



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:18 PM UTC

PDB ID : 4DV1 / pdb_00004dv1
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, U20G, bound with streptomycin
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on : 2012-02-22
Resolution : 3.85 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

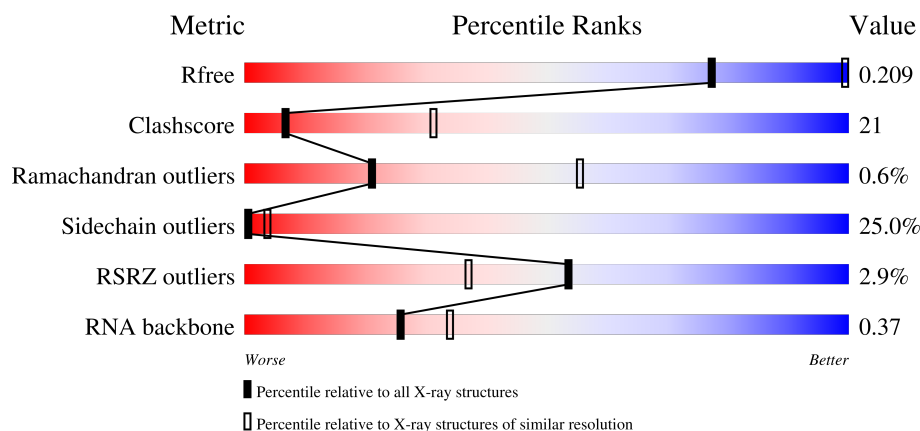
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)
RNA backbone	3983	1010 (4.56-3.10)

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	A	1522	2% 37% 45% 17% .
2	B	256	3% 34% 43% 13% . 9%
3	C	239	3% 32% 42% 11% . 14%

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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
23	MG	A	1695	-	-	-	X
23	MG	A	1712	-	-	-	X
23	MG	A	1730	-	-	-	X
23	MG	A	1751	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	P	101	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32510	14478	6014	10506	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	G	U	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	124	Total	C	N	O	S	0	0	0
			972	612	195	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	152	141	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called ribosomal protein S19.

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

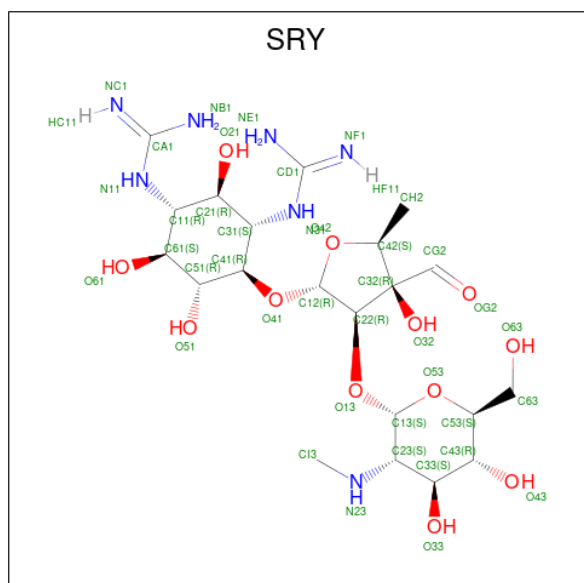
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

- Molecule 22 is STREPTOMYCIN (CCD ID: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 23 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	230	Total 230	Mg 230	0	0
23	B	1	Total 1	Mg 1	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	2	Total 2	Mg 2	0	0
23	I	1	Total 1	Mg 1	0	0
23	J	1	Total 1	Mg 1	0	0
23	K	1	Total 1	Mg 1	0	0
23	M	2	Total 2	Mg 2	0	0
23	N	2	Total 2	Mg 2	0	0
23	P	1	Total 1	Mg 1	0	0
23	S	2	Total 2	Mg 2	0	0
23	T	2	Total 2	Mg 2	0	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

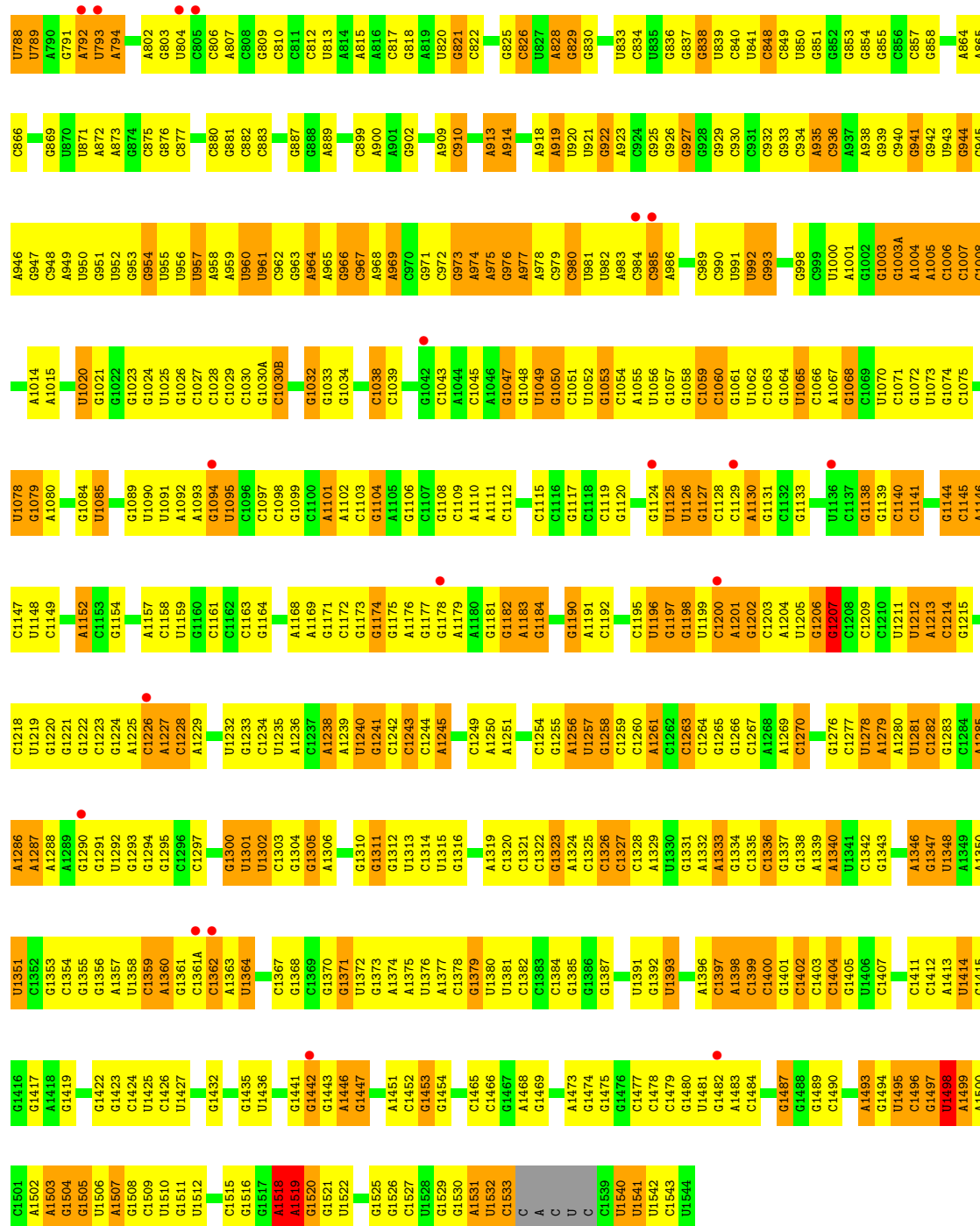
- Molecule 25 is water.

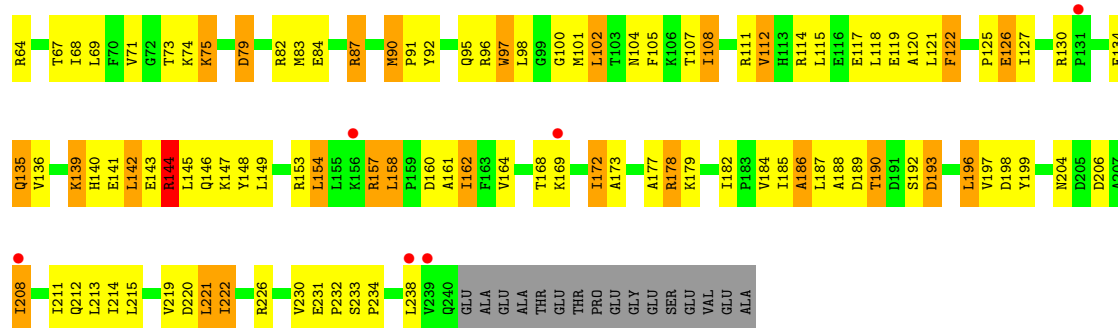
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	396	Total 396	O 396	0	0
25	E	6	Total 6	O 6	0	0

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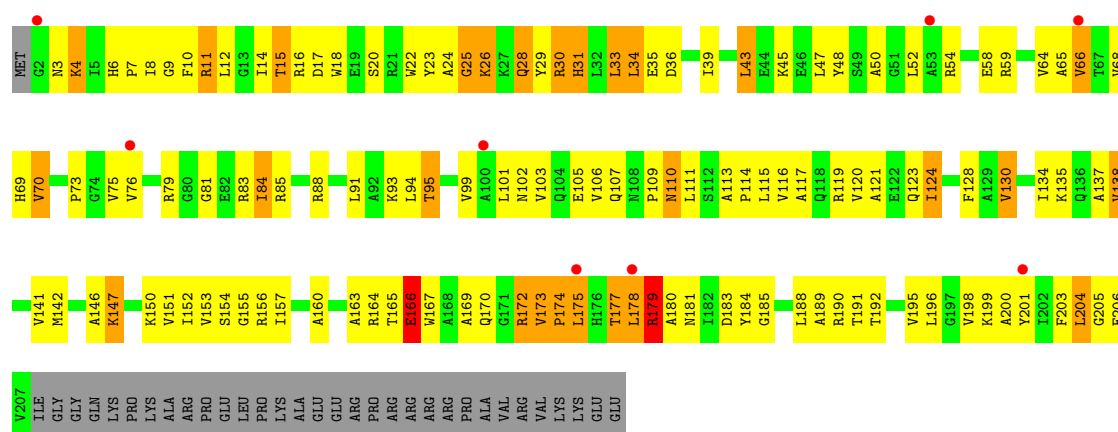
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total 1	O 1	0	0
25	J	1	Total 1	O 1	0	0
25	N	1	Total 1	O 1	0	0
25	Q	1	Total 1	O 1	0	0
25	T	3	Total 3	O 3	0	0
25	U	1	Total 1	O 1	0	0

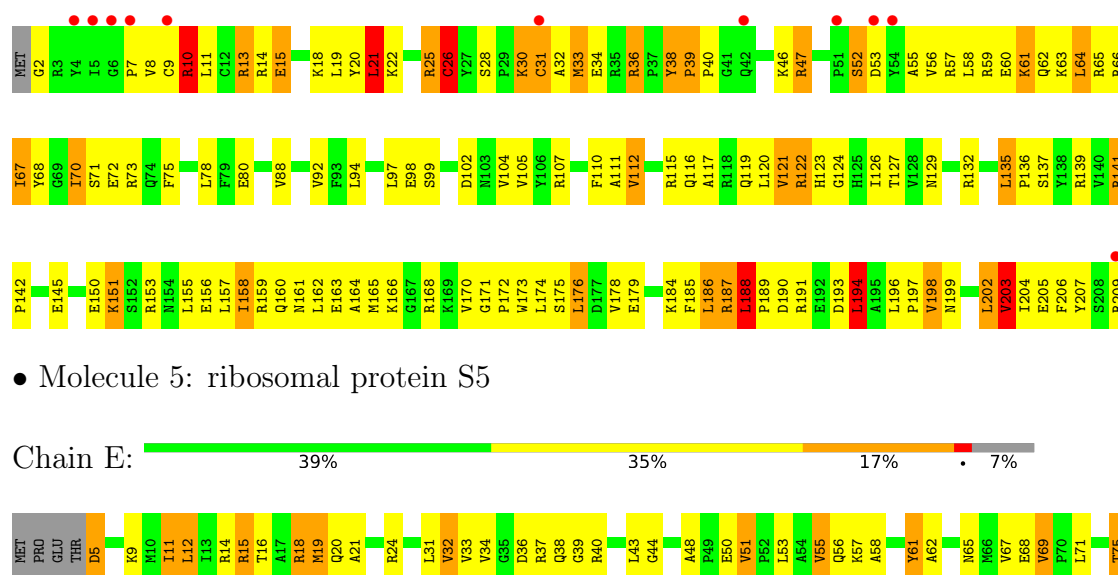




• Molecule 3: ribosomal protein S3

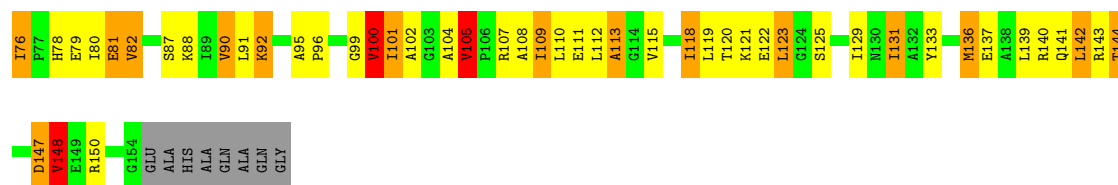


• Molecule 4: ribosomal protein S4



• Molecule 5: ribosomal protein S5

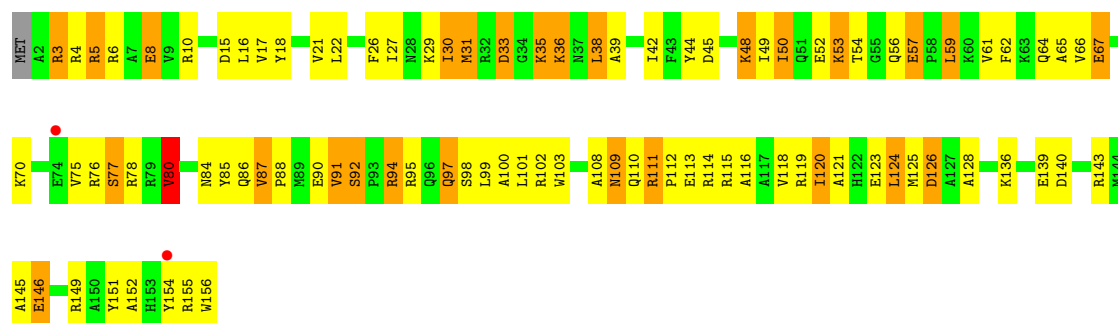




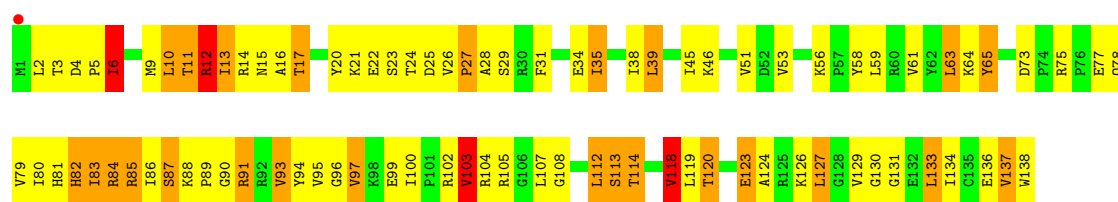
• Molecule 6: ribosomal protein S6



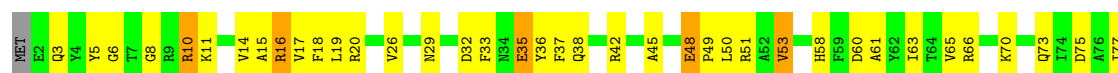
• Molecule 7: ribosomal protein S7

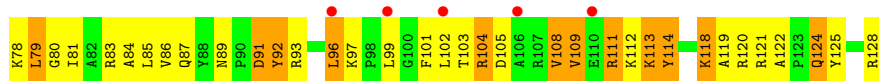


• Molecule 8: ribosomal protein S8

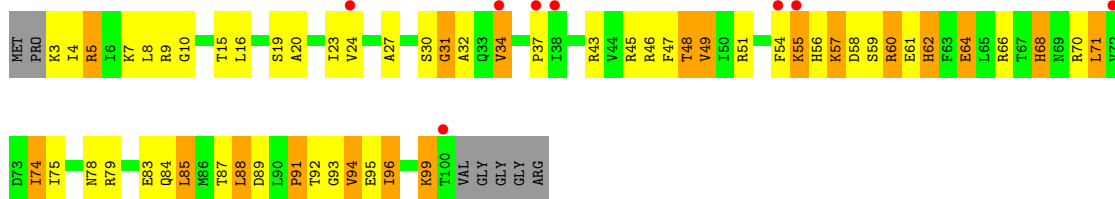


• Molecule 9: ribosomal protein S9

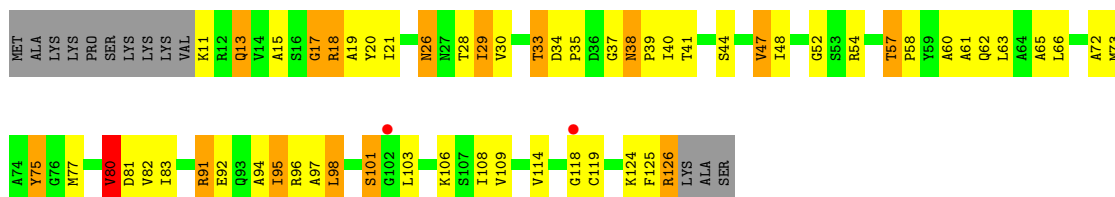
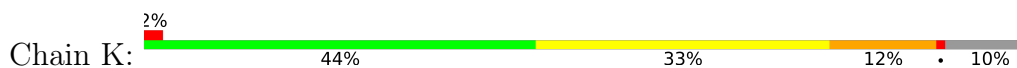




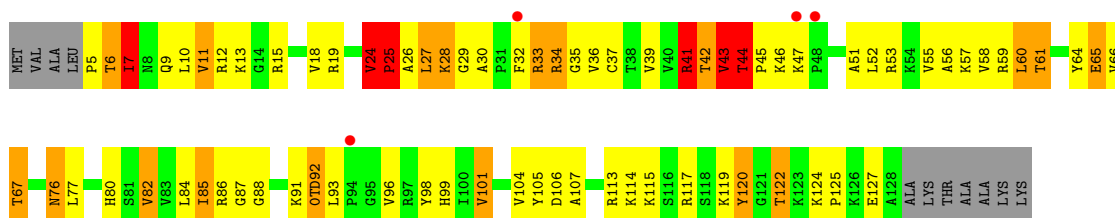
• Molecule 10: ribosomal protein S10



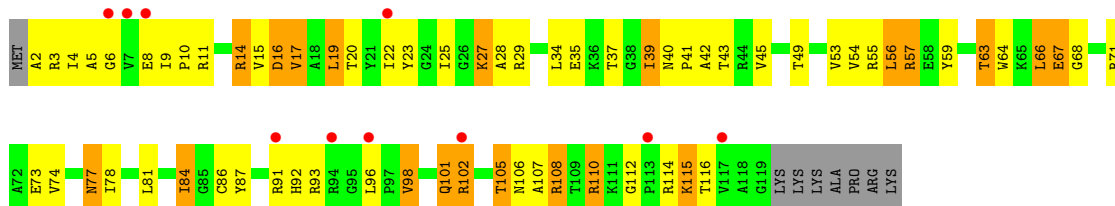
• Molecule 11: ribosomal protein S11



• Molecule 12: ribosomal protein S12



• Molecule 13: ribosomal protein S13



• Molecule 14: ribosomal protein S14

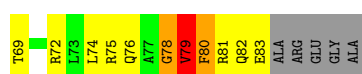




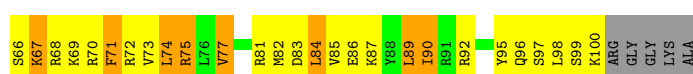
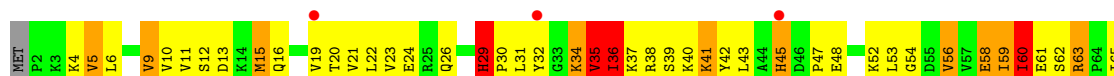
• Molecule 15: ribosomal protein S15



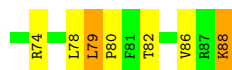
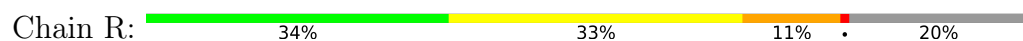
• Molecule 16: ribosomal protein S16



• Molecule 17: ribosomal protein S17

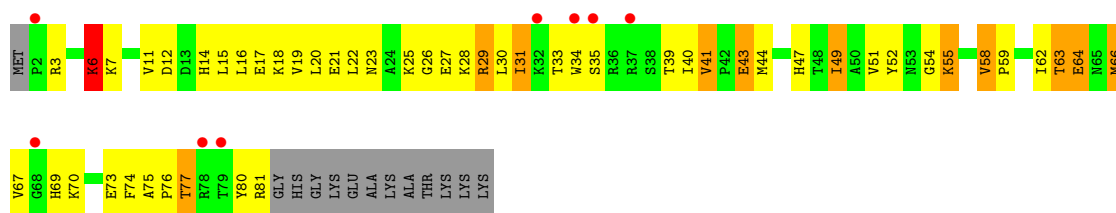


• Molecule 18: ribosomal protein S18

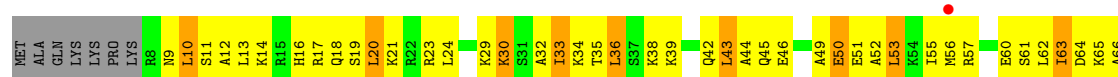


• Molecule 19: ribosomal protein S19

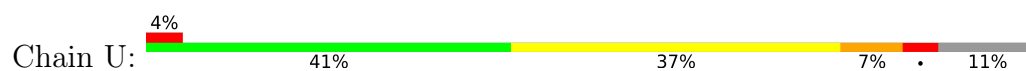




• Molecule 20: ribosomal protein S20



• Molecule 21: ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	403.45Å 403.45Å 173.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.85 34.93 – 3.85	Depositor EDS
% Data completeness (in resolution range)	97.3 (34.93-3.85) 96.9 (34.93-3.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 3.87Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.150 , 0.212 0.150 , 0.209	Depositor DCC
R_{free} test set	6514 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	161.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 153.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52297	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: 7MG, 2MG, 4OC, 5MC, 0TD, PSU, MA6, SRY, MG, M2G, UR3, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	1/36044 (0.0%)	0.61	0/56250
2	B	0.81	0/1935	1.21	12/2609 (0.5%)
3	C	0.81	0/1636	1.19	15/2205 (0.7%)
4	D	0.86	3/1733 (0.2%)	1.34	24/2318 (1.0%)
5	E	1.18	5/1162 (0.4%)	1.57	20/1564 (1.3%)
6	F	0.74	0/856	1.17	3/1154 (0.3%)
7	G	0.82	0/1276	1.31	14/1709 (0.8%)
8	H	1.26	6/1136 (0.5%)	1.50	16/1527 (1.0%)
9	I	0.83	0/1029	1.23	5/1379 (0.4%)
10	J	0.81	0/805	1.23	10/1082 (0.9%)
11	K	0.94	0/879	1.41	12/1187 (1.0%)
12	L	1.00	0/977	1.62	20/1306 (1.5%)
13	M	0.86	0/947	1.25	6/1270 (0.5%)
14	N	0.83	0/501	1.21	4/664 (0.6%)
15	O	0.96	1/740 (0.1%)	1.22	3/987 (0.3%)
16	P	1.01	0/716	1.44	12/963 (1.2%)
17	Q	1.24	7/836 (0.8%)	1.55	12/1117 (1.1%)
18	R	0.88	1/579 (0.2%)	1.23	4/768 (0.5%)
19	S	0.81	0/661	1.23	5/890 (0.6%)
20	T	0.96	1/765 (0.1%)	1.45	5/1007 (0.5%)
21	U	0.79	0/212	1.08	1/277 (0.4%)
All	All	0.73	25/55425 (0.0%)	0.90	203/82233 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1
12	L	0	1
13	M	0	1
16	P	0	2
20	T	0	1
All	All	0	9

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	11	VAL	CA-CB	-8.20	1.45	1.54
4	D	30	LYS	CA-C	7.07	1.61	1.52
17	Q	35	VAL	CA-CB	-6.32	1.46	1.54
5	E	90	VAL	CA-CB	-6.30	1.46	1.54
5	E	82	VAL	CA-CB	-6.03	1.46	1.54
17	Q	9	VAL	CA-CB	-5.91	1.47	1.54
8	H	118	VAL	CA-CB	-5.89	1.47	1.54
17	Q	56	VAL	CA-CB	-5.79	1.47	1.54
4	D	31	CYS	N-CA	5.75	1.53	1.46
5	E	148	VAL	CA-CB	-5.72	1.46	1.54
8	H	119	LEU	CA-C	-5.60	1.45	1.52
17	Q	36	ILE	CA-CB	-5.60	1.47	1.54
5	E	11	ILE	CA-CB	-5.58	1.46	1.54
1	A	1498	UR3	O3'-P	5.54	1.61	1.56
17	Q	99	SER	CA-C	5.54	1.60	1.52
4	D	203	VAL	CA-CB	-5.52	1.46	1.54
15	O	60	VAL	CA-CB	-5.42	1.47	1.54
8	H	124	ALA	CA-CB	-5.41	1.44	1.53
5	E	115	VAL	CA-CB	-5.21	1.48	1.54
20	T	63	ILE	CA-CB	-5.11	1.48	1.54
8	H	16	ALA	C-O	-5.09	1.18	1.24
8	H	6	ILE	CA-CB	-5.08	1.47	1.54
18	R	50	ILE	CA-CB	-5.06	1.48	1.54
8	H	61	VAL	CA-CB	-5.04	1.48	1.54
17	Q	65	ILE	CA-CB	-5.04	1.47	1.54

