



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:55 AM UTC

PDB ID : 4IO9 / pdb_00004io9
Title : Crystal structure of compound 4d bound to large ribosomal subunit (50S) from *Deinococcus radiodurans*
Authors : Han, S.; Marr, E.S.
Deposited on : 2013-01-07
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

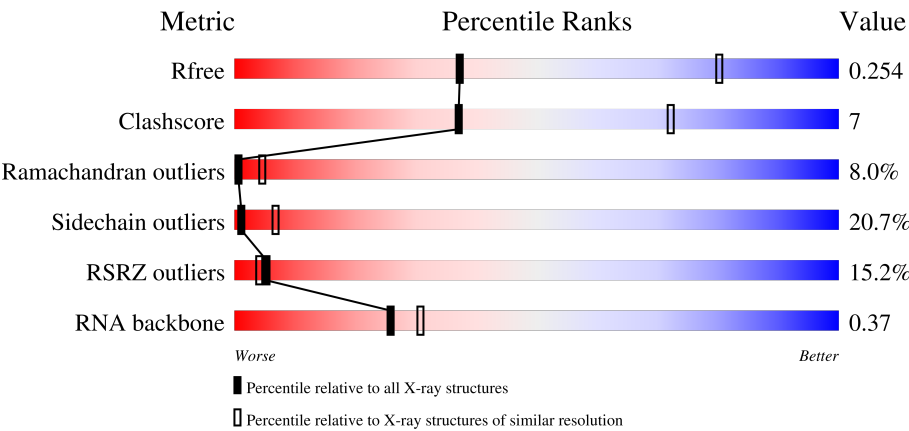
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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

Mol	Chain	Length	Quality of chain
1	X	2880	
2	Y	123	
3	A	274	
4	B	211	

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Mol	Chain	Length	Quality of chain
5	C	205	
6	D	180	
7	E	185	
8	F	144	
9	G	174	
10	H	134	
11	I	156	
12	J	141	
13	K	116	
14	L	114	
15	M	166	
16	N	118	
17	O	100	
18	P	134	
19	Q	95	
20	R	115	
21	S	237	
22	T	91	
23	U	81	
24	V	67	
25	W	55	
26	Z	60	
27	1	55	
28	2	47	
29	3	66	

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Mol	Chain	Length	Quality of chain
30	4	37	78% 73%24%

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
31	MG	X	2903	-	-	-	X
31	MG	X	2904	-	-	-	X
31	MG	X	2909	-	-	-	X
31	MG	X	2917	-	-	-	X
31	MG	X	2924	-	-	-	X
31	MG	Y	201	-	-	-	X

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 83875 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	2686	Total	C	N	O	P	0	0	0
			57651	25718	10642	18606	2685			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	122	Total	C	N	O	P	0	0	0
			2598	1161	476	840	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	0	0	0
			1826	1137	366	321	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	205	Total	C	N	O	S	0	0	0
			1539	965	295	271	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	197	Total	C	N	O	S	0	0	0
			1506	935	287	282	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	177	Total	C	N	O	S	0	0	0
			1400	892	247	254	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	171	Total	C	N	O	S	0	0	0
			1286	812	237	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	71	Total	C	N	O	S	0	0	0
			503	310	91	99	3			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	142	Total	C	N	O	S	0	0	0
			1114	704	209	198	3			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	141	Total	C	N	O	0	0	0
			1067	655	216	196			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	136	Total	C	N	O	S	0	0	0
			1090	696	202	185	7			

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	113	Total	C	N	O	S	0	0	0
			878	541	178	157	2			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	104	Total	C	N	O	0	0	0
			779	476	161	142			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	M	108	Total	C	N	O	0	0	0
			871	543	172	156			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	94	Total	C	N	O	0	0	0
			741	465	139	137			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	93	Total	C	N	O	S	0	0	0
			726	458	136	130	2			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	110	Total	C	N	O	S	0	0	0
			825	513	160	151	1			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	175	Total	C	N	O	S	0	0	0
			1345	849	236	254	6			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	84	Total	C	N	O	S	0	0	0
			625	393	122	109	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	72	Total	C	N	O		0	0	0
			552	341	116	95				

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	66	Total	C	N	O	S	0	0	0
			533	327	107	96	3			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	1	53	Total C	0	0	53
			53 53			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	2	46	Total C 46 46	0	0	46

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	3	63	Total C 63 63	0	0	63

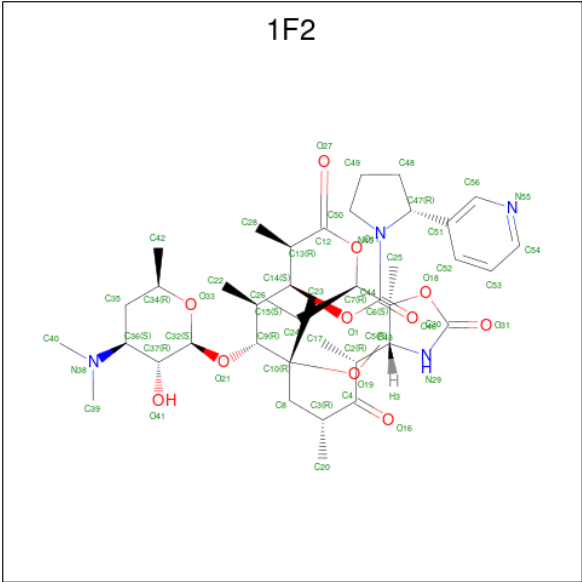
- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	4	37	Total C N O S 297 179 66 47 5	0	0	0

- Molecule 31 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	28	Total Mg 28 28	0	0
31	Y	5	Total Mg 5 5	0	0
31	J	1	Total Mg 1 1	0	0
31	M	1	Total Mg 1 1	0	0

- Molecule 32 is (3aS,4R,7R,8S,9S,10R,11R,13R,15R,15aR)-4-ethyl-11-methoxy-3a,7,9,11,13,15-hexamethyl-2,6,14-trioxo-10-{[3,4,6-trideoxy-3-(dimethylamino)-beta-D-xylo-hexopyranosyl]oxy}tetradecahydro-2H-oxacyclotetradecino[4,3-d][1,3]oxazol-8-yl (2R)-2-(pyridin-3-yl)pyrrolidine-1-carboxylate (CCD ID: 1F2) (formula: C₄₁H₆₄N₄O₁₁).

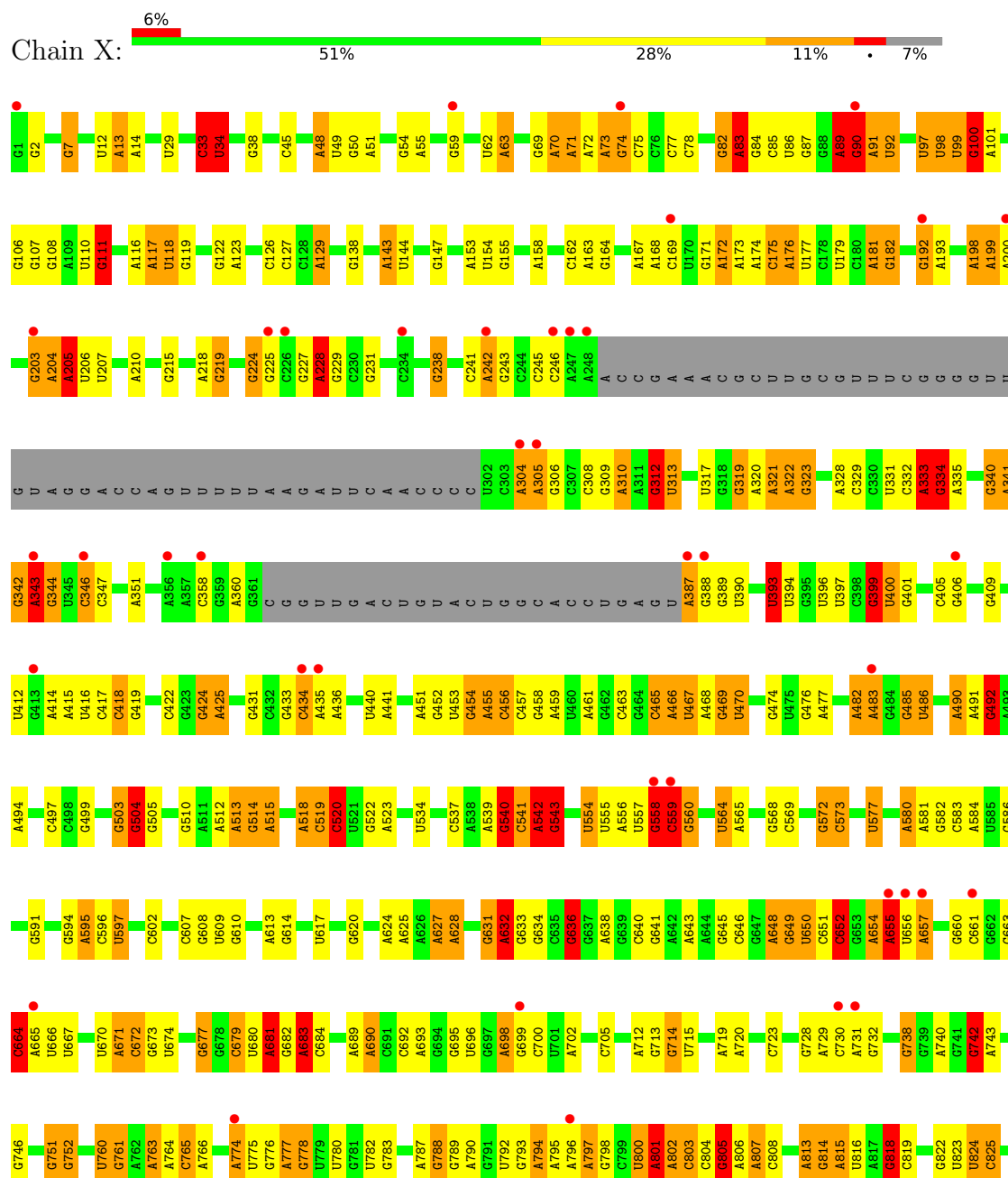


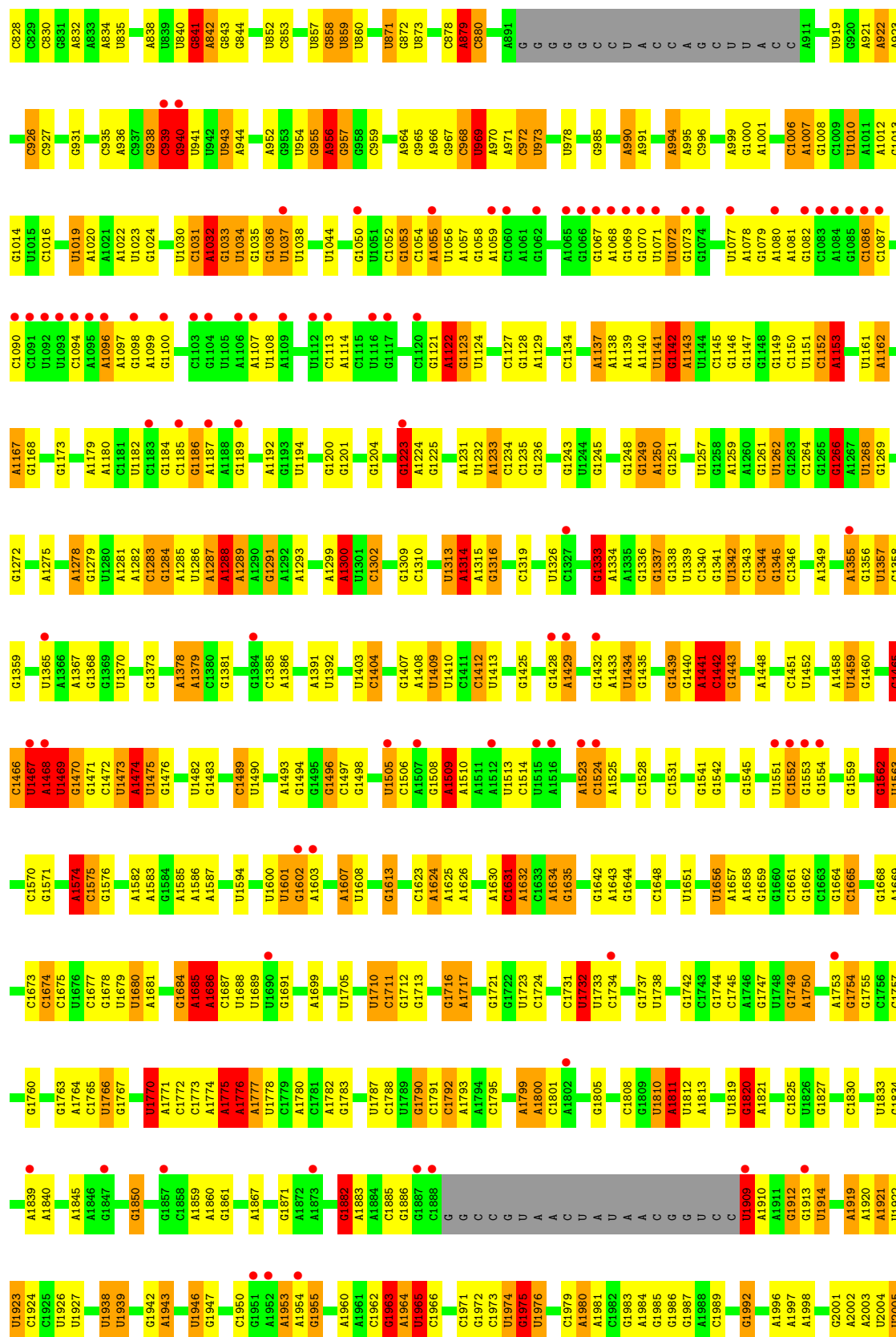
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	X	1	Total	C	N	O	0	0
			56	41	4	11		

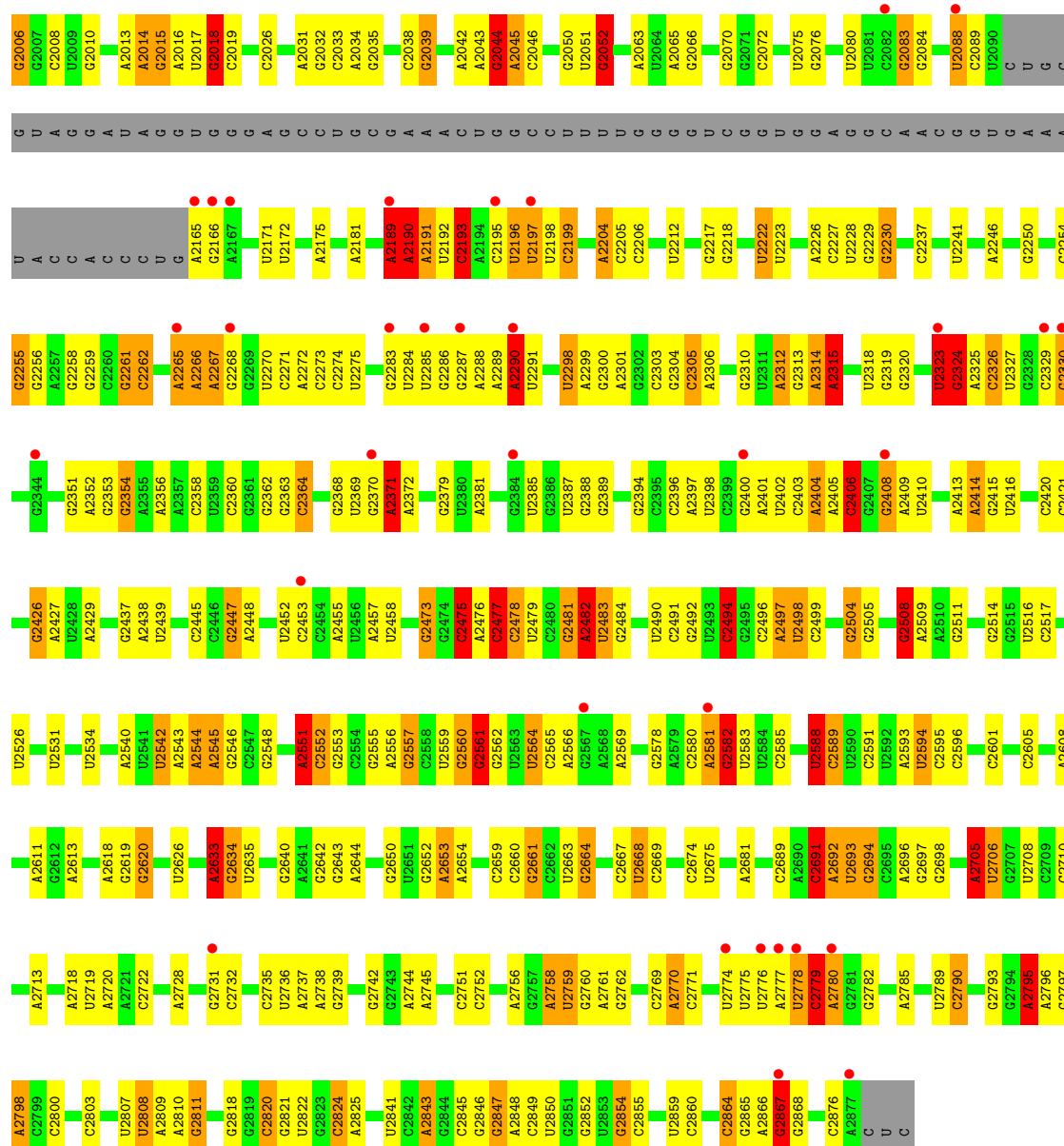
3 Residue-property plots

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

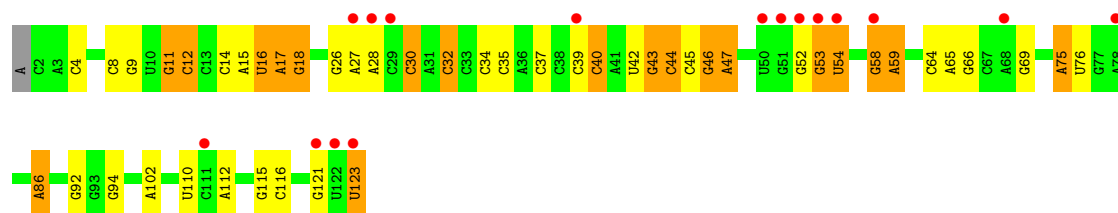
• Molecule 1: 23S ribosomal RNA





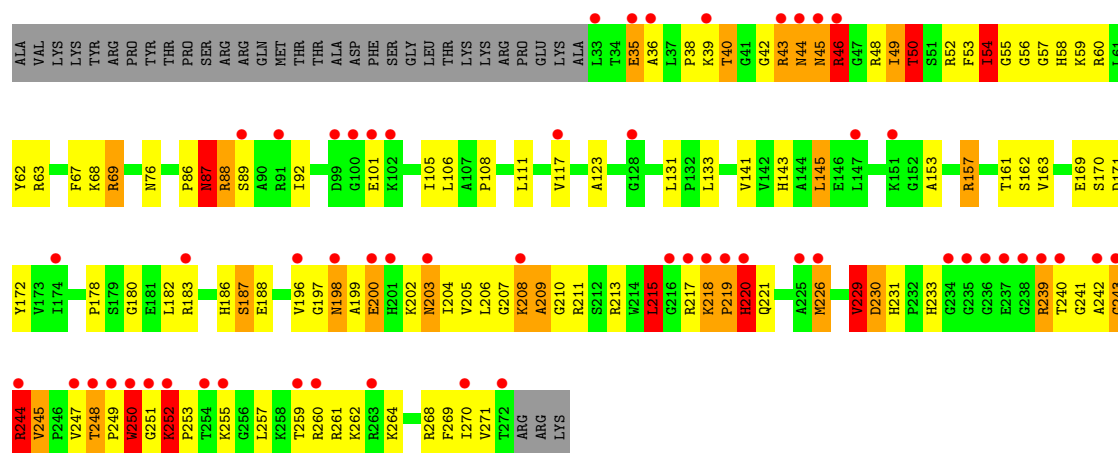


• Molecule 2: 5S ribosomal RNA

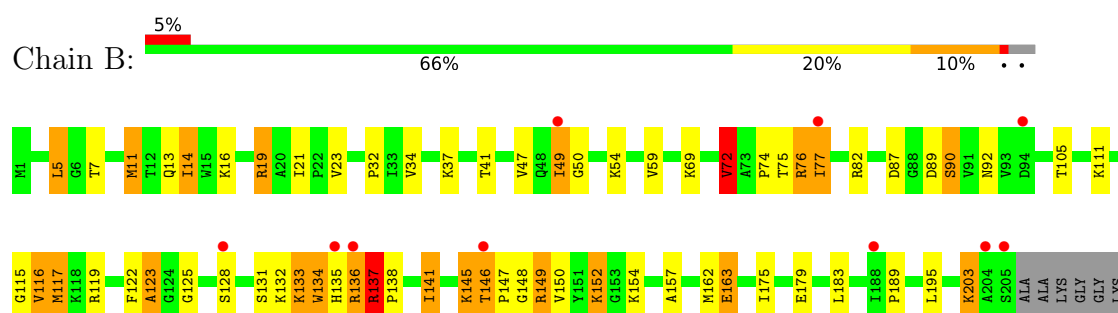


• Molecule 3: 50S ribosomal protein L2

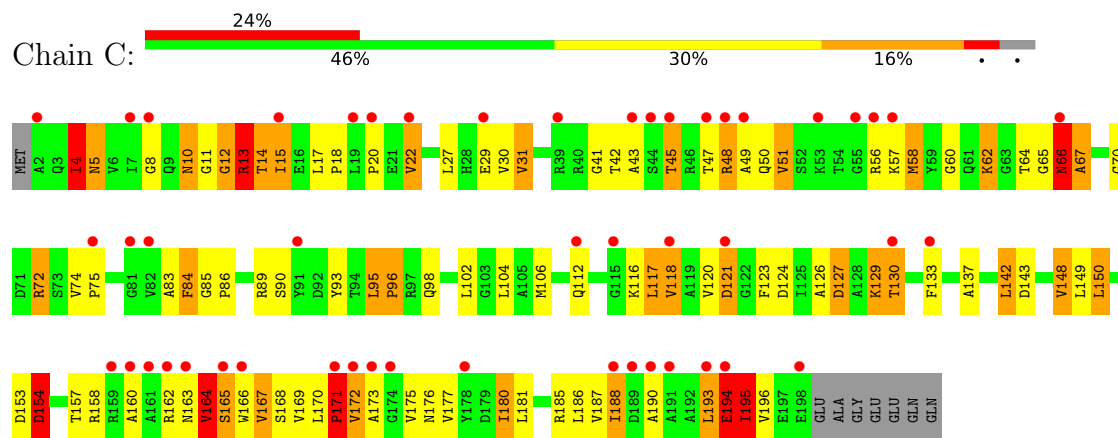




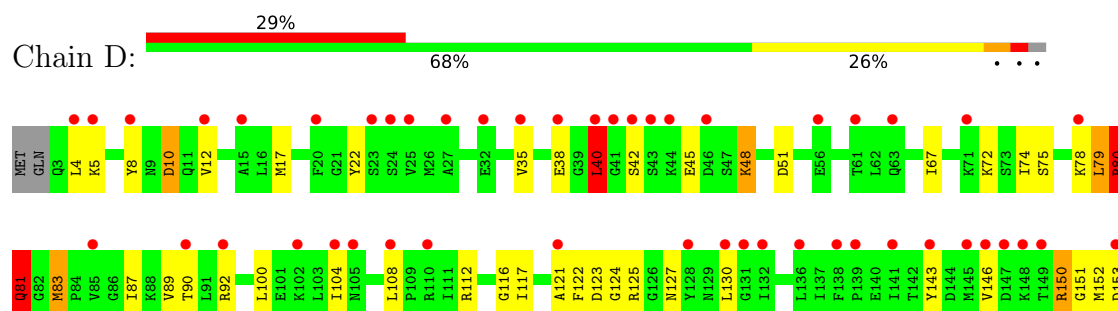
• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4

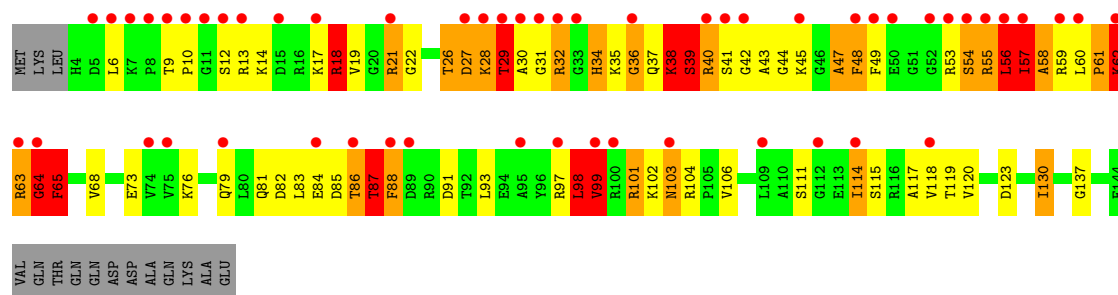


• Molecule 6: 50S ribosomal protein L5

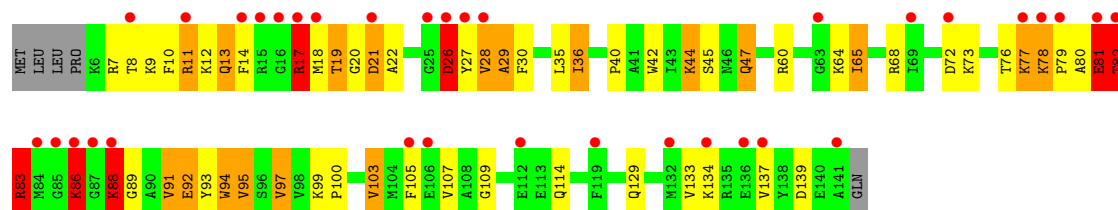




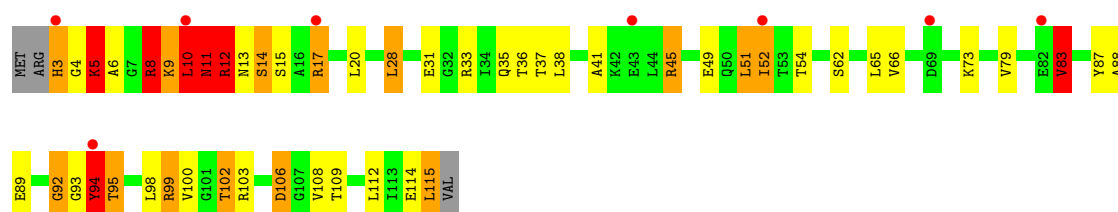
• Molecule 11: 50S ribosomal protein L15



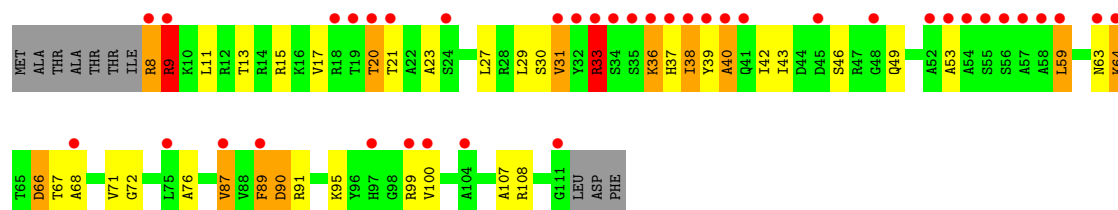
• Molecule 12: 50S ribosomal protein L16



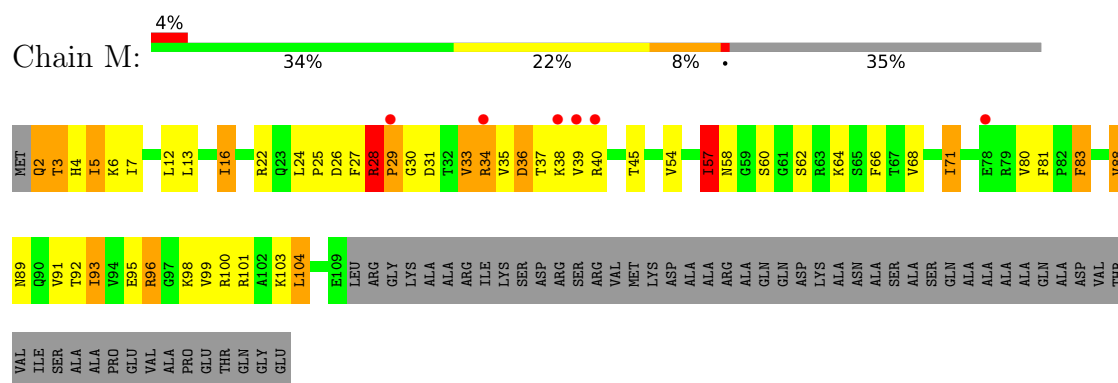
• Molecule 13: 50S ribosomal protein L17



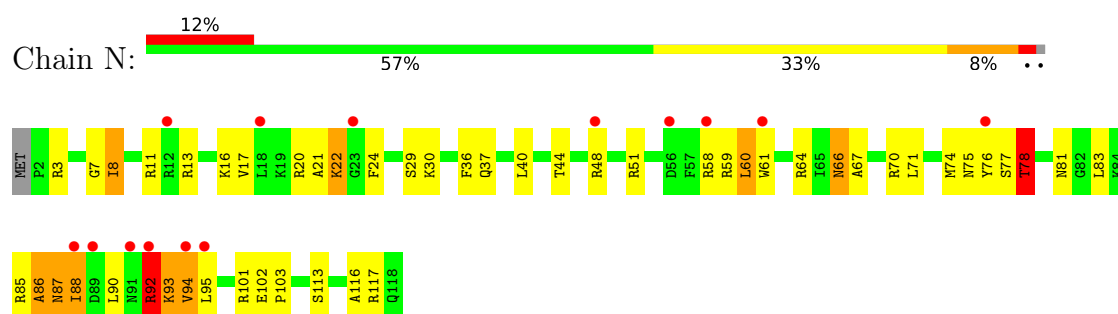
• Molecule 14: 50S ribosomal protein L18



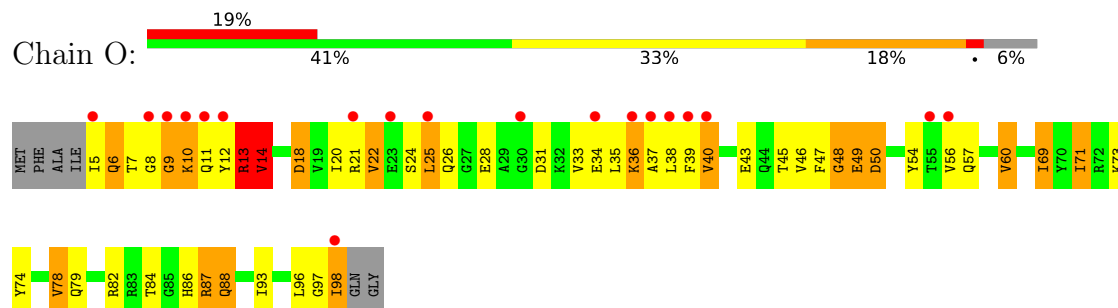
- Molecule 15: 50S ribosomal protein L19



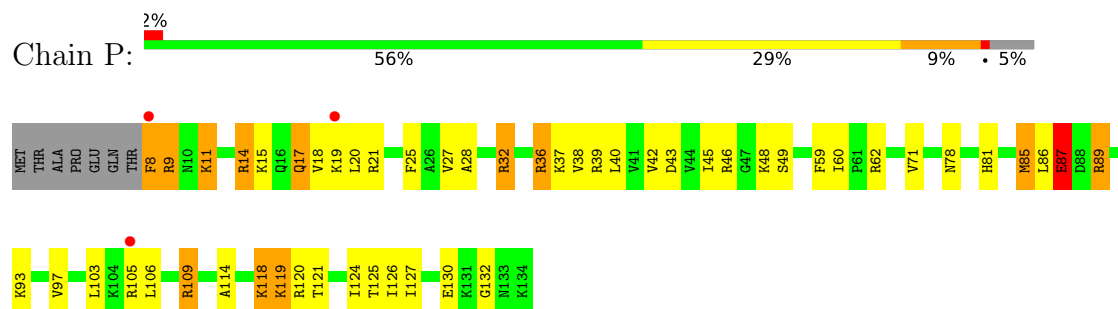
- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21

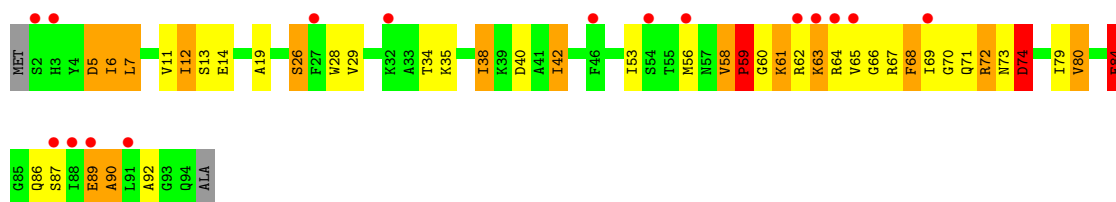


- Molecule 18: 50S ribosomal protein L22

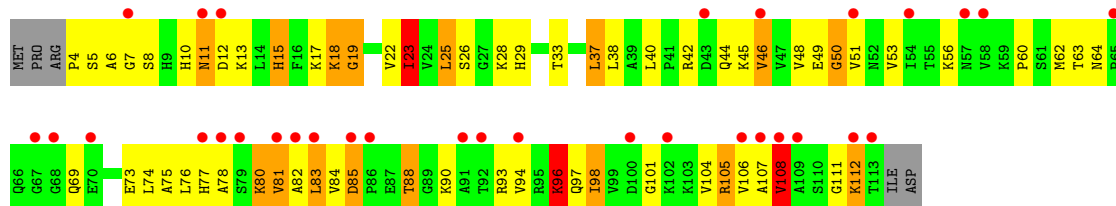


- Molecule 19: 50S ribosomal protein L23

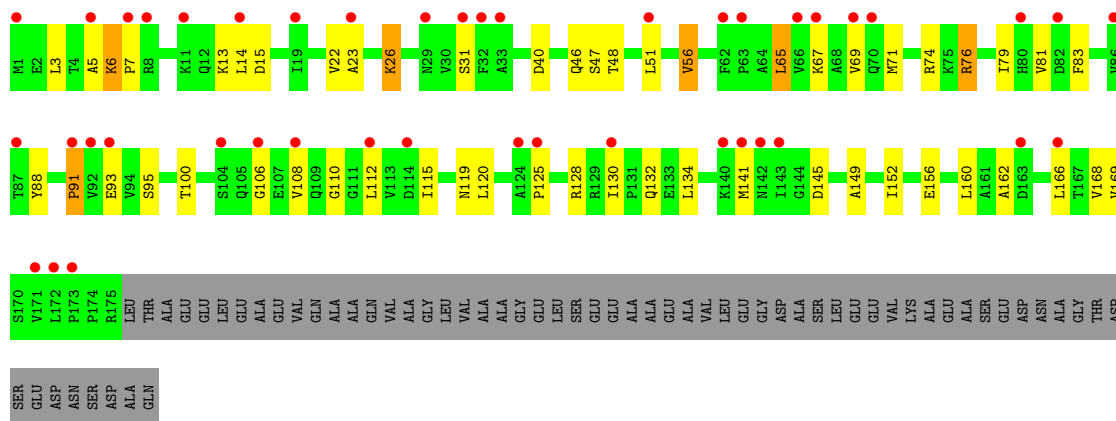




• Molecule 20: 50S ribosomal protein L24



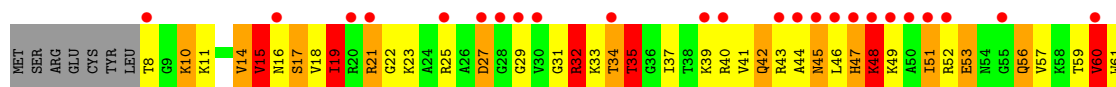
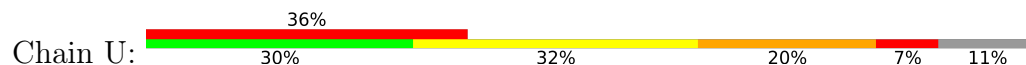
• Molecule 21: 50S ribosomal protein L25

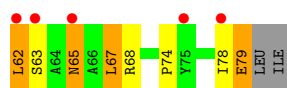


• Molecule 22: 50S ribosomal protein L27

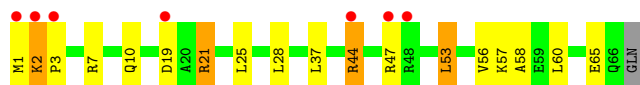


• Molecule 23: 50S ribosomal protein L28

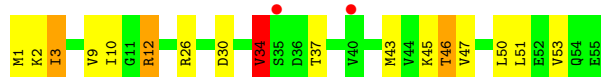




- Molecule 24: 50S ribosomal protein L29



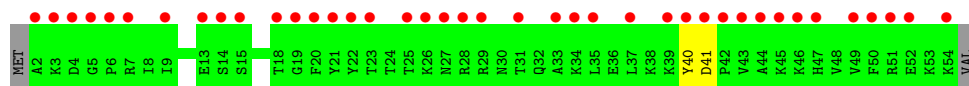
- Molecule 25: 50S ribosomal protein L30



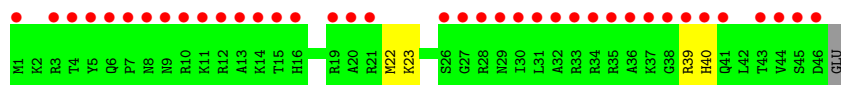
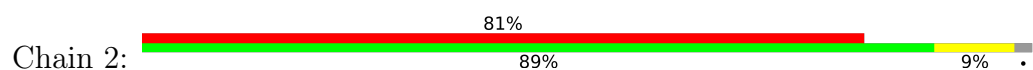
- Molecule 26: 50S ribosomal protein L32



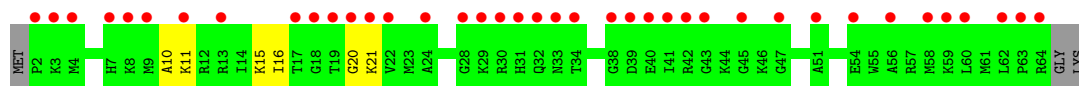
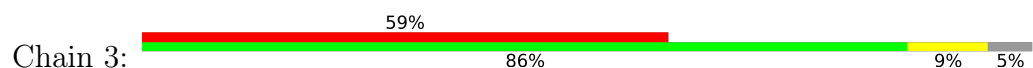
- Molecule 27: 50S ribosomal protein L33



