



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 07:54 AM UTC

PDB ID : 4DR6 / pdb_00004dr6
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with codon, near-cognate transfer RNA anticodon stem-loop mismatched at the first codon position and streptomycin bound
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Joglekar, G.
Deposited on : 2012-02-16
Resolution : 3.30 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](#) ①) were used in the production of this report:

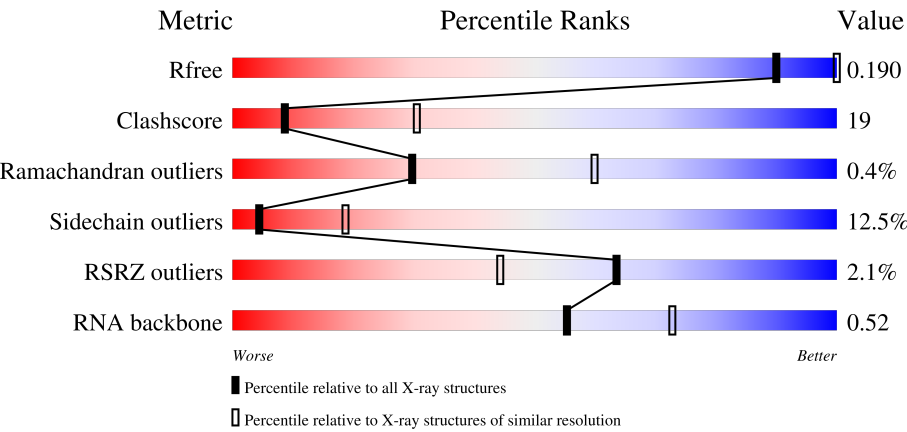
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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.



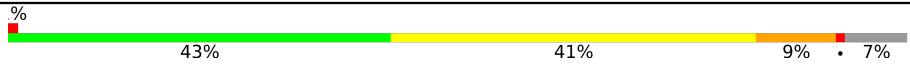
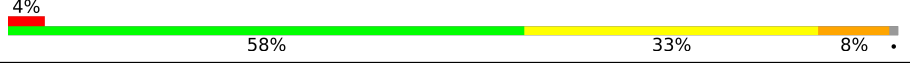
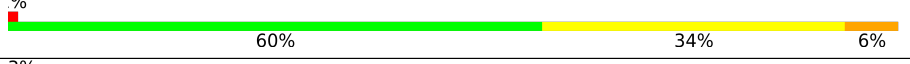
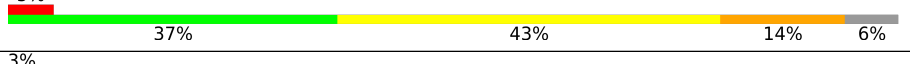
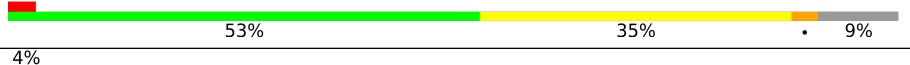
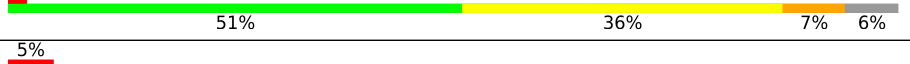
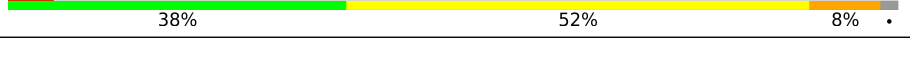
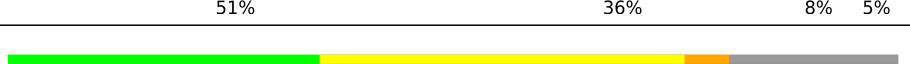
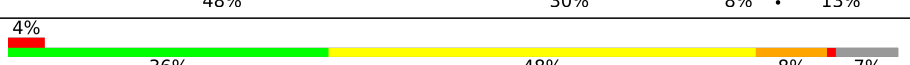
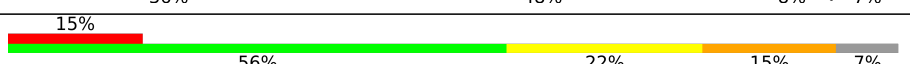
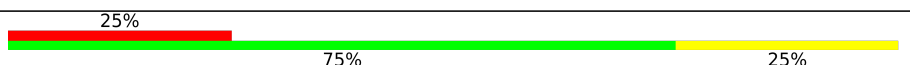
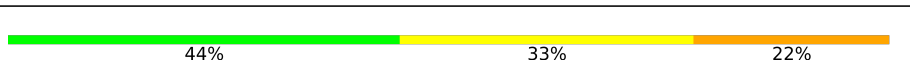
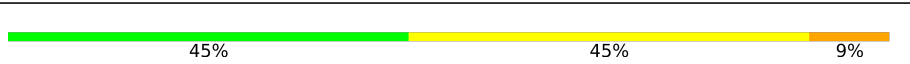
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	51%37%11%.
2	B	256	4% 45%38%9%8%
3	C	239	3% 41%36%9%13%
4	D	209	4% 54%39%6%.

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Mol	Chain	Length	Quality of chain
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	
22	V	4	
23	W	9	
24	a	11	
25	b	3	

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
26	MG	A	1630	-	-	-	X
26	MG	A	1728	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	MG	A	1758	-	-	-	X
26	MG	A	1774	-	-	-	X
26	MG	A	1926	-	-	-	X
26	MG	G	201[A]	-	-	-	X
26	MG	G	201[B]	-	-	-	X

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 53550 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	1514	Total	C	N	O	P	0	0	0
			32546	14496	6020	10517	1513			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1896	1211	337	343	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S 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 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S 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 30S ribosomal protein S7.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	117	Total	C	N	O	S	0	0	0
			873	543	166	161	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called 30S 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 30S 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 30S ribosomal protein S15.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	156	142	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 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	71	Total	C	N	O		0	0	0
			585	373	116	96				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called 5'-R(*UP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	4	Total	C	N	O	P	0	0	0
			77	36	8	30	3			

- Molecule 23 is a RNA chain called 5'-R(P*UP*UP*GP*AP*GP*GP*(PSU)P*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	9	Total	C	N	O	P	0	0	0
			197	87	36	65	9			

- Molecule 24 is a RNA chain called 5'-R(P*CP*UP*UP*GP*AP*GP*GP*(PSU)P*GP*GP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	a	11	Total	C	N	O	P	0	0	0
			237	105	41	80	11			

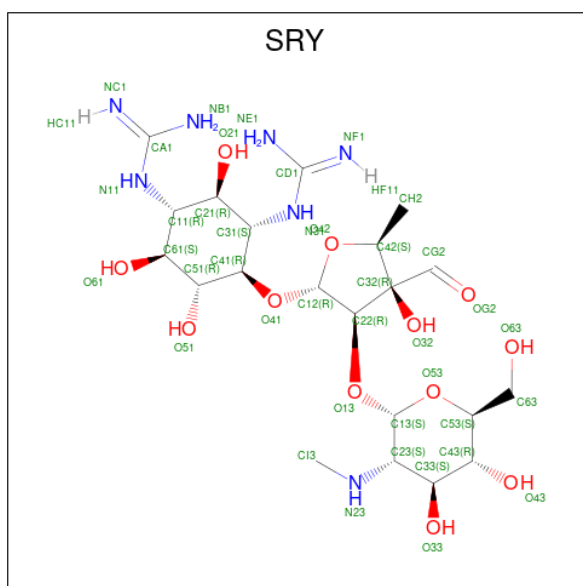
- Molecule 25 is a RNA chain called 5'-R(*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	b	2	Total	C	N	O	P	4	0	0
			40	18	4	16	2			

- Molecule 26 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	355	Total Mg 355 355	0	0
26	D	3	Total Mg 3 3	0	0
26	E	3	Total Mg 3 3	0	0
26	F	2	Total Mg 2 2	0	0
26	G	1	Total Mg 2 2	0	1
26	H	1	Total Mg 1 1	0	0
26	J	1	Total Mg 1 1	0	0
26	L	1	Total Mg 1 1	0	0
26	N	1	Total Mg 1 1	0	0
26	P	3	Total Mg 3 3	0	0
26	Q	1	Total Mg 1 1	0	0
26	S	3	Total Mg 3 3	0	0
26	T	1	Total Mg 1 1	0	0

- Molecule 27 is STREPTOMYCIN (CCD ID: SRY) (formula: $C_{21}H_{39}N_7O_{12}$).



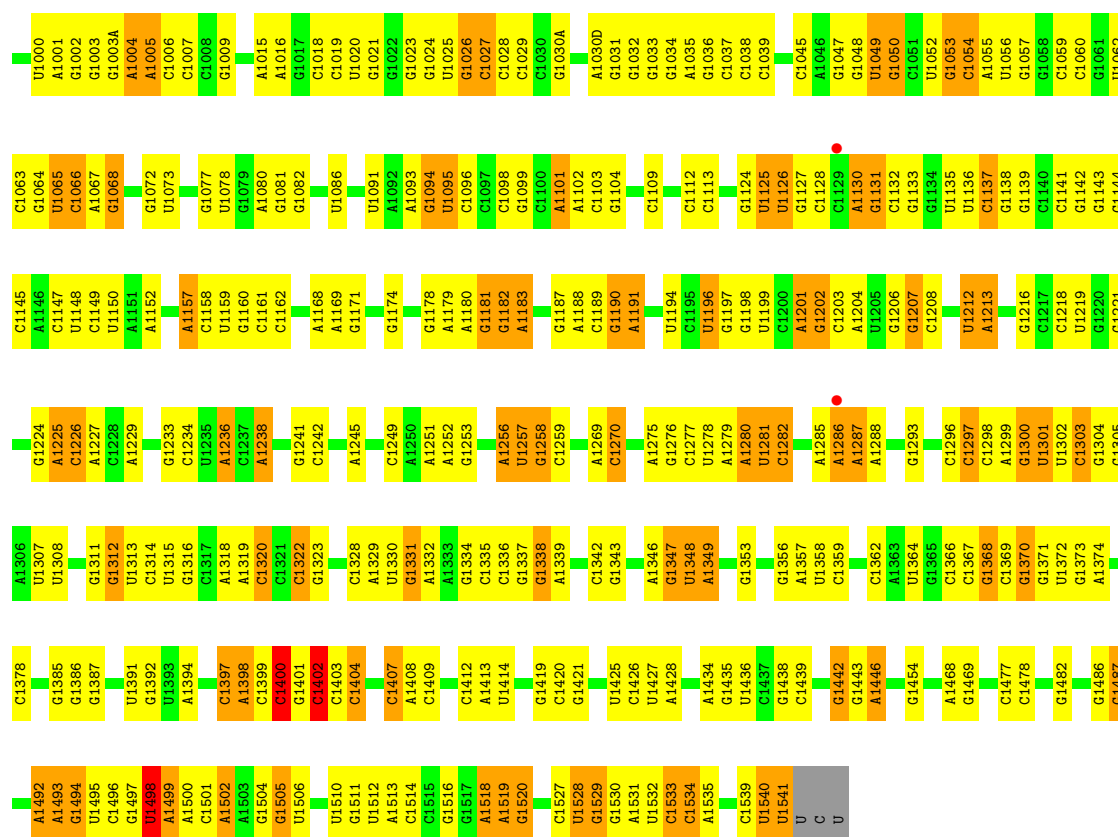
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
27	A	1	Total	C	N	O	0	0
			40	21	7	12		

- Molecule 28 is ZINC ION (CCD ID: ZN) (formula: Zn).

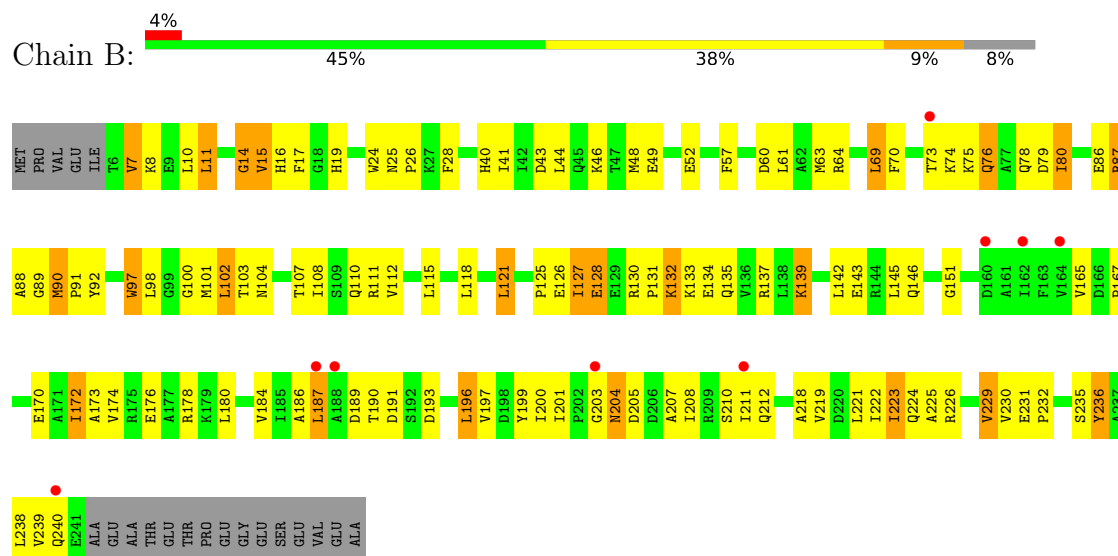
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	D	1	Total	Zn	0	0
			1	1		
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is water.

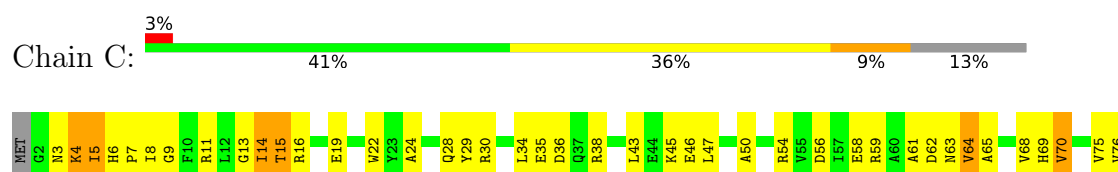
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	887	Total	O	0	0
			887	887		
29	C	1	Total	O	0	0
			1	1		
29	D	5	Total	O	0	0
			5	5		
29	E	5	Total	O	0	0
			5	5		
29	L	1	Total	O	0	0
			1	1		
29	N	1	Total	O	0	0
			1	1		
29	P	2	Total	O	0	0
			2	2		
29	S	2	Total	O	0	0
			2	2		
29	T	1	Total	O	0	0
			1	1		
29	U	2	Total	O	0	0
			2	2		