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	35	VAL	CB-CA-C	-14.85	93.70	111.08
12	L	24	VAL	CA-C-N	-13.92	102.44	119.84
12	L	24	VAL	C-N-CA	-13.92	102.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	111	ARG	CA-C-N	10.60	131.41	119.32
7	G	111	ARG	C-N-CA	10.60	131.41	119.32
4	D	38	TYR	CA-C-N	10.49	131.18	120.38
4	D	38	TYR	C-N-CA	10.49	131.18	120.38
16	P	62	VAL	N-CA-C	9.78	121.48	112.29
12	L	26	ALA	N-CA-C	-9.75	99.53	111.33
19	S	6	LYS	N-CA-C	9.66	122.29	108.00
4	D	26	CYS	N-CA-C	-9.54	100.91	112.54
17	Q	67	LYS	N-CA-C	-9.43	96.55	110.23
5	E	109	ILE	N-CA-C	9.20	120.02	110.36
6	F	11	ASN	CA-C-N	9.07	128.71	119.82
6	F	11	ASN	C-N-CA	9.07	128.71	119.82
20	T	94	ALA	N-CA-C	-8.99	92.24	107.80
14	N	25	VAL	N-CA-C	8.99	118.98	110.53
6	F	37	VAL	CB-CA-C	-8.91	100.65	111.08
5	E	105	VAL	CA-C-N	-8.69	110.79	119.56
5	E	105	VAL	C-N-CA	-8.69	110.79	119.56
7	G	87	VAL	N-CA-C	8.68	117.35	107.89
8	H	100	ILE	CA-C-N	8.68	128.74	119.89
8	H	100	ILE	C-N-CA	8.68	128.74	119.89
4	D	121	VAL	N-CA-C	-8.53	102.51	110.53
17	Q	60	ILE	N-CA-C	8.52	120.04	108.11
4	D	56	VAL	CB-CA-C	-8.43	101.18	111.97
4	D	30	LYS	N-CA-C	8.36	124.50	113.30
3	C	25	GLY	N-CA-C	8.33	126.30	114.64
5	E	76	ILE	CA-C-N	7.97	128.04	119.28
5	E	76	ILE	C-N-CA	7.97	128.04	119.28
10	J	99	LYS	N-CA-C	7.95	118.76	108.34
2	B	75	LYS	N-CA-C	-7.88	102.63	111.14
11	K	17	GLY	N-CA-C	7.84	122.10	110.42
17	Q	29	HIS	CA-C-N	7.84	127.48	119.56
17	Q	29	HIS	C-N-CA	7.84	127.48	119.56
12	L	105	TYR	CB-CA-C	-7.82	107.56	116.63
5	E	148	VAL	CB-CA-C	-7.72	101.90	112.24
3	C	166	GLU	N-CA-C	7.65	118.08	108.45
2	B	90	MET	CA-C-N	7.63	127.68	119.89
2	B	90	MET	C-N-CA	7.63	127.68	119.89
3	C	167	TRP	N-CA-C	7.53	117.15	108.49
12	L	6	THR	CA-C-N	-7.41	111.07	120.56
12	L	6	THR	C-N-CA	-7.41	111.07	120.56
2	B	16	HIS	N-CA-C	7.30	122.35	111.04
12	L	44	THR	CA-C-N	7.25	128.90	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	44	THR	C-N-CA	7.25	128.90	119.84
17	Q	90	ILE	CB-CA-C	-7.17	102.65	112.04
8	H	35	ILE	CB-CA-C	-7.16	102.54	111.70
7	G	114	ARG	N-CA-C	7.04	120.35	111.69
16	P	20	VAL	N-CA-C	7.02	117.61	108.35
16	P	5	ARG	N-CA-C	6.99	117.50	108.34
16	P	19	ILE	CB-CA-C	-6.94	102.31	110.91
16	P	80	PHE	N-CA-C	6.93	121.45	112.92
7	G	67	GLU	N-CA-C	6.93	119.43	111.11
10	J	66	ARG	N-CA-C	6.91	120.17	108.90
9	I	122	ALA	CA-C-N	6.90	126.87	119.76
9	I	122	ALA	C-N-CA	6.90	126.87	119.76
12	L	43	VAL	N-CA-C	6.89	119.97	108.81
5	E	48	ALA	CA-C-N	6.87	128.42	119.84
5	E	48	ALA	C-N-CA	6.87	128.42	119.84
13	M	67	GLU	CB-CA-C	-6.86	108.67	116.63
4	D	36	ARG	CA-C-N	6.80	126.48	119.82
4	D	36	ARG	C-N-CA	6.80	126.48	119.82
16	P	29	ASP	N-CA-C	6.78	121.72	113.17
12	L	30	ALA	CA-C-N	6.78	126.74	119.28
12	L	30	ALA	C-N-CA	6.78	126.74	119.28
5	E	51	VAL	CB-CA-C	-6.75	107.20	114.35
5	E	115	VAL	CB-CA-C	-6.71	101.11	111.71
2	B	193	ASP	CA-C-N	6.71	125.95	118.97
2	B	193	ASP	C-N-CA	6.71	125.95	118.97
13	M	108	ARG	N-CA-C	6.69	119.14	111.11
5	E	15	ARG	N-CA-C	6.59	121.53	112.90
8	H	17	THR	N-CA-C	6.52	119.21	111.71
11	K	91	ARG	N-CA-C	-6.50	104.05	112.23
5	E	50	GLU	CA-C-N	6.49	124.33	120.24
5	E	50	GLU	C-N-CA	6.49	124.33	120.24
4	D	171	GLY	CA-C-N	6.47	126.16	119.82
4	D	171	GLY	C-N-CA	6.47	126.16	119.82
16	P	79	VAL	N-CA-C	-6.47	104.59	113.00
18	R	50	ILE	CB-CA-C	-6.46	101.06	111.59
11	K	57	THR	CA-C-N	6.45	126.02	119.19
11	K	57	THR	C-N-CA	6.45	126.02	119.19
7	G	103	TRP	N-CA-C	6.44	118.09	111.14
4	D	204	ILE	CB-CA-C	-6.43	103.47	111.70
4	D	176	LEU	N-CA-C	6.42	119.07	108.99
8	H	114	THR	N-CA-C	6.41	117.90	108.86
7	G	36	LYS	N-CA-C	-6.41	103.81	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	92	LYS	N-CA-C	-6.40	100.47	110.14
12	L	85	ILE	CB-CA-C	-6.39	101.31	110.83
8	H	27	PRO	CA-C-N	-6.38	112.39	122.73
8	H	27	PRO	C-N-CA	-6.38	112.39	122.73
5	E	100	VAL	N-CA-C	-6.37	100.43	108.84
7	G	5	ARG	N-CA-C	6.36	118.34	109.31
19	S	70	LYS	N-CA-C	6.33	118.93	108.48
13	M	66	LEU	N-CA-C	6.32	119.48	109.50
3	C	124	ILE	N-CA-C	6.25	117.74	110.62
16	P	40	ASP	CA-C-N	6.22	125.78	119.19
16	P	40	ASP	C-N-CA	6.22	125.78	119.19
19	S	49	ILE	N-CA-C	6.21	117.06	108.12
4	D	188	LEU	CA-C-N	-6.20	114.34	120.98
4	D	188	LEU	C-N-CA	-6.20	114.34	120.98
16	P	9	PHE	N-CA-C	6.18	120.95	113.17
5	E	113	ALA	N-CA-C	-6.17	105.62	113.02
19	S	26	GLY	N-CA-C	-6.17	103.80	111.70
19	S	6	LYS	CB-CA-C	-6.11	107.78	116.34
8	H	103	VAL	N-CA-C	6.10	116.79	107.77
11	K	118	GLY	CA-C-N	-6.08	114.19	122.77
11	K	118	GLY	C-N-CA	-6.08	114.19	122.77
11	K	37	GLY	N-CA-C	6.07	123.14	114.64
3	C	174	PRO	CA-C-O	-6.04	116.84	121.31
12	L	119	LYS	N-CA-C	-6.03	102.15	110.35
15	O	27	VAL	CB-CA-C	-6.03	104.16	111.88
12	L	7	ILE	N-CA-CB	6.02	118.28	110.57
8	H	89	PRO	N-CA-C	-6.02	101.74	111.19
20	T	88	VAL	CB-CA-C	-5.98	104.05	111.70
9	I	96	LEU	N-CA-C	5.97	117.58	111.14
17	Q	5	VAL	CB-CA-C	-5.96	101.62	110.33
2	B	41	ILE	CB-CA-C	-5.96	102.82	110.98
16	P	51	VAL	N-CA-C	5.93	121.68	109.34
4	D	33	MET	N-CA-C	-5.92	104.90	111.71
4	D	21	LEU	N-CA-C	-5.91	105.73	113.17
12	L	82	VAL	CB-CA-C	-5.88	102.68	110.98
20	T	66	ALA	N-CA-C	-5.87	104.79	111.07
11	K	80	VAL	N-CA-C	5.84	116.41	107.77
4	D	10	ARG	N-CA-C	5.83	117.30	111.07
10	J	55	LYS	N-CA-C	5.79	116.58	108.00
12	L	18	VAL	N-CA-C	5.79	116.33	107.77
9	I	124	GLN	N-CA-C	5.76	118.06	108.20
4	D	196	LEU	CA-C-N	5.76	127.04	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	196	LEU	C-N-CA	5.76	127.04	119.84
7	G	91	VAL	N-CA-C	5.76	118.25	108.86
14	N	52	GLN	N-CA-C	5.75	120.42	113.17
2	B	8	LYS	N-CA-C	5.75	115.44	107.73
14	N	8	GLU	N-CA-C	5.75	118.29	111.33
2	B	187	LEU	N-CA-C	-5.74	101.14	110.20
17	Q	71	PHE	N-CA-C	5.72	118.39	109.52
15	O	11	VAL	N-CA-C	5.71	116.36	110.36
3	C	99	VAL	N-CA-C	5.71	116.99	108.54
3	C	173	VAL	CA-C-N	5.69	129.60	121.91
3	C	173	VAL	C-N-CA	5.69	129.60	121.91
7	G	87	VAL	CA-C-N	5.69	125.62	119.76
7	G	87	VAL	C-N-CA	5.69	125.62	119.76
4	D	39	PRO	CA-C-N	5.68	126.95	119.84
4	D	39	PRO	C-N-CA	5.68	126.95	119.84
3	C	179	ARG	N-CA-C	-5.67	98.73	110.80
18	R	79	LEU	CA-C-N	5.67	126.15	120.14
18	R	79	LEU	C-N-CA	5.67	126.15	120.14
2	B	214	ILE	N-CA-C	5.66	115.86	110.42
4	D	194	LEU	N-CA-C	5.65	118.68	109.59
17	Q	68	ARG	N-CA-C	5.64	120.11	113.23
13	M	11	ARG	N-CA-C	5.63	117.74	109.24
7	G	84	ASN	N-CA-C	5.63	118.39	110.23
8	H	24	THR	N-CA-C	5.63	118.65	108.69
5	E	90	VAL	N-CA-C	5.61	116.08	107.77
9	I	125	TYR	N-CA-C	-5.61	102.59	110.50
11	K	38	ASN	CA-C-N	5.58	125.78	120.31
11	K	38	ASN	C-N-CA	5.58	125.78	120.31
3	C	26	LYS	N-CA-C	-5.53	104.94	110.97
21	U	13	ILE	N-CA-C	-5.51	105.83	113.00
10	J	62	HIS	N-CA-C	5.50	117.83	110.35
10	J	91	PRO	N-CA-C	5.50	119.49	111.03
2	B	222	ILE	CB-CA-C	-5.46	104.87	112.02
2	B	144	ARG	N-CA-C	5.46	116.91	111.07
10	J	79	ARG	N-CA-C	5.42	117.19	111.28
12	L	41	ARG	N-CA-C	5.42	116.21	108.74
3	C	48	TYR	N-CA-C	5.41	117.87	111.33
4	D	112	VAL	CB-CA-C	-5.41	105.00	112.24
7	G	8	GLU	N-CA-C	5.40	118.47	110.48
8	H	88	LYS	CA-C-N	-5.38	114.38	119.76
8	H	88	LYS	C-N-CA	-5.38	114.38	119.76
10	J	60	ARG	N-CA-C	5.38	122.25	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	186	LEU	N-CA-C	5.35	119.92	113.17
20	T	73	HIS	CB-CA-C	-5.35	109.42	115.79
8	H	13	ILE	N-CA-C	5.33	116.70	110.62
17	Q	20	THR	CB-CA-C	-5.30	102.07	110.81
10	J	31	GLY	N-CA-C	5.29	121.98	112.77
7	G	120	ILE	CB-CA-C	-5.28	105.22	111.81
13	M	14	ARG	N-CA-C	-5.26	103.54	110.33
12	L	85	ILE	N-CA-C	5.26	115.53	108.17
10	J	94	VAL	N-CA-C	5.25	115.77	110.05
12	L	88	GLY	N-CA-C	-5.25	104.60	111.37
5	E	109	ILE	CB-CA-C	-5.23	105.19	111.88
12	L	114	LYS	N-CA-C	5.22	119.75	113.17
11	K	13	GLN	N-CA-C	5.22	117.02	110.91
10	J	89	ASP	N-CA-C	5.21	117.22	109.25
8	H	81	HIS	N-CA-C	-5.18	105.70	112.23
15	O	20	GLY	N-CA-C	5.18	122.25	115.36
18	R	58	LEU	N-CA-C	5.17	117.85	109.79
13	M	10	PRO	CA-C-O	-5.15	115.30	121.48
14	N	6	LEU	N-CA-C	5.14	119.25	112.92
17	Q	9	VAL	CB-CA-C	-5.13	102.84	110.33
5	E	142	LEU	N-CA-C	5.13	117.73	110.50
3	C	28	GLN	N-CA-C	5.11	119.61	113.17
3	C	4	LYS	N-CA-C	5.09	116.87	110.91
11	K	26	ASN	N-CA-C	5.09	119.64	113.38
8	H	12	ARG	NE-CZ-NH1	-5.07	116.43	121.50
16	P	76	GLN	N-CA-C	-5.05	105.67	111.07
3	C	95	THR	N-CA-C	5.04	117.61	110.50
20	T	75	ASN	N-CA-C	-5.03	107.19	113.38
17	Q	62	SER	N-CA-C	5.03	116.71	109.07
3	C	124	ILE	CB-CA-C	-5.02	105.46	112.04
8	H	87	SER	N-CA-C	-5.01	101.58	109.25
5	E	104	ALA	N-CA-C	-5.01	105.29	111.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	186	ALA	Peptide
2	B	8	LYS	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	Peptide

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Mol	Chain	Res	Type	Group
13	M	105	THR	Peptide
16	P	19	ILE	Peptide
16	P	78	GLY	Peptide
20	T	93	GLU	Peptide

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	A	32510	0	16434	861	0
2	B	1900	0	1951	102	0
3	C	1612	0	1677	121	0
4	D	1703	0	1763	108	0
5	E	1146	0	1207	62	0
6	F	843	0	857	48	0
7	G	1257	0	1296	73	0
8	H	1116	0	1177	65	0
9	I	1010	0	1037	76	0
10	J	792	0	835	50	0
11	K	864	0	881	39	0
12	L	972	0	1058	67	0
13	M	937	0	995	51	0
14	N	492	0	529	50	0
15	O	729	0	768	37	0
16	P	700	0	720	50	0
17	Q	823	0	893	57	0
18	R	574	0	644	43	0
19	S	647	0	673	36	0
20	T	763	0	861	51	0
21	U	208	0	221	15	0
22	A	40	0	37	7	0
23	A	230	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	2	0	0	0	0
23	I	1	0	0	0	0
23	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	1	0	0	0	0
23	M	2	0	0	0	0
23	N	2	0	0	0	0
23	P	1	0	0	0	0
23	S	2	0	0	0	0
23	T	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	396	0	0	5	0
25	E	6	0	0	0	0
25	G	1	0	0	1	0
25	J	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	3	0	0	1	0
25	U	1	0	0	0	0
All	All	52297	0	36514	1864	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 21.