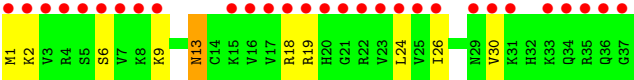
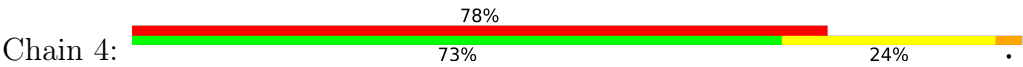
- Molecule 28: 50S ribosomal protein L34



- Molecule 29: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.94Å 409.69Å 694.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.20 30.00 – 3.21	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.20) 94.0 (30.00-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 3.24Å)	Xtriage
Refinement program	autoBUSTER	Depositor
R, R_{free}	0.199 , 0.235 0.214 , 0.254	Depositor DCC
R_{free} test set	18481 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.747	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 88.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	83875	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1F2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	X	0.69	22/64561 (0.0%)	1.39	808/100708 (0.8%)
2	Y	0.72	2/2904 (0.1%)	1.33	18/4525 (0.4%)
3	A	1.03	10/1862 (0.5%)	1.57	35/2510 (1.4%)
4	B	0.95	3/1567 (0.2%)	1.51	17/2105 (0.8%)
5	C	1.03	3/1529 (0.2%)	1.72	35/2070 (1.7%)
6	D	0.85	0/1419	1.31	3/1903 (0.2%)
7	E	0.85	0/1308	1.30	5/1771 (0.3%)
8	F	0.88	0/508	1.35	1/683 (0.1%)
9	G	0.96	2/1138 (0.2%)	1.65	19/1539 (1.2%)
10	H	0.93	0/1007	1.49	11/1352 (0.8%)
11	I	1.22	5/1081 (0.5%)	1.89	42/1448 (2.9%)
12	J	1.18	6/1113 (0.5%)	1.67	27/1486 (1.8%)
13	K	1.27	8/886 (0.9%)	1.82	28/1188 (2.4%)
14	L	0.92	0/785	1.63	10/1048 (1.0%)
15	M	1.05	3/884 (0.3%)	1.58	16/1186 (1.3%)
16	N	0.85	0/994	1.56	10/1323 (0.8%)
17	O	0.88	0/750	1.64	12/1000 (1.2%)
18	P	0.94	1/1027 (0.1%)	1.50	12/1373 (0.9%)
19	Q	0.99	2/737 (0.3%)	1.79	21/988 (2.1%)
20	R	1.11	1/835 (0.1%)	1.70	21/1121 (1.9%)
21	S	0.90	0/1370	1.37	4/1862 (0.2%)
22	T	0.94	0/633	1.42	6/838 (0.7%)
23	U	1.33	4/556 (0.7%)	1.92	21/741 (2.8%)
24	V	0.82	0/537	1.60	2/714 (0.3%)
25	W	0.85	0/426	1.50	3/568 (0.5%)
26	Z	1.04	1/469 (0.2%)	1.79	9/629 (1.4%)
30	4	0.87	0/298	1.20	0/390
All	All	0.78	73/91184 (0.1%)	1.44	1196/137069 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	0	6

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	19	THR	CA-C	11.68	1.67	1.52
13	K	52	ILE	CG1-CD1	11.10	1.95	1.51
20	R	77	HIS	CA-C	10.88	1.59	1.52
11	I	57	ILE	CG1-CD1	10.43	1.92	1.51
3	A	242	ALA	CA-C	8.22	1.63	1.52
13	K	94	TYR	CA-C	-8.21	1.43	1.53
13	K	12	ARG	CA-C	7.45	1.60	1.53
11	I	28	LYS	CA-C	7.38	1.61	1.53
4	B	136	ARG	CA-C	-7.31	1.43	1.52
11	I	29	THR	CA-C	7.10	1.62	1.52
15	M	57	ILE	CG1-CD1	7.00	1.79	1.51
13	K	3	HIS	CA-C	6.69	1.67	1.52
1	X	1467	U	C1'-N1	6.62	1.58	1.48
23	U	46	LEU	CA-C	6.58	1.61	1.52
1	X	1685	A	C3'-O3'	6.55	1.52	1.43
1	X	346	C	C1'-N1	6.54	1.58	1.48
23	U	47	HIS	C-N	6.44	1.42	1.33
15	M	33	VAL	CA-CB	6.41	1.61	1.54
1	X	1946	U	C1'-N1	6.36	1.57	1.48
3	A	54	ILE	CA-C	6.34	1.60	1.52
1	X	2189	A	C3'-O3'	6.32	1.51	1.42
15	M	29	PRO	CA-C	6.31	1.61	1.52
26	Z	53	ASP	CA-C	6.29	1.61	1.52
12	J	11	ARG	CA-C	6.26	1.61	1.52
3	A	241	GLY	C-N	6.15	1.42	1.33
11	I	28	LYS	C-N	6.07	1.42	1.33
3	A	239	ARG	CA-C	5.97	1.60	1.52
13	K	11	ASN	C-N	5.92	1.38	1.33
12	J	17	ARG	C-N	5.87	1.40	1.33
1	X	434	C	C1'-N1	5.82	1.56	1.47
1	X	661	C	C1'-N1	5.79	1.57	1.48
4	B	132	LYS	CA-C	5.79	1.60	1.52
23	U	46	LEU	C-N	5.77	1.41	1.33
1	X	559	C	C3'-O3'	5.77	1.50	1.42
1	X	646	C	C1'-N1	5.77	1.57	1.48
12	J	18	MET	C-N	5.72	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	393	U	C1'-N1	5.70	1.57	1.48
12	J	18	MET	CA-C	5.70	1.59	1.52
1	X	1909	U	C1'-N1	5.70	1.56	1.47
1	X	559	C	C1'-N1	5.67	1.56	1.48
1	X	656	U	O5'-C5'	5.64	1.50	1.42
5	C	66	ASN	C-N	5.64	1.41	1.33
1	X	2735	C	C1'-N1	5.59	1.56	1.48
3	A	242	ALA	N-CA	5.53	1.53	1.46
12	J	19	THR	N-CA	5.53	1.52	1.45
3	A	245	VAL	CA-C	5.52	1.58	1.52
3	A	35	GLU	CA-C	5.50	1.60	1.52
13	K	10	LEU	CB-CG	5.50	1.64	1.53
3	A	239	ARG	C-N	5.49	1.41	1.33
9	G	71	THR	C-N	5.46	1.38	1.33
1	X	483	A	O5'-C5'	5.44	1.50	1.42
18	P	60	ILE	C-N	5.43	1.38	1.33
3	A	215	LEU	CA-C	5.40	1.60	1.52
19	Q	71	GLN	CA-C	-5.38	1.45	1.52
1	X	927	C	C1'-N1	5.36	1.56	1.48
23	U	48	LYS	C-N	5.32	1.41	1.33
1	X	1688	U	C1'-N1	5.32	1.56	1.48
19	Q	72	ARG	CA-C	5.31	1.60	1.53
13	K	8	ARG	C-N	5.31	1.41	1.33
1	X	838	A	C3'-O3'	5.22	1.50	1.42
5	C	57	LYS	C-N	5.19	1.41	1.33
9	G	33	ILE	CA-C	5.19	1.58	1.52
2	Y	123	U	C1'-N1	5.16	1.56	1.48
5	C	57	LYS	N-CA	5.14	1.52	1.45
11	I	41	SER	CA-C	5.14	1.59	1.52
2	Y	32	C	C1'-N1	5.11	1.56	1.48
13	K	11	ASN	N-CA	5.10	1.52	1.46
3	A	46	ARG	CA-C	5.10	1.59	1.52
4	B	11	MET	SD-CE	5.09	1.92	1.79
1	X	2072	C	C1'-N1	5.09	1.56	1.48
1	X	422	C	C1'-N1	5.05	1.56	1.48
1	X	1975	G	C3'-O3'	5.04	1.50	1.43
1	X	78	C	C1'-N1	5.02	1.55	1.48