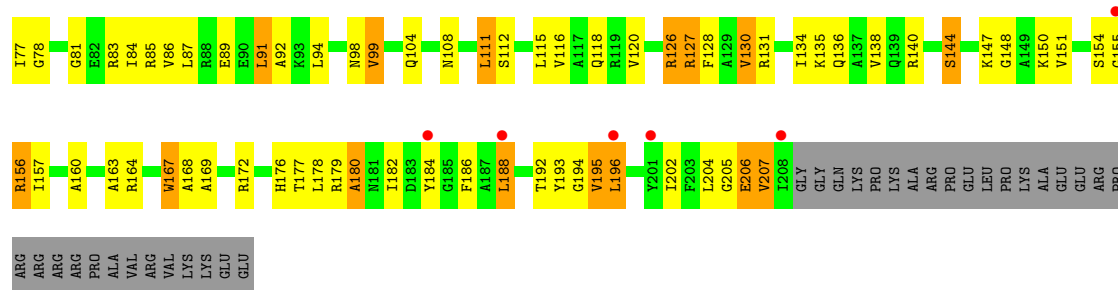


• Molecule 2: 30S ribosomal protein S2

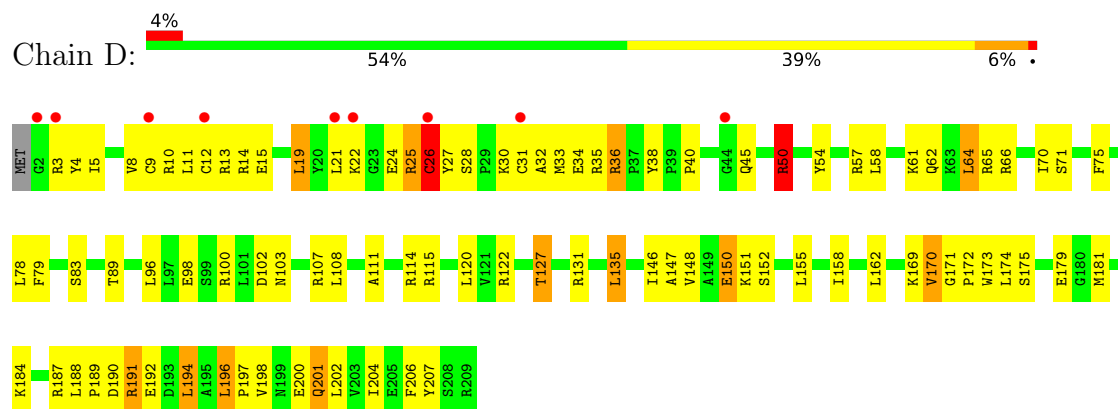


• Molecule 3: 30S ribosomal protein S3

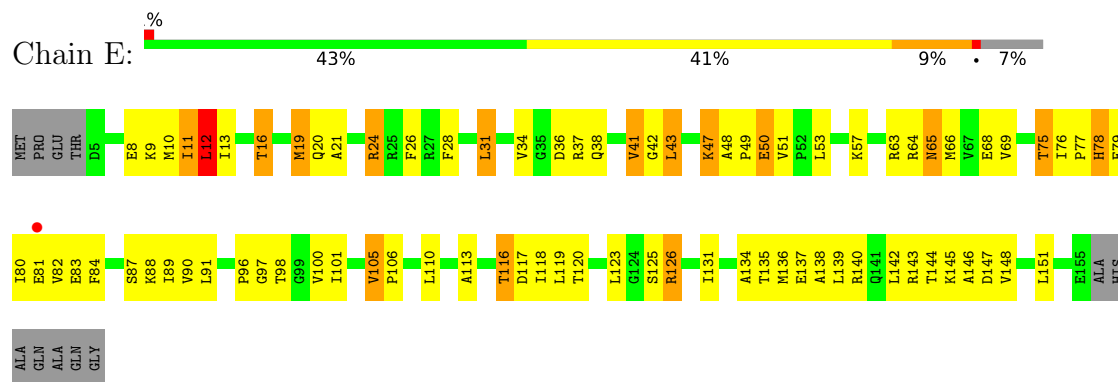




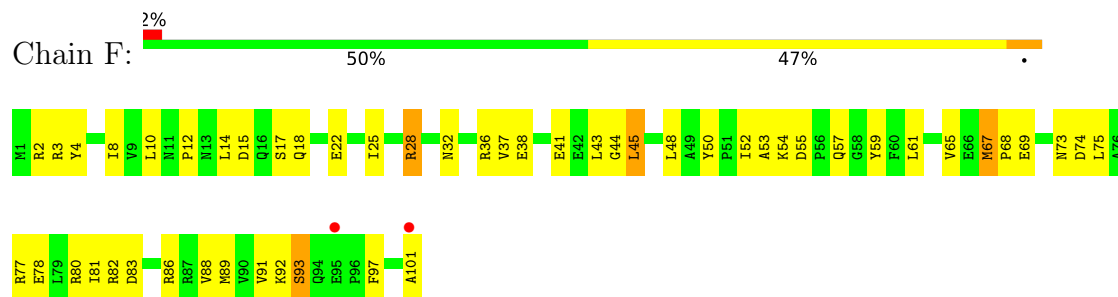
• Molecule 4: 30S ribosomal protein S4



• Molecule 5: 30S ribosomal protein S5

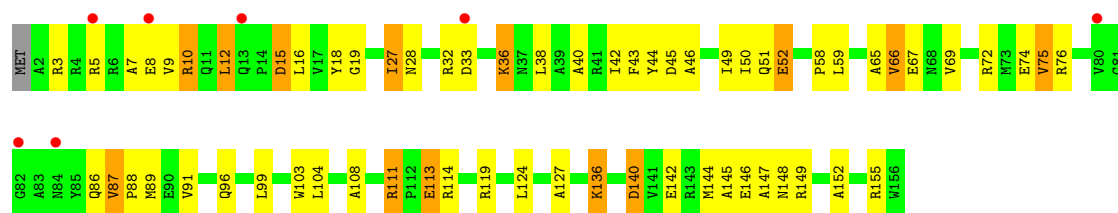


• Molecule 6: 30S ribosomal protein S6

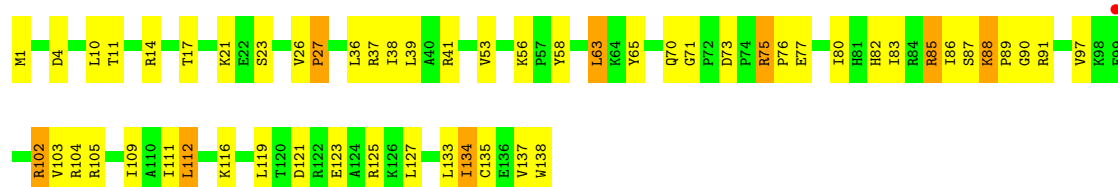


• Molecule 7: 30S ribosomal protein S7

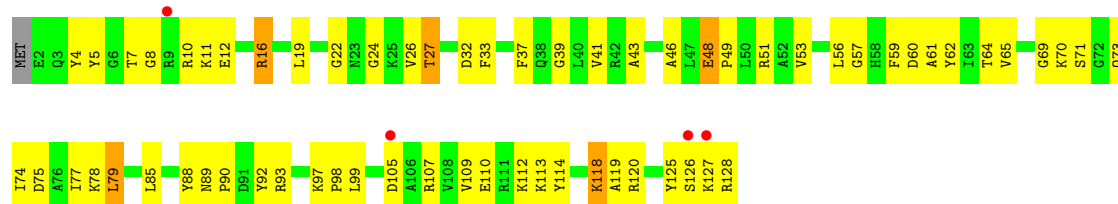




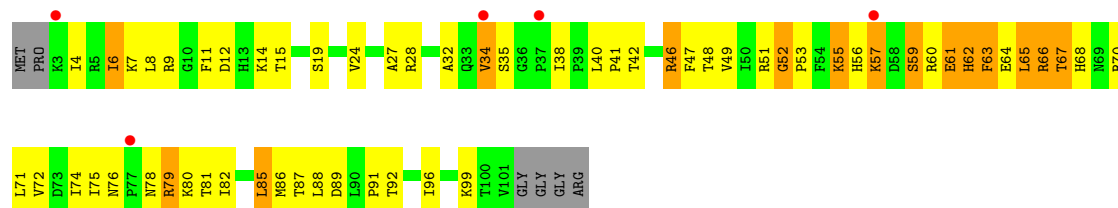
• Molecule 8: 30S ribosomal protein S8



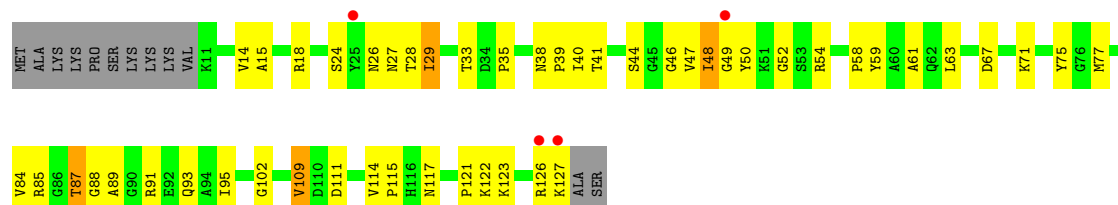
• Molecule 9: 30S ribosomal protein S9



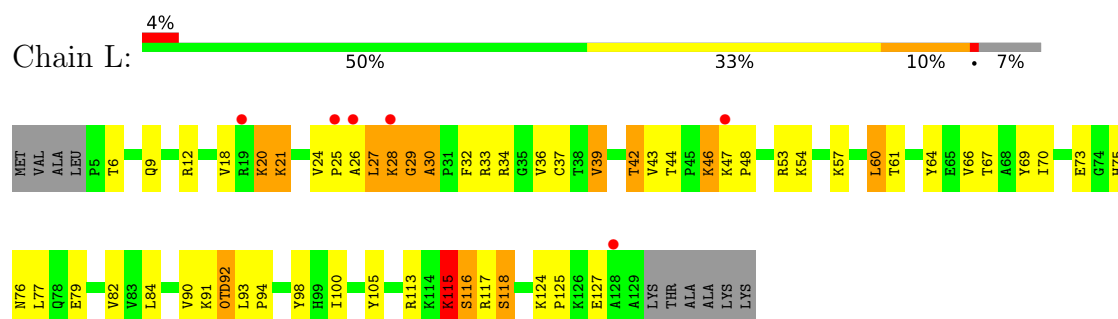
• Molecule 10: 30S ribosomal protein S10



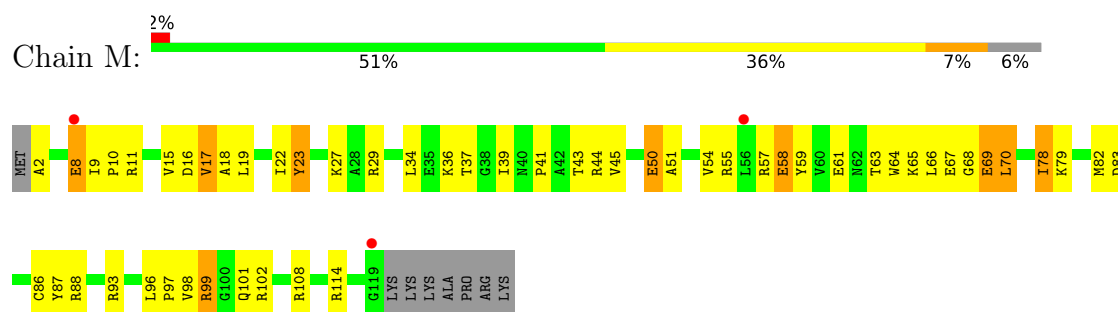
• Molecule 11: 30S ribosomal protein S11



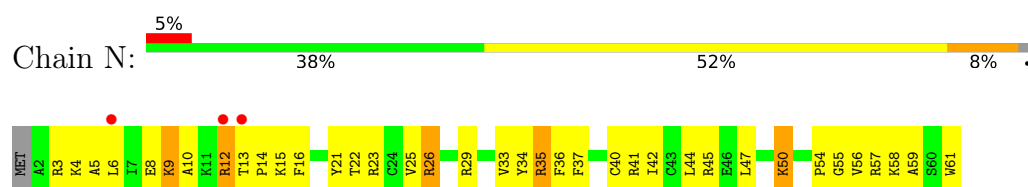
- Molecule 12: 30S ribosomal protein S12



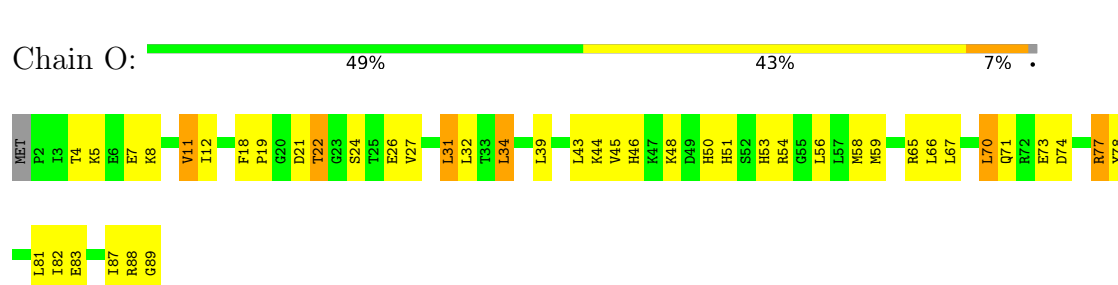
- Molecule 13: 30S ribosomal protein S13



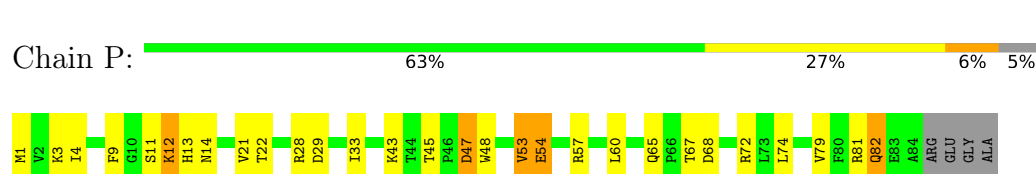
- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15

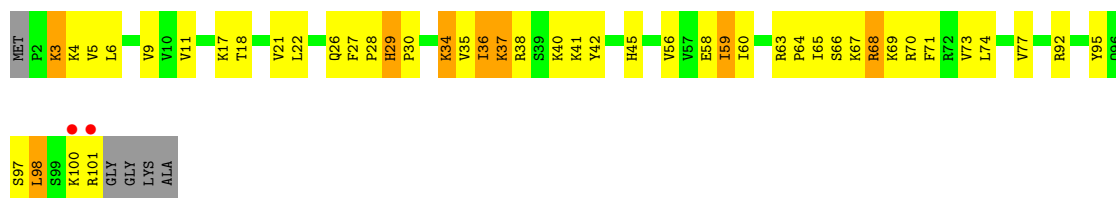


- Molecule 16: 30S ribosomal protein S16



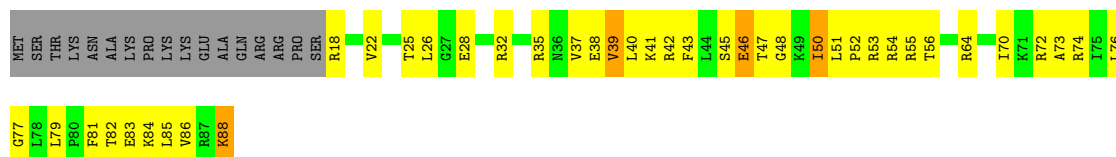
- Molecule 17: 30S ribosomal protein S17





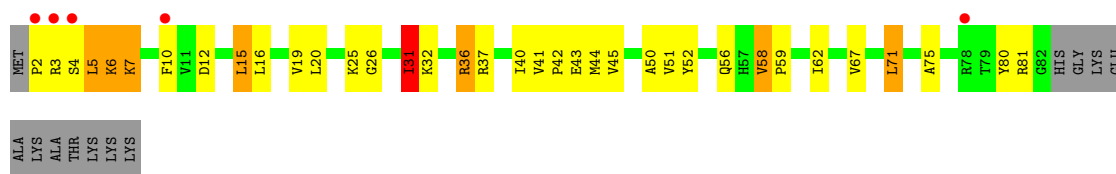
- Molecule 18: 30S ribosomal protein S18

Chain R: 35% 41% 5% 19%



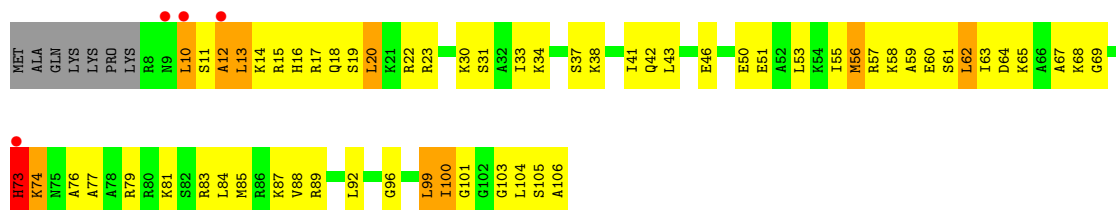
- Molecule 19: 30S ribosomal protein S19

Chain S: 5% 48% 30% 8% 13%



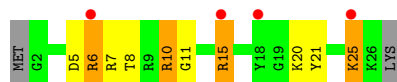
- Molecule 20: 30S ribosomal protein S20

Chain T: 4% 36% 48% 8% 7%



- Molecule 21: 30S ribosomal protein THX

Chain U: 15% 56% 22% 15% 7%



- Molecule 22: 5'-R(*UP*UP*UP*U)-3'

Chain V: 25% 75% 25%



- Molecule 23: 5'-R(P*UP*UP*GP*AP*GP*GP*(PSU)P*GP*G)-3'

Chain W: 44% 33% 22%



- Molecule 24: 5'-R(P*CP*UP*UP*GP*AP*GP*GP*(PSU)P*GP*GP*U)-3'

Chain a: 45% 45% 9%



- Molecule 25: 5'-R(*UP*UP*U)-3'

Chain b: 67% 67% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.60Å 402.60Å 174.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 3.30 49.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.48-3.30) 99.9 (49.48-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 3.33Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.153 , 0.192 0.153 , 0.190	Depositor DCC
R_{free} test set	10751 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	112.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	53550	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: M2G, 7MG, MA6, ZN, PSU, UR3, SRY, 4OC, 2MG, MG, 0TD, 5MC

