,96	0
30	MG	G	201	1/1	0.76	0.57	89,89,89,89	0
30	MG	X	3352	1/1	0.76	0.52	94,94,94,94	0
30	MG	X	3244	1/1	0.76	0.51	109,109,109,109	0
29	MN	X	3166	1/1	0.76	0.21	92,92,92,92	0
29	MN	X	3478	1/1	0.76	0.20	132,132,132,132	0
29	MN	X	3112	1/1	0.77	0.25	124,124,124,124	0
30	MG	X	3339	1/1	0.77	1.67	108,108,108,108	0
29	MN	X	3175	1/1	0.77	0.28	122,122,122,122	0
30	MG	A	302	1/1	0.78	0.57	92,92,92,92	0
30	MG	X	3346	1/1	0.78	0.47	68,68,68,68	0
32	MPD	J	201	8/8	0.78	0.30	125,125,125,125	0
30	MG	X	3336	1/1	0.78	0.91	99,99,99,99	0
33	SPD	Y	213	10/10	0.78	0.38	101,101,101,101	0
30	MG	X	3342	1/1	0.78	0.52	80,80,80,80	0
30	MG	X	3332	1/1	0.79	0.44	81,81,81,81	0
30	MG	X	3130	1/1	0.79	0.36	72,72,72,72	0
29	MN	X	3447	1/1	0.79	0.24	128,128,128,128	0
32	MPD	X	3004	8/8	0.79	0.30	135,135,135,135	0
29	MN	X	3186	1/1	0.79	0.45	143,143,143,143	0
30	MG	X	3286	1/1	0.79	0.47	77,77,77,77	0
29	MN	X	3379	1/1	0.79	0.19	158,158,158,158	0
30	MG	X	3365	1/1	0.79	0.69	76,76,76,76	0
29	MN	Z	102	1/1	0.80	0.36	112,112,112,112	0
30	MG	X	3394	1/1	0.80	0.19	98,98,98,98	0
29	MN	X	3454	1/1	0.80	0.49	126,126,126,126	0
30	MG	X	3382	1/1	0.80	0.66	126,126,126,126	0
29	MN	X	3158	1/1	0.80	0.30	117,117,117,117	0
30	MG	X	3413	1/1	0.80	0.56	90,90,90,90	0
29	MN	X	3231	1/1	0.80	0.26	161,161,161,161	0
30	MG	X	3423	1/1	0.81	0.32	79,79,79,79	0
30	MG	Y	207	1/1	0.81	0.27	78,78,78,78	0
30	MG	X	3385	1/1	0.81	1.06	88,88,88,88	0
30	MG	X	3229	1/1	0.81	0.20	98,98,98,98	0
29	MN	X	3468	1/1	0.81	0.25	104,104,104,104	0
29	MN	X	3469	1/1	0.81	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	3323	1/1	0.81	0.26	141,141,141,141	0
29	MN	X	3185	1/1	0.81	0.16	101,101,101,101	0
29	MN	X	3146	1/1	0.81	0.20	122,122,122,122	0
33	SPD	X	3496	10/10	0.81	0.48	102,102,102,102	0
29	MN	X	3314	1/1	0.81	0.30	147,147,147,147	0
30	MG	X	3375	1/1	0.81	0.24	76,76,76,76	0
30	MG	X	3228	1/1	0.81	0.30	150,150,150,150	0
30	MG	X	3260	1/1	0.82	0.14	123,123,123,123	0
30	MG	X	3378	1/1	0.82	0.59	83,83,83,83	0
29	MN	X	3456	1/1	0.82	0.24	113,113,113,113	0
30	MG	X	3354	1/1	0.82	0.71	75,75,75,75	0
29	MN	X	3154	1/1	0.82	0.35	124,124,124,124	0
30	MG	X	3212	1/1	0.82	0.97	78,78,78,78	0
30	MG	X	3288	1/1	0.82	0.32	81,81,81,81	0
29	MN	X	3479	1/1	0.82	0.24	171,171,171,171	0
30	MG	X	3363	1/1	0.82	0.36	82,82,82,82	0
29	MN	X	3162	1/1	0.82	0.24	118,118,118,118	0
30	MG	X	3305	1/1	0.82	0.43	123,123,123,123	0
30	MG	X	3406	1/1	0.82	0.29	71,71,71,71	0
30	MG	X	3408	1/1	0.82	1.48	97,97,97,97	0
30	MG	X	3429	1/1	0.83	0.23	102,102,102,102	0
30	MG	X	3477	1/1	0.83	0.32	80,80,80,80	0
30	MG	X	3123	1/1	0.83	0.49	69,69,69,69	0