All (1196) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1631	C	C1'-O4'-C4'	-26.78	82.92	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1288	A	C1'-O4'-C4'	-26.15	83.55	109.70
1	X	1288	A	C5'-C4'-O4'	16.54	133.91	109.10
1	X	1631	C	C4'-C3'-C2'	-16.28	86.32	102.60
1	X	1019	U	P-O3'-C3'	15.34	143.21	120.20
1	X	1631	C	C5'-C4'-O4'	14.77	131.26	109.10
1	X	1975	G	C2'-C3'-O3'	14.14	130.71	109.50
1	X	2705	A	P-O3'-C3'	13.27	140.11	120.20
1	X	1963	G	P-O3'-C3'	13.05	139.78	120.20
19	Q	61	LYS	N-CA-C	13.03	129.23	111.24
1	X	1716	G	P-O3'-C3'	12.92	139.58	120.20
19	Q	60	GLY	CA-C-N	12.65	141.28	122.68
19	Q	60	GLY	C-N-CA	12.65	141.28	122.68
1	X	1775	A	P-O3'-C3'	12.63	139.15	120.20
1	X	994	A	P-O3'-C3'	12.33	138.70	120.20
1	X	788	G	P-O3'-C3'	12.23	138.55	120.20
1	X	1634	A	P-O3'-C3'	12.18	138.47	120.20
1	X	2189	A	P-O3'-C3'	12.09	138.34	120.20
1	X	1288	A	C4'-C3'-C2'	-12.04	90.56	102.60
1	X	1631	C	O4'-C4'-C3'	-12.04	94.06	106.10
1	X	1475	U	P-O3'-C3'	12.02	138.22	120.20
1	X	1473	U	P-O3'-C3'	11.78	137.87	120.20
1	X	2497	A	P-O3'-C3'	11.59	137.58	120.20
1	X	2824	C	C2'-C3'-O3'	11.44	126.67	109.50
1	X	559	C	C4'-C3'-C2'	-11.37	91.23	102.60
1	X	1288	A	O4'-C4'-C3'	-11.35	94.75	106.10
1	X	2564	U	P-O3'-C3'	11.29	137.13	120.20
1	X	1468	A	O4'-C1'-C2'	-11.07	96.53	107.60
1	X	594	G	P-O3'-C3'	11.06	136.79	120.20
1	X	2190	A	P-O5'-C5'	11.04	137.45	120.90
1	X	1631	C	C2'-C3'-O3'	10.98	125.97	109.50
1	X	1288	A	O4'-C1'-N9	10.94	124.61	108.20
1	X	399	G	P-O3'-C3'	10.88	136.53	120.20
1	X	469	G	P-O3'-C3'	10.81	136.41	120.20
3	A	211	ARG	N-CA-C	-10.75	98.29	111.40
13	K	11	ASN	CA-C-N	10.74	136.34	122.16
13	K	11	ASN	C-N-CA	10.74	136.34	122.16
1	X	1355	A	P-O3'-C3'	10.71	136.26	120.20
13	K	93	GLY	CA-C-N	-10.68	106.96	122.77
13	K	93	GLY	C-N-CA	-10.68	106.96	122.77
1	X	558	G	P-O3'-C3'	10.64	136.16	120.20
1	X	73	A	P-O3'-C3'	10.56	136.04	120.20
1	X	1249	G	P-O3'-C3'	10.56	136.03	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	Z	37	HIS	CA-C-N	10.50	129.42	122.18
26	Z	37	HIS	C-N-CA	10.50	129.42	122.18
1	X	176	A	P-O3'-C3'	10.38	135.77	120.20
1	X	204	A	P-O3'-C3'	10.36	135.74	120.20
1	X	1142	G	O4'-C1'-C2'	-10.30	95.50	105.80
1	X	469	G	C5'-C4'-C3'	-10.29	99.76	115.20
1	X	1963	G	C2'-C3'-O3'	10.22	124.83	109.50
1	X	1574	A	C4'-C3'-C2'	-10.20	92.40	102.60
1	X	1261	G	P-O3'-C3'	10.12	135.39	120.20
1	X	467	U	P-O3'-C3'	10.00	135.20	120.20
1	X	1938	U	P-O3'-C3'	9.93	135.09	120.20
1	X	1770	U	O4'-C4'-C3'	-9.88	94.12	104.00
11	I	38	LYS	CA-C-N	9.86	140.36	121.54
11	I	38	LYS	C-N-CA	9.86	140.36	121.54
1	X	2312	A	P-O3'-C3'	9.84	134.96	120.20
1	X	841	G	O4'-C4'-C3'	-9.84	94.16	104.00
1	X	2551	A	P-O3'-C3'	9.80	134.91	120.20
1	X	2018	G	P-O3'-C3'	9.80	134.90	120.20
1	X	2014	A	P-O3'-C3'	9.75	134.82	120.20
2	Y	58	G	P-O3'-C3'	9.72	134.78	120.20
1	X	181	A	P-O3'-C3'	9.70	134.75	120.20
1	X	1036	G	P-O3'-C3'	9.70	134.75	120.20
1	X	100	G	P-O3'-C3'	9.69	134.74	120.20
1	X	99	U	P-O3'-C3'	9.69	134.73	120.20
1	X	2705	A	C4'-C3'-O3'	9.67	123.91	109.40
1	X	71	A	P-O3'-C3'	9.64	134.66	120.20
1	X	1820	G	P-O3'-C3'	9.62	134.63	120.20
11	I	57	ILE	N-CA-CB	9.56	121.12	110.51
1	X	1716	G	C2'-C3'-O3'	9.52	123.79	109.50
2	Y	16	U	P-O3'-C3'	9.50	134.45	120.20
1	X	334	G	P-O3'-C3'	9.48	134.42	120.20
1	X	2088	U	P-O3'-C3'	9.45	134.37	120.20
1	X	342	G	P-O3'-C3'	9.42	134.33	120.20
1	X	1142	G	C5'-C4'-O4'	9.39	123.19	109.10
1	X	2808	U	O4'-C1'-N1	9.38	122.57	108.50
1	X	1467	U	P-O3'-C3'	-9.37	106.15	120.20
1	X	1469	U	N1-C1'-C2'	9.31	125.97	112.00
1	X	33	C	P-O3'-C3'	9.24	134.06	120.20
1	X	2769	C	C1'-O4'-C4'	-9.20	100.70	109.90
1	X	1631	C	C5'-C4'-C3'	9.16	128.94	115.20
1	X	683	A	C2'-C3'-O3'	9.12	123.18	109.50
1	X	1790	G	P-O3'-C3'	9.10	133.85	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2691	C	O3'-P-O5'	-9.09	90.37	104.00
1	X	664	C	P-O3'-C3'	9.04	133.76	120.20
1	X	204	A	C2'-C3'-O3'	9.04	123.05	109.50
1	X	841	G	N9-C1'-C2'	9.03	125.55	112.00
12	J	19	THR	N-CA-C	9.03	123.17	108.99
1	X	2298	U	P-O3'-C3'	9.03	133.74	120.20
1	X	1278	A	O4'-C1'-N9	8.94	121.61	108.20
1	X	1574	A	C1'-O4'-C4'	-8.92	100.98	109.90
23	U	18	VAL	CA-C-N	8.91	138.02	121.97
23	U	18	VAL	C-N-CA	8.91	138.02	121.97
1	X	218	A	P-O3'-C3'	8.91	133.57	120.20
1	X	2736	U	P-O3'-C3'	8.90	133.56	120.20
1	X	454	G	P-O3'-C3'	8.89	133.53	120.20
1	X	1442	C	P-O3'-C3'	8.85	133.48	120.20
1	X	1631	C	N1-C1'-C2'	8.85	127.28	114.00
1	X	788	G	C2'-C3'-O3'	8.85	122.78	109.50
1	X	714	G	O4'-C4'-C3'	-8.78	95.22	104.00
4	B	132	LYS	CA-C-N	8.75	136.59	122.67
4	B	132	LYS	C-N-CA	8.75	136.59	122.67
3	A	203	ASN	CA-CB-CG	8.75	121.35	112.60
1	X	1953	A	P-O5'-C5'	-8.68	107.87	120.90
9	G	106	TYR	N-CA-CB	8.68	122.56	109.19
1	X	2044	G	O4'-C1'-C2'	-8.66	97.14	105.80
9	G	70	PHE	CA-CB-CG	8.64	122.44	113.80
1	X	1775	A	C2'-C3'-O3'	8.62	122.44	109.50
1	X	1680	U	C2'-C3'-O3'	8.62	126.63	113.70
1	X	1984	A	P-O5'-C5'	-8.62	107.97	120.90
1	X	1923	U	C2'-C3'-O3'	8.56	122.34	109.50
1	X	63	A	C5'-C4'-C3'	-8.54	103.18	116.00
1	X	1799	A	C1'-O4'-C4'	-8.54	101.17	109.70
3	A	209	ALA	CA-C-N	-8.50	113.33	123.44
3	A	209	ALA	C-N-CA	-8.50	113.33	123.44
1	X	518	A	P-O3'-C3'	8.49	132.93	120.20
1	X	1467	U	C4'-C3'-O3'	8.49	125.73	113.00
1	X	969	U	P-O3'-C3'	8.45	132.88	120.20
1	X	1152	C	P-O3'-C3'	8.44	132.86	120.20
19	Q	62	ARG	CA-C-N	8.44	137.66	121.54
19	Q	62	ARG	C-N-CA	8.44	137.66	121.54
9	G	120	SER	N-CA-C	-8.39	103.17	113.50
1	X	504	G	C3'-C2'-O2'	8.38	123.27	110.70
1	X	814	G	P-O3'-C3'	8.38	132.76	120.20
18	P	87	GLU	N-CA-C	8.36	121.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	26	ASN	CA-C-N	8.35	137.50	121.54
10	H	26	ASN	C-N-CA	8.35	137.50	121.54
1	X	341	A	P-O3'-C3'	8.35	132.72	120.20
1	X	2261	G	P-O3'-C3'	8.34	132.72	120.20
1	X	2481	G	P-O5'-C5'	8.34	133.41	120.90
1	X	2691	C	O4'-C1'-C2'	-8.33	99.27	107.60
1	X	1122	A	P-O3'-C3'	8.29	132.64	120.20
1	X	2204	A	P-O3'-C3'	8.29	132.63	120.20
1	X	2481	G	O3'-P-O5'	-8.28	91.58	104.00
1	X	343	A	O4'-C1'-N9	8.28	120.92	108.50
1	X	683	A	P-O3'-C3'	8.25	132.58	120.20
1	X	48	A	P-O3'-C3'	8.22	132.53	120.20
1	X	1552	C	P-O3'-C3'	8.22	132.53	120.20
3	A	171	ASP	N-CA-C	-8.22	103.39	113.50
9	G	94	LYS	N-CA-C	-8.19	103.11	113.43
1	X	198	A	P-O3'-C3'	8.17	132.46	120.20
1	X	469	G	C2'-C3'-O3'	8.16	121.75	109.50
1	X	564	U	C3'-C2'-O2'	8.14	122.91	110.70
1	X	454	G	C2'-C3'-O3'	8.13	121.70	109.50
1	X	1632	A	P-O3'-C3'	8.12	132.38	120.20
1	X	1850	G	P-O3'-C3'	8.11	132.36	120.20
1	X	2018	G	C5'-C4'-O4'	-8.09	96.97	109.10
1	X	1006	C	P-O5'-C5'	8.08	133.03	120.90
1	X	1096	A	P-O3'-C3'	8.08	132.32	120.20
1	X	2551	A	O3'-P-O5'	-8.08	91.88	104.00
5	C	49	ALA	N-CA-C	-8.07	102.53	112.38
1	X	466	A	C2'-C3'-O3'	8.05	121.58	109.50
1	X	399	G	C2'-C3'-O3'	8.05	121.58	109.50
1	X	803	C	P-O3'-C3'	8.04	132.26	120.20
1	X	2770	A	P-O3'-C3'	8.02	132.24	120.20
1	X	990	A	O4'-C4'-C3'	-8.00	96.00	104.00
1	X	182	G	P-O3'-C3'	7.98	132.18	120.20
1	X	418	C	C1'-O4'-C4'	-7.98	101.92	109.90
1	X	1938	U	C4'-C3'-C2'	7.97	110.57	102.60
1	X	655	A	P-O3'-C3'	7.96	132.14	120.20
1	X	581	A	P-O3'-C3'	-7.94	108.29	120.20
1	X	1142	G	O5'-C5'-C4'	7.94	123.61	111.70
1	X	1289	A	P-O5'-C5'	7.94	132.81	120.90
1	X	1053	G	P-O3'-C3'	7.93	132.10	120.20
1	X	2593	A	O3'-P-O5'	-7.93	92.11	104.00
1	X	1923	U	P-O3'-C3'	7.92	132.09	120.20
1	X	1613	G	C1'-O4'-C4'	-7.91	101.79	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1186	G	P-O3'-C3'	7.88	132.03	120.20
1	X	638	A	P-O3'-C3'	7.88	132.02	120.20
1	X	1980	A	C4'-C3'-C2'	-7.87	94.73	102.60
1	X	1985	G	C3'-C2'-O2'	7.87	122.51	110.70
1	X	1291	G	O4'-C4'-C3'	-7.86	96.14	104.00
2	Y	92	G	O4'-C4'-C3'	-7.86	96.14	104.00
1	X	1467	U	N1-C1'-C2'	7.86	123.79	112.00
1	X	1684	G	C4'-C3'-O3'	7.85	121.18	109.40
3	A	49	ILE	N-CA-CB	7.83	119.84	111.46
1	X	1223	G	C3'-C2'-C1'	7.83	109.33	101.50
1	X	1019	U	C2'-C3'-O3'	7.80	121.19	109.50
1	X	98	U	P-O3'-C3'	7.79	131.89	120.20
1	X	242	A	C1'-O4'-C4'	-7.79	102.11	109.90
17	O	6	GLN	CA-C-N	7.78	136.41	121.54
17	O	6	GLN	C-N-CA	7.78	136.41	121.54
9	G	96	ASP	CA-CB-CG	7.78	120.38	112.60
23	U	67	LEU	N-CA-C	-7.75	102.74	112.90
10	H	70	VAL	N-CA-CB	-7.75	101.67	112.52
1	X	1153	A	P-O5'-C5'	7.74	132.51	120.90
1	X	1288	A	C3'-C2'-C1'	-7.72	93.78	101.50
1	X	343	A	P-O5'-C5'	7.72	132.48	120.90
1	X	559	C	P-O3'-C3'	7.72	131.77	120.20
2	Y	52	G	P-O5'-C5'	7.68	132.42	120.90
1	X	751	G	C2'-C3'-O3'	7.68	125.22	113.70
1	X	1710	U	P-O3'-C3'	7.67	131.71	120.20
1	X	2189	A	O3'-P-O5'	7.66	115.49	104.00
1	X	2498	U	P-O3'-C3'	7.65	131.68	120.20
11	I	35	LYS	N-CA-C	-7.65	95.49	109.56
1	X	1680	U	C3'-C2'-O2'	7.64	122.16	110.70
1	X	1249	G	C2'-C3'-O3'	7.64	120.95	109.50
12	J	10	PHE	CA-CB-CG	7.63	121.43	113.80
11	I	28	LYS	CA-C-N	7.62	136.10	121.54
11	I	28	LYS	C-N-CA	7.62	136.10	121.54
11	I	32	ARG	N-CA-C	-7.62	96.81	109.46
1	X	89	A	P-O3'-C3'	7.62	131.63	120.20
12	J	88	LYS	N-CA-C	7.62	121.80	110.52
1	X	74	G	O4'-C4'-C3'	-7.61	96.39	104.00
1	X	1333	G	O4'-C1'-N9	7.61	119.61	108.20
3	A	50	THR	CB-CA-C	7.60	121.35	109.03
1	X	1142	G	P-O3'-C3'	7.60	131.60	120.20
1	X	577	U	C4'-C3'-C2'	-7.58	95.02	102.60
1	X	1496	G	P-O3'-C3'	7.58	131.57	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	132	LYS	N-CA-C	-7.57	105.21	114.75
1	X	751	G	O4'-C4'-C3'	-7.57	96.43	104.00
1	X	672	C	O4'-C4'-C3'	-7.57	96.43	104.00
1	X	765	C	P-O3'-C3'	7.56	131.54	120.20
1	X	2795	A	P-O3'-C3'	7.55	131.52	120.20
11	I	28	LYS	N-CA-C	7.53	122.29	108.58
1	X	955	G	N9-C1'-C2'	7.50	123.25	112.00
2	Y	11	G	C1'-O4'-C4'	-7.49	102.41	109.90
1	X	2016	A	P-O3'-C3'	7.49	131.43	120.20
1	X	1523	A	P-O3'-C3'	7.48	131.41	120.20
1	X	652	C	P-O5'-C5'	-7.47	109.70	120.90
18	P	19	LYS	N-CA-C	7.45	122.09	112.92
1	X	818	G	O4'-C1'-C2'	-7.44	98.36	105.80
1	X	1811	A	P-O3'-C3'	7.44	131.35	120.20
1	X	1820	G	C4'-C3'-O3'	7.42	120.53	109.40
11	I	55	ARG	CA-C-N	7.42	135.72	121.54
11	I	55	ARG	C-N-CA	7.42	135.72	121.54
1	X	1288	A	C2'-C3'-O3'	7.41	120.62	109.50
1	X	1266	G	P-O3'-C3'	7.41	131.31	120.20
1	X	1291	G	C3'-C2'-O2'	7.40	121.80	110.70
1	X	515	A	P-O3'-C3'	7.39	131.28	120.20
1	X	2018	G	N9-C1'-C2'	7.36	125.04	114.00
1	X	1391	A	P-O3'-C3'	7.35	131.22	120.20
1	X	765	C	C4'-C3'-O3'	7.34	120.42	109.40
1	X	1055	A	P-O3'-C3'	7.34	131.21	120.20
1	X	1469	U	P-O3'-C3'	7.32	131.19	120.20
1	X	1575	C	P-O3'-C3'	7.32	131.18	120.20
1	X	2204	A	C2'-C3'-O3'	7.32	120.48	109.50
1	X	2323	U	P-O3'-C3'	7.31	131.17	120.20
20	R	28	LYS	N-CA-C	-7.31	100.69	110.55
1	X	2426	G	P-O3'-C3'	7.30	131.15	120.20
11	I	27	ASP	CA-CB-CG	7.30	119.90	112.60
1	X	1975	G	C1'-C2'-O2'	-7.29	100.86	111.80
5	C	66	ASN	CA-CB-CG	7.28	119.88	112.60
1	X	2261	G	C2'-C3'-O3'	7.27	120.40	109.50
1	X	1409	U	P-O3'-C3'	7.26	131.09	120.20
1	X	1141	U	P-O3'-C3'	7.25	131.08	120.20
1	X	2808	U	P-O5'-C5'	7.25	131.77	120.90
1	X	2560	G	C2'-C3'-O3'	7.24	120.36	109.50
1	X	2045	A	C2'-C3'-O3'	7.24	120.35	109.50
1	X	1774	A	C4'-C3'-O3'	-7.23	102.15	113.00
1	X	1574	A	O4'-C1'-N9	7.22	119.33	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1770	U	C1'-O4'-C4'	-7.20	102.70	109.90
1	X	1412	C	C3'-C2'-C1'	-7.19	94.11	101.30
10	H	120	ASP	CA-CB-CG	7.18	119.78	112.60
5	C	167	VAL	N-CA-C	7.17	120.45	109.12
1	X	1986	G	O4'-C4'-C3'	-7.17	96.83	104.00
1	X	1355	A	C2'-C3'-O3'	7.15	120.23	109.50
1	X	777	A	P-O3'-C3'	7.14	130.92	120.20
1	X	2854	G	N9-C1'-C2'	7.14	124.72	114.00
1	X	334	G	C2'-C3'-O3'	7.14	120.21	109.50
1	X	1345	G	C1'-O4'-C4'	-7.13	102.57	109.70
1	X	1439	G	C2'-C3'-O3'	7.12	124.39	113.70
1	X	1732	U	P-O3'-C3'	7.12	130.88	120.20
1	X	2564	U	C2'-C3'-O3'	7.12	120.17	109.50
1	X	2258	G	C4'-C3'-C2'	-7.09	95.51	102.60
1	X	1634	A	C4'-C3'-C2'	7.09	109.69	102.60
1	X	2705	A	C4'-C3'-C2'	7.08	109.67	102.60
1	X	1470	G	P-O5'-C5'	-7.07	110.29	120.90
1	X	1679	U	O4'-C4'-C3'	-7.07	96.93	104.00
1	X	485	G	P-O5'-C5'	7.06	131.49	120.90
1	X	1468	A	N9-C1'-C2'	7.06	122.59	112.00
1	X	1469	U	O3'-P-O5'	7.05	114.58	104.00
1	X	465	C	O3'-P-O5'	-7.05	93.43	104.00
1	X	2437	G	P-O3'-C3'	7.05	130.77	120.20
1	X	2315	A	P-O5'-C5'	7.04	131.47	120.90
23	U	51	ILE	N-CA-C	7.04	117.56	108.12
1	X	514	G	P-O3'-C3'	7.04	130.76	120.20
1	X	955	G	P-O5'-C5'	-7.04	110.34	120.90
1	X	1086	C	P-O3'-C3'	7.03	130.75	120.20
1	X	1775	A	C4'-C3'-C2'	7.03	109.63	102.60
1	X	2811	G	C3'-C2'-O2'	7.03	121.24	110.70
19	Q	73	ASN	CA-C-N	7.02	134.95	121.54
19	Q	73	ASN	C-N-CA	7.02	134.95	121.54
1	X	2719	U	P-O5'-C5'	7.01	131.42	120.90
12	J	82	THR	CA-C-N	7.01	134.93	121.54
12	J	82	THR	C-N-CA	7.01	134.93	121.54
1	X	2620	G	C4'-C3'-C2'	-7.00	95.60	102.60
1	X	580	A	P-O3'-C3'	7.00	130.70	120.20
1	X	1601	U	P-O3'-C3'	7.00	130.69	120.20
20	R	88	THR	CA-C-N	6.99	126.62	119.92
20	R	88	THR	C-N-CA	6.99	126.62	119.92
1	X	967	G	P-O5'-C5'	6.97	131.36	120.90
5	C	18	PRO	N-CA-C	6.97	122.63	111.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	9	LYS	N-CA-C	6.97	118.67	111.14
1	X	2589	C	P-O3'-C3'	6.94	130.61	120.20
11	I	48	PHE	CA-C-N	6.94	134.80	121.54
11	I	48	PHE	C-N-CA	6.94	134.80	121.54
1	X	1678	G	O4'-C4'-C3'	-6.93	97.07	104.00
1	X	2323	U	N1-C1'-C2'	6.92	124.38	114.00
5	C	194	GLU	CA-C-N	6.92	134.42	121.97
5	C	194	GLU	C-N-CA	6.92	134.42	121.97
1	X	1938	U	C2'-C3'-O3'	6.91	119.86	109.50
1	X	175	C	P-O3'-C3'	6.91	130.56	120.20
1	X	1340	C	O3'-P-O5'	-6.90	93.65	104.00
1	X	1575	C	C2'-C3'-O3'	6.90	119.84	109.50
1	X	1674	C	C5'-C4'-O4'	-6.89	99.47	109.80
5	C	171	PRO	CA-C-N	6.88	134.36	121.97
5	C	171	PRO	C-N-CA	6.88	134.36	121.97
1	X	580	A	P-O5'-C5'	-6.88	110.58	120.90
1	X	2481	G	P-O3'-C3'	6.88	130.52	120.20
3	A	242	ALA	N-CA-C	6.88	125.46	110.80
1	X	1689	U	C3'-C2'-O2'	6.88	121.02	110.70
7	E	24	PHE	CA-C-N	6.88	131.56	121.31
7	E	24	PHE	C-N-CA	6.88	131.56	121.31
1	X	1200	G	P-O5'-C5'	6.87	131.21	120.90
1	X	2229	G	C4'-C3'-O3'	-6.87	99.10	109.40
1	X	2246	A	N9-C1'-C2'	6.87	122.30	112.00
1	X	2477	C	C5'-C4'-O4'	-6.86	99.50	109.80
1	X	731	A	P-O3'-C3'	6.85	130.48	120.20
1	X	1975	G	P-O3'-C3'	6.85	130.47	120.20
1	X	2795	A	C4'-C3'-O3'	-6.85	102.73	113.00
1	X	1467	U	O4'-C1'-C2'	-6.84	100.75	107.60
1	X	2808	U	C1'-O4'-C4'	-6.84	103.06	109.90
1	X	483	A	P-O3'-C3'	-6.84	109.95	120.20
1	X	957	G	P-O3'-C3'	6.83	130.45	120.20
1	X	1980	A	O4'-C4'-C3'	-6.83	97.17	104.00
26	Z	48	ASN	N-CA-C	6.82	118.41	110.97
1	X	1142	G	C4'-C3'-O3'	-6.82	99.17	109.40
1	X	1233	A	P-O3'-C3'	6.82	130.42	120.20
1	X	308	C	P-O5'-C5'	6.81	131.11	120.90
5	C	56	ARG	N-CA-C	6.81	122.48	114.04
1	X	98	U	C2'-C3'-O3'	6.81	119.71	109.50
20	R	12	ASP	N-CA-C	-6.80	102.55	111.74
1	X	2229	G	P-O3'-C3'	6.80	130.40	120.20
1	X	554	U	P-O3'-C3'	6.77	130.36	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2032	G	P-O3'-C3'	-6.77	110.05	120.20
1	X	1820	G	C4'-C3'-C2'	6.75	109.35	102.60
1	X	440	U	O3'-P-O5'	-6.74	93.89	104.00
1	X	1792	C	N1-C1'-C2'	6.73	124.10	114.00
1	X	2032	G	O4'-C4'-C3'	-6.73	97.27	104.00
1	X	346	C	N1-C1'-C2'	6.73	122.10	112.00
1	X	1757	C	C3'-C2'-O2'	6.72	120.78	110.70
1	X	2324	G	P-O3'-C3'	6.72	130.28	120.20
1	X	1656	U	C3'-C2'-O2'	6.71	120.77	110.70
1	X	2691	C	C1'-O4'-C4'	-6.71	103.19	109.90
1	X	1289	A	O4'-C4'-C3'	-6.71	97.29	104.00
1	X	1283	C	P-O3'-C3'	6.71	130.26	120.20
20	R	77	HIS	N-CA-C	6.70	119.53	108.48
13	K	102	THR	N-CA-C	6.70	120.20	110.42
1	X	1442	C	C2'-C3'-O3'	6.70	119.55	109.50
1	X	33	C	C4'-C3'-O3'	6.69	119.44	109.40
3	A	53	PHE	CA-CB-CG	-6.69	107.11	113.80
1	X	333	A	P-O3'-C3'	6.67	130.21	120.20
1	X	2582	G	P-O5'-C5'	6.67	130.91	120.90
1	X	1716	G	C4'-C3'-C2'	6.66	109.26	102.60
1	X	1141	U	C4'-C3'-O3'	6.66	119.39	109.40
1	X	1474	A	P-O3'-C3'	6.66	130.19	120.20
1	X	466	A	C4'-C3'-O3'	6.66	119.39	109.40
1	X	518	A	N9-C1'-C2'	6.65	123.98	114.00
1	X	656	U	P-O5'-C5'	6.65	130.88	120.90
1	X	387	A	P-O3'-C3'	6.65	130.17	120.20
14	L	20	THR	CA-C-N	6.63	134.21	121.54
14	L	20	THR	C-N-CA	6.63	134.21	121.54
24	V	44	ARG	CA-C-N	6.63	129.06	120.44
24	V	44	ARG	C-N-CA	6.63	129.06	120.44
1	X	2769	C	O4'-C1'-N1	6.62	118.43	108.50
1	X	939	C	P-O3'-C3'	6.62	130.13	120.20
1	X	469	G	C4'-C3'-O3'	6.62	119.32	109.40
1	X	242	A	O4'-C1'-N9	6.61	118.42	108.50
1	X	1992	G	C3'-C2'-O2'	6.61	120.62	110.70
1	X	2255	G	C3'-C2'-O2'	6.61	120.62	110.70
2	Y	123	U	N1-C1'-C2'	6.61	121.92	112.00
1	X	176	A	N9-C1'-C2'	6.61	123.91	114.00
1	X	1473	U	C2'-C3'-O3'	6.60	119.41	109.50
1	X	825	C	P-O3'-C3'	-6.60	110.30	120.20
1	X	1685	A	C2'-C3'-O3'	6.58	119.37	109.50
1	X	2305	C	C4'-C3'-O3'	-6.58	103.13	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2692	A	O3'-P-O5'	-6.58	94.13	104.00
1	X	2043	A	P-O5'-C5'	-6.58	111.03	120.90
1	X	1412	C	C4'-C3'-O3'	6.58	122.87	113.00
11	I	61	PRO	CA-C-N	6.57	134.08	121.54
11	I	61	PRO	C-N-CA	6.57	134.08	121.54
1	X	1409	U	C1'-O4'-C4'	-6.56	103.14	109.70
1	X	172	A	P-O3'-C3'	6.56	130.04	120.20
1	X	2633	A	P-O3'-C3'	6.55	130.03	120.20
1	X	399	G	C4'-C3'-C2'	6.54	109.14	102.60
1	X	1820	G	P-O5'-C5'	6.54	130.71	120.90
1	X	33	C	O4'-C1'-N1	6.52	117.98	108.20
1	X	2669	C	O4'-C1'-C2'	-6.52	99.28	105.80
1	X	1032	A	C4'-C3'-O3'	6.51	122.77	113.00
1	X	241	C	O4'-C4'-C3'	-6.51	97.49	104.00
9	G	103	TYR	CA-C-N	6.51	133.97	121.54
9	G	103	TYR	C-N-CA	6.51	133.97	121.54
1	X	242	A	C4'-C3'-C2'	-6.51	96.09	102.60
1	X	1664	G	C2'-C3'-O3'	6.51	119.26	109.50
1	X	1938	U	P-O5'-C5'	6.50	130.66	120.90
1	X	2691	C	C5'-C4'-C3'	-6.50	106.25	116.00
1	X	1288	A	C5'-C4'-C3'	6.50	124.94	115.20
1	X	505	G	N9-C1'-C2'	6.49	121.73	112.00
10	H	22	ILE	N-CA-C	-6.49	106.67	112.12
1	X	1631	C	O5'-C5'-C4'	-6.48	101.97	111.70
1	X	1685	A	C4'-C3'-O3'	6.48	119.12	109.40
1	X	1243	G	C3'-C2'-O2'	6.48	120.42	110.70
22	T	15	ASP	CA-C-N	6.48	133.92	121.54
22	T	15	ASP	C-N-CA	6.48	133.92	121.54
2	Y	30	C	P-O5'-C5'	6.48	130.62	120.90
19	Q	56	MET	N-CA-C	6.48	119.04	108.55
1	X	1496	G	C4'-C3'-O3'	6.47	122.70	113.00
1	X	1524	C	P-O3'-C3'	6.46	129.89	120.20
1	X	2852	G	O4'-C4'-C3'	-6.46	97.54	104.00
1	X	2719	U	C3'-C2'-O2'	6.45	120.38	110.70
11	I	99	VAL	N-CA-CB	6.44	121.86	111.23
5	C	163	ASN	N-CA-C	6.42	118.85	110.43
1	X	742	G	P-O3'-C3'	6.42	129.83	120.20
1	X	608	G	O4'-C4'-C3'	-6.42	97.58	104.00
1	X	2404	A	P-O3'-C3'	6.42	129.83	120.20
1	X	661	C	C4'-C3'-C2'	-6.42	96.18	102.60
1	X	652	C	C5'-C4'-C3'	-6.41	106.38	116.00
1	X	1019	U	C4'-C3'-O3'	6.41	119.02	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2479	U	P-O3'-C3'	6.40	129.81	120.20
1	X	1278	A	C3'-C2'-C1'	-6.40	95.10	101.50
1	X	2482	A	P-O5'-C5'	6.40	130.50	120.90
11	I	48	PHE	CA-CB-CG	6.40	120.20	113.80
1	X	1669	A	O4'-C4'-C3'	-6.39	97.61	104.00
1	X	2314	A	P-O5'-C5'	6.39	130.49	120.90
1	X	1268	U	P-O5'-C5'	6.39	130.48	120.90
20	R	78	ALA	N-CA-C	-6.39	102.90	112.54
1	X	304	A	P-O5'-C5'	6.38	130.47	120.90
1	X	879	A	C5'-C4'-C3'	-6.37	106.45	116.00
1	X	2265	A	P-O3'-C3'	6.37	129.75	120.20
11	I	62	LYS	CA-C-N	6.37	132.93	121.92
11	I	62	LYS	C-N-CA	6.37	132.93	121.92
1	X	492	G	C2'-C3'-O3'	6.36	119.04	109.50
3	A	250	TRP	CA-C-N	6.36	129.14	121.38
3	A	250	TRP	C-N-CA	6.36	129.14	121.38
1	X	1496	G	C2'-C3'-O3'	6.35	123.23	113.70
1	X	610	G	O3'-P-O5'	-6.35	94.48	104.00
1	X	176	A	C2'-C3'-O3'	6.34	119.02	109.50
1	X	752	G	O3'-P-O5'	-6.34	94.48	104.00
1	X	2511	G	P-O5'-C5'	6.34	130.40	120.90
26	Z	52	TYR	CA-C-N	6.32	133.62	121.54
26	Z	52	TYR	C-N-CA	6.32	133.62	121.54
1	X	2189	A	O4'-C1'-C2'	-6.32	101.28	107.60
1	X	2559	U	C4'-C3'-O3'	-6.32	103.53	113.00
1	X	1006	C	P-O3'-C3'	6.31	129.67	120.20
1	X	2605	C	C3'-C2'-O2'	6.30	120.15	110.70
23	U	53	GLU	N-CA-C	6.30	119.84	108.69
16	N	78	THR	CB-CA-C	6.30	120.66	110.96
1	X	1349	A	P-O5'-C5'	6.29	130.34	120.90
1	X	1468	A	C3'-C2'-C1'	-6.29	95.01	101.30
1	X	1278	A	C1'-O4'-C4'	-6.29	103.41	109.70
1	X	1656	U	P-O3'-C3'	6.29	129.63	120.20
5	C	58	MET	N-CA-C	6.29	124.20	110.80
1	X	2008	C	O3'-P-O5'	-6.29	94.57	104.00
12	J	83	ARG	CA-C-N	6.29	132.75	122.07
12	J	83	ARG	C-N-CA	6.29	132.75	122.07
1	X	2847	G	N9-C1'-C2'	6.28	121.42	112.00
1	X	1153	A	O5'-C5'-C4'	6.28	121.11	111.70
21	S	46	GLN	N-CA-C	6.27	120.13	112.23
1	X	838	A	O3'-P-O5'	-6.27	94.60	104.00
25	W	34	VAL	CA-C-N	6.26	130.20	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	W	34	VAL	C-N-CA	6.26	130.20	120.75
1	X	111	G	C5'-C4'-C3'	-6.26	106.61	116.00
23	U	45	ASN	CA-CB-CG	6.25	118.85	112.60
1	X	765	C	C2'-C3'-O3'	6.25	118.88	109.50
1	X	559	C	O4'-C1'-N1	6.25	117.87	108.50
1	X	801	A	P-O3'-C3'	6.25	129.57	120.20
12	J	86	LYS	N-CA-C	6.25	118.97	110.35
1	X	558	G	N9-C1'-C2'	6.25	123.37	114.00
1	X	1468	A	P-O3'-C3'	6.24	129.55	120.20
1	X	2015	G	N9-C1'-C2'	6.23	123.35	114.00
1	X	2744	A	P-O3'-C3'	6.23	129.55	120.20
1	X	1631	C	C3'-C2'-C1'	-6.23	95.27	101.50
20	R	81	VAL	N-CA-CB	6.23	117.93	110.95
1	X	1613	G	O4'-C4'-C3'	-6.23	99.87	106.10
1	X	2854	G	P-O3'-C3'	6.22	129.53	120.20
1	X	1974	U	C3'-C2'-O2'	6.22	120.03	110.70
22	T	15	ASP	CA-CB-CG	6.22	118.82	112.60
1	X	580	A	O5'-C5'-C4'	6.21	121.02	111.70
1	X	1010	U	P-O5'-C5'	6.21	130.21	120.90
1	X	1168	G	P-O5'-C5'	6.21	130.21	120.90
5	C	64	THR	N-CA-C	-6.21	104.97	112.54
1	X	1662	G	O3'-P-O5'	-6.20	94.69	104.00
1	X	490	A	P-O3'-C3'	6.20	129.50	120.20
1	X	1200	G	C3'-C2'-O2'	6.20	120.00	110.70
1	X	2667	C	P-O3'-C3'	6.20	129.50	120.20
1	X	2504	G	C3'-C2'-O2'	6.20	119.99	110.70
1	X	1607	A	C2'-C3'-O3'	6.19	122.99	113.70
1	X	2250	G	P-O5'-C5'	6.19	130.19	120.90
1	X	1412	C	C2'-C3'-O3'	6.19	122.98	113.70
1	X	343	A	O4'-C1'-C2'	-6.18	101.42	107.60
12	J	77	LYS	N-CA-C	6.18	118.17	108.96
13	K	52	ILE	N-CA-CB	6.18	117.78	110.55
1	X	126	C	N1-C1'-C2'	6.18	121.27	112.00
13	K	83	VAL	N-CA-C	6.18	116.29	110.30
17	O	50	ASP	N-CA-C	-6.18	104.45	112.23
4	B	90	SER	N-CA-C	6.17	123.94	110.80
1	X	1248	G	O3'-P-O5'	-6.16	94.76	104.00
1	X	677	G	C4'-C3'-C2'	-6.15	96.45	102.60
1	X	764	A	N9-C1'-C2'	6.15	121.23	112.00
1	X	978	U	C3'-C2'-O2'	6.15	119.93	110.70
1	X	959	C	P-O3'-C3'	-6.15	110.98	120.20
1	X	2564	U	N1-C1'-C2'	6.14	123.22	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1509	A	C1'-O4'-C4'	-6.13	103.77	109.90
1	X	1459	U	P-O3'-C3'	6.13	129.39	120.20
1	X	83	A	P-O3'-C3'	6.12	129.38	120.20
1	X	2406	C	P-O5'-C5'	6.12	130.08	120.90
21	S	141	MET	N-CA-C	6.12	119.87	110.20
23	U	47	HIS	N-CA-C	6.12	123.84	110.80
1	X	1662	G	N9-C1'-C2'	6.12	121.17	112.00
1	X	656	U	P-O3'-C3'	6.11	129.37	120.20
3	A	44	ASN	CA-CB-CG	6.11	118.71	112.60
5	C	57	LYS	CA-C-O	-6.11	113.86	121.55
20	R	77	HIS	CA-C-N	6.09	132.42	121.15
20	R	77	HIS	C-N-CA	6.09	132.42	121.15
1	X	1412	C	O4'-C4'-C3'	-6.09	97.91	104.00
1	X	683	A	N9-C1'-C2'	6.08	123.13	114.00
1	X	814	G	N9-C1'-C2'	6.08	123.12	114.00
1	X	2790	C	P-O3'-C3'	-6.08	111.08	120.20
1	X	2497	A	O3'-P-O5'	-6.08	94.88	104.00
1	X	2566	A	C3'-C2'-O2'	6.08	119.82	110.70
19	Q	60	GLY	N-CA-C	6.08	127.58	113.18
1	X	7	G	C5'-C4'-C3'	-6.07	106.89	116.00
1	X	2653	A	O3'-P-O5'	-6.07	94.89	104.00
13	K	3	HIS	CA-CB-CG	6.07	119.87	113.80
15	M	31	ASP	N-CA-C	6.07	118.61	110.35
13	K	94	TYR	N-CA-CB	6.07	120.61	110.53
16	N	87	ASN	CA-C-N	6.07	128.43	120.60
16	N	87	ASN	C-N-CA	6.07	128.43	120.60
1	X	843	G	P-O3'-C3'	6.07	129.30	120.20
1	X	2354	G	O4'-C4'-C3'	-6.06	97.94	104.00
1	X	632	A	C4'-C3'-C2'	-6.06	96.54	102.60
11	I	26	THR	CB-CA-C	6.06	120.67	110.79
1	X	1441	A	P-O3'-C3'	6.06	129.29	120.20
1	X	1631	C	C1'-C2'-O2'	-6.06	102.72	111.80
4	B	136	ARG	N-CA-CB	6.05	118.86	109.48
1	X	63	A	C4'-C3'-C2'	6.04	108.64	102.60
9	G	119	LEU	CA-C-N	6.04	132.37	121.92
9	G	119	LEU	C-N-CA	6.04	132.37	121.92
19	Q	89	GLU	CA-C-N	6.04	133.08	121.54
19	Q	89	GLU	C-N-CA	6.04	133.08	121.54
23	U	14	VAL	CA-C-N	6.04	132.85	121.97
23	U	14	VAL	C-N-CA	6.04	132.85	121.97
1	X	2477	C	P-O5'-C5'	6.04	129.96	120.90
11	I	63	ARG	N-CA-C	-6.04	106.08	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	319	G	N9-C1'-C2'	6.03	121.05	112.00
1	X	805	G	P-O5'-C5'	6.03	129.94	120.90
1	X	2199	C	P-O5'-C5'	6.03	129.94	120.90
12	J	10	PHE	CA-C-O	-6.02	115.00	121.45
1	X	1250	A	P-O3'-C3'	6.02	129.23	120.20
1	X	1313	U	C1'-O4'-C4'	-6.02	103.68	109.70
1	X	2793	G	C3'-C2'-O2'	6.02	119.73	110.70
1	X	467	U	N1-C1'-C2'	6.01	121.02	112.00
1	X	2002	A	P-O5'-C5'	6.01	129.92	120.90
1	X	2756	A	P-O3'-C3'	6.01	129.22	120.20
25	W	34	VAL	N-CA-C	6.01	118.11	108.85
1	X	1338	G	P-O3'-C3'	6.01	129.22	120.20
1	X	1942	G	O4'-C4'-C3'	-6.01	97.99	104.00
15	M	28	ARG	N-CA-C	-6.01	96.52	109.81
1	X	2237	C	P-O3'-C3'	6.01	129.21	120.20
1	X	2429	A	P-O3'-C3'	-6.00	111.19	120.20
1	X	2447	G	P-O3'-C3'	6.00	129.21	120.20
1	X	2190	A	O4'-C1'-N9	6.00	117.50	108.50
1	X	2496	C	O3'-P-O5'	-6.00	95.00	104.00
3	A	57	GLY	N-CA-C	6.00	119.74	112.48
2	Y	26	G	P-O3'-C3'	6.00	129.19	120.20
1	X	1749	G	O4'-C1'-C2'	-5.99	99.81	105.80
1	X	1763	G	C1'-C2'-O2'	5.99	117.39	108.40
1	X	1792	C	P-O3'-C3'	5.99	129.18	120.20
1	X	1333	G	C1'-C2'-O2'	-5.99	102.82	111.80
1	X	2652	G	O5'-C5'-C4'	-5.99	102.52	111.50
1	X	1684	G	P-O3'-C3'	5.98	129.18	120.20
1	X	966	A	P-O3'-C3'	-5.97	111.24	120.20
1	X	973	U	O3'-P-O5'	-5.97	95.04	104.00
1	X	1072	U	P-O3'-C3'	5.97	129.16	120.20
1	X	465	C	P-O5'-C5'	-5.97	111.94	120.90
1	X	2803	C	P-O5'-C5'	-5.97	111.94	120.90
1	X	2478	C	P-O3'-C3'	-5.97	111.25	120.20
11	I	87	THR	CA-C-N	5.97	132.94	121.54
11	I	87	THR	C-N-CA	5.97	132.94	121.54
14	L	72	GLY	CA-C-N	5.97	128.77	120.29
14	L	72	GLY	C-N-CA	5.97	128.77	120.29
1	X	940	G	P-O5'-C5'	5.97	129.85	120.90
1	X	1971	C	C1'-C2'-O2'	5.96	117.34	108.40
1	X	1574	A	C5'-C4'-O4'	5.96	118.74	109.80
1	X	1946	U	O4'-C1'-C2'	-5.96	101.64	107.60
12	J	89	GLY	CA-C-N	5.96	128.54	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	89	GLY	C-N-CA	5.96	128.54	120.38
1	X	1607	A	P-O3'-C3'	5.96	129.13	120.20
1	X	1680	U	O4'-C4'-C3'	-5.95	98.05	104.00
20	R	23	ILE	N-CA-CB	5.95	120.39	110.86
10	H	43	ARG	N-CA-C	5.95	119.73	112.23
1	X	179	U	C3'-C2'-O2'	5.95	119.62	110.70
1	X	609	U	O4'-C4'-C3'	-5.94	98.06	104.00
1	X	2018	G	C5'-C4'-C3'	-5.94	106.29	115.20
1	X	969	U	C4'-C3'-C2'	5.93	108.53	102.60
1	X	2692	A	P-O3'-C3'	5.93	129.10	120.20
1	X	483	A	C4'-C3'-C2'	5.93	108.53	102.60
1	X	972	C	C1'-O4'-C4'	-5.93	103.77	109.70
1	X	1272	G	O4'-C4'-C3'	-5.93	98.07	104.00
1	X	1811	A	C2'-C3'-O3'	5.93	118.39	109.50
1	X	636	G	O4'-C1'-C2'	-5.93	101.67	107.60
3	A	245	VAL	N-CA-C	5.92	115.70	109.01
1	X	483	A	O5'-C5'-C4'	5.92	120.38	111.50
1	X	2698	G	C4'-C3'-C2'	-5.92	96.68	102.60
4	B	89	ASP	CA-C-N	5.91	132.84	121.54
4	B	89	ASP	C-N-CA	5.91	132.84	121.54
1	X	1259	A	O3'-P-O5'	-5.91	95.14	104.00
19	Q	68	PHE	CA-C-N	5.90	132.60	121.97
19	Q	68	PHE	C-N-CA	5.90	132.60	121.97
17	O	34	GLU	CA-C-N	5.89	128.46	120.38
17	O	34	GLU	C-N-CA	5.89	128.46	120.38
1	X	634	G	P-O5'-C5'	5.89	129.74	120.90
11	I	36	GLY	CA-C-N	5.89	132.79	121.54
11	I	36	GLY	C-N-CA	5.89	132.79	121.54
1	X	609	U	C3'-C2'-O2'	5.88	119.52	110.70
1	X	2681	A	C4'-C3'-C2'	-5.88	96.72	102.60
5	C	193	LEU	N-CA-C	-5.88	104.82	112.23
1	X	705	C	C1'-C2'-O2'	5.88	117.22	108.40
1	X	824	U	O3'-P-O5'	-5.88	95.18	104.00
20	R	101	GLY	CA-C-N	5.88	128.96	120.38
20	R	101	GLY	C-N-CA	5.88	128.96	120.38
1	X	1987	G	O5'-C5'-C4'	-5.87	102.69	111.50
1	X	2196	U	P-O3'-C3'	5.87	129.01	120.20
5	C	12	GLY	CA-C-N	5.87	132.75	121.54
5	C	12	GLY	C-N-CA	5.87	132.75	121.54
1	X	1458	A	P-O3'-C3'	5.87	129.01	120.20
1	X	344	G	N9-C1'-C2'	5.87	120.80	112.00
1	X	2588	U	C2'-C3'-O3'	5.87	118.30	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	800	U	O3'-P-O5'	-5.87	95.20	104.00
1	X	1293	A	C1'-C2'-O2'	5.87	117.20	108.40
12	J	36	ILE	N-CA-C	5.87	116.32	108.11
12	J	103	VAL	N-CA-CB	5.86	117.11	110.72
1	X	596	C	P-O5'-C5'	-5.86	112.11	120.90
1	X	469	G	O4'-C1'-C2'	-5.86	99.94	105.80
1	X	1475	U	C2'-C3'-O3'	5.86	118.29	109.50
1	X	2039	G	O4'-C1'-C2'	-5.86	101.74	107.60
1	X	1559	G	P-O3'-C3'	5.86	128.98	120.20
1	X	1668	G	P-O3'-C3'	-5.86	111.42	120.20
1	X	2193	C	O4'-C4'-C3'	-5.85	98.15	104.00
1	X	1341	G	P-O5'-C5'	5.85	129.67	120.90
1	X	1754	G	P-O5'-C5'	5.85	129.67	120.90
4	B	179	GLU	N-CA-C	-5.85	106.15	113.28
1	X	167	A	P-O5'-C5'	5.84	129.66	120.90
1	X	1992	G	C5'-C4'-O4'	-5.84	101.04	109.80
1	X	943	U	N1-C1'-C2'	5.84	120.75	112.00
1	X	1344	C	O3'-P-O5'	-5.83	95.25	104.00
1	X	991	A	N9-C1'-C2'	5.83	120.75	112.00
8	F	101	TRP	N-CA-C	5.83	118.59	111.82
1	X	1820	G	C2'-C3'-O3'	5.83	118.24	109.50
1	X	2742	G	O4'-C4'-C3'	-5.83	98.17	104.00
3	A	243	GLY	CA-C-N	5.82	132.66	121.54
3	A	243	GLY	C-N-CA	5.82	132.66	121.54
4	B	128	SER	CA-C-N	-5.82	113.43	122.05
4	B	128	SER	C-N-CA	-5.82	113.43	122.05
1	X	1036	G	C2'-C3'-O3'	5.82	118.23	109.50
1	X	690	A	C2'-C3'-O3'	-5.82	104.97	113.70
1	X	1223	G	P-O3'-C3'	5.82	128.92	120.20
1	X	2044	G	C2'-C3'-O3'	5.82	118.22	109.50
1	X	1302	C	C3'-C2'-O2'	5.81	119.42	110.70
1	X	1783	G	O4'-C4'-C3'	-5.81	98.19	104.00
1	X	1983	G	O4'-C4'-C3'	-5.80	98.19	104.00
1	X	224	G	C3'-C2'-C1'	5.80	107.10	101.30
1	X	455	A	O3'-P-O5'	-5.80	95.30	104.00
1	X	1811	A	C4'-C3'-C2'	5.80	108.40	102.60
1	X	871	U	P-O5'-C5'	5.80	129.60	120.90
1	X	1674	C	C3'-C2'-O2'	5.80	119.39	110.70
5	C	130	THR	CA-C-N	5.80	128.84	120.38
5	C	130	THR	C-N-CA	5.80	128.84	120.38
1	X	1314	A	O4'-C1'-C2'	-5.79	100.01	105.80
1	X	1439	G	P-O3'-C3'	5.79	128.88	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1261	G	C4'-C3'-O3'	-5.78	100.73	109.40
10	H	44	TYR	N-CA-C	5.78	118.83	109.40
19	Q	19	ALA	CA-C-N	5.78	128.35	120.54
19	Q	19	ALA	C-N-CA	5.78	128.35	120.54
1	X	2778	U	P-O3'-C3'	5.78	128.87	120.20
23	U	15	VAL	N-CA-CB	5.78	120.76	111.23
13	K	99	ARG	CA-C-N	5.77	127.95	120.56
13	K	99	ARG	C-N-CA	5.77	127.95	120.56
1	X	968	C	C2'-C3'-O3'	5.77	118.15	109.50
1	X	2601	C	C4'-C3'-C2'	-5.77	96.83	102.60
1	X	2323	U	P-O5'-C5'	5.77	129.55	120.90
1	X	776	G	N9-C1'-C2'	5.77	120.65	112.00
1	X	1036	G	C4'-C3'-C2'	5.76	108.36	102.60
15	M	3	THR	N-CA-C	-5.76	99.13	108.41
1	X	702	A	O3'-P-O5'	-5.76	95.36	104.00
1	X	2230	G	C3'-C2'-O2'	5.76	119.34	110.70
5	C	163	ASN	CA-C-N	5.75	132.33	121.97
5	C	163	ASN	C-N-CA	5.75	132.33	121.97
1	X	198	A	C4'-C3'-O3'	5.75	118.03	109.40
1	X	1882	G	C3'-C2'-O2'	5.75	119.33	110.70
1	X	2508	G	N9-C1'-C2'	5.75	120.63	112.00
12	J	14	PHE	CA-CB-CG	5.75	119.55	113.80
15	M	36	ASP	CA-CB-CG	5.75	118.35	112.60
15	M	103	LYS	N-CA-C	5.75	120.95	113.88
13	K	5	LYS	CA-C-N	5.75	132.52	121.54
13	K	5	LYS	C-N-CA	5.75	132.52	121.54
1	X	1339	U	C3'-C2'-O2'	5.74	119.31	110.70
1	X	2033	C	N1-C1'-C2'	5.74	120.61	112.00
1	X	679	C	C3'-C2'-O2'	5.74	119.31	110.70
1	X	1766	U	P-O5'-C5'	-5.74	112.30	120.90
1	X	2303	C	C4'-C3'-O3'	-5.74	104.40	113.00
1	X	341	A	C2'-C3'-O3'	5.73	118.10	109.50
23	U	35	THR	CB-CA-C	5.73	120.00	111.17
1	X	2854	G	P-O5'-C5'	5.72	129.49	120.90
16	N	60	LEU	CA-C-N	5.72	128.21	120.65
16	N	60	LEU	C-N-CA	5.72	128.21	120.65
17	O	14	VAL	N-CA-CB	5.72	120.67	111.23
1	X	2275	U	P-O5'-C5'	5.72	129.47	120.90
16	N	66	ASN	CA-CB-CG	5.72	118.32	112.60
1	X	740	A	N9-C1'-C2'	5.71	120.57	112.00
4	B	152	LYS	N-CA-C	-5.71	102.44	110.50
1	X	943	U	O4'-C1'-N1	5.71	117.06	108.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2759	U	P-O3'-C3'	5.70	128.75	120.20
1	X	1407	G	N9-C1'-C2'	5.70	120.55	112.00
1	X	1466	C	C4'-C3'-C2'	-5.70	96.90	102.60
1	X	1459	U	C4'-C3'-C2'	5.69	108.29	102.60
1	X	2561	G	O4'-C1'-C2'	-5.69	101.91	107.60
1	X	129	A	P-O5'-C5'	5.69	129.44	120.90
3	A	220	HIS	CA-CB-CG	5.69	119.49	113.80
1	X	520	C	O3'-P-O5'	-5.69	95.47	104.00
11	I	64	GLY	CA-C-N	5.68	132.40	121.54
11	I	64	GLY	C-N-CA	5.68	132.40	121.54
1	X	540	G	N9-C1'-C2'	5.68	122.52	114.00
1	X	1245	G	C4'-C3'-C2'	-5.68	96.92	102.60
1	X	1184	G	P-O3'-C3'	5.68	128.72	120.20
1	X	696	U	P-O5'-C5'	5.68	129.42	120.90
1	X	2561	G	C5'-C4'-O4'	-5.68	101.28	109.80
1	X	2770	A	C4'-C3'-O3'	5.68	117.91	109.40
1	X	788	G	C1'-O4'-C4'	-5.67	104.03	109.70
1	X	1496	G	C3'-C2'-C1'	-5.67	95.63	101.30
1	X	418	C	C4'-C3'-C2'	-5.67	96.93	102.60
3	A	88	ARG	CA-C-N	5.67	132.36	121.54
3	A	88	ARG	C-N-CA	5.67	132.36	121.54
1	X	1644	G	C3'-C2'-O2'	5.66	119.20	110.70
1	X	1971	C	C3'-C2'-O2'	5.66	119.19	110.70
1	X	595	A	O3'-P-O5'	-5.66	95.51	104.00
13	K	38	LEU	CA-C-N	5.66	128.66	120.79
13	K	38	LEU	C-N-CA	5.66	128.66	120.79
1	X	2779	C	N1-C1'-C2'	5.66	120.49	112.00
1	X	469	G	O4'-C1'-N9	5.65	116.68	108.20
1	X	650	U	P-O5'-C5'	5.65	129.38	120.90
1	X	70	A	O4'-C4'-C3'	5.65	109.65	104.00
1	X	607	C	O4'-C4'-C3'	-5.65	98.35	104.00
1	X	343	A	P-O3'-C3'	5.65	128.67	120.20
1	X	1468	A	O4'-C1'-N9	5.65	116.97	108.50
11	I	41	SER	CA-C-N	5.65	132.48	121.41
11	I	41	SER	C-N-CA	5.65	132.48	121.41
1	X	738	G	N9-C1'-C2'	5.64	120.46	112.00
1	X	1408	A	C4'-C3'-O3'	-5.64	104.54	113.00
13	K	8	ARG	CA-C-N	5.64	132.31	121.54
13	K	8	ARG	C-N-CA	5.64	132.31	121.54
1	X	1429	A	O4'-C1'-N9	5.64	116.66	108.20
1	X	1465	G	O5'-C5'-C4'	-5.64	103.04	111.50
1	X	70	A	P-O5'-C5'	-5.64	112.45	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	681	A	C1'-C2'-O2'	5.64	116.86	108.40
1	X	1309	G	C2'-C3'-O3'	-5.63	105.25	113.70
12	J	81	GLU	CA-C-N	5.63	132.29	121.54
12	J	81	GLU	C-N-CA	5.63	132.29	121.54
13	K	94	TYR	N-CA-C	5.63	118.50	107.57
1	X	192	G	P-O3'-C3'	5.63	128.64	120.20
1	X	2642	G	P-O5'-C5'	5.62	129.34	120.90
1	X	1031	C	P-O3'-C3'	5.62	128.63	120.20
1	X	1233	A	C2'-C3'-O3'	5.62	117.93	109.50
1	X	1150	C	P-O3'-C3'	5.62	128.63	120.20
1	X	2476	A	C2'-C3'-O3'	5.62	117.93	109.50
23	U	16	ASN	N-CA-C	5.62	118.38	110.23
23	U	68	ARG	CA-C-N	5.61	128.58	120.38
23	U	68	ARG	C-N-CA	5.61	128.58	120.38
1	X	594	G	C4'-C3'-C2'	-5.61	96.99	102.60
1	X	2473	G	C3'-C2'-O2'	5.61	119.11	110.70
1	X	2793	G	O4'-C4'-C3'	-5.60	98.40	104.00
1	X	1147	G	C3'-C2'-O2'	5.60	119.10	110.70
1	X	540	G	P-O3'-C3'	5.60	128.59	120.20
1	X	2413	A	N9-C1'-C2'	5.59	120.39	112.00
3	A	229	VAL	CA-C-N	5.59	127.78	120.28
3	A	229	VAL	C-N-CA	5.59	127.78	120.28
1	X	2330	G	P-O3'-C3'	5.59	128.59	120.20
1	X	1071	U	P-O3'-C3'	5.59	128.58	120.20
1	X	1441	A	C2'-C3'-O3'	5.59	117.88	109.50
1	X	2548	G	O4'-C1'-C2'	-5.58	102.02	107.60
10	H	109	ARG	N-CA-C	5.58	117.67	109.24
15	M	3	THR	CA-C-N	-5.58	112.22	122.31
15	M	3	THR	C-N-CA	-5.58	112.22	122.31
1	X	85	C	C3'-C2'-O2'	5.58	119.06	110.70
1	X	308	C	P-O3'-C3'	-5.57	111.84	120.20
20	R	81	VAL	CB-CA-C	5.57	117.60	111.08
1	X	558	G	C2'-C3'-O3'	5.57	117.85	109.50
1	X	1830	C	P-O3'-C3'	5.57	128.55	120.20
12	J	97	VAL	N-CA-CB	5.56	117.00	110.82
1	X	2479	U	C4'-C3'-C2'	-5.56	97.04	102.60
1	X	2691	C	O4'-C1'-N1	5.56	116.84	108.50
20	R	8	SER	CA-C-N	5.56	129.59	120.63
20	R	8	SER	C-N-CA	5.56	129.59	120.63
1	X	610	G	C3'-C2'-C1'	-5.56	95.74	101.30
1	X	199	A	P-O3'-C3'	5.56	128.54	120.20
1	X	1452	U	O3'-P-O5'	-5.56	95.67	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	47	ALA	N-CA-C	5.56	122.64	110.80
1	X	71	A	C4'-C3'-O3'	5.55	117.73	109.40
1	X	921	A	P-O3'-C3'	5.55	128.53	120.20
3	A	200	GLU	N-CA-C	5.55	118.52	108.69
1	X	853	C	C3'-C2'-C1'	-5.55	95.75	101.30
1	X	2190	A	P-O3'-C3'	5.54	128.51	120.20
2	Y	11	G	O4'-C4'-C3'	-5.54	98.46	104.00
1	X	518	A	P-O5'-C5'	5.54	129.21	120.90
1	X	824	U	C2'-C3'-O3'	5.54	117.81	109.50
2	Y	75	A	P-O3'-C3'	5.54	128.51	120.20
1	X	1137	A	P-O3'-C3'	5.54	128.50	120.20
23	U	60	VAL	N-CA-C	5.54	120.86	109.34
1	X	117	A	C1'-O4'-C4'	-5.53	104.17	109.70
1	X	1283	C	C3'-C2'-O2'	5.52	118.98	110.70
1	X	2032	G	C2'-C3'-O3'	5.52	121.99	113.70
1	X	153	A	O3'-P-O5'	-5.52	95.72	104.00
1	X	794	A	O4'-C4'-C3'	-5.52	98.48	104.00
1	X	1249	G	C4'-C3'-C2'	5.52	108.12	102.60
1	X	2421	C	P-O5'-C5'	5.52	129.18	120.90
1	X	1006	C	C5'-C4'-C3'	5.52	123.47	115.20
15	M	28	ARG	CA-C-O	-5.52	112.60	120.16
22	T	19	LYS	N-CA-C	5.52	122.55	110.80
1	X	541	C	P-O3'-C3'	5.51	128.47	120.20
1	X	1037	U	N1-C1'-C2'	5.51	120.27	112.00
1	X	2569	A	P-O5'-C5'	-5.51	112.63	120.90
1	X	2824	C	P-O3'-C3'	5.51	128.46	120.20
3	A	230	ASP	N-CA-C	5.51	117.28	111.28
1	X	1250	A	C5'-C4'-O4'	5.50	117.36	109.10
12	J	17	ARG	N-CA-C	5.50	116.77	108.46
16	N	86	ALA	N-CA-C	-5.50	103.72	110.65
1	X	90	G	N9-C1'-C2'	5.49	120.24	112.00
1	X	802	A	P-O3'-C3'	5.49	128.43	120.20
11	I	34	HIS	CA-C-N	5.49	130.74	122.67
11	I	34	HIS	C-N-CA	5.49	130.74	122.67
4	B	34	VAL	CB-CA-C	5.48	116.86	110.88
1	X	308	C	C4'-C3'-C2'	5.48	108.08	102.60
1	X	1574	A	P-O5'-C5'	5.48	129.12	120.90
1	X	1467	U	C4'-C3'-C2'	5.47	108.07	102.60
1	X	312	G	C1'-O4'-C4'	-5.47	104.23	109.70
1	X	2555	G	O4'-C4'-C3'	-5.47	98.53	104.00
16	N	59	ARG	CA-C-N	5.47	127.61	120.28
16	N	59	ARG	C-N-CA	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1664	G	N9-C1'-C2'	5.46	122.20	114.00
1	X	2051	U	C4'-C3'-O3'	-5.46	104.80	113.00
1	X	1357	U	C1'-O4'-C4'	-5.46	104.24	109.70
1	X	765	C	C4'-C3'-C2'	5.46	108.06	102.60
5	C	123	PHE	N-CA-C	-5.46	106.46	113.01
1	X	825	C	P-O5'-C5'	5.46	129.08	120.90
1	X	1489	C	P-O3'-C3'	5.45	128.38	120.20
1	X	1279	G	C3'-C2'-C1'	-5.45	96.05	101.50
13	K	98	LEU	CA-C-N	-5.44	115.53	122.77
13	K	98	LEU	C-N-CA	-5.44	115.53	122.77
1	X	2785	A	C1'-C2'-O2'	5.44	116.56	108.40
1	X	2850	U	P-O5'-C5'	5.44	129.06	120.90
5	C	67	ALA	CA-C-N	5.44	131.92	121.54
5	C	67	ALA	C-N-CA	5.44	131.92	121.54
13	K	10	LEU	N-CA-C	-5.44	101.17	109.65
1	X	2018	G	C1'-O4'-C4'	-5.43	104.27	109.70
1	X	542	A	C3'-C2'-C1'	5.43	106.93	101.50
1	X	2290	A	P-O3'-C3'	5.43	128.35	120.20
5	C	142	LEU	CA-C-N	5.43	129.87	120.58
5	C	142	LEU	C-N-CA	5.43	129.87	120.58
3	A	49	ILE	CB-CA-C	5.43	117.27	111.35
19	Q	42	ILE	N-CA-CB	5.43	117.52	110.57
1	X	2789	U	C1'-C2'-O2'	5.42	116.53	108.40
2	Y	86	A	O4'-C4'-C3'	-5.42	98.58	104.00
1	X	2843	A	P-O5'-C5'	-5.42	112.77	120.90
1	X	956	A	O3'-P-O5'	-5.41	95.88	104.00
1	X	2323	U	C1'-C2'-O2'	-5.41	103.68	111.80
1	X	1505	U	P-O3'-C3'	5.41	128.31	120.20
1	X	698	A	O3'-P-O5'	-5.41	95.89	104.00
1	X	1772	C	C4'-C3'-O3'	-5.40	101.30	109.40
1	X	2526	U	C3'-C2'-O2'	5.40	118.81	110.70
14	L	23	ALA	CA-C-N	5.40	127.79	120.44
14	L	23	ALA	C-N-CA	5.40	127.79	120.44
1	X	205	A	C4'-C3'-O3'	5.40	121.10	113.00
23	U	19	ILE	N-CA-C	5.40	120.57	109.34
1	X	2619	G	C1'-C2'-O2'	5.40	116.49	108.40
1	X	2867	G	C1'-C2'-O2'	5.40	116.49	108.40
1	X	926	C	C1'-C2'-O2'	5.39	116.49	108.40
11	I	58	ALA	N-CA-C	-5.39	103.78	110.41
1	X	1800	A	P-O3'-C3'	5.39	128.29	120.20
1	X	172	A	P-O5'-C5'	5.39	128.99	120.90
6	D	163	ASP	CA-C-N	5.39	127.82	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	163	ASP	C-N-CA	5.39	127.82	120.54
20	R	94	VAL	N-CA-C	5.39	116.14	107.73
6	D	80	ARG	N-CA-C	5.39	115.50	108.07
1	X	1575	C	C4'-C3'-O3'	5.38	117.48	109.40
1	X	1938	U	O4'-C1'-C2'	5.38	111.19	105.80
1	X	1409	U	C5'-C4'-C3'	5.38	123.27	115.20
1	X	34	U	O4'-C1'-N1	5.38	116.27	108.20
1	X	71	A	C2'-C3'-O3'	5.38	117.57	109.50
1	X	2400	G	P-O3'-C3'	5.38	128.26	120.20
1	X	2492	G	N9-C1'-C2'	5.38	120.06	112.00
1	X	2013	A	C4'-C3'-O3'	-5.37	104.94	113.00
1	X	2560	G	C5'-C4'-O4'	5.37	117.16	109.10
1	X	1300	A	C4'-C3'-O3'	-5.36	104.96	113.00
1	X	559	C	C5'-C4'-O4'	5.36	117.84	109.80
1	X	238	G	C4'-C3'-C2'	-5.36	97.24	102.60
1	X	2800	C	C5'-C4'-C3'	-5.36	107.97	116.00
1	X	2552	C	C3'-C2'-O2'	5.35	118.73	110.70
1	X	543	G	N9-C1'-C2'	5.35	120.03	112.00
1	X	2534	U	C1'-O4'-C4'	-5.35	104.55	109.90
1	X	572	G	C3'-C2'-O2'	5.35	118.72	110.70
1	X	1774	A	C3'-C2'-O2'	5.35	118.72	110.70
19	Q	59	PRO	N-CA-C	5.35	123.49	112.47
1	X	645	G	P-O3'-C3'	5.34	128.22	120.20
1	X	1665	C	P-O5'-C5'	5.34	128.91	120.90
1	X	1776	A	C4'-C3'-C2'	-5.34	97.25	102.60
1	X	2414	A	P-O3'-C3'	5.34	128.22	120.20
23	U	25	ARG	CA-C-N	5.34	129.90	120.87
23	U	25	ARG	C-N-CA	5.34	129.90	120.87
1	X	674	U	C1'-C2'-O2'	5.34	116.41	108.40
1	X	2744	A	C3'-C2'-O2'	5.34	118.71	110.70
1	X	1434	U	N1-C1'-C2'	5.34	122.01	114.00
13	K	83	VAL	N-CA-CB	5.34	116.44	110.62
1	X	1562	G	O4'-C1'-C2'	5.33	111.13	105.80
1	X	2710	C	C1'-C2'-O2'	5.33	116.40	108.40
17	O	9	GLY	CA-C-N	5.33	131.73	121.54
17	O	9	GLY	C-N-CA	5.33	131.73	121.54
1	X	2566	A	C4'-C3'-O3'	-5.33	105.00	113.00
9	G	34	PRO	CA-C-N	5.33	131.13	122.39
9	G	34	PRO	C-N-CA	5.33	131.13	122.39
1	X	1976	U	P-O5'-C5'	-5.32	112.92	120.90
1	X	2050	G	P-O3'-C3'	5.32	128.19	120.20
3	A	45	ASN	CA-C-N	5.32	131.71	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	45	ASN	C-N-CA	5.32	131.71	121.54
12	J	11	ARG	N-CA-C	5.32	122.13	110.80
26	Z	47	PRO	CA-C-N	5.32	127.67	120.65
26	Z	47	PRO	C-N-CA	5.32	127.67	120.65
1	X	2668	U	O4'-C1'-C2'	5.32	111.12	105.80
1	X	1355	A	C4'-C3'-C2'	5.32	107.92	102.60
1	X	1439	G	O4'-C4'-C3'	-5.32	98.69	104.00
1	X	1602	G	P-O3'-C3'	5.32	128.17	120.20
12	J	76	THR	N-CA-C	5.31	117.95	110.14
1	X	1248	G	C4'-C3'-O3'	-5.31	105.03	113.00
1	X	2494	C	O5'-C5'-C4'	5.31	119.47	111.50
1	X	2722	C	C3'-C2'-O2'	5.31	118.67	110.70
15	M	33	VAL	N-CA-CB	5.31	117.05	111.00
1	X	1985	G	C2'-C3'-O3'	5.31	121.66	113.70
5	C	167	VAL	CA-C-N	5.31	130.48	123.00
5	C	167	VAL	C-N-CA	5.31	130.48	123.00
1	X	537	C	P-O3'-C3'	5.31	128.16	120.20
1	X	1938	U	N1-C1'-C2'	5.31	121.96	114.00
1	X	586	G	O4'-C4'-C3'	-5.30	98.69	104.00
1	X	1412	C	P-O3'-C3'	5.30	128.16	120.20
10	H	115	ALA	CA-C-N	5.30	128.12	120.38
10	H	115	ALA	C-N-CA	5.30	128.12	120.38
20	R	112	LYS	N-CA-C	5.30	117.06	108.26
1	X	2305	C	P-O3'-C3'	5.30	128.15	120.20
1	X	2618	A	O3'-P-O5'	-5.30	96.05	104.00
5	C	195	ILE	N-CA-CB	5.30	119.98	111.23
1	X	763	A	O3'-P-O5'	-5.30	96.05	104.00
1	X	1291	G	C2'-C3'-O3'	5.30	121.64	113.70
18	P	8	PHE	CA-CB-CG	5.30	119.10	113.80
1	X	765	C	P-O5'-C5'	5.29	128.84	120.90
1	X	2820	C	C3'-C2'-O2'	5.29	118.64	110.70
1	X	938	G	C1'-C2'-O2'	-5.29	103.87	111.80
5	C	29	GLU	CB-CG-CD	5.29	121.59	112.60
11	I	31	GLY	CA-C-N	-5.29	114.74	122.19
11	I	31	GLY	C-N-CA	-5.29	114.74	122.19
1	X	59	G	P-O3'-C3'	5.28	128.12	120.20
23	U	65	ASN	CA-C-N	5.28	128.31	120.17
23	U	65	ASN	C-N-CA	5.28	128.31	120.17
22	T	14	ARG	CA-C-N	5.28	129.80	121.56
22	T	14	ARG	C-N-CA	5.28	129.80	121.56
1	X	1960	A	C3'-C2'-O2'	5.28	118.62	110.70
2	Y	53	G	N9-C1'-C2'	5.28	119.91	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1686	A	N9-C1'-C2'	5.27	119.91	112.00
1	X	792	U	P-O5'-C5'	-5.27	112.99	120.90
1	X	1357	U	P-O5'-C5'	5.27	128.81	120.90
1	X	2323	U	O4'-C1'-N1	5.27	116.11	108.20
1	X	2552	C	N1-C1'-C2'	5.27	119.91	112.00
5	C	83	ALA	CA-C-N	5.27	131.61	121.54
5	C	83	ALA	C-N-CA	5.27	131.61	121.54
5	C	96	PRO	CA-C-N	5.27	129.57	121.19
5	C	96	PRO	C-N-CA	5.27	129.57	121.19
9	G	93	LYS	N-CA-C	5.27	117.01	108.26
1	X	1882	G	C3'-C2'-C1'	5.27	106.57	101.30
1	X	2544	A	O3'-P-O5'	-5.27	96.09	104.00
1	X	2458	U	C5'-C4'-C3'	-5.27	108.10	116.00
13	K	100	VAL	N-CA-C	5.27	115.48	110.53
1	X	1790	G	C2'-C3'-O3'	5.26	117.39	109.50
1	X	2697	G	P-O3'-C3'	-5.26	112.31	120.20
1	X	813	A	P-O3'-C3'	5.26	128.09	120.20
1	X	965	G	C1'-C2'-O2'	5.26	116.29	108.40
1	X	1750	A	C3'-C2'-O2'	5.26	118.59	110.70
1	X	1162	A	C4'-C3'-C2'	-5.26	97.34	102.60
1	X	1669	A	O5'-C5'-C4'	-5.26	103.61	111.50
1	X	1469	U	C4'-C3'-O3'	-5.26	105.11	113.00
1	X	1201	G	C4'-C3'-O3'	-5.25	105.12	113.00
1	X	499	G	P-O3'-C3'	-5.25	112.33	120.20
1	X	2578	G	C1'-C2'-O2'	5.25	116.27	108.40
2	Y	12	C	O4'-C4'-C3'	-5.25	98.75	104.00
1	X	774	A	O4'-C1'-C2'	-5.25	102.36	107.60
4	B	136	ARG	N-CA-C	5.25	117.95	110.24
1	X	1634	A	O3'-P-O5'	-5.24	96.14	104.00
9	G	108	GLY	N-CA-C	-5.24	100.75	113.18
1	X	597	U	O4'-C4'-C3'	-5.24	98.76	104.00
1	X	2860	C	P-O5'-C5'	5.24	128.76	120.90
1	X	2267	A	P-O3'-C3'	5.24	128.06	120.20
17	O	18	ASP	CA-CB-CG	5.24	117.84	112.60
14	L	90	ASP	CA-CB-CG	5.24	117.83	112.60
7	E	12	PRO	CA-C-N	5.23	131.53	121.54
7	E	12	PRO	C-N-CA	5.23	131.53	121.54
4	B	19	ARG	N-CA-C	5.23	117.49	109.07
13	K	52	ILE	CB-CG1-CD1	5.23	124.78	113.80
1	X	698	A	P-O3'-C3'	5.22	128.03	120.20
1	X	1142	G	C5'-C4'-C3'	5.22	123.03	115.20
1	X	1562	G	C4'-C3'-C2'	5.22	107.82	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	2752	C	C3'-C2'-O2'	5.22	118.53	110.70
3	A	252	LYS	N-CA-C	5.22	121.35	109.81
15	M	83	PHE	CA-CB-CG	5.22	119.02	113.80
1	X	2371	A	O4'-C1'-N9	5.22	116.33	108.50
1	X	652	C	C4'-C3'-C2'	5.21	107.81	102.60
4	B	92	ASN	N-CA-C	5.21	117.70	111.71
1	X	1721	G	O4'-C4'-C3'	-5.21	98.79	104.00
1	X	2001	G	P-O5'-C5'	-5.21	113.08	120.90
26	Z	54	GLY	N-CA-C	-5.21	105.62	112.81
2	Y	54	U	O4'-C1'-N1	5.21	116.31	108.50
5	C	13	ARG	N-CA-C	5.21	121.90	110.80
1	X	859	U	C5'-C4'-O4'	5.21	116.91	109.10
1	X	456	C	C5'-C4'-O4'	-5.20	102.00	109.80
1	X	2439	U	C3'-C2'-O2'	5.20	118.50	110.70
1	X	97	U	C5'-C4'-C3'	-5.20	108.20	116.00
1	X	503	G	O4'-C4'-C3'	-5.20	98.80	104.00
1	X	573	C	C3'-C2'-O2'	5.20	118.50	110.70
1	X	1262	U	C5'-C4'-O4'	-5.19	102.01	109.80
1	X	1429	A	C1'-C2'-O2'	-5.19	104.01	111.80
1	X	1489	C	N1-C1'-C2'	5.19	119.79	112.00
1	X	2008	C	C4'-C3'-O3'	-5.19	105.21	113.00
18	P	11	LYS	CA-C-N	5.19	127.55	120.54
18	P	11	LYS	C-N-CA	5.19	127.55	120.54
11	I	41	SER	N-CA-C	5.18	121.84	110.80
1	X	13	A	P-O5'-C5'	5.18	128.67	120.90
1	X	761	G	N9-C1'-C2'	5.18	119.77	112.00
1	X	1505	U	N1-C1'-C2'	5.18	119.77	112.00
18	P	14	ARG	CA-C-N	5.18	127.74	120.28
18	P	14	ARG	C-N-CA	5.18	127.74	120.28
1	X	71	A	C4'-C3'-C2'	5.18	107.78	102.60
13	K	54	THR	CA-C-N	5.18	127.74	120.28
13	K	54	THR	C-N-CA	5.18	127.74	120.28
1	X	470	U	N1-C1'-C2'	5.18	119.76	112.00
1	X	1326	U	C3'-C2'-O2'	5.18	118.47	110.70
1	X	824	U	N1-C1'-C2'	5.17	121.76	114.00
1	X	2426	G	O3'-P-O5'	-5.17	96.24	104.00
1	X	1336	G	P-O5'-C5'	-5.17	113.14	120.90
1	X	483	A	C5'-C4'-O4'	5.17	117.56	109.80
1	X	2006	G	C2'-C3'-O3'	-5.17	105.95	113.70
3	A	180	GLY	CA-C-N	5.17	128.05	120.71
3	A	180	GLY	C-N-CA	5.17	128.05	120.71
1	X	14	A	C4'-C3'-O3'	-5.17	105.25	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	86	LEU	CA-C-N	5.17	127.97	120.79
18	P	86	LEU	C-N-CA	5.17	127.97	120.79
1	X	683	A	C4'-C3'-C2'	5.17	107.77	102.60
1	X	938	G	O4'-C1'-N9	5.16	115.94	108.20
12	J	20	GLY	CA-C-N	5.16	131.40	121.54
12	J	20	GLY	C-N-CA	5.16	131.40	121.54
9	G	110	LEU	CA-C-N	5.16	130.41	122.77
9	G	110	LEU	C-N-CA	5.16	130.41	122.77
3	A	87	ASN	CA-CB-CG	5.16	117.76	112.60
1	X	822	G	C4'-C3'-C2'	-5.16	97.44	102.60
1	X	1204	G	C3'-C2'-O2'	5.16	118.43	110.70
1	X	965	G	P-O3'-C3'	-5.15	112.47	120.20
1	X	2052	G	O5'-C5'-C4'	-5.15	103.77	111.50
10	H	36	THR	CB-CA-C	5.15	118.03	109.53
16	N	20	ARG	N-CA-C	-5.15	105.84	111.82
18	P	89	ARG	CA-C-N	5.15	128.19	120.87
18	P	89	ARG	C-N-CA	5.15	128.19	120.87
1	X	2668	U	O3'-P-O5'	-5.15	96.28	104.00
15	M	29	PRO	N-CA-C	5.15	123.08	112.47
18	P	93	LYS	N-CA-C	-5.15	105.36	110.97
1	X	317	U	O3'-P-O5'	-5.15	96.28	104.00
1	X	780	U	C3'-C2'-O2'	5.15	118.42	110.70
1	X	1677	C	C4'-C3'-C2'	-5.15	97.45	102.60
1	X	1032	A	C3'-C2'-C1'	-5.14	96.16	101.30
1	X	2758	A	C4'-C3'-O3'	-5.14	101.68	109.40
17	O	78	VAL	N-CA-CB	-5.14	105.62	112.26
9	G	129	HIS	CA-C-N	5.14	131.36	121.54
9	G	129	HIS	C-N-CA	5.14	131.36	121.54
1	X	483	A	C3'-C2'-O2'	5.14	118.41	110.70
1	X	2634	G	C1'-O4'-C4'	-5.14	104.56	109.70
11	I	40	ARG	CA-C-N	5.14	131.36	121.54
11	I	40	ARG	C-N-CA	5.14	131.36	121.54
15	M	4	HIS	N-CA-C	5.14	120.19	113.20
1	X	1300	A	N9-C1'-C2'	5.14	119.71	112.00
1	X	1404	C	C1'-O4'-C4'	-5.14	104.56	109.70
4	B	163	GLU	CB-CG-CD	5.13	121.33	112.60
1	X	2526	U	P-O5'-C5'	5.13	128.60	120.90
1	X	2416	U	N1-C1'-C2'	5.13	119.69	112.00
19	Q	73	ASN	CA-CB-CG	5.13	117.73	112.60
1	X	1037	U	C1'-O4'-C4'	-5.12	104.78	109.90
13	K	31	GLU	CB-CG-CD	5.12	121.31	112.60
1	X	838	A	OP1-P-O3'	5.12	123.37	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	139	ASP	N-CA-C	-5.12	105.11	112.13
1	X	788	G	N9-C1'-C2'	5.12	121.68	114.00
14	L	9	ARG	CA-C-N	5.12	127.66	120.28
14	L	9	ARG	C-N-CA	5.12	127.66	120.28
15	M	54	VAL	N-CA-CB	5.12	116.69	110.95
15	M	30	GLY	CA-C-N	5.12	128.48	120.75
15	M	30	GLY	C-N-CA	5.12	128.48	120.75
1	X	2689	C	O3'-P-O5'	-5.12	96.32	104.00
1	X	1965	U	P-O5'-C5'	-5.12	113.22	120.90
1	X	999	A	P-O5'-C5'	-5.11	113.23	120.90
1	X	1434	U	C1'-O4'-C4'	-5.11	104.59	109.70
1	X	763	A	P-O3'-C3'	5.11	127.86	120.20
19	Q	74	ASP	N-CA-C	5.11	121.68	110.80
1	X	1288	A	P-O3'-C3'	-5.11	112.54	120.20
1	X	1459	U	O4'-C1'-C2'	5.11	110.91	105.80
1	X	1149	G	C4'-C3'-C2'	-5.10	97.50	102.60
15	M	71	ILE	CB-CA-C	5.10	117.62	110.99
1	X	418	C	C5'-C4'-C3'	5.10	123.65	116.00
1	X	1287	A	P-O5'-C5'	-5.10	113.26	120.90
12	J	22	ALA	N-CA-C	5.10	117.86	110.42
1	X	577	U	O4'-C1'-C2'	-5.09	102.51	107.60
1	X	591	G	C3'-C2'-O2'	5.09	118.34	110.70
1	X	805	G	O4'-C1'-N9	-5.09	100.56	108.20
1	X	879	A	O5'-C5'-C4'	5.09	119.14	111.50
1	X	1964	A	N9-C1'-C2'	5.09	119.64	112.00
1	X	1167	A	C2'-C3'-O3'	5.09	117.13	109.50
1	X	2018	G	C4'-C3'-O3'	5.09	117.04	109.40
1	X	2303	C	P-O3'-C3'	5.09	127.83	120.20
2	Y	11	G	C3'-C2'-O2'	5.09	118.33	110.70
5	C	154	ASP	CA-CB-CG	5.09	117.69	112.60
2	Y	9	G	C3'-C2'-C1'	-5.09	96.21	101.30
1	X	2457	A	O3'-P-O5'	-5.08	96.38	104.00
1	X	2475	C	O4'-C1'-N1	5.08	116.13	108.50
1	X	321	A	P-O3'-C3'	5.08	127.82	120.20
1	X	2720	A	O4'-C4'-C3'	-5.08	98.92	104.00
1	X	2818	G	C4'-C3'-C2'	-5.08	97.52	102.60
12	J	92	GLU	CB-CG-CD	5.08	121.23	112.60
1	X	2807	U	C4'-C3'-O3'	-5.07	105.39	113.00
2	Y	86	A	C1'-O4'-C4'	-5.07	104.83	109.90
20	R	74	LEU	CA-C-N	5.07	131.23	121.54
20	R	74	LEU	C-N-CA	5.07	131.23	121.54
1	X	742	G	C1'-O4'-C4'	-5.07	104.83	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	1882	G	P-O3'-C3'	5.07	127.81	120.20
21	S	162	ALA	CA-C-N	5.07	127.44	120.39
21	S	162	ALA	C-N-CA	5.07	127.44	120.39
1	X	1635	G	C1'-C2'-O2'	5.07	116.00	108.40
1	X	1742	G	C3'-C2'-O2'	5.07	118.31	110.70
1	X	1711	C	C1'-O4'-C4'	-5.07	104.63	109.70
1	X	228	A	C3'-C2'-O2'	5.07	118.30	110.70
1	X	2031	A	N9-C1'-C2'	5.07	119.60	112.00
1	X	1664	G	P-O5'-C5'	5.07	128.50	120.90
11	I	42	GLY	N-CA-C	-5.06	101.18	113.18
1	X	1316	G	C3'-C2'-O2'	5.06	118.29	110.70
13	K	10	LEU	CD1-CG-CD2	-5.06	99.67	110.80
7	E	13	SER	N-CA-C	5.06	121.57	110.80
14	L	20	THR	CB-CA-C	5.06	120.48	110.42
3	A	69	ARG	CA-C-N	5.06	127.37	120.54
3	A	69	ARG	C-N-CA	5.06	127.37	120.54
1	X	122	G	C3'-C2'-O2'	5.05	118.28	110.70
1	X	1067	G	P-O3'-C3'	5.05	127.78	120.20
1	X	117	A	P-O3'-C3'	5.05	127.78	120.20
1	X	990	A	C3'-C2'-O2'	5.05	118.27	110.70
19	Q	64	ARG	CA-C-N	5.05	130.09	123.17
19	Q	64	ARG	C-N-CA	5.05	130.09	123.17
1	X	203	G	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	322	A	P-O3'-C3'	5.05	127.77	120.20
1	X	778	G	C4'-C3'-C2'	-5.05	97.55	102.60
1	X	1980	A	C5'-C4'-O4'	5.05	117.37	109.80
2	Y	18	G	P-O5'-C5'	5.05	128.47	120.90
9	G	91	THR	CA-C-N	5.04	125.68	120.03
9	G	91	THR	C-N-CA	5.04	125.68	120.03
17	O	25	LEU	CA-C-N	5.04	128.23	120.82
17	O	25	LEU	C-N-CA	5.04	128.23	120.82
1	X	466	A	P-O3'-C3'	5.04	127.75	120.20
1	X	828	C	C4'-C3'-O3'	-5.04	105.45	113.00
1	X	1541	G	C4'-C3'-C2'	-5.04	97.56	102.60
11	I	26	THR	CA-C-N	5.03	129.38	122.84
11	I	26	THR	C-N-CA	5.03	129.38	122.84
1	X	2841	U	P-O5'-C5'	5.03	128.45	120.90
1	X	1006	C	O5'-C5'-C4'	5.03	119.25	111.70
1	X	2696	A	P-O5'-C5'	-5.03	113.35	120.90
3	A	40	THR	CA-C-N	5.03	124.88	120.10
3	A	40	THR	C-N-CA	5.03	124.88	120.10
26	Z	37	HIS	N-CA-C	5.03	118.33	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	351	A	N9-C1'-C2'	5.03	119.54	112.00
11	I	103	ASN	N-CA-C	5.03	121.50	110.80
23	U	18	VAL	N-CA-C	5.02	117.24	108.90
20	R	4	PRO	CA-C-N	5.02	131.13	121.54
20	R	4	PRO	C-N-CA	5.02	131.13	121.54
1	X	2476	A	P-O3'-C3'	5.02	127.73	120.20
1	X	2542	U	C3'-C2'-O2'	5.02	118.22	110.70
1	X	7	G	C4'-C3'-C2'	5.01	107.61	102.60
1	X	656	U	C5'-C4'-C3'	5.01	123.52	116.00
1	X	2669	C	C2'-C3'-O3'	5.01	117.01	109.50
1	X	543	G	C3'-C2'-O2'	5.01	118.21	110.70
1	X	1310	C	P-O5'-C5'	-5.01	113.39	120.90
1	X	1439	G	C3'-C2'-C1'	-5.01	96.29	101.30
1	X	2596	C	O4'-C1'-N1	5.00	116.01	108.50
1	X	497	C	O3'-P-O5'	-5.00	96.49	104.00
4	B	89	ASP	N-CA-C	5.00	116.75	107.60
1	X	342	G	C4'-C3'-O3'	5.00	116.90	109.40
1	X	1771	A	P-O3'-C3'	5.00	127.70	120.20
3	A	261	ARG	N-CA-C	5.00	117.92	110.52