All (1864) 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)
1:A:1443:G:H5''	1:A:1446:A:H5'	1.37	1.01
1:A:103:C:OP1	20:T:17:ARG:NH1	1.98	0.95
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.50	0.91
3:C:142:MET:HE2	3:C:170:GLN:HB2	1.52	0.90
1:A:279:A:OP2	17:Q:95:TYR:OH	1.89	0.90
4:D:68:TYR:OH	4:D:98:GLU:OE1	1.91	0.89
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.53	0.89
1:A:1255:G:H2'	1:A:1279:A:H61	1.37	0.88
1:A:1498:UR3:O2'	1:A:1499:A:OP2	1.92	0.88
6:F:100:ASN:HD22	18:R:28:GLU:HG3	1.38	0.87
19:S:33:THR:HG22	19:S:35:SER:H	1.40	0.87
1:A:1316:G:N2	1:A:1319:A:OP2	2.08	0.86
12:L:57:LYS:HD2	12:L:67:THR:HG23	1.57	0.86
7:G:111:ARG:HD3	7:G:112:PRO:HD2	1.58	0.85
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.09	0.85
1:A:235:C:N4	25:A:1969:HOH:O	2.09	0.85
1:A:147:G:H1	1:A:175:C:H42	1.20	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1412:C:H2'	1:A:1413:A:C8	2.10	0.85
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.42	0.85
6:F:101:ALA:HA	18:R:28:GLU:HB3	1.60	0.84
10:J:31:GLY:HA2	10:J:78:ASN:HB2	1.57	0.84
1:A:419:C:N3	1:A:424:G:N2	2.26	0.84
2:B:17:PHE:HA	2:B:44:LEU:HD11	1.60	0.84
3:C:6:HIS:HD2	3:C:9:GLY:H	1.25	0.83
1:A:1008:C:H42	1:A:1021:G:H22	1.23	0.83
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.83
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.61	0.83
1:A:1376:U:O4	7:G:10:ARG:NH1	2.13	0.82
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.60	0.82
1:A:998:G:N2	1:A:1043:C:N3	2.28	0.81
8:H:83:ILE:HB	8:H:137:VAL:HG22	1.62	0.81
1:A:1055:A:N6	1:A:1205:U:O2	2.14	0.81
1:A:1124:G:N2	1:A:1126:U:O4	2.13	0.80
1:A:1404:5MC:H1'	1:A:1499:A:C2	2.17	0.80
1:A:113:G:H1'	1:A:354:G:H5'	1.63	0.79
3:C:156:ARG:H	3:C:163:ALA:HA	1.45	0.79
4:D:155:LEU:HB2	4:D:158:ILE:HD11	1.63	0.79
2:B:60:ASP:OD2	2:B:64:ARG:NH2	2.15	0.79
1:A:106:C:H2'	1:A:107:G:H5'	1.65	0.79
10:J:3:LYS:HG2	10:J:75:ILE:HD12	1.65	0.79
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.48	0.79
2:B:82:ARG:NH1	2:B:92:TYR:OH	2.15	0.79
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	1.65	0.78
1:A:1007:C:H1'	1:A:1023:G:H1	1.48	0.78
1:A:563:A:N6	25:A:1931:HOH:O	2.13	0.77
5:E:100:VAL:O	5:E:107:ARG:NH2	2.17	0.77
15:O:35:ARG:NH1	15:O:59:MET:SD	2.57	0.77
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.66	0.77
1:A:936:C:O2	1:A:1382:C:N4	2.16	0.77
1:A:1124:G:N2	1:A:1149:C:N3	2.32	0.77
1:A:613:C:H42	1:A:627:G:H1	1.32	0.76
2:B:157:ARG:HG2	2:B:158:LEU:HD12	1.68	0.76
1:A:1510:U:H2'	1:A:1511:G:C8	2.20	0.76
1:A:584:G:OP2	17:Q:87:LYS:NZ	2.17	0.76
4:D:13:ARG:NH1	4:D:38:TYR:O	2.18	0.76
1:A:1195:C:H3'	1:A:1196:U:H5''	1.67	0.76
3:C:75:VAL:O	3:C:83:ARG:NH1	2.18	0.76
1:A:1426:C:H42	1:A:1474:G:H1	1.32	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.13	0.76
4:D:190:ASP:H	4:D:193:ASP:HB2	1.51	0.75
1:A:1053:G:H4'	1:A:1054:C:H5'	1.69	0.75
1:A:1266:G:N2	1:A:1269:A:OP2	2.20	0.75
1:A:1130:A:H4'	9:I:20:ARG:HH22	1.52	0.75
6:F:22:GLU:OE2	6:F:82:ARG:NH1	2.19	0.75
1:A:501:C:H2'	1:A:502:G:H8	1.51	0.75
1:A:1112:C:O2	3:C:179:ARG:NH1	2.20	0.75
1:A:1255:G:N2	1:A:1259:C:O2	2.18	0.75
1:A:1303:C:H2'	1:A:1304:G:H5'	1.69	0.74
13:M:5:ALA:HB2	13:M:22:ILE:HD13	1.68	0.74
18:R:46:GLU:N	18:R:46:GLU:OE1	2.20	0.74
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.21	0.74
1:A:1255:G:O2'	1:A:1258:G:H1'	1.87	0.74
1:A:409:G:H1	1:A:433:C:H42	1.36	0.74
15:O:6:GLU:OE1	15:O:6:GLU:N	2.17	0.74
21:U:12:LYS:O	21:U:22:ARG:NH1	2.20	0.74
1:A:836:G:OP1	18:R:61:LYS:NZ	2.19	0.73
1:A:1119:C:N3	1:A:1154:G:N2	2.31	0.73
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.71	0.73
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.70	0.73
1:A:250:A:H4'	1:A:251:G:O5'	1.88	0.73
1:A:1505:G:C8	1:A:1505:G:H3'	2.24	0.73
12:L:46:LYS:HG2	12:L:47:LYS:H	1.52	0.73
1:A:948:C:H42	1:A:1233:G:H1	1.35	0.73
1:A:953:G:H5'	1:A:965:A:H61	1.54	0.73
4:D:173:TRP:CE2	4:D:189:PRO:HG3	2.24	0.72
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.71	0.72
1:A:1357:A:H2'	1:A:1358:U:C6	2.24	0.72
1:A:1258:G:H1	1:A:1277:C:H42	1.37	0.72
1:A:938:A:H5'	7:G:76:ARG:HH22	1.54	0.72
19:S:11:VAL:HG22	19:S:39:THR:HB	1.72	0.72
21:U:10:ARG:HD3	21:U:13:ILE:HG21	1.70	0.72
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.71	0.72
1:A:1120:G:N1	1:A:1154:G:N3	2.38	0.72
20:T:12:ALA:HA	25:T:303:HOH:O	1.88	0.72
3:C:25:GLY:H	3:C:28:GLN:HB2	1.53	0.71
19:S:47:HIS:HB2	19:S:49:ILE:HD11	1.72	0.71
1:A:1195:C:H3'	1:A:1196:U:C5'	2.20	0.71
1:A:1328:C:H2'	1:A:1329:A:H8	1.55	0.71
5:E:32:VAL:HG22	5:E:58:ALA:HB1	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:39:LEU:HD22	15:O:56:LEU:HB2	1.72	0.71
1:A:759:A:H2'	1:A:760:G:H5'	1.71	0.71
7:G:38:LEU:O	7:G:42:ILE:HG13	1.90	0.71
3:C:156:ARG:NH1	3:C:160:ALA:O	2.24	0.71
1:A:106:C:C2'	1:A:107:G:H5'	2.20	0.70
1:A:419:C:H42	1:A:424:G:H1	1.38	0.70
7:G:53:LYS:HZ2	7:G:125:MET:HE1	1.56	0.70
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.26	0.70
1:A:393:A:OP2	16:P:12:LYS:NZ	2.23	0.70
1:A:1240:U:OP2	7:G:116:ALA:N	2.23	0.70
1:A:103:C:P	20:T:17:ARG:HH12	2.14	0.70
1:A:1435:G:H2'	1:A:1436:U:C6	2.27	0.70
3:C:6:HIS:CD2	3:C:9:GLY:H	2.08	0.70
1:A:80:G:H1	1:A:89:C:H42	1.40	0.69
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.75	0.69
12:L:53:ARG:NH1	12:L:92:OTD:OD2	2.25	0.69
1:A:442:C:H42	1:A:492:G:H1	1.41	0.69
1:A:13:U:O2	1:A:914:A:H3'	1.92	0.69
10:J:30:SER:O	10:J:78:ASN:ND2	2.24	0.69
16:P:15:PRO:HG2	16:P:41:PRO:HG3	1.72	0.69
1:A:129(A):G:N3	1:A:190(E):U:H5''	2.07	0.69
1:A:390:C:O3'	16:P:28:ARG:NH2	2.25	0.69
5:E:118:ILE:O	5:E:119:LEU:HD23	1.93	0.69
8:H:120:THR:N	8:H:123:GLU:OE1	2.26	0.69
1:A:517:G:N1	1:A:533:A:OP2	2.24	0.69
1:A:147:G:H1	1:A:175:C:N4	1.91	0.69
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.74	0.68
7:G:16:LEU:HD21	9:I:42:ARG:HG2	1.75	0.68
1:A:1103:C:H5'	2:B:98:LEU:HD12	1.76	0.68
1:A:1158:C:N3	1:A:1181:G:N2	2.41	0.68
12:L:27:LEU:C	12:L:29:GLY:H	2.01	0.68
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.09	0.68
9:I:45:ALA:HA	9:I:48:GLU:HB3	1.74	0.68
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.76	0.68
18:R:32:ARG:HA	18:R:69:THR:HG21	1.76	0.68
8:H:64:LYS:HG3	8:H:79:VAL:HG21	1.74	0.68
1:A:677:U:H3	1:A:713:G:H22	1.39	0.68
1:A:978:A:H62	1:A:1360:A:N6	1.92	0.68
1:A:1063:C:H2'	1:A:1064:G:C8	2.29	0.68
4:D:150:GLU:HA	4:D:153:ARG:HE	1.59	0.68
1:A:1412:C:H2'	1:A:1413:A:H8	1.55	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:84:ILE:HG23	3:C:88:ARG:HH21	1.59	0.67
1:A:1048:G:H2'	1:A:1050:G:C8	2.28	0.67
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.67
1:A:615:C:H42	1:A:625:G:H1	1.39	0.67
1:A:1368:G:OP2	9:I:112:LYS:NZ	2.24	0.67
3:C:11:ARG:NH1	3:C:177:THR:O	2.20	0.67
3:C:150:LYS:HE3	3:C:173:VAL:HB	1.76	0.67
4:D:57:ARG:HA	4:D:202:LEU:HD12	1.77	0.67
1:A:789:U:O2'	1:A:791:G:N7	2.27	0.67
1:A:1505:G:H3'	1:A:1505:G:H8	1.58	0.67
1:A:192:U:H4'	20:T:57:ARG:HD2	1.77	0.67
4:D:68:TYR:CE2	4:D:97:LEU:HB3	2.30	0.67
1:A:107:G:C2	1:A:108:G:H1'	2.30	0.67
1:A:501:C:OP1	12:L:117:ARG:NH2	2.28	0.67
1:A:409:G:N2	1:A:433:C:N3	2.36	0.67
1:A:485:G:O2'	1:A:486:U:O5'	2.13	0.67
3:C:142:MET:HA	3:C:146:ALA:HB3	1.77	0.66
1:A:664:G:H22	1:A:741:G:H1	1.43	0.66
2:B:98:LEU:HD23	2:B:101:MET:HE3	1.76	0.66
3:C:111:LEU:HD13	3:C:204:LEU:HD13	1.78	0.66
12:L:124:LYS:HD2	12:L:125:PRO:HD2	1.76	0.66
1:A:411:A:C5	1:A:413:G:H1'	2.31	0.66
1:A:481:G:HO2'	1:A:482:A:H8	1.41	0.66
3:C:106:VAL:HG12	3:C:109:PRO:HA	1.77	0.66
16:P:53:VAL:O	16:P:56:ALA:N	2.28	0.66
17:Q:87:LYS:HA	17:Q:90:ILE:HD12	1.77	0.66
1:A:1236:A:H4'	1:A:1304:G:H4'	1.77	0.66
22:A:1601:SRY:O61	12:L:46:LYS:HD3	1.95	0.66
9:I:108:VAL:HG12	9:I:109:VAL:H	1.61	0.66
1:A:617:G:H1	1:A:623:C:H42	1.44	0.66
1:A:1245:A:H61	1:A:1292:U:H3	1.43	0.66
14:N:24:CYS:SG	14:N:28:GLY:N	2.68	0.66
1:A:946:A:O2'	1:A:1333:A:N3	2.24	0.66
1:A:968:A:C8	1:A:1062:U:H4'	2.31	0.66
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.11	0.66
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.36	0.66
13:M:37:THR:O	13:M:55:ARG:NH1	2.27	0.66
3:C:138:VAL:HG13	3:C:151:VAL:HG23	1.77	0.65
11:K:57:THR:HG23	11:K:60:ALA:H	1.62	0.65
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.76	0.65
15:O:55:GLY:HA2	15:O:58:MET:HE2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:U:H2'	1:A:96:G:H8	1.60	0.65
1:A:518:C:H5''	1:A:519:C:C6	2.32	0.65
1:A:837:G:H1	1:A:849:C:H42	1.44	0.65
1:A:1065:U:H5''	1:A:1190:G:N2	2.12	0.65
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.78	0.65
13:M:14:ARG:HE	13:M:42:ALA:HA	1.61	0.65
17:Q:81:ARG:HB3	17:Q:84:LEU:HD11	1.76	0.65
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.78	0.65
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.78	0.65
1:A:1183:A:O2'	1:A:1184:G:OP1	2.14	0.65
4:D:18:LYS:HG2	4:D:33:MET:HG2	1.77	0.65
1:A:527:7MG:H5''	1:A:527:7MG:H81	1.79	0.65
15:O:70:LEU:HB3	15:O:78:TYR:HB2	1.79	0.65
1:A:714:G:H2'	1:A:715:A:C8	2.31	0.65
1:A:1290:G:H2'	1:A:1291:G:H8	1.61	0.65
1:A:76:C:O2'	1:A:77:G:H5'	1.97	0.64
1:A:1008:C:H42	1:A:1021:G:N2	1.94	0.64
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.45	0.64
1:A:547:A:OP2	4:D:2:GLY:N	2.31	0.64
3:C:150:LYS:HG2	3:C:169:ALA:HB2	1.80	0.64
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.79	0.64
18:R:51:LEU:HD13	18:R:52:PRO:HD2	1.79	0.64
1:A:115:G:O2'	1:A:116:A:OP2	2.12	0.64
1:A:1347:G:N2	1:A:1374:A:OP2	2.19	0.64
18:R:59:SER:OG	18:R:60:ALA:N	2.30	0.64
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.16	0.64
3:C:23:TYR:HD2	10:J:95:GLU:HG3	1.63	0.64
12:L:85:ILE:CG2	12:L:98:TYR:HB3	2.28	0.64
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.78	0.64
1:A:539:A:H2'	1:A:540:G:H8	1.62	0.64
1:A:539:A:H2'	1:A:540:G:C8	2.31	0.64
1:A:1347:G:H3'	9:I:108:VAL:O	1.97	0.64
1:A:1465:C:H2'	1:A:1466:C:O4'	1.98	0.64
3:C:130:VAL:O	3:C:134:ILE:HG12	1.98	0.64
5:E:18:ARG:HG2	5:E:19:MET:N	2.12	0.64
6:F:100:ASN:ND2	18:R:28:GLU:HG3	2.12	0.63
1:A:1111:A:N1	3:C:177:THR:OG1	2.32	0.63
1:A:1257:U:H4'	1:A:1258:G:O5'	1.97	0.63
4:D:57:ARG:NH2	5:E:107:ARG:HD3	2.13	0.63
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.81	0.63
2:B:79:ASP:OD1	2:B:79:ASP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.33	0.63
9:I:93:ARG:HD2	9:I:97:LYS:NZ	2.14	0.63
20:T:63:ILE:HG21	20:T:81:LYS:HG3	1.80	0.63
1:A:1255:G:H2'	1:A:1279:A:N6	2.12	0.63
8:H:46:LYS:HG3	8:H:64:LYS:HB3	1.81	0.63
18:R:59:SER:N	18:R:62:GLU:OE1	2.32	0.63
1:A:1202:G:O4'	14:N:29:ARG:NH1	2.32	0.62
1:A:1174:G:H2'	1:A:1175:G:H8	1.64	0.62
4:D:191:ARG:HH12	4:D:198:VAL:HG12	1.64	0.62
9:I:53:VAL:HG21	9:I:85:LEU:HD23	1.80	0.62
14:N:40:CYS:C	14:N:44:LEU:HD22	2.24	0.62
21:U:10:ARG:HA	21:U:13:ILE:HB	1.80	0.62
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.32	0.62
3:C:47:LEU:HG	3:C:76:VAL:HG11	1.80	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.16	0.62
16:P:57:ARG:HH21	16:P:79:VAL:HA	1.63	0.62
20:T:10:LEU:HD13	20:T:12:ALA:H	1.64	0.62
1:A:1242:C:H42	1:A:1295:G:H1	1.46	0.62
6:F:14:LEU:HD21	6:F:84:ASN:ND2	2.14	0.62
12:L:117:ARG:HB3	12:L:122:THR:HG23	1.82	0.62
13:M:4:ILE:HG23	13:M:57:ARG:HA	1.81	0.62
15:O:41:GLU:OE2	15:O:44:LYS:NZ	2.33	0.62
1:A:1405:G:H1	1:A:1496:C:H5	1.48	0.62
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.80	0.62
12:L:84:LEU:HD23	12:L:101:VAL:HG21	1.81	0.62
1:A:737:A:O2'	6:F:73:ASN:ND2	2.32	0.62
1:A:973:G:H3'	1:A:974:A:H5''	1.82	0.62
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.64	0.62
12:L:85:ILE:HG21	12:L:98:TYR:HB3	1.80	0.62
16:P:78:GLY:C	16:P:80:PHE:H	2.07	0.62
1:A:384:G:H2'	1:A:385:C:C6	2.35	0.62
1:A:958:A:O2'	1:A:985:C:O2'	2.17	0.62
6:F:74:ASP:OD1	6:F:74:ASP:N	2.31	0.62
13:M:29:ARG:HD3	13:M:64:TRP:CE2	2.35	0.62
19:S:22:LEU:HD22	19:S:28:LYS:HG3	1.82	0.62
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.82	0.62
1:A:838:G:O6	1:A:848:C:N4	2.33	0.61
1:A:1028:C:N3	1:A:1034:G:N2	2.47	0.61
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.82	0.61
1:A:731:G:OP1	1:A:766:A:H1'	2.00	0.61
20:T:77:ALA:O	20:T:80:ARG:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1239:A:H4'	1:A:1240:U:H5''	1.81	0.61
1:A:1300:G:OP2	1:A:1335:C:N4	2.32	0.61
16:P:32:TYR:HE2	16:P:35:LYS:HB2	1.63	0.61
1:A:1030:C:H5	1:A:1030(A):G:C6	2.18	0.61
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.82	0.61
5:E:147:ASP:O	5:E:150:ARG:HB3	2.01	0.61
1:A:74:C:H42	1:A:96:G:H1	1.48	0.61
1:A:1058:G:OP1	3:C:199:LYS:NZ	2.30	0.61
20:T:10:LEU:HD22	20:T:11:SER:H	1.66	0.61
1:A:1359:C:O2'	1:A:1361(A):C:N4	2.33	0.61
1:A:1397:C:O2'	1:A:1398:A:OP1	2.19	0.61
1:A:1496:C:O2'	1:A:1497:G:O4'	2.17	0.61
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.81	0.61
1:A:1432:G:O2'	1:A:1468:A:N6	2.34	0.61
1:A:1504:G:OP1	1:A:1507:A:H4'	2.01	0.61
7:G:48:LYS:HG2	7:G:49:ILE:HD12	1.82	0.61
7:G:78:ARG:HD2	7:G:156:TRP:CE3	2.36	0.61
7:G:88:PRO:HG2	7:G:155:ARG:NH1	2.16	0.61
1:A:1243:C:OP2	21:U:10:ARG:NH2	2.32	0.61
1:A:1375:A:H4'	7:G:29:LYS:HE3	1.82	0.61
5:E:65:ASN:ND2	5:E:65:ASN:O	2.34	0.61
6:F:12:PRO:HG3	6:F:57:GLN:HG3	1.83	0.61
17:Q:47:PRO:HG2	17:Q:48:GLU:HG2	1.83	0.61
16:P:8:ARG:NH1	16:P:15:PRO:HB3	2.16	0.60
1:A:935:A:H61	7:G:3:ARG:HG3	1.66	0.60
1:A:953:G:H2'	1:A:954:G:O4'	2.02	0.60
3:C:26:LYS:HG2	10:J:45:ARG:HH12	1.65	0.60
7:G:30:ILE:HG22	7:G:39:ALA:HB1	1.83	0.60
7:G:70:LYS:HG3	7:G:100:ALA:HB2	1.83	0.60
13:M:16:ASP:OD1	13:M:16:ASP:N	2.26	0.60
1:A:143:A:H2	1:A:220:G:H22	1.47	0.60
3:C:101:LEU:HG	3:C:102:ASN:H	1.66	0.60
6:F:4:TYR:HB2	6:F:65:VAL:HG22	1.82	0.60
14:N:39:LEU:HD13	14:N:43:CYS:HB3	1.82	0.60
1:A:1234:C:H1'	1:A:1364:U:O2	2.01	0.60
4:D:47:ARG:NE	4:D:47:ARG:O	2.33	0.60
10:J:84:GLN:HG3	10:J:85:LEU:HD12	1.83	0.60
1:A:392:G:H2'	1:A:393:A:H8	1.67	0.60
1:A:1346:A:H5''	9:I:120:ARG:HH12	1.66	0.60
4:D:65:ARG:HB2	4:D:75:PHE:CE1	2.36	0.60
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:G:H2'	1:A:36:C:C6	2.37	0.60
12:L:6:THR:HG1	12:L:9:GLN:H	1.48	0.60
1:A:1338:G:H2'	1:A:1339:A:C8	2.36	0.60
3:C:150:LYS:HB2	3:C:201:TYR:HB2	1.83	0.60
7:G:108:ALA:HB2	7:G:123:GLU:HG2	1.83	0.60
14:N:8:GLU:O	14:N:12:ARG:N	2.32	0.60
1:A:620:C:H2'	1:A:621:A:O4'	2.02	0.60
1:A:144:G:H1	1:A:178:C:H42	1.49	0.60
2:B:164:VAL:HG23	2:B:186:ALA:HA	1.83	0.60
1:A:102:G:H2'	1:A:103:C:H6	1.65	0.59
1:A:285:G:H2'	1:A:286:G:H8	1.67	0.59
1:A:636:U:H2'	1:A:637:G:C8	2.36	0.59
1:A:826:C:O2	8:H:15:ASN:ND2	2.34	0.59
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.31	0.59
1:A:1222:G:OP1	19:S:77:THR:HG21	2.02	0.59
1:A:79:G:C6	1:A:80:G:C6	2.90	0.59
2:B:73:THR:HG23	2:B:95:GLN:O	2.01	0.59
3:C:14:ILE:HD11	14:N:57:ARG:HH22	1.67	0.59
9:I:91:ASP:OD1	9:I:91:ASP:N	2.31	0.59
13:M:101:GLN:OE1	13:M:101:GLN:N	2.34	0.59
14:N:52:GLN:O	14:N:53:LEU:HD23	2.03	0.59
20:T:92:LEU:O	20:T:96:GLY:HA2	2.02	0.59
1:A:571:U:O4	1:A:864:A:N6	2.35	0.59
5:E:144:THR:O	5:E:148:VAL:HG23	2.03	0.59
6:F:35:ALA:HA	6:F:67:MET:HB3	1.83	0.59
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.38	0.59
1:A:439:A:OP2	1:A:494:G:N1	2.36	0.59
1:A:1400:5MC:H3'	1:A:1401:G:H5'	1.85	0.59
2:B:139:LYS:HZ2	2:B:143:GLU:HG3	1.67	0.59
3:C:6:HIS:HD2	3:C:9:GLY:N	1.98	0.59
1:A:913:A:OP2	12:L:91:LYS:NZ	2.36	0.59
1:A:1518:MA6:H102	1:A:1519:MA6:H103	1.84	0.59
8:H:73:ASP:OD1	8:H:75:ARG:HB2	2.03	0.59
1:A:512:U:OP1	4:D:46:LYS:NZ	2.34	0.59
1:A:1267:C:N3	1:A:1327:C:O2'	2.36	0.59
1:A:1376:U:H2'	1:A:1377:A:C8	2.38	0.59
19:S:15:LEU:HD13	19:S:44:MET:HE1	1.85	0.59
20:T:35:THR:HA	20:T:38:LYS:HE2	1.84	0.59
20:T:50:GLU:HG3	20:T:51:GLU:HG2	1.83	0.59
1:A:578:C:O2'	1:A:728:A:N3	2.35	0.59
1:A:918:A:H2'	1:A:919:A:C8	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:A:H4'	1:A:1202:G:O5'	2.03	0.59
1:A:1255:G:C6	1:A:1279:A:N7	2.71	0.59
3:C:25:GLY:HA2	3:C:29:TYR:N	2.17	0.59
3:C:188:LEU:HD22	3:C:195:VAL:HG22	1.84	0.59
11:K:81:ASP:CG	11:K:106:LYS:HB2	2.27	0.59
1:A:109:A:H62	1:A:324:G:H21	1.48	0.58
1:A:394:G:H2'	1:A:395:C:H6	1.68	0.58
1:A:1238:A:H5'	1:A:1336:C:H41	1.66	0.58
3:C:155:GLY:HA2	3:C:164:ARG:O	2.03	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.68	0.58
8:H:123:GLU:HA	8:H:126:LYS:HB3	1.84	0.58
1:A:452:A:O2'	16:P:72:ARG:HD2	2.03	0.58
2:B:162:ILE:O	2:B:185:ILE:HD12	2.03	0.58
20:T:71:THR:O	20:T:72:LEU:HD23	2.03	0.58
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.38	0.58
3:C:14:ILE:HG22	3:C:15:THR:HG23	1.84	0.58
3:C:153:VAL:H	3:C:166:GLU:HB3	1.67	0.58
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.21	0.58
12:L:33:ARG:O	12:L:85:ILE:HD12	2.02	0.58
18:R:58:LEU:HD23	18:R:58:LEU:H	1.68	0.58
1:A:376:G:O3'	16:P:5:ARG:NH1	2.36	0.58
9:I:19:LEU:HD11	9:I:81:ILE:HA	1.83	0.58
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.85	0.58
1:A:90:U:H2'	1:A:91:C:O4'	2.03	0.58
1:A:200:G:H1	1:A:217:C:H42	1.51	0.58
1:A:407:G:OP1	4:D:115:ARG:NH2	2.31	0.58
3:C:123:GLN:O	3:C:128:PHE:HB2	2.03	0.58
13:M:63:THR:HG23	13:M:64:TRP:H	1.68	0.58
16:P:75:ARG:HB2	16:P:80:PHE:HD1	1.69	0.58
20:T:69:GLY:O	20:T:73:HIS:ND1	2.37	0.58
1:A:95:U:H2'	1:A:96:G:C8	2.37	0.58
1:A:1255:G:C4	1:A:1279:A:N6	2.71	0.58
1:A:1007:C:H2'	1:A:1008:C:C5	2.39	0.58
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.84	0.58
9:I:103:THR:HG22	9:I:104:ARG:O	2.04	0.58
13:M:14:ARG:HB2	13:M:17:VAL:HG23	1.86	0.58
19:S:69:HIS:HB3	19:S:73:GLU:CD	2.28	0.58
1:A:943:U:C2'	1:A:944:G:H5'	2.34	0.58
1:A:1360:A:H2	14:N:18:VAL:HB	1.68	0.58
1:A:112:G:O2'	1:A:113:G:H5'	2.04	0.58
1:A:192:U:O4'	20:T:103:GLY:HA2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.85	0.58
5:E:118:ILE:HG12	5:E:119:LEU:H	1.69	0.58
10:J:57:LYS:NZ	10:J:60:ARG:HH22	2.02	0.58
1:A:642:A:N3	8:H:113:SER:OG	2.37	0.57
6:F:80:ARG:HH12	6:F:88:VAL:H	1.51	0.57
17:Q:24:GLU:HA	17:Q:39:SER:HB3	1.86	0.57
1:A:707:C:H2'	1:A:708:C:C6	2.39	0.57
1:A:972:C:OP2	10:J:57:LYS:HE3	2.04	0.57
1:A:1030(A):G:H2'	1:A:1030(B):C:H5''	1.86	0.57
9:I:15:ALA:HA	9:I:65:VAL:HG12	1.87	0.57
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.87	0.57
5:E:102:ALA:HA	5:E:120:THR:HB	1.86	0.57
1:A:1479:C:H2'	1:A:1480:G:H8	1.68	0.57
9:I:16:ARG:HB2	9:I:16:ARG:HH11	1.68	0.57
18:R:46:GLU:H	18:R:46:GLU:CD	2.10	0.57
1:A:598:U:H4'	8:H:94:TYR:CD1	2.40	0.57
1:A:836:G:C6	1:A:851:G:C6	2.93	0.57
1:A:1202:G:O2'	14:N:27:CYS:SG	2.62	0.57
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.37	0.57
3:C:180:ALA:HB1	3:C:205:GLY:O	2.05	0.57
6:F:80:ARG:NH1	6:F:88:VAL:H	2.02	0.57
14:N:24:CYS:SG	14:N:29:ARG:N	2.71	0.57
1:A:184:G:H2'	1:A:185:A:H8	1.70	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
1:A:451:A:H2	1:A:480:U:C5	2.22	0.57
1:A:452:A:O2'	1:A:453:A:O5'	2.22	0.57
1:A:646:U:H2'	1:A:647:C:C6	2.39	0.57
1:A:1520:G:H2'	1:A:1521:G:H8	1.68	0.57
5:E:99:GLY:O	5:E:101:ILE:HD12	2.03	0.57
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.86	0.57
16:P:5:ARG:HE	16:P:22:THR:HG21	1.69	0.57
1:A:1379:G:OP2	7:G:6:ARG:NH2	2.38	0.57
2:B:114:ARG:NH1	2:B:117:GLU:OE2	2.33	0.57
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.04	0.57
1:A:687:A:H4'	1:A:688:G:O5'	2.04	0.57
1:A:825:G:H1	1:A:875:C:H42	1.52	0.57
9:I:20:ARG:O	9:I:60:ASP:N	2.38	0.57
1:A:992:U:O2'	1:A:993:G:OP2	2.20	0.57
1:A:1328:C:H2'	1:A:1329:A:C8	2.37	0.57
2:B:19:HIS:CG	2:B:20:GLU:H	2.23	0.57
3:C:10:PHE:CE1	3:C:178:LEU:HD21	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:93:ARG:HD2	9:I:97:LYS:HZ2	1.68	0.57
1:A:216:G:O2'	1:A:217:C:O4'	2.17	0.57
1:A:1163:C:H2'	1:A:1164:G:C8	2.40	0.57
2:B:118:LEU:HB2	2:B:142:LEU:HD23	1.86	0.57
7:G:26:PHE:HA	7:G:101:LEU:HD23	1.87	0.57
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.87	0.57
7:G:90:GLU:N	7:G:90:GLU:OE2	2.38	0.57
1:A:129:U:O3'	1:A:129(A):G:H3'	2.04	0.56
1:A:1168:A:H2'	1:A:1169:A:C8	2.40	0.56
3:C:88:ARG:HA	3:C:91:LEU:HB3	1.86	0.56
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.87	0.56
4:D:60:GLU:OE1	4:D:60:GLU:HA	2.05	0.56
5:E:20:GLN:CD	5:E:21:ALA:H	2.13	0.56
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.87	0.56
1:A:411:A:N7	1:A:413:G:H1'	2.20	0.56
1:A:545:C:OP2	4:D:62:GLN:NE2	2.27	0.56
1:A:914:A:OP1	22:A:1601:SRY:HI33	2.04	0.56
1:A:975:A:H5'	1:A:975:A:H8	1.70	0.56
1:A:1095:U:OP1	1:A:1108:G:N2	2.32	0.56
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.39	0.56
1:A:1270:C:HO2'	1:A:1313:U:HO2'	1.42	0.56
1:A:1399:C:O2	1:A:1401:G:C5	2.58	0.56
4:D:98:GLU:HG2	4:D:189:PRO:HG2	1.87	0.56
7:G:50:ILE:O	7:G:54:THR:OG1	2.17	0.56
8:H:2:LEU:HD23	8:H:3:THR:N	2.19	0.56
9:I:32:ASP:OD2	9:I:33:PHE:N	2.38	0.56
2:B:87:ARG:HH21	2:B:233:SER:HB2	1.68	0.56
8:H:91:ARG:NH1	17:Q:32:TYR:O	2.38	0.56
10:J:19:SER:HB2	10:J:91:PRO:HG3	1.87	0.56
14:N:39:LEU:HD22	14:N:43:CYS:CB	2.35	0.56
16:P:49:LEU:HD12	16:P:50:LYS:H	1.71	0.56
1:A:1281:U:H4'	1:A:1282:C:OP2	2.05	0.56
3:C:35:GLU:O	3:C:39:ILE:HG13	2.06	0.56
5:E:95:ALA:HB1	5:E:96:PRO:HD2	1.87	0.56
9:I:10:ARG:HH21	9:I:11:LYS:HE3	1.71	0.56
1:A:1227:A:O3'	13:M:115:LYS:HG2	2.06	0.56
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.41	0.56
1:A:83:U:O2'	1:A:84:U:H5'	2.05	0.56
1:A:613:C:N4	1:A:627:G:H1	2.02	0.56
1:A:1477:C:H2'	1:A:1478:C:H6	1.70	0.56
1:A:1198:G:H2'	1:A:1199:U:C6	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:80:ILE:H	8:H:80:ILE:HD12	1.71	0.56
19:S:64:GLU:O	19:S:67:VAL:HG23	2.06	0.56
1:A:463:A:H2'	1:A:474:G:H8	1.71	0.56
1:A:981:U:H2'	1:A:982:U:C5	2.41	0.56
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.18	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.41	0.56
1:A:1414:U:H2'	1:A:1415:G:H8	1.70	0.56
20:T:36:LEU:O	20:T:39:LYS:HB3	2.06	0.56
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.88	0.56
1:A:451:A:N7	1:A:481:G:C2	2.74	0.56
4:D:99:SER:HB2	4:D:139:ARG:HD3	1.87	0.56
12:L:86:ARG:HH11	12:L:86:ARG:HG3	1.71	0.56
1:A:142:G:O2'	1:A:196:A:N1	2.31	0.55
1:A:254:G:OP1	17:Q:67:LYS:O	2.24	0.55
1:A:327:A:O2'	1:A:328:C:O4'	2.22	0.55
4:D:31:CYS:C	4:D:33:MET:H	2.13	0.55
1:A:76:C:H2'	1:A:77:G:C8	2.40	0.55
1:A:651:C:H2'	1:A:652:U:C6	2.41	0.55
1:A:1103:C:H5'	2:B:98:LEU:CD1	2.36	0.55
1:A:1347:G:O2'	1:A:1348:U:P	2.64	0.55
6:F:80:ARG:NH2	6:F:88:VAL:O	2.40	0.55
1:A:9:G:OP2	5:E:121:LYS:NZ	2.28	0.55
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.88	0.55
1:A:562:C:H1'	12:L:15:ARG:HD2	1.88	0.55
1:A:973:G:O3'	14:N:41:ARG:NH2	2.35	0.55
2:B:178:ARG:HD3	2:B:196:LEU:HD22	1.88	0.55
8:H:63:LEU:HD22	8:H:63:LEU:H	1.71	0.55
8:H:65:TYR:N	8:H:65:TYR:CD1	2.75	0.55
13:M:14:ARG:NE	13:M:42:ALA:HA	2.21	0.55
1:A:1020:U:H2'	1:A:1021:G:H8	1.72	0.55
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.89	0.55
10:J:57:LYS:HZ1	10:J:60:ARG:HH22	1.55	0.55
1:A:478:A:H2'	1:A:479:C:C6	2.42	0.55
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.55
1:A:1071:C:H42	1:A:1104:G:H1	1.53	0.55
1:A:1205:U:H5''	3:C:190:ARG:HE	1.71	0.55
4:D:191:ARG:NH1	4:D:198:VAL:HG12	2.21	0.55
6:F:98:LEU:HD22	6:F:101:ALA:HB2	1.88	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.40	0.55
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.89	0.55
9:I:86:VAL:HG21	9:I:102:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:U:O4	1:A:20:G:N2	2.34	0.55
1:A:164:U:H2'	1:A:165:C:C6	2.42	0.55
1:A:1279:A:OP2	10:J:9:ARG:NH2	2.40	0.55
1:A:1405:G:N2	1:A:1497:G:C4	2.74	0.55
1:A:1442:G:C2	1:A:1446:A:N7	2.75	0.55
2:B:53:ARG:HA	2:B:56:ARG:NH1	2.21	0.55
12:L:41:ARG:HH12	12:L:43:VAL:HG13	1.72	0.55
1:A:658:G:H2'	1:A:659:U:H6	1.72	0.55
1:A:960:U:H4'	1:A:961:U:C5'	2.37	0.55
1:A:1355:G:H2'	1:A:1356:G:C8	2.41	0.55
6:F:97:PHE:CE2	6:F:99:ALA:HB2	2.42	0.55
8:H:123:GLU:O	8:H:127:LEU:HB2	2.07	0.55
1:A:509:A:C8	1:A:509:A:H3'	2.42	0.55
1:A:538:G:OP1	12:L:115:LYS:N	2.40	0.55
4:D:55:ALA:O	4:D:59:ARG:HG2	2.06	0.55
16:P:53:VAL:O	16:P:54:GLU:C	2.50	0.55
19:S:21:GLU:O	19:S:25:LYS:HD3	2.06	0.55
5:E:40:ARG:HG2	5:E:68:GLU:HA	1.89	0.55
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.42	0.55
1:A:706:A:O2'	11:K:29:ILE:HD11	2.07	0.54
1:A:1494:G:C2	1:A:1495:U:C5	2.95	0.54
3:C:43:LEU:HD13	3:C:47:LEU:HD13	1.88	0.54
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.72	0.54
1:A:384:G:H2'	1:A:385:C:H6	1.70	0.54
1:A:1007:C:O2'	1:A:1023:G:N2	2.38	0.54
1:A:1068:G:OP2	1:A:1068:G:H8	1.89	0.54
1:A:1419:G:H1	1:A:1481:U:H3	1.55	0.54
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.89	0.54
3:C:117:ALA:HB2	3:C:200:ALA:HB2	1.89	0.54
7:G:123:GLU:O	7:G:126:ASP:N	2.39	0.54
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.89	0.54
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.89	0.54
14:N:39:LEU:HD13	14:N:43:CYS:C	2.33	0.54
17:Q:29:HIS:CE1	17:Q:31:LEU:H	2.24	0.54
1:A:887:G:H1	1:A:910:C:H42	1.55	0.54
1:A:954:G:H21	1:A:1227:A:H62	1.55	0.54
1:A:1376:U:H2'	1:A:1377:A:H8	1.72	0.54
1:A:1413:A:H2	1:A:1487:G:H22	1.53	0.54
2:B:12:GLU:HB2	2:B:213:LEU:HD11	1.89	0.54
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.54
12:L:85:ILE:HG23	12:L:99:HIS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:18:LYS:O	19:S:22:LEU:HG	2.06	0.54
1:A:451:A:N7	1:A:481:G:N2	2.55	0.54
5:E:109:ILE:HG22	5:E:110:LEU:HD23	1.89	0.54
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.40	0.54
9:I:19:LEU:HD12	9:I:84:ALA:HB3	1.89	0.54
13:M:86:CYS:SG	13:M:87:TYR:N	2.80	0.54
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.23	0.54
15:O:61:GLY:O	15:O:65:ARG:HD3	2.06	0.54
17:Q:10:VAL:HG21	17:Q:52:LYS:O	2.08	0.54
20:T:49:ALA:HB3	20:T:99:LEU:HB2	1.90	0.54
2:B:172:ILE:HD12	2:B:173:ALA:H	1.72	0.54
14:N:18:VAL:HG22	14:N:19:ARG:HD2	1.90	0.54
1:A:474:G:H4'	16:P:81:ARG:HH21	1.72	0.54
1:A:770:C:H42	1:A:809:G:H1	1.55	0.54
1:A:788:U:H5''	1:A:789:U:OP2	2.08	0.54
1:A:1004:A:O2'	1:A:1005:A:OP1	2.24	0.54
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.54
11:K:66:LEU:HD21	11:K:97:ALA:HB1	1.89	0.54
1:A:35:G:H2'	1:A:36:C:H6	1.71	0.54
1:A:1097:C:H2'	1:A:1098:C:C6	2.42	0.54
5:E:37:ARG:HH22	5:E:111:GLU:HG2	1.73	0.54
7:G:53:LYS:NZ	7:G:125:MET:HE1	2.20	0.54
9:I:10:ARG:NH1	9:I:105:ASP:OD2	2.40	0.54
12:L:87:GLY:H	12:L:99:HIS:H	1.55	0.54
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.43	0.54
1:A:113:G:C1'	1:A:354:G:H5'	2.34	0.54
1:A:130:A:H5'	17:Q:63:ARG:NH2	2.22	0.54
8:H:17:THR:HB	8:H:78:GLN:HE22	1.73	0.54
14:N:39:LEU:HB3	14:N:44:LEU:HD13	1.88	0.54
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.40	0.54
1:A:1305:G:N2	1:A:1331:G:H1'	2.23	0.54
22:A:1601:SRY:O21	22:A:1601:SRY:NE1	2.41	0.54
4:D:25:ARG:HA	4:D:28:SER:HB2	1.90	0.54
6:F:11:ASN:HB2	6:F:86:ARG:NE	2.23	0.54
1:A:75:G:H2'	1:A:76:C:C6	2.43	0.54
1:A:90:U:C4	1:A:91:C:C4	2.96	0.54
1:A:952:U:H2'	1:A:953:G:H8	1.72	0.54
1:A:1049:U:O2'	14:N:3:ARG:NH1	2.41	0.54
1:A:1172:C:H2'	1:A:1173:G:C8	2.43	0.54
4:D:8:VAL:O	4:D:11:LEU:N	2.40	0.54
6:F:95:GLU:O	18:R:32:ARG:NH1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.89	0.54
20:T:78:ALA:HA	20:T:81:LYS:HD3	1.90	0.54
1:A:792:A:N6	1:A:794:A:C2	2.76	0.53
13:M:39:ILE:HD12	13:M:40:ASN:H	1.74	0.53
17:Q:56:VAL:O	17:Q:77:VAL:HG23	2.08	0.53
1:A:369:C:H42	1:A:392:G:H1	1.55	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.06	0.53
1:A:1056:U:O2'	1:A:1057:G:H5'	2.08	0.53
1:A:1290:G:H2'	1:A:1291:G:C8	2.41	0.53
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.72	0.53
4:D:63:LYS:O	4:D:67:ILE:HG13	2.08	0.53
4:D:187:ARG:NH1	4:D:188:LEU:HD23	2.24	0.53
10:J:16:LEU:HD21	10:J:94:VAL:HA	1.90	0.53
1:A:1006:C:H2'	1:A:1007:C:C6	2.43	0.53
2:B:16:HIS:CD2	2:B:204:ASN:H	2.27	0.53
15:O:21:ASP:OD1	15:O:24:SER:OG	2.20	0.53
1:A:1329:A:P	13:M:28:ALA:HB3	2.49	0.53
3:C:188:LEU:HD23	3:C:196:LEU:O	2.08	0.53
16:P:9:PHE:CE2	16:P:18:ARG:HD2	2.43	0.53
17:Q:81:ARG:NH2	17:Q:83:ASP:OD2	2.41	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.09	0.53
1:A:914:A:P	22:A:1601:SRY:HI33	2.49	0.53
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.08	0.53
1:A:1258:G:H1	1:A:1277:C:N4	2.03	0.53
1:A:1531:A:O5'	1:A:1531:A:H8	1.91	0.53
4:D:10:ARG:HA	4:D:13:ARG:HG2	1.89	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.43	0.53
1:A:200:G:H2'	1:A:201:C:O2	2.07	0.53
1:A:1163:C:H2'	1:A:1164:G:H8	1.74	0.53
7:G:139:GLU:O	7:G:143:ARG:HB3	2.09	0.53
8:H:87:SER:HA	8:H:93:VAL:HG23	1.90	0.53
1:A:505:G:H1	1:A:526:C:H42	1.57	0.53
1:A:965:A:C2	1:A:969:A:C2	2.97	0.53
1:A:1061:G:H1'	10:J:56:HIS:CE1	2.44	0.53
7:G:5:ARG:NH2	25:G:201:HOH:O	2.37	0.53
8:H:85:ARG:NE	8:H:87:SER:O	2.42	0.53
13:M:96:LEU:O	13:M:110:ARG:NH1	2.41	0.53
15:O:2:PRO:O	15:O:38:ARG:NH2	2.41	0.53
1:A:451:A:N6	1:A:481:G:C4	2.77	0.53
1:A:1145:C:H1'	1:A:1146:A:N7	2.24	0.53
4:D:162:LEU:HA	4:D:165:MET:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:775:G:C2'	1:A:776:G:H5'	2.39	0.53
3:C:81:GLY:O	3:C:84:ILE:HG22	2.08	0.53
3:C:180:ALA:CB	3:C:203:PHE:HE1	2.22	0.53
4:D:190:ASP:OD1	4:D:191:ARG:N	2.42	0.53
5:E:122:GLU:O	5:E:123:LEU:HD23	2.09	0.53
8:H:9:MET:O	8:H:13:ILE:HD12	2.09	0.53
1:A:392:G:H2'	1:A:393:A:C8	2.44	0.53
3:C:66:VAL:HG12	3:C:68:VAL:HG23	1.91	0.53
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.90	0.53
7:G:140:ASP:HA	7:G:143:ARG:HD2	1.89	0.53
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.44	0.53
16:P:68:ASP:OD1	16:P:68:ASP:N	2.42	0.53
1:A:1014:A:H2'	1:A:1015:A:O4'	2.08	0.52
1:A:1204:A:C5	1:A:1205:U:C5	2.97	0.52
1:A:1278:U:H4'	1:A:1279:A:N3	2.24	0.52
1:A:1392:G:N2	1:A:1502:A:H8	2.07	0.52
1:A:1493:A:H2'	1:A:1494:G:H8	1.74	0.52
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.15	0.52
12:L:6:THR:OG1	12:L:9:GLN:N	2.37	0.52
14:N:40:CYS:O	14:N:44:LEU:N	2.30	0.52
16:P:9:PHE:HE2	16:P:18:ARG:HD2	1.74	0.52
16:P:58:TYR:CD1	16:P:58:TYR:C	2.85	0.52
1:A:463:A:OP1	16:P:75:ARG:NH1	2.37	0.52
1:A:760:G:H2'	1:A:761:G:O4'	2.08	0.52
1:A:1057:G:H5''	3:C:154:SER:HB2	1.92	0.52
1:A:1064:G:N2	1:A:1191:A:OP2	2.36	0.52
1:A:1354:C:H2'	1:A:1355:G:H8	1.74	0.52
1:A:1392:G:H21	1:A:1502:A:H8	1.57	0.52
13:M:59:TYR:O	13:M:63:THR:HG22	2.09	0.52
1:A:403:C:O2'	4:D:122:ARG:NH1	2.43	0.52
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.52
1:A:1355:G:H2'	1:A:1356:G:H8	1.73	0.52
13:M:22:ILE:HG22	13:M:23:TYR:N	2.25	0.52
14:N:2:ALA:HB2	14:N:28:GLY:HA3	1.91	0.52
1:A:89:C:H2'	1:A:90:U:C6	2.44	0.52
1:A:1482:G:HO2'	1:A:1483:A:H8	1.54	0.52
1:A:1525:G:H2'	1:A:1526:G:H8	1.74	0.52
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.24	0.52
4:D:119:GLN:HG3	4:D:123:HIS:CD2	2.44	0.52
7:G:80:VAL:HG11	7:G:154:TYR:HE2	1.75	0.52
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:114:THR:HG22	8:H:131:GLY:HA3	1.92	0.52
4:D:10:ARG:O	4:D:13:ARG:HG2	2.08	0.52
10:J:8:LEU:HD21	10:J:96:ILE:HG23	1.90	0.52
13:M:2:ALA:O	13:M:4:ILE:HD12	2.10	0.52
14:N:24:CYS:O	14:N:28:GLY:HA2	2.10	0.52
1:A:75:G:C6	1:A:96:G:N1	2.77	0.52
1:A:767:A:H2'	1:A:768:A:O4'	2.09	0.52
22:A:1601:SRY:O21	22:A:1601:SRY:NB1	2.42	0.52
2:B:136:VAL:O	2:B:140:HIS:ND1	2.41	0.52
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.25	0.52
6:F:2:ARG:O	6:F:66:GLU:HA	2.09	0.52
6:F:41:GLU:O	6:F:62:TRP:HB3	2.09	0.52
6:F:70:ASP:OD1	6:F:71:ARG:HG2	2.09	0.52
13:M:74:VAL:O	13:M:78:ILE:HG13	2.10	0.52
1:A:37:U:H2'	1:A:38:G:O4'	2.10	0.52
1:A:130:A:H5'	17:Q:63:ARG:CZ	2.40	0.52
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.52
1:A:372:C:H4'	1:A:373:A:O5'	2.10	0.52
1:A:975:A:H4'	1:A:976:G:O5'	2.09	0.52
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.52
3:C:150:LYS:HZ3	3:C:175:LEU:HD11	1.75	0.52
8:H:82:HIS:CE1	8:H:138:TRP:NE1	2.77	0.52
8:H:86:ILE:HG21	8:H:133:LEU:HD13	1.91	0.52
9:I:48:GLU:N	9:I:49:PRO:HD2	2.25	0.52
1:A:463:A:H1'	16:P:82:GLN:HG3	1.92	0.52
1:A:609:A:N6	25:A:2089:HOH:O	2.42	0.52
1:A:644:G:C5	1:A:645:C:C5	2.98	0.52
1:A:1256:A:H4'	1:A:1257:U:O5'	2.10	0.52
1:A:1328:C:OP2	21:U:7:ARG:NH1	2.43	0.52
2:B:168:THR:HG22	2:B:169:LYS:HD2	1.92	0.52
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.92	0.52
12:L:86:ARG:HG3	12:L:86:ARG:NH1	2.23	0.52
17:Q:58:GLU:HB3	17:Q:74:LEU:HB3	1.92	0.52
1:A:411:A:H62	1:A:413:G:N2	2.08	0.52
1:A:721:G:C6	1:A:733:A:C2	2.98	0.52
3:C:23:TYR:CD2	10:J:95:GLU:HG3	2.44	0.52
8:H:12:ARG:NH1	8:H:27:PRO:HD3	2.24	0.52
8:H:82:HIS:CE1	8:H:138:TRP:CD1	2.98	0.52
1:A:269:C:H2'	1:A:270:A:C8	2.45	0.51
1:A:1197:G:H5''	1:A:1198:G:OP2	2.11	0.51
1:A:1404:5MC:H1'	1:A:1499:A:H2	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:LYS:HD3	2:B:193:ASP:OD1	2.10	0.51
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.51
3:C:36:ASP:O	3:C:39:ILE:HB	2.11	0.51
4:D:163:GLU:HG3	4:D:166:LYS:HE2	1.91	0.51
9:I:50:LEU:O	9:I:53:VAL:HG12	2.10	0.51
1:A:422:C:H4'	1:A:423:G:O5'	2.10	0.51
1:A:1052:U:C2	1:A:1200:C:N4	2.78	0.51
25:A:2110:HOH:O	2:B:96:ARG:HG2	2.11	0.51
11:K:72:ALA:HA	11:K:75:TYR:HB2	1.91	0.51
1:A:750:G:N3	15:O:23:GLY:HA3	2.25	0.51
1:A:757:U:H5''	1:A:822:C:O2	2.10	0.51
1:A:974:A:H8	1:A:974:A:OP1	1.94	0.51
2:B:55:PHE:HA	2:B:58:ILE:HD12	1.91	0.51
14:N:47:LEU:O	14:N:53:LEU:HG	2.11	0.51
1:A:633:G:H2'	1:A:634:C:C6	2.46	0.51
1:A:1357:A:H2'	1:A:1358:U:H6	1.71	0.51
2:B:68:ILE:H	2:B:90:MET:HG2	1.74	0.51
3:C:26:LYS:HG2	10:J:45:ARG:NH1	2.26	0.51
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.93	0.51
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.74	0.51
8:H:82:HIS:CE1	8:H:138:TRP:HE1	2.28	0.51
1:A:230:G:H2'	1:A:231:G:O4'	2.11	0.51
1:A:1030:C:N3	1:A:1032:G:N1	2.58	0.51
1:A:1172:C:H2'	1:A:1173:G:H8	1.76	0.51
3:C:120:VAL:HG12	3:C:124:ILE:HD11	1.92	0.51
7:G:145:ALA:O	7:G:146:GLU:HG2	2.10	0.51
10:J:91:PRO:HB2	10:J:94:VAL:HG13	1.91	0.51
1:A:132:C:O3'	20:T:74:LYS:NZ	2.43	0.51
1:A:658:G:H1	1:A:747:C:H42	1.59	0.51
3:C:16:ARG:HG3	3:C:17:ASP:H	1.76	0.51
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.45	0.51
1:A:279:A:OP1	1:A:280:C:O2'	2.17	0.51
1:A:710:G:H5''	6:F:54:LYS:HE3	1.91	0.51
1:A:1029:C:N3	1:A:1033:G:N2	2.58	0.51
1:A:1095:U:H5''	1:A:1109:C:O2	2.11	0.51
1:A:1316:G:H1	19:S:6:LYS:HZ3	1.59	0.51
5:E:39:GLY:O	5:E:69:VAL:HG23	2.11	0.51
12:L:6:THR:HG23	12:L:9:GLN:OE1	2.10	0.51
15:O:56:LEU:O	15:O:60:VAL:HG23	2.10	0.51
1:A:575:G:OP1	1:A:575:G:H4'	2.11	0.51
1:A:1094:G:O2'	1:A:1108:G:N2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:GLY:HA2	2:B:42:ILE:HG12	1.93	0.51
4:D:111:ALA:HA	4:D:161:ASN:ND2	2.25	0.51
5:E:5:ASP:OD1	5:E:5:ASP:N	2.43	0.51
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.45	0.51
20:T:43:LEU:HD12	20:T:52:ALA:HA	1.93	0.51
1:A:552:U:H2'	1:A:553:A:C8	2.46	0.51
1:A:1302:U:O4	13:M:14:ARG:NH1	2.44	0.51
1:A:1368:G:OP1	9:I:111:ARG:NH1	2.44	0.51
1:A:1505:G:C8	1:A:1505:G:C3'	2.91	0.51
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.92	0.51
4:D:15:GLU:CD	4:D:59:ARG:HH21	2.18	0.51
9:I:118:LYS:O	9:I:120:ARG:N	2.43	0.51
11:K:95:ILE:HA	11:K:98:LEU:CD1	2.41	0.51
12:L:87:GLY:HA2	12:L:98:TYR:CA	2.32	0.51
1:A:789:U:H2'	1:A:791:G:OP2	2.11	0.50
1:A:984:C:N3	1:A:1221:G:N2	2.54	0.50
1:A:1003:G:H2'	1:A:1003(A):G:C8	2.46	0.50
1:A:1120:G:H22	1:A:1154:G:H1'	1.75	0.50
2:B:49:GLU:O	2:B:52:GLU:HB3	2.11	0.50
3:C:116:VAL:O	3:C:120:VAL:HG23	2.11	0.50
7:G:77:SER:HA	7:G:86:GLN:HA	1.91	0.50
16:P:53:VAL:O	16:P:55:ARG:N	2.44	0.50
17:Q:4:LYS:HG3	17:Q:5:VAL:N	2.24	0.50
1:A:738:C:OP1	6:F:92:LYS:HD3	2.11	0.50
1:A:1074:G:C6	1:A:1075:C:C4	2.99	0.50
3:C:30:ARG:HG2	3:C:31:HIS:H	1.76	0.50
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.91	0.50
5:E:36:ASP:C	5:E:38:GLN:H	2.19	0.50
8:H:104:ARG:CZ	8:H:138:TRP:CZ2	2.95	0.50
9:I:53:VAL:HG22	9:I:92:TYR:CZ	2.46	0.50
15:O:39:LEU:CD2	15:O:56:LEU:HB2	2.41	0.50
17:Q:13:ASP:O	17:Q:15:MET:N	2.44	0.50
1:A:93:G:C2	1:A:95:U:C2	2.99	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.47	0.50
10:J:37:PRO:HA	10:J:71:LEU:H	1.75	0.50
1:A:502:G:C2	1:A:503:C:C2	2.99	0.50
1:A:803:G:C6	1:A:804:U:C4	2.99	0.50
1:A:882:C:O2'	1:A:883:C:H5'	2.11	0.50
5:E:44:GLY:HA3	5:E:62:ALA:HB2	1.93	0.50
7:G:62:PHE:O	7:G:66:VAL:HG23	2.11	0.50
8:H:25:ASP:OD1	8:H:25:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:125:PHE:C	11:K:126:ARG:HG3	2.37	0.50
12:L:25:PRO:C	12:L:27:LEU:N	2.64	0.50
20:T:29:LYS:O	20:T:32:ALA:HB3	2.11	0.50
1:A:247:G:OP2	17:Q:100:LYS:HD3	2.11	0.50
1:A:909:A:H2'	1:A:910:C:O4'	2.11	0.50
1:A:962:C:H1'	1:A:1201:A:N1	2.26	0.50
1:A:1112:C:H1'	3:C:179:ARG:HH12	1.76	0.50
1:A:1279:A:OP1	10:J:7:LYS:NZ	2.45	0.50
1:A:1411:C:H42	1:A:1489:G:H1	1.60	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HG2	1.92	0.50
8:H:84:ARG:HD2	8:H:85:ARG:O	2.12	0.50
9:I:61:ALA:HB1	9:I:63:ILE:HG12	1.94	0.50
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.27	0.50
19:S:34:TRP:HA	19:S:52:TYR:HB3	1.92	0.50
1:A:435:C:H2'	1:A:436:C:H6	1.77	0.50
1:A:1211:U:O2'	1:A:1212:U:OP2	2.26	0.50
4:D:173:TRP:NE1	4:D:189:PRO:HG3	2.25	0.50
5:E:81:GLU:OE2	5:E:81:GLU:N	2.38	0.50
7:G:57:GLU:OE1	7:G:59:LEU:HB3	2.11	0.50
16:P:74:LEU:HD22	16:P:79:VAL:HG21	1.94	0.50
18:R:58:LEU:HD23	18:R:58:LEU:N	2.26	0.50
1:A:299:G:C6	1:A:300:A:C6	2.99	0.50
1:A:741:G:H2'	1:A:742:G:O4'	2.12	0.50
1:A:932:C:H5'	7:G:4:ARG:HG2	1.94	0.50
1:A:1078:U:H5''	1:A:1079:G:OP2	2.11	0.50
1:A:1526:G:O2'	1:A:1527:C:H5'	2.12	0.50
6:F:97:PHE:HE2	6:F:99:ALA:HB2	1.76	0.50
11:K:92:GLU:HG3	11:K:96:ARG:NH1	2.26	0.50
1:A:559:A:O2'	1:A:560:U:OP2	2.24	0.50
4:D:170:VAL:HG11	4:D:175:SER:HA	1.92	0.50
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.50
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.50
1:A:90:U:O4	1:A:91:C:N4	2.45	0.50
1:A:232:G:H2'	1:A:233:C:H6	1.77	0.50
1:A:450:G:OP1	16:P:43:LYS:NZ	2.45	0.50
2:B:83:MET:HE2	2:B:234:PRO:HB2	1.93	0.50
15:O:33:THR:HG21	15:O:85:LEU:HD13	1.94	0.50
17:Q:58:GLU:O	17:Q:59:ILE:HD13	2.12	0.50
20:T:35:THR:HA	20:T:38:LYS:NZ	2.27	0.50
20:T:50:GLU:HG3	20:T:51:GLU:H	1.77	0.50
1:A:945:G:N1	1:A:1337:G:C2	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:G:OP1	13:M:77:ASN:ND2	2.44	0.49
1:A:1483:A:H2'	1:A:1484:C:O4'	2.12	0.49
4:D:155:LEU:HB2	4:D:158:ILE:CD1	2.37	0.49
7:G:65:ALA:HB2	7:G:128:ALA:HB2	1.94	0.49
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.94	0.49
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.92	0.49
15:O:6:GLU:HA	15:O:9:GLN:HB2	1.94	0.49
1:A:337:C:H2'	1:A:338:A:C8	2.46	0.49
1:A:394:G:H2'	1:A:395:C:C6	2.47	0.49
1:A:429:U:H1'	1:A:430:A:H5''	1.95	0.49
1:A:948:C:N4	1:A:1233:G:H1	2.07	0.49
1:A:954:G:C5	1:A:955:U:C4	3.00	0.49
1:A:1119:C:H42	1:A:1154:G:H1	1.60	0.49
7:G:115:ARG:HD2	7:G:118:VAL:HG21	1.94	0.49
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.45	0.49
12:L:19:ARG:H	12:L:19:ARG:HD2	1.77	0.49
17:Q:22:LEU:HD12	17:Q:23:VAL:H	1.77	0.49
1:A:942:G:H21	9:I:124:GLN:HE22	1.59	0.49
1:A:1285:A:H4'	1:A:1286:A:O5'	2.12	0.49
1:A:922:G:C6	1:A:923:A:C6	3.01	0.49
1:A:945:G:C6	1:A:1337:G:C2	3.00	0.49
1:A:954:G:N2	1:A:1227:A:H62	2.11	0.49
1:A:1174:G:H2'	1:A:1175:G:C8	2.45	0.49
1:A:1258:G:OP2	1:A:1258:G:H8	1.96	0.49
2:B:177:ALA:HB1	2:B:182:ILE:HB	1.94	0.49
5:E:43:LEU:HD22	5:E:136:MET:HG2	1.93	0.49
10:J:71:LEU:HD22	10:J:71:LEU:N	2.26	0.49
12:L:59:ARG:NH1	12:L:65:GLU:HB3	2.27	0.49
1:A:49:U:H6	1:A:49:U:H5''	1.76	0.49
1:A:533:A:O2'	1:A:535:A:OP2	2.28	0.49
1:A:983:A:OP1	14:N:3:ARG:NH2	2.44	0.49
1:A:1220:G:H2'	1:A:1221:G:O4'	2.13	0.49
3:C:25:GLY:N	3:C:28:GLN:HB2	2.26	0.49
4:D:63:LYS:NZ	4:D:197:PRO:O	2.40	0.49
5:E:43:LEU:HD11	5:E:133:TYR:HD2	1.77	0.49
11:K:17:GLY:HA2	11:K:35:PRO:HG3	1.95	0.49
1:A:232:G:H1'	1:A:262:A:N1	2.28	0.49
1:A:748:C:H4'	1:A:749:C:O5'	2.12	0.49
1:A:967:5MC:H4'	9:I:128:ARG:NE	2.26	0.49
1:A:1301:U:O2'	1:A:1302:U:O5'	2.30	0.49
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:30:LYS:C	4:D:32:ALA:H	2.20	0.49
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.46	0.49
19:S:80:TYR:CG	19:S:81:ARG:N	2.81	0.49
1:A:443:C:H2'	1:A:444:C:H6	1.78	0.49
1:A:737:A:H1'	6:F:73:ASN:HD21	1.78	0.49
1:A:942:G:C2	1:A:943:U:C2	3.00	0.49
1:A:1326:C:H5''	21:U:18:TYR:O	2.12	0.49
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.48	0.49
7:G:87:VAL:HG13	7:G:151:TYR:HB3	1.93	0.49
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.46	0.49
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.48	0.49
11:K:62:GLN:O	11:K:66:LEU:HG	2.13	0.49
13:M:84:ILE:HG13	13:M:86:CYS:H	1.78	0.49
20:T:75:ASN:N	20:T:75:ASN:OD1	2.46	0.49
1:A:344:A:H4'	1:A:345:C:OP2	2.13	0.49
2:B:143:GLU:O	2:B:147:LYS:HG3	2.12	0.49
2:B:184:VAL:O	2:B:198:ASP:HB2	2.12	0.49
15:O:76:GLU:N	15:O:79:ARG:HH21	2.10	0.49
16:P:57:ARG:HH21	16:P:79:VAL:CA	2.24	0.49
19:S:63:THR:HG22	19:S:64:GLU:H	1.77	0.49
1:A:691:G:H2'	1:A:692:U:H6	1.77	0.49
1:A:881:G:OP2	12:L:12:ARG:NH2	2.46	0.49
1:A:1206:G:H2'	1:A:1207:2MG:C8	2.48	0.49
5:E:75:THR:OG1	5:E:76:ILE:N	2.29	0.49
7:G:66:VAL:HG12	7:G:70:LYS:HZ3	1.77	0.49
7:G:88:PRO:HG2	7:G:155:ARG:HH12	1.75	0.49
18:R:61:LYS:O	18:R:65:ILE:HG13	2.13	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.48
1:A:485:G:O2'	1:A:486:U:P	2.71	0.48
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.28	0.48
9:I:8:GLY:HA2	9:I:79:LEU:HD12	1.94	0.48
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.48
1:A:1190:G:OP1	3:C:4:LYS:HA	2.13	0.48
1:A:1203:C:OP1	14:N:2:ALA:N	2.46	0.48
4:D:141:ARG:HG2	4:D:142:PRO:HD2	1.95	0.48
13:M:5:ALA:CB	13:M:22:ILE:HD13	2.40	0.48
16:P:6:LEU:HD12	16:P:6:LEU:HA	1.60	0.48
3:C:10:PHE:CD1	3:C:178:LEU:HD21	2.48	0.48
3:C:137:ALA:O	3:C:141:VAL:HG23	2.12	0.48
5:E:82:VAL:O	5:E:88:LYS:HA	2.14	0.48
5:E:142:LEU:HA	5:E:142:LEU:HD23	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:34:GLU:HB3	8:H:118:VAL:HG21	1.94	0.48
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.95	0.48
12:L:27:LEU:C	12:L:29:GLY:N	2.66	0.48
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.96	0.48
1:A:217:C:H2'	1:A:218:C:H6	1.77	0.48
1:A:455:C:H2'	1:A:456:C:H6	1.78	0.48
1:A:828:A:H4'	1:A:828:A:OP1	2.14	0.48
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.93	0.48
12:L:58:VAL:O	12:L:65:GLU:HA	2.13	0.48
1:A:484:G:H5'	1:A:486:U:H1'	1.95	0.48
1:A:517:G:H5'	1:A:519:C:C2	2.49	0.48
3:C:147:LYS:HB3	3:C:203:PHE:CE2	2.48	0.48
12:L:56:ALA:O	12:L:58:VAL:HG23	2.12	0.48
20:T:35:THR:HA	20:T:38:LYS:CE	2.43	0.48
1:A:76:C:H2'	1:A:77:G:H8	1.77	0.48