30	MG	X	3307	1/1	0.83	0.52	71,71,71,71	0
29	MN	X	3133	1/1	0.83	0.28	133,133,133,133	0
32	MPD	Q	101	8/8	0.83	0.20	137,137,137,137	0
30	MG	X	3167	1/1	0.83	0.34	62,62,62,62	0
30	MG	X	3213	1/1	0.83	1.50	86,86,86,86	0
30	MG	X	3356	1/1	0.83	0.13	83,83,83,83	0
30	MG	C	302	1/1	0.83	0.29	78,78,78,78	0
29	MN	X	3208	1/1	0.84	0.29	141,141,141,141	0
29	MN	X	3168	1/1	0.84	0.29	115,115,115,115	0
30	MG	X	3345	1/1	0.84	0.30	65,65,65,65	0
29	MN	X	3360	1/1	0.84	0.12	146,146,146,146	0
30	MG	X	3387	1/1	0.84	0.34	175,175,175,175	0
30	MG	X	3246	1/1	0.84	0.90	72,72,72,72	0
29	MN	X	3463	1/1	0.84	0.17	134,134,134,134	0
29	MN	X	3174	1/1	0.84	0.18	121,121,121,121	0
30	MG	X	3489	1/1	0.84	0.70	62,62,62,62	0
30	MG	X	3283	1/1	0.84	0.22	129,129,129,129	0
29	MN	X	3139	1/1	0.84	0.45	117,117,117,117	0
30	MG	X	3440	1/1	0.84	0.42	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3316	1/1	0.85	0.10	173,173,173,173	0
30	MG	X	3002	1/1	0.85	1.02	100,100,100,100	0
30	MG	X	3280	1/1	0.85	0.33	159,159,159,159	0
30	MG	X	3300	1/1	0.85	0.25	94,94,94,94	0
32	MPD	X	3008	8/8	0.85	0.26	94,94,94,94	0
30	MG	X	3371	1/1	0.85	0.49	88,88,88,88	0
30	MG	Y	205	1/1	0.85	0.82	94,94,94,94	0
33	SPD	X	3492	10/10	0.85	0.27	105,105,105,105	0
30	MG	X	3372	1/1	0.85	0.50	78,78,78,78	0
33	SPD	X	3497	10/10	0.85	0.18	96,96,96,96	0
30	MG	X	3419	1/1	0.85	0.70	107,107,107,107	0
29	MN	X	3319	1/1	0.85	0.10	158,158,158,158	0
29	MN	X	3150	1/1	0.85	0.18	110,110,110,110	0
30	MG	X	3224	1/1	0.86	0.78	66,66,66,66	0
30	MG	X	3242	1/1	0.86	0.69	65,65,65,65	0
32	MPD	Z	101	8/8	0.86	0.21	145,145,145,145	0
30	MG	X	3329	1/1	0.86	0.52	63,63,63,63	0
33	SPD	X	3494	10/10	0.86	0.27	87,87,87,87	0
29	MN	X	3178	1/1	0.86	0.11	126,126,126,126	0
30	MG	X	3444	1/1	0.86	0.40	100,100,100,100	0
29	MN	X	3262	1/1	0.86	0.12	143,143,143,143	0
29	MN	X	3148	1/1	0.86	0.25	144,144,144,144	0
30	MG	X	3233	1/1	0.86	0.34	68,68,68,68	0
30	MG	X	3129	1/1	0.87	0.60	79,79,79,79	0
29	MN	Y	208	1/1	0.87	0.19	164,164,164,164	0
29	MN	X	3380	1/1	0.87	0.26	151,151,151,151	0
29	MN	X	3194	1/1	0.87	0.21	138,138,138,138	0
29	MN	X	3422	1/1	0.87	0.23	154,154,154,154	0
30	MG	X	3328	1/1	0.87	0.53	103,103,103,103	0
29	MN	X	3058	1/1	0.87	0.39	101,101,101,101	0
30	MG	X	3347	1/1	0.87	1.25	108,108,108,108	0
30	MG	X	3411	1/1	0.87	0.42	82,82,82,82	0
30	MG	X	3241	1/1	0.87	1.25	78,78,78,78	0
30	MG	X	3334	1/1	0.87	0.70	89,89,89,89	0
30	MG	X	3350	1/1	0.87	0.39	100,100,100,100	0
33	SPD	X	3495	10/10	0.87	0.24	83,83,83,83	0
30	MG	X	3504	1/1	0.87	0.57	74,74,74,74	0
30	MG	X	3295	1/1	0.87	0.45	100,100,100,100	0
29	MN	X	3376	1/1	0.87	0.10	119,119,119,119	0