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1143	A	Sidechain
1	X	1337	G	Sidechain
1	X	474	G	Sidechain
1	X	671	A	Sidechain
1	X	683	A	Sidechain
1	X	805	G	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	57651	0	29049	404	0
2	Y	2598	0	1328	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1826	0	1885	66	0
4	B	1539	0	1600	62	0
5	C	1506	0	1525	51	0
6	D	1400	0	1481	24	0
7	E	1286	0	1336	10	0
8	F	503	0	520	5	0
9	G	1114	0	1144	70	0
10	H	997	0	1046	31	0
11	I	1067	0	1103	37	0
12	J	1090	0	1125	36	0
13	K	878	0	930	37	0
14	L	779	0	820	25	0
15	M	871	0	894	25	0
16	N	978	0	1020	34	0
17	O	741	0	756	34	0
18	P	1014	0	1096	22	0
19	Q	726	0	753	17	0
20	R	825	0	881	27	0
21	S	1345	0	1372	18	0
22	T	625	0	655	11	0
23	U	552	0	604	26	0
24	V	533	0	558	5	0
25	W	424	0	470	8	0
26	Z	457	0	462	12	0
27	1	53	0	0	1	0
28	2	46	0	0	2	0
29	3	63	0	0	3	0
30	4	297	0	330	5	0
31	J	1	0	0	0	0
31	M	1	0	0	0	0
31	X	28	0	0	0	0
31	Y	5	0	0	0	0
32	X	56	0	64	3	0
All	All	83875	0	54807	971	0