1:A:191:G:H1'	20:T:105:SER:HA	1.94	0.48
1:A:781:A:C4	1:A:802:A:C2	3.02	0.48
1:A:1426:C:H2'	1:A:1427:U:H6	1.78	0.48
20:T:51:GLU:O	20:T:55:ILE:HG12	2.13	0.48
1:A:695:A:C2	1:A:787:A:H1'	2.49	0.48
1:A:865:A:O5'	1:A:865:A:H8	1.97	0.48
1:A:1520:G:O2'	1:A:1521:G:H5'	2.14	0.48
3:C:12:LEU:HD22	3:C:18:TRP:CD1	2.48	0.48
4:D:9:CYS:SG	4:D:31:CYS:O	2.72	0.48
4:D:156:GLU:HG3	4:D:160:GLN:HE22	1.78	0.48
5:E:90:VAL:C	5:E:91:LEU:HD23	2.39	0.48
9:I:50:LEU:HD23	9:I:85:LEU:HD21	1.95	0.48
13:M:108:ARG:HD3	13:M:114:ARG:NH2	2.29	0.48
1:A:35:G:C6	1:A:36:C:N4	2.81	0.48
1:A:1020:U:C2	1:A:1021:G:C8	3.02	0.48
1:A:1126:U:H3	1:A:1149:C:H1'	1.79	0.48
1:A:1363:A:H4'	1:A:1364:U:H5''	1.93	0.48
1:A:1373:G:H5''	7:G:36:LYS:HD3	1.95	0.48
1:A:1508:G:C5	1:A:1509:C:C5	3.01	0.48
12:L:84:LEU:O	12:L:101:VAL:HG23	2.14	0.48
16:P:51:VAL:HG12	16:P:53:VAL:N	2.29	0.48
1:A:79:G:N1	1:A:80:G:C6	2.82	0.48
1:A:721:G:H4'	1:A:722:A:O4'	2.13	0.48
1:A:956:U:H4'	19:S:80:TYR:HE1	1.79	0.48
2:B:47:THR:HG22	2:B:51:LEU:HD12	1.96	0.48
6:F:28:ARG:O	6:F:32:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:5:ARG:H	10:J:5:ARG:HG3	1.44	0.48
15:O:26:GLU:OE2	15:O:77:ARG:HD2	2.13	0.48
16:P:8:ARG:CZ	16:P:15:PRO:HB3	2.44	0.48
18:R:43:PHE:CD2	18:R:56:THR:HG22	2.33	0.48
1:A:113:G:H2'	1:A:114:U:C6	2.49	0.48
1:A:411:A:N6	1:A:413:G:N3	2.61	0.48
1:A:785:G:C2	1:A:786:G:C8	3.02	0.48
1:A:946:A:H2'	1:A:947:G:C8	2.49	0.48
1:A:949:A:C2	1:A:1233:G:N3	2.82	0.48
1:A:1130:A:N6	1:A:1144:G:H21	2.12	0.48
1:A:1240:U:H5	7:G:109:ASN:HD21	1.59	0.48
1:A:1242:C:N4	1:A:1295:G:H1	2.09	0.48
1:A:1254:C:H2'	1:A:1255:G:C8	2.49	0.48
2:B:84:GLU:O	2:B:87:ARG:HB2	2.14	0.48
9:I:104:ARG:HD2	9:I:105:ASP:H	1.79	0.48
14:N:39:LEU:CD2	14:N:43:CYS:HB3	2.44	0.48
1:A:478:A:H2'	1:A:479:C:H6	1.79	0.47
1:A:837:G:H1	1:A:849:C:N4	2.11	0.47
1:A:1510:U:H2'	1:A:1511:G:H8	1.75	0.47
7:G:31:MET:HB2	7:G:35:LYS:O	2.14	0.47
10:J:46:ARG:HD2	10:J:64:GLU:HB3	1.96	0.47
1:A:376:G:H2'	1:A:377:G:H8	1.79	0.47
1:A:505:G:C6	1:A:535:A:C2	3.01	0.47
1:A:679:C:H2'	1:A:680:C:C6	2.48	0.47
1:A:933:G:OP2	7:G:3:ARG:HB3	2.15	0.47
1:A:975:A:O2'	14:N:32:SER:HB2	2.15	0.47
1:A:1191:A:H2'	1:A:1192:C:C6	2.49	0.47
2:B:95:GLN:HG3	2:B:148:TYR:HA	1.95	0.47
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.39	0.47
17:Q:38:ARG:HD3	17:Q:38:ARG:HA	1.55	0.47
1:A:90:U:C4	1:A:91:C:N4	2.83	0.47
1:A:558:G:H5''	1:A:559:A:H3'	1.95	0.47
1:A:663:A:H2'	1:A:664:G:O4'	2.14	0.47
1:A:691:G:H2'	1:A:692:U:C6	2.49	0.47
1:A:943:U:H2'	1:A:944:G:H5'	1.96	0.47
1:A:976:G:OP2	1:A:1358:U:H1'	2.14	0.47
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.29	0.47
1:A:1452:C:H4'	1:A:1453:G:O5'	2.14	0.47
2:B:36:ARG:CG	2:B:41:ILE:HD11	2.45	0.47
4:D:8:VAL:O	4:D:10:ARG:N	2.47	0.47
11:K:39:PRO:O	11:K:40:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:70:LEU:HD22	15:O:70:LEU:HA	1.38	0.47
1:A:968:A:H8	1:A:968:A:OP1	1.98	0.47
16:P:43:LYS:HB2	16:P:43:LYS:HE2	1.72	0.47
1:A:956:U:H2'	1:A:957:U:O4'	2.15	0.47
1:A:1004:A:O2'	1:A:1005:A:P	2.71	0.47
1:A:1120:G:C2	1:A:1154:G:N3	2.82	0.47
2:B:25:ASN:HD22	2:B:25:ASN:C	2.22	0.47
2:B:96:ARG:HH12	2:B:172:ILE:HD11	1.80	0.47
3:C:84:ILE:HG23	3:C:88:ARG:NH2	2.28	0.47
6:F:48:LEU:HG	6:F:57:GLN:HA	1.96	0.47
9:I:6:GLY:HA3	9:I:83:ARG:HB3	1.97	0.47
9:I:114:TYR:H	9:I:114:TYR:HD2	1.60	0.47
15:O:36:ILE:HG13	15:O:59:MET:HE3	1.97	0.47
19:S:11:VAL:HG13	19:S:39:THR:O	2.15	0.47
1:A:979:C:H42	14:N:18:VAL:HG23	1.78	0.47
1:A:1263:C:H2'	1:A:1264:C:O4'	2.14	0.47
1:A:1442:G:C6	1:A:1446:A:N6	2.78	0.47
1:A:1493:A:H2'	1:A:1494:G:C8	2.49	0.47
2:B:71:VAL:HB	2:B:164:VAL:HG12	1.96	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HG2	2.50	0.47
3:C:110:ASN:N	3:C:110:ASN:OD1	2.47	0.47
9:I:79:LEU:HD13	9:I:83:ARG:HD3	1.97	0.47
15:O:29:VAL:O	15:O:33:THR:HB	2.14	0.47
20:T:87:LYS:HD3	20:T:90:GLN:HE21	1.79	0.47
1:A:75:G:C6	1:A:96:G:C6	3.02	0.47
1:A:484:G:O2'	1:A:485:G:OP2	2.22	0.47
1:A:653:A:O4'	8:H:56:LYS:HE2	2.14	0.47
1:A:877:C:O2	8:H:3:THR:HG21	2.15	0.47
1:A:1007:C:O2	1:A:1023:G:N1	2.48	0.47
1:A:1392:G:C2'	1:A:1393:U:H5'	2.45	0.47
1:A:1500:A:OP2	1:A:1505:G:OP1	2.33	0.47
2:B:17:PHE:HD1	2:B:18:GLY:N	2.13	0.47
2:B:112:VAL:HG23	2:B:149:LEU:HD13	1.96	0.47
2:B:122:PHE:CZ	2:B:139:LYS:HE2	2.50	0.47
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.97	0.47
7:G:75:VAL:HG22	7:G:88:PRO:HA	1.96	0.47
13:M:108:ARG:NH2	13:M:112:GLY:O	2.48	0.47
14:N:41:ARG:HG3	14:N:42:ILE:N	2.30	0.47
17:Q:29:HIS:C	17:Q:29:HIS:ND1	2.73	0.47
19:S:41:VAL:HG23	19:S:44:MET:HG3	1.96	0.47
1:A:60:A:H4'	1:A:61:G:O5'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:G:C2	1:A:850:U:O2	2.68	0.47
1:A:853:G:C2	1:A:854:G:C8	3.03	0.47
1:A:952:U:H2'	1:A:953:G:C8	2.49	0.47
2:B:196:LEU:HA	2:B:196:LEU:HD23	1.66	0.47
3:C:190:ARG:HG3	3:C:195:VAL:HB	1.96	0.47
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.96	0.47
8:H:96:GLY:HA2	8:H:130:GLY:HA3	1.96	0.47
10:J:51:ARG:HG3	10:J:59:SER:HB2	1.97	0.47
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.47	0.47
19:S:34:TRP:HD1	19:S:52:TYR:CG	2.32	0.47
1:A:161:A:N1	1:A:347:G:O2'	2.42	0.47
1:A:219:C:O2'	1:A:381:C:H5'	2.15	0.47
1:A:260:G:C4	1:A:261:U:C5	3.03	0.47
1:A:344:A:H5'	1:A:345:C:C5	2.50	0.47
1:A:690:G:C6	1:A:691:G:C6	3.03	0.47
1:A:1339:A:H5''	1:A:1340:A:OP2	2.14	0.47
7:G:57:GLU:H	7:G:57:GLU:HG3	1.48	0.47
9:I:75:ASP:O	9:I:78:LYS:HB3	2.15	0.47
11:K:65:ALA:HB1	11:K:98:LEU:HB3	1.97	0.47
13:M:105:THR:O	13:M:107:ALA:N	2.48	0.47
18:R:55:ARG:HB3	18:R:55:ARG:CZ	2.45	0.47
1:A:694:A:N1	1:A:787:A:O2'	2.46	0.47
1:A:792:A:O2'	1:A:793:U:OP2	2.23	0.47
1:A:986:A:H1'	19:S:54:GLY:O	2.15	0.47
1:A:1070:U:O2	1:A:1106:G:C2	2.69	0.47
1:A:1499:A:H1'	1:A:1520:G:OP1	2.13	0.47
3:C:36:ASP:HA	3:C:39:ILE:CD1	2.43	0.47
6:F:38:GLU:HB2	6:F:64:GLN:O	2.15	0.47
14:N:23:ARG:HH12	14:N:30:ALA:HB2	1.80	0.47
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.73	0.47
17:Q:61:GLU:HA	17:Q:71:PHE:CE1	2.50	0.47
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.97	0.47
1:A:315:A:O2'	1:A:330:C:O2'	2.26	0.46
1:A:1145:C:H1'	1:A:1146:A:C8	2.49	0.46
1:A:1303:C:H2'	1:A:1304:G:C5'	2.42	0.46
1:A:1347:G:O2'	1:A:1348:U:O5'	2.33	0.46
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.97	0.46
2:B:7:VAL:HG21	2:B:221:LEU:HD23	1.97	0.46
2:B:119:GLU:HG3	2:B:142:LEU:HD11	1.97	0.46
4:D:124:GLY:O	4:D:132:ARG:HG3	2.16	0.46
8:H:31:PHE:O	8:H:35:ILE:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:47:VAL:HG12	11:K:48:ILE:N	2.30	0.46
11:K:77:MET:HE3	11:K:80:VAL:HG22	1.96	0.46
1:A:131:C:H2'	1:A:132:C:C6	2.50	0.46
1:A:457:C:H2'	1:A:458:C:C6	2.50	0.46
1:A:544:G:C5	1:A:545:C:C5	3.02	0.46
1:A:953:G:C5'	1:A:965:A:H61	2.23	0.46
1:A:1232:U:H5''	9:I:124:GLN:O	2.15	0.46
1:A:1325:C:H4'	21:U:17:THR:HG21	1.97	0.46
1:A:1399:C:C2	1:A:1401:G:C4	3.04	0.46
3:C:172:ARG:HB2	3:C:172:ARG:NH1	2.29	0.46
4:D:61:LYS:HE2	4:D:72:GLU:OE1	2.15	0.46
4:D:187:ARG:CZ	4:D:188:LEU:HB2	2.45	0.46
9:I:111:ARG:HH11	9:I:113:LYS:HA	1.80	0.46
12:L:11:VAL:HG22	17:Q:29:HIS:CD2	2.51	0.46
16:P:1:MET:HE3	16:P:1:MET:HB3	1.65	0.46
1:A:102:G:H2'	1:A:103:C:C6	2.49	0.46
1:A:1003:G:N2	1:A:1039:C:N3	2.62	0.46
1:A:1261:A:H1'	1:A:1283:G:H5''	1.96	0.46
2:B:82:ARG:NH1	2:B:82:ARG:HB2	2.30	0.46
2:B:115:LEU:HD23	2:B:153:ARG:NE	2.30	0.46
6:F:12:PRO:HD3	6:F:58:GLY:HA2	1.97	0.46
13:M:17:VAL:O	13:M:20:THR:HB	2.14	0.46
15:O:17:ARG:HB2	15:O:18:PHE:CD2	2.51	0.46
17:Q:10:VAL:HG23	17:Q:54:GLY:H	1.79	0.46
1:A:707:C:H4'	11:K:20:TYR:CD2	2.51	0.46
3:C:113:ALA:HA	3:C:116:VAL:HG23	1.96	0.46
16:P:51:VAL:HG12	16:P:52:ASP:C	2.40	0.46
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.50	0.46
19:S:29:ARG:H	19:S:29:ARG:HD2	1.80	0.46
1:A:268:C:H2'	1:A:269:C:H6	1.80	0.46
1:A:1030:C:N4	1:A:1032:G:O6	2.47	0.46
1:A:1065:U:C5	1:A:1190:G:H1'	2.50	0.46
4:D:205:GLU:CD	5:E:100:VAL:HG23	2.40	0.46
7:G:16:LEU:HD11	9:I:45:ALA:HB2	1.97	0.46
12:L:60:LEU:HA	12:L:60:LEU:HD13	1.60	0.46
18:R:53:ARG:NH1	18:R:58:LEU:O	2.49	0.46
19:S:15:LEU:O	19:S:19:VAL:HG12	2.16	0.46
1:A:406:G:H21	4:D:119:GLN:HE22	1.63	0.46
1:A:666:G:H5'	1:A:726:C:H1'	1.96	0.46
1:A:1003:G:H22	1:A:1039:C:H42	1.64	0.46
1:A:1124:G:H5''	1:A:1125:U:OP1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:TRP:CE3	2:B:26:PRO:HA	2.51	0.46
5:E:75:THR:C	5:E:76:ILE:HD12	2.41	0.46
7:G:50:ILE:HD11	7:G:125:MET:HB2	1.97	0.46
8:H:77:GLU:HG2	8:H:78:GLN:N	2.30	0.46
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.63	0.46
1:A:184:G:H2'	1:A:185:A:C8	2.48	0.46
1:A:691:G:H3'	11:K:26:ASN:HD21	1.79	0.46
1:A:792:A:N6	1:A:794:A:N1	2.63	0.46
1:A:935:A:N6	7:G:3:ARG:HG3	2.29	0.46
1:A:986:A:O2'	19:S:52:TYR:OH	2.26	0.46
4:D:64:LEU:HD22	4:D:67:ILE:HD12	1.98	0.46
1:A:694:A:C2	1:A:695:A:H1'	2.50	0.46
1:A:781:A:C5	1:A:802:A:C2	3.04	0.46
1:A:792:A:C6	1:A:794:A:C2	3.04	0.46
1:A:881:G:OP1	12:L:13:LYS:NZ	2.48	0.46
3:C:105:GLU:O	3:C:107:GLN:NE2	2.49	0.46
9:I:19:LEU:HD11	9:I:81:ILE:HD13	1.98	0.46
12:L:25:PRO:HB3	12:L:27:LEU:HD12	1.98	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.80	0.46
1:A:370:C:N3	1:A:392:G:C2	2.84	0.46
1:A:788:U:H3'	1:A:789:U:O4'	2.16	0.46
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.16	0.46
3:C:70:VAL:O	3:C:106:VAL:HG23	2.16	0.46
4:D:30:LYS:O	4:D:32:ALA:N	2.48	0.46
4:D:107:ARG:NH1	4:D:194:LEU:HD11	2.31	0.46
5:E:110:LEU:HD12	5:E:118:ILE:HG21	1.98	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.54	0.46
12:L:82:VAL:O	12:L:106:ASP:HB2	2.16	0.46
1:A:78:G:N1	1:A:92:C:C4	2.84	0.46
1:A:268:C:H2'	1:A:269:C:C6	2.51	0.46
1:A:701:C:O2'	1:A:702:A:OP2	2.24	0.46
1:A:738:C:P	6:F:92:LYS:HD3	2.56	0.46
1:A:923:A:O4'	1:A:1398:A:C2	2.68	0.46
1:A:940:C:H2'	1:A:941:G:O4'	2.16	0.46
1:A:1323:G:H2'	1:A:1324:A:C8	2.51	0.46
1:A:1542:U:H2'	1:A:1543:C:C6	2.51	0.46
10:J:27:ALA:O	10:J:31:GLY:N	2.44	0.46
11:K:94:ALA:O	11:K:98:LEU:HD12	2.16	0.46
13:M:91:ARG:HB3	13:M:98:VAL:HG22	1.97	0.46
18:R:54:ARG:HE	18:R:54:ARG:HB2	1.58	0.46
1:A:350:G:O2'	1:A:351:G:H5'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:A:C6	1:A:390:C:H1'	2.51	0.45
1:A:459:G:H1'	1:A:463:A:H61	1.81	0.45
1:A:479:C:H2'	1:A:480:U:O4'	2.16	0.45
1:A:806:C:H2'	1:A:807:A:H8	1.81	0.45
1:A:942:G:N2	1:A:943:U:C2	2.83	0.45
1:A:1060:C:C2	1:A:1198:G:C2	3.04	0.45
2:B:44:LEU:O	2:B:47:THR:HB	2.16	0.45
2:B:52:GLU:HG2	2:B:56:ARG:HH22	1.81	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.51	0.45
7:G:17:VAL:HG11	7:G:44:TYR:CE2	2.51	0.45
9:I:8:GLY:H	9:I:83:ARG:NH1	2.14	0.45
10:J:57:LYS:HG3	10:J:58:ASP:OD2	2.15	0.45
11:K:101:SER:HG	11:K:103:LEU:H	1.63	0.45
1:A:345:C:OP2	1:A:345:C:H6	1.98	0.45
1:A:485:G:HO2'	1:A:486:U:P	2.39	0.45
1:A:945:G:N1	1:A:1337:G:N2	2.63	0.45
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.16	0.45
1:A:1360:A:C2	14:N:18:VAL:HB	2.49	0.45
4:D:94:LEU:O	4:D:97:LEU:HB2	2.17	0.45
10:J:8:LEU:HA	10:J:95:GLU:O	2.16	0.45
15:O:85:LEU:HD23	15:O:85:LEU:N	2.31	0.45
1:A:152:A:N6	1:A:170:U:C2	2.85	0.45
1:A:337:C:H2'	1:A:338:A:H8	1.82	0.45
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.45
1:A:983:A:P	14:N:3:ARG:HH22	2.39	0.45
4:D:112:VAL:HG23	4:D:116:GLN:OE1	2.16	0.45
4:D:194:LEU:HD13	4:D:194:LEU:HA	1.63	0.45
6:F:26:ILE:O	6:F:30:LEU:HD12	2.16	0.45
17:Q:74:LEU:HD22	17:Q:74:LEU:HA	1.66	0.45
1:A:459:G:H1'	1:A:463:A:N6	2.32	0.45
1:A:550:G:C5	1:A:551:U:C5	3.04	0.45
1:A:671:G:H1	1:A:735:C:H42	1.63	0.45
1:A:825:G:H21	8:H:11:THR:HG21	1.80	0.45
1:A:1014:A:N6	1:A:1015:A:N1	2.64	0.45
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.45
1:A:1053:G:OP1	1:A:1054:C:H5''	2.16	0.45
1:A:1094:G:OP2	1:A:1095:U:H5	2.00	0.45
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.35	0.45
5:E:55:VAL:HG12	5:E:56:GLN:N	2.32	0.45
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.55	0.45
9:I:32:ASP:HB3	9:I:35:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:20:ALA:O	10:J:24:VAL:HG12	2.16	0.45
14:N:3:ARG:HE	14:N:6:LEU:HD23	1.82	0.45
1:A:75:G:O6	1:A:96:G:C6	2.70	0.45
1:A:951:G:OP2	13:M:102:ARG:NH2	2.47	0.45
1:A:977:A:H8	1:A:1223:C:N3	2.14	0.45
3:C:150:LYS:NZ	3:C:175:LEU:HD11	2.30	0.45
4:D:13:ARG:HB2	4:D:38:TYR:O	2.16	0.45
4:D:102:ASP:HA	4:D:121:VAL:HG21	1.99	0.45
7:G:5:ARG:HB3	7:G:6:ARG:H	1.62	0.45
18:R:56:THR:HB	18:R:58:LEU:CD2	2.46	0.45
1:A:77:G:C6	1:A:93:G:N1	2.85	0.45
1:A:89:C:H2'	1:A:90:U:O4'	2.16	0.45
1:A:718:G:O6	18:R:74:ARG:NH1	2.48	0.45
1:A:723:U:O2	1:A:723:U:H2'	2.16	0.45
1:A:880:C:OP2	12:L:6:THR:HG21	2.17	0.45
1:A:1422:G:C2	1:A:1423:G:C8	3.05	0.45
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.99	0.45
3:C:175:LEU:HD22	3:C:201:TYR:CD2	2.52	0.45
16:P:78:GLY:C	16:P:80:PHE:N	2.66	0.45
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.98	0.45
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.52	0.45
20:T:45:GLN:N	20:T:45:GLN:OE1	2.49	0.45
1:A:435:C:H2'	1:A:436:C:C6	2.51	0.45
1:A:661:G:H1	1:A:744:C:H42	1.63	0.45
1:A:975:A:H5'	1:A:975:A:C8	2.49	0.45
1:A:1058:G:H2'	1:A:1059:C:C6	2.51	0.45
1:A:1089:G:C6	1:A:1090:U:C4	3.05	0.45
1:A:1202:G:H2'	1:A:1203:C:O4'	2.16	0.45
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.17	0.45
3:C:30:ARG:H	3:C:30:ARG:HD3	1.80	0.45
3:C:85:ARG:HH11	3:C:88:ARG:HH12	1.63	0.45
5:E:92:LYS:O	5:E:118:ILE:HG12	2.17	0.45
7:G:75:VAL:HG13	7:G:87:VAL:C	2.41	0.45
9:I:86:VAL:HG23	9:I:96:LEU:HD22	1.98	0.45
12:L:42:THR:HA	12:L:53:ARG:O	2.16	0.45
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.98	0.45
14:N:16:PHE:HD1	14:N:19:ARG:NE	2.15	0.45
1:A:79:G:C2	1:A:80:G:C4	3.05	0.45
1:A:457:C:H2'	1:A:458:C:H6	1.82	0.45
1:A:977:A:H8	1:A:1223:C:C4	2.34	0.45
1:A:1267:C:O2	21:U:20:LYS:HD2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1511:G:H2'	1:A:1512:U:O4'	2.15	0.45
4:D:173:TRP:CE2	4:D:174:LEU:HD11	2.51	0.45
5:E:11:ILE:HB	5:E:31:LEU:CB	2.46	0.45
9:I:20:ARG:HB2	9:I:60:ASP:HB3	1.99	0.45
12:L:92:0TD:OD1	12:L:92:0TD:N	2.49	0.45
18:R:56:THR:HB	18:R:58:LEU:HD21	1.99	0.45
1:A:6:G:O2'	1:A:7:G:H5'	2.17	0.45
1:A:489:C:OP1	4:D:132:ARG:NH2	2.49	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
1:A:922:G:C2	1:A:1396:A:C6	3.05	0.45
1:A:946:A:N1	1:A:1236:A:C2	2.85	0.45
1:A:974:A:P	14:N:41:ARG:HH22	2.39	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.05	0.45
1:A:1496:C:O2'	1:A:1497:G:O5'	2.35	0.45
3:C:175:LEU:H	3:C:175:LEU:HG	1.46	0.45
4:D:20:TYR:HA	4:D:26:CYS:SG	2.57	0.45
8:H:6:ILE:HG13	8:H:31:PHE:HE2	1.81	0.45
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.52	0.45
8:H:112:LEU:H	8:H:112:LEU:HD12	1.82	0.45
11:K:44:SER:H	11:K:47:VAL:HB	1.81	0.45
13:M:27:LYS:HD2	13:M:27:LYS:HA	1.36	0.45
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.99	0.45
13:M:102:ARG:O	13:M:102:ARG:HG3	2.17	0.45
13:M:105:THR:OG1	13:M:106:ASN:HB2	2.16	0.45
14:N:41:ARG:HG3	14:N:42:ILE:H	1.82	0.45
16:P:39:TYR:HE2	16:P:41:PRO:HB3	1.82	0.45
18:R:22:VAL:HG23	18:R:56:THR:HA	1.99	0.45
18:R:60:ALA:O	18:R:64:ARG:HG3	2.17	0.45
1:A:92:C:H2'	1:A:93:G:H8	1.81	0.45
1:A:456:C:C2	1:A:457:C:C5	3.04	0.45
1:A:1080:A:H5''	5:E:16:THR:OG1	2.17	0.45
1:A:1202:G:C4	14:N:42:ILE:HD12	2.52	0.45
4:D:31:CYS:O	4:D:31:CYS:SG	2.75	0.45
4:D:159:ARG:O	4:D:163:GLU:HB2	2.17	0.45
18:R:43:PHE:O	18:R:51:LEU:HD23	2.16	0.45
19:S:15:LEU:HD12	19:S:16:LEU:N	2.32	0.45
20:T:30:LYS:O	20:T:33:ILE:HB	2.17	0.45
1:A:1342:C:H2'	1:A:1343:G:C8	2.51	0.44
6:F:27:GLN:O	6:F:31:GLU:HG3	2.17	0.44
7:G:121:ALA:O	7:G:124:LEU:HD12	2.16	0.44
9:I:6:GLY:CA	9:I:83:ARG:HB3	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:G:N7	1:A:481:G:O6	2.50	0.44
1:A:517:G:H5'	1:A:519:C:O2	2.16	0.44
1:A:1265:G:C6	1:A:1266:G:C6	3.05	0.44
1:A:1329:A:OP1	13:M:28:ALA:HB3	2.17	0.44
3:C:150:LYS:HG2	3:C:169:ALA:CB	2.46	0.44
4:D:34:GLU:C	4:D:36:ARG:H	2.25	0.44
14:N:39:LEU:CD1	14:N:43:CYS:HB3	2.47	0.44
17:Q:43:LEU:HD23	17:Q:43:LEU:HA	1.69	0.44
18:R:52:PRO:O	18:R:56:THR:OG1	2.29	0.44
20:T:51:GLU:HG2	20:T:51:GLU:H	1.56	0.44
1:A:92:C:O2'	1:A:93:G:H5'	2.17	0.44
1:A:328:C:O2	1:A:328:C:H2'	2.17	0.44
1:A:370:C:H2'	1:A:371:G:O4'	2.17	0.44
1:A:401:C:H1'	1:A:622:A:H1'	1.99	0.44
1:A:451:A:H2	1:A:480:U:C4	2.35	0.44
1:A:546:G:OP1	4:D:73:ARG:HG2	2.16	0.44
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.44
1:A:712:A:H2'	1:A:713:G:O4'	2.18	0.44
1:A:1196:U:H3'	1:A:1196:U:OP1	2.18	0.44
3:C:181:ASN:O	3:C:181:ASN:ND2	2.50	0.44
5:E:65:ASN:OD1	5:E:140:ARG:NH2	2.49	0.44
6:F:73:ASN:HD22	6:F:73:ASN:N	2.14	0.44
7:G:88:PRO:HG2	7:G:155:ARG:CZ	2.47	0.44
12:L:120:TYR:N	12:L:120:TYR:CD2	2.85	0.44
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.98	0.44
1:A:279:A:H5'	1:A:279:A:H8	1.82	0.44
1:A:411:A:H62	1:A:413:G:H21	1.65	0.44
1:A:1423:G:N2	1:A:1477:C:O2	2.40	0.44
1:A:1532:U:H2'	1:A:1533:C:H3'	2.00	0.44
5:E:65:ASN:O	5:E:65:ASN:CG	2.60	0.44
10:J:57:LYS:HE2	10:J:57:LYS:HB2	1.86	0.44
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.81	0.44
13:M:3:ARG:HA	13:M:8:GLU:O	2.17	0.44
1:A:263:A:OP2	20:T:79:ARG:NH1	2.48	0.44
1:A:429:U:H4'	1:A:430:A:O5'	2.17	0.44
1:A:602:A:C2	1:A:637:G:C2	3.06	0.44
1:A:658:G:H2'	1:A:659:U:C6	2.52	0.44
1:A:803:G:H8	1:A:803:G:O5'	1.99	0.44
1:A:829:G:O2'	1:A:830:G:H5'	2.18	0.44
1:A:1235:U:O3'	21:U:3:LYS:HB2	2.18	0.44
1:A:1391:U:H2'	1:A:1392:G:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:5MC:H3'	1:A:1401:G:C5'	2.46	0.44
2:B:36:ARG:HG3	2:B:41:ILE:HD11	1.99	0.44
2:B:100:GLY:O	2:B:104:ASN:N	2.49	0.44
2:B:114:ARG:NE	2:B:141:GLU:OE2	2.46	0.44
8:H:28:ALA:HB2	8:H:59:LEU:HG	1.99	0.44
9:I:5:TYR:CE2	9:I:18:PHE:HE2	2.35	0.44
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.53	0.44
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.32	0.44
12:L:34:ARG:O	12:L:34:ARG:HG3	2.18	0.44
20:T:77:ALA:O	20:T:78:ALA:C	2.60	0.44
1:A:222:U:H2'	1:A:223:U:C6	2.53	0.44
1:A:642:A:C5	1:A:643:C:C5	3.05	0.44
1:A:956:U:HO2'	19:S:80:TYR:HD1	1.63	0.44
1:A:1342:C:H2'	1:A:1343:G:H8	1.82	0.44
1:A:1540:PSU:HN1	1:A:1541:PSU:HN1	1.64	0.44
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.17	0.44
6:F:4:TYR:HE1	6:F:92:LYS:HG2	1.79	0.44
12:L:5:PRO:HG2	12:L:10:LEU:HD11	1.99	0.44
17:Q:95:TYR:O	17:Q:97:SER:N	2.50	0.44
1:A:410:G:OP2	4:D:25:ARG:HG3	2.17	0.44
1:A:538:G:OP2	12:L:115:LYS:HB2	2.17	0.44
1:A:695:A:OP2	11:K:52:GLY:HA3	2.18	0.44
2:B:31:TYR:CD2	2:B:31:TYR:N	2.85	0.44
2:B:48:MET:HA	2:B:51:LEU:HB2	1.99	0.44
6:F:67:MET:HB2	6:F:67:MET:HE3	1.76	0.44
7:G:50:ILE:HD13	7:G:50:ILE:HA	1.61	0.44
7:G:149:ARG:C	7:G:151:TYR:H	2.26	0.44
8:H:134:ILE:HA	8:H:134:ILE:HD13	1.70	0.44
1:A:69:G:H1	1:A:99:C:H42	1.66	0.44
1:A:815:A:N6	1:A:1509:C:H1'	2.33	0.44
1:A:838:G:C2	1:A:849:C:C2	3.05	0.44
1:A:1004:A:HO2'	1:A:1005:A:P	2.41	0.44
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.53	0.44
1:A:1424:C:H2'	1:A:1425:U:H6	1.83	0.44
2:B:87:ARG:HB3	2:B:87:ARG:HH11	1.82	0.44
15:O:42:HIS:CD2	15:O:43:LEU:HD23	2.53	0.44
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.57	0.44
17:Q:58:GLU:HB3	17:Q:74:LEU:CB	2.47	0.44
17:Q:83:ASP:OD1	17:Q:83:ASP:N	2.50	0.44
19:S:18:LYS:HD2	19:S:31:ILE:HD11	2.00	0.44
1:A:61:G:H2'	1:A:62:U:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:G:C6	1:A:1073:U:C4	3.06	0.44
1:A:1228:C:O3'	13:M:116:THR:HG23	2.18	0.44
1:A:1494:G:C2	1:A:1495:U:C4	3.05	0.44
2:B:15:VAL:HG11	2:B:213:LEU:HD12	2.00	0.44
3:C:7:PRO:HG2	3:C:184:TYR:CD1	2.53	0.44
3:C:11:ARG:HD3	3:C:181:ASN:HA	1.99	0.44
4:D:70:ILE:HA	4:D:70:ILE:HD13	1.63	0.44
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.50	0.44
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.99	0.44
6:F:78:GLU:O	6:F:81:ILE:HG22	2.18	0.44
11:K:73:MET:HG3	11:K:103:LEU:HD21	1.98	0.44
13:M:19:LEU:HD11	13:M:56:LEU:CD1	2.48	0.44
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.18	0.44
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.52	0.44
1:A:16:A:O2'	1:A:17:U:H5'	2.18	0.43
1:A:434:U:H2'	1:A:435:C:C6	2.53	0.43
1:A:667:G:H4'	15:O:51:HIS:ND1	2.32	0.43
1:A:673:G:H2'	1:A:674:G:C8	2.53	0.43
1:A:838:G:N2	1:A:849:C:C2	2.86	0.43
1:A:1244:C:H42	1:A:1293:G:H1	1.64	0.43
1:A:1426:C:H2'	1:A:1427:U:C6	2.52	0.43
2:B:62:ALA:HB1	2:B:222:ILE:HG23	1.99	0.43
3:C:22:TRP:CH2	3:C:33:LEU:HD21	2.53	0.43
5:E:110:LEU:HD23	5:E:110:LEU:N	2.33	0.43
6:F:11:ASN:HA	6:F:12:PRO:HD2	1.73	0.43
8:H:35:ILE:HG12	8:H:35:ILE:H	1.61	0.43
10:J:5:ARG:HD3	10:J:99:LYS:HB3	1.98	0.43
12:L:51:ALA:O	12:L:52:LEU:HD23	2.18	0.43
12:L:113:ARG:HH12	12:L:115:LYS:HB3	1.83	0.43
19:S:43:GLU:OE1	19:S:43:GLU:N	2.49	0.43
20:T:65:LYS:O	20:T:68:LYS:HB3	2.18	0.43
1:A:77:G:C6	1:A:93:G:C6	3.06	0.43
1:A:1293:G:H2'	1:A:1294:G:O4'	2.18	0.43
3:C:173:VAL:HG12	3:C:175:LEU:HD23	2.00	0.43
4:D:57:ARG:HG3	4:D:202:LEU:CD1	2.48	0.43
5:E:43:LEU:HD22	5:E:136:MET:HE2	2.00	0.43
8:H:12:ARG:HH11	8:H:26:VAL:HA	1.82	0.43
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.66	0.43
12:L:53:ARG:HG2	12:L:93:LEU:HD11	2.00	0.43
1:A:146:G:C2	1:A:147:G:C4	3.06	0.43
1:A:448:A:P	1:A:485:G:H22	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:C:H2'	1:A:680:C:H6	1.83	0.43
1:A:1133:G:N2	1:A:1141:C:N3	2.63	0.43
1:A:1178:G:P	9:I:97:LYS:HZ3	2.41	0.43
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.18	0.43
3:C:114:PRO:N	3:C:185:GLY:HA3	2.33	0.43
5:E:90:VAL:O	5:E:91:LEU:HD23	2.19	0.43
1:A:83:U:C2'	1:A:84:U:H5'	2.48	0.43
1:A:109:A:H2'	1:A:326:G:N2	2.33	0.43
1:A:357:G:C2	1:A:358:U:C5	3.07	0.43
1:A:445:G:H2'	1:A:446:G:H8	1.83	0.43
1:A:959:A:O2'	1:A:984:C:O2'	2.34	0.43
3:C:73:PRO:HG3	3:C:105:GLU:OE1	2.19	0.43
7:G:124:LEU:H	7:G:124:LEU:HG	1.44	0.43
15:O:85:LEU:HB2	15:O:87:ILE:HD12	2.01	0.43
17:Q:63:ARG:CB	17:Q:63:ARG:HH11	2.32	0.43
20:T:53:LEU:HA	20:T:56:MET:HE2	1.99	0.43
21:U:5:ASP:O	21:U:8:THR:OG1	2.35	0.43
1:A:90:U:C4	1:A:91:C:C5	3.06	0.43
1:A:321:A:N6	1:A:329:A:OP2	2.49	0.43
1:A:946:A:C6	1:A:1236:A:C2	3.06	0.43
1:A:964:A:O2'	10:J:55:LYS:NZ	2.22	0.43
1:A:1084:G:O2'	1:A:1085:U:OP1	2.34	0.43
1:A:1226:C:H4'	1:A:1227:A:OP1	2.18	0.43
1:A:1474:G:H2'	1:A:1475:G:C8	2.54	0.43
4:D:25:ARG:HA	4:D:28:SER:H	1.83	0.43
7:G:17:VAL:HG21	7:G:44:TYR:CZ	2.53	0.43
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.54	0.43
9:I:17:VAL:HG22	9:I:63:ILE:HD12	2.00	0.43
9:I:48:GLU:HA	9:I:51:ARG:HD2	2.00	0.43
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.99	0.43
17:Q:45:HIS:ND1	17:Q:45:HIS:C	2.76	0.43
20:T:61:SER:O	20:T:62:LEU:C	2.61	0.43
1:A:279:A:H5'	1:A:279:A:C8	2.53	0.43
1:A:410:G:N1	1:A:429:U:O2	2.51	0.43
1:A:920:U:H2'	1:A:921:U:C6	2.54	0.43
1:A:1054:C:OP1	1:A:1197:G:OP1	2.37	0.43
1:A:1117:G:H5''	9:I:104:ARG:NH2	2.33	0.43
1:A:1301:U:O2'	1:A:1302:U:P	2.77	0.43
2:B:54:THR:O	2:B:58:ILE:HG13	2.19	0.43
4:D:119:GLN:HG3	4:D:123:HIS:NE2	2.33	0.43
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:59:ARG:HA	12:L:59:ARG:HH11	1.84	0.43
15:O:4:THR:O	15:O:7:GLU:HB2	2.19	0.43
17:Q:6:LEU:O	17:Q:58:GLU:HG3	2.17	0.43
20:T:33:ILE:HG12	20:T:62:LEU:CD2	2.48	0.43
20:T:50:GLU:H	20:T:50:GLU:HG2	1.34	0.43
1:A:190:C:O2'	1:A:190(A):C:H5'	2.18	0.43
1:A:284:G:H2'	1:A:285:G:C8	2.53	0.43
1:A:391:G:C6	1:A:392:G:C5	3.07	0.43
1:A:1008:C:N4	1:A:1021:G:H22	2.04	0.43
1:A:1347:G:H2'	1:A:1373:G:C6	2.53	0.43
1:A:1521:G:H2'	1:A:1522:U:C6	2.54	0.43
2:B:188:ALA:HB1	2:B:192:SER:OG	2.18	0.43
4:D:88:VAL:O	4:D:92:VAL:HG23	2.17	0.43
4:D:126:ILE:O	4:D:132:ARG:HA	2.18	0.43
10:J:8:LEU:CD2	10:J:96:ILE:HG23	2.49	0.43
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.00	0.43
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.33	0.43
18:R:37:VAL:HG13	18:R:41:LYS:HD3	2.00	0.43
18:R:88:LYS:HB3	18:R:88:LYS:NZ	2.33	0.43
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.66	0.43
1:A:1094:G:O2'	1:A:1095:U:OP1	2.37	0.43
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.33	0.43
22:A:1601:SRY:HI32	22:A:1601:SRY:C22	2.49	0.43
4:D:150:GLU:CD	4:D:150:GLU:H	2.26	0.43
4:D:190:ASP:HB3	4:D:193:ASP:OD2	2.18	0.43
6:F:100:ASN:HB2	18:R:23:LYS:HD2	1.99	0.43
9:I:89:ASN:HB3	9:I:92:TYR:HB2	2.01	0.43
10:J:88:LEU:HD23	10:J:88:LEU:HA	1.85	0.43
13:M:92:HIS:CD2	13:M:98:VAL:HG21	2.53	0.43
1:A:854:G:H3'	1:A:871:U:O4	2.18	0.43
1:A:927:G:O2'	1:A:1503:A:N7	2.46	0.43
1:A:1015:A:O2'	1:A:1218:C:O2'	2.26	0.43
1:A:1326:C:H2'	1:A:1327:C:C6	2.53	0.43
2:B:226:ARG:HE	2:B:226:ARG:HB2	1.64	0.43
4:D:187:ARG:NH2	4:D:188:LEU:O	2.51	0.43
5:E:43:LEU:HD11	5:E:133:TYR:CD2	2.53	0.43
11:K:29:ILE:C	11:K:29:ILE:HD12	2.43	0.43
17:Q:89:LEU:HD23	17:Q:89:LEU:HA	1.77	0.43
19:S:75:ALA:HA	19:S:76:PRO:HD2	1.82	0.43
1:A:585:G:C6	1:A:586:C:C4	3.06	0.43
1:A:1157:A:H4'	1:A:1158:C:O4'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1206:G:H4'	3:C:192:THR:O	2.19	0.43
1:A:1384:C:H2'	1:A:1385:G:C8	2.54	0.43
4:D:11:LEU:HD13	4:D:66:ARG:CD	2.49	0.43
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.77	0.43
9:I:36:TYR:CD2	9:I:37:PHE:CE2	3.07	0.43
9:I:104:ARG:HD2	9:I:105:ASP:N	2.34	0.43
11:K:58:PRO:O	11:K:61:ALA:HB3	2.19	0.43
12:L:98:TYR:CD1	12:L:98:TYR:N	2.87	0.43
14:N:14:PRO:C	14:N:16:PHE:H	2.27	0.43
1:A:24:U:H2'	1:A:25:C:C6	2.54	0.42
1:A:77:G:N1	1:A:93:G:C6	2.87	0.42
1:A:386:C:C2'	1:A:387:U:H5'	2.49	0.42
1:A:474:G:C2	1:A:475:G:N7	2.87	0.42
1:A:865:A:C6	1:A:866:C:C4	3.07	0.42
1:A:1303:C:C2'	1:A:1304:G:H5'	2.44	0.42
1:A:1502:A:H2	1:A:1505:G:H1	1.66	0.42
11:K:33:THR:HB	11:K:39:PRO:HA	2.01	0.42
12:L:115:LYS:HD2	12:L:115:LYS:HA	1.87	0.42
14:N:44:LEU:O	14:N:48:ALA:HB2	2.19	0.42
16:P:41:PRO:O	16:P:43:LYS:HD3	2.19	0.42
1:A:113:G:H2'	1:A:114:U:H6	1.84	0.42
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.19	0.42
1:A:448:A:C4	1:A:487:A:C2	3.07	0.42
1:A:981:U:H2'	1:A:982:U:C6	2.54	0.42
1:A:1060:C:N3	1:A:1198:G:C6	2.87	0.42
3:C:113:ALA:N	3:C:114:PRO:HD2	2.33	0.42
4:D:18:LYS:HB3	4:D:20:TYR:HE2	1.84	0.42
5:E:100:VAL:HG12	5:E:118:ILE:HG22	2.01	0.42
15:O:15:PHE:HE2	15:O:85:LEU:HD21	1.83	0.42
16:P:54:GLU:C	16:P:54:GLU:CD	2.87	0.42
1:A:825:G:H1	1:A:875:C:N4	2.16	0.42
1:A:833:U:H2'	1:A:834:C:H6	1.84	0.42
1:A:1092:A:H1'	1:A:1183:A:N6	2.34	0.42
1:A:1376:U:C2	1:A:1377:A:N7	2.87	0.42
1:A:1518:MA6:H102	1:A:1519:MA6:C6	2.49	0.42
2:B:91:PRO:HA	2:B:154:LEU:HD12	2.01	0.42
3:C:113:ALA:HB3	3:C:184:TYR:C	2.44	0.42
5:E:78:HIS:ND1	8:H:104:ARG:HG3	2.33	0.42
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.59	0.42
7:G:136:LYS:HE2	7:G:136:LYS:HB2	1.76	0.42
7:G:152:ALA:HA	7:G:155:ARG:CZ	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:15:THR:HG21	10:J:93:GLY:HA3	2.00	0.42
16:P:4:ILE:HA	16:P:20:VAL:O	2.19	0.42
20:T:18:GLN:O	20:T:21:LYS:HB2	2.18	0.42
1:A:162:A:H1'	1:A:348:G:O2'	2.19	0.42
1:A:200:G:N2	1:A:218:C:C2	2.87	0.42
1:A:279:A:H5''	1:A:281:G:O4'	2.18	0.42
1:A:945:G:O6	1:A:1236:A:N1	2.52	0.42
1:A:1201:A:H1'	1:A:1202:G:OP2	2.20	0.42
1:A:1213:A:N6	1:A:1215:G:N3	2.67	0.42
1:A:1479:C:H2'	1:A:1480:G:C8	2.52	0.42
2:B:115:LEU:HD11	2:B:146:GLN:HG3	2.02	0.42
3:C:94:LEU:HA	3:C:94:LEU:HD13	1.73	0.42
3:C:106:VAL:CG1	3:C:109:PRO:HA	2.45	0.42
5:E:11:ILE:HG22	5:E:12:LEU:N	2.33	0.42
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.54	0.42
8:H:39:LEU:HD13	8:H:39:LEU:HA	1.72	0.42
11:K:34:ASP:HA	11:K:35:PRO:HD3	1.81	0.42
12:L:76:ASN:OD1	12:L:76:ASN:C	2.62	0.42
13:M:6:GLY:O	13:M:67:GLU:HG2	2.19	0.42
13:M:23:TYR:CZ	13:M:71:ARG:HG2	2.55	0.42
1:A:216:G:H2'	1:A:217:C:C6	2.54	0.42
1:A:217:C:H2'	1:A:218:C:C6	2.54	0.42
1:A:647:C:H2'	1:A:648:A:C8	2.55	0.42
1:A:1241:G:H2'	1:A:1242:C:H6	1.84	0.42
1:A:1249:C:H2'	1:A:1250:A:H5'	2.01	0.42
1:A:1361(A):C:O2'	1:A:1362:C:H6	2.01	0.42
1:A:1387:G:O2'	25:A:2035:HOH:O	2.21	0.42
2:B:28:PHE:HD2	2:B:32:ILE:HD11	1.84	0.42
2:B:108:ILE:HD13	2:B:108:ILE:HA	1.83	0.42
3:C:135:LYS:HB3	3:C:135:LYS:HE2	1.84	0.42
4:D:57:ARG:NH1	4:D:202:LEU:HD11	2.35	0.42
5:E:76:ILE:N	5:E:76:ILE:HD12	2.34	0.42
9:I:15:ALA:CB	9:I:65:VAL:HG12	2.48	0.42
10:J:37:PRO:HB2	10:J:70:ARG:HB3	2.02	0.42
18:R:53:ARG:NH1	18:R:59:SER:HA	2.34	0.42
19:S:39:THR:HG22	19:S:40:ILE:O	2.18	0.42
20:T:53:LEU:HA	20:T:53:LEU:HD22	1.79	0.42
20:T:88:VAL:O	20:T:92:LEU:HD23	2.20	0.42
1:A:7:G:O6	5:E:92:LYS:HE3	2.19	0.42
1:A:219:C:C4	1:A:220:G:C8	3.07	0.42
1:A:460:A:C6	1:A:462:G:C5	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:C:C2	1:A:1329:A:C8	3.08	0.42
2:B:157:ARG:HG2	2:B:158:LEU:N	2.34	0.42
4:D:156:GLU:O	4:D:160:GLN:NE2	2.53	0.42
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.55	0.42
7:G:10:ARG:NH1	7:G:10:ARG:HB2	2.34	0.42
11:K:19:ALA:HB2	11:K:80:VAL:CG1	2.50	0.42
11:K:48:ILE:HD13	11:K:63:LEU:HB3	2.02	0.42
14:N:12:ARG:HD2	14:N:14:PRO:HG3	2.02	0.42
15:O:28:GLN:O	15:O:32:LEU:HB2	2.19	0.42
16:P:38:TYR:O	16:P:49:LEU:HD12	2.20	0.42
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.45	0.42
19:S:30:LEU:HB3	19:S:31:ILE:H	1.67	0.42
1:A:809:G:C6	1:A:810:C:C5	3.08	0.42
3:C:175:LEU:HD22	3:C:201:TYR:CE2	2.54	0.42
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.80	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB2	2.01	0.42
9:I:50:LEU:HD21	9:I:85:LEU:HD11	2.02	0.42
9:I:79:LEU:O	9:I:83:ARG:HB2	2.20	0.42
10:J:49:VAL:CG1	14:N:41:ARG:HB2	2.50	0.42
11:K:18:ARG:HB2	11:K:33:THR:HG23	2.01	0.42
16:P:65:GLN:HA	16:P:66:PRO:HD2	1.84	0.42
20:T:33:ILE:HG12	20:T:62:LEU:HD23	2.01	0.42
1:A:33:A:N3	12:L:32:PHE:HE2	2.17	0.42
1:A:1276:G:H2'	1:A:1277:C:C6	2.55	0.42
3:C:17:ASP:O	3:C:54:ARG:NH2	2.53	0.42
11:K:21:ILE:HD12	11:K:95:ILE:HG12	2.02	0.42
13:M:92:HIS:NE2	13:M:98:VAL:HG21	2.35	0.42
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.02	0.42
1:A:35:G:C4	1:A:36:C:C5	3.07	0.42
1:A:232:G:H2'	1:A:233:C:C6	2.54	0.42
1:A:707:C:O3'	11:K:20:TYR:HE2	2.03	0.42
1:A:1138:G:O2'	1:A:1140:C:H5'	2.20	0.42
3:C:134:ILE:HD13	3:C:134:ILE:N	2.34	0.42
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.02	0.42
7:G:92:SER:HG	7:G:95:ARG:H	1.59	0.42
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.35	0.42
16:P:53:VAL:HG23	16:P:54:GLU:H	1.84	0.42
1:A:522:C:H5''	12:L:120:TYR:OH	2.19	0.42
1:A:538:G:P	12:L:115:LYS:HB2	2.60	0.42
1:A:980:C:C5	1:A:981:U:C4	3.08	0.42
1:A:1321:C:H5'	13:M:87:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:203:PHE:HE1	1.85	0.42
6:F:55:ASP:HA	6:F:56:PRO:HD3	1.83	0.42
18:R:32:ARG:HA	18:R:69:THR:CG2	2.46	0.42
18:R:46:GLU:N	18:R:46:GLU:CD	2.76	0.42
19:S:12:ASP:H	19:S:15:LEU:HD11	1.84	0.42
1:A:460:A:H8	1:A:460:A:OP1	2.03	0.41
1:A:663:A:H5'	18:R:61:LYS:HE3	2.01	0.41
1:A:1474:G:H2'	1:A:1475:G:H8	1.85	0.41
22:A:1601:SRV:HI32	22:A:1601:SRV:H22	2.02	0.41
4:D:11:LEU:HD13	4:D:66:ARG:HD3	2.02	0.41
8:H:11:THR:O	8:H:12:ARG:C	2.63	0.41
14:N:41:ARG:HA	14:N:44:LEU:HB2	2.02	0.41
16:P:39:TYR:CZ	16:P:41:PRO:HA	2.55	0.41
1:A:9:G:OP1	5:E:122:GLU:HG3	2.19	0.41
1:A:78:G:C5	1:A:79:G:N7	2.88	0.41
1:A:491:G:C4	1:A:492:G:C8	3.07	0.41
1:A:778:G:C5	1:A:779:C:C5	3.08	0.41
1:A:960:U:H4'	1:A:961:U:O5'	2.21	0.41
1:A:1198:G:H2'	1:A:1199:U:C5	2.56	0.41
1:A:1347:G:H2'	1:A:1373:G:O6	2.20	0.41
2:B:23:ARG:O	2:B:24:TRP:CD1	2.74	0.41
3:C:150:LYS:HG3	3:C:173:VAL:HG21	2.01	0.41
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.08	0.41
9:I:96:LEU:HA	9:I:99:LEU:HD12	2.01	0.41
16:P:50:LYS:HE2	16:P:50:LYS:HB2	1.81	0.41
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	2.01	0.41
18:R:20:ALA:HA	18:R:21:LYS:NZ	2.35	0.41
20:T:10:LEU:HD22	20:T:11:SER:N	2.32	0.41
1:A:881:G:P	12:L:12:ARG:HH22	2.43	0.41
1:A:1060:C:H4'	10:J:51:ARG:HB3	2.01	0.41
1:A:1061:G:C6	1:A:1197:G:C6	3.08	0.41
1:A:1354:C:H2'	1:A:1355:G:C8	2.54	0.41
1:A:1497:G:H2'	1:A:1498:UR3:H5'	2.01	0.41
2:B:172:ILE:H	2:B:172:ILE:HG13	1.46	0.41
3:C:26:LYS:HG2	10:J:45:ARG:HH22	1.85	0.41
4:D:117:ALA:O	4:D:121:VAL:HG23	2.21	0.41
4:D:199:ASN:ND2	4:D:202:LEU:HD23	2.36	0.41
5:E:18:ARG:HE	5:E:18:ARG:HB3	1.45	0.41
12:L:37:CYS:SG	12:L:56:ALA:HB1	2.61	0.41
15:O:38:ARG:O	15:O:41:GLU:HB3	2.20	0.41
1:A:412:A:O2'	1:A:413:G:O4'	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:G:H2'	1:A:930:C:O4'	2.20	0.41
1:A:986:A:C6	1:A:1220:G:C6	3.09	0.41
1:A:1092:A:H5''	7:G:4:ARG:CZ	2.50	0.41
1:A:1098:C:H2'	1:A:1099:G:O4'	2.21	0.41
1:A:1277:C:H1'	1:A:1282:C:H1'	2.02	0.41
1:A:1346:A:C5'	9:I:120:ARG:HH12	2.30	0.41
1:A:1350:A:OP2	9:I:118:LYS:HD3	2.19	0.41
1:A:1516:G:N2	1:A:1519:MA6:OP2	2.47	0.41
2:B:22:LYS:HE2	2:B:22:LYS:HB2	1.90	0.41
2:B:23:ARG:C	2:B:24:TRP:HD1	2.28	0.41
2:B:40:HIS:HD1	2:B:190:THR:HG21	1.85	0.41
2:B:135:GLN:HE21	2:B:135:GLN:HB2	1.55	0.41
2:B:189:ASP:N	2:B:189:ASP:OD1	2.53	0.41
3:C:116:VAL:O	3:C:119:ARG:HB3	2.20	0.41
4:D:157:LEU:HD23	4:D:157:LEU:HA	1.81	0.41
5:E:71:LEU:HD11	5:E:113:ALA:O	2.20	0.41
17:Q:75:ARG:HD2	17:Q:75:ARG:C	2.45	0.41
19:S:66:MET:H	19:S:66:MET:HG2	1.63	0.41
1:A:89:C:N3	1:A:90:U:C4	2.89	0.41
1:A:101:A:C2	1:A:102:G:C8	3.09	0.41
1:A:682:G:N2	1:A:708:C:O2	2.51	0.41
1:A:837:G:N2	1:A:850:U:C2	2.89	0.41
1:A:1133:G:N2	1:A:1141:C:C2	2.84	0.41
1:A:1306:A:C6	1:A:1332:A:C8	3.07	0.41
2:B:73:THR:HG22	2:B:73:THR:O	2.21	0.41
2:B:105:PHE:HD1	2:B:105:PHE:HA	1.71	0.41
5:E:11:ILE:HG23	5:E:11:ILE:HD12	1.67	0.41
7:G:30:ILE:HA	7:G:30:ILE:HD13	1.74	0.41
7:G:94:ARG:HA	7:G:97:GLN:HB2	2.02	0.41
8:H:103:VAL:HG12	8:H:108:GLY:C	2.46	0.41
10:J:48:THR:HB	10:J:62:HIS:CD2	2.55	0.41
11:K:15:ALA:HA	11:K:77:MET:HA	2.02	0.41
16:P:32:TYR:CD1	16:P:32:TYR:N	2.88	0.41
17:Q:60:ILE:C	17:Q:71:PHE:HD1	2.29	0.41
17:Q:82:MET:HE2	17:Q:82:MET:HB3	1.92	0.41
20:T:73:HIS:HB3	20:T:74:LYS:H	1.56	0.41
1:A:146:G:N2	1:A:147:G:C4	2.88	0.41
1:A:284:G:H2'	1:A:285:G:H8	1.84	0.41
1:A:544:G:C6	1:A:545:C:C4	3.08	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.20	0.41
1:A:1314:C:H2'	1:A:1315:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.36	0.41
1:A:1372:U:H2'	1:A:1373:G:H5'	2.02	0.41
2:B:220:ASP:HA	2:B:230:VAL:HG21	2.02	0.41
3:C:59:ARG:O	10:J:92:THR:HG23	2.21	0.41
4:D:58:LEU:HA	4:D:58:LEU:HD22	1.74	0.41
4:D:174:LEU:HA	4:D:184:LYS:O	2.20	0.41
9:I:49:PRO:O	9:I:53:VAL:HB	2.21	0.41
10:J:10:GLY:HA3	10:J:16:LEU:HD11	2.02	0.41
10:J:32:ALA:O	10:J:34:VAL:HG23	2.20	0.41
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.21	0.41
18:R:37:VAL:O	18:R:40:LEU:N	2.54	0.41
1:A:79:G:H2'	1:A:80:G:C8	2.55	0.41
1:A:389:A:C5	1:A:390:C:H1'	2.56	0.41
1:A:969:A:H8	1:A:969:A:H5'	1.85	0.41
1:A:986:A:H4'	19:S:55:LYS:NZ	2.36	0.41
1:A:1061:G:H5''	1:A:1062:U:OP2	2.21	0.41
1:A:1109:C:H2'	1:A:1110:A:O4'	2.21	0.41
1:A:1254:C:H2'	1:A:1255:G:H8	1.86	0.41
1:A:1360:A:H8	1:A:1361:G:O4'	2.04	0.41
1:A:1473:A:H2'	1:A:1474:G:O4'	2.21	0.41
2:B:208:ILE:HG12	2:B:211:ILE:HD11	2.03	0.41
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.03	0.41
4:D:52:SER:O	4:D:53:ASP:C	2.62	0.41
4:D:64:LEU:HD22	4:D:64:LEU:HA	1.83	0.41
5:E:9:LYS:NZ	5:E:108:ALA:HA	2.36	0.41
7:G:140:ASP:HA	7:G:143:ARG:CD	2.50	0.41
9:I:89:ASN:O	9:I:92:TYR:HB2	2.21	0.41
9:I:111:ARG:NH1	9:I:113:LYS:HA	2.36	0.41
11:K:92:GLU:HG3	11:K:96:ARG:HH11	1.85	0.41
16:P:58:TYR:CD1	16:P:59:TRP:N	2.88	0.41
1:A:81:U:C6	1:A:81:U:H3'	2.55	0.41
1:A:144:G:H2'	1:A:145:G:O4'	2.21	0.41
1:A:413:G:H2'	1:A:428:G:N2	2.36	0.41
1:A:426:G:OP1	4:D:38:TYR:OH	2.28	0.41
1:A:1004:A:H1'	1:A:1038:C:H42	1.84	0.41
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.02	0.41
3:C:93:LYS:C	3:C:94:LEU:HD22	2.46	0.41
3:C:174:PRO:HB2	3:C:177:THR:HG22	2.03	0.41
3:C:195:VAL:O	3:C:196:LEU:HD23	2.21	0.41
4:D:151:LYS:H	4:D:151:LYS:HD2	1.84	0.41
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:20:TYR:CD1	11:K:83:ILE:HB	2.55	0.41
13:M:108:ARG:HD3	13:M:114:ARG:HH21	1.85	0.41
16:P:78:GLY:HA2	16:P:80:PHE:H	1.86	0.41
1:A:35:G:C4	1:A:550:G:N2	2.88	0.41
1:A:140:A:H2'	1:A:141:A:O4'	2.21	0.41
1:A:363:A:OP2	12:L:61:THR:HG21	2.21	0.41
1:A:363:A:OP2	12:L:34:ARG:HG2	2.20	0.41
1:A:371:G:C2'	1:A:372:C:H5'	2.51	0.41
1:A:669:U:H2'	1:A:670:G:H8	1.86	0.41
1:A:922:G:H5''	1:A:922:G:H8	1.86	0.41
1:A:963:G:N2	1:A:973:G:C5	2.89	0.41
1:A:974:A:P	14:N:41:ARG:HH12	2.44	0.41
1:A:998:G:H1	1:A:1043:C:H42	1.69	0.41
1:A:1060:C:H2'	1:A:1061:G:H8	1.86	0.41
1:A:1091:U:O2	1:A:1093:A:H8	2.03	0.41
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.56	0.41
1:A:1351:U:H3	1:A:1371:G:H1	1.67	0.41
1:A:1356:G:H2'	1:A:1357:A:C8	2.56	0.41
1:A:1417:G:O5'	1:A:1417:G:H8	2.04	0.41
1:A:1507:A:H2'	1:A:1508:G:O4'	2.21	0.41
2:B:25:ASN:HD21	2:B:27:LYS:HG3	1.86	0.41
2:B:130:ARG:HD2	2:B:134:GLU:OE2	2.21	0.41
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.73	0.41
3:C:43:LEU:HD13	3:C:47:LEU:CD1	2.51	0.41
3:C:151:VAL:HG12	3:C:152:ILE:N	2.35	0.41
4:D:72:GLU:O	4:D:72:GLU:HG3	2.21	0.41
8:H:95:VAL:O	8:H:131:GLY:N	2.43	0.41
9:I:49:PRO:HD3	9:I:101:PHE:CE2	2.56	0.41
1:A:114:U:H1'	1:A:353:A:H1'	2.02	0.41
1:A:297:G:N2	1:A:300:A:OP2	2.53	0.41
1:A:406:G:H21	4:D:119:GLN:NE2	2.18	0.41
1:A:830:G:N2	1:A:857:C:C2	2.89	0.41
1:A:837:G:N2	1:A:850:U:O2	2.54	0.41
1:A:921:U:O2'	5:E:19:MET:O	2.26	0.41
1:A:939:G:H5''	7:G:102:ARG:NH1	2.36	0.41
1:A:946:A:H2'	1:A:947:G:H8	1.85	0.41
1:A:954:G:C6	1:A:955:U:C4	3.09	0.41
1:A:1075:C:H5''	2:B:179:LYS:NZ	2.36	0.41
1:A:1347:G:N2	1:A:1373:G:H2'	2.36	0.41
1:A:1399:C:H4'	1:A:1400:5MC:H5''	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:131:ILE:HA	5:E:131:ILE:HD13	1.55	0.41
8:H:83:ILE:HG21	8:H:83:ILE:HD13	1.74	0.41
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.40	0.41
14:N:25:VAL:HG12	14:N:38:GLY:O	2.21	0.41
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.02	0.41
16:P:34:GLU:OE2	16:P:55:ARG:HD2	2.21	0.41
17:Q:4:LYS:O	17:Q:60:ILE:HD13	2.22	0.41
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.75	0.41
20:T:14:LYS:HA	20:T:17:ARG:NH2	2.36	0.41
20:T:20:LEU:O	20:T:23:ARG:HB3	2.20	0.41
1:A:597:G:C4	1:A:644:G:C2	3.09	0.40
1:A:720:C:H5'	18:R:52:PRO:HA	2.03	0.40
1:A:925:G:C2	1:A:927:G:C8	3.09	0.40
1:A:1229:A:OP1	13:M:116:THR:OG1	2.26	0.40
1:A:1425:U:H2'	1:A:1426:C:C6	2.56	0.40
3:C:22:TRP:HH2	3:C:33:LEU:HD21	1.84	0.40
3:C:52:LEU:O	3:C:115:LEU:HD21	2.21	0.40
6:F:4:TYR:CD1	6:F:92:LYS:HA	2.56	0.40
7:G:64:GLN:HA	7:G:67:GLU:HB3	2.03	0.40
8:H:96:GLY:O	8:H:97:VAL:C	2.63	0.40
10:J:7:LYS:HD3	10:J:9:ARG:HE	1.86	0.40
10:J:49:VAL:HG23	14:N:34:TYR:OH	2.21	0.40
18:R:20:ALA:HA	18:R:21:LYS:HZ2	1.87	0.40
18:R:79:LEU:CD2	18:R:80:PRO:HD2	2.51	0.40
1:A:246:A:O3'	1:A:247:G:H4'	2.21	0.40
1:A:285:G:C4	1:A:286:G:C8	3.09	0.40
1:A:373:A:H1'	1:A:481:G:H1'	2.02	0.40
1:A:775:G:H2'	1:A:776:G:H5'	2.03	0.40
1:A:1090:U:O2'	1:A:1091:U:H5'	2.20	0.40
1:A:1214:C:H3'	1:A:1215:G:H8	1.86	0.40
1:A:1447:G:N3	1:A:1447:G:H2'	2.36	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.36	0.40
4:D:111:ALA:HA	4:D:161:ASN:HD22	1.85	0.40
7:G:70:LYS:NZ	7:G:97:GLN:HA	2.36	0.40
8:H:120:THR:HG23	8:H:123:GLU:CD	2.46	0.40
9:I:15:ALA:CA	9:I:65:VAL:HG12	2.51	0.40
11:K:82:VAL:HB	11:K:108:ILE:CD1	2.51	0.40
1:A:820:U:H4'	1:A:821:G:OP2	2.20	0.40
1:A:899:C:H2'	1:A:900:A:O4'	2.20	0.40
1:A:919:A:O5'	1:A:919:A:H8	2.04	0.40
1:A:1000:U:H2'	1:A:1001:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:G:O2'	1:A:1199:U:H5	2.04	0.40
1:A:1125:U:P	1:A:1145:C:H41	2.42	0.40
2:B:117:GLU:O	2:B:120:ALA:HB3	2.21	0.40
3:C:20:SER:HB3	3:C:22:TRP:NE1	2.37	0.40
4:D:164:ALA:O	4:D:168:ARG:HD2	2.21	0.40
6:F:39:LYS:NZ	6:F:39:LYS:HB2	2.37	0.40
8:H:39:LEU:HB3	8:H:45:ILE:HG12	2.04	0.40
13:M:40:ASN:HB3	13:M:43:THR:HG23	2.03	0.40
20:T:33:ILE:O	20:T:34:LYS:C	2.64	0.40
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.68	0.40
1:A:79:G:C2	1:A:80:G:C5	3.10	0.40
1:A:474:G:N2	1:A:475:G:C5	2.90	0.40
1:A:580:U:H2'	1:A:581:G:O4'	2.21	0.40
1:A:633:G:H2'	1:A:634:C:H6	1.86	0.40
1:A:778:G:C6	1:A:779:C:C4	3.10	0.40
1:A:1005:A:N6	1:A:1024:G:O2'	2.55	0.40
1:A:1181:G:C4	1:A:1182:G:N1	2.90	0.40
1:A:1311:G:N2	1:A:1327:C:C2	2.89	0.40
1:A:1311:G:N3	1:A:1311:G:H2'	2.36	0.40
1:A:1519:MA6:H8	1:A:1519:MA6:O5'	2.20	0.40
3:C:34:LEU:HG	14:N:25:VAL:HG11	2.03	0.40
3:C:58:GLU:H	3:C:65:ALA:HB3	1.86	0.40
5:E:61:TYR:HD2	5:E:61:TYR:HA	1.77	0.40
7:G:21:VAL:H	7:G:21:VAL:HG22	1.57	0.40
9:I:104:ARG:NH1	9:I:105:ASP:O	2.54	0.40
10:J:16:LEU:HB3	10:J:70:ARG:HE	1.85	0.40
13:M:34:LEU:HA	13:M:34:LEU:HD23	1.58	0.40
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	2.02	0.40
17:Q:29:HIS:CE1	17:Q:32:TYR:H	2.40	0.40
1:A:75:G:O2'	1:A:76:C:H5'	2.21	0.40
1:A:136:C:H1'	16:P:1:MET:HG3	2.03	0.40
1:A:260:G:C6	1:A:261:U:C4	3.10	0.40
1:A:945:G:H2'	1:A:945:G:N3	2.36	0.40
1:A:1047:G:C2'	1:A:1048:G:H5'	2.51	0.40
1:A:1126:U:H2'	1:A:1127:G:H5'	2.03	0.40
1:A:1179:A:OP2	9:I:93:ARG:NH1	2.54	0.40
1:A:1290:G:O2'	1:A:1291:G:H5'	2.21	0.40
1:A:1478:C:O2	1:A:1478:C:H2'	2.22	0.40
2:B:100:GLY:O	2:B:101:MET:C	2.64	0.40
3:C:93:LYS:O	3:C:94:LEU:HD13	2.20	0.40
4:D:203:VAL:O	4:D:206:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:62:GLU:O	18:R:65:ILE:N	2.55	0.40
19:S:74:PHE:CD1	19:S:74:PHE:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	200 (86%)	30 (13%)	2 (1%)	14	47
3	C	204/239 (85%)	179 (88%)	25 (12%)	0	100	100
4	D	206/209 (99%)	186 (90%)	20 (10%)	0	100	100
5	E	148/162 (91%)	136 (92%)	11 (7%)	1 (1%)	18	53
6	F	99/101 (98%)	90 (91%)	8 (8%)	1 (1%)	12	45
7	G	153/156 (98%)	136 (89%)	16 (10%)	1 (1%)	18	53
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	16	50
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	12	45
11	K	114/129 (88%)	103 (90%)	11 (10%)	0	100	100
12	L	121/135 (90%)	107 (88%)	12 (10%)	2 (2%)	7	35
13	M	116/126 (92%)	103 (89%)	12 (10%)	1 (1%)	14	47
14	N	58/61 (95%)	49 (84%)	9 (16%)	0	100	100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	10	41
16	P	81/88 (92%)	75 (93%)	5 (6%)	1 (1%)	10	41
17	Q	97/105 (92%)	89 (92%)	8 (8%)	0	100	100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100	100
19	S	78/93 (84%)	67 (86%)	10 (13%)	1 (1%)	9	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	12	45
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2541 (92%)	2089 (89%)	233 (10%)	14 (1%)	21	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
12	L	28	LYS
2	B	21	ARG
2	B	24	TRP
9	I	119	ALA
20	T	99	LEU
5	E	129	ILE
16	P	53	VAL
7	G	80	VAL
6	F	68	PRO
10	J	34	VAL
13	M	84	ILE
12	L	25	PRO
15	O	45	VAL