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	0.33	1/36085 (0.0%)	0.42	0/56316
2	B	0.47	0/1931	0.92	6/2607 (0.2%)
3	C	0.45	0/1637	0.88	2/2207 (0.1%)
4	D	0.50	0/1733	0.95	10/2318 (0.4%)
5	E	0.66	0/1163	1.07	3/1566 (0.2%)
6	F	0.39	0/856	0.87	1/1154 (0.1%)
7	G	0.43	0/1276	0.93	4/1709 (0.2%)
8	H	0.66	0/1136	1.11	8/1527 (0.5%)
9	I	0.41	0/1029	0.95	2/1379 (0.1%)
10	J	0.44	0/806	0.99	5/1084 (0.5%)
11	K	0.55	0/888	1.03	3/1198 (0.3%)
12	L	0.60	0/978	1.13	7/1308 (0.5%)
13	M	0.44	0/947	0.84	0/1270
14	N	0.43	0/501	0.89	1/664 (0.2%)
15	O	0.52	0/745	0.85	0/992
16	P	0.63	0/717	0.98	1/965 (0.1%)
17	Q	0.62	0/847	1.11	2/1131 (0.2%)
18	R	0.49	0/590	0.93	1/782 (0.1%)
19	S	0.41	0/662	0.88	1/892 (0.1%)
20	T	0.59	0/765	1.00	2/1007 (0.2%)
21	U	0.46	0/213	0.80	0/279
22	V	0.21	0/84	0.36	0/128
23	W	0.18	0/198	0.26	0/308
24	a	0.23	0/242	0.35	0/376
25	b	0.22	0/43	0.32	0/64
All	All	0.40	1/56072 (0.0%)	0.64	59/83231 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
8	H	0	2
10	J	0	1
12	L	0	1
20	T	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.18	1.61	1.56

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-13.02	97.28	114.85
12	L	26	ALA	N-CA-C	-10.32	100.87	113.15
4	D	26	CYS	N-CA-C	-9.24	102.02	113.20
11	K	14	VAL	N-CA-C	8.62	118.64	110.53
17	Q	29	HIS	CA-C-N	8.41	128.06	119.56
17	Q	29	HIS	C-N-CA	8.41	128.06	119.56
2	B	15	VAL	N-CA-C	8.00	118.05	110.53
12	L	29	GLY	N-CA-C	-7.95	105.09	115.59
8	H	75	ARG	CA-C-N	7.73	128.19	119.92
8	H	75	ARG	C-N-CA	7.73	128.19	119.92
7	G	111	ARG	CA-C-N	7.61	127.24	119.56
7	G	111	ARG	C-N-CA	7.61	127.24	119.56
8	H	88	LYS	CA-C-N	-7.40	112.16	119.78
8	H	88	LYS	C-N-CA	-7.40	112.16	119.78
20	T	96	GLY	N-CA-C	7.29	121.03	111.70
2	B	87	ARG	N-CA-C	-7.22	101.24	110.19
9	I	22	GLY	N-CA-C	7.14	119.52	110.38
10	J	59	SER	N-CA-C	7.04	121.58	112.92
19	S	36	ARG	N-CA-C	-6.84	104.94	113.28
12	L	115	LYS	CA-C-N	-6.49	113.33	123.13
12	L	115	LYS	C-N-CA	-6.49	113.33	123.13
10	J	62	HIS	N-CA-C	6.17	118.98	110.35
14	N	12	ARG	N-CA-C	-6.13	105.56	113.16
3	C	194	GLY	N-CA-C	5.97	118.64	110.58
2	B	76	GLN	N-CA-C	-5.83	104.52	111.69
20	T	76	ALA	N-CA-C	-5.81	104.87	111.14
11	K	91	ARG	N-CA-C	-5.75	104.61	111.69
12	L	105	TYR	CB-CA-C	-5.72	110.00	116.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	87	VAL	CA-C-N	5.63	125.81	119.90
7	G	87	VAL	C-N-CA	5.63	125.81	119.90
5	E	69	VAL	CB-CA-C	-5.58	105.75	110.94
5	E	12	LEU	N-CA-C	5.57	116.92	108.07
11	K	102	GLY	N-CA-C	-5.54	108.10	114.69
4	D	188	LEU	CA-C-N	5.53	125.46	119.76
4	D	188	LEU	C-N-CA	5.53	125.46	119.76
8	H	134	ILE	CB-CA-C	-5.46	104.87	112.02
10	J	52	GLY	CA-C-N	5.43	125.26	119.28
10	J	52	GLY	C-N-CA	5.43	125.26	119.28
4	D	196	LEU	CA-C-N	5.35	126.53	119.84
4	D	196	LEU	C-N-CA	5.35	126.53	119.84
18	R	50	ILE	CB-CA-C	-5.32	104.24	111.15
8	H	73	ASP	CA-C-N	5.29	125.37	119.87
8	H	73	ASP	C-N-CA	5.29	125.37	119.87
10	J	55	LYS	CB-CA-C	-5.26	108.95	115.89
12	L	30	ALA	CA-C-N	5.25	125.06	119.28
12	L	30	ALA	C-N-CA	5.25	125.06	119.28
5	E	41	VAL	CB-CA-C	-5.23	102.60	110.55
4	D	190	ASP	N-CA-C	-5.20	103.82	110.53
8	H	80	ILE	CB-CA-C	-5.20	104.65	111.25
2	B	7	VAL	N-CA-C	5.19	120.14	109.34
2	B	90	MET	CA-C-N	5.14	125.58	120.14
2	B	90	MET	C-N-CA	5.14	125.58	120.14
6	F	67	MET	N-CA-C	5.06	114.12	108.25
4	D	50	ARG	CA-C-N	5.04	124.94	119.85
4	D	50	ARG	C-N-CA	5.04	124.94	119.85
4	D	36	ARG	CA-C-N	5.03	124.69	119.56
4	D	36	ARG	C-N-CA	5.03	124.69	119.56
16	P	9	PHE	N-CA-C	5.02	121.50	110.80
3	C	180	ALA	N-CA-C	5.01	117.39	111.33

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	14	GLY	Peptide
2	B	89	GLY	Peptide
8	H	27	PRO	Peptide
8	H	90	GLY	Peptide
10	J	61	GLU	Peptide
12	L	46	LYS	Peptide

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Mol	Chain	Res	Type	Group
20	T	12	ALA	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	32546	0	16456	744	0
2	B	1896	0	1936	105	0
3	C	1613	0	1677	110	0
4	D	1703	0	1763	82	0
5	E	1147	0	1207	82	0
6	F	843	0	857	42	0
7	G	1257	0	1296	53	0
8	H	1116	0	1177	40	0
9	I	1010	0	1037	57	0
10	J	793	0	835	69	0
11	K	873	0	894	36	0
12	L	973	0	1058	51	0
13	M	937	0	995	47	0
14	N	492	0	529	52	0
15	O	734	0	771	39	0
16	P	701	0	720	24	0
17	Q	834	0	906	42	0
18	R	585	0	657	39	0
19	S	648	0	673	44	0
20	T	763	0	861	70	0
21	U	209	0	221	12	0
22	V	77	0	42	1	0
23	W	197	0	97	6	0
24	a	237	0	118	3	0
25	b	40	0	21	3	0
26	A	355	0	0	0	0
26	D	3	0	0	0	0
26	E	3	0	0	0	0
26	F	2	0	0	0	0
26	G	2	0	0	0	0
26	H	1	0	0	0	0
26	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	L	1	0	0	0	0
26	N	1	0	0	0	0
26	P	3	0	0	0	0
26	Q	1	0	0	0	0
26	S	3	0	0	0	0
26	T	1	0	0	0	0
27	A	40	0	37	9	0
28	D	1	0	0	0	0
28	N	1	0	0	0	0
29	A	887	0	0	41	0
29	C	1	0	0	0	0
29	D	5	0	0	0	0
29	E	5	0	0	0	0
29	L	1	0	0	0	0
29	N	1	0	0	0	0
29	P	2	0	0	0	0
29	S	2	0	0	0	0
29	T	1	0	0	0	0
29	U	2	0	0	0	0
All	All	53550	0	36841	1676	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 19.