29	MN	X	3116	1/1	0.87	0.42	111,111,111,111	0
30	MG	X	3338	1/1	0.87	0.34	82,82,82,82	0
29	MN	X	3176	1/1	0.88	0.31	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3287	1/1	0.88	1.56	102,102,102,102	0
30	MG	J	202	1/1	0.88	0.18	92,92,92,92	0
29	MN	X	3320	1/1	0.88	0.31	107,107,107,107	0
30	MG	X	3290	1/1	0.88	0.59	98,98,98,98	0
30	MG	X	3412	1/1	0.88	0.53	106,106,106,106	0
32	MPD	X	3010	8/8	0.88	0.22	113,113,113,113	0
30	MG	X	3144	1/1	0.88	0.32	71,71,71,71	0
30	MG	X	3226	1/1	0.88	0.82	102,102,102,102	0
30	MG	X	3359	1/1	0.88	0.51	91,91,91,91	0
30	MG	X	3420	1/1	0.88	0.47	75,75,75,75	0
29	MN	X	3113	1/1	0.88	0.23	96,96,96,96	0
29	MN	X	3461	1/1	0.88	0.26	149,149,149,149	0
29	MN	X	3151	1/1	0.88	0.25	97,97,97,97	0
30	MG	X	3282	1/1	0.88	0.25	85,85,85,85	0
30	MG	X	3368	1/1	0.88	0.54	87,87,87,87	0
30	MG	X	3397	1/1	0.88	0.21	78,78,78,78	0
29	MN	X	3182	1/1	0.88	0.13	133,133,133,133	0
30	MG	X	3298	1/1	0.89	0.40	95,95,95,95	0
29	MN	X	3060	1/1	0.89	0.23	90,90,90,90	0
29	MN	X	3025	1/1	0.89	0.31	128,128,128,128	0
30	MG	X	3484	1/1	0.89	0.17	77,77,77,77	0
30	MG	X	3238	1/1	0.89	0.86	85,85,85,85	0
30	MG	X	3424	1/1	0.89	1.44	89,89,89,89	0
29	MN	X	3153	1/1	0.89	0.09	123,123,123,123	0
29	MN	X	3019	1/1	0.89	0.32	109,109,109,109	0
29	MN	X	3124	1/1	0.89	0.13	147,147,147,147	0
33	SPD	X	3493	10/10	0.89	0.27	83,83,83,83	0
30	MG	X	3291	1/1	0.89	0.47	86,86,86,86	0
30	MG	X	3355	1/1	0.89	0.19	91,91,91,91	0
30	MG	X	3205	1/1	0.89	0.15	98,98,98,98	0
30	MG	X	3343	1/1	0.89	0.63	73,73,73,73	0
29	MN	X	3326	1/1	0.89	0.21	145,145,145,145	0
30	MG	X	3249	1/1	0.89	0.98	109,109,109,109	0
30	MG	X	3473	1/1	0.89	0.19	82,82,82,82	0
29	MN	X	3084	1/1	0.90	0.14	123,123,123,123	0
30	MG	X	3138	1/1	0.90	0.53	72,72,72,72	0
29	MN	X	3198	1/1	0.90	0.18	125,125,125,125	0
30	MG	X	3381	1/1	0.90	0.71	97,97,97,97	0
30	MG	X	3416	1/1	0.90	0.27	90,90,90,90	0
30	MG	X	3232	1/1	0.90	1.01	74,74,74,74	0
29	MN	R	201	1/1	0.90	0.28	123,123,123,123	0
30	MG	X	3486	1/1	0.90	0.60	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3147	1/1	0.90	0.11	119,119,119,119	0
29	MN	X	3465	1/1	0.90	0.24	117,117,117,117	0
29	MN	X	3117	1/1	0.90	0.26	107,107,107,107	0
30	MG	X	3207	1/1	0.90	0.28	66,66,66,66	0
30	MG	A	304	1/1	0.90	0.49	105,105,105,105	0
29	MN	X	3119	1/1	0.90	0.20	140,140,140,140	0
30	MG	X	3214	1/1	0.90	0.77	86,86,86,86	0
29	MN	X	3034	1/1	0.90	0.26	77,77,77,77	0
30	MG	Y	211	1/1	0.90	0.42	115,115,115,115	0
29	MN	X	3027	1/1	0.90	0.36	68,68,68,68	0
34	EOH	X	3500	3/3	0.90	0.34	99,99,99,99	0
29	MN	X	3073	1/1	0.90	0.36	95,95,95,95	0
30	MG	X	3443	1/1	0.91	0.24	118,118,118,118	0