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	
2	B	202/220 (92%)	159 (79%)	43 (21%)	1	6
3	C	160/188 (85%)	127 (79%)	33 (21%)	1	8
4	D	180/181 (99%)	139 (77%)	41 (23%)	1	5
5	E	115/123 (94%)	79 (69%)	36 (31%)	0	2
6	F	90/90 (100%)	73 (81%)	17 (19%)	1	10
7	G	126/127 (99%)	93 (74%)	33 (26%)	0	3
8	H	119/119 (100%)	84 (71%)	35 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	98/99 (99%)	75 (76%)	23 (24%)	1	5
10	J	87/92 (95%)	70 (80%)	17 (20%)	1	9
11	K	88/99 (89%)	69 (78%)	19 (22%)	1	6
12	L	103/110 (94%)	76 (74%)	27 (26%)	0	3
13	M	94/101 (93%)	69 (73%)	25 (27%)	0	3
14	N	49/50 (98%)	37 (76%)	12 (24%)	1	4
15	O	79/80 (99%)	50 (63%)	29 (37%)	0	1
16	P	72/74 (97%)	55 (76%)	17 (24%)	1	5
17	Q	94/97 (97%)	66 (70%)	28 (30%)	0	2
18	R	61/77 (79%)	45 (74%)	16 (26%)	0	3
19	S	71/80 (89%)	53 (75%)	18 (25%)	0	3
20	T	76/82 (93%)	53 (70%)	23 (30%)	0	2
21	U	19/22 (86%)	16 (84%)	3 (16%)	2	14
All	All	1983/2111 (94%)	1488 (75%)	495 (25%)	0	4