All (1676) 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:451:A:O2'	29:A:2771:HOH:O	1.63	1.17
5:E:126:ARG:HG2	5:E:126:ARG:HH11	1.10	1.09
13:M:99:ARG:HB2	13:M:101:GLN:HE22	1.14	1.06
1:A:1535:A:N1	24:a:37:G:N1	2.03	1.05
5:E:11:ILE:HG22	5:E:31:LEU:HB3	1.41	1.03
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	1.93	1.02
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.41	1.00
20:T:67:ALA:O	20:T:73:HIS:HB3	1.61	1.00
11:K:15:ALA:HA	11:K:77:MET:HA	1.42	0.98
1:A:279:A:OP2	17:Q:95:TYR:OH	1.79	0.98
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.44	0.97
10:J:48:THR:HA	10:J:62:HIS:HB3	1.42	0.97
1:A:542:G:OP1	4:D:10:ARG:NH2	1.98	0.96
1:A:413:G:N2	1:A:429:U:OP2	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:8:GLU:HG2	13:M:22:ILE:HA	1.46	0.95
12:L:27:LEU:O	12:L:29:GLY:N	2.00	0.94
1:A:664:G:H22	1:A:741:G:H1	1.04	0.94
1:A:975:A:H4'	1:A:976:G:H5''	1.51	0.93
1:A:1256:A:H4'	1:A:1257:U:O5'	1.68	0.93
11:K:18:ARG:NH1	11:K:35:PRO:O	2.03	0.91
1:A:298:A:N6	29:A:2233:HOH:O	2.02	0.91
21:U:10:ARG:HH11	21:U:10:ARG:HG3	1.32	0.91
1:A:328:C:O2	1:A:328:C:H2'	1.70	0.89
1:A:834:C:N4	29:A:2826:HOH:O	2.04	0.89
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.55	0.89
1:A:975:A:H5'	1:A:975:A:H8	1.37	0.87
1:A:1124:G:N7	1:A:1145:C:O2'	2.05	0.87
1:A:1147:C:O2	9:I:16:ARG:NH2	2.07	0.87
13:M:37:THR:HG23	13:M:39:ILE:HG13	1.55	0.87
1:A:1054:C:O2	1:A:1054:C:H3'	1.75	0.86
19:S:80:TYR:CE1	19:S:81:ARG:HG2	2.10	0.86
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.55	0.86
10:J:55:LYS:HG2	10:J:56:HIS:H	1.39	0.86
1:A:372:C:O2'	29:A:2764:HOH:O	1.94	0.85
5:E:144:THR:O	5:E:148:VAL:HG23	1.76	0.85
1:A:1057:G:H5''	3:C:154:SER:HB2	1.58	0.85
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.10	0.84
14:N:3:ARG:NH2	14:N:6:LEU:HD21	1.92	0.84
1:A:1314:C:OP2	19:S:6:LYS:HD3	1.78	0.83
7:G:152:ALA:O	7:G:155:ARG:NH1	2.11	0.83
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.44	0.83
20:T:74:LYS:HB3	20:T:74:LYS:NZ	1.91	0.83
1:A:1305:G:N2	1:A:1331:G:H1'	1.93	0.83
5:E:24:ARG:HH11	5:E:24:ARG:HG3	1.42	0.83
2:B:80:ILE:HD12	2:B:80:ILE:H	1.42	0.82
12:L:27:LEU:C	12:L:29:GLY:H	1.84	0.82
1:A:835:U:OP1	18:R:64:ARG:NH2	2.12	0.82
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.13	0.82
7:G:38:LEU:O	7:G:42:ILE:HG13	1.79	0.82
1:A:1143:G:H2'	1:A:1144:G:C8	2.14	0.82
1:A:353:A:H5'	1:A:353:A:H8	1.42	0.82
5:E:126:ARG:HG2	5:E:126:ARG:NH1	1.89	0.82
1:A:266:G:O2'	1:A:267:C:OP2	1.98	0.82
12:L:6:THR:OG1	12:L:9:GLN:HG3	1.79	0.81
1:A:499:A:H4'	1:A:500:G:OP1	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1366:C:H2'	1:A:1367:C:H6	1.45	0.81
1:A:1347:G:O2'	1:A:1348:U:OP2	1.97	0.81
10:J:63:PHE:HB2	14:N:57:ARG:O	1.80	0.81
1:A:61:G:O2'	29:A:2002:HOH:O	2.00	0.80
1:A:1225:A:H5'	1:A:1226:C:OP2	1.82	0.80
3:C:54:ARG:NH2	3:C:56:ASP:OD1	2.15	0.79
10:J:24:VAL:HG13	10:J:34:VAL:HG11	1.63	0.79
12:L:28:LYS:HE2	12:L:33:ARG:HH12	1.47	0.79
4:D:201:GLN:NE2	5:E:116:THR:HG22	1.98	0.79
1:A:991:U:O2'	1:A:992:U:O5'	1.98	0.78
1:A:1125:U:H3'	1:A:1126:U:C5	2.19	0.78
1:A:1412:C:H2'	1:A:1413:A:C8	2.19	0.78
7:G:45:ASP:O	7:G:49:ILE:HG13	1.84	0.78
1:A:953:G:H5'	1:A:965:A:H61	1.49	0.78
19:S:40:ILE:HG22	19:S:67:VAL:HA	1.65	0.78
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.67	0.77
3:C:130:VAL:O	3:C:134:ILE:HG13	1.83	0.77
1:A:580:U:H2'	1:A:581:G:O4'	1.85	0.77
5:E:24:ARG:HH11	5:E:24:ARG:CG	1.96	0.77
15:O:45:VAL:HG12	15:O:46:HIS:N	1.98	0.77
1:A:1148:U:H2'	1:A:1149:C:O4'	1.84	0.77
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.66	0.77
1:A:1003:G:N2	1:A:1039:C:O2	2.18	0.77
11:K:33:THR:HG22	11:K:39:PRO:HA	1.67	0.77
1:A:975:A:H5'	1:A:975:A:C8	2.20	0.77
1:A:1281:U:H4'	1:A:1282:C:OP2	1.85	0.77
13:M:99:ARG:HB2	13:M:101:GLN:NE2	1.96	0.77
1:A:793:U:H3'	1:A:794:A:H5''	1.65	0.76
1:A:1196:U:O2'	29:A:2247:HOH:O	2.03	0.76
1:A:1314:C:C5	19:S:6:LYS:HE2	2.18	0.76
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.83	0.76
19:S:15:LEU:HD13	19:S:16:LEU:N	2.00	0.76
3:C:155:GLY:O	3:C:196:LEU:HD22	1.86	0.76
1:A:677:U:H3	1:A:713:G:H22	1.33	0.76
1:A:560:U:H5''	1:A:566:G:N2	2.00	0.76
1:A:664:G:OP1	18:R:64:ARG:NH1	2.19	0.76
18:R:47:THR:HG22	18:R:48:GLY:N	2.00	0.75
19:S:40:ILE:HG23	19:S:62:ILE:HD11	1.67	0.75
8:H:102:ARG:H	8:H:102:ARG:CD	1.98	0.75
19:S:36:ARG:NH2	19:S:75:ALA:O	2.19	0.75
2:B:101:MET:HA	2:B:108:ILE:HG13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:G:OP2	29:A:2018:HOH:O	2.04	0.75
7:G:10:ARG:HG2	7:G:10:ARG:HH11	1.49	0.75
1:A:1003(A):G:N2	1:A:1038:C:O2	2.19	0.75
2:B:75:LYS:HA	2:B:78:GLN:HG3	1.66	0.75
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.01	0.74
1:A:1347:G:O2'	1:A:1348:U:P	2.45	0.74
1:A:1124:G:H5'	10:J:35:SER:HB2	1.68	0.74
10:J:48:THR:HA	10:J:62:HIS:CB	2.17	0.74
1:A:254:G:OP1	17:Q:67:LYS:O	2.05	0.74
3:C:130:VAL:HG11	3:C:157:ILE:HG23	1.67	0.74
5:E:83:GLU:HG2	5:E:88:LYS:HD2	1.69	0.74
7:G:136:LYS:NZ	7:G:140:ASP:OD1	2.16	0.74
17:Q:101:ARG:HD3	17:Q:101:ARG:H	1.50	0.74
20:T:56:MET:HE2	20:T:85:MET:HA	1.69	0.74
1:A:235:C:N4	29:A:2119:HOH:O	2.20	0.74
1:A:839:U:O2	1:A:839:U:H2'	1.88	0.74
17:Q:67:LYS:O	17:Q:68:ARG:HB2	1.85	0.74
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.23	0.74
10:J:78:ASN:OD1	10:J:79:ARG:NH1	2.21	0.74
1:A:1338:G:H2'	1:A:1339:A:C8	2.24	0.73
1:A:1391:U:H2'	1:A:1392:G:C8	2.23	0.73
1:A:1287:A:H2'	1:A:1288:A:C8	2.22	0.73
1:A:130:A:OP2	1:A:190(E):U:O2'	2.06	0.73
1:A:1502:A:H2	1:A:1505:G:H1	1.34	0.73
5:E:41:VAL:HG13	5:E:113:ALA:HA	1.70	0.73
13:M:78:ILE:HG22	13:M:79:LYS:N	2.03	0.73
10:J:55:LYS:CG	10:J:56:HIS:H	2.01	0.73
13:M:79:LYS:NZ	13:M:83:ASP:OD1	2.21	0.73
20:T:13:LEU:HD12	20:T:14:LYS:N	2.04	0.73
3:C:13:GLY:HA3	14:N:57:ARG:HH22	1.54	0.73
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.70	0.72
1:A:1001:A:H2'	1:A:1002:G:H8	1.52	0.72
1:A:1143:G:H2'	1:A:1144:G:H8	1.55	0.72
2:B:16:HIS:HB3	2:B:44:LEU:HD21	1.72	0.72
1:A:527:7MG:OP2	27:A:1956:SRV:O32	2.05	0.72
17:Q:27:PHE:CZ	17:Q:36:ILE:HD11	2.23	0.72
1:A:1366:C:H2'	1:A:1367:C:C6	2.24	0.72
1:A:1279:A:H5''	1:A:1280:A:OP1	1.90	0.72
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.72	0.72
13:M:15:VAL:HG23	13:M:43:THR:O	1.90	0.72
1:A:1387:G:O2'	29:A:2237:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.72	0.71
1:A:1435:G:H2'	1:A:1436:U:C6	2.24	0.71
4:D:32:ALA:HA	4:D:35:ARG:HB2	1.73	0.71
15:O:56:LEU:HA	15:O:59:MET:HE3	1.70	0.71
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.71	0.71
2:B:74:LYS:C	2:B:76:GLN:H	1.98	0.71
18:R:47:THR:HG22	18:R:48:GLY:H	1.53	0.71
1:A:92:C:O2'	1:A:93:G:H5'	1.90	0.71
1:A:640:A:N6	29:A:2098:HOH:O	2.23	0.71
4:D:201:GLN:HE22	5:E:116:THR:HG22	1.55	0.70
12:L:25:PRO:C	12:L:27:LEU:H	1.99	0.70
1:A:353:A:H5'	1:A:353:A:C8	2.26	0.70
1:A:192:U:O4'	20:T:103:GLY:HA2	1.91	0.70
10:J:48:THR:CA	10:J:62:HIS:HB3	2.20	0.70
1:A:1392:G:H21	1:A:1502:A:H8	1.38	0.70
21:U:6:ARG:HB2	21:U:15:ARG:NH1	2.06	0.70
1:A:328:C:O2'	1:A:329:A:OP2	2.10	0.70
12:L:20:LYS:H	12:L:20:LYS:HD2	1.55	0.70
20:T:67:ALA:HA	20:T:73:HIS:H	1.55	0.70
1:A:1304:G:OP2	29:A:2277:HOH:O	2.09	0.70
1:A:1502:A:H2	1:A:1505:G:N1	1.90	0.70
1:A:421:U:H5'	1:A:422:C:C5	2.27	0.70
1:A:914:A:OP1	27:A:1956:SRY:HI33	1.91	0.69
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.74	0.69
5:E:42:GLY:HA2	5:E:136:MET:HE1	1.73	0.69
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.10	0.69
2:B:223:ILE:HD13	2:B:230:VAL:H	1.57	0.69
1:A:1002:G:H2'	1:A:1003:G:C8	2.25	0.69
1:A:1190:G:HO2'	1:A:1191:A:P	2.15	0.69
1:A:192:U:C1'	20:T:103:GLY:HA2	2.22	0.69
20:T:83:ARG:O	20:T:87:LYS:HD2	1.92	0.69
10:J:86:MET:HA	10:J:86:MET:HE3	1.73	0.69
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.74	0.69
1:A:103:C:OP1	20:T:17:ARG:NH1	2.26	0.69
1:A:1251:A:H4'	9:I:12:GLU:OE1	1.92	0.69
3:C:156:ARG:H	3:C:163:ALA:HA	1.58	0.69
3:C:77:ILE:HG22	3:C:78:GLY:O	1.93	0.69
2:B:103:THR:HG23	2:B:176:GLU:OE1	1.93	0.69
4:D:70:ILE:HG22	4:D:71:SER:O	1.93	0.69
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.74	0.69
12:L:60:LEU:HB2	12:L:64:TYR:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:G:H5'	1:A:298:A:O4'	1.93	0.68
1:A:299:G:H2'	1:A:300:A:C8	2.28	0.68
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.33	0.68
10:J:7:LYS:HD3	10:J:9:ARG:HH21	1.57	0.68
1:A:453:A:H4'	16:P:72:ARG:HG3	1.76	0.68
2:B:107:THR:O	2:B:110:GLN:HB2	1.92	0.68
8:H:82:HIS:ND1	8:H:138:TRP:NE1	2.42	0.68
1:A:653:A:OP1	8:H:56:LYS:NZ	2.26	0.68
1:A:820:U:H4'	1:A:821:G:OP2	1.92	0.68
1:A:290:C:N4	29:A:2818:HOH:O	2.26	0.68
1:A:409:G:OP1	4:D:24:GLU:O	2.12	0.68
17:Q:40:LYS:HD2	17:Q:42:TYR:CZ	2.29	0.68
19:S:5:LEU:HG	19:S:6:LYS:H	1.59	0.68
16:P:22:THR:HA	16:P:33:ILE:HG13	1.76	0.68
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.76	0.68
1:A:1229:A:OP2	13:M:114:ARG:HD3	1.94	0.67
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.76	0.67
1:A:620:C:N1	4:D:135:LEU:HD13	2.10	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.29	0.67
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.29	0.67
1:A:496:A:H4'	1:A:497:A:OP1	1.92	0.67
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.76	0.67
19:S:58:VAL:HG12	19:S:59:PRO:HD2	1.75	0.67
9:I:48:GLU:OE1	9:I:48:GLU:HA	1.93	0.67
13:M:51:ALA:O	13:M:54:VAL:HG12	1.94	0.67
13:M:82:MET:HE3	13:M:93:ARG:HG2	1.76	0.67
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.77	0.67
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.60	0.67
1:A:1300:G:O2'	1:A:1301:U:P	2.52	0.67
8:H:102:ARG:H	8:H:102:ARG:HD2	1.57	0.67
1:A:509:A:O2'	1:A:510:A:OP1	2.13	0.67
1:A:1049:U:H4'	1:A:1050:G:O5'	1.93	0.67
1:A:1149:C:H2'	1:A:1150:U:C6	2.30	0.67
11:K:27:ASN:OD1	11:K:28:THR:N	2.27	0.67
20:T:13:LEU:HD12	20:T:13:LEU:C	2.20	0.67
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.75	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.93	0.67
10:J:63:PHE:HB3	14:N:58:LYS:HA	1.77	0.67
1:A:89:C:C5	1:A:90:U:C4	2.84	0.67
1:A:951:G:OP2	13:M:102:ARG:NH2	2.28	0.67
1:A:972:C:OP1	10:J:57:LYS:NZ	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:U:O3'	1:A:129(A):G:H3'	1.95	0.66
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.28	0.66
5:E:12:LEU:HD23	5:E:12:LEU:C	2.20	0.66
1:A:737:A:H1'	6:F:73:ASN:HD21	1.60	0.66
3:C:43:LEU:HD12	3:C:47:LEU:HD13	1.77	0.66
21:U:6:ARG:HB2	21:U:15:ARG:HH12	1.59	0.66
1:A:442:C:H42	1:A:492:G:H1	1.42	0.66
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.76	0.66
14:N:41:ARG:HG3	14:N:42:ILE:N	2.10	0.66
1:A:795:C:H5''	1:A:796:C:OP2	1.95	0.66
1:A:1125:U:H3'	1:A:1126:U:H5	1.59	0.66
2:B:239:VAL:O	2:B:240:GLN:HB3	1.95	0.66
1:A:1305:G:H22	1:A:1331:G:H1'	1.58	0.66
1:A:1482:G:N1	29:A:2391:HOH:O	2.17	0.66
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.76	0.66
1:A:1212:U:O2	1:A:1212:U:H2'	1.95	0.66
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.78	0.66
3:C:147:LYS:HD3	3:C:205:GLY:H	1.61	0.66
15:O:74:ASP:HB3	15:O:77:ARG:HG3	1.76	0.66
19:S:51:VAL:HG11	19:S:71:LEU:HD22	1.77	0.66
10:J:32:ALA:O	10:J:34:VAL:HG23	1.95	0.66
17:Q:58:GLU:O	17:Q:59:ILE:HD13	1.95	0.66
19:S:7:LYS:HD2	19:S:7:LYS:O	1.95	0.66
1:A:1101:A:H4'	1:A:1102:A:O5'	1.96	0.66
6:F:28:ARG:O	6:F:32:ASN:ND2	2.29	0.66
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.78	0.66
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.30	0.66
1:A:126:G:N7	29:A:2422:HOH:O	2.29	0.66
10:J:27:ALA:HB1	10:J:81:THR:HG23	1.78	0.66
1:A:804:U:H5''	1:A:805:C:OP2	1.95	0.65