29	MN	X	3453	1/1	0.91	0.33	126,126,126,126	0
29	MN	X	3184	1/1	0.91	0.13	128,128,128,128	0
30	MG	X	3448	1/1	0.91	0.65	72,72,72,72	0
30	MG	X	3268	1/1	0.91	0.36	62,62,62,62	0
30	MG	X	3304	1/1	0.91	0.46	117,117,117,117	0
30	MG	M	201	1/1	0.91	0.42	68,68,68,68	0
30	MG	O	201	1/1	0.91	0.27	51,51,51,51	0
29	MN	X	3045	1/1	0.91	0.27	96,96,96,96	0
29	MN	X	3110	1/1	0.91	0.19	117,117,117,117	0
32	MPD	X	3006	8/8	0.91	0.22	82,82,82,82	0
29	MN	X	3480	1/1	0.91	0.57	175,175,175,175	0
30	MG	X	3481	1/1	0.91	0.23	82,82,82,82	0
30	MG	X	3285	1/1	0.91	0.21	75,75,75,75	0
30	MG	X	3485	1/1	0.91	0.23	102,102,102,102	0
29	MN	A	301	1/1	0.91	0.39	138,138,138,138	0
29	MN	X	3315	1/1	0.91	0.18	104,104,104,104	0
29	MN	X	3462	1/1	0.91	0.28	152,152,152,152	0
29	MN	X	3439	1/1	0.91	0.28	94,94,94,94	0
30	MG	X	3490	1/1	0.91	0.30	100,100,100,100	0
30	MG	X	3396	1/1	0.91	0.60	108,108,108,108	0
29	MN	X	3059	1/1	0.91	0.24	111,111,111,111	0
29	MN	X	3159	1/1	0.91	0.17	118,118,118,118	0
30	MG	Y	206	1/1	0.91	0.86	104,104,104,104	0
30	MG	X	3399	1/1	0.91	0.47	79,79,79,79	0
29	MN	X	3452	1/1	0.91	0.08	120,120,120,120	0
35	EPE	N	201	15/15	0.91	0.20	73,73,73,73	0
30	MG	X	3165	1/1	0.92	0.79	84,84,84,84	0
29	MN	T	101	1/1	0.92	0.18	121,121,121,121	0
29	MN	X	3077	1/1	0.92	0.32	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3111	1/1	0.92	0.32	130,130,130,130	0
30	MG	X	3483	1/1	0.92	0.29	91,91,91,91	0
30	MG	X	3333	1/1	0.92	0.77	97,97,97,97	0
30	MG	X	3259	1/1	0.92	0.49	122,122,122,122	0
32	MPD	X	3007	8/8	0.92	0.36	132,132,132,132	0
30	MG	X	3383	1/1	0.92	0.46	75,75,75,75	0
29	MN	X	3177	1/1	0.92	0.16	125,125,125,125	0
32	MPD	X	3011	8/8	0.92	0.30	75,75,75,75	0
29	MN	X	3044	1/1	0.92	0.37	116,116,116,116	0
29	MN	X	3405	1/1	0.92	0.17	103,103,103,103	0
29	MN	X	3455	1/1	0.92	0.43	116,116,116,116	0
30	MG	X	3302	1/1	0.92	0.16	100,100,100,100	0
30	MG	X	3303	1/1	0.92	0.72	101,101,101,101	0
30	MG	Y	204	1/1	0.92	0.37	78,78,78,78	0
30	MG	X	3272	1/1	0.92	0.46	104,104,104,104	0
29	MN	X	3101	1/1	0.92	0.48	131,131,131,131	0
29	MN	X	3322	1/1	0.92	0.15	137,137,137,137	0
29	MN	X	3199	1/1	0.92	0.20	143,143,143,143	0
30	MG	X	3367	1/1	0.92	0.39	83,83,83,83	0
29	MN	X	3173	1/1	0.92	0.25	129,129,129,129	0
30	MG	X	3369	1/1	0.92	0.74	70,70,70,70	0
29	MN	X	3109	1/1	0.92	0.14	92,92,92,92	0
29	MN	X	3024	1/1	0.93	0.18	120,120,120,120	0
29	MN	X	3470	1/1	0.93	0.18	148,148,148,148	0
29	MN	X	3163	1/1	0.93	0.13	124,124,124,124	0
29	MN	X	3190	1/1	0.93	0.20	124,124,124,124	0
29	MN	X	3317	1/1	0.93	0.14	137,137,137,137	0
30	MG	X	3388	1/1	0.93	0.85	85,85,85,85	0