All (495) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	10	LEU
2	B	16	HIS
2	B	17	PHE
2	B	21	ARG
2	B	23	ARG
2	B	39	ILE
2	B	45	GLN
2	B	48	MET
2	B	53	ARG
2	B	61	LEU
2	B	67	THR
2	B	69	LEU
2	B	75	LYS
2	B	79	ASP
2	B	87	ARG
2	B	97	TRP
2	B	102	LEU

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Mol	Chain	Res	Type
2	B	107	THR
2	B	108	ILE
2	B	112	VAL
2	B	121	LEU
2	B	122	PHE
2	B	126	GLU
2	B	127	ILE
2	B	135	GLN
2	B	139	LYS
2	B	142	LEU
2	B	144	ARG
2	B	154	LEU
2	B	157	ARG
2	B	158	LEU
2	B	160	ASP
2	B	162	ILE
2	B	172	ILE
2	B	178	ARG
2	B	190	THR
2	B	196	LEU
2	B	208	ILE
2	B	212	GLN
2	B	221	LEU
2	B	238	LEU
3	C	3	ASN
3	C	11	ARG
3	C	15	THR
3	C	30	ARG
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	43	LEU
3	C	45	LYS
3	C	64	VAL
3	C	66	VAL
3	C	69	HIS
3	C	70	VAL
3	C	79	ARG
3	C	84	ILE
3	C	95	THR
3	C	103	VAL
3	C	110	ASN