1:A:502:G:OP1	12:L:118:SER:OG	2.14	0.65
12:L:28:LYS:C	12:L:30:ALA:H	2.05	0.65
3:C:151:VAL:O	3:C:167:TRP:O	2.15	0.65
14:N:3:ARG:HH21	14:N:6:LEU:HD21	1.57	0.65
1:A:1005:A:C6	1:A:1026:G:N2	2.65	0.65
10:J:55:LYS:HG2	10:J:56:HIS:N	2.08	0.65
21:U:10:ARG:HG3	21:U:10:ARG:NH1	2.08	0.65
3:C:134:ILE:O	3:C:138:VAL:HG23	1.96	0.65
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.77	0.65
8:H:111:ILE:O	8:H:134:ILE:HB	1.97	0.65
1:A:1347:G:C2'	1:A:1348:U:OP2	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:90:PRO:O	9:I:93:ARG:HG3	1.97	0.65
1:A:1368:G:OP2	9:I:112:LYS:HD3	1.96	0.65
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.79	0.65
9:I:10:ARG:HG3	9:I:11:LYS:HG2	1.77	0.65
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.78	0.65
1:A:812:C:H4'	1:A:813:U:O5'	1.97	0.65
1:A:1197:G:OP1	29:A:2249:HOH:O	2.15	0.65
5:E:144:THR:HG22	5:E:146:ALA:H	1.62	0.65
10:J:75:ILE:HG22	10:J:76:ASN:H	1.60	0.65
10:J:82:ILE:O	10:J:85:LEU:HB2	1.96	0.65
1:A:1065:U:H1'	1:A:1066:C:OP2	1.97	0.65
1:A:1157:A:H4'	1:A:1158:C:O5'	1.97	0.65
1:A:1212:U:H4'	1:A:1213:A:O5'	1.96	0.64
3:C:34:LEU:O	3:C:38:ARG:HG3	1.97	0.64
5:E:12:LEU:HD23	5:E:13:ILE:N	2.13	0.64
1:A:35:G:H2'	1:A:36:C:C6	2.33	0.64
1:A:89:C:H2'	1:A:90:U:O5'	1.98	0.64
1:A:1126:U:C4	1:A:1127:G:N2	2.66	0.64
1:A:1425:U:H2'	1:A:1426:C:H6	1.62	0.64
10:J:74:ILE:O	10:J:74:ILE:HG13	1.98	0.64
13:M:36:LYS:HD2	13:M:59:TYR:OH	1.97	0.64
13:M:99:ARG:CB	13:M:101:GLN:HE22	2.00	0.64
1:A:1068:G:P	29:A:2237:HOH:O	2.55	0.64
1:A:1136:U:H5''	1:A:1137:C:OP2	1.97	0.64
3:C:195:VAL:C	3:C:196:LEU:HD23	2.23	0.64
1:A:974:A:OP2	14:N:41:ARG:NH1	2.25	0.64
1:A:1001:A:H2'	1:A:1002:G:C8	2.31	0.64
1:A:1028:C:N3	1:A:1034:G:C2	2.66	0.64
3:C:47:LEU:HG	3:C:76:VAL:HG12	1.79	0.64
22:V:1:U:H3	23:W:36:G:H1	1.46	0.64
1:A:673:G:H2'	1:A:674:G:C8	2.32	0.64
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.28	0.64
2:B:170:GLU:OE2	2:B:170:GLU:HA	1.97	0.64
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.80	0.64
3:C:126:ARG:HG2	3:C:128:PHE:HB2	1.78	0.64
3:C:126:ARG:HG3	3:C:128:PHE:H	1.63	0.64
4:D:191:ARG:HH11	4:D:191:ARG:HG3	1.63	0.64
1:A:1152:A:OP1	10:J:68:HIS:ND1	2.28	0.64
2:B:240:GLN:HG2	2:B:240:GLN:O	1.97	0.63
10:J:61:GLU:HG2	10:J:61:GLU:O	1.97	0.63
1:A:977:A:H2'	1:A:978:A:H5'	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:50:ALA:HA	19:S:58:VAL:O	1.98	0.63
7:G:5:ARG:HG3	7:G:7:ALA:H	1.63	0.63
1:A:1241:G:H2'	1:A:1242:C:C6	2.34	0.63
5:E:43:LEU:HD12	5:E:136:MET:HE2	1.80	0.63
1:A:299:G:O6	29:A:2235:HOH:O	2.11	0.63
1:A:1064:G:N2	1:A:1190:G:H2'	2.13	0.63
20:T:74:LYS:HB3	20:T:74:LYS:HZ2	1.63	0.63
3:C:6:HIS:HD2	3:C:9:GLY:H	1.44	0.63
4:D:32:ALA:O	4:D:36:ARG:N	2.29	0.63
1:A:1086:U:H3	1:A:1099:G:H22	1.47	0.62
1:A:1225:A:H2'	1:A:1225:A:N3	2.14	0.62
1:A:755:G:OP2	15:O:65:ARG:HD2	1.99	0.62
1:A:1329:A:C2'	1:A:1330:U:H5'	2.30	0.62
13:M:88:ARG:HD2	19:S:3:ARG:HH21	1.63	0.62
3:C:85:ARG:HG2	3:C:85:ARG:HH11	1.63	0.62
1:A:23:C:N4	29:A:2692:HOH:O	2.33	0.62
1:A:229:U:O2'	1:A:230:G:H5'	1.98	0.62
1:A:390:C:H2'	1:A:391:G:C8	2.35	0.62
1:A:579:G:H5'	1:A:728:A:H1'	1.79	0.62
1:A:1190:G:O2'	1:A:1191:A:P	2.58	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.12	0.62
8:H:23:SER:HA	8:H:63:LEU:HD22	1.81	0.62
12:L:28:LYS:HE2	12:L:33:ARG:NH1	2.13	0.62
13:M:19:LEU:O	13:M:22:ILE:HG12	1.99	0.62
1:A:814:A:H2'	1:A:816:A:C5'	2.30	0.62
1:A:1004:A:N7	1:A:1037:C:N3	2.47	0.62
3:C:86:VAL:O	3:C:89:GLU:HB3	2.00	0.62
4:D:102:ASP:OD1	4:D:103:ASN:N	2.32	0.62
20:T:16:HIS:O	20:T:19:SER:OG	2.13	0.62
1:A:814:A:H2'	1:A:816:A:H5'	1.82	0.62
1:A:1112:C:H1'	3:C:179:ARG:HH11	1.63	0.62
9:I:5:TYR:OH	9:I:7:THR:OG1	2.17	0.62
1:A:328:C:O2	1:A:328:C:C2'	2.43	0.62
1:A:616:G:O2'	1:A:617:G:H5'	2.00	0.62
3:C:30:ARG:HG2	14:N:36:PHE:O	2.00	0.62
4:D:150:GLU:CD	4:D:150:GLU:N	2.57	0.62
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.80	0.62
3:C:46:GLU:HG3	3:C:83:ARG:HH21	1.65	0.62
1:A:89:C:H6	1:A:89:C:H3'	1.63	0.61
1:A:965:A:H4'	1:A:966:M2G:O5'	1.99	0.61
27:A:1956:SRY:HI32	27:A:1956:SRY:O13	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:182:ILE:HG13	1.82	0.61
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.33	0.61
10:J:40:LEU:HB3	10:J:41:PRO:HD2	1.81	0.61
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.82	0.61
5:E:98:THR:HB	5:E:117:ASP:HB3	1.82	0.61
16:P:74:LEU:O	16:P:79:VAL:HG23	2.00	0.61
18:R:47:THR:HA	18:R:83:GLU:HB2	1.80	0.61
1:A:1533:C:HO2'	1:A:1534:C:P	2.22	0.61
3:C:116:VAL:O	3:C:120:VAL:HG23	1.99	0.61
1:A:1278:U:H5''	1:A:1279:A:C8	2.36	0.61
20:T:58:LYS:HE2	20:T:62:LEU:CD2	2.31	0.61
1:A:850:U:H2'	1:A:851:G:H5''	1.81	0.61
2:B:10:LEU:HD22	2:B:15:VAL:HG21	1.81	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.83	0.61
1:A:289:G:P	29:A:2015:HOH:O	2.58	0.61
1:A:539:A:H2'	1:A:540:G:C8	2.36	0.61
1:A:1103:C:H5''	2:B:98:LEU:HD12	1.82	0.61
3:C:46:GLU:HG2	3:C:87:LEU:HD21	1.83	0.61
1:A:1054:C:O2	1:A:1054:C:C3'	2.48	0.61
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.82	0.61
1:A:89:C:C4	1:A:90:U:N3	2.69	0.61
1:A:99:C:H2'	1:A:101:A:C8	2.36	0.61
1:A:1035:A:H2'	1:A:1036:G:C8	2.36	0.61
6:F:97:PHE:HB2	18:R:32:ARG:HH11	1.65	0.61
14:N:3:ARG:HB2	14:N:6:LEU:HD23	1.82	0.61
19:S:7:LYS:HD2	19:S:7:LYS:C	2.25	0.61
1:A:1003:G:N2	1:A:1039:C:C2	2.69	0.60
1:A:1391:U:H2'	1:A:1392:G:H8	1.63	0.60
1:A:972:C:OP1	10:J:57:LYS:HD2	2.01	0.60
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.15	0.60
11:K:50:TYR:HE2	11:K:54:ARG:HH11	1.49	0.60
1:A:1027:C:H5	1:A:1035:A:N1	1.99	0.60
1:A:1269:A:H5''	1:A:1270:C:OP2	2.01	0.60
1:A:1412:C:H2'	1:A:1413:A:H8	1.66	0.60
3:C:14:ILE:C	3:C:16:ARG:H	2.09	0.60
3:C:126:ARG:CG	3:C:128:PHE:HB2	2.32	0.60
1:A:1316:G:N1	1:A:1319:A:OP2	2.34	0.60
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.83	0.60
4:D:62:GLN:O	4:D:66:ARG:HD3	2.02	0.60
8:H:112:LEU:N	8:H:112:LEU:HD23	2.16	0.60
10:J:6:ILE:HG23	10:J:96:ILE:HG23	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:LYS:HZ3	2:B:143:GLU:HG3	1.66	0.60
1:A:1427:U:H2'	1:A:1428:A:C8	2.37	0.60
2:B:98:LEU:O	2:B:101:MET:HG3	2.02	0.60
16:P:47:ASP:CG	16:P:47:ASP:O	2.44	0.60
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.32	0.60
1:A:706:A:O4'	11:K:29:ILE:HD11	2.02	0.60
1:A:1256:A:H1'	1:A:1257:U:OP2	2.00	0.60
1:A:1535:A:C2	24:a:37:G:N2	2.69	0.60
4:D:25:ARG:HG2	4:D:25:ARG:O	2.02	0.60
1:A:1004:A:H5'	29:A:2351:HOH:O	2.01	0.59
12:L:53:ARG:HG3	12:L:93:LEU:HD21	1.83	0.59
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.84	0.59
1:A:1528:U:O2'	1:A:1529:G:OP2	2.13	0.59
16:P:3:LYS:HD2	16:P:65:GLN:O	2.02	0.59
1:A:1313:U:O4	19:S:4:SER:OG	2.19	0.59
10:J:79:ARG:HB2	10:J:80:LYS:HD2	1.83	0.59
1:A:88:A:C5	1:A:89:C:N3	2.70	0.59
1:A:501:C:H2'	1:A:502:G:C8	2.37	0.59
1:A:1131:G:H8	1:A:1131:G:OP2	1.84	0.59
3:C:34:LEU:HD22	14:N:25:VAL:HG21	1.84	0.59
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.51	0.59
1:A:828:A:H4'	1:A:828:A:OP1	2.00	0.59
1:A:1277:C:O2'	1:A:1279:A:H1'	2.03	0.59
1:A:707:C:OP1	11:K:85:ARG:NH1	2.35	0.59
20:T:59:ALA:O	20:T:63:ILE:HG13	2.02	0.59
1:A:89:C:C2'	1:A:90:U:O5'	2.50	0.59
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.85	0.59
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.85	0.59
10:J:47:PHE:O	10:J:62:HIS:HB2	2.02	0.59
12:L:70:ILE:HG21	12:L:75:HIS:CD2	2.37	0.59
17:Q:101:ARG:HD3	17:Q:101:ARG:N	2.16	0.59
1:A:79:G:C2	1:A:91:C:C2	2.91	0.59
1:A:397:A:H5'	1:A:398:C:OP1	2.02	0.59
1:A:594:G:C2'	1:A:595:G:H5'	2.33	0.59
1:A:1053:G:HO2'	1:A:1199:U:H5	1.48	0.59
1:A:1125:U:C3'	1:A:1126:U:H5	2.15	0.59
1:A:1356:G:H2'	1:A:1357:A:C8	2.37	0.59
1:A:1399:C:O2	1:A:1401:G:C5	2.56	0.59
6:F:3:ARG:O	6:F:93:SER:HB2	2.01	0.59
1:A:1004:A:H62	1:A:1037:C:H42	1.50	0.59
1:A:45:U:H2'	1:A:46:G:C8	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:C:N4	29:A:2482:HOH:O	2.34	0.58
1:A:667:G:H4'	15:O:51:HIS:ND1	2.19	0.58
3:C:180:ALA:CB	3:C:182:ILE:HG13	2.34	0.58
5:E:11:ILE:HD11	5:E:105:VAL:HA	1.85	0.58
1:A:1027:C:OP1	1:A:1027:C:C4'	2.51	0.58
1:A:1126:U:O4	1:A:1127:G:N2	2.36	0.58
4:D:150:GLU:N	4:D:150:GLU:OE2	2.36	0.58
7:G:108:ALA:O	7:G:119:ARG:HB3	2.02	0.58
8:H:4:ASP:CG	8:H:85:ARG:HH21	2.11	0.58
13:M:2:ALA:O	13:M:9:ILE:HA	2.03	0.58
13:M:8:GLU:CG	13:M:22:ILE:HA	2.27	0.58
18:R:46:GLU:H	18:R:46:GLU:CD	2.11	0.58
1:A:141:A:H1'	1:A:182:U:O2	2.03	0.58
1:A:251:G:H4'	1:A:252:U:O5'	2.03	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
1:A:1052:U:H2'	1:A:1055:A:OP1	2.03	0.58
1:A:1179:A:H2'	1:A:1180:A:O4'	2.02	0.58
2:B:172:ILE:HD13	2:B:172:ILE:H	1.68	0.58
3:C:91:LEU:HD23	3:C:92:ALA:N	2.19	0.58
5:E:144:THR:HG22	5:E:145:LYS:N	2.17	0.58
8:H:112:LEU:HD23	8:H:112:LEU:H	1.68	0.58
1:A:31:G:N2	1:A:48:C:OP1	2.27	0.58
1:A:914:A:P	27:A:1956:SRY:HI33	2.42	0.58
4:D:170:VAL:HG13	4:D:171:GLY:N	2.18	0.58
14:N:9:LYS:HD2	14:N:9:LYS:O	2.04	0.58
1:A:1047:G:C2'	1:A:1048:G:H5'	2.32	0.58
1:A:1131:G:H2'	1:A:1132:C:C6	2.38	0.58
6:F:22:GLU:OE2	6:F:82:ARG:HD3	2.04	0.58
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.84	0.58
9:I:26:VAL:HG12	9:I:61:ALA:HB3	1.84	0.58
15:O:45:VAL:CG1	15:O:46:HIS:N	2.66	0.58
1:A:976:G:H5'	1:A:1358:U:O2'	2.03	0.58
6:F:80:ARG:NH1	6:F:88:VAL:O	2.36	0.58
20:T:10:LEU:HG	20:T:12:ALA:H	1.69	0.58
2:B:80:ILE:H	2:B:80:ILE:CD1	2.14	0.58
15:O:39:LEU:HG	15:O:59:MET:HE1	1.83	0.58
1:A:35:G:H2'	1:A:36:C:H6	1.66	0.58
3:C:14:ILE:O	3:C:16:ARG:N	2.36	0.58
8:H:82:HIS:ND1	8:H:138:TRP:CE2	2.71	0.58
1:A:421:U:H5'	1:A:422:C:H5	1.68	0.58
2:B:125:PRO:HG2	2:B:126:GLU:OE1	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:19:SER:OG	10:J:91:PRO:HG2	2.04	0.58
11:K:48:ILE:HG22	11:K:49:GLY:H	1.68	0.58
1:A:501:C:H2'	1:A:502:G:H8	1.69	0.57
1:A:1035:A:C6	1:A:1036:G:C6	2.92	0.57
5:E:126:ARG:HH11	5:E:126:ARG:CG	2.00	0.57
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.69	0.57
12:L:36:VAL:HG22	12:L:82:VAL:HG22	1.85	0.57
19:S:5:LEU:HG	19:S:6:LYS:N	2.19	0.57
1:A:1004:A:O2'	1:A:1005:A:OP1	2.14	0.57
1:A:1300:G:O2'	1:A:1301:U:OP2	2.21	0.57
6:F:28:ARG:HG2	6:F:32:ASN:HD21	1.67	0.57
8:H:103:VAL:HG21	8:H:109:ILE:O	2.04	0.57
9:I:32:ASP:OD1	9:I:33:PHE:N	2.37	0.57
1:A:1057:G:C5'	3:C:154:SER:HB2	2.33	0.57
1:A:1112:C:N4	3:C:178:LEU:HD23	2.19	0.57
4:D:172:PRO:HD2	4:D:173:TRP:CZ3	2.39	0.57
15:O:11:VAL:HG11	15:O:34:LEU:HD12	1.86	0.57
1:A:972:C:P	10:J:57:LYS:HD2	2.44	0.57
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.34	0.57
13:M:86:CYS:SG	13:M:87:TYR:N	2.76	0.57
20:T:51:GLU:O	20:T:55:ILE:HG12	2.04	0.57
20:T:69:GLY:O	20:T:73:HIS:CE1	2.57	0.57
1:A:714:G:H2'	1:A:715:A:C8	2.39	0.57
1:A:860:A:H2'	1:A:861:G:O4'	2.04	0.57
2:B:212:GLN:HE21	2:B:235:SER:CB	2.14	0.57
15:O:45:VAL:HG12	15:O:46:HIS:H	1.69	0.57
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.84	0.57
21:U:10:ARG:HH11	21:U:10:ARG:CG	2.11	0.57
1:A:17:U:H2'	1:A:18:C:C6	2.40	0.57
1:A:1054:C:O2'	1:A:1055:A:H5''	2.04	0.57
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.86	0.57
13:M:16:ASP:OD2	13:M:17:VAL:N	2.34	0.57
1:A:250:A:H1'	1:A:251:G:OP2	2.04	0.57
1:A:1072:G:H2'	1:A:1073:U:C6	2.39	0.57
14:N:41:ARG:HG3	14:N:42:ILE:H	1.69	0.57
1:A:757:U:H2'	1:A:758:G:O4'	2.04	0.57
1:A:895:G:H2'	1:A:896:C:H6	1.70	0.57
3:C:127:ARG:NH2	3:C:193:TYR:HE2	2.03	0.57
10:J:12:ASP:OD2	10:J:15:THR:HG23	2.05	0.57
12:L:24:VAL:O	12:L:24:VAL:HG12	2.04	0.57
18:R:26:LEU:HD11	18:R:42:ARG:HH11	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:58:VAL:CG1	19:S:59:PRO:HD2	2.35	0.57