30	MG	X	3137	1/1	0.93	1.13	63,63,63,63	0
32	MPD	X	3009	8/8	0.93	0.39	129,129,129,129	0
29	MN	X	3104	1/1	0.93	0.14	94,94,94,94	0
29	MN	X	3157	1/1	0.93	0.24	108,108,108,108	0
30	MG	X	3434	1/1	0.93	0.21	64,64,64,64	0
29	MN	X	3321	1/1	0.93	0.07	159,159,159,159	0
29	MN	X	3122	1/1	0.93	0.23	99,99,99,99	0
30	MG	X	3258	1/1	0.93	0.26	80,80,80,80	0
30	MG	X	3292	1/1	0.93	0.36	89,89,89,89	0
29	MN	X	3243	1/1	0.93	0.18	114,114,114,114	0
29	MN	X	3071	1/1	0.93	0.21	98,98,98,98	0
29	MN	X	3161	1/1	0.93	0.23	93,93,93,93	0
30	MG	X	3373	1/1	0.93	0.33	97,97,97,97	0
30	MG	X	3297	1/1	0.93	0.19	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3353	1/1	0.93	0.17	79,79,79,79	0
34	EOH	X	3499	3/3	0.93	0.40	80,80,80,80	0
29	MN	X	3311	1/1	0.93	0.16	124,124,124,124	0
30	MG	I	201	1/1	0.93	0.57	80,80,80,80	0
30	MG	X	3415	1/1	0.93	0.24	81,81,81,81	0
30	MG	X	3274	1/1	0.94	0.34	99,99,99,99	0
29	MN	X	3037	1/1	0.94	0.26	90,90,90,90	0
29	MN	X	3149	1/1	0.94	0.26	109,109,109,109	0
30	MG	X	3390	1/1	0.94	0.56	63,63,63,63	0
30	MG	X	3427	1/1	0.94	0.15	59,59,59,59	0
29	MN	X	3082	1/1	0.94	0.20	112,112,112,112	0
29	MN	X	3125	1/1	0.94	0.13	123,123,123,123	0
29	MN	X	3318	1/1	0.94	0.08	128,128,128,128	0
30	MG	X	3501	1/1	0.94	0.83	64,64,64,64	0
30	MG	X	3366	1/1	0.94	0.66	99,99,99,99	0
30	MG	X	3142	1/1	0.94	0.51	72,72,72,72	0
30	MG	X	3309	1/1	0.94	0.34	105,105,105,105	0
29	MN	X	3193	1/1	0.94	0.09	110,110,110,110	0
29	MN	X	3115	1/1	0.94	0.32	116,116,116,116	0
29	MN	X	3237	1/1	0.94	0.07	167,167,167,167	0
29	MN	X	3179	1/1	0.94	0.12	106,106,106,106	0
29	MN	X	3041	1/1	0.94	0.18	77,77,77,77	0
29	MN	X	3094	1/1	0.94	0.14	124,124,124,124	0
30	MG	X	3450	1/1	0.94	0.75	132,132,132,132	0
30	MG	X	3239	1/1	0.94	0.39	91,91,91,91	0
30	MG	X	3240	1/1	0.94	0.67	78,78,78,78	0
29	MN	X	3264	1/1	0.94	0.12	117,117,117,117	0
29	MN	X	3047	1/1	0.94	0.26	70,70,70,70	0
30	MG	X	3301	1/1	0.94	0.19	72,72,72,72	0
29	MN	X	3192	1/1	0.95	0.09	138,138,138,138	0
29	MN	X	3036	1/1	0.95	0.30	86,86,86,86	0
29	MN	X	3464	1/1	0.95	0.56	149,149,149,149	0
29	MN	X	3017	1/1	0.95	0.08	92,92,92,92	0
30	MG	X	3247	1/1	0.95	0.52	85,85,85,85	0
30	MG	X	3432	1/1	0.95	0.24	71,71,71,71	0
29	MN	X	3404	1/1	0.95	0.15	131,131,131,131	0
29	MN	X	3197	1/1	0.95	0.26	138,138,138,138	0
30	MG	X	3384	1/1	0.95	0.26	102,102,102,102	0
30	MG	X	3438	1/1	0.95	0.20	84,84,84,84	0
29	MN	X	3407	1/1	0.95	0.20	83,83,83,83	0
30	MG	X	3299	1/1	0.95	0.22	149,149,149,149	0
29	MN	X	3418	1/1	0.95	0.13	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MG	X	3204	1/1	0.95	0.14	100,100,100,100	0
29	MN	X	3090	1/1	0.95	0.26	97,97,97,97	0