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Mol	Chain	Res	Type
3	C	130	VAL
3	C	138	VAL
3	C	147	LYS
3	C	165	THR
3	C	166	GLU
3	C	172	ARG
3	C	175	LEU
3	C	177	THR
3	C	178	LEU
3	C	179	ARG
3	C	183	ASP
3	C	191	THR
3	C	198	VAL
3	C	204	LEU
3	C	206	GLU
4	D	10	ARG
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	39	PRO
4	D	47	ARG
4	D	52	SER
4	D	61	LYS
4	D	64	LEU
4	D	67	ILE
4	D	70	ILE
4	D	71	SER
4	D	78	LEU
4	D	80	GLU
4	D	104	VAL
4	D	120	LEU
4	D	122	ARG
4	D	127	THR
4	D	129	ASN
4	D	135	LEU
4	D	137	SER
4	D	141	ARG
4	D	145	GLU

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Mol	Chain	Res	Type
4	D	151	LYS
4	D	158	ILE
4	D	176	LEU
4	D	178	VAL
4	D	179	GLU
4	D	185	PHE
4	D	186	LEU
4	D	187	ARG
4	D	188	LEU
4	D	194	LEU
4	D	198	VAL
4	D	202	LEU
4	D	203	VAL
4	D	209	ARG
5	E	5	ASP
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	18	ARG
5	E	19	MET
5	E	24	ARG
5	E	32	VAL
5	E	33	VAL
5	E	34	VAL
5	E	51	VAL
5	E	53	LEU
5	E	55	VAL
5	E	61	TYR
5	E	67	VAL
5	E	69	VAL
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	87	SER
5	E	100	VAL
5	E	101	ILE
5	E	105	VAL
5	E	112	LEU
5	E	118	ILE
5	E	123	LEU
5	E	125	SER

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Mol	Chain	Res	Type
5	E	131	ILE
5	E	136	MET
5	E	137	GLU
5	E	141	GLN
5	E	143	ARG
5	E	144	THR
5	E	147	ASP
5	E	148	VAL
6	F	19	LEU
6	F	24	GLU
6	F	30	LEU
6	F	39	LYS
6	F	43	LEU
6	F	45	LEU
6	F	47	ARG
6	F	65	VAL
6	F	66	GLU
6	F	73	ASN
6	F	74	ASP
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	88	VAL
6	F	94	GLN
6	F	98	LEU
7	G	3	ARG
7	G	8	GLU
7	G	22	LEU
7	G	27	ILE
7	G	30	ILE
7	G	31	MET
7	G	33	ASP
7	G	35	LYS
7	G	38	LEU
7	G	45	ASP
7	G	48	LYS
7	G	50	ILE
7	G	52	GLU
7	G	53	LYS
7	G	56	GLN
7	G	57	GLU
7	G	59	LEU

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Mol	Chain	Res	Type
7	G	61	VAL
7	G	77	SER
7	G	80	VAL
7	G	85	TYR
7	G	91	VAL
7	G	92	SER
7	G	94	ARG
7	G	97	GLN
7	G	98	SER
7	G	99	LEU
7	G	109	ASN
7	G	110	GLN
7	G	113	GLU
7	G	124	LEU
7	G	126	ASP
7	G	146	GLU
8	H	5	PRO
8	H	6	ILE
8	H	10	LEU
8	H	11	THR
8	H	12	ARG
8	H	14	ARG
8	H	22	GLU
8	H	23	SER
8	H	29	SER
8	H	38	ILE
8	H	39	LEU
8	H	51	VAL
8	H	63	LEU
8	H	65	TYR
8	H	82	HIS
8	H	83	ILE
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG
8	H	93	VAL
8	H	97	VAL
8	H	102	ARG
8	H	103	VAL
8	H	105	ARG
8	H	107	LEU
8	H	112	LEU

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Mol	Chain	Res	Type
8	H	113	SER
8	H	118	VAL
8	H	120	THR
8	H	123	GLU
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
8	H	136	GLU
8	H	137	VAL
9	I	3	GLN
9	I	10	ARG
9	I	14	VAL
9	I	16	ARG
9	I	29	ASN
9	I	35	GLU
9	I	38	GLN
9	I	48	GLU
9	I	53	VAL
9	I	58	HIS
9	I	70	LYS
9	I	79	LEU
9	I	87	GLN
9	I	91	ASP
9	I	92	TYR
9	I	104	ARG
9	I	108	VAL
9	I	109	VAL
9	I	111	ARG
9	I	113	LYS
9	I	114	TYR
9	I	118	LYS
9	I	121	ARG
10	J	4	ILE
10	J	5	ARG
10	J	23	ILE
10	J	43	ARG
10	J	47	PHE
10	J	48	THR
10	J	49	VAL
10	J	54	PHE
10	J	57	LYS
10	J	64	GLU

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Mol	Chain	Res	Type
10	J	68	HIS
10	J	71	LEU
10	J	74	ILE
10	J	83	GLU
10	J	85	LEU
10	J	88	LEU
10	J	96	ILE
11	K	11	LYS
11	K	13	GLN
11	K	18	ARG
11	K	28	THR
11	K	29	ILE
11	K	33	THR
11	K	47	VAL
11	K	54	ARG
11	K	75	TYR
11	K	80	VAL
11	K	91	ARG
11	K	95	ILE
11	K	98	LEU
11	K	101	SER
11	K	109	VAL
11	K	114	VAL
11	K	119	CYS
11	K	124	LYS
11	K	126	ARG
12	L	7	ILE
12	L	11	VAL
12	L	24	VAL
12	L	27	LEU
12	L	33	ARG
12	L	34	ARG
12	L	36	VAL
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	55	VAL
12	L	60	LEU
12	L	61	THR
12	L	64	TYR

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Mol	Chain	Res	Type
12	L	65	GLU
12	L	66	VAL
12	L	67	THR
12	L	76	ASN
12	L	80	HIS
12	L	96	VAL
12	L	101	VAL
12	L	104	VAL
12	L	120	TYR
12	L	122	THR
12	L	127	GLU
13	M	9	ILE
13	M	15	VAL
13	M	16	ASP
13	M	17	VAL
13	M	19	LEU
13	M	27	LYS
13	M	35	GLU
13	M	39	ILE
13	M	45	VAL
13	M	49	THR
13	M	53	VAL
13	M	54	VAL
13	M	56	LEU
13	M	57	ARG
13	M	63	THR
13	M	66	LEU
13	M	73	GLU
13	M	77	ASN
13	M	81	LEU
13	M	93	ARG
13	M	98	VAL
13	M	101	GLN
13	M	102	ARG
13	M	110	ARG
13	M	115	LYS
14	N	9	LYS
14	N	12	ARG
14	N	18	VAL
14	N	21	TYR
14	N	22	THR
14	N	25	VAL

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Mol	Chain	Res	Type
14	N	27	CYS
14	N	31	ARG
14	N	42	ILE
14	N	44	LEU
14	N	45	ARG
14	N	47	LEU
15	O	4	THR
15	O	5	LYS
15	O	9	GLN
15	O	26	GLU
15	O	27	VAL
15	O	31	LEU
15	O	32	LEU
15	O	33	THR
15	O	34	LEU
15	O	36	ILE
15	O	38	ARG
15	O	39	LEU
15	O	42	HIS
15	O	44	LYS
15	O	45	VAL
15	O	47	LYS
15	O	56	LEU
15	O	60	VAL
15	O	64	ARG
15	O	67	LEU
15	O	68	ARG
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	78	TYR
15	O	81	LEU
15	O	84	LYS
15	O	87	ILE
15	O	88	ARG
16	P	1	MET
16	P	2	VAL
16	P	5	ARG
16	P	6	LEU
16	P	20	VAL
16	P	33	ILE
16	P	44	THR

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Mol	Chain	Res	Type
16	P	45	THR
16	P	50	LYS
16	P	53	VAL
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	68	ASP
16	P	69	THR
16	P	79	VAL
16	P	83	GLU
17	Q	9	VAL
17	Q	12	SER
17	Q	15	MET
17	Q	19	VAL
17	Q	21	VAL
17	Q	29	HIS
17	Q	34	LYS
17	Q	35	VAL
17	Q	36	ILE
17	Q	41	LYS
17	Q	45	HIS
17	Q	53	LEU
17	Q	58	GLU
17	Q	59	ILE
17	Q	60	ILE
17	Q	63	ARG
17	Q	72	ARG
17	Q	73	VAL
17	Q	74	LEU
17	Q	75	ARG
17	Q	77	VAL
17	Q	84	LEU
17	Q	85	VAL
17	Q	86	GLU
17	Q	89	LEU
17	Q	92	ARG
17	Q	96	GLN
17	Q	98	LEU
18	R	21	LYS
18	R	22	VAL
18	R	28	GLU
18	R	31	LEU

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Mol	Chain	Res	Type
18	R	35	ARG
18	R	37	VAL
18	R	40	LEU
18	R	42	ARG
18	R	46	GLU
18	R	47	THR
18	R	53	ARG
18	R	56	THR
18	R	58	LEU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	3	ARG
19	S	6	LYS
19	S	7	LYS
19	S	17	GLU
19	S	20	LEU
19	S	23	ASN
19	S	27	GLU
19	S	29	ARG
19	S	41	VAL
19	S	43	GLU
19	S	51	VAL
19	S	55	LYS
19	S	58	VAL
19	S	62	ILE
19	S	63	THR
19	S	64	GLU
19	S	66	MET
19	S	77	THR
20	T	9	ASN
20	T	10	LEU
20	T	13	LEU
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	30	LYS
20	T	33	ILE
20	T	36	LEU
20	T	42	GLN
20	T	43	LEU
20	T	46	GLU

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Mol	Chain	Res	Type
20	T	50	GLU
20	T	53	LEU
20	T	64	ASP
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	85	MET
20	T	86	ARG
20	T	90	GLN
20	T	91	LEU
21	U	8	THR
21	U	12	LYS
21	U	13	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	45	GLN
2	B	113	HIS
2	B	135	GLN
2	B	212	GLN
3	C	6	HIS
3	C	139	GLN
4	D	45	GLN
4	D	119	GLN
6	F	73	ASN
6	F	100	ASN
7	G	84	ASN
9	I	73	GLN
10	J	56	HIS
10	J	76	ASN
15	O	53	HIS
15	O	71	GLN
19	S	69	HIS
20	T	16	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	395 (26%)	45 (2%)

All (395) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	19	C
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	41	G
1	A	45	U
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	58	C
1	A	66	G
1	A	68	G
1	A	69	G
1	A	76	C
1	A	81	U
1	A	89	C
1	A	91	C
1	A	92	C
1	A	97	G
1	A	99	C
1	A	106	C
1	A	107	G
1	A	108	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	141	A
1	A	145	G
1	A	157	G

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Mol	Chain	Res	Type
1	A	163	C
1	A	175	C
1	A	178	C
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
1	A	190(G)	G
1	A	195	A
1	A	197	A
1	A	199	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	217	C
1	A	220	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	246	A
1	A	247	G
1	A	251	G
1	A	252	U
1	A	254	G
1	A	257	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	299	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	324	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	344	A
1	A	345	C
1	A	346	G

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Mol	Chain	Res	Type
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	374	A
1	A	384	G
1	A	388	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	405	U
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	450	G
1	A	455	C
1	A	460	A
1	A	461	C
1	A	475	G
1	A	476	G
1	A	478	A
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	487	A
1	A	497	A
1	A	498	U
1	A	505	G

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Mol	Chain	Res	Type
1	A	509	A
1	A	510	A
1	A	511	C
1	A	513	C
1	A	518	C
1	A	519	C
1	A	524	G
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	541	G
1	A	547	A
1	A	558	G
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	597	G
1	A	598	U
1	A	607	A
1	A	615	C
1	A	618	C
1	A	624	C
1	A	630	G
1	A	631	G
1	A	652	U
1	A	653	A
1	A	656	C
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	694	A
1	A	701	C

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Mol	Chain	Res	Type
1	A	702	A
1	A	703	G
1	A	718	G
1	A	722	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	733	A
1	A	734	G
1	A	749	C
1	A	755	G
1	A	759	A
1	A	760	G
1	A	773	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	784	C
1	A	787	A
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	812	C
1	A	813	U
1	A	817	C
1	A	818	G
1	A	821	G
1	A	826	C
1	A	828	A
1	A	829	G
1	A	838	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	855	G
1	A	858	G
1	A	869	G
1	A	872	A
1	A	873	A

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Mol	Chain	Res	Type
1	A	876	G
1	A	889	A
1	A	902	G
1	A	910	C
1	A	914	A
1	A	919	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	936	C
1	A	941	G
1	A	944	G
1	A	950	U
1	A	954	G
1	A	957	U
1	A	960	U
1	A	961	U
1	A	964	A
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	973	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	980	C
1	A	985	C
1	A	989	C
1	A	990	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003	G
1	A	1003(A)	G
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1008	C
1	A	1020	U

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Mol	Chain	Res	Type
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1030(B)	C
1	A	1032	G
1	A	1038	C
1	A	1045	C
1	A	1047	G
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1059	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1079	G
1	A	1085	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1104	G
1	A	1115	C
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1144	G
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1161	C
1	A	1171	G
1	A	1174	G

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Mol	Chain	Res	Type
1	A	1176	A
1	A	1177	G
1	A	1183	A
1	A	1184	G
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1206	G
1	A	1207	2MG
1	A	1209	C
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1243	C
1	A	1245	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1263	C
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1297	C
1	A	1300	G

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Mol	Chain	Res	Type
1	A	1301	U
1	A	1302	U
1	A	1305	G
1	A	1311	G
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1326	C
1	A	1327	C
1	A	1334	G
1	A	1336	C
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1359	C
1	A	1360	A
1	A	1362	C
1	A	1364	U
1	A	1370	G
1	A	1371	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1393	U
1	A	1397	C
1	A	1398	A
1	A	1399	C
1	A	1402	4OC
1	A	1414	U
1	A	1441	G
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1453	G
1	A	1454	G
1	A	1469	G
1	A	1487	G

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Mol	Chain	Res	Type
1	A	1490	C
1	A	1493	A
1	A	1495	U
1	A	1496	C
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1515	C
1	A	1518	MA6
1	A	1519	MA6
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1532	U
1	A	1533	C

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	65	U
1	A	115	G
1	A	129(A)	G
1	A	173	U
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	509	A
1	A	518	C

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Mol	Chain	Res	Type
1	A	559	A
1	A	597	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1301	U
1	A	1333	A
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1540	1	18,21,22	1.41	1 (5%)	21,30,33	1.64	4 (19%)
1	5MC	A	1400	1	19,22,23	1.56	4 (21%)	26,32,35	1.09	4 (15%)
1	5MC	A	1407	1	19,22,23	2.27	5 (26%)	26,32,35	1.29	4 (15%)
1	PSU	A	516	1	18,21,22	1.39	3 (16%)	21,30,33	1.39	4 (19%)
1	7MG	A	527	1	23,26,27	3.80	7 (30%)	27,39,42	2.62	9 (33%)
1	M2G	A	966	1	24,27,28	1.47	5 (20%)	33,40,43	0.94	2 (6%)
1	MA6	A	1518	1	23,26,27	2.02	7 (30%)	33,38,41	1.45	6 (18%)
1	MA6	A	1519	1	23,26,27	2.31	10 (43%)	33,38,41	0.93	1 (3%)
1	5MC	A	1404	1	19,22,23	1.54	4 (21%)	26,32,35	1.45	5 (19%)
1	4OC	A	1402	1	20,23,24	1.25	1 (5%)	25,32,35	0.72	0
12	0TD	L	92	12	8,9,10	1.02	0	6,11,13	3.36	3 (50%)
1	PSU	A	1541	1	18,21,22	1.27	1 (5%)	21,30,33	1.91	4 (19%)
1	5MC	A	967	1	19,22,23	1.09	2 (10%)	26,32,35	0.90	1 (3%)
1	UR3	A	1498	1	19,22,23	1.18	1 (5%)	26,32,35	1.14	1 (3%)
1	2MG	A	1207	1	23,26,27	1.52	5 (21%)	33,38,41	1.13	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/11/29/30	0/3/3/3
1	MA6	A	1518	1	-	4/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	6/11/29/30	0/3/3/3
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
12	0TD	L	92	12	-	4/7/12/14	-
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-16.09	1.35	1.45
1	A	1407	5MC	C5-C4	6.98	1.49	1.44
1	A	527	7MG	C5-N7	5.84	1.43	1.35
1	A	1519	MA6	C5-C4	5.39	1.48	1.39
1	A	1540	PSU	C6-C5	5.05	1.40	1.35
1	A	1518	MA6	C8-N9	4.95	1.46	1.37
1	A	1541	PSU	C6-C5	4.68	1.40	1.35
1	A	1519	MA6	C2-N1	4.36	1.41	1.33
1	A	516	PSU	C6-C5	4.35	1.40	1.35
1	A	1518	MA6	C5-N7	4.22	1.46	1.39
1	A	1407	5MC	C2-N1	4.22	1.48	1.40
1	A	1400	5MC	C2-N1	3.93	1.48	1.40
1	A	1519	MA6	C8-N9	3.92	1.44	1.37
1	A	1402	4OC	C2-N3	3.88	1.44	1.36
1	A	1518	MA6	C9-N6	3.76	1.54	1.45
1	A	1404	5MC	C5-C4	3.74	1.46	1.44
1	A	966	M2G	C8-N9	3.65	1.45	1.37
1	A	1519	MA6	C6-N6	3.58	1.46	1.36
1	A	1518	MA6	C4-N3	3.57	1.41	1.34
1	A	1404	5MC	C1'-N1	-3.55	1.37	1.47
1	A	1519	MA6	C6-N1	3.40	1.40	1.34
1	A	1498	UR3	C4-N3	-3.36	1.33	1.40
1	A	1207	2MG	C2-N2	3.32	1.40	1.33
1	A	1407	5MC	C2-N3	3.30	1.42	1.36
1	A	966	M2G	C4-N3	3.25	1.41	1.34
1	A	1207	2MG	C2-N1	3.19	1.41	1.36
1	A	1519	MA6	C5-N7	3.11	1.44	1.39
1	A	1404	5MC	C6-N1	-2.91	1.33	1.38
1	A	1400	5MC	C1'-N1	2.83	1.55	1.47
1	A	1400	5MC	C6-C5	2.83	1.39	1.34
1	A	1207	2MG	C8-N9	2.81	1.43	1.37
1	A	1400	5MC	C2-N3	2.78	1.41	1.36
1	A	1519	MA6	C9-N6	2.76	1.51	1.45
1	A	966	M2G	O6-C6	-2.73	1.18	1.23
1	A	527	7MG	C2-N1	-2.68	1.31	1.37
1	A	966	M2G	C2-N2	2.62	1.39	1.35
1	A	1207	2MG	C4-N3	2.60	1.40	1.34
1	A	1207	2MG	C6-N1	2.57	1.43	1.38
1	A	527	7MG	C2-N2	2.51	1.40	1.34
1	A	1519	MA6	C4-N3	2.45	1.39	1.34
1	A	527	7MG	O6-C6	-2.44	1.18	1.23
1	A	967	5MC	C4-N4	2.42	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C4-N3	2.38	1.39	1.34
1	A	967	5MC	C2-N3	2.34	1.41	1.36
1	A	1407	5MC	C1'-N1	2.32	1.54	1.47
1	A	966	M2G	C4-N9	2.31	1.44	1.38
1	A	1519	MA6	C8-N7	2.27	1.36	1.31
1	A	1518	MA6	C8-N7	2.25	1.36	1.31
1	A	1518	MA6	C5-C4	2.23	1.43	1.39
1	A	1407	5MC	C4-N4	2.14	1.39	1.34
1	A	1519	MA6	C5-C6	2.07	1.46	1.41
1	A	1518	MA6	C5-C6	2.05	1.46	1.41
1	A	516	PSU	O4'-C1'	-2.04	1.41	1.43
1	A	1404	5MC	C2-N3	2.04	1.40	1.36
1	A	516	PSU	C2-N1	2.03	1.39	1.36
1	A	527	7MG	C8-N7	-2.00	1.32	1.42

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	6.42	122.24	110.94
12	L	92	0TD	CSB-SB-CB	-6.04	91.51	102.36
1	A	527	7MG	N9-C4-N3	5.74	133.87	125.46
1	A	1541	PSU	N1-C2-N3	5.03	120.48	115.17
1	A	527	7MG	C5-C4-N3	-4.51	119.67	128.13
1	A	527	7MG	N9-C8-N7	4.31	109.47	103.37
1	A	527	7MG	C2-N3-C4	4.19	119.52	112.30
1	A	527	7MG	C2-N1-C6	-3.91	118.02	125.11
1	A	1541	PSU	C4-N3-C2	-3.85	121.07	126.37
1	A	1540	PSU	N1-C2-N3	3.82	119.20	115.17
1	A	1540	PSU	C4-N3-C2	-3.80	121.14	126.37
1	A	1518	MA6	C4-N9-C1'	-3.72	117.92	126.63
12	L	92	0TD	CB-CA-N	-3.63	101.75	109.10
1	A	1518	MA6	C1'-N9-C8	3.60	135.09	127.09
1	A	1541	PSU	O2-C2-N1	-3.58	119.10	122.79
1	A	527	7MG	O6-C6-C5	-3.58	118.84	127.62
1	A	1541	PSU	C6-N1-C2	-3.55	119.39	122.69
1	A	1404	5MC	N4-C4-N3	-3.53	112.12	118.51
1	A	527	7MG	C6-C5-C4	-3.38	116.45	122.40
1	A	516	PSU	C4-N3-C2	-3.38	121.72	126.37
1	A	1498	UR3	C6-N1-C2	-3.34	119.07	121.80
12	L	92	0TD	OD1-CG-CB	-3.22	115.69	122.44
1	A	1540	PSU	C6-N1-C2	-2.91	119.99	122.69
1	A	1404	5MC	C5-C4-N3	2.91	124.73	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1404	5MC	C5-C6-N1	-2.83	120.24	123.31
1	A	1519	MA6	C2-N1-C6	2.82	118.72	111.83
1	A	1404	5MC	C4-N3-C2	-2.81	116.90	120.81
1	A	1518	MA6	C6-C5-N7	2.69	137.73	133.43
1	A	966	M2G	C5-C4-N3	-2.66	124.16	128.39
1	A	1518	MA6	C4-C5-C6	-2.64	113.19	115.91
1	A	1207	2MG	C5-C4-N3	-2.63	124.20	128.39
1	A	527	7MG	C6-C5-N7	2.63	136.01	131.93
1	A	1407	5MC	N4-C4-N3	-2.52	113.94	118.51
1	A	1407	5MC	C4-N3-C2	-2.51	117.32	120.81
1	A	966	M2G	O6-C6-N1	-2.50	115.41	120.11
1	A	1518	MA6	C2-N1-C6	2.39	117.67	111.83
1	A	1540	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	A	516	PSU	N1-C2-N3	2.33	117.63	115.17
1	A	1207	2MG	N9-C4-N3	2.33	130.62	125.95
1	A	1404	5MC	C6-N1-C2	2.32	124.05	120.95
1	A	1400	5MC	O2-C2-N3	-2.32	118.67	122.33
1	A	1407	5MC	O2-C2-N3	-2.31	118.68	122.33
1	A	1207	2MG	C6-C5-N7	-2.30	126.10	130.29
1	A	516	PSU	O4'-C1'-C2'	2.26	108.28	105.15
1	A	516	PSU	O2-C2-N1	-2.23	120.49	122.79
1	A	1400	5MC	N4-C4-N3	-2.19	114.55	118.51
1	A	1400	5MC	C6-N1-C2	-2.17	118.06	120.95
1	A	1407	5MC	CM5-C5-C6	-2.16	119.93	122.85
1	A	967	5MC	N4-C4-N3	-2.13	114.65	118.51
1	A	1400	5MC	C5-C4-N3	2.07	123.88	121.75
1	A	1518	MA6	N1-C6-N6	-2.03	114.38	116.86

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C9
1	A	1541	PSU	C2'-C1'-C5-C4
1	A	1541	PSU	C2'-C1'-C5-C6
1	A	1518	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C9
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C10
12	L	92	0TD	CA-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD2
1	A	1540	PSU	O4'-C1'-C5-C6
1	A	967	5MC	C2'-C1'-N1-C6
12	L	92	0TD	CG-CB-SB-CSB
1	A	967	5MC	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1540	PSU	1	0
1	A	1400	5MC	3	0
1	A	527	7MG	1	0
1	A	1518	MA6	2	0
1	A	1519	MA6	4	0
1	A	1404	5MC	3	0
12	L	92	0TD	2	0
1	A	1541	PSU	1	0
1	A	967	5MC	1	0
1	A	1498	UR3	3	0
1	A	1207	2MG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 250 ligands modelled in this entry, 249 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	$\# Z > 2$
22	SRY	A	1601	-	40,42,42	2.42	13 (32%)	49,63,63	2.32	11 (22%)

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
22	SRY	A	1601	-	-	5/20/87/87	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.49	1.49	1.33
22	A	1601	SRY	CA1-N11	6.03	1.43	1.33
22	A	1601	SRY	C11-N11	-3.42	1.40	1.45
22	A	1601	SRY	O53-C53	-3.38	1.36	1.44
22	A	1601	SRY	CA1-NB1	3.10	1.45	1.34
22	A	1601	SRY	C21-C11	-2.91	1.47	1.53
22	A	1601	SRY	C23-N23	-2.87	1.42	1.47
22	A	1601	SRY	CD1-NE1	2.82	1.44	1.34
22	A	1601	SRY	C32-CG2	-2.42	1.48	1.52
22	A	1601	SRY	C21-C31	-2.27	1.48	1.53
22	A	1601	SRY	O51-C51	-2.25	1.37	1.43
22	A	1601	SRY	O32-C32	-2.21	1.40	1.44
22	A	1601	SRY	O43-C43	-2.11	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	C13-O13-C22	-6.04	105.98	116.26
22	A	1601	SRY	C61-C11-N11	-6.02	99.52	110.62
22	A	1601	SRY	C12-O42-C42	-5.83	99.07	108.48
22	A	1601	SRY	O41-C12-O42	-4.52	106.75	111.37
22	A	1601	SRY	CI3-N23-C23	-4.51	108.41	114.23
22	A	1601	SRY	C43-C33-C23	-4.20	104.28	110.40
22	A	1601	SRY	O13-C13-C23	3.93	114.44	108.07
22	A	1601	SRY	C12-O41-C41	-3.18	110.45	117.98
22	A	1601	SRY	C21-C31-N31	3.07	116.27	110.62
22	A	1601	SRY	O13-C13-O53	-2.28	104.69	110.69
22	A	1601	SRY	C61-C51-C41	2.02	114.27	109.68

There are no chirality outliers.