20:T:74:LYS:HB3	20:T:74:LYS:HZ3	1.68	0.57
1:A:144:G:H1	1:A:178:C:H42	1.52	0.57
1:A:628:G:C2'	1:A:629:G:H5'	2.35	0.57
1:A:1015:A:N3	1:A:1218:C:O2'	2.37	0.57
1:A:1407:5MC:C2'	1:A:1408:A:H5'	2.35	0.57
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.38	0.57
20:T:13:LEU:C	20:T:13:LEU:CD1	2.77	0.57
1:A:1178:G:N2	1:A:1180:A:H3'	2.20	0.56
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.35	0.56
13:M:57:ARG:HD3	13:M:61:GLU:OE2	2.05	0.56
19:S:16:LEU:O	19:S:20:LEU:HG	2.05	0.56
1:A:501:C:OP1	12:L:117:ARG:NH2	2.38	0.56
4:D:8:VAL:HG11	4:D:21:LEU:HB2	1.88	0.56
18:R:37:VAL:O	18:R:40:LEU:N	2.38	0.56
1:A:664:G:N2	1:A:741:G:H1	1.88	0.56
1:A:1027:C:OP1	1:A:1027:C:O4'	2.23	0.56
1:A:1064:G:H22	1:A:1190:G:H2'	1.70	0.56
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.89	0.56
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.87	0.56
9:I:105:ASP:OD2	9:I:107:ARG:HG3	2.05	0.56
10:J:34:VAL:HG13	10:J:74:ILE:HG22	1.88	0.56
18:R:47:THR:CG2	18:R:48:GLY:N	2.68	0.56
1:A:149:A:H2'	1:A:150:C:C6	2.41	0.56
1:A:628:G:O2'	1:A:629:G:H5'	2.04	0.56
1:A:1004:A:H5''	29:A:2349:HOH:O	2.06	0.56
1:A:1053:G:C3'	1:A:1054:C:H5'	2.35	0.56
2:B:97:TRP:CZ3	2:B:176:GLU:OE2	2.57	0.56
1:A:187:C:N3	20:T:105:SER:CB	2.69	0.56
2:B:134:GLU:HA	2:B:137:ARG:CG	2.36	0.56
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.87	0.56
1:A:1277:C:H2'	1:A:1279:A:H8	1.71	0.56
2:B:87:ARG:HG2	2:B:88:ALA:H	1.70	0.56
3:C:127:ARG:HH22	3:C:193:TYR:HE2	1.52	0.56
6:F:45:LEU:C	6:F:45:LEU:HD12	2.31	0.56
10:J:63:PHE:HA	14:N:59:ALA:HB3	1.86	0.56
12:L:20:LYS:H	12:L:20:LYS:CD	2.17	0.56
12:L:54:LYS:N	12:L:54:LYS:HD2	2.19	0.56
1:A:975:A:H4'	1:A:976:G:C5'	2.33	0.56
1:A:1286:A:H3'	1:A:1287:A:H5''	1.86	0.56
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:ASN:OD1	7:G:36:LYS:HE3	2.05	0.56
1:A:777:A:OP1	29:A:2573:HOH:O	2.17	0.56
2:B:132:LYS:NZ	2:B:132:LYS:HB3	2.21	0.56
10:J:47:PHE:CZ	14:N:37:PHE:CE1	2.94	0.56
1:A:428:G:H1'	1:A:429:U:OP2	2.06	0.56
1:A:250:A:H4'	1:A:251:G:O5'	2.06	0.56
1:A:503:C:OP2	12:L:116:SER:HB3	2.06	0.56
1:A:946:A:H2'	1:A:947:G:C8	2.41	0.56
1:A:1442:G:C6	1:A:1446:A:N6	2.73	0.56
2:B:14:GLY:HA3	2:B:210:SER:HB2	1.87	0.56
1:A:1026:G:N7	1:A:1027:C:N3	2.53	0.55
7:G:12:LEU:H	7:G:12:LEU:HD12	1.69	0.55
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.40	0.55
11:K:15:ALA:CA	11:K:77:MET:HA	2.27	0.55
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.54	0.55
1:A:983:A:O2'	1:A:1050:G:OP2	2.23	0.55
1:A:1054:C:N3	23:W:34:G:O4'	2.40	0.55
10:J:24:VAL:O	10:J:28:ARG:HB2	2.06	0.55
1:A:1495:U:H2'	1:A:1496:C:O4'	2.06	0.55
1:A:187:C:N3	20:T:105:SER:HB2	2.21	0.55
1:A:539:A:H2'	1:A:540:G:H8	1.70	0.55
1:A:91:C:H2'	1:A:92:C:H6	1.71	0.55
1:A:895:G:H2'	1:A:896:C:C6	2.41	0.55
1:A:1027:C:N4	29:A:2347:HOH:O	2.39	0.55
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.20	0.55
2:B:90:MET:HB3	2:B:91:PRO:HD2	1.87	0.55
5:E:76:ILE:HG23	5:E:142:LEU:CD1	2.37	0.55
1:A:1160:G:C6	1:A:1181:G:O6	2.60	0.55
1:A:1181:G:C2	1:A:1182:G:N2	2.75	0.55
14:N:9:LYS:HG3	14:N:10:ALA:N	2.20	0.55
19:S:43:GLU:OE2	19:S:43:GLU:N	2.24	0.55
1:A:129(A):G:H1'	1:A:190(E):U:H2'	1.88	0.55
1:A:1002:G:C6	1:A:1003:G:C6	2.95	0.55
1:A:1003:G:N2	1:A:1003(A):G:C6	2.74	0.55
1:A:1275:A:H2'	1:A:1276:G:O4'	2.06	0.55
12:L:73:GLU:OE1	12:L:73:GLU:HA	2.07	0.55
1:A:620:C:H2'	1:A:621:A:O4'	2.07	0.55
8:H:102:ARG:CD	8:H:102:ARG:N	2.65	0.55
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.89	0.55
9:I:70:LYS:O	9:I:74:ILE:HG13	2.06	0.55
1:A:421:U:O2	1:A:421:U:O4'	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1065:U:H5''	1:A:1190:G:N2	2.22	0.55
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.88	0.55
5:E:97:GLY:N	5:E:117:ASP:OD1	2.40	0.55
13:M:59:TYR:O	13:M:63:THR:HB	2.07	0.55
1:A:192:U:H1'	20:T:103:GLY:HA2	1.89	0.55
1:A:459:G:H1'	1:A:463:A:H61	1.71	0.55
1:A:526:C:O3'	27:A:1956:SRV:HI31	2.06	0.55
1:A:1532:U:H2'	1:A:1533:C:C6	2.41	0.55
3:C:127:ARG:NH2	3:C:193:TYR:CE2	2.75	0.55
10:J:63:PHE:HA	14:N:59:ALA:CB	2.37	0.55
15:O:8:LYS:O	15:O:12:ILE:HG12	2.06	0.55
19:S:80:TYR:CD1	19:S:81:ARG:N	2.76	0.55
2:B:74:LYS:C	2:B:76:GLN:N	2.64	0.54
3:C:156:ARG:NH1	3:C:193:TYR:O	2.40	0.54
4:D:175:SER:HB2	4:D:184:LYS:HB2	1.90	0.54
21:U:7:ARG:O	21:U:21:TYR:CD2	2.61	0.54
1:A:1312:G:N7	19:S:4:SER:HB3	2.21	0.54
11:K:67:ASP:O	11:K:71:LYS:HG3	2.08	0.54
14:N:14:PRO:HB2	14:N:16:PHE:O	2.07	0.54
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.42	0.54
1:A:56:U:H2'	1:A:57:G:C8	2.41	0.54
1:A:353:A:H8	1:A:353:A:C5'	2.15	0.54
1:A:1286:A:H8	1:A:1287:A:H5''	1.71	0.54
2:B:115:LEU:HD11	2:B:146:GLN:HG3	1.89	0.54
3:C:6:HIS:CD2	3:C:9:GLY:H	2.25	0.54
3:C:46:GLU:HG2	3:C:87:LEU:CD2	2.37	0.54
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.89	0.54
7:G:72:ARG:HD3	7:G:142:GLU:OE1	2.07	0.54
9:I:118:LYS:O	9:I:120:ARG:N	2.39	0.54
20:T:67:ALA:HA	20:T:73:HIS:N	2.21	0.54
1:A:594:G:H2'	1:A:595:G:H5'	1.88	0.54
1:A:960:U:H4'	1:A:961:U:C5'	2.37	0.54
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.90	0.54
18:R:47:THR:CG2	18:R:48:GLY:H	2.18	0.54
20:T:33:ILE:O	20:T:34:LYS:C	2.51	0.54
1:A:1256:A:N6	1:A:1277:C:C5	2.76	0.54
19:S:25:LYS:HG3	19:S:26:GLY:H	1.73	0.54
1:A:722:A:O2'	1:A:723:U:C2	2.61	0.54
20:T:89:ARG:HB2	20:T:104:LEU:HD11	1.90	0.54
2:B:224:GLN:HG2	2:B:229:VAL:HG22	1.89	0.54
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.43	0.54
1:A:60:A:H4'	1:A:61:G:O5'	2.08	0.54
1:A:179:A:O2'	1:A:180:U:H5'	2.08	0.54
1:A:838:G:N2	1:A:849:C:C2	2.75	0.54
1:A:1533:C:O2'	1:A:1534:C:OP1	2.21	0.54
17:Q:59:ILE:CD1	17:Q:73:VAL:HA	2.38	0.54
18:R:39:VAL:O	18:R:42:ARG:HB2	2.08	0.54
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.43	0.54
1:A:667:G:H4'	15:O:51:HIS:CE1	2.43	0.53
1:A:981:U:H5'	14:N:21:TYR:CE1	2.42	0.53
1:A:1277:C:C2'	1:A:1279:A:H8	2.21	0.53
2:B:16:HIS:CB	2:B:44:LEU:HD21	2.37	0.53
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.08	0.53
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.90	0.53
5:E:105:VAL:HG12	5:E:106:PRO:N	2.23	0.53
7:G:51:GLN:O	7:G:52:GLU:CD	2.52	0.53
9:I:27:THR:HG23	9:I:62:TYR:HA	1.89	0.53
19:S:15:LEU:HD13	19:S:16:LEU:H	1.73	0.53
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.43	0.53
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.44	0.53
1:A:1095:U:H2'	1:A:1096:C:O4'	2.08	0.53
1:A:1168:A:H2'	1:A:1169:A:C8	2.43	0.53
1:A:1241:G:H2'	1:A:1242:C:H6	1.72	0.53
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.43	0.53
9:I:11:LYS:O	9:I:12:GLU:HB2	2.07	0.53
10:J:55:LYS:CG	10:J:56:HIS:N	2.71	0.53
1:A:620:C:C2	4:D:135:LEU:HD13	2.44	0.53
1:A:684:A:N6	1:A:685:G:C6	2.77	0.53
1:A:792:A:H4'	1:A:793:U:H5''	1.91	0.53
2:B:80:ILE:HD12	2:B:80:ILE:N	2.16	0.53
9:I:128:ARG:HG3	9:I:128:ARG:OXT	2.07	0.53
10:J:51:ARG:HG3	10:J:59:SER:O	2.08	0.53
12:L:28:LYS:C	12:L:30:ALA:N	2.61	0.53
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.90	0.53
1:A:509:A:H5'	4:D:54:TYR:HD2	1.73	0.53
12:L:47:LYS:N	12:L:48:PRO:HD2	2.23	0.53
20:T:56:MET:HE2	20:T:85:MET:HG2	1.89	0.53
1:A:1142:G:H5'	1:A:1143:G:OP2	2.08	0.53
1:A:1402:4OC:O2	1:A:1500:A:N1	2.42	0.53
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.44	0.53
2:B:133:LYS:O	2:B:137:ARG:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:53:VAL:CG2	9:I:85:LEU:HD21	2.38	0.53
19:S:51:VAL:O	19:S:58:VAL:HG23	2.08	0.53
1:A:1486:G:H2'	1:A:1487:G:O4'	2.09	0.53
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.09	0.53
6:F:89:MET:HE2	18:R:76:LEU:HG	1.90	0.53
1:A:204:U:H4'	1:A:216:G:OP1	2.06	0.53
1:A:421:U:H4'	1:A:422:C:OP2	2.09	0.53
6:F:41:GLU:OE1	18:R:35:ARG:NH1	2.35	0.53
20:T:74:LYS:NZ	20:T:74:LYS:CB	2.68	0.53
1:A:538:G:OP2	12:L:115:LYS:HG3	2.08	0.53
1:A:609:A:N6	29:A:2344:HOH:O	2.40	0.53
17:Q:100:LYS:HB2	17:Q:101:ARG:HH11	1.74	0.53
1:A:112:G:C2'	1:A:113:G:H5'	2.39	0.52
1:A:630:G:H5'	1:A:631:G:OP2	2.09	0.52
1:A:1073:U:OP2	5:E:57:LYS:HE2	2.08	0.52
1:A:1329:A:H5'	13:M:29:ARG:HD2	1.91	0.52
27:A:1956:SRV:O51	12:L:46:LYS:HE3	2.10	0.52
17:Q:34:LYS:HG3	17:Q:35:VAL:N	2.24	0.52
2:B:108:ILE:O	2:B:111:ARG:HB2	2.09	0.52
3:C:59:ARG:HG2	3:C:64:VAL:HG13	1.90	0.52
11:K:85:ARG:HE	11:K:111:ASP:HB3	1.74	0.52
1:A:248:C:C2'	1:A:249:U:H5'	2.39	0.52
1:A:983:A:H1'	1:A:1049:U:O2	2.09	0.52
1:A:1296:C:H5''	1:A:1297:C:OP2	2.09	0.52
1:A:1533:C:O2'	1:A:1534:C:P	2.66	0.52
3:C:61:ALA:C	3:C:63:ASN:H	2.17	0.52
5:E:76:ILE:HG23	5:E:142:LEU:HD13	1.89	0.52
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.91	0.52
12:L:76:ASN:O	12:L:77:LEU:HD23	2.09	0.52
14:N:5:ALA:O	14:N:8:GLU:HG3	2.09	0.52
1:A:261:U:C5	20:T:79:ARG:NH1	2.78	0.52
1:A:315:A:OP1	29:A:2618:HOH:O	2.18	0.52
1:A:914:A:OP1	27:A:1956:SRV:CI3	2.58	0.52
1:A:1286:A:C8	1:A:1287:A:H5''	2.44	0.52
2:B:11:LEU:HD23	2:B:16:HIS:CE1	2.45	0.52
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.91	0.52
3:C:11:ARG:NH1	3:C:177:THR:O	2.43	0.52
5:E:43:LEU:O	5:E:65:ASN:ND2	2.42	0.52
16:P:28:ARG:HG2	16:P:28:ARG:HH11	1.75	0.52
14:N:9:LYS:HD2	14:N:9:LYS:C	2.35	0.52
20:T:43:LEU:HD13	20:T:51:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:A:H3'	27:A:1956:SRV:HG21	1.91	0.52
1:A:1003:G:C2	1:A:1003(A):G:C6	2.96	0.52
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.91	0.52
1:A:192:U:H4'	20:T:57:ARG:HD3	1.92	0.52
1:A:1442:G:C5	1:A:1446:A:N6	2.78	0.52
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.91	0.52
3:C:111:LEU:HD21	3:C:144:SER:O	2.10	0.52
6:F:74:ASP:O	6:F:77:ARG:HB3	2.10	0.52
13:M:8:GLU:HG2	13:M:22:ILE:HD13	1.92	0.52
1:A:1068:G:OP2	1:A:1068:G:H8	1.93	0.52
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.92	0.52
18:R:46:GLU:OE2	18:R:46:GLU:N	2.31	0.52
1:A:992:U:O2'	29:A:2728:HOH:O	2.19	0.52
1:A:1062:U:H2'	1:A:1063:C:C6	2.45	0.52
3:C:130:VAL:HG11	3:C:157:ILE:CG2	2.40	0.52
5:E:117:ASP:OD2	5:E:117:ASP:N	2.43	0.52
1:A:190(F):G:H4'	1:A:190(G):G:OP2	2.09	0.52
1:A:1053:G:O2'	1:A:1199:U:H5	1.92	0.52
1:A:1407:5MC:H2'	1:A:1408:A:H5'	1.90	0.52
2:B:207:ALA:O	2:B:211:ILE:HG13	2.09	0.52
4:D:162:LEU:HD13	4:D:181:MET:HG2	1.91	0.52
5:E:101:ILE:HD12	5:E:101:ILE:N	2.23	0.52
15:O:26:GLU:CD	15:O:77:ARG:HH12	2.18	0.52
17:Q:100:LYS:CB	17:Q:101:ARG:HH11	2.23	0.52
1:A:983:A:H3'	1:A:983:A:N3	2.25	0.51
1:A:1112:C:N3	3:C:178:LEU:HB2	2.24	0.51
1:A:1258:G:H2'	1:A:1259:C:C6	2.45	0.51
1:A:1269:A:H2	1:A:1312:G:N3	2.08	0.51
1:A:1434:A:H2'	1:A:1435:G:O4'	2.10	0.51
4:D:21:LEU:HD21	4:D:66:ARG:O	2.11	0.51
13:M:58:GLU:HA	13:M:58:GLU:OE2	2.09	0.51
1:A:984:C:H42	1:A:1221:G:H1	1.58	0.51
3:C:7:PRO:HG2	3:C:184:TYR:HB2	1.92	0.51
3:C:64:VAL:HB	3:C:99:VAL:HB	1.91	0.51
4:D:24:GLU:O	4:D:25:ARG:HB3	2.11	0.51
9:I:8:GLY:CA	9:I:79:LEU:HB3	2.40	0.51
10:J:66:ARG:HH11	10:J:66:ARG:HG3	1.75	0.51
12:L:113:ARG:HH11	12:L:116:SER:H	1.57	0.51
21:U:10:ARG:NH1	21:U:10:ARG:CG	2.72	0.51
1:A:390:C:H2'	1:A:391:G:H8	1.75	0.51
1:A:563:A:H2'	1:A:567:G:C8	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:A:H1'	6:F:73:ASN:ND2	2.25	0.51
1:A:1256:A:H4'	1:A:1257:U:C5'	2.40	0.51
10:J:61:GLU:O	10:J:61:GLU:CG	2.59	0.51
20:T:67:ALA:CB	20:T:73:HIS:HA	2.40	0.51
1:A:328:C:H1'	1:A:329:A:OP2	2.11	0.51
1:A:509:A:C8	1:A:509:A:H3'	2.45	0.51
5:E:36:ASP:CG	5:E:38:GLN:HB2	2.35	0.51
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.91	0.51
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.91	0.51
19:S:12:ASP:OD2	19:S:37:ARG:NH2	2.40	0.51
1:A:1000:U:H2'	1:A:1001:A:C8	2.46	0.51
10:J:46:ARG:HH11	10:J:46:ARG:HG3	1.76	0.51