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

All (971) 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)
15:M:57:ILE:CD1	15:M:57:ILE:CG1	1.79	1.58
11:I:57:ILE:CD1	11:I:57:ILE:CG1	1.92	1.45
13:K:52:ILE:CD1	13:K:52:ILE:CG1	1.95	1.45
9:G:100:TYR:HB2	9:G:116:ARG:NH1	1.66	1.08
11:I:62:LYS:HE2	11:I:64:GLY:HA2	1.34	1.03
1:X:787:A:H2	1:X:800:U:HO2'	1.06	1.03
1:X:1333:G:N2	1:X:1344:C:H41	1.55	1.03
1:X:1882:G:N2	1:X:1885:C:H41	1.55	1.03
23:U:31:GLY:HA2	23:U:32:ARG:HH11	1.18	1.02
4:B:152:LYS:HB2	9:G:106:TYR:HB3	1.42	1.01
1:X:617:U:H5	1:X:632:A:C2	1.82	0.97
3:A:43:ARG:N	3:A:43:ARG:HD2	1.82	0.95
11:I:62:LYS:CE	11:I:64:GLY:HA2	1.97	0.95
1:X:1919:A:H2	1:X:1926:U:H3	0.97	0.94
26:Z:4:HIS:HB3	26:Z:5:PRO:HD3	1.49	0.94
17:O:87:ARG:HG2	17:O:87:ARG:HH11	1.32	0.94
1:X:1030:U:H3	1:X:1153:A:H62	1.12	0.91
3:A:247:VAL:HG23	3:A:248:THR:HG23	1.52	0.91
1:X:1033:G:H22	1:X:1153:A:H2	1.20	0.90
1:X:2371:A:H2	1:X:2403:C:H42	1.19	0.90
1:X:1466:C:H2'	1:X:1467:U:O4'	1.73	0.89
9:G:61:ARG:HH11	9:G:66:HIS:H	1.15	0.89
9:G:100:TYR:HB2	9:G:116:ARG:HH12	1.35	0.89
4:B:116:VAL:HG22	4:B:136:ARG:HE	1.36	0.88
14:L:38:ILE:HG13	14:L:39:TYR:H	1.37	0.87
17:O:5:ILE:HD12	17:O:6:GLN:H	1.41	0.86
1:X:1542:G:H22	1:X:1562:G:H1	0.92	0.86
3:A:43:ARG:HD2	3:A:43:ARG:H	1.39	0.85
4:B:32:PRO:HB3	4:B:72:VAL:HG11	1.55	0.85
13:K:17:ARG:NH1	13:K:20:LEU:HD23	1.91	0.85
32:X:2929:1F2:H9	32:X:2929:1F2:H54	1.58	0.85
3:A:231:HIS:HD2	3:A:233:HIS:H	1.24	0.85
1:X:1030:U:H3	1:X:1153:A:N6	1.75	0.84
3:A:210:GLY:HA2	3:A:213:ARG:HB2	1.59	0.84
1:X:1919:A:H2	1:X:1926:U:N3	1.74	0.84
1:X:559:C:H2'	1:X:560:G:C1'	2.08	0.83
19:Q:61:LYS:H	19:Q:72:ARG:HA	1.42	0.83
1:X:215:G:H21	1:X:632:A:H8	1.25	0.83
1:X:1468:A:H5'	1:X:1472:C:N4	1.94	0.83
1:X:1007:A:H1'	17:O:6:GLN:HG2	1.61	0.83
1:X:1333:G:H22	1:X:1344:C:H41	1.26	0.82
9:G:33:ILE:HB	9:G:34:PRO:HD3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:108:GLY:H	9:G:110:LEU:HG	1.45	0.82
1:X:1333:G:H22	1:X:1344:C:N4	1.78	0.82
13:K:17:ARG:HH11	13:K:20:LEU:HD23	1.41	0.81
4:B:116:VAL:HG22	4:B:136:ARG:NE	1.95	0.81
1:X:1333:G:N2	1:X:1344:C:N4	2.28	0.81
4:B:147:PRO:C	4:B:149:ARG:H	1.88	0.81
13:K:3:HIS:HB3	13:K:5:LYS:HD2	1.62	0.79
1:X:774:A:O5'	1:X:774:A:H8	1.65	0.78
1:X:559:C:H2'	1:X:560:G:H1'	1.66	0.78
9:G:93:LYS:HG2	9:G:96:ASP:HB3	1.65	0.78
1:X:2266:A:H62	1:X:2323:U:H3	1.29	0.77
12:J:78:LYS:HA	12:J:88:LYS:HZ3	1.48	0.77
3:A:231:HIS:CD2	3:A:233:HIS:H	2.03	0.77
9:G:106:TYR:O	9:G:110:LEU:HG	1.85	0.77
1:X:1142:G:H21	9:G:101:THR:CG2	1.99	0.76
10:H:13:ASN:HD21	10:H:109:ARG:HG2	1.50	0.76
23:U:48:LYS:HG2	23:U:49:LYS:H	1.50	0.76
5:C:148:VAL:HG13	5:C:185:ARG:HB2	1.66	0.76
9:G:61:ARG:NH1	9:G:66:HIS:H	1.84	0.76
1:X:2797:G:OP2	13:K:3:HIS:NE2	2.18	0.76
13:K:11:ASN:OD1	13:K:17:ARG:NH2	2.18	0.76
20:R:107:ALA:HB1	20:R:111:GLY:HA2	1.68	0.75
23:U:31:GLY:HA2	23:U:32:ARG:NH1	1.99	0.74
1:X:2042:A:H5''	5:C:65:GLY:HA2	1.70	0.74
1:X:83:A:H5''	20:R:17:LYS:HG2	1.70	0.74
9:G:132:PHE:CZ	9:G:145:HIS:HB2	2.23	0.74
4:B:54:LYS:HB2	4:B:75:THR:O	1.88	0.74
1:X:1882:G:H22	1:X:1885:C:H41	1.31	0.73
1:X:631:G:H4'	1:X:632:A:H5'	1.70	0.73
4:B:152:LYS:CB	9:G:106:TYR:HB3	2.18	0.73
16:N:61:TRP:HH2	16:N:94:VAL:H	1.37	0.73
25:W:12:ARG:CG	25:W:12:ARG:HH11	2.01	0.73
16:N:66:ASN:HB3	16:N:76:TYR:HB2	1.70	0.73
1:X:1770:U:H5	1:X:1775:A:N7	1.86	0.72
1:X:1373:G:H22	1:X:2192:U:H3	1.37	0.72
12:J:40:PRO:HB3	12:J:99:LYS:HD2	1.71	0.72
9:G:100:TYR:HB2	9:G:116:ARG:HH11	1.52	0.72
1:X:1266:G:N7	11:I:32:ARG:NH1	2.38	0.71
17:O:87:ARG:HG2	17:O:87:ARG:NH1	2.01	0.71
1:X:1142:G:H21	9:G:101:THR:HG22	1.54	0.71
5:C:43:ALA:HB1	5:C:86:PRO:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2691:C:OP1	1:X:2694:G:H4'	1.90	0.71
12:J:27:TYR:HB2	12:J:137:VAL:HG21	1.72	0.71
1:X:1542:G:N2	1:X:1562:G:H1	1.78	0.70
4:B:134:TRP:H	4:B:134:TRP:CD1	2.08	0.70
1:X:512:A:H4'	18:P:15:LYS:HB3	1.73	0.70
1:X:823:U:OP1	11:I:32:ARG:NH1	2.24	0.70
6:D:4:LEU:HG	6:D:5:LYS:H	1.57	0.70
1:X:1448:A:H61	1:X:1574:A:H61	1.37	0.70
29:3:15:LYS:CA	29:3:16:ILE:CA	2.70	0.70
1:X:2241:U:H5	22:T:17:ASN:OD1	1.75	0.70
4:B:7:THR:HG21	15:M:5:ILE:HD11	1.74	0.70
1:X:542:A:C2	1:X:2004:U:H2'	2.27	0.69
1:X:227:G:H2'	1:X:228:A:C8	2.27	0.69
14:L:8:ARG:HG3	14:L:9:ARG:N	2.06	0.69
4:B:152:LYS:HB2	9:G:106:TYR:CB	2.22	0.69
9:G:104:THR:OG1	9:G:110:LEU:HB3	1.93	0.69
1:X:2561:G:H5'	1:X:2561:G:H8	1.55	0.69
3:A:172:TYR:HA	3:A:186:HIS:HA	1.73	0.69
7:E:107:ILE:HD11	7:E:151:VAL:HG12	1.74	0.69
1:X:2368:G:H5''	1:X:2369:U:H5'	1.72	0.69
25:W:12:ARG:HH11	25:W:12:ARG:HG2	1.57	0.69
12:J:27:TYR:CB	12:J:137:VAL:HG21	2.22	0.69
14:L:8:ARG:HG3	14:L:9:ARG:H	1.57	0.69
1:X:558:G:H4'	1:X:559:C:H5'	1.76	0.68
1:X:1673:C:H5''	4:B:136:ARG:HD3	1.76	0.68
17:O:88:GLN:HE21	17:O:88:GLN:HA	1.58	0.68
1:X:1745:C:P	15:M:101:ARG:HH22	2.16	0.68
15:M:34:ARG:NH2	15:M:88:VAL:HG13	2.08	0.68
17:O:12:TYR:HB2	17:O:40:VAL:H	1.58	0.68
22:T:23:VAL:HA	22:T:38:VAL:HG23	1.74	0.68
26:Z:4:HIS:HB3	26:Z:5:PRO:CD	2.24	0.68
11:I:62:LYS:NZ	11:I:64:GLY:HA2	2.09	0.68
23:U:32:ARG:HG2	23:U:33:LYS:H	1.58	0.68
1:X:1675:C:OP1	4:B:134:TRP:CE2	2.46	0.68
1:X:2653:A:O2'	10:H:41:ASN:ND2	2.27	0.68
1:X:504:G:H21	18:P:78:ASN:HD21	1.42	0.67
1:X:2561:G:H5'	1:X:2561:G:C8	2.29	0.67
20:R:23:ILE:HG22	20:R:33:THR:HB	1.75	0.67
5:C:45:THR:HG21	5:C:85:GLY:HA3	1.75	0.67
10:H:13:ASN:ND2	10:H:109:ARG:HG2	2.09	0.67
11:I:32:ARG:HD2	17:O:79:GLN:NE2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:652:C:H42	1:X:657:A:H61	1.42	0.67
1:X:2387:U:H2'	1:X:2388:G:H8	1.58	0.67
9:G:67:ARG:HG2	9:G:70:PHE:HA	1.77	0.67
4:B:16:LYS:HB2	4:B:21:ILE:HD11	1.77	0.66
1:X:1257:U:H5''	11:I:17:LYS:HG3	1.77	0.66
1:X:1882:G:H21	1:X:1885:C:H41	1.43	0.66
1:X:323:G:OP1	1:X:343:A:H5''	1.94	0.66
1:X:1673:C:H5''	4:B:136:ARG:CD	2.26	0.66
1:X:1673:C:C5'	4:B:136:ARG:HD2	2.25	0.66
3:A:218:LYS:HE3	3:A:221:GLN:HB2	1.76	0.66
5:C:137:ALA:HB1	5:C:142:LEU:HB2	1.77	0.66
5:C:112:GLN:HA	5:C:116:LYS:HD3	1.78	0.66
17:O:57:GLN:H	17:O:97:GLY:HA3	1.61	0.66
1:X:1673:C:C5'	4:B:136:ARG:CD	2.74	0.66
1:X:1744:G:OP1	15:M:100:ARG:HD2	1.96	0.66
1:X:1770:U:C5	1:X:1775:A:N7	2.64	0.65
1:X:617:U:C5	1:X:632:A:C2	2.74	0.65
1:X:1673:C:H5'	4:B:136:ARG:HD2	1.79	0.65
1:X:2319:G:H2'	1:X:2320:G:H8	1.61	0.65
1:X:2594:U:H2'	1:X:2595:C:H6	1.61	0.65
20:R:90:LYS:HB2	20:R:108:VAL:HG21	1.78	0.65
1:X:640:C:H4'	1:X:660:G:H21	1.62	0.65
1:X:320:A:N3	1:X:340:G:O2'	2.29	0.64
14:L:38:ILE:HG13	14:L:39:TYR:N	2.11	0.64
1:X:1753:A:O5'	1:X:1753:A:H8	1.81	0.64
4:B:134:TRP:H	4:B:134:TRP:HD1	1.45	0.64
3:A:45:ASN:CG	3:A:46:ARG:H	2.05	0.64
9:G:33:ILE:HB	9:G:34:PRO:CD	2.27	0.64
20:R:10:HIS:HD2	20:R:44:GLN:NE2	1.96	0.64
3:A:200:GLU:HG3	3:A:202:LYS:HB2	1.80	0.64
5:C:164:VAL:C	5:C:166:TRP:H	2.05	0.64
6:D:80:ARG:HD3	6:D:83:MET:HB2	1.80	0.63
23:U:52:ARG:HG3	23:U:79:GLU:HA	1.80	0.63
1:X:1468:A:H5'	1:X:1472:C:H42	1.64	0.63
1:X:482:A:H2'	1:X:483:A:O4'	1.98	0.63
1:X:564:U:H2'	1:X:565:A:C8	2.34	0.63
13:K:3:HIS:CG	13:K:5:LYS:HZ2	2.15	0.63
1:X:1113:C:H2'	1:X:1114:A:H8	1.64	0.63
3:A:86:PRO:O	3:A:87:ASN:HB2	1.97	0.63
17:O:87:ARG:HH11	17:O:87:ARG:CG	2.10	0.62
5:C:148:VAL:O	5:C:167:VAL:HA	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:11:ASN:ND2	13:K:12:ARG:HE	1.97	0.62
23:U:22:GLY:HA3	23:U:39:LYS:HD2	1.82	0.62
9:G:107:GLN:HA	9:G:110:LEU:HB2	1.81	0.62
1:X:2477:C:H6	1:X:2477:C:H5'	1.65	0.62
1:X:2042:A:H5''	5:C:65:GLY:CA	2.30	0.62
2:Y:30:C:OP1	14:L:37:HIS:HB3	2.00	0.62
11:I:18:ARG:HB3	11:I:21:ARG:HB2	1.81	0.62
1:X:504:G:H4'	18:P:27:VAL:HG13	1.81	0.62
1:X:971:A:H61	12:J:83:ARG:HH22	1.47	0.62
10:H:98:ILE:HG22	10:H:106:ARG:HG3	1.81	0.62
13:K:79:VAL:HA	13:K:83:VAL:HG13	1.81	0.62
19:Q:53:ILE:HD13	19:Q:80:VAL:HG13	1.80	0.62
1:X:1737:G:H2'	1:X:1738:U:C6	2.36	0.61
1:X:2659:C:H5'	4:B:189:PRO:HA	1.82	0.61
1:X:2790:C:O2'	26:Z:43:HIS:HD2	1.83	0.61
11:I:17:LYS:O	11:I:18:ARG:HB2	2.00	0.61
1:X:2779:C:H2'	1:X:2780:A:C8	2.36	0.61
1:X:2222:U:H2'	1:X:2223:U:C6	2.35	0.61
11:I:62:LYS:HG2	11:I:64:GLY:H	1.66	0.61
23:U:31:GLY:C	23:U:32:ARG:HE	2.08	0.61
1:X:559:C:H2'	1:X:560:G:O4'	2.01	0.60
4:B:152:LYS:H	9:G:106:TYR:HB3	1.65	0.60
17:O:73:LYS:HB2	17:O:82:ARG:HB2	1.82	0.60
16:N:93:LYS:HD3	17:O:5:ILE:HB	1.84	0.60
23:U:22:GLY:HA3	23:U:39:LYS:CD	2.31	0.60
3:A:226:MET:HG2	3:A:230:ASP:HB2	1.84	0.60
2:Y:45:C:H2'	6:D:92:ARG:NH1	2.17	0.60
9:G:105:GLY:O	9:G:106:TYR:C	2.42	0.60
32:X:2929:1F2:H9	32:X:2929:1F2:C43	2.29	0.60
1:X:857:U:H3'	1:X:858:G:C8	2.37	0.60
3:A:58:HIS:O	3:A:58:HIS:ND1	2.35	0.60
4:B:75:THR:O	4:B:76:ARG:HB2	2.00	0.60
14:L:38:ILE:HG21	14:L:71:VAL:HG21	1.84	0.60
1:X:954:U:OP2	11:I:38:LYS:HG2	2.01	0.60
1:X:636:G:H5''	1:X:636:G:H8	1.67	0.59
1:X:689:A:H8	1:X:2052:G:H21	1.50	0.59
10:H:83:ARG:HH21	10:H:89:ILE:HD11	1.67	0.59
1:X:2845:C:H5''	13:K:65:LEU:HD11	1.84	0.59
4:B:147:PRO:C	4:B:149:ARG:N	2.58	0.59
1:X:2044:G:OP1	5:C:62:LYS:NZ	2.36	0.59
1:X:1811:A:H5''	3:A:161:THR:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:19:THR:HG23	12:J:99:LYS:HD3	1.84	0.59
1:X:2795:A:H4'	13:K:5:LYS:HG2	1.83	0.59
6:D:75:SER:HB2	6:D:79:LEU:HD13	1.82	0.59
1:X:793:G:H21	1:X:796:A:H62	1.50	0.59
9:G:157:PRO:C	9:G:159:SER:H	2.10	0.59
1:X:172:A:H61	1:X:175:C:H3'	1.68	0.59
1:X:1173:G:H21	17:O:88:GLN:HE22	1.50	0.59
14:L:33:ARG:CZ	14:L:38:ILE:HB	2.33	0.59
1:X:1466:C:C2'	1:X:1467:U:O4'	2.47	0.59
1:X:2310:G:H4'	22:T:43:THR:H	1.68	0.59
13:K:3:HIS:CG	13:K:5:LYS:NZ	2.70	0.59
16:N:37:GLN:HA	16:N:40:LEU:HD12	1.85	0.59
1:X:1448:A:H61	1:X:1574:A:N6	2.01	0.59
3:A:243:GLY:C	3:A:244:ARG:HD3	2.28	0.59
14:L:38:ILE:HG13	14:L:40:ALA:H	1.67	0.59
1:X:692:C:H2'	1:X:693:A:H8	1.68	0.58
23:U:27:ASP:H	23:U:32:ARG:HH21	1.51	0.58
1:X:746:G:N7	1:X:774:A:C6	2.71	0.58
1:X:1142:G:OP1	9:G:107:GLN:O	2.21	0.58
4:B:122:PHE:O	4:B:123:ALA:HB2	2.02	0.58
1:X:333:A:H2'	5:C:162:ARG:HH12	1.68	0.58
9:G:132:PHE:HB2	9:G:145:HIS:CE1	2.38	0.58
16:N:93:LYS:CE	17:O:5:ILE:HD13	2.34	0.58
16:N:93:LYS:HE3	17:O:5:ILE:HD13	1.85	0.58
19:Q:29:VAL:HG11	19:Q:38:ILE:HD11	1.85	0.58
20:R:105:ARG:HH12	20:R:112:LYS:HA	1.69	0.58
10:H:132:GLU:HG2	10:H:134:LEU:HG	1.84	0.58
3:A:133:LEU:HB2	3:A:187:SER:HA	1.86	0.58
1:X:1675:C:OP1	4:B:134:TRP:NE1	2.36	0.58
11:I:38:LYS:HD2	11:I:40:ARG:O	2.04	0.58
1:X:2594:U:H2'	1:X:2595:C:C6	2.39	0.57
12:J:36:ILE:HD11	12:J:103:VAL:HG22	1.86	0.57
23:U:17:SER:HB2	23:U:44:ALA:HA	1.86	0.57
1:X:405:C:H2'	1:X:406:G:H8	1.69	0.57
1:X:2387:U:H2'	1:X:2388:G:C8	2.39	0.57
13:K:87:TYR:HE1	13:K:94:TYR:HD2	1.51	0.57
16:N:66:ASN:HB3	16:N:76:TYR:CB	2.35	0.57
19:Q:66:GLY:C	19:Q:68:PHE:H	2.10	0.57
1:X:1342:U:H5''	1:X:1343:C:H5	1.68	0.57
3:A:42:GLY:C	3:A:43:ARG:HH11	2.12	0.57
12:J:44:LYS:HD2	12:J:47:GLN:HE22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:692:C:H2'	1:X:693:A:C8	2.40	0.57
1:X:939:C:H5'	1:X:939:C:H6	1.70	0.57
1:X:1467:U:H2'	1:X:1468:A:OP1	2.05	0.57
1:X:1773:C:H1'	1:X:2588:U:H5''	1.87	0.57
9:G:67:ARG:CG	9:G:70:PHE:HA	2.35	0.57
18:P:28:ALA:HB2	18:P:71:VAL:HG22	1.87	0.56
1:X:1142:G:C1'	9:G:103:TYR:HD2	2.18	0.56
1:X:794:A:H5'	3:A:218:LYS:HZ2	1.71	0.56
18:P:14:ARG:HA	18:P:17:GLN:HG2	1.87	0.56
21:S:95:SER:HB3	21:S:119:ASN:HB3	1.87	0.56
1:X:333:A:H2'	5:C:162:ARG:NH1	2.20	0.56
20:R:25:LEU:HD12	20:R:81:VAL:N	2.20	0.56
6:D:150:ARG:HE	6:D:151:GLY:H	1.54	0.56
8:F:117:ALA:HB1	8:F:122:ALA:HB1	1.87	0.56
13:K:13:ASN:ND2	13:K:15:SER:OG	2.38	0.56
26:Z:35:GLN:O	26:Z:37:HIS:N	2.39	0.56
1:X:1805:G:H1'	3:A:50:THR:CG2	2.36	0.56
1:X:1673:C:H5'	4:B:136:ARG:CD	2.36	0.56
9:G:103:TYR:CG	9:G:111:LYS:HA	2.40	0.56
1:X:485:G:C6	1:X:520:C:N4	2.74	0.56
21:S:6:LYS:H	21:S:7:PRO:HD3	1.71	0.56
1:X:38:G:H21	5:C:42:THR:HG21	1.71	0.56
1:X:794:A:H2	1:X:1767:G:N3	2.04	0.56
9:G:162:LYS:H	9:G:163:PRO:HD3	1.71	0.56
1:X:794:A:H5'	3:A:218:LYS:NZ	2.21	0.55
1:X:2490:U:H2'	1:X:2491:C:O4'	2.06	0.55
4:B:147:PRO:HB2	4:B:149:ARG:HD2	1.87	0.55
4:B:149:ARG:NH2	9:G:106:TYR:HD1	2.04	0.55
1:X:2319:G:H2'	1:X:2320:G:C8	2.42	0.55
1:X:1673:C:C5'	4:B:136:ARG:HD3	2.36	0.55
1:X:2620:G:H5''	9:G:104:THR:HB	1.89	0.55
11:I:10:PRO:HA	11:I:14:LYS:HB2	1.89	0.55
23:U:62:LEU:HD23	23:U:67:LEU:HD12	1.89	0.55
3:A:86:PRO:O	3:A:87:ASN:CB	2.54	0.55
1:X:1122:A:O2'	1:X:1123:G:H4'	2.07	0.55
9:G:68:PRO:HD2	9:G:76:GLN:HB3	1.88	0.55
25:W:1:MET:HB3	25:W:34:VAL:HG12	1.89	0.55
30:4:19:ARG:HD2	30:4:24:LEU:HD22	1.89	0.55
1:X:38:G:H1	1:X:453:U:H3	1.53	0.55
1:X:940:G:N2	25:W:43:MET:HE2	2.22	0.55
1:X:2516:U:H2'	1:X:2517:C:C6	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:43:ARG:HB3	3:A:54:ILE:HG13	1.89	0.55
16:N:66:ASN:HB3	16:N:76:TYR:H	1.71	0.55
1:X:1008:G:H5''	16:N:92:ARG:HB3	1.89	0.54
1:X:1268:U:C2	5:C:66:ASN:HA	2.42	0.54
1:X:1278:A:H61	1:X:1996:A:H5''	1.72	0.54
2:Y:53:G:H21	2:Y:54:U:H5''	1.72	0.54
16:N:101:ARG:O	16:N:103:PRO:HD3	2.08	0.54
17:O:10:LYS:HG3	17:O:11:GLN:HG2	1.90	0.54
1:X:742:G:N1	3:A:208:LYS:HD3	2.23	0.54
11:I:97:ARG:O	11:I:98:LEU:HB2	2.05	0.54
1:X:654:A:H2'	1:X:655:A:H5'	1.89	0.54
1:X:1962:C:H2'	1:X:1963:G:H5'	1.90	0.54
5:C:158:ARG:HA	5:C:169:VAL:HG21	1.90	0.54
1:X:494:A:C8	20:R:56:LYS:HD2	2.43	0.54
8:F:79:ARG:HG2	8:F:84:ILE:HB	1.89	0.54
1:X:219:G:N2	1:X:231:G:H2'	2.22	0.54
1:X:1337:G:OP2	18:P:105:ARG:NH1	2.41	0.54
9:G:106:TYR:O	9:G:110:LEU:CG	2.56	0.54
24:V:25:LEU:HD21	24:V:47:ARG:HG2	1.90	0.54
1:X:224:G:H4'	1:X:399:G:C5	2.42	0.53
1:X:797:A:C5	3:A:229:VAL:HG21	2.43	0.53
1:X:969:U:C4	12:J:17:ARG:HB2	2.43	0.53
4:B:116:VAL:HG13	4:B:136:ARG:HH21	1.73	0.53
13:K:49:GLU:O	13:K:52:ILE:HG12	2.08	0.53
23:U:53:GLU:HB2	23:U:56:GLN:O	2.09	0.53
5:C:133:PHE:HB2	5:C:160:ALA:HB1	1.89	0.53
11:I:54:SER:C	11:I:56:LEU:H	2.17	0.53
1:X:2761:A:H5''	1:X:2762:G:H5'	1.89	0.53
1:X:617:U:H5	1:X:632:A:N1	2.04	0.53
1:X:1033:G:N2	1:X:1153:A:H2	1.98	0.53
1:X:1810:U:H2'	3:A:157:ARG:HD3	1.90	0.53
4:B:149:ARG:CZ	9:G:106:TYR:HD1	2.21	0.53
5:C:41:GLY:HA3	5:C:89:ARG:O	2.09	0.53
9:G:55:ALA:C	9:G:134:MET:HE1	2.34	0.53
11:I:58:ALA:O	11:I:59:ARG:HB3	2.08	0.53
12:J:28:VAL:HG12	12:J:29:ALA:H	1.72	0.53
16:N:21:ALA:HB1	16:N:29:SER:HA	1.91	0.53
1:X:2241:U:C5	22:T:17:ASN:OD1	2.59	0.53
6:D:40:LEU:HD21	6:D:87:ILE:HD12	1.91	0.53
12:J:28:VAL:HG23	12:J:137:VAL:HB	1.91	0.53
1:X:617:U:H5	1:X:632:A:H2	1.50	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:69:ILE:HG22	17:O:86:HIS:HB3	1.90	0.53
18:P:38:VAL:HG12	18:P:97:VAL:HG21	1.90	0.53
21:S:91:PRO:HG2	21:S:125:PRO:HD2	1.90	0.53
1:X:1373:G:N2	1:X:2192:U:H3	2.04	0.53
3:A:45:ASN:CG	3:A:46:ARG:N	2.67	0.53
4:B:152:LYS:H	9:G:106:TYR:CB	2.22	0.53
14:L:76:ALA:HB2	14:L:107:ALA:HA	1.91	0.53
2:Y:32:C:H1'	2:Y:59:A:H61	1.73	0.53
12:J:109:GLY:HA3	21:S:112:LEU:HD21	1.90	0.52
16:N:66:ASN:HB2	16:N:70:ARG:HH11	1.73	0.52
1:X:1033:G:N2	1:X:1153:A:C2	2.75	0.52
4:B:183:LEU:HD11	15:M:16:ILE:HG21	1.90	0.52
1:X:760:U:C6	26:Z:3:LYS:HG3	2.44	0.52
1:X:2545:A:H61	10:H:40:GLY:HA3	1.74	0.52
1:X:1468:A:H5'	1:X:1472:C:H41	1.73	0.52
1:X:1765:C:N3	3:A:208:LYS:HE2	2.24	0.52
2:Y:16:U:H3'	2:Y:17:A:H5''	1.90	0.52
10:H:41:ASN:ND2	10:H:41:ASN:H	2.08	0.52
17:O:38:LEU:HD23	17:O:47:PHE:HB3	1.91	0.52
19:Q:5:ASP:O	19:Q:7:LEU:N	2.43	0.52
10:H:27:SER:HA	10:H:50:ILE:HD12	1.91	0.52
22:T:50:GLY:O	22:T:62:LEU:HB2	2.10	0.52
1:X:879:A:H2'	1:X:879:A:N3	2.25	0.52
1:X:2397:A:H2'	1:X:2398:U:O4'	2.10	0.52
9:G:62:ILE:HG22	9:G:135:LEU:HD21	1.90	0.52
12:J:12:LYS:O	12:J:13:GLN:HB2	2.08	0.52
12:J:100:PRO:HB2	21:S:74:ARG:HG2	1.91	0.52
15:M:99:VAL:HG11	15:M:104:LEU:HD22	1.90	0.52
1:X:415:A:H61	1:X:436:A:H61	1.58	0.52
1:X:1845:A:N1	1:X:2070:G:H1'	2.25	0.52
5:C:30:VAL:HG11	5:C:177:VAL:HG21	1.92	0.52
10:H:2:ILE:HB	10:H:45:ALA:HB3	1.92	0.52
18:P:25:PHE:HD1	18:P:127:ILE:HD11	1.74	0.52
1:X:1939:U:H1'	1:X:2531:U:OP1	2.10	0.52
1:X:1943:A:H8	1:X:1943:A:H5''	1.74	0.52
10:H:24:VAL:HA	10:H:51:ILE:HG22	1.92	0.52
14:L:29:LEU:HB3	14:L:89:PHE:HA	1.92	0.52
24:V:56:VAL:C	24:V:58:ALA:H	2.18	0.52
1:X:1686:A:H5''	1:X:1687:C:OP2	2.09	0.52
9:G:98:LYS:HB3	9:G:116:ARG:HB2	1.92	0.52
19:Q:66:GLY:O	19:Q:68:PHE:N	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1630:A:N1	18:P:114:ALA:HB2	2.26	0.51
1:X:1643:A:H61	1:X:1656:U:H3	1.59	0.51
1:X:1805:G:H1'	3:A:50:THR:HG21	1.90	0.51
1:X:2368:G:H5''	1:X:2369:U:C5'	2.39	0.51
16:N:24:PHE:O	16:N:29:SER:HB3	2.11	0.51
1:X:118:U:H4'	1:X:119:G:H5''	1.93	0.51
16:N:74:MET:HE2	16:N:78:THR:HG23	1.93	0.51
1:X:305:A:H5'	1:X:305:A:H8	1.75	0.51
1:X:1342:U:H5''	1:X:1343:C:C5	2.46	0.51
1:X:1586:A:H2'	1:X:1587:A:C8	2.45	0.51
1:X:2551:A:H62	4:B:145:LYS:HG3	1.74	0.51
13:K:10:LEU:HA	13:K:17:ARG:HG2	1.93	0.51
14:L:33:ARG:NH1	14:L:38:ILE:HB	2.25	0.51
20:R:105:ARG:HH22	20:R:111:GLY:C	2.17	0.51
3:A:182:LEU:HB2	3:A:268:ARG:O	2.10	0.51
6:D:8:TYR:O	6:D:12:VAL:HB	2.11	0.51
6:D:123:ASP:HB3	6:D:127:ASN:HB2	1.92	0.51
9:G:57:LEU:HD22	9:G:170:PRO:HA	1.92	0.51
14:L:36:LYS:HB3	14:L:64:LYS:HB2	1.93	0.51
16:N:81:ASN:HD22	16:N:117:ARG:HH21	1.58	0.51
21:S:51:LEU:HB3	21:S:65:LEU:HD12	1.92	0.51
1:X:486:U:H4'	1:X:519:C:H2'	1.92	0.51
20:R:51:VAL:HG21	20:R:76:LEU:HD21	1.92	0.51
1:X:504:G:N2	18:P:78:ASN:HD21	2.08	0.51
11:I:21:ARG:HH11	11:I:22:GLY:HA3	1.76	0.51
1:X:1737:G:H2'	1:X:1738:U:H6	1.75	0.51
9:G:70:PHE:HB2	16:N:64:ARG:HG2	1.93	0.51
13:K:45:ARG:HD2	13:K:95:THR:HG22	1.92	0.51
14:L:8:ARG:CG	14:L:9:ARG:H	2.22	0.51
1:X:2475:C:OP1	12:J:83:ARG:HB3	2.11	0.50
5:C:8:GLY:HA3	5:C:120:VAL:HB	1.93	0.50
9:G:103:TYR:HB3	9:G:107:GLN:HE21	1.76	0.50
24:V:7:ARG:HB2	24:V:60:LEU:HD11	1.92	0.50
3:A:43:ARG:N	3:A:43:ARG:CD	2.64	0.50
6:D:78:LYS:HG2	6:D:80:ARG:HH11	1.76	0.50
1:X:2083:G:H1	1:X:2172:U:H3	1.58	0.50
9:G:162:LYS:N	9:G:163:PRO:CD	2.74	0.50
23:U:48:LYS:HG2	23:U:49:LYS:N	2.21	0.50
23:U:49:LYS:HA	23:U:62:LEU:H	1.75	0.50
3:A:36:ALA:HB1	3:A:62:TYR:O	2.12	0.50
5:C:148:VAL:HB	5:C:167:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:25:LEU:HD11	10:H:52:VAL:HG23	1.93	0.50
1:X:954:U:P	11:I:38:LYS:HG2	2.52	0.50
12:J:92:GLU:HG3	12:J:93:TYR:CD2	2.46	0.50
18:P:17:GLN:HG3	18:P:18:VAL:HG23	1.94	0.50
6:D:143:TYR:HA	6:D:146:VAL:HG22	1.94	0.50
9:G:124:GLU:O	9:G:128:GLU:HB2	2.11	0.50
13:K:17:ARG:NH1	13:K:20:LEU:CD2	2.71	0.50
20:R:29:HIS:CD2	20:R:51:VAL:HG22	2.47	0.50
1:X:490:A:N3	1:X:492:G:H5''	2.27	0.50
1:X:670:U:H2'	1:X:671:A:C8	2.46	0.50
1:X:1142:G:N2	9:G:101:THR:HG22	2.22	0.50
1:X:654:A:H2'	1:X:655:A:C5'	2.42	0.50
16:N:44:THR:O	16:N:48:ARG:HG3	2.12	0.50
21:S:69:VAL:HG22	21:S:81:VAL:HG13	1.93	0.50
1:X:922:A:N1	1:X:2256:G:H1'	2.27	0.50
1:X:2034:A:O4'	4:B:141:ILE:HD12	2.12	0.50
4:B:50:GLY:HA3	4:B:75:THR:HG21	1.94	0.50
4:B:146:THR:OG1	4:B:147:PRO:HD3	2.12	0.50
7:E:154:PRO:HA	7:E:160:LYS:O	2.11	0.50
11:I:28:LYS:NZ	11:I:36:GLY:HA3	2.27	0.50
12:J:65:ILE:HG23	12:J:107:VAL:HG12	1.94	0.50
1:X:2272:A:H5''	14:L:15:ARG:HH21	1.77	0.49
1:X:2508:G:C8	1:X:2508:G:H5'	2.47	0.49
2:Y:45:C:H2'	6:D:92:ARG:HH11	1.77	0.49
4:B:147:PRO:O	4:B:149:ARG:N	2.45	0.49
5:C:22:VAL:HG13	5:C:106:MET:HG2	1.94	0.49
9:G:140:GLN:HG2	9:G:144:MET:HE3	1.94	0.49
20:R:80:LYS:NZ	20:R:80:LYS:O	2.45	0.49
21:S:6:LYS:HB2	21:S:31:SER:HB3	1.94	0.49
23:U:14:VAL:O	23:U:15:VAL:HG22	2.12	0.49
1:X:742:G:N7	3:A:209:ALA:O	2.45	0.49
1:X:1134:C:H1'	30:4:18:ARG:HH12	1.77	0.49
1:X:1467:U:H6	1:X:1467:U:H3'	1.77	0.49
1:X:1493:A:H2'	1:X:1494:G:O4'	2.12	0.49
4:B:5:LEU:HG	4:B:195:LEU:HD11	1.94	0.49
9:G:132:PHE:HZ	9:G:142:ARG:HA	1.77	0.49
14:L:31:VAL:HG21	14:L:100:VAL:HG23	1.93	0.49
1:X:2352:A:H2'	1:X:2353:G:C8	2.46	0.49
7:E:6:LYS:HB3	7:E:69:ARG:HD3	1.92	0.49
7:E:11:VAL:HB	7:E:15:VAL:HG21	1.93	0.49
17:O:12:TYR:CB	17:O:40:VAL:H	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:71:ILE:HD11	17:O:86:HIS:HB2	1.94	0.49
23:U:51:ILE:HG23	23:U:59:THR:HA	1.94	0.49
1:X:2266:A:H2	1:X:2325:A:H62	1.58	0.49
11:I:117:ALA:HA	11:I:137:GLY:O	2.13	0.49
1:X:649:G:H1	1:X:660:G:H1	1.60	0.49
10:H:78:SER:HA	10:H:91:PHE:O	2.11	0.49
23:U:48:LYS:CG	23:U:49:LYS:H	2.24	0.49
23:U:49:LYS:HB2	23:U:61:TRP:CE3	2.48	0.49
1:X:2867:G:O5'	1:X:2867:G:H8	1.95	0.49
12:J:77:LYS:O	12:J:79:PRO:HD3	2.12	0.49
13:K:11:ASN:HD22	13:K:12:ARG:HE	1.60	0.49
18:P:36:ARG:HA	18:P:39:ARG:HD2	1.93	0.49
1:X:29:U:H4'	16:N:11:ARG:HH22	1.78	0.49
1:X:2017:U:H2'	1:X:2018:G:H5''	1.95	0.49
10:H:110:VAL:HG23	10:H:129:LEU:HB2	1.94	0.49
16:N:88:ILE:HG12	17:O:49:GLU:HB2	1.94	0.49
18:P:32:ARG:HA	18:P:121:THR:HG22	1.94	0.49
23:U:23:LYS:HD2	23:U:35:THR:HG21	1.95	0.49
1:X:389:G:H2'	1:X:390:U:C6	2.47	0.49
12:J:27:TYR:HB3	12:J:137:VAL:HG21	1.93	0.49
1:X:2080:U:H3	1:X:2175:A:H61	1.60	0.49
1:X:2661:G:O6	1:X:2708:U:H1'	2.13	0.49
10:H:28:GLY:HA3	10:H:35:THR:OG1	2.13	0.49
1:X:91:A:H2'	1:X:92:U:C6	2.48	0.48
1:X:649:G:N2	1:X:660:G:N2	2.60	0.48
1:X:818:G:H1'	1:X:844:G:O2'	2.13	0.48
14:L:15:ARG:HH11	14:L:15:ARG:HA	1.78	0.48
1:X:2505:G:H1'	30:4:1:MET:HB2	1.93	0.48
4:B:13:GLN:O	4:B:14:ILE:HD12	2.13	0.48
4:B:195:LEU:H	15:M:2:GLN:HG2	1.78	0.48
13:K:10:LEU:HD23	13:K:17:ARG:HB2	1.95	0.48
16:N:83:LEU:HD12	16:N:113:SER:HB2	1.93	0.48
18:P:103:LEU:HB2	18:P:119:LYS:HB2	1.96	0.48
21:S:6:LYS:N	21:S:7:PRO:HD3	2.27	0.48
1:X:12:U:O2	1:X:12:U:H2'	2.13	0.48
6:D:72:LYS:HE2	6:D:81:GLN:HE21	1.79	0.48
7:E:38:ASN:HB3	7:E:40:GLU:HG2	1.95	0.48
1:X:2352:A:H2'	1:X:2353:G:H8	1.78	0.48
14:L:27:LEU:HB2	14:L:87:VAL:HG22	1.95	0.48
1:X:89:A:H4'	1:X:90:G:H5''	1.96	0.48
1:X:1494:G:O2'	1:X:1574:A:H2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:164:VAL:O	5:C:166:TRP:N	2.40	0.48
27:1:40:TYR:CA	27:1:41:ASP:CA	2.91	0.48
1:X:1562:G:H5''	1:X:1563:U:H5'	1.94	0.48
1:X:1705:U:O2	1:X:1717:A:H8	1.97	0.48
9:G:157:PRO:O	9:G:159:SER:N	2.46	0.48
11:I:32:ARG:HD2	17:O:79:GLN:HE22	1.77	0.48
1:X:1278:A:H2	1:X:1997:A:H62	1.61	0.48
1:X:2270:U:H2'	1:X:2271:C:C6	2.47	0.48
5:C:5:ASN:HB2	5:C:10:ASN:HA	1.95	0.48
10:H:116:ARG:HH11	15:M:38:LYS:HD3	1.78	0.48
17:O:10:LYS:HD2	17:O:37:ALA:HB3	1.95	0.48
1:X:617:U:C5	1:X:632:A:N1	2.81	0.48
1:X:627:A:H2'	1:X:628:A:C8	2.49	0.48
1:X:1685:A:H5''	10:H:5:GLN:HG2	1.96	0.48
17:O:33:VAL:HG12	17:O:57:GLN:HE21	1.79	0.48
1:X:1997:A:H2'	1:X:1998:A:C8	2.49	0.48
4:B:133:LYS:HD2	4:B:137:ARG:HB3	1.96	0.48
18:P:85:MET:HE2	18:P:130:GLU:HG3	1.95	0.48
23:U:51:ILE:HA	23:U:59:THR:O	2.13	0.48
1:X:1833:U:H2'	1:X:1834:G:C8	2.49	0.48
1:X:2289:A:H3'	1:X:2290:A:H8	1.78	0.48
3:A:43:ARG:H	3:A:43:ARG:CD	2.18	0.48
30:4:19:ARG:HB2	30:4:24:LEU:HD13	1.96	0.48
1:X:1777:A:H1'	1:X:1921:A:N6	2.28	0.47
4:B:117:MET:H	4:B:136:ARG:HG3	1.79	0.47
20:R:105:ARG:HH21	20:R:107:ALA:HB2	1.77	0.47
1:X:712:A:H2'	1:X:713:G:O4'	2.15	0.47
1:X:1820:G:OP2	3:A:239:ARG:NH1	2.47	0.47
3:A:244:ARG:HB3	3:A:252:LYS:NZ	2.29	0.47
8:F:101:TRP:HZ3	8:F:140:GLY:HA3	1.78	0.47
1:X:1776:A:OP1	1:X:1965:U:H5'	2.15	0.47
11:I:88:PHE:HE2	11:I:119:THR:HB	1.79	0.47
18:P:40:LEU:HB3	26:Z:25:LEU:HD13	1.96	0.47
1:X:738:G:O5'	1:X:738:G:H8	1.98	0.47
1:X:1787:U:H2'	1:X:1788:C:C6	2.49	0.47
12:J:81:GLU:HG2	12:J:82:THR:H	1.79	0.47
1:X:1992:G:H1'	13:K:106:ASP:O	2.13	0.47
26:Z:16:ARG:HD3	26:Z:20:ARG:CZ	2.44	0.47
1:X:334:G:C8	5:C:164:VAL:HG13	2.49	0.47
1:X:1859:A:H2'	1:X:1860:A:C8	2.50	0.47
4:B:59:VAL:HG21	4:B:74:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:137:ARG:HG3	4:B:138:PRO:HD2	1.97	0.47
5:C:118:VAL:HG22	5:C:188:ILE:HD12	1.97	0.47
5:C:149:LEU:HD23	5:C:180:ILE:HG22	1.96	0.47
18:P:59:PHE:HD2	26:Z:41:LEU:HD22	1.79	0.47
23:U:27:ASP:N	23:U:32:ARG:HH21	2.12	0.47
1:X:33:C:O2'	1:X:34:U:H5''	2.14	0.47
1:X:143:A:H2'	1:X:144:U:C6	2.49	0.47
1:X:1137:A:H4'	1:X:1138:A:O5'	2.15	0.47
1:X:2189:A:C2	1:X:2190:A:C4	3.02	0.47
9:G:106:TYR:O	9:G:110:LEU:CD1	2.62	0.47
11:I:43:ALA:C	11:I:45:LYS:H	2.23	0.47
1:X:86:U:H5''	1:X:87:G:H5'	1.95	0.47
1:X:774:A:O5'	1:X:774:A:C8	2.56	0.47
1:X:879:A:H5'	1:X:880:C:OP2	2.14	0.47
11:I:62:LYS:NZ	11:I:64:GLY:CA	2.76	0.47
16:N:61:TRP:CZ3	16:N:94:VAL:N	2.82	0.47
1:X:203:G:H21	1:X:205:A:H62	1.62	0.47
1:X:1586:A:H5'	3:A:38:PRO:HG3	1.95	0.47
1:X:2654:A:H5'	10:H:42:LYS:H	1.80	0.47
22:T:3:HIS:CD2	22:T:5:LYS:HB2	2.50	0.47
23:U:19:ILE:HA	23:U:42:GLN:HA	1.95	0.47
1:X:935:C:H2'	1:X:936:A:C8	2.50	0.47
1:X:1173:G:H4'	17:O:22:VAL:HG23	1.97	0.47
4:B:122:PHE:O	4:B:123:ALA:CB	2.63	0.47
10:H:77:THR:HA	10:H:94:ASN:HB3	1.96	0.47
10:H:83:ARG:NH2	10:H:89:ILE:HD11	2.28	0.47
1:X:577:U:OP1	11:I:40:ARG:NH2	2.48	0.46
3:A:106:LEU:H	3:A:106:LEU:HD12	1.79	0.46
5:C:186:LEU:HG	5:C:188:ILE:HG12	1.95	0.46
6:D:35:VAL:HG22	6:D:90:THR:HG23	1.97	0.46
1:X:2289:A:H3'	1:X:2290:A:C8	2.49	0.46
9:G:103:TYR:CZ	9:G:111:LYS:HB2	2.51	0.46
10:H:112:GLY:O	10:H:131:PRO:HD2	2.15	0.46
12:J:26:ASP:O	12:J:27:TYR:HD1	1.97	0.46
1:X:650:U:H2'	1:X:651:C:C6	2.50	0.46
1:X:923:A:C6	12:J:12:LYS:HG2	2.50	0.46
1:X:1469:U:OP2	1:X:1471:G:OP2	2.33	0.46
1:X:2581:A:H2'	1:X:2582:G:C4'	2.46	0.46
6:D:72:LYS:HG2	6:D:81:GLN:HG2	1.98	0.46
18:P:118:LYS:HD2	18:P:120:ARG:HH21	1.80	0.46
20:R:23:ILE:HG23	20:R:84:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:R:40:LEU:HB2	20:R:45:LYS:HB2	1.97	0.46
1:X:542:A:C2	1:X:2004:U:C2'	2.97	0.46
1:X:1030:U:N3	1:X:1153:A:N6	2.54	0.46
11:I:76:LYS:HB3	11:I:79:GLN:HG2	1.98	0.46
12:J:77:LYS:HG3	12:J:78:LYS:H	1.80	0.46
25:W:46:THR:HG22	25:W:47:VAL:HG13	1.97	0.46
1:X:1142:G:O5'	9:G:107:GLN:HB3	2.15	0.46
1:X:2705:A:H1'	1:X:2706:U:H2'	1.97	0.46
8:F:77:LEU:HD13	8:F:107:ILE:HG23	1.98	0.46
9:G:67:ARG:HE	9:G:70:PHE:HA	1.80	0.46
9:G:69:ASP:H	9:G:76:GLN:HE21	1.62	0.46
12:J:27:TYR:HB2	12:J:137:VAL:HG11	1.98	0.46
13:K:87:TYR:CE1	13:K:94:TYR:HD2	2.30	0.46
7:E:164:PHE:O	7:E:166:GLY:N	2.48	0.46
1:X:1922:U:OP1	1:X:2583:U:O2'	2.33	0.46
3:A:270:ILE:HG13	3:A:271:VAL:H	1.81	0.46
10:H:28:GLY:O	10:H:29:ILE:HB	2.16	0.46
1:X:334:G:H5'	5:C:162:ARG:NH2	2.31	0.46
1:X:673:G:H5'	5:C:93:TYR:CD1	2.51	0.46
1:X:719:A:H2'	1:X:720:A:O4'	2.16	0.46
16:N:74:MET:HB3	16:N:75:ASN:H	1.59	0.46
1:X:641:G:N2	1:X:643:A:H3'	2.31	0.46
9:G:156:HIS:N	9:G:157:PRO:CD	2.79	0.46
13:K:3:HIS:HB3	13:K:5:LYS:CD	2.42	0.46
1:X:510:G:N1	1:X:513:A:OP2	2.45	0.45
1:X:1469:U:P	1:X:1471:G:OP2	2.74	0.45
1:X:2326:C:H2'	1:X:2327:U:H6	1.81	0.45
8:F:104:VAL:HA	8:F:107:ILE:HD12	1.98	0.45
13:K:3:HIS:ND1	13:K:5:LYS:NZ	2.47	0.45
13:K:36:THR:HG23	13:K:41:ALA:HB2	1.98	0.45
20:R:105:ARG:HH22	20:R:112:LYS:HA	1.80	0.45
1:X:568:G:H2'	1:X:569:C:O4'	2.15	0.45
1:X:652:C:H5''	1:X:652:C:H6	1.81	0.45
1:X:834:A:H5'	1:X:835:U:H6	1.81	0.45
1:X:1744:G:H5''	15:M:100:ARG:HD3	1.98	0.45
3:A:182:LEU:HD12	3:A:269:PHE:HB2	1.97	0.45
12:J:42:TRP:CG	12:J:95:VAL:HG11	2.52	0.45
20:R:45:LYS:HA	20:R:76:LEU:O	2.16	0.45
28:2:39:ARG:CA	28:2:40:HIS:CA	2.95	0.45
5:C:4:ILE:HG23	5:C:13:ARG:HH22	1.80	0.45
17:O:48:GLY:C	17:O:50:ASP:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:597:U:O4	1:X:683:A:H1'	2.16	0.45
1:X:2372:A:H5''	11:I:61:PRO:HB3	1.98	0.45
2:Y:46:G:H4'	6:D:92:ARG:HH12	1.82	0.45
5:C:74:VAL:HB	5:C:75:PRO:HD2	1.97	0.45
5:C:170:LEU:HA	5:C:171:PRO:HD3	1.84	0.45
24:V:21:ARG:HH11	24:V:53:LEU:HD11	1.81	0.45
1:X:2790:C:O2'	26:Z:43:HIS:CD2	2.65	0.45
6:D:152:MET:HE2	6:D:154:ILE:HD11	1.99	0.45
10:H:123:PHE:HB3	10:H:126:ILE:HG13	1.98	0.45
1:X:1974:U:H2'	1:X:1975:G:H5''	1.99	0.45
1:X:2273:C:H2'	1:X:2274:C:H6	1.82	0.45
5:C:127:ASP:HB2	5:C:129:LYS:HG3	1.99	0.45
12:J:26:ASP:O	12:J:27:TYR:CD1	2.70	0.45
1:X:347:C:H4'	20:R:15:HIS:CD2	2.52	0.45
1:X:1012:A:H2'	1:X:1013:G:O4'	2.16	0.45
1:X:2226:A:H2'	1:X:2227:C:H6	1.81	0.45
1:X:2821:G:H2'	1:X:2822:U:C6	2.51	0.45
3:A:217:ARG:O	3:A:218:LYS:C	2.60	0.45
4:B:59:VAL:HG21	4:B:74:PRO:CB	2.46	0.45
25:W:3:ILE:HD12	25:W:51:LEU:HD13	1.99	0.45
26:Z:16:ARG:O	26:Z:20:ARG:HD2	2.17	0.45
1:X:1882:G:H22	1:X:1885:C:N4	2.08	0.45
1:X:1963:G:O2'	1:X:1965:U:OP2	2.35	0.45
6:D:8:TYR:HB2	6:D:173:MET:HE1	1.97	0.45
15:M:93:ILE:HG21	15:M:96:ARG:HG2	1.99	0.45
25:W:47:VAL:HB	25:W:50:LEU:HD12	1.99	0.45
1:X:2189:A:H2	1:X:2190:A:C5	2.35	0.45
1:X:2691:C:O2'	1:X:2693:U:H5'	2.17	0.45
3:A:252:LYS:HD2	3:A:253:PRO:HD3	1.98	0.45
4:B:23:VAL:HG21	4:B:183:LEU:HD13	1.98	0.45
9:G:66:HIS:HA	16:N:67:ALA:HB1	1.98	0.45
12:J:27:TYR:CZ	21:S:76:ARG:HB3	2.52	0.45
4:B:146:THR:CB	4:B:147:PRO:HD3	2.47	0.45
14:L:38:ILE:CG1	14:L:39:TYR:H	2.18	0.45
1:X:649:G:H22	1:X:660:G:N2	2.15	0.44
1:X:763:A:OP1	1:X:1631:C:N4	2.43	0.44
1:X:1167:A:C8	16:N:51:ARG:HG3	2.52	0.44
1:X:1474:A:H2'	1:X:1474:A:N3	2.32	0.44
13:K:33:ARG:HD3	13:K:112:LEU:HD22	2.00	0.44
15:M:5:ILE:H	15:M:5:ILE:HG13	1.62	0.44
1:X:1142:G:O4'	9:G:107:GLN:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:40:C:H42	2:Y:46:G:H1	1.65	0.44
5:C:45:THR:HG22	5:C:47:THR:OG1	2.17	0.44
7:E:25:LYS:HG3	7:E:34:THR:HG22	1.98	0.44
12:J:77:LYS:HG3	12:J:78:LYS:N	2.32	0.44
17:O:36:LYS:HD2	17:O:54:TYR:HB2	1.99	0.44
20:R:96:LYS:CG	20:R:97:GLN:H	2.31	0.44
1:X:679:C:H2'	1:X:680:U:C6	2.52	0.44
1:X:1833:U:H2'	1:X:1834:G:H8	1.80	0.44
4:B:115:GLY:HA2	4:B:157:ALA:CB	2.47	0.44
6:D:116:GLY:HA2	6:D:176:PRO:HB2	1.99	0.44
7:E:43:VAL:HB	7:E:52:VAL:HG13	1.99	0.44
9:G:58:ILE:HG12	9:G:80:VAL:HG11	1.99	0.44
16:N:75:ASN:ND2	16:N:77:SER:HB3	2.33	0.44
25:W:12:ARG:CG	25:W:12:ARG:NH1	2.72	0.44
1:X:577:U:H5''	1:X:956:A:N6	2.32	0.44
1:X:857:U:H3'	1:X:858:G:H8	1.79	0.44
1:X:2751:C:H5'	4:B:203:LYS:HD3	1.98	0.44
19:Q:11:VAL:HB	19:Q:26:SER:HB2	1.98	0.44
1:X:680:U:H2'	1:X:681:A:H5''	1.99	0.44
1:X:1032:A:C8	1:X:1032:A:H3'	2.52	0.44
3:A:67:PHE:HD2	3:A:153:ALA:HB3	1.83	0.44
3:A:145:LEU:HD13	3:A:163:VAL:HG11	2.00	0.44
1:X:1509:A:H8	1:X:1510:A:C8	2.36	0.44
1:X:1827:G:H1'	1:X:1914:U:C2	2.53	0.44
2:Y:47:A:H8	6:D:92:ARG:CZ	2.30	0.44
3:A:123:ALA:HB3	3:A:131:LEU:HB3	2.00	0.44
9:G:158:HIS:HA	9:G:161:GLN:HB2	2.00	0.44
1:X:1007:A:H4'	16:N:93:LYS:HB3	2.00	0.44
1:X:1465:G:H2'	1:X:1466:C:C6	2.53	0.44
1:X:2445:C:H5''	30:4:6:SER:HB3	2.00	0.44
5:C:164:VAL:HB	5:C:165:SER:H	1.42	0.44
22:T:38:VAL:HG13	22:T:40:GLN:HG2	1.98	0.44
1:X:168:A:H2'	1:X:169:C:C6	2.53	0.44
1:X:400:U:H5	23:U:21:ARG:HH12	1.64	0.44
1:X:1050:G:H1	1:X:1127:C:H42	1.65	0.44
1:X:1385:C:H2'	1:X:1386:A:O4'	2.17	0.44
1:X:457:C:H5''	16:N:3:ARG:HB3	1.99	0.44
1:X:663:G:C5	1:X:664:C:H1'	2.52	0.44
1:X:1583:A:H3'	3:A:86:PRO:HG3	2.00	0.44
2:Y:116:C:H4'	14:L:49:GLN:HG2	2.00	0.44
3:A:67:PHE:CE2	3:A:106:LEU:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:67:PHE:HB3	3:A:153:ALA:H	1.83	0.44
4:B:11:MET:HA	4:B:23:VAL:O	2.17	0.44
4:B:32:PRO:CB	4:B:72:VAL:HG11	2.38	0.44
10:H:105:PRO:HG3	10:H:126:ILE:HD13	1.99	0.44
20:R:22:VAL:HG13	20:R:82:ALA:HA	2.00	0.44
14:L:42:ILE:HD12	14:L:87:VAL:HG21	2.00	0.43
1:X:834:A:H5'	1:X:835:U:C6	2.53	0.43
1:X:1811:A:H3'	3:A:178:PRO:HB2	1.99	0.43
12:J:73:LYS:H	12:J:94:TRP:HD1	1.66	0.43
1:X:465:C:O2'	1:X:483:A:N6	2.52	0.43
5:C:47:THR:HG23	5:C:84:PHE:H	1.83	0.43
5:C:154:ASP:HB2	5:C:157:THR:OG1	2.17	0.43
12:J:86:LYS:H	12:J:86:LYS:HG2	1.68	0.43
1:X:800:U:H5''	1:X:801:A:H5'	2.01	0.43
1:X:1113:C:H2'	1:X:1114:A:C8	2.48	0.43
1:X:1630:A:C2	18:P:114:ALA:HB2	2.54	0.43
1:X:1745:C:OP1	15:M:101:ARG:NH2	2.51	0.43
1:X:1955:G:OP2	3:A:239:ARG:NH1	2.49	0.43
1:X:1973:C:H2'	1:X:1974:U:O4'	2.18	0.43
10:H:28:GLY:HA3	10:H:35:THR:H	1.84	0.43
11:I:81:GLN:HG2	11:I:114:ILE:HG22	1.99	0.43
13:K:11:ASN:OD1	13:K:17:ARG:CZ	2.66	0.43
20:R:56:LYS:HD3	20:R:69:GLN:HG2	1.99	0.43
1:X:534:U:H4'	1:X:564:U:H4'	2.00	0.43
1:X:1731:C:H2'	1:X:1732:U:H3'	1.98	0.43
5:C:58:MET:HB2	5:C:70:GLY:O	2.18	0.43
9:G:103:TYR:CB	9:G:107:GLN:HE21	2.32	0.43
11:I:38:LYS:HB3	11:I:39:SER:H	1.65	0.43
22:T:20:TYR:HB3	22:T:21:LEU:H	1.72	0.43
23:U:33:LYS:O	23:U:34:THR:HB	2.18	0.43
1:X:82:G:N2	1:X:100:G:O2'	2.51	0.43
1:X:224:G:H4'	1:X:399:G:C6	2.53	0.43
1:X:841:G:H2'	1:X:842:A:C8	2.53	0.43
1:X:1674:C:H2'	1:X:1675:C:C6	2.54	0.43
29:3:20:GLY:CA	29:3:21:LYS:CA	2.97	0.43
1:X:163:A:H2'	1:X:164:G:C8	2.54	0.43
1:X:2197:U:H2'	1:X:2198:U:C6	2.54	0.43
3:A:219:PRO:O	3:A:220:HIS:C	2.62	0.43
1:X:1223:G:H5'	1:X:1225:G:O4'	2.18	0.43
1:X:1314:A:H2	1:X:1642:G:N3	2.16	0.43
1:X:1674:C:H2'	1:X:1675:C:H6	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2543:A:C2	1:X:2626:U:H4'	2.54	0.43
9:G:67:ARG:HB3	9:G:70:PHE:HA	2.01	0.43
20:R:37:LEU:HD21	20:R:49:GLU:HG3	2.01	0.43
1:X:310:A:N1	1:X:333:A:O2'	2.42	0.43
1:X:476:G:H2'	1:X:477:A:C8	2.54	0.43
1:X:2189:A:H2	1:X:2190:A:C4	2.37	0.43
1:X:2356:A:H1'	14:L:89:PHE:CZ	2.54	0.43
3:A:213:ARG:C	3:A:215:LEU:H	2.27	0.43
3:A:250:TRP:HB3	3:A:251:GLY:H	1.61	0.43
14:L:89:PHE:CD1	14:L:89:PHE:N	2.71	0.43
28:2:22:MET:CA	28:2:23:LYS:CA	2.97	0.43
1:X:1966:C:H4'	1:X:2585:C:H4'	2.01	0.43
1:X:2633:A:N1	1:X:2644:A:H5''	2.34	0.43
2:Y:43:G:H5'	2:Y:44:C:H5'	2.00	0.43
7:E:17:VAL:HG22	7:E:26:VAL:HG22	2.00	0.43
9:G:70:PHE:CB	16:N:64:ARG:HG2	2.49	0.43
19:Q:58:VAL:HA	19:Q:59:PRO:HD3	1.81	0.43
19:Q:68:PHE:O	19:Q:70:GLY:N	2.51	0.43
1:X:77:C:H42	1:X:106:G:H1	1.66	0.42
1:X:807:A:H2'	1:X:808:C:C6	2.53	0.42
1:X:1699:A:H61	1:X:1723:U:H3	1.66	0.42
4:B:115:GLY:HA2	4:B:157:ALA:HB2	2.00	0.42
10:H:124:MET:O	10:H:127:VAL:HG12	2.18	0.42
18:P:87:GLU:C	18:P:89:ARG:H	2.27	0.42
1:X:312:G:HO2'	1:X:313:U:H6	1.66	0.42
1:X:331:U:O2'	5:C:162:ARG:NH1	2.52	0.42
1:X:830:C:O2'	1:X:852:U:H5''	2.19	0.42
1:X:1367:A:H2'	1:X:1368:G:O4'	2.19	0.42
1:X:1623:C:H4'	1:X:1624:A:O5'	2.19	0.42
4:B:125:GLY:H	4:B:135:HIS:HA	1.84	0.42
10:H:88:THR:HB	15:M:80:VAL:HB	2.00	0.42
17:O:36:LYS:HD3	17:O:39:PHE:HB3	2.01	0.42
1:X:540:G:C5	1:X:2005:U:H5''	2.54	0.42
1:X:2324:G:N3	1:X:2360:C:H2'	2.35	0.42
1:X:2394:G:H4'	11:I:65:PHE:HB3	2.02	0.42
1:X:2581:A:H2'	1:X:2582:G:H4'	2.00	0.42
2:Y:65:A:H2'	2:Y:66:G:H8	1.84	0.42
13:K:8:ARG:O	13:K:9:LYS:HB3	2.19	0.42
13:K:13:ASN:O	13:K:14:SER:C	2.62	0.42
17:O:13:ARG:HB3	17:O:14:VAL:H	1.71	0.42
19:Q:84:GLU:HA	19:Q:86:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1989:C:O2'	1:X:2798:A:N3	2.49	0.42
14:L:66:ASP:C	14:L:68:ALA:H	2.26	0.42
17:O:98:ILE:H	17:O:98:ILE:HG13	1.75	0.42
1:X:334:G:H8	5:C:164:VAL:HG13	1.83	0.42
1:X:1142:G:H5'	9:G:111:LYS:HB3	2.02	0.42
1:X:1658:A:H2'	1:X:1659:G:O4'	2.19	0.42
2:Y:34:C:H2'	2:Y:35:C:C6	2.54	0.42
2:Y:94:G:H5'	21:S:74:ARG:HH12	1.84	0.42
4:B:16:LYS:HB2	4:B:21:ILE:CD1	2.46	0.42
10:H:27:SER:HB3	10:H:50:ILE:HG13	2.01	0.42
11:I:130:ILE:H	11:I:130:ILE:HG13	1.65	0.42
12:J:27:TYR:CE2	21:S:76:ARG:HB3	2.55	0.42
12:J:27:TYR:HE2	21:S:76:ARG:HD3	1.84	0.42
1:X:82:G:N1	1:X:100:G:H2'	2.34	0.42
1:X:636:G:H8	1:X:636:G:C5'	2.33	0.42
1:X:1030:U:C4	1:X:1031:C:H5	2.37	0.42
1:X:2191:A:OP1	1:X:2193:C:N4	2.52	0.42
3:A:186:HIS:HB2	3:A:188:GLU:HG3	2.01	0.42
3:A:247:VAL:HG23	3:A:248:THR:N	2.34	0.42
5:C:27:LEU:O	5:C:31:VAL:HG22	2.19	0.42
5:C:150:LEU:HB3	5:C:169:VAL:HG23	2.00	0.42
5:C:194:GLU:O	5:C:195:ILE:HG12	2.20	0.42
9:G:69:ASP:H	9:G:76:GLN:NE2	2.17	0.42
9:G:106:TYR:CE2	9:G:108:GLY:CA	3.03	0.42
10:H:26:ASN:HB3	10:H:38:GLY:H	1.84	0.42
13:K:28:LEU:HD13	13:K:115:LEU:HD23	2.00	0.42
19:Q:28:TRP:HZ3	19:Q:58:VAL:HG21	1.84	0.42
20:R:46:VAL:HG21	20:R:80:LYS:HE3	2.02	0.42
21:S:23:ALA:HA	21:S:83:PHE:O	2.18	0.42
1:X:110:U:H3'	1:X:111:G:H5''	2.01	0.42
1:X:451:A:H2'	1:X:452:G:C8	2.55	0.42
1:X:1909:U:P	1:X:1912:G:H1	2.42	0.42
1:X:2540:A:O2'	10:H:23:ARG:HG3	2.19	0.42
1:X:2663:U:C4	1:X:2664:G:N7	2.88	0.42
3:A:43:ARG:N	3:A:43:ARG:HH11	2.17	0.42
3:A:108:PRO:HB3	3:A:143:HIS:HE1	1.84	0.42
5:C:95:LEU:HD23	5:C:96:PRO:HD2	2.00	0.42
6:D:17:MET:HG2	6:D:22:TYR:HB2	2.01	0.42
7:E:19:ALA:HB1	7:E:24:PHE:HD2	1.84	0.42
9:G:65:LYS:HD2	9:G:66:HIS:CD2	2.54	0.42
14:L:63:ASN:HB3	14:L:66:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:39:VAL:HA	15:M:45:THR:HA	2.02	0.42
20:R:105:ARG:HH22	20:R:112:LYS:CA	2.33	0.42
26:Z:36:CYS:HB3	26:Z:49:CYS:HB3	1.91	0.42
29:3:10:ALA:CA	29:3:11:LYS:CA	2.98	0.42
1:X:503:G:H2'	1:X:504:G:O4'	2.20	0.42
1:X:648:A:H4'	1:X:649:G:O4'	2.20	0.42
1:X:1441:A:H4'	1:X:1442:C:O5'	2.19	0.42
1:X:1766:U:O4	1:X:1780:A:H2	2.02	0.42
19:Q:59:PRO:HA	19:Q:74:ASP:OD1	2.19	0.42
1:X:2542:U:O2	1:X:2544:A:H8	2.03	0.42
3:A:231:HIS:HD2	3:A:233:HIS:N	2.04	0.42
19:Q:35:LYS:HA	19:Q:38:ILE:HG22	2.01	0.42
1:X:543:G:H5'	16:N:24:PHE:CE1	2.55	0.42
1:X:760:U:O2	1:X:1997:A:H1'	2.20	0.42
1:X:1845:A:N3	1:X:2212:U:O2'	2.50	0.42
1:X:2674:C:H2'	1:X:2675:U:H6	1.85	0.42
9:G:43:VAL:HB	9:G:167:LYS:HG2	2.02	0.42
1:X:1151:U:H3'	9:G:91:THR:HG21	2.01	0.41
1:X:1378:A:H3'	1:X:1379:A:H8	1.85	0.41
1:X:1939:U:O2	1:X:1939:U:H2'	2.18	0.41
1:X:2315:A:H2	1:X:2364:C:O2	2.03	0.41
2:Y:8:C:H4'	2:Y:30:C:H5'	2.01	0.41
3:A:208:LYS:HE3	3:A:208:LYS:HA	2.01	0.41
4:B:183:LEU:HD11	15:M:16:ILE:CG2	2.50	0.41
12:J:36:ILE:HD12	12:J:133:VAL:HG21	2.01	0.41
15:M:34:ARG:HB2	15:M:91:VAL:HG23	2.02	0.41
21:S:168:VAL:HG12	21:S:169:VAL:HG23	2.01	0.41
1:X:171:G:H2'	1:X:172:A:O4'	2.20	0.41
1:X:1300:A:H5'	13:K:103:ARG:HD2	2.01	0.41
1:X:2065:A:H2'	1:X:2066:G:O4'	2.20	0.41
1:X:2326:C:H2'	1:X:2327:U:C6	2.55	0.41
1:X:2326:C:C2	1:X:2327:U:C5	3.08	0.41
5:C:164:VAL:C	5:C:166:TRP:N	2.77	0.41
15:M:66:PHE:CE2	15:M:81:PHE:HB2	2.55	0.41
1:X:577:U:C5'	1:X:956:A:N6	2.84	0.41
4:B:134:TRP:CD1	4:B:134:TRP:N	2.83	0.41
6:D:38:GLU:HG3	6:D:40:LEU:HD23	2.01	0.41
9:G:162:LYS:H	9:G:163:PRO:CD	2.33	0.41
22:T:46:LYS:HB2	22:T:78:PHE:CE2	2.56	0.41
23:U:49:LYS:HB2	23:U:61:TRP:CD2	2.56	0.41
1:X:1231:A:H2'	1:X:1232:U:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2820:C:H5''	15:M:60:SER:HB3	2.02	0.41
5:C:48:ARG:C	5:C:50:GLN:N	2.78	0.41
5:C:62:LYS:HE2	5:C:62:LYS:HB3	1.72	0.41
14:L:30:SER:O	14:L:40:ALA:HA	2.21	0.41
17:O:60:VAL:HA	17:O:93:ILE:HG22	2.03	0.41
4:B:5:LEU:HD22	4:B:49:ILE:HG22	2.02	0.41
6:D:48:LYS:H	6:D:48:LYS:HG3	1.67	0.41
11:I:87:THR:HB	11:I:97:ARG:HD3	2.02	0.41
24:V:2:LYS:H	24:V:3:PRO:CD	2.34	0.41
1:X:558:G:H4'	1:X:559:C:C5'	2.48	0.41
1:X:573:C:HO2'	1:X:1266:G:H1	1.68	0.41
1:X:636:G:C5'	1:X:636:G:C8	3.04	0.41
1:X:1442:C:O2'	1:X:1443:G:H5'	2.19	0.41
1:X:2406:C:C5'	1:X:2408:G:H5'	2.50	0.41
3:A:141:VAL:HG13	3:A:162:SER:HB3	2.02	0.41
5:C:12:GLY:O	5:C:14:THR:N	2.49	0.41
13:K:51:LEU:HD12	13:K:66:VAL:HG22	2.02	0.41
15:M:39:VAL:HG12	15:M:45:THR:HG23	2.01	0.41
19:Q:90:ALA:C	19:Q:92:ALA:H	2.28	0.41
1:X:346:C:O2	1:X:347:C:C5	2.73	0.41
1:X:564:U:H2'	1:X:565:A:H8	1.83	0.41
1:X:1283:C:H5''	1:X:1284:G:O5'	2.21	0.41
1:X:1813:A:O5'	1:X:1813:A:H8	2.04	0.41
4:B:149:ARG:CZ	9:G:106:TYR:CD1	3.03	0.41
6:D:104:ILE:HA	6:D:108:LEU:HD12	2.03	0.41
15:M:24:LEU:HD12	15:M:83:PHE:CG	2.56	0.41
15:M:58:ASN:HD22	15:M:58:ASN:H	1.67	0.41
16:N:93:LYS:HE2	17:O:5:ILE:HD13	2.03	0.41
18:P:43:ASP:OD2	18:P:46:ARG:NH2	2.54	0.41
21:S:47:SER:OG	21:S:48:THR:N	2.51	0.41
1:X:393:U:H2'	1:X:394:U:H6	1.85	0.41
1:X:1919:A:C2	1:X:1926:U:N3	2.67	0.41
4:B:183:LEU:HD21	15:M:16:ILE:HD13	2.02	0.41
5:C:173:ALA:HB1	5:C:193:LEU:HD13	2.02	0.41
23:U:10:LYS:HD2	23:U:60:VAL:HG11	2.02	0.41
1:X:162:C:H2'	1:X:163:A:H8	1.85	0.41
1:X:172:A:N6	1:X:175:C:H3'	2.34	0.41
1:X:405:C:H2'	1:X:406:G:C8	2.53	0.41
1:X:1032:A:H2'	1:X:1034:U:H5''	2.03	0.41
1:X:1179:A:H2'	1:X:1180:A:C8	2.56	0.41
1:X:1687:C:O5'	1:X:1687:C:H6	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2206:C:H1'	3:A:262:LYS:HE2	2.03	0.41
3:A:202:LYS:C	3:A:204:ILE:H	2.29	0.41
5:C:117:LEU:HB3	5:C:187:VAL:HA	2.02	0.41
10:H:114:VAL:HG22	10:H:133:VAL:HG22	2.02	0.41
11:I:102:LYS:O	11:I:104:ARG:N	2.37	0.41
13:K:106:ASP:OD1	13:K:108:VAL:HB	2.21	0.41
17:O:40:VAL:HG13	17:O:45:THR:HG22	2.01	0.41
21:S:149:ALA:HB1	21:S:160:LEU:HD13	2.02	0.41
1:X:1467:U:C6	1:X:1467:U:C5'	3.04	0.41
1:X:1795:C:H5'	3:A:257:LEU:HD13	2.02	0.41
1:X:2189:A:C2	1:X:2190:A:C5	3.09	0.41
11:I:30:ALA:HB3	11:I:34:HIS:CE1	2.56	0.41
11:I:54:SER:O	11:I:56:LEU:N	2.50	0.41
13:K:3:HIS:CE1	13:K:5:LYS:HZ2	2.31	0.41
16:N:17:VAL:HG11	16:N:36:PHE:HB2	2.02	0.41
19:Q:72:ARG:H	19:Q:72:ARG:HG2	1.65	0.41
22:T:21:LEU:HD11	22:T:41:ARG:CZ	2.51	0.41
1:X:82:G:H1	1:X:100:G:H2'	1.86	0.40
1:X:219:G:O2'	1:X:231:G:O6	2.37	0.40
1:X:573:C:H5''	17:O:74:TYR:OH	2.21	0.40
1:X:689:A:H2	1:X:815:A:H61	1.68	0.40
1:X:2262:C:C2	1:X:2368:G:C2	3.10	0.40
3:A:205:VAL:O	3:A:207:GLY:N	2.54	0.40
11:I:76:LYS:HG2	11:I:111:SER:HB2	2.03	0.40
12:J:35:LEU:HD23	12:J:105:PHE:HD2	1.86	0.40
12:J:133:VAL:HG12	21:S:76:ARG:CZ	2.51	0.40
13:K:49:GLU:OE1	13:K:95:THR:HB	2.21	0.40
16:N:93:LYS:H	16:N:93:LYS:HG3	1.69	0.40
20:R:93:ARG:HE	20:R:108:VAL:HG12	1.86	0.40
22:T:3:HIS:HD2	22:T:5:LYS:HB2	1.85	0.40
1:X:1235:C:H2'	1:X:1236:G:C8	2.57	0.40
1:X:1467:U:C2'	1:X:1468:A:OP1	2.68	0.40
1:X:2855:C:H1'	13:K:92:GLY:O	2.22	0.40
1:X:2864:C:H2'	1:X:2865:G:C8	2.57	0.40
2:Y:64:C:H2'	2:Y:65:A:H8	1.85	0.40
3:A:202:LYS:C	3:A:204:ILE:N	2.79	0.40
4:B:77:ILE:HD13	15:M:3:THR:HG22	2.02	0.40
9:G:119:LEU:HD23	9:G:122:HIS:HD2	1.85	0.40
12:J:26:ASP:HB3	12:J:27:TYR:H	1.60	0.40
16:N:22:LYS:C	16:N:24:PHE:H	2.29	0.40
16:N:86:ALA:HB2	16:N:116:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:424:G:H4'	1:X:425:A:O5'	2.21	0.40
1:X:636:G:H5''	1:X:636:G:C8	2.53	0.40
1:X:1142:G:OP2	1:X:2494:C:H5''	2.21	0.40
1:X:2551:A:N7	4:B:145:LYS:HB2	2.37	0.40
15:M:27:PHE:CE2	15:M:91:VAL:HG11	2.56	0.40
1:X:309:G:H5''	1:X:310:A:OP1	2.21	0.40
1:X:2556:A:H5''	1:X:2557:G:H5'	2.04	0.40
3:A:244:ARG:C	3:A:252:LYS:HE3	2.46	0.40
6:D:177:PHE:HB2	6:D:179:LYS:HE3	2.02	0.40
9:G:62:ILE:CG2	9:G:135:LEU:HD21	2.50	0.40
9:G:67:ARG:HE	9:G:70:PHE:C	2.30	0.40
17:O:10:LYS:HA	17:O:36:LYS:HA	2.03	0.40
20:R:17:LYS:C	20:R:19:GLY:H	2.29	0.40
1:X:89:A:C4'	1:X:90:G:H5''	2.52	0.40
1:X:393:U:H2'	1:X:394:U:C6	2.57	0.40
1:X:761:G:OP2	18:P:109:ARG:HG3	2.21	0.40
1:X:1151:U:H4'	1:X:1153:A:H5''	2.04	0.40
1:X:1287:A:H2'	1:X:1288:A:H5''	2.03	0.40
1:X:2482:A:H4'	1:X:2483:U:OP1	2.21	0.40
32:X:2929:1F2:H46	32:X:2929:1F2:O41	2.21	0.40
3:A:60:ARG:HD3	3:A:86:PRO:HB2	2.04	0.40
5:C:48:ARG:HB2	5:C:51:VAL:HG22	2.02	0.40
13:K:17:ARG:HD3	13:K:17:ARG:HA	2.00	0.40
19:Q:6:ILE:HG22	19:Q:7:LEU:HD23	2.01	0.40
19:Q:66:GLY:C	19:Q:68:PHE:N	2.77	0.40
20:R:48:VAL:HG12	20:R:50:GLY:H	1.86	0.40
26:Z:45:ILE:HG21	26:Z:57:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	238/274 (87%)	178 (75%)	39 (16%)	21 (9%)	0	3
4	B	203/211 (96%)	171 (84%)	24 (12%)	8 (4%)	2	18
5	C	195/205 (95%)	129 (66%)	45 (23%)	21 (11%)	0	2
6	D	175/180 (97%)	141 (81%)	27 (15%)	7 (4%)	2	17
7	E	169/185 (91%)	139 (82%)	20 (12%)	10 (6%)	1	10
8	F	69/144 (48%)	57 (83%)	10 (14%)	2 (3%)	3	24
9	G	140/174 (80%)	105 (75%)	21 (15%)	14 (10%)	0	2
10	H	132/134 (98%)	115 (87%)	11 (8%)	6 (4%)	2	15
11	I	139/156 (89%)	85 (61%)	28 (20%)	26 (19%)	0	0
12	J	134/141 (95%)	101 (75%)	19 (14%)	14 (10%)	0	2
13	K	111/116 (96%)	92 (83%)	11 (10%)	8 (7%)	1	6
14	L	102/114 (90%)	75 (74%)	19 (19%)	8 (8%)	1	5
15	M	106/166 (64%)	89 (84%)	13 (12%)	4 (4%)	2	18
16	N	115/118 (98%)	92 (80%)	17 (15%)	6 (5%)	1	12
17	O	92/100 (92%)	67 (73%)	13 (14%)	12 (13%)	0	1
18	P	125/134 (93%)	108 (86%)	12 (10%)	5 (4%)	2	17
19	Q	91/95 (96%)	64 (70%)	14 (15%)	13 (14%)	0	1
20	R	108/115 (94%)	66 (61%)	24 (22%)	18 (17%)	0	0
21	S	173/237 (73%)	135 (78%)	28 (16%)	10 (6%)	1	10
22	T	82/91 (90%)	64 (78%)	11 (13%)	7 (8%)	0	3
23	U	70/81 (86%)	43 (61%)	16 (23%)	11 (16%)	0	0
24	V	64/67 (96%)	58 (91%)	4 (6%)	2 (3%)	3	22
25	W	53/55 (96%)	50 (94%)	3 (6%)	0	100	100
26	Z	56/60 (93%)	48 (86%)	5 (9%)	3 (5%)	1	12
30	4	35/37 (95%)	31 (89%)	3 (9%)	1 (3%)	3	24
All	All	2977/3390 (88%)	2303 (77%)	437 (15%)	237 (8%)	1	4