All (5) torsion outliers are listed below:

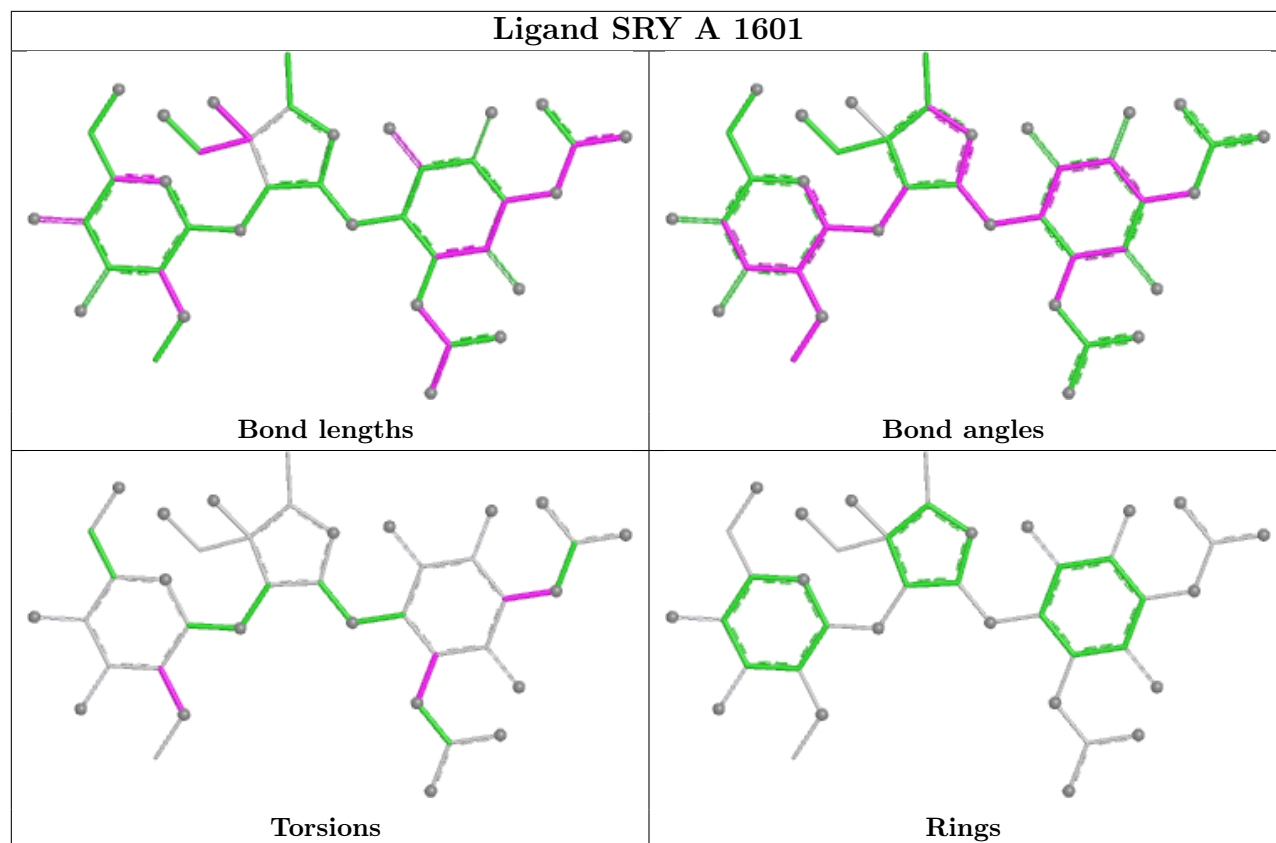
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C41-C31-N31-CD1
22	A	1601	SRY	C21-C31-N31-CD1
22	A	1601	SRY	C21-C11-N11-CA1
22	A	1601	SRY	C61-C11-N11-CA1

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	7	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(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.02	31 (2%) 63 44	106, 179, 327, 407	0
2	B	234/256 (91%)	-0.15	8 (3%) 48 34	145, 211, 332, 358	0
3	C	206/239 (86%)	0.09	8 (3%) 43 31	181, 265, 316, 365	0
4	D	208/209 (99%)	0.21	11 (5%) 32 25	124, 193, 249, 283	0
5	E	150/162 (92%)	-0.31	0 100 100	104, 150, 199, 232	0
6	F	101/101 (100%)	-0.26	0 100 100	155, 212, 246, 277	0
7	G	155/156 (99%)	-0.02	2 (1%) 75 53	172, 228, 288, 335	0
8	H	138/138 (100%)	-0.26	1 (0%) 84 66	94, 135, 187, 218	0
9	I	127/128 (99%)	0.09	5 (3%) 43 31	201, 250, 303, 322	0
10	J	98/105 (93%)	0.44	8 (8%) 17 17	220, 277, 355, 391	0
11	K	116/129 (89%)	-0.17	2 (1%) 69 48	130, 171, 224, 258	0
12	L	123/135 (91%)	0.18	4 (3%) 49 34	107, 175, 218, 248	0
13	M	118/126 (93%)	0.26	10 (8%) 16 17	162, 214, 254, 309	0
14	N	60/61 (98%)	0.15	2 (3%) 49 34	187, 249, 314, 329	0
15	O	87/89 (97%)	0.08	1 (1%) 78 57	113, 171, 213, 232	0
16	P	83/88 (94%)	0.04	4 (4%) 35 27	130, 180, 220, 274	0
17	Q	99/105 (94%)	0.07	3 (3%) 52 36	116, 150, 201, 232	0
18	R	70/88 (79%)	-0.10	0 100 100	116, 183, 244, 259	0
19	S	80/93 (86%)	0.52	8 (10%) 12 15	234, 284, 341, 352	0
20	T	99/106 (93%)	-0.08	2 (2%) 65 45	124, 172, 240, 267	0
21	U	24/27 (88%)	0.52	1 (4%) 40 30	198, 248, 286, 302	0
All	All	3874/4063 (95%)	0.01	111 (2%) 53 37	94, 194, 306, 407	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	4	TYR	6.0
7	G	154	TYR	5.5
20	T	106	ALA	5.4
1	A	532	A	5.1
1	A	984	C	5.0
3	C	2	GLY	4.9
1	A	353	A	4.7
10	J	37	PRO	4.6
1	A	1361(A)	C	4.6
12	L	47	LYS	4.6
1	A	1129	C	4.3
13	M	8	GLU	4.3
4	D	6	GLY	4.2
1	A	81	U	4.1
2	B	208	ILE	4.1
21	U	25	LYS	4.0
13	M	94	ARG	3.9
1	A	760	G	3.9
1	A	1042	G	3.9
19	S	68	GLY	3.9
10	J	34	VAL	3.8
1	A	202	U	3.8
3	C	76	VAL	3.7
1	A	792	A	3.7
1	A	723	U	3.6
1	A	805	C	3.6
9	I	102	LEU	3.5
1	A	793	U	3.4
2	B	19	HIS	3.4
8	H	1	MET	3.3
1	A	985	C	3.3
4	D	5	ILE	3.2
19	S	2	PRO	3.2
12	L	32	PHE	3.2
2	B	14	GLY	3.2
13	M	102	ARG	3.1
2	B	239	VAL	3.1
19	S	32	LYS	3.1
4	D	31	CYS	3.1
4	D	209	ARG	3.0
13	M	6	GLY	3.0
9	I	99	LEU	3.0
4	D	54	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
10	J	100	THR	3.0
17	Q	32	TYR	2.9
16	P	59	TRP	2.9
4	D	7	PRO	2.9
10	J	38	ILE	2.8
2	B	238	LEU	2.8
2	B	169	LYS	2.8
9	I	110	GLU	2.8
4	D	9	CYS	2.8
3	C	100	ALA	2.8
1	A	1482	G	2.8
10	J	54	PHE	2.8
10	J	24	VAL	2.7
7	G	74	GLU	2.7
3	C	66	VAL	2.7
14	N	4	LYS	2.7
20	T	56	MET	2.7
1	A	1362	C	2.7
1	A	1178	G	2.7
13	M	96	LEU	2.7
4	D	42	GLN	2.7
14	N	55	GLY	2.6
9	I	96	LEU	2.5
11	K	102	GLY	2.5
19	S	79	THR	2.5
19	S	37	ARG	2.5
1	A	1124	G	2.5
1	A	82	U	2.5
3	C	178	LEU	2.5
12	L	48	PRO	2.4
16	P	25	ARG	2.4
19	S	78	ARG	2.4
15	O	54	ARG	2.4
13	M	22	ILE	2.4
1	A	190(B)	C	2.4
1	A	1200	C	2.4
1	A	60	A	2.4
17	Q	19	VAL	2.4
3	C	201	TYR	2.4
13	M	91	ARG	2.4
13	M	113	PRO	2.3
19	S	35	SER	2.3

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Mol	Chain	Res	Type	RSRZ
17	Q	45	HIS	2.3
1	A	1136	U	2.3
11	K	118	GLY	2.3
1	A	1226	C	2.3
16	P	23	ASP	2.3
12	L	94	PRO	2.2
1	A	1442	G	2.2
16	P	68	ASP	2.2
1	A	804	U	2.2
19	S	34	TRP	2.1
1	A	159	G	2.1
3	C	175	LEU	2.1
9	I	106	ALA	2.1
3	C	53	ALA	2.1
13	M	117	VAL	2.1
1	A	1094	G	2.1
4	D	51	PRO	2.1
10	J	55	LYS	2.1
1	A	1290	G	2.1
2	B	131	PRO	2.1
4	D	53	ASP	2.1
2	B	156	LYS	2.1
10	J	72	VAL	2.1
1	A	452	A	2.0
1	A	578	C	2.0
13	M	7	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
1	PSU	A	1541	20/21	0.73	0.18	297,305,321,325	0
1	PSU	A	1540	20/21	0.75	0.21	235,263,334,335	0
1	MA6	A	1518	24/25	0.92	0.10	151,187,221,227	0
1	M2G	A	966	25/26	0.93	0.11	177,182,207,211	0
1	PSU	A	516	20/21	0.93	0.10	163,188,214,220	0
1	7MG	A	527	24/25	0.94	0.13	125,146,165,180	0
1	MA6	A	1519	24/25	0.96	0.13	144,181,202,206	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	1407	21/22	0.96	0.09	171,191,202,207	0
1	5MC	A	1400	21/22	0.96	0.11	142,169,178,182	0
12	0TD	L	92	10/11	0.96	0.10	121,166,173,350	0
1	UR3	A	1498	21/22	0.97	0.09	160,183,204,223	0
1	4OC	A	1402	22/23	0.97	0.11	150,156,180,192	0
1	2MG	A	1207	24/25	0.97	0.15	231,289,310,316	0
1	5MC	A	1404	21/22	0.98	0.08	166,182,196,204	0
1	5MC	A	967	21/22	0.98	0.07	182,192,200,205	0

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($\text{\AA}^2$)	Q<0.9
23	MG	A	1681	1/1	0.31	0.20	243,243,243,243	0
23	MG	A	1831	1/1	0.38	0.18	484,484,484,484	0
23	MG	K	201	1/1	0.40	0.23	181,181,181,181	0
23	MG	S	102	1/1	0.48	0.33	156,156,156,156	0
23	MG	N	103	1/1	0.57	0.25	156,156,156,156	0
23	MG	E	201	1/1	0.57	0.14	435,435,435,435	0
23	MG	B	301	1/1	0.60	0.27	181,181,181,181	0
23	MG	A	1659	1/1	0.65	0.29	142,142,142,142	0
23	MG	A	1757	1/1	0.65	0.99	143,143,143,143	0
23	MG	A	1763	1/1	0.69	0.36	181,181,181,181	0
23	MG	A	1712	1/1	0.70	0.54	138,138,138,138	0
23	MG	A	1778	1/1	0.70	0.34	156,156,156,156	0
23	MG	P	101	1/1	0.71	0.42	122,122,122,122	0
23	MG	A	1788	1/1	0.72	0.27	156,156,156,156	0
23	MG	A	1696	1/1	0.72	0.12	245,245,245,245	0
23	MG	A	1773	1/1	0.73	0.31	162,162,162,162	0
23	MG	A	1710	1/1	0.73	0.22	161,161,161,161	0
23	MG	A	1817	1/1	0.74	0.10	197,197,197,197	0
23	MG	A	1787	1/1	0.79	0.38	102,102,102,102	0
23	MG	A	1695	1/1	0.79	0.65	245,245,245,245	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1693	1/1	0.79	0.37	179,179,179,179	0
23	MG	A	1730	1/1	0.79	0.70	134,134,134,134	0
23	MG	A	1751	1/1	0.79	0.43	133,133,133,133	0
23	MG	H	201	1/1	0.80	0.21	131,131,131,131	0
23	MG	A	1623	1/1	0.81	0.31	170,170,170,170	0
23	MG	A	1736	1/1	0.81	0.53	125,125,125,125	0
23	MG	A	1765	1/1	0.81	0.16	372,372,372,372	0
23	MG	A	1668	1/1	0.81	0.51	173,173,173,173	0
23	MG	A	1714	1/1	0.82	0.20	143,143,143,143	0
23	MG	A	1728	1/1	0.82	0.16	150,150,150,150	0
23	MG	A	1758	1/1	0.82	0.56	128,128,128,128	0
23	MG	A	1784	1/1	0.82	0.32	145,145,145,145	0
23	MG	A	1744	1/1	0.82	0.17	176,176,176,176	0
23	MG	A	1718	1/1	0.83	0.61	144,144,144,144	0
23	MG	A	1692	1/1	0.83	0.64	142,142,142,142	0
23	MG	M	202	1/1	0.83	0.32	148,148,148,148	0
23	MG	A	1782	1/1	0.83	0.35	131,131,131,131	0
23	MG	A	1770	1/1	0.83	0.40	141,141,141,141	0
23	MG	A	1771	1/1	0.83	0.41	138,138,138,138	0
23	MG	A	1755	1/1	0.84	0.56	190,190,190,190	0
23	MG	A	1785	1/1	0.84	0.51	142,142,142,142	0
23	MG	A	1626	1/1	0.85	0.58	118,118,118,118	0
23	MG	A	1738	1/1	0.85	0.43	123,123,123,123	0
23	MG	A	1739	1/1	0.85	0.27	162,162,162,162	0
23	MG	A	1720	1/1	0.85	0.32	139,139,139,139	0
23	MG	A	1727	1/1	0.85	0.28	138,138,138,138	0
23	MG	A	1802	1/1	0.85	0.14	457,457,457,457	0
23	MG	A	1704	1/1	0.85	0.20	118,118,118,118	0
23	MG	A	1706	1/1	0.85	0.41	163,163,163,163	0
23	MG	A	1746	1/1	0.86	0.22	282,282,282,282	0
23	MG	A	1636	1/1	0.86	0.29	186,186,186,186	0
23	MG	A	1822	1/1	0.86	0.25	374,374,374,374	0
23	MG	A	1783	1/1	0.87	0.32	133,133,133,133	0
23	MG	M	201	1/1	0.87	0.44	163,163,163,163	0
23	MG	A	1750	1/1	0.87	0.19	125,125,125,125	0
23	MG	A	1777	1/1	0.88	0.28	107,107,107,107	0
23	MG	A	1672	1/1	0.88	0.25	102,102,102,102	0
23	MG	A	1747	1/1	0.88	0.15	296,296,296,296	0
23	MG	A	1679	1/1	0.88	0.63	133,133,133,133	0
23	MG	A	1772	1/1	0.88	0.14	121,121,121,121	0
23	MG	A	1643	1/1	0.88	0.26	135,135,135,135	0
23	MG	A	1774	1/1	0.88	0.39	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1661	1/1	0.89	0.45	124,124,124,124	0
23	MG	A	1813	1/1	0.89	0.55	146,146,146,146	0
23	MG	A	1781	1/1	0.89	0.20	145,145,145,145	0
23	MG	A	1819	1/1	0.89	0.21	483,483,483,483	0
23	MG	A	1759	1/1	0.89	0.14	161,161,161,161	0
23	MG	A	1768	1/1	0.89	0.06	550,550,550,550	0
23	MG	A	1795	1/1	0.89	0.39	457,457,457,457	0
23	MG	D	302	1/1	0.89	0.15	186,186,186,186	0
23	MG	A	1667	1/1	0.90	0.47	143,143,143,143	0
23	MG	A	1637	1/1	0.90	0.41	143,143,143,143	0
23	MG	A	1618	1/1	0.90	0.22	152,152,152,152	0
23	MG	I	201	1/1	0.90	0.17	204,204,204,204	0
23	MG	A	1794	1/1	0.90	0.23	206,206,206,206	0
23	MG	A	1721	1/1	0.91	0.20	135,135,135,135	0
23	MG	A	1737	1/1	0.91	0.25	140,140,140,140	0
23	MG	A	1725	1/1	0.91	0.22	153,153,153,153	0
23	MG	A	1682	1/1	0.91	0.08	365,365,365,365	0
23	MG	A	1769	1/1	0.91	0.15	209,209,209,209	0
23	MG	A	1779	1/1	0.91	0.49	146,146,146,146	0
23	MG	A	1656	1/1	0.91	0.27	173,173,173,173	0
23	MG	A	1677	1/1	0.91	0.24	191,191,191,191	0
23	MG	A	1702	1/1	0.92	0.08	126,126,126,126	0
23	MG	A	1638	1/1	0.92	0.18	170,170,170,170	0
23	MG	A	1754	1/1	0.92	0.07	177,177,177,177	0
23	MG	A	1658	1/1	0.92	0.10	146,146,146,146	0
23	MG	A	1651	1/1	0.92	0.48	140,140,140,140	0
23	MG	A	1697	1/1	0.92	0.29	135,135,135,135	0
23	MG	A	1820	1/1	0.92	0.12	265,265,265,265	0
23	MG	A	1701	1/1	0.92	0.22	129,129,129,129	0
23	MG	A	1760	1/1	0.92	0.06	130,130,130,130	0
23	MG	A	1715	1/1	0.92	0.34	151,151,151,151	0
23	MG	A	1694	1/1	0.93	0.21	180,180,180,180	0
23	MG	A	1776	1/1	0.93	0.26	111,111,111,111	0
23	MG	A	1731	1/1	0.93	0.42	148,148,148,148	0
23	MG	A	1700	1/1	0.93	0.12	134,134,134,134	0
23	MG	A	1633	1/1	0.93	0.23	125,125,125,125	0
23	MG	A	1818	1/1	0.93	0.44	483,483,483,483	0
23	MG	A	1676	1/1	0.93	0.31	133,133,133,133	0
23	MG	A	1825	1/1	0.94	0.12	377,377,377,377	0
23	MG	A	1827	1/1	0.94	0.12	391,391,391,391	0
23	MG	A	1829	1/1	0.94	0.09	323,323,323,323	0
23	MG	A	1621	1/1	0.94	0.16	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1707	1/1	0.94	0.56	120,120,120,120	0
23	MG	A	1699	1/1	0.94	0.10	135,135,135,135	0
23	MG	A	1654	1/1	0.94	0.31	201,201,201,201	0
23	MG	A	1713	1/1	0.94	0.10	133,133,133,133	0
23	MG	A	1811	1/1	0.94	0.16	346,346,346,346	0
23	MG	A	1660	1/1	0.94	0.06	194,194,194,194	0
23	MG	A	1648	1/1	0.94	0.14	230,230,230,230	0
23	MG	A	1732	1/1	0.94	0.52	131,131,131,131	0
23	MG	A	1752	1/1	0.94	0.33	147,147,147,147	0
23	MG	A	1735	1/1	0.94	0.22	155,155,155,155	0
23	MG	A	1683	1/1	0.94	0.10	422,422,422,422	0
23	MG	T	201	1/1	0.94	0.09	142,142,142,142	0
23	MG	A	1645	1/1	0.95	0.09	146,146,146,146	0
23	MG	A	1652	1/1	0.95	0.08	141,141,141,141	0
23	MG	A	1809	1/1	0.95	0.23	281,281,281,281	0
23	MG	A	1734	1/1	0.95	0.29	163,163,163,163	0
23	MG	A	1723	1/1	0.95	0.25	109,109,109,109	0
23	MG	A	1724	1/1	0.95	0.35	176,176,176,176	0
23	MG	A	1670	1/1	0.95	0.28	173,173,173,173	0
23	MG	A	1647	1/1	0.95	0.20	180,180,180,180	0
23	MG	A	1756	1/1	0.95	0.10	213,213,213,213	0
23	MG	A	1673	1/1	0.95	0.11	118,118,118,118	0
23	MG	A	1741	1/1	0.95	0.16	145,145,145,145	0
23	MG	A	1789	1/1	0.95	0.11	152,152,152,152	0
22	SRY	A	1601	40/40	0.95	0.09	123,154,201,206	0
23	MG	A	1733	1/1	0.96	0.07	126,126,126,126	0
23	MG	A	1749	1/1	0.96	0.34	126,126,126,126	0
23	MG	A	1641	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1786	1/1	0.96	0.81	145,145,145,145	0
23	MG	A	1616	1/1	0.96	0.22	107,107,107,107	0
23	MG	A	1619	1/1	0.96	0.19	253,253,253,253	0
23	MG	A	1686	1/1	0.96	0.11	150,150,150,150	0
23	MG	A	1791	1/1	0.96	0.05	144,144,144,144	0
23	MG	A	1691	1/1	0.96	0.10	187,187,187,187	0
23	MG	A	1663	1/1	0.96	0.15	138,138,138,138	0
23	MG	A	1617	1/1	0.96	0.08	129,129,129,129	0
23	MG	A	1803	1/1	0.96	0.14	342,342,342,342	0
23	MG	A	1807	1/1	0.96	0.15	427,427,427,427	0
23	MG	A	1742	1/1	0.96	0.05	134,134,134,134	0
23	MG	A	1703	1/1	0.96	0.11	180,180,180,180	0
23	MG	A	1745	1/1	0.96	0.46	235,235,235,235	0
23	MG	A	1816	1/1	0.96	0.04	262,262,262,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1639	1/1	0.96	0.23	126,126,126,126	0
23	MG	A	1764	1/1	0.96	0.14	308,308,308,308	0
23	MG	A	1709	1/1	0.97	0.14	141,141,141,141	0
23	MG	A	1814	1/1	0.97	0.19	128,128,128,128	0
23	MG	A	1622	1/1	0.97	0.06	138,138,138,138	0
23	MG	A	1780	1/1	0.97	0.11	111,111,111,111	0
23	MG	A	1604	1/1	0.97	0.19	133,133,133,133	0
23	MG	A	1624	1/1	0.97	0.16	210,210,210,210	0
23	MG	A	1657	1/1	0.97	0.23	177,177,177,177	0
23	MG	A	1675	1/1	0.97	0.18	121,121,121,121	0
23	MG	A	1716	1/1	0.97	0.10	121,121,121,121	0
23	MG	A	1608	1/1	0.97	0.15	118,118,118,118	0
23	MG	A	1740	1/1	0.97	0.25	123,123,123,123	0
23	MG	A	1628	1/1	0.97	0.28	191,191,191,191	0
23	MG	A	1632	1/1	0.97	0.07	91,91,91,91	0
23	MG	A	1790	1/1	0.97	0.16	148,148,148,148	0
23	MG	A	1610	1/1	0.97	0.24	193,193,193,193	0
23	MG	A	1793	1/1	0.97	0.05	302,302,302,302	0
23	MG	H	202	1/1	0.97	0.04	137,137,137,137	0
23	MG	A	1635	1/1	0.97	0.13	214,214,214,214	0
23	MG	J	201	1/1	0.97	0.14	138,138,138,138	0
23	MG	A	1665	1/1	0.97	0.12	247,247,247,247	0
23	MG	A	1800	1/1	0.97	0.35	400,400,400,400	0
23	MG	A	1726	1/1	0.97	0.34	130,130,130,130	0
23	MG	N	102	1/1	0.97	0.16	214,214,214,214	0
23	MG	A	1684	1/1	0.97	0.14	124,124,124,124	0
23	MG	A	1705	1/1	0.97	0.25	153,153,153,153	0
23	MG	A	1666	1/1	0.97	0.40	187,187,187,187	0
23	MG	A	1603	1/1	0.97	0.10	128,128,128,128	0
23	MG	T	202	1/1	0.97	0.13	450,450,450,450	0
23	MG	A	1662	1/1	0.98	0.13	162,162,162,162	0
23	MG	A	1808	1/1	0.98	0.15	444,444,444,444	0
23	MG	A	1650	1/1	0.98	0.13	155,155,155,155	0
23	MG	A	1664	1/1	0.98	0.22	226,226,226,226	0
23	MG	A	1812	1/1	0.98	0.06	226,226,226,226	0
23	MG	A	1775	1/1	0.98	0.09	123,123,123,123	0
23	MG	A	1615	1/1	0.98	0.08	129,129,129,129	0
23	MG	A	1815	1/1	0.98	0.15	190,190,190,190	0
23	MG	A	1685	1/1	0.98	0.09	263,263,263,263	0
23	MG	A	1607	1/1	0.98	0.10	161,161,161,161	0
23	MG	A	1708	1/1	0.98	0.13	119,119,119,119	0
23	MG	A	1753	1/1	0.98	0.12	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1653	1/1	0.98	0.11	185,185,185,185	0
23	MG	A	1821	1/1	0.98	0.09	236,236,236,236	0
23	MG	A	1605	1/1	0.98	0.10	148,148,148,148	0
23	MG	A	1823	1/1	0.98	0.08	194,194,194,194	0
23	MG	A	1711	1/1	0.98	0.14	187,187,187,187	0
23	MG	A	1669	1/1	0.98	0.27	138,138,138,138	0
23	MG	A	1655	1/1	0.98	0.30	181,181,181,181	0
23	MG	A	1830	1/1	0.98	0.12	494,494,494,494	0
23	MG	A	1640	1/1	0.98	0.18	129,129,129,129	0
23	MG	A	1606	1/1	0.98	0.43	126,126,126,126	0
23	MG	A	1761	1/1	0.98	0.21	158,158,158,158	0
23	MG	A	1762	1/1	0.98	0.10	109,109,109,109	0
23	MG	A	1611	1/1	0.98	0.07	223,223,223,223	0
23	MG	A	1717	1/1	0.98	0.09	110,110,110,110	0
23	MG	A	1620	1/1	0.98	0.44	197,197,197,197	0
23	MG	A	1766	1/1	0.98	0.04	220,220,220,220	0
23	MG	A	1613	1/1	0.98	0.11	126,126,126,126	0
23	MG	A	1796	1/1	0.98	0.24	372,372,372,372	0
23	MG	A	1797	1/1	0.98	0.16	429,429,429,429	0
23	MG	A	1614	1/1	0.98	0.08	94,94,94,94	0
23	MG	A	1801	1/1	0.98	0.29	423,423,423,423	0
23	MG	A	1743	1/1	0.98	0.16	183,183,183,183	0
23	MG	S	101	1/1	0.98	0.11	138,138,138,138	0
23	MG	A	1722	1/1	0.98	0.09	116,116,116,116	0
23	MG	A	1805	1/1	0.98	0.25	426,426,426,426	0
23	MG	A	1806	1/1	0.98	0.19	392,392,392,392	0
23	MG	A	1644	1/1	0.99	0.12	175,175,175,175	0
23	MG	A	1671	1/1	0.99	0.16	208,208,208,208	0
23	MG	A	1634	1/1	0.99	0.02	112,112,112,112	0
23	MG	A	1646	1/1	0.99	0.05	131,131,131,131	0
23	MG	A	1674	1/1	0.99	0.14	112,112,112,112	0
23	MG	A	1602	1/1	0.99	0.20	180,180,180,180	0
23	MG	A	1792	1/1	0.99	0.08	127,127,127,127	0
23	MG	A	1767	1/1	0.99	0.08	327,327,327,327	0
23	MG	A	1824	1/1	0.99	0.09	366,366,366,366	0
23	MG	A	1627	1/1	0.99	0.12	160,160,160,160	0
23	MG	A	1826	1/1	0.99	0.16	458,458,458,458	0
23	MG	A	1698	1/1	0.99	0.11	131,131,131,131	0
23	MG	A	1828	1/1	0.99	0.19	356,356,356,356	0
23	MG	A	1649	1/1	0.99	0.04	192,192,192,192	0
23	MG	A	1678	1/1	0.99	0.07	136,136,136,136	0
23	MG	A	1798	1/1	0.99	0.11	454,454,454,454	0

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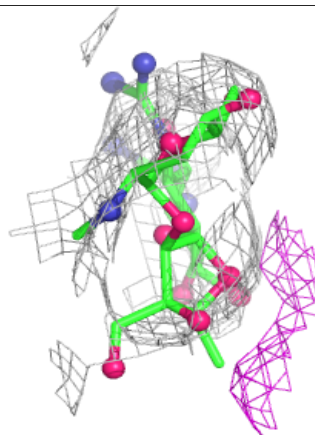
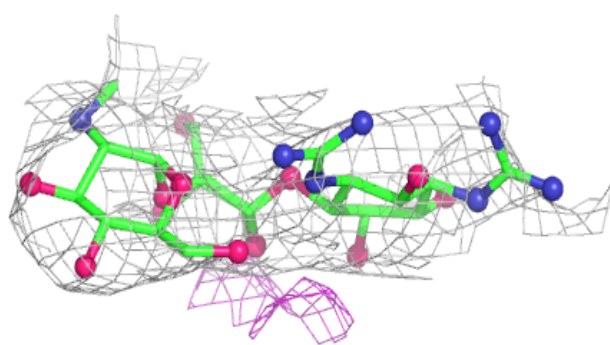
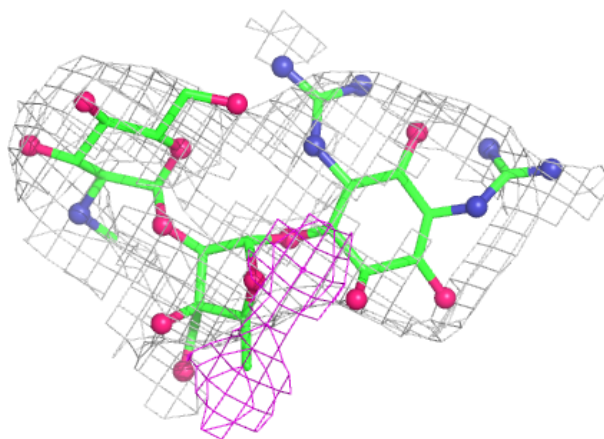
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	MG	A	1799	1/1	0.99	0.12	242,242,242,242	0
23	MG	A	1609	1/1	0.99	0.13	155,155,155,155	0
23	MG	A	1748	1/1	0.99	0.18	204,204,204,204	0
23	MG	A	1680	1/1	0.99	0.11	306,306,306,306	0
23	MG	A	1629	1/1	0.99	0.06	125,125,125,125	0
23	MG	A	1804	1/1	0.99	0.14	420,420,420,420	0
23	MG	A	1630	1/1	0.99	0.11	92,92,92,92	0
23	MG	A	1631	1/1	0.99	0.36	127,127,127,127	0
23	MG	A	1729	1/1	0.99	0.36	123,123,123,123	0
23	MG	A	1612	1/1	0.99	0.07	123,123,123,123	0
23	MG	A	1642	1/1	0.99	0.10	107,107,107,107	0
23	MG	A	1810	1/1	0.99	0.04	117,117,117,117	0
23	MG	A	1625	1/1	0.99	0.12	134,134,134,134	0
23	MG	A	1687	1/1	0.99	0.05	96,96,96,96	0
23	MG	A	1688	1/1	0.99	0.20	301,301,301,301	0
23	MG	A	1689	1/1	0.99	0.12	151,151,151,151	0
23	MG	A	1690	1/1	0.99	0.10	216,216,216,216	0
24	ZN	D	301	1/1	0.99	0.20	159,159,159,159	0
24	ZN	N	101	1/1	0.99	0.08	336,336,336,336	0
23	MG	A	1719	1/1	1.00	0.17	105,105,105,105	0

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

Electron density around SRY A 1601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.