31	62B	X	3003	35/35	0.95	0.29	65,65,65,65	0
29	MN	X	3128	1/1	0.95	0.24	93,93,93,93	0
32	MPD	X	3005	8/8	0.95	0.23	78,78,78,78	0
29	MN	X	3013	1/1	0.95	0.25	70,70,70,70	0
29	MN	X	3436	1/1	0.95	0.17	119,119,119,119	0
30	MG	X	3451	1/1	0.95	0.30	115,115,115,115	0
29	MN	Y	202	1/1	0.95	0.15	105,105,105,105	0
30	MG	X	3261	1/1	0.95	0.23	91,91,91,91	0
29	MN	X	3095	1/1	0.95	0.20	79,79,79,79	0
30	MG	X	3476	1/1	0.95	0.15	64,64,64,64	0
29	MN	X	3096	1/1	0.95	0.38	100,100,100,100	0
29	MN	X	3100	1/1	0.95	0.25	96,96,96,96	0
30	MG	X	3482	1/1	0.95	0.26	90,90,90,90	0
29	MN	X	3074	1/1	0.95	0.52	113,113,113,113	0
29	MN	X	3103	1/1	0.95	0.21	85,85,85,85	0
30	MG	X	3277	1/1	0.95	0.62	97,97,97,97	0
30	MG	X	3331	1/1	0.95	0.36	86,86,86,86	0
29	MN	X	3223	1/1	0.95	0.17	119,119,119,119	0
29	MN	X	3062	1/1	0.95	0.14	87,87,87,87	0
29	MN	X	3171	1/1	0.95	0.21	114,114,114,114	0
29	MN	X	3325	1/1	0.95	0.16	187,187,187,187	0
29	MN	X	3189	1/1	0.95	0.07	154,154,154,154	0
29	MN	X	3330	1/1	0.95	0.15	104,104,104,104	0
29	MN	X	3120	1/1	0.95	0.21	166,166,166,166	0
29	MN	X	3089	1/1	0.96	0.14	113,113,113,113	0
29	MN	X	3046	1/1	0.96	0.29	91,91,91,91	0
29	MN	X	3093	1/1	0.96	0.22	81,81,81,81	0
30	MG	X	3389	1/1	0.96	0.37	94,94,94,94	0
30	MG	X	3442	1/1	0.96	0.16	71,71,71,71	0
29	MN	X	3068	1/1	0.96	0.35	94,94,94,94	0
30	MG	X	3218	1/1	0.96	0.18	75,75,75,75	0
29	MN	X	3070	1/1	0.96	0.33	129,129,129,129	0
29	MN	X	3021	1/1	0.96	0.21	91,91,91,91	0
29	MN	X	3097	1/1	0.96	0.26	109,109,109,109	0
30	MG	X	3227	1/1	0.96	0.71	95,95,95,95	0
29	MN	X	3220	1/1	0.96	0.08	103,103,103,103	0
29	MN	X	3049	1/1	0.96	0.30	93,93,93,93	0
29	MN	X	3052	1/1	0.96	0.31	90,90,90,90	0
30	MG	X	3278	1/1	0.96	0.23	82,82,82,82	0
29	MN	X	3102	1/1	0.96	0.56	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3054	1/1	0.96	0.35	97,97,97,97	0
29	MN	X	3160	1/1	0.96	0.15	100,100,100,100	0
30	MG	X	3284	1/1	0.96	0.17	72,72,72,72	0
29	MN	X	3029	1/1	0.96	0.39	69,69,69,69	0
29	MN	X	3131	1/1	0.96	0.23	126,126,126,126	0
29	MN	X	3392	1/1	0.96	0.11	89,89,89,89	0
30	MG	X	3141	1/1	0.96	0.24	85,85,85,85	0
30	MG	X	3289	1/1	0.96	0.24	110,110,110,110	0
29	MN	X	3401	1/1	0.96	0.13	104,104,104,104	0
30	MG	X	3143	1/1	0.96	0.44	59,59,59,59	0
29	MN	X	3081	1/1	0.96	0.28	109,109,109,109	0
29	MN	X	3135	1/1	0.96	0.15	115,115,115,115	0
29	MN	X	3312	1/1	0.96	0.26	115,115,115,115	0
29	MN	X	3313	1/1	0.96	0.10	117,117,117,117	0
30	MG	X	3431	1/1	0.96	0.38	55,55,55,55	0
29	MN	X	3015	1/1	0.96	0.09	80,80,80,80	0
29	MN	X	3140	1/1	0.96	0.12	105,105,105,105	0
29	MN	X	3016	1/1	0.96	0.12	75,75,75,75	0
30	MG	Y	209	1/1	0.96	0.91	153,153,153,153	0