All (237) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	56	GLY
3	A	89	SER
3	A	198	ASN
3	A	199	ALA

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Mol	Chain	Res	Type
3	A	249	PRO
3	A	250	TRP
4	B	116	VAL
4	B	146	THR
5	C	13	ARG
5	C	20	PRO
5	C	60	GLY
5	C	67	ALA
5	C	121	ASP
5	C	129	LYS
5	C	164	VAL
5	C	165	SER
5	C	172	VAL
5	C	195	ILE
6	D	81	GLN
7	E	55	PRO
7	E	126	PRO
7	E	165	VAL
9	G	34	PRO
9	G	67	ARG
9	G	91	THR
9	G	104	THR
9	G	107	GLN
9	G	158	HIS
10	H	27	SER
10	H	29	ILE
11	I	18	ARG
11	I	37	GLN
11	I	39	SER
11	I	55	ARG
11	I	62	LYS
11	I	98	LEU
11	I	99	VAL
11	I	103	ASN
12	J	13	GLN
12	J	21	ASP
12	J	26	ASP
13	K	6	ALA
13	K	9	LYS
14	L	21	THR
15	M	26	ASP
15	M	29	PRO

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Mol	Chain	Res	Type
16	N	7	GLY
16	N	87	ASN
17	O	7	THR
17	O	9	GLY
17	O	10	LYS
17	O	14	VAL
17	O	31	ASP
17	O	48	GLY
19	Q	6	ILE
19	Q	12	ILE
19	Q	67	ARG
19	Q	69	ILE
19	Q	90	ALA
20	R	5	SER
20	R	11	ASN
21	S	26	LYS
22	T	19	LYS
23	U	15	VAL
23	U	19	ILE
23	U	29	GLY
23	U	60	VAL
24	V	2	LYS
26	Z	4	HIS
26	Z	36	CYS
26	Z	53	ASP
3	A	87	ASN
3	A	206	LEU
3	A	248	THR
4	B	76	ARG
4	B	123	ALA
4	B	148	GLY
5	C	22	VAL
5	C	84	PHE
6	D	124	GLY
7	E	13	SER
9	G	64	GLY
9	G	97	ASP
9	G	170	PRO
11	I	47	ALA
11	I	49	PHE
11	I	54	SER
11	I	56	LEU

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Mol	Chain	Res	Type
11	I	64	GLY
11	I	86	THR
12	J	11	ARG
12	J	80	ALA
12	J	83	ARG
13	K	4	GLY
13	K	92	GLY
14	L	33	ARG
14	L	40	ALA
14	L	46	SER
17	O	8	GLY
17	O	60	VAL
18	P	9	ARG
19	Q	74	ASP
19	Q	84	GLU
19	Q	87	SER
19	Q	89	GLU
20	R	7	GLY
20	R	60	PRO
20	R	83	LEU
20	R	85	ASP
20	R	98	ILE
20	R	108	VAL
21	S	5	ALA
21	S	88	TYR
21	S	91	PRO
21	S	156	GLU
22	T	21	LEU
22	T	74	LYS
23	U	27	ASP
23	U	32	ARG
23	U	41	VAL
23	U	56	GLN
24	V	57	LYS
3	A	170	SER
3	A	220	HIS
3	A	244	ARG
4	B	90	SER
5	C	15	ILE
5	C	190	ALA
6	D	122	PHE
7	E	19	ALA

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Mol	Chain	Res	Type
7	E	58	ALA
7	E	173	ALA
8	F	120	VAL
9	G	33	ILE
9	G	37	ASP
10	H	5	GLN
10	H	37	GLY
11	I	29	THR
11	I	65	PHE
11	I	82	ASP
11	I	88	PHE
11	I	115	SER
12	J	60	ARG
12	J	81	GLU
13	K	11	ASN
14	L	20	THR
16	N	92	ARG
16	N	95	LEU
17	O	13	ARG
17	O	36	LYS
17	O	49	GLU
18	P	132	GLY
19	Q	5	ASP
19	Q	59	PRO
19	Q	63	LYS
20	R	6	ALA
20	R	18	LYS
20	R	26	SER
20	R	50	GLY
20	R	62	MET
20	R	63	THR
20	R	96	LYS
21	S	76	ARG
21	S	106	GLY
3	A	59	LYS
4	B	137	ARG
5	C	72	ARG
5	C	196	VAL
6	D	42	SER
7	E	7	GLN
9	G	163	PRO
11	I	91	ASP

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Mol	Chain	Res	Type
13	K	8	ARG
13	K	14	SER
13	K	88	ALA
14	L	59	LEU
15	M	25	PRO
16	N	94	VAL
19	Q	13	SER
21	S	6	LYS
22	T	13	GLY
22	T	73	GLY
23	U	34	THR
23	U	48	LYS
3	A	35	GLU
3	A	54	ILE
3	A	55	GLY
3	A	187	SER
3	A	219	PRO
5	C	4	ILE
5	C	11	GLY
5	C	66	ASN
5	C	126	ALA
6	D	10	ASP
6	D	40	LEU
7	E	80	SER
9	G	68	PRO
10	H	41	ASN
10	H	42	LYS
11	I	19	VAL
11	I	101	ARG
12	J	29	ALA
12	J	30	PHE
12	J	78	LYS
14	L	53	ALA
16	N	8	ILE
18	P	20	LEU
18	P	81	HIS
18	P	85	MET
21	S	56	VAL
22	T	11	LYS
22	T	27	GLY
30	4	13	ASN
3	A	252	LYS

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Mol	Chain	Res	Type
3	A	255	LYS
5	C	171	PRO
6	D	121	ALA
9	G	105	GLY
11	I	9	THR
11	I	84	GLU
12	J	28	VAL
12	J	82	THR
20	R	75	ALA
21	S	110	GLY
23	U	74	PRO
4	B	72	VAL
8	F	118	GLY
11	I	44	GLY
11	I	68	VAL
12	J	91	VAL
20	R	19	GLY
14	L	38	ILE
15	M	28	ARG
17	O	22	VAL
20	R	64	ASN
3	A	197	GLY
7	E	136	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	185/215 (86%)	146 (79%)	39 (21%)	1	6
4	B	155/157 (99%)	126 (81%)	29 (19%)	1	9
5	C	157/163 (96%)	119 (76%)	38 (24%)	1	4
6	D	153/156 (98%)	132 (86%)	21 (14%)	3	18
7	E	136/144 (94%)	122 (90%)	14 (10%)	7	28
8	F	51/107 (48%)	47 (92%)	4 (8%)	11	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	118/146 (81%)	93 (79%)	25 (21%)	1	6
10	H	103/103 (100%)	81 (79%)	22 (21%)	1	6
11	I	108/121 (89%)	75 (69%)	33 (31%)	0	1
12	J	110/115 (96%)	87 (79%)	23 (21%)	1	6
13	K	90/93 (97%)	67 (74%)	23 (26%)	0	3
14	L	74/82 (90%)	54 (73%)	20 (27%)	0	2
15	M	94/134 (70%)	66 (70%)	28 (30%)	0	1
16	N	96/97 (99%)	81 (84%)	15 (16%)	2	13
17	O	75/79 (95%)	53 (71%)	22 (29%)	0	1
18	P	109/115 (95%)	88 (81%)	21 (19%)	1	8
19	Q	75/76 (99%)	61 (81%)	14 (19%)	1	9
20	R	91/96 (95%)	69 (76%)	22 (24%)	1	4
21	S	149/192 (78%)	125 (84%)	24 (16%)	2	13
22	T	62/67 (92%)	55 (89%)	7 (11%)	5	24
23	U	57/66 (86%)	36 (63%)	21 (37%)	0	0
24	V	54/55 (98%)	45 (83%)	9 (17%)	2	11
25	W	48/48 (100%)	36 (75%)	12 (25%)	0	3
26	Z	51/53 (96%)	38 (74%)	13 (26%)	0	3
30	4	35/35 (100%)	30 (86%)	5 (14%)	3	16
All	All	2436/2715 (90%)	1932 (79%)	504 (21%)	1	7

All (504) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	39	LYS
3	A	40	THR
3	A	43	ARG
3	A	44	ASN
3	A	46	ARG
3	A	48	ARG
3	A	49	ILE
3	A	50	THR
3	A	52	ARG
3	A	54	ILE
3	A	63	ARG

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Mol	Chain	Res	Type
3	A	68	LYS
3	A	69	ARG
3	A	76	ASN
3	A	88	ARG
3	A	92	ILE
3	A	101	GLU
3	A	105	ILE
3	A	111	LEU
3	A	117	VAL
3	A	145	LEU
3	A	157	ARG
3	A	169	GLU
3	A	183	ARG
3	A	196	VAL
3	A	198	ASN
3	A	203	ASN
3	A	208	LYS
3	A	215	LEU
3	A	218	LYS
3	A	226	MET
3	A	229	VAL
3	A	240	THR
3	A	244	ARG
3	A	245	VAL
3	A	252	LYS
3	A	259	THR
3	A	260	ARG
3	A	264	LYS
4	B	5	LEU
4	B	14	ILE
4	B	19	ARG
4	B	37	LYS
4	B	41	THR
4	B	47	VAL
4	B	49	ILE
4	B	69	LYS
4	B	72	VAL
4	B	77	ILE
4	B	82	ARG
4	B	87	ASP
4	B	105	THR
4	B	111	LYS

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Mol	Chain	Res	Type
4	B	117	MET
4	B	119	ARG
4	B	131	SER
4	B	133	LYS
4	B	134	TRP
4	B	137	ARG
4	B	141	ILE
4	B	145	LYS
4	B	149	ARG
4	B	150	VAL
4	B	154	LYS
4	B	162	MET
4	B	163	GLU
4	B	175	ILE
4	B	203	LYS
5	C	4	ILE
5	C	5	ASN
5	C	10	ASN
5	C	13	ARG
5	C	14	THR
5	C	15	ILE
5	C	17	LEU
5	C	31	VAL
5	C	45	THR
5	C	48	ARG
5	C	51	VAL
5	C	62	LYS
5	C	72	ARG
5	C	90	SER
5	C	95	LEU
5	C	98	GLN
5	C	102	LEU
5	C	104	LEU
5	C	117	LEU
5	C	118	VAL
5	C	121	ASP
5	C	124	ASP
5	C	127	ASP
5	C	130	THR
5	C	143	ASP
5	C	148	VAL
5	C	150	LEU

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Mol	Chain	Res	Type
5	C	153	ASP
5	C	154	ASP
5	C	164	VAL
5	C	168	SER
5	C	172	VAL
5	C	175	VAL
5	C	176	ASN
5	C	180	ILE
5	C	181	LEU
5	C	188	ILE
5	C	194	GLU
6	D	10	ASP
6	D	40	LEU
6	D	45	GLU
6	D	48	LYS
6	D	51	ASP
6	D	67	ILE
6	D	74	ILE
6	D	79	LEU
6	D	80	ARG
6	D	81	GLN
6	D	83	MET
6	D	89	VAL
6	D	100	LEU
6	D	112	ARG
6	D	117	ILE
6	D	125	ARG
6	D	130	LEU
6	D	150	ARG
6	D	153	ASP
6	D	171	GLN
6	D	175	LEU
7	E	7	GLN
7	E	35	VAL
7	E	39	THR
7	E	48	ASP
7	E	50	LEU
7	E	53	GLU
7	E	59	GLN
7	E	67	LEU
7	E	69	ARG
7	E	98	LEU

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Mol	Chain	Res	Type
7	E	106	ASN
7	E	130	ARG
7	E	140	LEU
7	E	143	GLN
8	F	78	ILE
8	F	84	ILE
8	F	110	THR
8	F	111	LYS
9	G	31	THR
9	G	37	ASP
9	G	38	GLU
9	G	43	VAL
9	G	53	ARG
9	G	56	THR
9	G	62	ILE
9	G	63	ARG
9	G	70	PHE
9	G	71	THR
9	G	75	ILE
9	G	90	LEU
9	G	98	LYS
9	G	101	THR
9	G	104	THR
9	G	112	THR
9	G	113	GLU
9	G	127	ILE
9	G	132	PHE
9	G	145	HIS
9	G	154	GLU
9	G	165	VAL
9	G	166	LEU
9	G	168	THR
9	G	169	GLN
10	H	7	ARG
10	H	8	LEU
10	H	20	MET
10	H	22	ILE
10	H	23	ARG
10	H	27	SER
10	H	29	ILE
10	H	36	THR
10	H	41	ASN