1:A:1126:U:N3	1:A:1127:G:N2	2.58	0.51
4:D:152:SER:O	4:D:155:LEU:HB2	2.11	0.51
5:E:137:GLU:OE2	5:E:140:ARG:HD2	2.11	0.51
24:a:31:C:O2'	24:a:32:U:O5'	2.22	0.51
1:A:560:U:H5'	1:A:560:U:C6	2.45	0.51
1:A:910:C:OP2	12:L:21:LYS:NZ	2.31	0.51
1:A:1527:C:C2'	1:A:1528:U:H5'	2.41	0.51
12:L:6:THR:HG1	12:L:9:GLN:HG3	1.76	0.51
1:A:179:A:H2'	1:A:180:U:C6	2.45	0.51
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.41	0.51
13:M:2:ALA:O	13:M:10:PRO:HD2	2.11	0.51
1:A:991:U:HO2'	1:A:992:U:P	2.33	0.51
1:A:1109:C:OP2	3:C:176:HIS:ND1	2.43	0.51
1:A:1206:G:C6	1:A:1207:2MG:C5	2.98	0.51
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.93	0.51
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.92	0.51
4:D:9:CYS:O	4:D:13:ARG:HG3	2.10	0.51
19:S:12:ASP:CG	19:S:37:ARG:HH21	2.19	0.51
1:A:687:A:H4'	1:A:688:G:O5'	2.11	0.51
1:A:767:A:H2'	1:A:768:A:O4'	2.10	0.51
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.38	0.51
18:R:22:VAL:O	18:R:26:LEU:HD13	2.11	0.51
1:A:383:A:C5	1:A:384:G:H1'	2.46	0.50
1:A:510:A:H5''	1:A:511:C:P	2.50	0.50
2:B:204:ASN:C	2:B:204:ASN:OD1	2.52	0.50
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.46	0.50
20:T:56:MET:HE3	20:T:88:VAL:HG11	1.92	0.50
1:A:328:C:C2'	1:A:329:A:OP2	2.59	0.50
1:A:1054:C:N4	23:W:34:G:C8	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:G:C2'	1:A:1301:U:OP2	2.59	0.50
3:C:47:LEU:CD2	3:C:68:VAL:HG11	2.42	0.50
13:M:96:LEU:HB3	13:M:97:PRO:CD	2.40	0.50
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.10	0.50
17:Q:5:VAL:HG22	17:Q:60:ILE:HD12	1.94	0.50
19:S:10:PHE:C	19:S:10:PHE:CD2	2.89	0.50
1:A:1347:G:H22	1:A:1374:A:P	2.35	0.50
2:B:139:LYS:NZ	2:B:143:GLU:HG3	2.26	0.50
13:M:37:THR:O	13:M:55:ARG:HD2	2.11	0.50
15:O:18:PHE:HB2	15:O:19:PRO:CD	2.41	0.50
20:T:69:GLY:O	20:T:73:HIS:ND1	2.44	0.50
1:A:1226:C:H4'	19:S:80:TYR:CE2	2.47	0.50
5:E:75:THR:HG23	5:E:76:ILE:O	2.10	0.50
9:I:126:SER:C	9:I:128:ARG:H	2.19	0.50
12:L:39:VAL:HG23	12:L:57:LYS:HB2	1.93	0.50
1:A:83:U:H3'	1:A:83:U:H6	1.76	0.50
1:A:117:G:O5'	1:A:117:G:H8	1.94	0.50
1:A:715:A:H2'	1:A:716:A:C8	2.47	0.50
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.94	0.50
1:A:1233:G:H2'	1:A:1234:C:C6	2.46	0.50
2:B:28:PHE:CD2	2:B:190:THR:HA	2.46	0.50
9:I:125:TYR:CE1	9:I:127:LYS:HB2	2.47	0.50
13:M:108:ARG:NH2	13:M:114:ARG:HA	2.27	0.50
19:S:15:LEU:O	19:S:19:VAL:HG12	2.11	0.50
2:B:24:TRP:O	2:B:24:TRP:CG	2.64	0.50
8:H:104:ARG:O	8:H:105:ARG:C	2.55	0.50
21:U:5:ASP:O	21:U:11:GLY:HA3	2.11	0.50
1:A:1190:G:OP1	3:C:4:LYS:HA	2.12	0.50
1:A:1203:C:O5'	1:A:1203:C:H6	1.94	0.50
1:A:1330:U:OP1	13:M:23:TYR:O	2.28	0.50
3:C:58:GLU:HB2	3:C:65:ALA:CB	2.42	0.50
7:G:145:ALA:C	7:G:147:ALA:H	2.19	0.50
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.50
1:A:933:G:O6	7:G:3:ARG:NH2	2.45	0.50
1:A:1425:U:H2'	1:A:1426:C:C6	2.45	0.50
1:A:130:A:C8	17:Q:63:ARG:HG3	2.47	0.50
1:A:1053:G:C4'	1:A:1054:C:H5'	2.42	0.50
2:B:139:LYS:HE2	2:B:139:LYS:HA	1.93	0.50
7:G:9:VAL:HG12	7:G:10:ARG:O	2.11	0.50
14:N:61:TRP:O	14:N:61:TRP:CD1	2.65	0.50
1:A:112:G:O2'	1:A:113:G:H5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:U:H4'	1:A:216:G:O4'	2.11	0.49
1:A:1202:G:O2'	14:N:29:ARG:HB3	2.12	0.49
1:A:1212:U:H5''	1:A:1213:A:C8	2.47	0.49
4:D:170:VAL:CG1	4:D:171:GLY:N	2.75	0.49
11:K:87:THR:O	11:K:87:THR:OG1	2.30	0.49
13:M:65:LYS:O	13:M:70:LEU:HG	2.12	0.49
15:O:67:LEU:HD13	15:O:82:ILE:HD11	1.94	0.49
17:Q:40:LYS:HG2	17:Q:41:LYS:N	2.26	0.49
1:A:953:G:C5'	1:A:965:A:H61	2.23	0.49
1:A:1004:A:H62	1:A:1037:C:N4	2.10	0.49
2:B:19:HIS:CD2	2:B:191:ASP:OD1	2.65	0.49
3:C:85:ARG:HG2	3:C:85:ARG:NH1	2.27	0.49
5:E:8:GLU:HB3	5:E:34:VAL:HG12	1.93	0.49
5:E:36:ASP:C	5:E:38:GLN:H	2.19	0.49
5:E:100:VAL:C	5:E:101:ILE:HD12	2.37	0.49
9:I:48:GLU:OE1	9:I:51:ARG:NE	2.42	0.49
18:R:25:THR:C	18:R:26:LEU:HD12	2.37	0.49
1:A:1063:C:H3'	1:A:1064:G:H2'	1.95	0.49
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.47	0.49
6:F:101:ALA:HA	18:R:28:GLU:HB3	1.93	0.49
12:L:28:LYS:HG2	12:L:30:ALA:HB2	1.94	0.49
1:A:840:C:H4'	1:A:848:C:O2	2.12	0.49
1:A:980:C:H5''	1:A:981:U:OP2	2.13	0.49
9:I:118:LYS:C	9:I:120:ARG:H	2.19	0.49
12:L:34:ARG:O	12:L:61:THR:HG23	2.13	0.49
16:P:12:LYS:C	16:P:14:ASN:H	2.20	0.49
1:A:399:G:OP1	29:A:2090:HOH:O	2.20	0.49
1:A:665:A:N3	1:A:732:C:H2'	2.27	0.49
1:A:858:G:O2'	1:A:859:A:H5'	2.12	0.49
1:A:1149:C:O2'	1:A:1280:A:N1	2.42	0.49
9:I:4:TYR:CZ	9:I:88:TYR:HD1	2.30	0.49
1:A:872:A:H4'	1:A:873:A:OP1	2.13	0.49
1:A:961:U:C2'	1:A:962:C:H5'	2.43	0.49
1:A:575:G:O2'	1:A:821:G:H5'	2.11	0.49
7:G:15:ASP:O	7:G:19:GLY:HA2	2.12	0.49
7:G:111:ARG:HB3	7:G:113:GLU:HG2	1.94	0.49
2:B:48:MET:O	2:B:52:GLU:HG3	2.12	0.49
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.90	0.49
4:D:83:SER:HA	4:D:89:THR:HG23	1.94	0.49
6:F:82:ARG:HA	6:F:82:ARG:HE	1.76	0.49
7:G:16:LEU:H	7:G:16:LEU:HD22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.40	0.49
20:T:50:GLU:HG3	20:T:100:ILE:HG12	1.93	0.49
1:A:524:G:H2'	1:A:525:C:C6	2.48	0.49
1:A:741:G:H2'	1:A:742:G:O4'	2.13	0.49
4:D:31:CYS:O	4:D:32:ALA:HB3	2.13	0.49
6:F:69:GLU:H	6:F:69:GLU:CD	2.21	0.49
7:G:5:ARG:HH12	7:G:8:GLU:HG2	1.77	0.49
7:G:43:PHE:O	7:G:46:ALA:HB3	2.13	0.49
12:L:46:LYS:C	12:L:48:PRO:HD2	2.37	0.49
1:A:1047:G:H5''	14:N:4:LYS:CD	2.39	0.49
1:A:1095:U:H2'	1:A:1096:C:C6	2.48	0.49
3:C:126:ARG:O	3:C:127:ARG:CB	2.60	0.49
3:C:136:GLN:O	3:C:140:ARG:HG3	2.13	0.49
1:A:88:A:C6	1:A:89:C:N3	2.81	0.48
1:A:1073:U:P	5:E:57:LYS:HE2	2.53	0.48
1:A:1198:G:H2'	1:A:1199:U:C6	2.48	0.48
1:A:1540:PSU:C2	1:A:1541:PSU:C2	3.01	0.48
2:B:75:LYS:CA	2:B:78:GLN:HG3	2.39	0.48
9:I:69:GLY:O	9:I:73:GLN:HG3	2.13	0.48
19:S:5:LEU:O	19:S:6:LYS:HB2	2.13	0.48
1:A:1047:G:O2'	1:A:1048:G:H5'	2.13	0.48
8:H:70:GLN:OE1	8:H:70:GLN:HA	2.13	0.48
1:A:461:C:H4'	1:A:462:G:OP2	2.13	0.48
1:A:608:A:OP2	29:A:2345:HOH:O	2.20	0.48
1:A:959:A:H3'	1:A:960:U:H5''	1.94	0.48
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.95	0.48
1:A:1281:U:H5'	1:A:1282:C:H5	1.77	0.48
1:A:1378:C:O2	7:G:76:ARG:NH1	2.42	0.48
3:C:6:HIS:HD2	3:C:8:ILE:HB	1.75	0.48
4:D:50:ARG:HH22	5:E:9:LYS:NZ	2.11	0.48
15:O:22:THR:O	15:O:27:VAL:HG11	2.13	0.48
1:A:56:U:H2'	1:A:57:G:H8	1.78	0.48
1:A:1065:U:C1'	1:A:1066:C:OP2	2.62	0.48
1:A:1072:G:C5	1:A:1073:U:C4	3.02	0.48
1:A:1112:C:C2	3:C:178:LEU:HB2	2.48	0.48
3:C:126:ARG:HG3	3:C:128:PHE:N	2.27	0.48
4:D:150:GLU:CD	4:D:150:GLU:H	2.19	0.48
1:A:80:G:C2	1:A:81:U:N3	2.79	0.48
1:A:519:C:H2'	1:A:520:A:C8	2.49	0.48
1:A:1103:C:C5'	2:B:98:LEU:HD12	2.43	0.48
1:A:1300:G:C6	1:A:1335:C:C5	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:U:H2'	1:A:1496:C:C6	2.48	0.48
4:D:79:PHE:HE1	4:D:204:ILE:HD12	1.79	0.48
5:E:98:THR:N	5:E:117:ASP:OD1	2.42	0.48
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.96	0.48
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.49	0.48
9:I:26:VAL:HG23	9:I:33:PHE:HB2	1.94	0.48
9:I:75:ASP:O	9:I:78:LYS:HB3	2.14	0.48
1:A:179:A:H2'	1:A:180:U:H6	1.78	0.48
1:A:256:U:OP1	17:Q:17:LYS:NZ	2.46	0.48
1:A:1064:G:H22	1:A:1190:G:C2'	2.26	0.48
10:J:99:LYS:HG3	10:J:99:LYS:O	2.13	0.48
16:P:74:LEU:N	16:P:74:LEU:HD23	2.28	0.48
1:A:250:A:C4'	1:A:251:G:O5'	2.61	0.48
6:F:53:ALA:C	6:F:54:LYS:HG2	2.39	0.48
7:G:75:VAL:CG1	7:G:144:MET:HE3	2.43	0.48
10:J:6:ILE:HB	10:J:72:VAL:HG21	1.94	0.48
1:A:89:C:H3'	1:A:89:C:C6	2.47	0.48
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.94	0.48
5:E:78:HIS:HE1	5:E:142:LEU:HD23	1.78	0.48
10:J:38:ILE:O	10:J:70:ARG:HA	2.14	0.48
11:K:24:SER:C	11:K:26:ASN:N	2.71	0.48
11:K:24:SER:C	11:K:26:ASN:H	2.22	0.48
11:K:88:GLY:O	11:K:89:ALA:C	2.57	0.48
1:A:359:U:H2'	1:A:360:A:C8	2.49	0.48
1:A:376:G:P	16:P:67:THR:HG21	2.53	0.48
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.48
1:A:1018:C:H2'	1:A:1019:C:C6	2.48	0.48
10:J:47:PHE:HD2	14:N:34:TYR:CD2	2.32	0.48
11:K:29:ILE:HB	11:K:44:SER:HB3	1.95	0.48
14:N:5:ALA:O	14:N:8:GLU:CG	2.62	0.48
14:N:26:ARG:HE	14:N:47:LEU:HD11	1.79	0.48
17:Q:68:ARG:N	17:Q:70:ARG:HH11	2.11	0.48
17:Q:95:TYR:O	17:Q:98:LEU:HD12	2.13	0.48
1:A:118:U:H3'	1:A:288:A:H61	1.78	0.48
1:A:502:G:H2'	1:A:503:C:O4'	2.14	0.48
1:A:976:G:C8	1:A:1358:U:O2	2.67	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.96	0.48
3:C:112:SER:O	3:C:116:VAL:HG23	2.14	0.48
4:D:4:TYR:O	4:D:4:TYR:CD2	2.66	0.48
6:F:3:ARG:NH1	6:F:38:GLU:OE2	2.47	0.48
8:H:88:LYS:O	8:H:89:PRO:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:59:TYR:C	13:M:59:TYR:CD2	2.92	0.48
18:R:40:LEU:HD23	18:R:40:LEU:HA	1.65	0.48
1:A:991:U:O2'	1:A:992:U:P	2.71	0.47
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.56	0.47
5:E:90:VAL:O	5:E:91:LEU:HD23	2.13	0.47
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.32	0.47
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.31	0.47
10:J:48:THR:O	14:N:34:TYR:OH	2.31	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.49	0.47
16:P:28:ARG:NH1	16:P:29:ASP:OD2	2.47	0.47
1:A:695:A:OP1	11:K:52:GLY:HA3	2.14	0.47
1:A:738:C:OP1	6:F:92:LYS:HD3	2.14	0.47
1:A:983:A:H5'	1:A:984:C:OP2	2.14	0.47
1:A:1064:G:N2	1:A:1190:G:C2'	2.77	0.47
1:A:1493:A:H5''	1:A:1494:G:OP2	2.15	0.47
2:B:229:VAL:O	2:B:229:VAL:HG12	2.14	0.47
8:H:103:VAL:HG21	8:H:109:ILE:C	2.39	0.47
11:K:33:THR:HG22	11:K:39:PRO:CA	2.41	0.47
12:L:28:LYS:HB3	12:L:30:ALA:HB2	1.96	0.47
13:M:10:PRO:O	13:M:11:ARG:HB2	2.15	0.47
18:R:22:VAL:HG23	18:R:55:ARG:O	2.14	0.47
1:A:89:C:C6	1:A:89:C:C3'	2.97	0.47
1:A:191:G:N2	20:T:103:GLY:O	2.42	0.47
1:A:1190:G:O2'	1:A:1191:A:OP2	2.17	0.47
4:D:169:LYS:HE2	4:D:169:LYS:HB2	1.62	0.47
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.97	0.47
19:S:5:LEU:CG	19:S:6:LYS:N	2.77	0.47
1:A:510:A:P	29:A:2174:HOH:O	2.71	0.47
1:A:862:C:H5''	29:A:2651:HOH:O	2.14	0.47
1:A:1133:G:H1	1:A:1141:C:H42	1.62	0.47
1:A:1346:A:N1	1:A:1374:A:H5''	2.29	0.47
1:A:1397:C:H4'	1:A:1398:A:OP2	2.14	0.47
5:E:81:GLU:OE2	5:E:88:LYS:NZ	2.40	0.47
6:F:25:ILE:HD13	6:F:82:ARG:HD2	1.96	0.47
7:G:5:ARG:NH1	7:G:8:GLU:HG2	2.30	0.47
17:Q:18:THR:HG23	17:Q:69:LYS:HD3	1.97	0.47
1:A:180:U:H2'	1:A:181:G:H5'	1.96	0.47
1:A:1281:U:H5'	1:A:1282:C:C5	2.50	0.47
3:C:14:ILE:C	3:C:15:THR:HG23	2.39	0.47
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.97	0.47
5:E:8:GLU:CB	5:E:34:VAL:HG12	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:66:LEU:O	13:M:69:GLU:HG2	2.13	0.47
15:O:87:ILE:HG22	15:O:88:ARG:HG2	1.97	0.47
1:A:47:C:H4'	1:A:48:C:OP1	2.14	0.47
1:A:890:G:O2'	1:A:906:G:O6	2.22	0.47
1:A:993:G:H4'	1:A:994:A:OP2	2.14	0.47
2:B:41:ILE:HD12	2:B:41:ILE:N	2.29	0.47
3:C:19:GLU:HG2	3:C:54:ARG:HE	1.79	0.47
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.43	0.47
6:F:78:GLU:O	6:F:81:ILE:HG12	2.15	0.47
10:J:82:ILE:O	10:J:82:ILE:HG22	2.15	0.47
13:M:16:ASP:HB3	13:M:34:LEU:HD12	1.97	0.47
14:N:21:TYR:HE2	14:N:23:ARG:NE	2.12	0.47
1:A:577:G:H1'	1:A:816:A:C4	2.50	0.47
1:A:689:C:OP1	11:K:27:ASN:ND2	2.48	0.47
1:A:1098:C:H2'	1:A:1099:G:O4'	2.15	0.47
1:A:1236:A:H4'	1:A:1304:G:H4'	1.95	0.47
1:A:1372:U:H5''	9:I:71:SER:HB2	1.95	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.77	0.47
1:A:1494:G:OP2	1:A:1494:G:H8	1.98	0.47
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.22	0.47
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.47
4:D:28:SER:O	4:D:30:LYS:N	2.44	0.47
4:D:70:ILE:HD11	4:D:100:ARG:NE	2.29	0.47
5:E:66:MET:HE3	5:E:66:MET:HB3	1.88	0.47
7:G:10:ARG:HG2	7:G:10:ARG:NH1	2.25	0.47
8:H:36:LEU:O	8:H:37:ARG:C	2.56	0.47