29	MN	X	3134	1/1	0.97	0.17	121,121,121,121	0
29	MN	X	3020	1/1	0.97	0.28	107,107,107,107	0
30	MG	X	3414	1/1	0.97	0.18	89,89,89,89	0
30	MG	Y	201	1/1	0.97	0.28	66,66,66,66	0
29	MN	X	3200	1/1	0.97	0.19	123,123,123,123	0
29	MN	X	3172	1/1	0.97	0.14	114,114,114,114	0
29	MN	X	3105	1/1	0.97	0.19	97,97,97,97	0
29	MN	X	3206	1/1	0.97	0.07	95,95,95,95	0
30	MG	X	3364	1/1	0.97	0.73	83,83,83,83	0
29	MN	X	3108	1/1	0.97	0.19	89,89,89,89	0
29	MN	X	3078	1/1	0.97	0.44	111,111,111,111	0
30	MG	X	3426	1/1	0.97	0.25	104,104,104,104	0
29	MN	X	3035	1/1	0.97	0.23	74,74,74,74	0
30	MG	C	301	1/1	0.97	0.40	64,64,64,64	0
29	MN	X	3026	1/1	0.97	0.29	66,66,66,66	0
29	MN	X	3374	1/1	0.97	0.12	104,104,104,104	0
30	MG	X	3267	1/1	0.97	0.26	72,72,72,72	0
29	MN	X	3048	1/1	0.97	0.43	93,93,93,93	0
29	MN	X	3086	1/1	0.97	0.47	92,92,92,92	0
29	MN	X	3088	1/1	0.97	0.28	101,101,101,101	0
30	MG	X	3276	1/1	0.97	0.23	67,67,67,67	0
30	MG	X	3377	1/1	0.97	0.43	121,121,121,121	0
30	MG	X	3221	1/1	0.97	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3063	1/1	0.97	0.31	70,70,70,70	0
29	MN	X	3234	1/1	0.97	0.05	144,144,144,144	0
30	MG	X	3281	1/1	0.97	0.71	113,113,113,113	0
29	MN	X	3402	1/1	0.97	0.13	108,108,108,108	0
29	MN	X	3502	1/1	0.97	0.26	88,88,88,88	0
29	MN	X	3235	1/1	0.97	0.11	155,155,155,155	0
29	MN	X	3064	1/1	0.97	0.18	84,84,84,84	0
29	MN	X	3065	1/1	0.97	0.37	97,97,97,97	0
29	MN	X	3409	1/1	0.97	0.17	87,87,87,87	0
29	MN	X	3245	1/1	0.97	0.21	129,129,129,129	0
29	MN	X	3067	1/1	0.97	0.42	104,104,104,104	0
29	MN	X	3012	1/1	0.97	0.38	79,79,79,79	0
29	MN	X	3187	1/1	0.97	0.09	137,137,137,137	0
29	MN	X	3069	1/1	0.97	0.29	103,103,103,103	0
29	MN	X	3051	1/1	0.97	0.24	97,97,97,97	0
29	MN	X	3191	1/1	0.97	0.06	138,138,138,138	0
29	MN	X	3001	1/1	0.97	0.38	97,97,97,97	0
30	MG	X	3296	1/1	0.97	0.21	45,45,45,45	0
29	MN	X	3031	1/1	0.97	0.24	68,68,68,68	0
29	MN	X	3056	1/1	0.97	0.18	88,88,88,88	0
29	MN	X	3195	1/1	0.97	0.22	139,139,139,139	0
30	MG	X	3410	1/1	0.97	0.16	95,95,95,95	0
29	MN	X	3057	1/1	0.97	0.23	68,68,68,68	0
29	MN	X	3216	1/1	0.98	0.04	94,94,94,94	0
29	MN	X	3106	1/1	0.98	0.14	100,100,100,100	0
29	MN	X	3107	1/1	0.98	0.29	73,73,73,73	0
29	MN	X	3055	1/1	0.98	0.26	86,86,86,86	0
29	MN	X	3091	1/1	0.98	0.16	92,92,92,92	0
29	MN	X	3075	1/1	0.98	0.23	71,71,71,71	0
30	MG	X	3269	1/1	0.98	0.17	132,132,132,132	0
30	MG	X	3271	1/1	0.98	0.26	92,92,92,92	0
29	MN	X	3076	1/1	0.98	0.30	90,90,90,90	0
30	MG	X	3273	1/1	0.98	0.46	124,124,124,124	0
29	MN	X	3038	1/1	0.98	0.31	106,106,106,106	0
29	MN	X	3039	1/1	0.98	0.34	79,79,79,79	0