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Mol	Chain	Res	Type
10	H	47	VAL
10	H	81	ILE
10	H	89	ILE
10	H	94	ASN
10	H	97	VAL
10	H	99	ILE
10	H	102	GLN
10	H	106	ARG
10	H	114	VAL
10	H	120	ASP
10	H	122	ARG
10	H	126	ILE
10	H	127	VAL
11	I	6	LEU
11	I	12	SER
11	I	13	ARG
11	I	18	ARG
11	I	21	ARG
11	I	26	THR
11	I	27	ASP
11	I	29	THR
11	I	38	LYS
11	I	39	SER
11	I	48	PHE
11	I	53	ARG
11	I	56	LEU
11	I	57	ILE
11	I	60	LEU
11	I	62	LYS
11	I	63	ARG
11	I	65	PHE
11	I	73	GLU
11	I	83	LEU
11	I	85	ASP
11	I	86	THR
11	I	87	THR
11	I	93	LEU
11	I	98	LEU
11	I	99	VAL
11	I	101	ARG
11	I	106	VAL
11	I	114	ILE

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Mol	Chain	Res	Type
11	I	118	VAL
11	I	120	VAL
11	I	123	ASP
11	I	130	ILE
12	J	7	ARG
12	J	8	THR
12	J	17	ARG
12	J	21	ASP
12	J	26	ASP
12	J	44	LYS
12	J	45	SER
12	J	47	GLN
12	J	64	LYS
12	J	65	ILE
12	J	68	ARG
12	J	72	ASP
12	J	81	GLU
12	J	82	THR
12	J	86	LYS
12	J	88	LYS
12	J	91	VAL
12	J	94	TRP
12	J	95	VAL
12	J	97	VAL
12	J	114	GLN
12	J	129	GLN
12	J	134	LYS
13	K	5	LYS
13	K	8	ARG
13	K	10	LEU
13	K	11	ASN
13	K	12	ARG
13	K	17	ARG
13	K	28	LEU
13	K	35	GLN
13	K	37	THR
13	K	45	ARG
13	K	51	LEU
13	K	62	SER
13	K	73	LYS
13	K	83	VAL
13	K	89	GLU

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Mol	Chain	Res	Type
13	K	94	TYR
13	K	95	THR
13	K	99	ARG
13	K	102	THR
13	K	106	ASP
13	K	109	THR
13	K	114	GLU
13	K	115	LEU
14	L	8	ARG
14	L	9	ARG
14	L	11	LEU
14	L	13	THR
14	L	17	VAL
14	L	31	VAL
14	L	33	ARG
14	L	36	LYS
14	L	43	ILE
14	L	59	LEU
14	L	64	LYS
14	L	66	ASP
14	L	67	THR
14	L	87	VAL
14	L	89	PHE
14	L	90	ASP
14	L	91	ARG
14	L	95	LYS
14	L	99	ARG
14	L	108	ARG
15	M	2	GLN
15	M	5	ILE
15	M	6	LYS
15	M	7	ILE
15	M	12	LEU
15	M	13	LEU
15	M	16	ILE
15	M	22	ARG
15	M	28	ARG
15	M	33	VAL
15	M	34	ARG
15	M	35	VAL
15	M	36	ASP
15	M	37	THR

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Mol	Chain	Res	Type
15	M	40	ARG
15	M	57	ILE
15	M	62	SER
15	M	64	LYS
15	M	68	VAL
15	M	71	ILE
15	M	88	VAL
15	M	89	ASN
15	M	92	THR
15	M	93	ILE
15	M	95	GLU
15	M	96	ARG
15	M	98	LYS
15	M	104	LEU
16	N	8	ILE
16	N	13	ARG
16	N	16	LYS
16	N	22	LYS
16	N	30	LYS
16	N	58	ARG
16	N	60	LEU
16	N	71	LEU
16	N	78	THR
16	N	85	ARG
16	N	88	ILE
16	N	90	LEU
16	N	92	ARG
16	N	93	LYS
16	N	102	GLU
17	O	13	ARG
17	O	14	VAL
17	O	18	ASP
17	O	20	ILE
17	O	21	ARG
17	O	24	SER
17	O	25	LEU
17	O	26	GLN
17	O	28	GLU
17	O	35	LEU
17	O	40	VAL
17	O	43	GLU
17	O	46	VAL

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Mol	Chain	Res	Type
17	O	56	VAL
17	O	69	ILE
17	O	71	ILE
17	O	78	VAL
17	O	84	THR
17	O	87	ARG
17	O	88	GLN
17	O	96	LEU
17	O	98	ILE
18	P	8	PHE
18	P	9	ARG
18	P	11	LYS
18	P	17	GLN
18	P	21	ARG
18	P	32	ARG
18	P	36	ARG
18	P	37	LYS
18	P	42	VAL
18	P	45	ILE
18	P	48	LYS
18	P	49	SER
18	P	62	ARG
18	P	87	GLU
18	P	106	LEU
18	P	109	ARG
18	P	118	LYS
18	P	119	LYS
18	P	124	ILE
18	P	125	THR
18	P	126	ILE
19	Q	7	LEU
19	Q	12	ILE
19	Q	14	GLU
19	Q	26	SER
19	Q	34	THR
19	Q	38	ILE
19	Q	40	ASP
19	Q	42	ILE
19	Q	58	VAL
19	Q	63	LYS
19	Q	65	VAL
19	Q	79	ILE

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Mol	Chain	Res	Type
19	Q	80	VAL
19	Q	84	GLU
20	R	11	ASN
20	R	13	LYS
20	R	15	HIS
20	R	18	LYS
20	R	23	ILE
20	R	25	LEU
20	R	37	LEU
20	R	38	LEU
20	R	42	ARG
20	R	46	VAL
20	R	53	VAL
20	R	73	GLU
20	R	80	LYS
20	R	83	LEU
20	R	85	ASP
20	R	88	THR
20	R	96	LYS
20	R	98	ILE
20	R	104	VAL
20	R	105	ARG
20	R	106	VAL
20	R	108	VAL
21	S	3	LEU
21	S	13	LYS
21	S	14	LEU
21	S	15	ASP
21	S	22	VAL
21	S	26	LYS
21	S	40	ASP
21	S	56	VAL
21	S	65	LEU
21	S	67	LYS
21	S	71	MET
21	S	79	ILE
21	S	93	GLU
21	S	100	THR
21	S	108	VAL
21	S	115	ILE
21	S	120	LEU
21	S	128	ARG

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Mol	Chain	Res	Type
21	S	130	ILE
21	S	132	GLN
21	S	134	LEU
21	S	145	ASP
21	S	152	ILE
21	S	166	LEU
22	T	16	SER
22	T	17	ASN
22	T	37	LEU
22	T	38	VAL
22	T	46	LYS
22	T	49	GLN
22	T	62	LEU
23	U	8	THR
23	U	10	LYS
23	U	11	LYS
23	U	17	SER
23	U	19	ILE
23	U	21	ARG
23	U	32	ARG
23	U	35	THR
23	U	37	ILE
23	U	40	ARG
23	U	42	GLN
23	U	43	ARG
23	U	45	ASN
23	U	47	HIS
23	U	57	VAL
23	U	60	VAL
23	U	62	LEU
23	U	63	SER
23	U	65	ASN
23	U	78	ILE
23	U	79	GLU
24	V	1	MET
24	V	10	GLN
24	V	19	ASP
24	V	21	ARG
24	V	28	LEU
24	V	37	LEU
24	V	44	ARG
24	V	53	LEU

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Mol	Chain	Res	Type
24	V	65	GLU
25	W	2	LYS
25	W	3	ILE
25	W	9	VAL
25	W	10	ILE
25	W	12	ARG
25	W	26	ARG
25	W	30	ASP
25	W	34	VAL
25	W	37	THR
25	W	45	LYS
25	W	46	THR
25	W	53	VAL
26	Z	4	HIS
26	Z	6	VAL
26	Z	8	LYS
26	Z	11	THR
26	Z	18	MET
26	Z	26	THR
26	Z	31	THR
26	Z	35	GLN
26	Z	40	LYS
26	Z	41	LEU
26	Z	53	ASP
26	Z	57	VAL
26	Z	58	LEU
30	4	2	LYS
30	4	9	LYS
30	4	13	ASN
30	4	26	ILE
30	4	30	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	154	GLN
3	A	164	GLN
3	A	231	HIS
4	B	129	HIS
4	B	192	ASN
5	C	5	ASN
5	C	61	GLN

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Mol	Chain	Res	Type
5	C	66	ASN
6	D	37	ASN
6	D	81	GLN
6	D	129	ASN
7	E	20	GLN
7	E	106	ASN
7	E	143	GLN
7	E	147	ASN
9	G	36	ASN
9	G	73	ASN
9	G	76	GLN
9	G	122	HIS
10	H	41	ASN
11	I	34	HIS
11	I	37	GLN
11	I	66	ASN
12	J	47	GLN
12	J	58	HIS
12	J	124	HIS
13	K	13	ASN
14	L	41	GLN
14	L	49	GLN
16	N	31	GLN
16	N	41	ASN
16	N	52	ASN
16	N	66	ASN
16	N	72	HIS
16	N	91	ASN
17	O	11	GLN
17	O	79	GLN
17	O	88	GLN
18	P	78	ASN
18	P	81	HIS
19	Q	8	GLN
19	Q	86	GLN
20	R	10	HIS
20	R	29	HIS
20	R	44	GLN
20	R	52	ASN
21	S	29	ASN
22	T	3	HIS
22	T	17	ASN

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Mol	Chain	Res	Type
22	T	57	HIS
23	U	16	ASN
23	U	42	GLN
25	W	49	HIS
25	W	54	GLN
26	Z	29	ASN
26	Z	35	GLN
26	Z	43	HIS
26	Z	44	HIS
30	4	29	ASN
30	4	34	GLN
30	4	36	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2683/2880 (93%)	712 (26%)	252 (9%)
2	Y	121/123 (98%)	27 (22%)	7 (5%)
All	All	2804/3003 (93%)	739 (26%)	259 (9%)

All (739) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	G
1	X	7	G
1	X	34	U
1	X	45	C
1	X	48	A
1	X	49	U
1	X	50	G
1	X	51	A
1	X	54	G
1	X	55	A
1	X	63	A
1	X	69	G
1	X	70	A
1	X	71	A
1	X	72	A
1	X	74	G
1	X	75	C
1	X	82	G

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Mol	Chain	Res	Type
1	X	83	A
1	X	84	G
1	X	89	A
1	X	90	G
1	X	91	A
1	X	92	U
1	X	97	U
1	X	98	U
1	X	99	U
1	X	100	G
1	X	101	A
1	X	107	G
1	X	108	G
1	X	111	G
1	X	116	A
1	X	117	A
1	X	118	U
1	X	123	A
1	X	127	C
1	X	129	A
1	X	138	G
1	X	143	A
1	X	147	G
1	X	154	U
1	X	155	G
1	X	158	A
1	X	173	A
1	X	174	A
1	X	176	A
1	X	177	U
1	X	181	A
1	X	182	G
1	X	192	G
1	X	193	A
1	X	198	A
1	X	199	A
1	X	200	A
1	X	204	A
1	X	205	A
1	X	206	U
1	X	207	U
1	X	210	A

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Mol	Chain	Res	Type
1	X	219	G
1	X	225	G
1	X	228	A
1	X	229	G
1	X	238	G
1	X	242	A
1	X	243	G
1	X	245	C
1	X	246	C
1	X	304	A
1	X	305	A
1	X	306	G
1	X	310	A
1	X	312	G
1	X	313	U
1	X	319	G
1	X	321	A
1	X	322	A
1	X	323	G
1	X	329	C
1	X	332	C
1	X	333	A
1	X	334	G
1	X	335	A
1	X	340	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	344	G
1	X	358	C
1	X	360	A
1	X	388	G
1	X	393	U
1	X	396	U
1	X	397	U
1	X	399	G
1	X	400	U
1	X	401	G
1	X	409	G
1	X	412	U
1	X	414	A
1	X	416	U

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Mol	Chain	Res	Type
1	X	418	C
1	X	419	G
1	X	424	G
1	X	425	A
1	X	431	G
1	X	433	G
1	X	434	C
1	X	435	A
1	X	441	A
1	X	454	G
1	X	455	A
1	X	456	C
1	X	458	G
1	X	459	A
1	X	461	A
1	X	463	C
1	X	467	U
1	X	468	A
1	X	469	G
1	X	470	U
1	X	482	A
1	X	486	U
1	X	491	A
1	X	492	G
1	X	504	G
1	X	513	A
1	X	514	G
1	X	515	A
1	X	518	A
1	X	519	C
1	X	520	C
1	X	522	G
1	X	523	A
1	X	539	A
1	X	540	G
1	X	541	C
1	X	542	A
1	X	543	G
1	X	554	U
1	X	555	U
1	X	556	A
1	X	557	U

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Mol	Chain	Res	Type
1	X	558	G
1	X	559	C
1	X	560	G
1	X	572	G
1	X	580	A
1	X	582	G
1	X	583	C
1	X	584	A
1	X	595	A
1	X	602	C
1	X	613	A
1	X	614	G
1	X	620	G
1	X	624	A
1	X	625	A
1	X	627	A
1	X	628	A
1	X	631	G
1	X	632	A
1	X	633	G
1	X	636	G
1	X	648	A
1	X	649	G
1	X	652	C
1	X	654	A
1	X	655	A
1	X	657	A
1	X	664	C
1	X	665	A
1	X	666	U
1	X	667	U
1	X	681	A
1	X	682	G
1	X	683	A
1	X	684	C
1	X	690	A
1	X	695	G
1	X	698	A
1	X	699	G
1	X	700	C
1	X	714	G
1	X	715	U

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Mol	Chain	Res	Type
1	X	723	C
1	X	728	G
1	X	729	A
1	X	730	C
1	X	732	G
1	X	742	G
1	X	743	A
1	X	751	G
1	X	752	G
1	X	760	U
1	X	766	A
1	X	777	A
1	X	778	G
1	X	782	U
1	X	783	G
1	X	788	G
1	X	789	G
1	X	790	A
1	X	795	A
1	X	797	A
1	X	798	G
1	X	801	A
1	X	802	A
1	X	803	C
1	X	804	C
1	X	805	G
1	X	806	A
1	X	807	A
1	X	814	G
1	X	815	A
1	X	816	U
1	X	818	G
1	X	819	C
1	X	824	U
1	X	825	C
1	X	832	A
1	X	840	U
1	X	841	G
1	X	858	G
1	X	859	U
1	X	860	U
1	X	871	U

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Mol	Chain	Res	Type
1	X	872	G
1	X	873	U
1	X	878	C
1	X	879	A
1	X	880	C
1	X	919	U
1	X	922	A
1	X	926	C
1	X	931	G
1	X	938	G
1	X	939	C
1	X	940	G
1	X	941	U
1	X	943	U
1	X	944	A
1	X	952	A
1	X	955	G
1	X	956	A
1	X	957	G
1	X	964	A
1	X	968	C
1	X	969	U
1	X	970	A
1	X	972	C
1	X	973	U
1	X	985	G
1	X	994	A
1	X	995	A
1	X	996	C
1	X	1000	G
1	X	1001	A
1	X	1006	C
1	X	1007	A
1	X	1010	U
1	X	1014	G
1	X	1016	C
1	X	1019	U
1	X	1020	A
1	X	1022	A
1	X	1023	U
1	X	1024	G
1	X	1033	G

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Mol	Chain	Res	Type
1	X	1034	U
1	X	1035	G
1	X	1036	G
1	X	1037	U
1	X	1038	U
1	X	1044	U
1	X	1052	C
1	X	1053	G
1	X	1054	C
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1058	G
1	X	1059	A
1	X	1068	A
1	X	1069	G
1	X	1070	G
1	X	1072	U
1	X	1073	G
1	X	1077	U
1	X	1078	A
1	X	1079	G
1	X	1081	A
1	X	1082	G
1	X	1086	C
1	X	1087	C
1	X	1090	C
1	X	1094	C
1	X	1097	A
1	X	1098	G
1	X	1099	A
1	X	1100	G
1	X	1107	A
1	X	1108	U
1	X	1121	G
1	X	1122	A
1	X	1123	G
1	X	1124	U
1	X	1128	G
1	X	1129	A
1	X	1139	A
1	X	1140	A

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Mol	Chain	Res	Type
1	X	1141	U
1	X	1142	G
1	X	1143	A
1	X	1145	C
1	X	1146	G
1	X	1152	C
1	X	1153	A
1	X	1161	U
1	X	1162	A
1	X	1182	U
1	X	1185	C
1	X	1187	A
1	X	1189	G
1	X	1192	A
1	X	1194	U
1	X	1223	G
1	X	1224	A
1	X	1233	A
1	X	1234	C
1	X	1250	A
1	X	1251	G
1	X	1262	U
1	X	1264	C
1	X	1266	G
1	X	1269	G
1	X	1275	A
1	X	1281	A
1	X	1282	A
1	X	1284	G
1	X	1285	A
1	X	1286	U
1	X	1288	A
1	X	1289	A
1	X	1299	A
1	X	1300	A
1	X	1302	C
1	X	1313	U
1	X	1314	A
1	X	1315	A
1	X	1316	G
1	X	1319	C
1	X	1334	A

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Mol	Chain	Res	Type
1	X	1342	U
1	X	1345	G
1	X	1346	C
1	X	1356	G
1	X	1357	U
1	X	1358	C
1	X	1359	G
1	X	1365	U
1	X	1370	U
1	X	1378	A
1	X	1379	A
1	X	1381	G
1	X	1392	U
1	X	1404	C
1	X	1409	U
1	X	1410	U
1	X	1412	C
1	X	1413	U
1	X	1425	G
1	X	1428	G
1	X	1429	A
1	X	1432	G
1	X	1433	A
1	X	1434	U
1	X	1435	G
1	X	1439	G
1	X	1440	G
1	X	1441	A
1	X	1442	C
1	X	1443	G
1	X	1451	C
1	X	1459	U
1	X	1460	G
1	X	1465	G
1	X	1467	U
1	X	1468	A
1	X	1469	U
1	X	1470	G
1	X	1474	A
1	X	1475	U
1	X	1476	G
1	X	1482	U

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Mol	Chain	Res	Type
1	X	1483	G
1	X	1489	C
1	X	1490	U
1	X	1496	G
1	X	1497	C
1	X	1498	G
1	X	1505	U
1	X	1506	C
1	X	1508	G
1	X	1509	A
1	X	1513	U
1	X	1514	C
1	X	1523	A
1	X	1524	C
1	X	1525	A
1	X	1528	C
1	X	1531	C
1	X	1545	G
1	X	1551	U
1	X	1552	C
1	X	1553	G
1	X	1554	G
1	X	1562	G
1	X	1563	U
1	X	1570	C
1	X	1571	G
1	X	1574	A
1	X	1575	C
1	X	1576	G
1	X	1582	A
1	X	1585	A
1	X	1594	U
1	X	1600	U
1	X	1601	U
1	X	1602	G
1	X	1603	A
1	X	1607	A
1	X	1608	U
1	X	1613	G
1	X	1624	A
1	X	1625	A
1	X	1626	A

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Mol	Chain	Res	Type
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1635	G
1	X	1648	C
1	X	1651	U
1	X	1657	A
1	X	1661	C
1	X	1665	C
1	X	1680	U
1	X	1681	A
1	X	1685	A
1	X	1686	A
1	X	1691	G
1	X	1710	U
1	X	1711	C
1	X	1712	G
1	X	1713	G
1	X	1716	G
1	X	1717	A
1	X	1724	C
1	X	1732	U
1	X	1733	U
1	X	1734	C
1	X	1747	G
1	X	1749	G
1	X	1750	A
1	X	1754	G
1	X	1755	G
1	X	1760	G
1	X	1764	A
1	X	1775	A
1	X	1776	A
1	X	1777	A
1	X	1778	U
1	X	1782	A
1	X	1790	G
1	X	1791	C
1	X	1792	C
1	X	1793	A
1	X	1799	A
1	X	1800	A

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Mol	Chain	Res	Type
1	X	1801	C
1	X	1808	C
1	X	1810	U
1	X	1811	A
1	X	1812	U
1	X	1819	U
1	X	1821	A
1	X	1825	C
1	X	1839	A
1	X	1840	A
1	X	1850	G
1	X	1861	G
1	X	1867	A
1	X	1882	G
1	X	1883	A
1	X	1886	G
1	X	1910	A
1	X	1912	G
1	X	1913	G
1	X	1914	U
1	X	1919	A
1	X	1920	A
1	X	1921	A
1	X	1923	U
1	X	1924	C
1	X	1927	U
1	X	1938	U
1	X	1939	U
1	X	1943	A
1	X	1946	U
1	X	1947	G
1	X	1950	C
1	X	1953	A
1	X	1954	A
1	X	1955	G
1	X	1964	A
1	X	1965	U
1	X	1972	G
1	X	1975	G
1	X	1976	U
1	X	1979	C
1	X	1980	A

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Mol	Chain	Res	Type
1	X	1981	A
1	X	2003	A
1	X	2005	U
1	X	2006	G
1	X	2010	G
1	X	2014	A
1	X	2015	G
1	X	2018	G
1	X	2019	C
1	X	2026	C
1	X	2035	G
1	X	2038	C
1	X	2039	G
1	X	2044	G
1	X	2045	A
1	X	2046	C
1	X	2052	G
1	X	2063	A
1	X	2075	U
1	X	2076	G
1	X	2084	G
1	X	2089	C
1	X	2166	G
1	X	2171	U
1	X	2181	A
1	X	2189	A
1	X	2190	A
1	X	2191	A
1	X	2195	C
1	X	2196	U
1	X	2197	U
1	X	2199	C
1	X	2204	A
1	X	2205	C
1	X	2217	G
1	X	2218	G
1	X	2222	U
1	X	2230	G
1	X	2254	C
1	X	2255	G
1	X	2259	G
1	X	2262	C

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Mol	Chain	Res	Type
1	X	2265	A
1	X	2266	A
1	X	2267	A
1	X	2268	G
1	X	2283	G
1	X	2284	U
1	X	2285	U
1	X	2286	G
1	X	2287	G
1	X	2288	A
1	X	2290	A
1	X	2291	U
1	X	2298	U
1	X	2299	A
1	X	2300	G
1	X	2301	A
1	X	2304	G
1	X	2305	C
1	X	2306	A
1	X	2313	G
1	X	2314	A
1	X	2315	A
1	X	2318	U
1	X	2323	U
1	X	2324	G
1	X	2326	C
1	X	2329	C
1	X	2330	G
1	X	2351	G
1	X	2358	C
1	X	2362	G
1	X	2363	G
1	X	2364	C
1	X	2370	G
1	X	2371	A
1	X	2379	G
1	X	2381	A
1	X	2385	U
1	X	2389	G
1	X	2396	C
1	X	2401	A
1	X	2402	U

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Mol	Chain	Res	Type
1	X	2404	A
1	X	2405	A
1	X	2406	C
1	X	2408	G
1	X	2409	A
1	X	2410	U
1	X	2414	A
1	X	2415	G
1	X	2420	C
1	X	2426	G
1	X	2427	A
1	X	2438	A
1	X	2447	G
1	X	2448	A
1	X	2452	U
1	X	2453	C
1	X	2455	A
1	X	2473	G
1	X	2475	C
1	X	2477	C
1	X	2478	C
1	X	2481	G
1	X	2482	A
1	X	2483	U
1	X	2484	G
1	X	2494	C
1	X	2497	A
1	X	2498	U
1	X	2499	C
1	X	2504	G
1	X	2508	G
1	X	2509	A
1	X	2514	G
1	X	2545	A
1	X	2546	G
1	X	2552	C
1	X	2553	G
1	X	2557	G
1	X	2560	G
1	X	2561	G
1	X	2562	G
1	X	2565	C

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Mol	Chain	Res	Type
1	X	2581	A
1	X	2582	G
1	X	2588	U
1	X	2589	C
1	X	2591	C
1	X	2594	U
1	X	2608	A
1	X	2611	A
1	X	2613	A
1	X	2633	A
1	X	2635	U
1	X	2640	G
1	X	2643	G
1	X	2650	G
1	X	2661	G
1	X	2664	G
1	X	2668	U
1	X	2691	C
1	X	2692	A
1	X	2693	U
1	X	2694	G
1	X	2705	A
1	X	2706	U
1	X	2713	A
1	X	2718	A
1	X	2728	A
1	X	2731	G
1	X	2732	C
1	X	2737	A
1	X	2738	A
1	X	2739	G
1	X	2745	A
1	X	2758	A
1	X	2759	U
1	X	2760	G
1	X	2770	A
1	X	2771	C
1	X	2774	U
1	X	2775	U
1	X	2776	U
1	X	2777	A
1	X	2778	U

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Mol	Chain	Res	Type
1	X	2779	C
1	X	2780	A
1	X	2782	G
1	X	2795	A
1	X	2796	A
1	X	2798	A
1	X	2808	U
1	X	2809	A
1	X	2810	A
1	X	2811	G
1	X	2824	C
1	X	2825	A
1	X	2843	A
1	X	2846	G
1	X	2847	G
1	X	2848	A
1	X	2849	C
1	X	2854	G
1	X	2859	U
1	X	2864	C
1	X	2866	A
1	X	2868	G
2	Y	4	C
2	Y	11	G
2	Y	12	C
2	Y	14	C
2	Y	15	A
2	Y	17	A
2	Y	18	G
2	Y	27	A
2	Y	28	A
2	Y	37	C
2	Y	39	C
2	Y	40	C
2	Y	42	U
2	Y	43	G
2	Y	44	C
2	Y	46	G
2	Y	47	A
2	Y	59	A
2	Y	69	G
2	Y	75	A

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Mol	Chain	Res	Type
2	Y	76	U
2	Y	102	A
2	Y	110	U
2	Y	112	A
2	Y	115	G
2	Y	121	G
2	Y	123	U

All (259) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	13	A
1	X	33	C
1	X	34	U
1	X	48	A
1	X	49	U
1	X	50	G
1	X	62	U
1	X	70	A
1	X	71	A
1	X	73	A
1	X	74	G
1	X	82	G
1	X	83	A
1	X	89	A
1	X	98	U
1	X	99	U
1	X	100	G
1	X	117	A
1	X	154	U
1	X	173	A
1	X	176	A
1	X	181	A
1	X	182	G
1	X	198	A
1	X	199	A
1	X	204	A
1	X	242	A
1	X	312	G
1	X	321	A
1	X	322	A
1	X	328	A

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Mol	Chain	Res	Type
1	X	332	C
1	X	334	G
1	X	341	A
1	X	342	G
1	X	343	A
1	X	387	A
1	X	396	U
1	X	399	G
1	X	416	U
1	X	417	C
1	X	418	C
1	X	419	G
1	X	434	C
1	X	454	G
1	X	458	G
1	X	466	A
1	X	467	U
1	X	469	G
1	X	504	G
1	X	513	A
1	X	522	G
1	X	539	A
1	X	540	G
1	X	542	A
1	X	557	U
1	X	558	G
1	X	559	C
1	X	580	A
1	X	631	G
1	X	648	A
1	X	652	C
1	X	664	C
1	X	672	C
1	X	677	G
1	X	681	A
1	X	682	G
1	X	683	A
1	X	698	A
1	X	714	G
1	X	751	G
1	X	765	C
1	X	775	U

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Mol	Chain	Res	Type
1	X	777	A
1	X	788	G
1	X	803	C
1	X	806	A
1	X	813	A
1	X	814	G
1	X	818	G
1	X	824	U
1	X	840	U
1	X	842	A
1	X	858	G
1	X	859	U
1	X	860	U
1	X	871	U
1	X	872	G
1	X	878	C
1	X	938	G
1	X	939	C
1	X	955	G
1	X	969	U
1	X	972	C
1	X	990	A
1	X	994	A
1	X	995	A
1	X	1000	G
1	X	1006	C
1	X	1007	A
1	X	1019	U
1	X	1032	A
1	X	1036	G
1	X	1038	U
1	X	1053	G
1	X	1055	A
1	X	1056	U
1	X	1057	A
1	X	1069	G
1	X	1072	U
1	X	1080	A
1	X	1081	A
1	X	1086	C
1	X	1096	A
1	X	1099	A

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Mol	Chain	Res	Type
1	X	1122	A
1	X	1141	U
1	X	1142	G
1	X	1152	C
1	X	1185	C
1	X	1186	G
1	X	1223	G
1	X	1233	A
1	X	1249	G
1	X	1266	G
1	X	1288	A
1	X	1289	A
1	X	1291	G
1	X	1299	A
1	X	1314	A
1	X	1315	A
1	X	1333	G
1	X	1345	G
1	X	1355	A
1	X	1357	U
1	X	1403	U
1	X	1404	C
1	X	1409	U
1	X	1412	C
1	X	1429	A
1	X	1433	A
1	X	1434	U
1	X	1439	G
1	X	1441	A
1	X	1442	C
1	X	1459	U
1	X	1473	U
1	X	1475	U
1	X	1482	U
1	X	1496	G
1	X	1508	G
1	X	1513	U
1	X	1552	C
1	X	1562	G
1	X	1570	C
1	X	1574	A
1	X	1575	C

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Mol	Chain	Res	Type
1	X	1601	U
1	X	1602	G
1	X	1607	A
1	X	1613	G
1	X	1624	A
1	X	1631	C
1	X	1632	A
1	X	1634	A
1	X	1680	U
1	X	1684	G
1	X	1685	A
1	X	1710	U
1	X	1711	C
1	X	1716	G
1	X	1732	U
1	X	1749	G
1	X	1770	U
1	X	1775	A
1	X	1777	A
1	X	1790	G
1	X	1799	A
1	X	1800	A
1	X	1810	U
1	X	1811	A
1	X	1820	G
1	X	1839	A
1	X	1871	G
1	X	1882	G
1	X	1883	A
1	X	1909	U
1	X	1920	A
1	X	1923	U
1	X	1938	U
1	X	1953	A
1	X	1963	G
1	X	1975	G
1	X	1980	A
1	X	2005	U
1	X	2014	A
1	X	2018	G
1	X	2045	A
1	X	2075	U

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Mol	Chain	Res	Type
1	X	2083	G
1	X	2088	U
1	X	2165	A
1	X	2189	A
1	X	2193	C
1	X	2204	A
1	X	2217	G
1	X	2228	U
1	X	2254	C
1	X	2261	G
1	X	2265	A
1	X	2290	A
1	X	2298	U
1	X	2299	A
1	X	2305	C
1	X	2312	A
1	X	2314	A
1	X	2323	U
1	X	2354	G
1	X	2363	G
1	X	2370	G
1	X	2381	A
1	X	2401	A
1	X	2447	G
1	X	2477	C
1	X	2482	A
1	X	2497	A
1	X	2498	U
1	X	2508	G
1	X	2551	A
1	X	2560	G
1	X	2561	G
1	X	2564	U
1	X	2565	C
1	X	2580	C
1	X	2634	G
1	X	2660	C
1	X	2691	C
1	X	2705	A
1	X	2731	G
1	X	2738	A
1	X	2758	A

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Mol	Chain	Res	Type
1	X	2770	A
1	X	2777	A
1	X	2778	U
1	X	2808	U
1	X	2810	A
1	X	2824	C
1	X	2846	G
1	X	2848	A
1	X	2854	G
1	X	2867	G
1	X	2876	C
2	Y	4	C
2	Y	11	G
2	Y	14	C
2	Y	46	G
2	Y	58	G
2	Y	59	A
2	Y	86	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 35 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	1F2	X	2929	-	59,60,60	2.06	14 (23%)	80,90,90	2.18	26 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	1F2	X	2929	-	-	1/74/115/115	0/5/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	2929	1F2	C30-N29	9.38	1.46	1.33
32	X	2929	1F2	C8-C10	4.40	1.59	1.52
32	X	2929	1F2	C5-N29	3.70	1.52	1.45
32	X	2929	1F2	O11-C12	-3.57	1.26	1.34
32	X	2929	1F2	C10-C9	-3.31	1.46	1.55
32	X	2929	1F2	C17-C2	3.27	1.60	1.53
32	X	2929	1F2	O11-C7	3.18	1.51	1.46
32	X	2929	1F2	C2-C5	-3.09	1.50	1.54
32	X	2929	1F2	O18-C6	-2.93	1.43	1.47
32	X	2929	1F2	C13-C12	-2.83	1.45	1.51
32	X	2929	1F2	C25-C6	2.51	1.57	1.52
32	X	2929	1F2	C15-C14	-2.36	1.48	1.54
32	X	2929	1F2	C15-C9	-2.25	1.49	1.54
32	X	2929	1F2	O18-C30	-2.25	1.33	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F2	C5-N29-C30	-6.77	103.55	112.39
32	X	2929	1F2	C24-C7-C6	-5.42	107.76	115.23
32	X	2929	1F2	C48-C47-N45	5.06	107.56	101.93
32	X	2929	1F2	O16-C4-C2	-4.41	114.51	120.64
32	X	2929	1F2	O31-C30-N29	-4.18	124.25	129.19
32	X	2929	1F2	O46-C44-N45	-4.03	119.63	124.21
32	X	2929	1F2	O11-C12-C13	3.76	119.57	111.53
32	X	2929	1F2	C3-C4-C2	3.74	125.44	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	X	2929	1F2	C22-C15-C14	3.59	117.73	111.40
32	X	2929	1F2	C22-C15-C9	3.33	119.72	112.42
32	X	2929	1F2	C50-N45-C47	-2.97	108.54	111.88
32	X	2929	1F2	O19-C10-C9	2.92	113.59	107.82
32	X	2929	1F2	C10-C9-C15	2.89	117.95	113.54
32	X	2929	1F2	C8-C10-C9	-2.87	106.72	110.18
32	X	2929	1F2	C32-C37-C36	2.81	113.66	109.15
32	X	2929	1F2	O1-C14-C13	-2.66	103.12	107.84
32	X	2929	1F2	C54-N55-C56	2.63	121.46	116.85
32	X	2929	1F2	C32-O21-C9	-2.61	111.82	116.26
32	X	2929	1F2	O27-C12-C13	-2.52	117.57	124.11
32	X	2929	1F2	C7-O11-C12	2.39	122.38	118.20
32	X	2929	1F2	O19-C10-C8	2.38	110.72	105.71
32	X	2929	1F2	O18-C30-O31	2.23	124.53	121.64
32	X	2929	1F2	C28-C13-C14	-2.18	108.12	113.00
32	X	2929	1F2	O33-C34-C42	-2.12	102.90	106.88
32	X	2929	1F2	O11-C7-C6	2.08	110.18	105.48
32	X	2929	1F2	O1-C44-O46	-2.06	120.66	124.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	X	2929	1F2	C35-C36-N38-C40

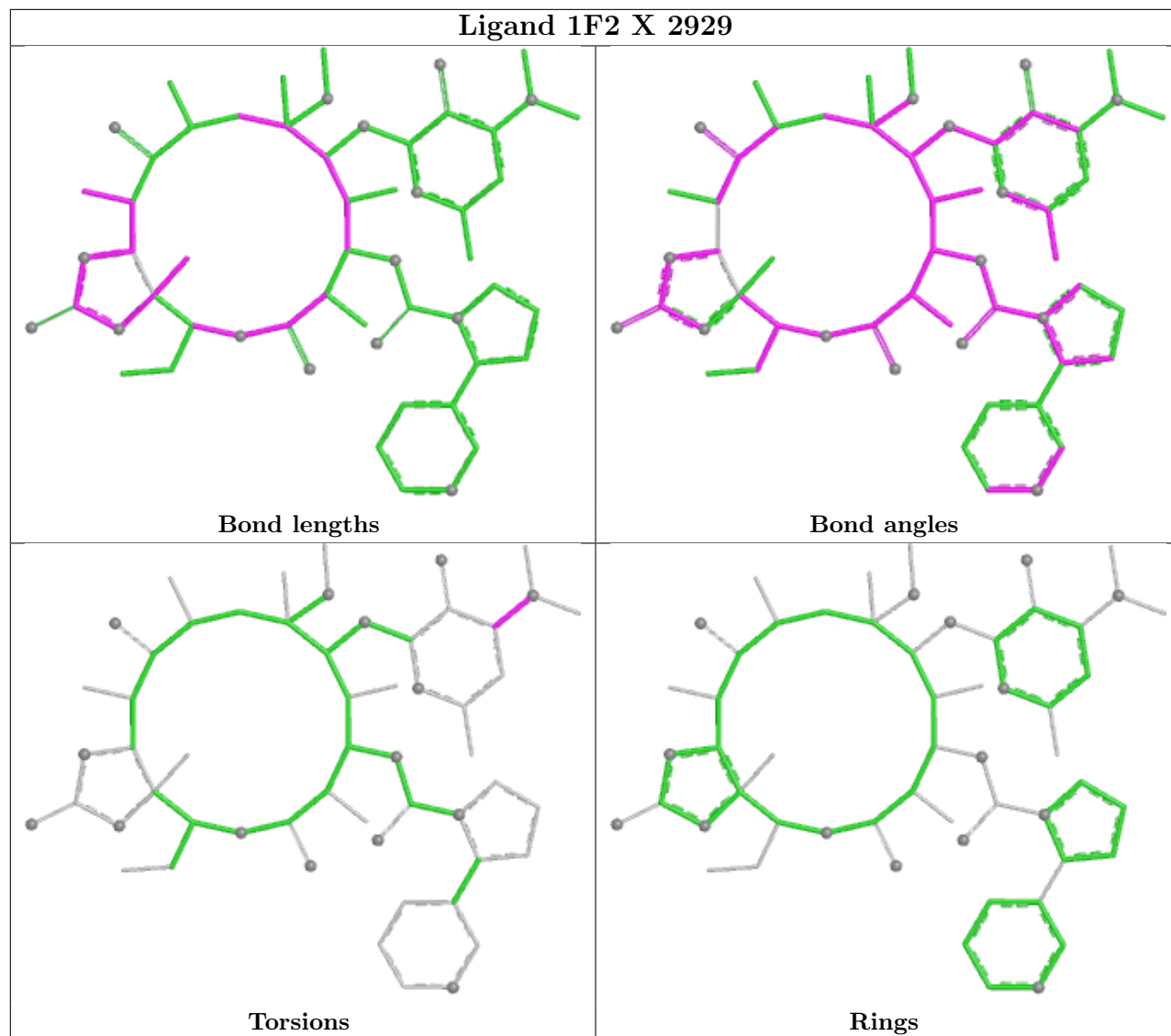
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	2929	1F2	3	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	X	2686/2880 (93%)	0.31	159 (5%)	28	18	43, 92, 197, 276	0
2	Y	122/123 (99%)	0.87	16 (13%)	7	6	83, 136, 170, 192	0
3	A	240/274 (87%)	1.30	56 (23%)	2	2	68, 116, 146, 173	0
4	B	205/211 (97%)	0.35	10 (4%)	35	22	45, 73, 106, 154	0
5	C	197/205 (96%)	1.40	49 (24%)	2	2	57, 114, 155, 187	0
6	D	177/180 (98%)	1.42	53 (29%)	1	1	146, 183, 216, 227	0
7	E	171/185 (92%)	1.00	23 (13%)	7	5	92, 143, 192, 206	0
8	F	71/144 (49%)	1.99	30 (42%)	0	1	211, 236, 252, 257	0
9	G	142/174 (81%)	1.37	37 (26%)	1	2	73, 97, 145, 161	0
10	H	134/134 (100%)	0.22	5 (3%)	45	28	50, 70, 96, 120	0
11	I	141/156 (90%)	2.20	54 (38%)	1	1	67, 129, 174, 204	0
12	J	136/141 (96%)	1.20	34 (25%)	2	2	74, 103, 149, 184	0
13	K	113/116 (97%)	0.28	8 (7%)	22	14	35, 60, 79, 91	0
14	L	104/114 (91%)	1.69	39 (37%)	1	1	98, 134, 156, 168	0
15	M	108/166 (65%)	0.31	6 (5%)	30	19	50, 73, 111, 144	0
16	N	117/118 (99%)	0.75	14 (11%)	9	6	60, 90, 127, 160	0
17	O	94/100 (94%)	1.11	19 (20%)	3	2	67, 115, 156, 173	0
18	P	127/134 (94%)	0.11	3 (2%)	59	40	50, 67, 108, 158	0
19	Q	93/95 (97%)	0.91	16 (17%)	4	3	73, 106, 162, 195	0
20	R	110/115 (95%)	1.40	32 (29%)	1	1	88, 117, 170, 178	0
21	S	175/237 (73%)	1.25	43 (24%)	2	2	121, 155, 175, 190	0
22	T	84/91 (92%)	1.29	18 (21%)	2	2	80, 108, 186, 199	0
23	U	72/81 (88%)	2.04	29 (40%)	0	1	92, 128, 153, 162	0
24	V	66/67 (98%)	0.68	7 (10%)	11	8	100, 132, 211, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
25	W	55/55 (100%)	0.27	2 (3%)	46	28	81, 98, 126, 152	0
26	Z	58/60 (96%)	0.57	4 (6%)	23	14	49, 71, 105, 113	0
27	1	53/55 (96%)	5.73	40 (75%)	0	0	8, 32, 61, 96	0
28	2	46/47 (97%)	6.41	38 (82%)	0	0	3, 16, 37, 59	0
29	3	63/66 (95%)	6.05	39 (61%)	0	0	3, 25, 40, 60	0
30	4	37/37 (100%)	4.91	29 (78%)	0	0	227, 254, 265, 269	0
All	All	5997/6561 (91%)	0.88	912 (15%)	5	4	3, 100, 196, 276	0

All (912) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	3	28	GLY	41.9
27	1	2	ALA	32.4
27	1	7	ARG	31.8
29	3	60	LEU	23.0
28	2	46	ASP	21.9
29	3	63	PRO	21.5
29	3	2	PRO	20.9
29	3	13	ARG	17.5
27	1	52	GLU	16.9
27	1	44	ALA	16.4
29	3	19	THR	14.7
29	3	22	VAL	14.5
29	3	3	LYS	14.3
28	2	14	LYS	13.5
29	3	38	GLY	13.3
29	3	17	THR	13.3
29	3	9	MET	13.2
28	2	21	ARG	13.1
28	2	26	SER	12.9
29	3	39	ASP	12.9
28	2	34	ARG	12.7
29	3	51	ALA	12.6
28	2	4	THR	12.5
9	G	97	ASP	12.4
28	2	27	GLY	11.9
28	2	31	LEU	11.7
27	1	3	LYS	11.5
27	1	46	LYS	11.3
30	4	6	SER	11.3

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Mol	Chain	Res	Type	RSRZ
26	Z	2	ALA	11.3
28	2	1	MET	11.0
30	4	5	SER	10.7
29	3	43	GLY	10.6
30	4	4	ARG	10.4
11	I	52	GLY	10.3
27	1	43	VAL	10.1
27	1	33	ALA	10.0
11	I	29	THR	9.9
29	3	34	THR	9.7
27	1	4	ASP	9.7
27	1	5	GLY	9.6
27	1	21	TYR	9.5
28	2	15	THR	9.4
6	D	42	SER	9.3
30	4	23	VAL	9.2
5	C	44	SER	9.1
1	X	248	A	9.1
30	4	31	LYS	9.0
11	I	48	PHE	9.0
27	1	14	SER	8.8
29	3	33	ASN	8.8
28	2	38	GLY	8.7
11	I	63	ARG	8.7
30	4	2	LYS	8.7
28	2	9	ASN	8.6
3	A	220	HIS	8.5
27	1	27	ASN	8.4
12	J	84	MET	8.4
8	F	126	THR	8.4
12	J	141	ALA	8.4
30	4	8	LYS	8.3
30	4	19	ARG	8.3
28	2	13	ALA	8.2
23	U	47	HIS	8.1
28	2	36	ALA	7.9
8	F	115	LEU	7.9
11	I	9	THR	7.9
17	O	36	LYS	7.8
28	2	43	THR	7.7
30	4	17	VAL	7.7
30	4	21	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
29	3	4	MET	7.7
3	A	203	ASN	7.7
30	4	3	VAL	7.6
29	3	40	GLU	7.6
28	2	35	ARG	7.6
5	C	47	THR	7.5
11	I	6	LEU	7.5
22	T	9	SER	7.4
28	2	11	LYS	7.3
28	2	41	GLN	7.3
30	4	36	GLN	7.1
11	I	53	ARG	7.1
6	D	43	SER	7.0
27	1	54	LYS	6.9
28	2	10	ARG	6.8
11	I	8	PRO	6.8
30	4	18	ARG	6.8
29	3	41	ILE	6.7
1	X	731	A	6.7
28	2	32	ALA	6.6
28	2	3	ARG	6.6
29	3	18	GLY	6.6
30	4	37	GLY	6.6
2	Y	123	U	6.4
28	2	30	ILE	6.4
1	X	940	G	6.3
29	3	58	MET	6.2
11	I	32	ARG	6.1
17	O	5	ILE	6.1
23	U	39	LYS	6.0
4	B	135	HIS	6.0
11	I	31	GLY	5.9
23	U	52	ARG	5.9
30	4	20	HIS	5.9
14	L	58	ALA	5.9
9	G	129	HIS	5.8
9	G	110	LEU	5.8
29	3	30	ARG	5.8
20	R	77	HIS	5.8
16	N	48	ARG	5.8
9	G	103	TYR	5.6
29	3	31	HIS	5.6

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Mol	Chain	Res	Type	RSRZ
5	C	57	LYS	5.6
6	D	153	ASP	5.5
27	1	18	THR	5.5
3	A	219	PRO	5.5
23	U	8	THR	5.5
6	D	85	VAL	5.5
27	1	45	LYS	5.5
3	A	33	LEU	5.5
27	1	15	SER	5.4
5	C	66	ASN	5.3
29	3	45	GLY	5.3
17	O	34	GLU	5.3
14	L	54	ALA	5.3
11	I	12	SER	5.3
5	C	19	LEU	5.3
8	F	127	VAL	5.2
17	O	10	LYS	5.2
9	G	40	ASN	5.2
14	L	41	GLN	5.2
30	4	1	MET	5.2
17	O	11	GLN	5.2
11	I	30	ALA	5.2
27	1	51	ARG	5.2
1	X	1552	C	5.2
14	L	57	ALA	5.2
13	K	17	ARG	5.1
1	X	1092	U	5.1
28	2	40	HIS	5.1
11	I	54	SER	5.1
11	I	28	LYS	5.1
28	2	7	PRO	5.0
20	R	78	ALA	5.0
11	I	64	GLY	5.0
3	A	151	LYS	5.0
1	X	1083	C	5.0
9	G	100	TYR	5.0
1	X	558	G	5.0
30	4	15	LYS	5.0
28	2	8	ASN	4.9
11	I	56	LEU	4.9
14	L	97	HIS	4.9
28	2	12	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
22	T	10	SER	4.9
1	X	2290	A	4.9
1	X	1065	A	4.9
1	X	1095	A	4.9
5	C	190	ALA	4.9
28	2	37	LYS	4.9
1	X	2323	U	4.9
3	A	100	GLY	4.8
11	I	11	GLY	4.8
29	3	32	GLN	4.8
28	2	28	ARG	4.8
16	N	94	VAL	4.8
5	C	48	ARG	4.8
23	U	40	ARG	4.8
30	4	26	ILE	4.8
8	F	123	ALA	4.8
1	X	434	C	4.8
17	O	39	PHE	4.8
30	4	16	VAL	4.8
1	X	1059	A	4.7
1	X	1071	U	4.7
28	2	5	TYR	4.7
22	T	8	GLY	4.7
23	U	50	ALA	4.7
1	X	1066	G	4.7
1	X	2330	G	4.7
20	R	57	ASN	4.7
12	J	27	TYR	4.6
3	A	101	GLU	4.6
1	X	665	A	4.6
7	E	5	GLY	4.6
28	2	16	HIS	4.6
8	F	124	ALA	4.6
11	I	15	ASP	4.6
21	S	93	GLU	4.6
3	A	46	ARG	4.6
8	F	125	ASN	4.6
30	4	24	LEU	4.6
28	2	20	ALA	4.6
5	C	82	VAL	4.5
11	I	27	ASP	4.5
14	L	53	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
20	R	58	VAL	4.5
23	U	48	LYS	4.5
30	4	22	ARG	4.5
16	N	91	ASN	4.4
27	1	47	HIS	4.4
1	X	1091	C	4.4
12	J	72	ASP	4.4
1	X	1080	A	4.4
11	I	36	GLY	4.4
29	3	21	LYS	4.4
7	E	37	TYR	4.4
30	4	30	VAL	4.4
23	U	62	LEU	4.3
14	L	99	ARG	4.3
21	S	31	SER	4.3
5	C	55	GLY	4.3
9	G	162	LYS	4.3
22	T	11	LYS	4.2
19	Q	56	MET	4.2
23	U	27	ASP	4.2
11	I	41	SER	4.2
1	X	346	C	4.2
27	1	13	GLU	4.2
15	M	34	ARG	4.2
1	X	1067	G	4.2
14	L	33	ARG	4.2
29	3	42	ARG	4.2
27	1	39	LYS	4.2
29	3	20	GLY	4.2
12	J	16	GLY	4.1
19	Q	62	ARG	4.1
11	I	33	GLY	4.1
8	F	86	LYS	4.1
27	1	6	PRO	4.1
16	N	56	ASP	4.0
28	2	45	SER	4.0
22	T	20	TYR	4.0
1	X	1037	U	4.0
22	T	15	ASP	4.0
29	3	8	LYS	4.0
21	S	1	MET	4.0
5	C	194	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
23	U	49	LYS	4.0
3	A	250	TRP	4.0
22	T	19	LYS	4.0
22	T	7	VAL	3.9
20	R	7	GLY	3.9
3	A	237	GLU	3.9
1	X	1060	C	3.9
22	T	13	GLY	3.9
1	X	774	A	3.9
1	X	1086	C	3.9
11	I	17	LYS	3.9
23	U	16	ASN	3.9
20	R	102	LYS	3.9
14	L	9	ARG	3.9
20	R	94	VAL	3.9
29	3	64	ARG	3.8
30	4	7	VAL	3.8
12	J	21	ASP	3.8
5	C	161	ALA	3.8
23	U	30	VAL	3.8
27	1	34	LYS	3.8
3	A	44	ASN	3.8
1	X	483	A	3.8
5	C	189	ASP	3.8
1	X	656	U	3.8
1	X	2776	U	3.8
21	S	86	VAL	3.8
9	G	106	TYR	3.8
10	H	104	GLU	3.8
14	L	21	THR	3.8
6	D	40	LEU	3.8
9	G	119	LEU	3.8
17	O	23	GLU	3.8
5	C	159	ARG	3.8
21	S	32	PHE	3.8
27	1	28	ARG	3.8
9	G	160	ALA	3.8
8	F	104	VAL	3.8
11	I	5	ASP	3.8
23	U	21	ARG	3.8
11	I	10	PRO	3.7
1	X	939	C	3.7

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Mol	Chain	Res	Type	RSRZ
12	J	86	LYS	3.7
3	A	201	HIS	3.7
11	I	57	ILE	3.7
14	L	89	PHE	3.7
6	D	148	LYS	3.7
20	R	81	VAL	3.7
5	C	193	LEU	3.7
20	R	43	ASP	3.7
11	I	100	ARG	3.7
14	L	111	GLY	3.7
11	I	7	LYS	3.6
24	V	2	LYS	3.6
7	E	17	VAL	3.6
13	K	94	TYR	3.6
22	T	14	ARG	3.6
6	D	4	LEU	3.6
1	X	1553	G	3.6
27	1	50	PHE	3.6
22	T	12	ASN	3.6
11	I	99	VAL	3.6
4	B	205	SER	3.6
20	R	12	ASP	3.6
11	I	62	LYS	3.6
1	X	1074	G	3.6
14	L	39	TYR	3.6
8	F	133	SER	3.6
1	X	1077	U	3.6
8	F	116	ASN	3.5
23	U	51	ILE	3.5
16	N	76	TYR	3.5
27	1	22	TYR	3.5
13	K	3	HIS	3.5
23	U	28	GLY	3.5
27	1	19	GLY	3.5
19	Q	65	VAL	3.5
1	X	1753	A	3.5
20	R	79	SER	3.5
30	4	33	LYS	3.5
27	1	40	TYR	3.5
3	A	248	THR	3.5
1	X	1093	U	3.5
11	I	55	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
12	J	14	PHE	3.5
23	U	46	LEU	3.5
3	A	249	PRO	3.5
21	S	163	ASP	3.5
16	N	61	TRP	3.5
1	X	1112	U	3.5
3	A	102	LYS	3.4
5	C	91	TYR	3.4
21	S	92	VAL	3.4
19	Q	69	ILE	3.4
14	L	24	SER	3.4
1	X	1084	A	3.4
3	A	239	ARG	3.4
11	I	21	ARG	3.4
1	X	2197	U	3.4
1	X	2285	U	3.4
16	N	88	ILE	3.4
17	O	98	ILE	3.4
15	M	29	PRO	3.4
1	X	2283	G	3.4
14	L	34	SER	3.4
14	L	45	ASP	3.4
17	O	25	LEU	3.4
1	X	1107	A	3.4
1	X	1120	C	3.4
4	B	128	SER	3.4
12	J	28	VAL	3.4
16	N	89	ASP	3.4
1	X	2731	G	3.4
3	A	243	GLY	3.4
3	A	252	LYS	3.4
1	X	1954	A	3.3
18	P	8	PHE	3.3
1	X	559	C	3.3
7	E	43	VAL	3.3
11	I	59	ARG	3.3
27	1	9	ILE	3.3
9	G	71	THR	3.3
11	I	74	VAL	3.3
1	X	1073	G	3.3
21	S	104	SER	3.3
21	S	114	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
27	1	42	PRO	3.3
9	G	66	HIS	3.3
12	J	17	ARG	3.3
5	C	133	PHE	3.3
8	F	77	LEU	3.3
11	I	60	LEU	3.3
20	R	82	ALA	3.3
30	4	35	ARG	3.3
23	U	34	THR	3.3
8	F	117	ALA	3.3
28	2	6	GLN	3.2
14	L	20	THR	3.2
1	X	2166	G	3.2
3	A	235	GLY	3.2
12	J	15	ARG	3.2
3	A	238	GLY	3.2
22	T	73	GLY	3.2
14	L	36	LYS	3.2
9	G	34	PRO	3.2
1	X	247	A	3.2
1	X	1050	G	3.2
5	C	165	SER	3.2
20	R	112	LYS	3.2
3	A	254	THR	3.2
27	1	31	THR	3.2
1	X	657	A	3.2
29	3	54	GLU	3.2
12	J	11	ARG	3.2
16	N	58	ARG	3.2
19	Q	2	SER	3.2
27	1	25	THR	3.2
1	X	2778	U	3.1
9	G	41	TRP	3.1
19	Q	89	GLU	3.1
7	E	59	GLN	3.1
14	L	56	SER	3.1
5	C	178	TYR	3.1
6	D	149	THR	3.1
1	X	1104	G	3.1
28	2	19	ARG	3.1
9	G	163	PRO	3.1
5	C	49	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
6	D	108	LEU	3.1
1	X	1468	A	3.1
1	X	1087	C	3.1
21	S	7	PRO	3.1
5	C	174	GLY	3.1
7	E	68	THR	3.1
20	R	92	THR	3.1
3	A	91	ARG	3.1
9	G	53	ARG	3.1
8	F	134	MET	3.1
29	3	7	HIS	3.0
1	X	1085	G	3.0
15	M	40	ARG	3.0
14	L	55	SER	3.0
20	R	54	ILE	3.0
6	D	8	TYR	3.0
20	R	91	ALA	3.0
4	B	146	THR	3.0
7	E	175	LYS	3.0
3	A	270	ILE	3.0
9	G	74	MET	3.0
21	S	19	ILE	3.0
29	3	24	ALA	3.0
24	V	47	ARG	3.0
3	A	128	GLY	3.0
12	J	78	LYS	3.0
1	X	2167	A	3.0
5	C	118	VAL	3.0
8	F	78	ILE	3.0
5	C	2	ALA	3.0
24	V	44	ARG	3.0
7	E	111	HIS	3.0
5	C	115	GLY	3.0
6	D	131	GLY	3.0
11	I	42	GLY	3.0
1	X	1069	G	3.0
1	X	1117	G	3.0
1	X	1428	G	3.0
1	X	1432	G	3.0
17	O	40	VAL	3.0
21	S	70	GLN	3.0
8	F	130	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	X	435	A	3.0
1	X	1055	A	3.0
20	R	83	LEU	3.0
12	J	134	LYS	3.0
8	F	107	ILE	3.0
13	K	52	ILE	3.0
5	C	56	ARG	2.9
5	C	162	ARG	2.9
17	O	21	ARG	2.9
1	X	1062	G	2.9
19	Q	3	HIS	2.9
20	R	51	VAL	2.9
19	Q	46	PHE	2.9
3	A	240	THR	2.9
6	D	136	LEU	2.9
8	F	99	LEU	2.9
5	C	29	GLU	2.9
3	A	36	ALA	2.9
14	L	59	LEU	2.9
29	3	62	LEU	2.9
1	X	1090	C	2.9
6	D	32	GLU	2.9
14	L	40	ALA	2.9
21	S	171	VAL	2.9
6	D	20	PHE	2.9
9	G	107	GLN	2.9
14	L	18	ARG	2.9
24	V	1	MET	2.9
12	J	26	ASP	2.9
27	1	26	LYS	2.9
12	J	82	THR	2.9
5	C	160	ALA	2.9
1	X	1429	A	2.9
3	A	244	ARG	2.9
9	G	116	ARG	2.9
6	D	5	LYS	2.9
16	N	18	LEU	2.9
26	Z	3	LYS	2.9
30	4	34	GLN	2.9
6	D	139	PRO	2.9
27	1	23	THR	2.9
1	X	1106	A	2.9

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Mol	Chain	Res	Type	RSRZ
12	J	132	MET	2.9
21	S	143	ILE	2.9
29	3	11	LYS	2.9
13	K	82	GLU	2.8
3	A	174	ILE	2.8
7	E	33	LEU	2.8
10	H	134	LEU	2.8
23	U	75	TYR	2.8
1	X	304	A	2.8
1	X	343	A	2.8
1	X	2265	A	2.8
1	X	406	G	2.8
1	X	1365	U	2.8
1	X	1551	U	2.8
1	X	1913	G	2.8
2	Y	58	G	2.8
1	X	246	C	2.8
6	D	35	VAL	2.8
19	Q	64	ARG	2.8
23	U	43	ARG	2.8
5	C	53	LYS	2.8
6	D	161	LYS	2.8
7	E	25	LYS	2.8
6	D	154	ILE	2.8
7	E	65	HIS	2.8
17	O	37	ALA	2.8
23	U	63	SER	2.8
28	2	33	ARG	2.8
12	J	106	GLU	2.8
1	X	1515	U	2.8
1	X	2774	U	2.8
9	G	171	LEU	2.8
1	X	1951	G	2.8
26	Z	56	GLN	2.8
18	P	19	LYS	2.8
1	X	1068	A	2.8
1	X	1094	C	2.8
2	Y	39	C	2.8
7	E	58	ALA	2.8
6	D	130	LEU	2.8
5	C	81	GLY	2.7
17	O	9	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
20	R	67	GLY	2.7
5	C	39	ARG	2.7
11	I	40	ARG	2.7
1	X	1116	U	2.7
1	X	1523	A	2.7
1	X	2581	A	2.7
2	Y	28	A	2.7
7	E	143	GLN	2.7
20	R	86	PRO	2.7
11	I	109	LEU	2.7
13	K	10	LEU	2.7
27	1	35	LEU	2.7
1	X	1103	C	2.7
3	A	251	GLY	2.7
27	1	29	ARG	2.7
3	A	242	ALA	2.7
5	C	112	GLN	2.7
1	X	2088	U	2.7
1	X	305	A	2.7
3	A	216	GLY	2.7
1	X	1524	C	2.7
1	X	1847	G	2.7
11	I	88	PHE	2.7
27	1	20	PHE	2.7
12	J	85	GLY	2.7
23	U	20	ARG	2.7
3	A	218	LYS	2.7
6	D	24	SER	2.7
8	F	93	LYS	2.7
30	4	9	LYS	2.7
8	F	108	ALA	2.7
7	E	98	LEU	2.7
14	L	100	VAL	2.7
2	Y	53	G	2.7
8	F	138	VAL	2.7
5	C	163	ASN	2.7
9	G	73	ASN	2.7
12	J	105	PHE	2.6
22	T	55	ARG	2.6
3	A	208	LYS	2.6
6	D	56	GLU	2.6
14	L	48	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
6	D	23	SER	2.6
11	I	95	ALA	2.6
17	O	56	VAL	2.6
1	X	1082	G	2.6
27	1	41	ASP	2.6
4	B	136	ARG	2.6
9	G	36	ASN	2.6
1	X	356	A	2.6
1	X	2189	A	2.6
1	X	2877	A	2.6
14	L	19	THR	2.6
6	D	146	VAL	2.6
23	U	44	ALA	2.6
6	D	102	LYS	2.6
12	J	69	ILE	2.6
14	L	37	HIS	2.6
26	Z	4	HIS	2.6
6	D	138	PHE	2.6
3	A	99	ASP	2.6
4	B	94	ASP	2.6
2	Y	54	U	2.6
1	X	699	G	2.6
1	X	1100	G	2.6
1	X	1554	G	2.6
5	C	22	VAL	2.6
6	D	27	ALA	2.6
1	X	1109	A	2.6
6	D	169	LEU	2.6
9	G	54	LEU	2.6
3	A	247	VAL	2.6
12	J	137	VAL	2.6
3	A	272	THR	2.6
14	L	104	ALA	2.6
6	D	44	LYS	2.6
14	L	38	ILE	2.6
1	X	192	G	2.6
3	A	89	SER	2.6
1	X	1802	A	2.6
1	X	1952	A	2.6
22	T	17	ASN	2.6
5	C	43	ALA	2.6
8	F	128	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
20	R	109	ALA	2.6
5	C	188	ILE	2.5
11	I	114	ILE	2.5
8	F	74	MET	2.5
20	R	65	PRO	2.5
9	G	39	GLN	2.5
17	O	8	GLY	2.5
1	X	2268	G	2.5
1	X	2344	G	2.5
5	C	172	VAL	2.5
6	D	71	LYS	2.5
7	E	6	LYS	2.5
22	T	74	LYS	2.5
1	X	226	C	2.5
2	Y	111	C	2.5
5	C	75	PRO	2.5
12	J	63	GLY	2.5
17	O	30	GLY	2.5
7	E	60	LYS	2.5
12	J	88	LYS	2.5
15	M	39	VAL	2.5
20	R	46	VAL	2.5
13	K	69	ASP	2.5
21	S	23	ALA	2.5
12	J	18	MET	2.5
19	Q	27	PHE	2.5
1	X	1113	C	2.5
10	H	28	GLY	2.5
21	S	5	ALA	2.5
5	C	45	THR	2.5
11	I	13	ARG	2.5
21	S	172	LEU	2.5
1	X	2165	A	2.5
27	1	49	VAL	2.5
1	X	413	G	2.5
21	S	33	ALA	2.5
7	E	131	ILE	2.5
1	X	730	C	2.5
21	S	141	MET	2.5
3	A	255	LYS	2.5
17	O	38	LEU	2.5
21	S	14	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
23	U	78	ILE	2.4
25	W	35	SER	2.4
1	X	796	A	2.4
1	X	1096	A	2.4
1	X	1507	A	2.4
1	X	1070	G	2.4
9	G	68	PRO	2.4
1	X	1690	U	2.4
5	C	191	ALA	2.4
11	I	49	PHE	2.4
3	A	45	ASN	2.4
14	L	63	ASN	2.4
23	U	65	ASN	2.4
28	2	29	ASN	2.4
1	X	200	A	2.4
6	D	25	VAL	2.4
6	D	128	TYR	2.4
7	E	26	VAL	2.4
23	U	60	VAL	2.4
1	X	358	C	2.4
1	X	1327	C	2.4
1	X	225	G	2.4
1	X	2287	G	2.4
4	B	188	ILE	2.4
9	G	94	LYS	2.4
16	N	92	ARG	2.4
6	D	155	THR	2.4
23	U	45	ASN	2.4
29	3	47	GLY	2.4
1	X	1355	A	2.4
6	D	92	ARG	2.4
1	X	2329	C	2.4
13	K	43	GLU	2.4
1	X	1098	G	2.4
1	X	2867	G	2.4
5	C	130	THR	2.4
9	G	130	ALA	2.4
17	O	12	TYR	2.4
11	I	45	LYS	2.4
3	A	263	ARG	2.4
3	A	35	GLU	2.4
5	C	8	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	198	ASN	2.3
6	D	78	LYS	2.3
9	G	111	LYS	2.3
21	S	80	HIS	2.3
16	N	12	ARG	2.3
21	S	8	ARG	2.3
1	X	1602	G	2.3
1	X	2370	G	2.3
2	Y	121	G	2.3
9	G	164	GLN	2.3
11	I	84	GLU	2.3
21	S	108	VAL	2.3
6	D	41	GLY	2.3
11	I	86	THR	2.3
21	S	11	LYS	2.3
11	I	97	ARG	2.3
22	T	6	GLY	2.3
23	U	25	ARG	2.3
9	G	156	HIS	2.3
21	S	124	ALA	2.3
9	G	69	ASP	2.3
21	S	82	ASP	2.3
21	S	112	LEU	2.3
1	X	1384	G	2.3
25	W	40	VAL	2.3
24	V	48	ARG	2.3
3	A	225	ALA	2.3
11	I	103	ASN	2.3
1	X	242	A	2.3
2	Y	68	A	2.3
1	X	1505	U	2.3
2	Y	122	U	2.3
14	L	64	LYS	2.3
28	2	39	ARG	2.3
6	D	104	ILE	2.3
9	G	108	GLY	2.3
12	J	25	GLY	2.3
1	X	59	G	2.3
1	X	90	G	2.3
11	I	89	ASP	2.3
21	S	140	LYS	2.3
1	X	2777	A	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	43	ARG	2.3
3	A	217	ARG	2.3
6	D	38	GLU	2.3
1	X	1888	C	2.3
1	X	2453	C	2.3
21	S	87	THR	2.3
6	D	143	TYR	2.3
7	E	83	TYR	2.3
12	J	119	PHE	2.3
14	L	35	SER	2.3
14	L	32	TYR	2.3
9	G	102	ARG	2.3
8	F	136	VAL	2.3
20	R	100	ASP	2.3
1	X	1887	G	2.2
4	B	77	ILE	2.2
6	D	121	ALA	2.2
8	F	122	ALA	2.2
20	R	68	GLY	2.2
1	X	1187	A	2.2
1	X	1512	A	2.2
1	X	1909	U	2.2
3	A	39	LYS	2.2
1	X	169	C	2.2
6	D	12	VAL	2.2
3	A	200	GLU	2.2
21	S	130	ILE	2.2
12	J	79	PRO	2.2
21	S	173	PRO	2.2
16	N	95	LEU	2.2
21	S	166	LEU	2.2
29	3	56	ALA	2.2
1	X	388	G	2.2
1	X	2384	G	2.2
1	X	1467	U	2.2
1	X	1603	A	2.2
11	I	118	VAL	2.2
22	T	68	VAL	2.2
30	4	29	ASN	2.2
20	R	70	GLU	2.2
2	Y	29	C	2.2
3	A	236	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
5	C	20	PRO	2.2
6	D	15	ALA	2.2
14	L	52	ALA	2.2
23	U	29	GLY	2.2
5	C	166	TRP	2.2
12	J	8	THR	2.2
8	F	75	SER	2.2
1	X	74	G	2.2
1	X	655	A	2.2
1	X	2567	G	2.2
8	F	100	ASN	2.2
3	A	147	LEU	2.2
29	3	59	LYS	2.2
1	X	1183	C	2.2
1	X	2082	C	2.2
14	L	31	VAL	2.2
5	C	7	ILE	2.2
10	H	27	SER	2.2
19	Q	54	SER	2.2
19	Q	87	SER	2.2
7	E	38	ASN	2.2
12	J	81	GLU	2.2
5	C	171	PRO	2.2
8	F	129	GLY	2.2
12	J	87	GLY	2.2
21	S	63	PRO	2.2
21	S	106	GLY	2.2
1	X	1857	G	2.2
2	Y	51	G	2.2
11	I	75	VAL	2.1
21	S	66	VAL	2.1
1	X	661	C	2.1
3	A	260	ARG	2.1
12	J	112	GLU	2.1
14	L	8	ARG	2.1
5	C	121	ASP	2.1
24	V	19	ASP	2.1
14	L	87	VAL	2.1
9	G	101	THR	2.1
1	X	1516	A	2.1
1	X	2780	A	2.1
6	D	132	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
4	B	204	ALA	2.1
7	E	80	SER	2.1
10	H	117	GLU	2.1
11	I	50	GLU	2.1
11	I	112	GLY	2.1
1	X	1185	C	2.1
21	S	91	PRO	2.1
24	V	3	PRO	2.1
6	D	105	ASN	2.1
3	A	196	VAL	2.1
7	E	52	VAL	2.1
20	R	108	VAL	2.1
30	4	25	VAL	2.1
2	Y	50	U	2.1
4	B	49	ILE	2.1
17	O	55	THR	2.1
6	D	173	MET	2.1
1	X	387	A	2.1
2	Y	27	A	2.1
2	Y	78	A	2.1
3	A	234	GLY	2.1
1	X	203	G	2.1
8	F	120	VAL	2.1
20	R	106	VAL	2.1
21	S	51	LEU	2.1
6	D	145	MET	2.1
14	L	68	ALA	2.1
6	D	63	GLN	2.1
12	J	136	GLU	2.1
21	S	62	PHE	2.1
22	T	18	PRO	2.1
7	E	141	VAL	2.1
1	X	1873	A	2.1
12	J	77	LYS	2.1
21	S	29	ASN	2.1
6	D	141	ILE	2.1
18	P	105	ARG	2.1
19	Q	88	ILE	2.1
20	R	85	ASP	2.1
6	D	61	THR	2.1
6	D	90	THR	2.1
1	X	234	C	2.1

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Mol	Chain	Res	Type	RSRZ
1	X	1734	C	2.1
1	X	2195	C	2.1
1	X	1189	G	2.1
1	X	1223	G	2.1
11	I	79	GLN	2.1
16	N	23	GLY	2.1
5	C	198	GLU	2.1
8	F	142	PRO	2.1
9	G	157	PRO	2.1
15	M	78	GLU	2.1
3	A	117	VAL	2.0
9	G	165	VAL	2.0
19	Q	32	LYS	2.0
3	A	183	ARG	2.0
14	L	75	LEU	2.0
19	Q	91	LEU	2.0
21	S	142	ASN	2.0
27	1	37	LEU	2.0
1	X	1839	A	2.0
6	D	147	ASP	2.0
20	R	107	ALA	2.0
23	U	55	GLY	2.0
29	3	29	LYS	2.0
21	S	69	VAL	2.0
28	2	44	VAL	2.0
1	X	1	G	2.0
1	X	2400	G	2.0
1	X	2408	G	2.0
2	Y	52	G	2.0
6	D	110	ARG	2.0
5	C	15	ILE	2.0
3	A	226	MET	2.0
20	R	11	ASN	2.0
3	A	259	THR	2.0
5	C	173	ALA	2.0
20	R	113	THR	2.0
6	D	46	ASP	2.0
8	F	111	LYS	2.0
15	M	38	LYS	2.0
19	Q	63	LYS	2.0
21	S	67	LYS	2.0
21	S	125	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
9	G	90	LEU	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 oligosaccharides 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.

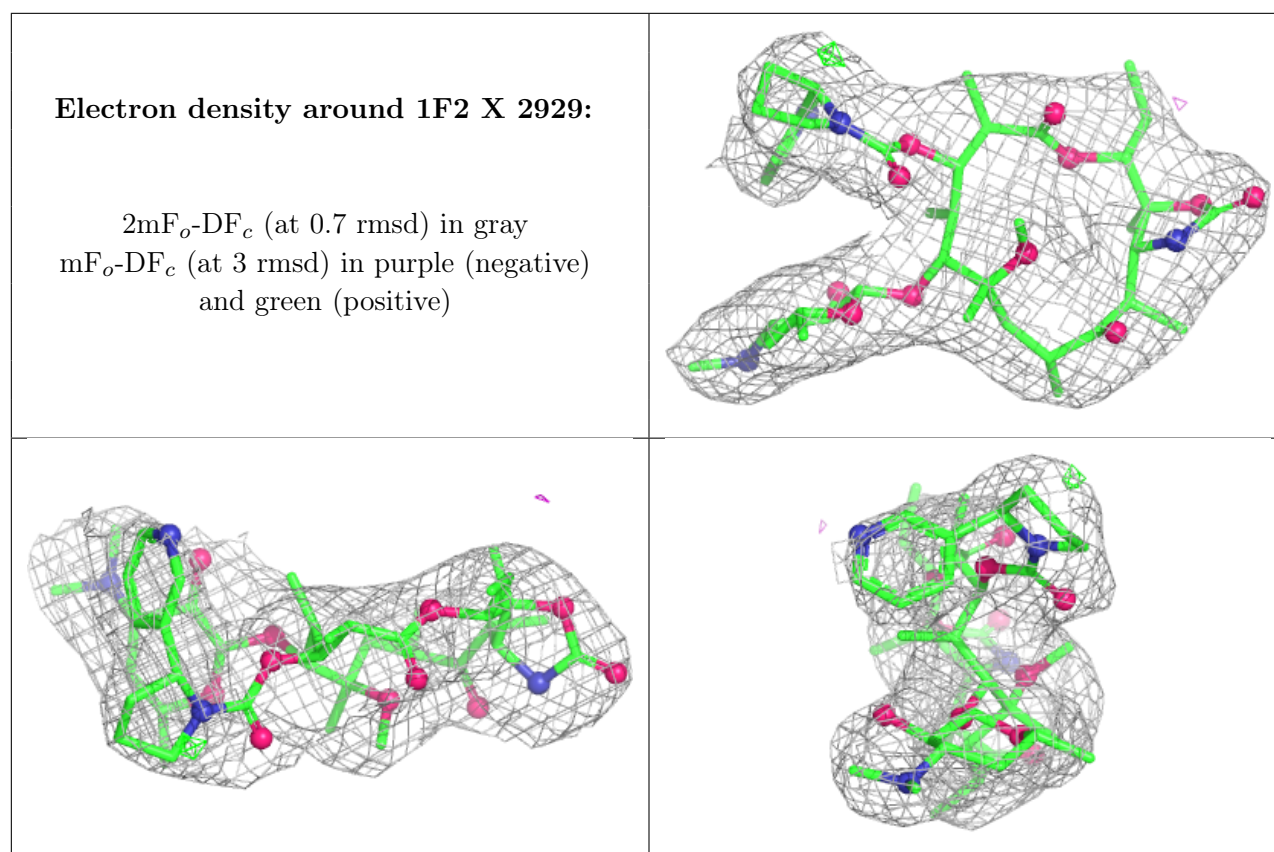
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	MG	X	2903	1/1	0.49	1.47	89,89,89,89	0
31	MG	X	2909	1/1	0.68	0.82	96,96,96,96	0
31	MG	X	2924	1/1	0.71	0.59	69,69,69,69	0
31	MG	X	2904	1/1	0.76	0.68	107,107,107,107	0
31	MG	X	2917	1/1	0.77	0.62	55,55,55,55	0
31	MG	Y	201	1/1	0.77	0.90	89,89,89,89	0
31	MG	X	2902	1/1	0.80	0.34	94,94,94,94	0
31	MG	X	2907	1/1	0.80	0.65	51,51,51,51	0
31	MG	Y	205	1/1	0.81	0.15	79,79,79,79	0
31	MG	X	2906	1/1	0.82	0.46	58,58,58,58	0
31	MG	X	2910	1/1	0.84	0.44	42,42,42,42	0
31	MG	X	2911	1/1	0.84	0.31	68,68,68,68	0
31	MG	Y	203	1/1	0.85	0.63	87,87,87,87	0
31	MG	X	2905	1/1	0.86	0.30	65,65,65,65	0
31	MG	X	2920	1/1	0.87	0.37	115,115,115,115	0
31	MG	X	2928	1/1	0.91	0.92	62,62,62,62	0
31	MG	X	2914	1/1	0.92	0.31	27,27,27,27	0
31	MG	X	2912	1/1	0.93	0.32	71,71,71,71	0
31	MG	Y	202	1/1	0.93	0.54	58,58,58,58	0
31	MG	X	2925	1/1	0.94	0.21	122,122,122,122	0
31	MG	Y	204	1/1	0.94	0.55	82,82,82,82	0
31	MG	X	2913	1/1	0.94	0.71	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	MG	J	201	1/1	0.94	0.39	100,100,100,100	0
31	MG	X	2918	1/1	0.95	0.56	42,42,42,42	0
31	MG	X	2915	1/1	0.95	0.62	57,57,57,57	0
31	MG	X	2921	1/1	0.95	0.53	81,81,81,81	0
31	MG	X	2908	1/1	0.95	0.51	37,37,37,37	0
31	MG	X	2919	1/1	0.96	0.35	30,30,30,30	0
31	MG	X	2901	1/1	0.96	0.79	50,50,50,50	0
31	MG	X	2916	1/1	0.96	0.52	37,37,37,37	0
31	MG	M	201	1/1	0.96	0.30	23,23,23,23	0
32	1F2	X	2929	56/56	0.96	0.09	42,68,77,83	0
31	MG	X	2922	1/1	0.97	0.58	44,44,44,44	0
31	MG	X	2926	1/1	0.98	0.56	45,45,45,45	0
31	MG	X	2927	1/1	0.99	0.12	62,62,62,62	0
31	MG	X	2923	1/1	0.99	0.32	34,34,34,34	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.