29	MN	X	3169	1/1	0.98	0.19	107,107,107,107	0
29	MN	X	3459	1/1	0.98	0.34	161,161,161,161	0
30	MG	X	3279	1/1	0.98	0.34	67,67,67,67	0
29	MN	X	3257	1/1	0.98	0.06	93,93,93,93	0
29	MN	X	3170	1/1	0.98	0.17	104,104,104,104	0
29	MN	X	3080	1/1	0.98	0.23	78,78,78,78	0
29	MN	X	3099	1/1	0.98	0.28	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3028	1/1	0.98	0.26	53,53,53,53	0
29	MN	X	3403	1/1	0.98	0.10	114,114,114,114	0
29	MN	X	3014	1/1	0.98	0.27	53,53,53,53	0
29	MN	X	3467	1/1	0.98	0.38	72,72,72,72	0
29	MN	X	3118	1/1	0.98	0.19	65,65,65,65	0
29	MN	X	3030	1/1	0.98	0.38	69,69,69,69	0
29	MN	X	3152	1/1	0.98	0.16	75,75,75,75	0
30	MG	X	3491	1/1	0.98	0.15	86,86,86,86	0
29	MN	X	3061	1/1	0.98	0.13	92,92,92,92	0
29	MN	X	3472	1/1	0.98	0.21	110,110,110,110	0
29	MN	X	3121	1/1	0.98	0.17	104,104,104,104	0
30	MG	X	3430	1/1	0.98	0.40	74,74,74,74	0
29	MN	X	3053	1/1	0.98	0.22	58,58,58,58	0
29	MN	X	3156	1/1	0.98	0.21	77,77,77,77	0
30	MG	X	3256	1/1	0.98	0.37	69,69,69,69	0
29	MN	X	3022	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3503	1/1	0.98	0.25	68,68,68,68	0
29	MN	X	3042	1/1	0.99	0.23	74,74,74,74	0
29	MN	X	3132	1/1	0.99	0.20	104,104,104,104	0
29	MN	X	3079	1/1	0.99	0.27	58,58,58,58	0
29	MN	X	3092	1/1	0.99	0.22	90,90,90,90	0
29	MN	X	3457	1/1	0.99	0.45	135,135,135,135	0
29	MN	X	3251	1/1	0.99	0.12	81,81,81,81	0
29	MN	X	3043	1/1	0.99	0.34	81,81,81,81	0
29	MN	X	3136	1/1	0.99	0.25	55,55,55,55	0
29	MN	X	3201	1/1	0.99	0.15	88,88,88,88	0
29	MN	X	3050	1/1	0.99	0.25	98,98,98,98	0
29	MN	X	3270	1/1	0.99	0.12	110,110,110,110	0
29	MN	X	3032	1/1	0.99	0.33	64,64,64,64	0
29	MN	X	3145	1/1	0.99	0.19	69,69,69,69	0
29	MN	X	3083	1/1	0.99	0.31	73,73,73,73	0
29	MN	X	3164	1/1	0.99	0.28	111,111,111,111	0
29	MN	X	3066	1/1	0.99	0.24	80,80,80,80	0
29	MN	X	3098	1/1	0.99	0.19	92,92,92,92	0
30	MG	X	3275	1/1	0.99	0.16	71,71,71,71	0
29	MN	X	3215	1/1	0.99	0.14	87,87,87,87	0
29	MN	X	3188	1/1	0.99	0.25	114,114,114,114	0
29	MN	X	3217	1/1	0.99	0.14	86,86,86,86	0
29	MN	X	3219	1/1	0.99	0.15	85,85,85,85	0
29	MN	X	3033	1/1	0.99	0.27	78,78,78,78	0
29	MN	X	3040	1/1	0.99	0.36	81,81,81,81	0
29	MN	X	3126	1/1	0.99	0.21	74,74,74,74	0

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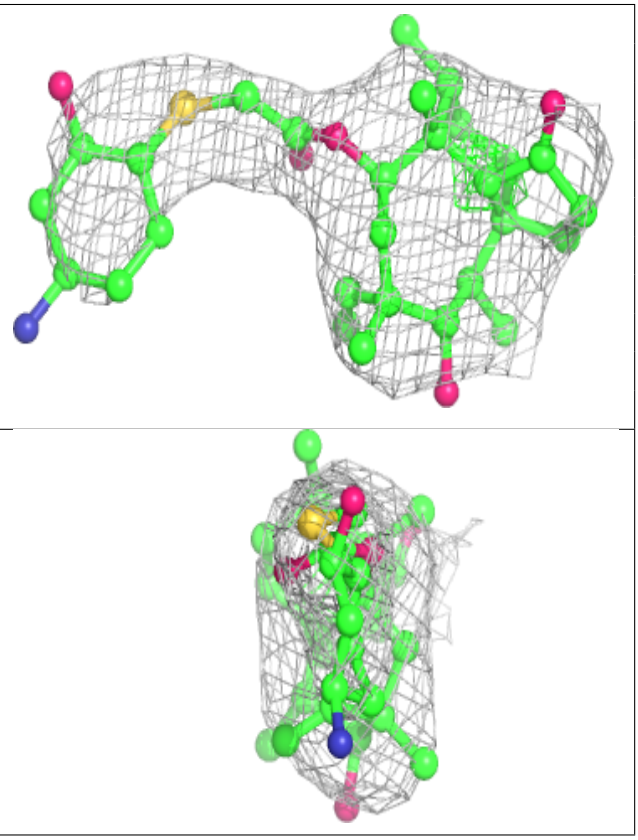
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	MN	X	3127	1/1	0.99	0.17	94,94,94,94	0
29	MN	X	3023	1/1	0.99	0.27	92,92,92,92	0
29	MN	X	3018	1/1	1.00	0.12	86,86,86,86	0
29	MN	X	3085	1/1	1.00	0.27	59,59,59,59	0

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

Electron density around 62B X 3003:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.