8:H:116:LYS:HD3	8:H:127:LEU:HD13	1.97	0.47
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.47	0.47
11:K:59:TYR:CE2	11:K:63:LEU:HD11	2.49	0.47
13:M:88:ARG:HG2	13:M:98:VAL:HG12	1.97	0.47
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.97	0.47
20:T:20:LEU:HD13	20:T:20:LEU:HA	1.65	0.47
20:T:57:ARG:NH2	20:T:100:ILE:HD12	2.30	0.47
1:A:922:G:H1'	5:E:19:MET:HB3	1.95	0.47
1:A:1035:A:N6	1:A:1036:G:O6	2.48	0.47
1:A:1349:A:C2	1:A:1374:A:C4	3.03	0.47
2:B:100:GLY:O	2:B:104:ASN:N	2.44	0.47
2:B:186:ALA:HB3	2:B:197:VAL:HG11	1.95	0.47
3:C:64:VAL:HG12	3:C:65:ALA:H	1.80	0.47
4:D:146:ILE:N	4:D:146:ILE:HD12	2.29	0.47
7:G:10:ARG:HH11	7:G:10:ARG:CG	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:THR:HB	11:K:38:ASN:O	2.14	0.47
1:A:58:C:O5'	1:A:58:C:H6	1.97	0.47
1:A:90:U:C2'	1:A:91:C:O5'	2.63	0.47
1:A:527:7MG:O2'	1:A:535:A:N1	2.42	0.47
1:A:695:A:H61	1:A:797:C:H1'	1.80	0.47
1:A:1358:U:OP1	14:N:35:ARG:HG3	2.14	0.47
3:C:54:ARG:HB2	3:C:54:ARG:HH11	1.79	0.47
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.97	0.47
7:G:91:VAL:HG12	7:G:96:GLN:HG3	1.96	0.47
8:H:27:PRO:HA	8:H:58:TYR:CD2	2.50	0.47
19:S:31:ILE:O	19:S:50:ALA:HB3	2.14	0.47
1:A:558:G:H3'	1:A:559:A:H3'	1.97	0.47
1:A:1529:G:OP2	1:A:1529:G:H3'	2.15	0.47
2:B:44:LEU:N	2:B:44:LEU:HD22	2.30	0.47
5:E:11:ILE:O	5:E:12:LEU:HB2	2.13	0.47
14:N:13:THR:N	14:N:14:PRO:HD3	2.30	0.47
1:A:187:C:O2	20:T:105:SER:HB3	2.15	0.46
1:A:344:A:H5''	1:A:345:C:H5	1.80	0.46
1:A:499:A:C4'	1:A:500:G:OP1	2.56	0.46
1:A:736:C:H2'	1:A:737:A:C8	2.50	0.46
1:A:1091:U:O2	1:A:1093:A:C8	2.68	0.46
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.96	0.46
1:A:1347:G:N2	1:A:1373:G:H2'	2.30	0.46
1:A:1392:G:N2	1:A:1502:A:C8	2.80	0.46
1:A:1477:C:H2'	1:A:1478:C:H6	1.80	0.46
3:C:186:PHE:C	3:C:186:PHE:CD2	2.93	0.46
4:D:8:VAL:O	4:D:11:LEU:N	2.41	0.46
4:D:206:PHE:CE2	4:D:207:TYR:CE2	3.03	0.46
6:F:12:PRO:HG3	6:F:57:GLN:O	2.15	0.46
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.69	0.46
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.50	0.46
1:A:853:G:C2'	1:A:854:G:H5'	2.46	0.46
1:A:1077:G:N2	1:A:1080:A:OP2	2.43	0.46
2:B:128:GLU:HA	2:B:135:GLN:NE2	2.30	0.46
1:A:115:G:H1'	1:A:116:A:N7	2.31	0.46
1:A:960:U:O2	1:A:960:U:H2'	2.13	0.46
1:A:1329:A:OP2	21:U:7:ARG:NH2	2.47	0.46
2:B:46:LYS:HD3	2:B:49:GLU:OE1	2.15	0.46
20:T:79:ARG:HD2	20:T:83:ARG:NH1	2.31	0.46
1:A:126:G:N1	29:A:2119:HOH:O	2.34	0.46
1:A:1112:C:C4	3:C:178:LEU:HD23	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1420:C:H2'	1:A:1421:G:O4'	2.15	0.46
3:C:14:ILE:C	3:C:16:ARG:N	2.74	0.46
4:D:127:THR:HG23	4:D:147:ALA:O	2.15	0.46
6:F:14:LEU:HD22	6:F:18:GLN:CB	2.45	0.46
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.96	0.46
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.31	0.46
19:S:40:ILE:CG2	19:S:62:ILE:HD11	2.43	0.46
1:A:586:C:C2'	1:A:587:G:H5'	2.45	0.46
1:A:1311:G:N7	19:S:2:PRO:HA	2.30	0.46
3:C:179:ARG:HD2	3:C:207:VAL:HG22	1.97	0.46
5:E:48:ALA:HB1	5:E:49:PRO:HD2	1.96	0.46
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.50	0.46
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.69	0.46
15:O:43:LEU:HD11	15:O:53:HIS:HA	1.97	0.46
17:Q:4:LYS:HD2	17:Q:6:LEU:HD21	1.98	0.46
20:T:53:LEU:HD13	20:T:100:ILE:HG22	1.96	0.46
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.98	0.46
1:A:186:C:H2'	1:A:187:C:C6	2.51	0.46
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.37	0.46
1:A:1080:A:H4'	5:E:16:THR:HG21	1.97	0.46
1:A:1439:C:OP1	20:T:38:LYS:HE3	2.15	0.46
1:A:1468:A:H2'	1:A:1469:G:O4'	2.16	0.46
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.96	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.78	0.46
11:K:121:PRO:HB2	11:K:126:ARG:HG3	1.98	0.46
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.97	0.46
18:R:39:VAL:CG1	18:R:40:LEU:N	2.79	0.46
20:T:67:ALA:HB1	20:T:73:HIS:HA	1.98	0.46
1:A:1251:A:C4'	9:I:12:GLU:OE1	2.63	0.46
2:B:230:VAL:HG12	2:B:231:GLU:O	2.15	0.46
6:F:45:LEU:HD12	6:F:45:LEU:O	2.15	0.46
1:A:262:A:C6	1:A:263:A:C6	3.03	0.46
1:A:629:G:H2'	1:A:630:G:O4'	2.16	0.46
1:A:984:C:N4	1:A:1221:G:H1	2.14	0.46
1:A:1320:C:O2	19:S:36:ARG:NH1	2.49	0.46
2:B:112:VAL:O	2:B:115:LEU:HB3	2.16	0.46
3:C:112:SER:HB3	3:C:115:LEU:HD12	1.97	0.46
5:E:144:THR:HB	5:E:147:ASP:OD1	2.16	0.46
16:P:57:ARG:HD3	16:P:79:VAL:O	2.16	0.46
1:A:614:A:H2'	1:A:615:C:H6	1.81	0.46
1:A:1032:G:H2'	1:A:1033:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:U:C4	1:A:1127:G:C2	3.04	0.46
1:A:1540:PSU:H6	1:A:1540:PSU:O5'	1.99	0.46
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.45	0.46
7:G:10:ARG:NH1	7:G:10:ARG:CG	2.77	0.46
14:N:14:PRO:O	14:N:15:LYS:HB3	2.16	0.46
1:A:151:A:H2'	1:A:152:A:O4'	2.15	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.46
2:B:69:LEU:C	2:B:69:LEU:CD2	2.89	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.81	0.45
1:A:614:A:H2'	1:A:615:C:C6	2.50	0.45
1:A:1329:A:O2'	1:A:1330:U:H5'	2.15	0.45
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.51	0.45
12:L:76:ASN:O	12:L:76:ASN:OD1	2.34	0.45
25:b:1:U:O5'	25:b:1:U:H6	2.00	0.45
1:A:21:G:H2'	1:A:22:G:C8	2.51	0.45
1:A:68:G:C2'	1:A:69:G:O5'	2.65	0.45
1:A:411:A:C6	1:A:429:U:C5	3.04	0.45
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.31	0.45
2:B:165:VAL:O	2:B:187:LEU:O	2.34	0.45
3:C:8:ILE:HG13	3:C:184:TYR:HB3	1.98	0.45
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.42	0.45
5:E:24:ARG:CG	5:E:24:ARG:NH1	2.64	0.45
5:E:96:PRO:HA	5:E:117:ASP:OD1	2.17	0.45
9:I:16:ARG:HD3	9:I:64:THR:HB	1.97	0.45
10:J:48:THR:CB	10:J:62:HIS:HB3	2.46	0.45
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.45
13:M:67:GLU:HB3	13:M:68:GLY:H	1.48	0.45
19:S:52:TYR:HA	19:S:56:GLN:O	2.17	0.45
1:A:22:G:H2'	1:A:23:C:C6	2.52	0.45
1:A:130:A:OP2	1:A:190(E):U:C2'	2.64	0.45
1:A:176:C:O2'	1:A:177:C:H5'	2.16	0.45
1:A:1029:C:N3	1:A:1033:G:N2	2.64	0.45
2:B:73:THR:O	2:B:73:THR:HG22	2.16	0.45
4:D:31:CYS:C	4:D:33:MET:H	2.24	0.45
5:E:144:THR:CG2	5:E:145:LYS:N	2.79	0.45
10:J:99:LYS:HB2	10:J:99:LYS:HE3	1.85	0.45
11:K:39:PRO:O	11:K:40:ILE:HD13	2.16	0.45
15:O:31:LEU:HD12	15:O:31:LEU:HA	1.74	0.45
1:A:114:U:H1'	1:A:353:A:H1'	1.97	0.45
1:A:162:A:H5''	1:A:163:C:OP2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:A:H4'	1:A:548:G:O5'	2.16	0.45
1:A:811:C:H4'	1:A:900:A:N6	2.31	0.45
1:A:1053:G:H4'	1:A:1054:C:H5'	1.98	0.45
10:J:71:LEU:HA	10:J:71:LEU:HD23	1.74	0.45
1:A:107:G:H2'	1:A:108:G:H5''	1.99	0.45
1:A:128:G:H4'	17:Q:3:LYS:HG3	1.99	0.45
1:A:737:A:H2'	1:A:738:C:C6	2.51	0.45
1:A:981:U:H2'	1:A:982:U:C5	2.51	0.45
1:A:1003(A):G:C2	1:A:1038:C:O2	2.69	0.45
1:A:1277:C:H2'	1:A:1279:A:C8	2.51	0.45
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.52	0.45
7:G:69:VAL:HG12	7:G:69:VAL:O	2.16	0.45
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.71	0.45
9:I:37:PHE:HB3	9:I:43:ALA:HB2	1.98	0.45
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.34	0.45
11:K:58:PRO:O	11:K:61:ALA:HB3	2.16	0.45
21:U:25:LYS:NZ	21:U:25:LYS:HB3	2.32	0.45
1:A:560:U:C5'	1:A:566:G:N2	2.77	0.45
1:A:922:G:N3	1:A:1398:A:H2	2.15	0.45
1:A:961:U:H2'	1:A:962:C:H5'	1.97	0.45
1:A:1065:U:C2'	1:A:1066:C:OP2	2.64	0.45
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.97	0.45
2:B:174:VAL:O	2:B:178:ARG:HG3	2.17	0.45
4:D:12:CYS:HA	4:D:19:LEU:CD2	2.46	0.45
4:D:38:TYR:CE1	4:D:45:GLN:HG3	2.51	0.45
19:S:40:ILE:CG2	19:S:67:VAL:HA	2.41	0.45
1:A:243:A:C2	1:A:246:A:C8	3.04	0.45
1:A:793:U:H3'	1:A:794:A:C5'	2.39	0.45
1:A:1055:A:C2	1:A:1056:U:H1'	2.51	0.45
1:A:1128:C:O2'	1:A:1130:A:C8	2.65	0.45
1:A:1493:A:H4'	1:A:1494:G:OP1	2.15	0.45
1:A:229:U:H5''	16:P:33:ILE:HD13	1.99	0.45
1:A:1003(A):G:N1	1:A:1004:A:H1'	2.32	0.45
1:A:1047:G:H2'	1:A:1048:G:H5'	1.97	0.45
2:B:57:PHE:CD1	2:B:199:TYR:CZ	3.05	0.45
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.23	0.45
2:B:239:VAL:O	2:B:240:GLN:CB	2.65	0.45
3:C:91:LEU:HD21	3:C:99:VAL:HG13	1.99	0.45
4:D:172:PRO:HD2	4:D:173:TRP:CE3	2.51	0.45
1:A:1298:C:H4'	1:A:1299:A:O4'	2.16	0.45
3:C:94:LEU:HD12	3:C:94:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ALA:HB1	3:C:182:ILE:CG1	2.45	0.45
4:D:62:GLN:OE1	4:D:62:GLN:HA	2.17	0.45
8:H:85:ARG:HD2	8:H:87:SER:O	2.17	0.45
10:J:75:ILE:HG22	10:J:76:ASN:N	2.27	0.45
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.97	0.45
13:M:63:THR:HG23	13:M:64:TRP:N	2.32	0.45
1:A:1258:G:H2'	1:A:1259:C:H6	1.79	0.45
3:C:34:LEU:HG	3:C:38:ARG:NE	2.32	0.45
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.85	0.45
9:I:99:LEU:HD22	9:I:99:LEU:H	1.82	0.45
1:A:392:G:H2'	1:A:393:A:C8	2.52	0.44
1:A:1006:C:H2'	1:A:1007:C:H6	1.82	0.44
1:A:1300:G:C5	1:A:1335:C:C5	3.04	0.44
3:C:148:GLY:HA3	3:C:172:ARG:O	2.17	0.44
4:D:107:ARG:NH1	4:D:114:ARG:HH22	2.15	0.44
4:D:206:PHE:HE2	4:D:207:TYR:CE2	2.35	0.44
5:E:101:ILE:N	5:E:101:ILE:CD1	2.80	0.44
7:G:51:GLN:O	7:G:52:GLU:OE2	2.35	0.44
13:M:102:ARG:O	13:M:102:ARG:HG3	2.17	0.44
16:P:1:MET:O	16:P:1:MET:HG2	2.12	0.44
19:S:7:LYS:C	19:S:7:LYS:CD	2.90	0.44
20:T:10:LEU:HD23	20:T:13:LEU:H	1.82	0.44
1:A:266:G:H5''	1:A:268:C:H41	1.82	0.44
1:A:814:A:H2'	1:A:816:A:H5''	1.99	0.44
1:A:1158:C:H3'	1:A:1158:C:O2	2.16	0.44
1:A:1413:A:H2'	1:A:1414:U:O4'	2.17	0.44
3:C:167:TRP:HZ3	3:C:169:ALA:HB3	1.82	0.44
9:I:89:ASN:O	9:I:92:TYR:HB2	2.17	0.44
13:M:65:LYS:HB2	13:M:65:LYS:HE3	1.72	0.44
1:A:114:U:O2'	1:A:115:G:H5'	2.18	0.44
1:A:259:G:O2'	1:A:260:G:H5'	2.18	0.44
1:A:540:G:H2'	1:A:541:G:O4'	2.17	0.44
1:A:661:G:H8	1:A:661:G:H5''	1.82	0.44
2:B:40:HIS:C	2:B:41:ILE:HD12	2.42	0.44
2:B:92:TYR:O	2:B:92:TYR:CD1	2.71	0.44
2:B:97:TRP:CE3	2:B:98:LEU:O	2.71	0.44
3:C:81:GLY:O	3:C:84:ILE:HG22	2.17	0.44
3:C:156:ARG:NE	3:C:160:ALA:O	2.50	0.44
15:O:45:VAL:CG1	15:O:46:HIS:H	2.29	0.44
1:A:187:C:C2	20:T:105:SER:HB3	2.52	0.44
1:A:463:A:H2'	1:A:474:G:O4'	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:913:A:OP1	12:L:91:LYS:HE2	2.17	0.44
1:A:1054:C:C2'	1:A:1055:A:H5''	2.48	0.44
1:A:1130:A:OP1	1:A:1131:G:OP2	2.34	0.44
1:A:1373:G:H5''	7:G:36:LYS:CG	2.47	0.44
1:A:1518:MA6:H2'	1:A:1519:MA6:C8	2.47	0.44
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.98	0.44
2:B:193:ASP:C	2:B:193:ASP:OD1	2.59	0.44
12:L:53:ARG:HH12	12:L:92:OTD:CG	2.25	0.44
15:O:18:PHE:HB2	15:O:19:PRO:HD2	1.98	0.44
20:T:12:ALA:O	20:T:15:ARG:HB2	2.18	0.44
1:A:229:U:C2'	1:A:230:G:H5'	2.47	0.44
1:A:262:A:H5'	20:T:74:LYS:HD3	2.00	0.44
1:A:526:C:OP1	12:L:91:LYS:HE3	2.18	0.44
1:A:587:G:N2	1:A:754:C:OP2	2.49	0.44
1:A:685:G:C2	1:A:686:U:C4	3.06	0.44
1:A:1314:C:C6	19:S:6:LYS:HE2	2.53	0.44
1:A:1316:G:N2	1:A:1318:A:H3'	2.32	0.44
13:M:63:THR:HG23	13:M:64:TRP:H	1.83	0.44
15:O:74:ASP:HB3	15:O:77:ARG:CG	2.46	0.44
20:T:57:ARG:HH21	20:T:100:ILE:HG21	1.83	0.44
1:A:89:C:C5	1:A:90:U:N3	2.86	0.44
1:A:162:A:C5	1:A:163:C:H1'	2.53	0.44
1:A:765:G:H5''	1:A:766:A:OP1	2.16	0.44
1:A:1202:G:C2	14:N:42:ILE:HG21	2.53	0.44
1:A:57:G:H2'	1:A:58:C:C6	2.51	0.44
1:A:201:C:H42	1:A:216:G:H1	1.64	0.44
1:A:269:C:H2'	1:A:270:A:C8	2.52	0.44
1:A:952:U:H2'	1:A:953:G:H8	1.82	0.44
1:A:1112:C:H5''	1:A:1113:C:OP2	2.18	0.44
1:A:1307:U:H2'	1:A:1308:U:O4'	2.18	0.44
5:E:143:ARG:NH1	8:H:77:GLU:CD	2.75	0.44
9:I:7:THR:HG22	9:I:8:GLY:N	2.32	0.44
9:I:127:LYS:HG2	9:I:127:LYS:O	2.17	0.44
18:R:76:LEU:HA	18:R:76:LEU:HD23	1.58	0.44
1:A:1125:U:O2'	1:A:1126:U:P	2.76	0.44
4:D:108:LEU:HA	4:D:108:LEU:HD23	1.83	0.44
7:G:18:TYR:CD2	7:G:59:LEU:HD13	2.52	0.44
7:G:113:GLU:HG2	7:G:113:GLU:H	1.55	0.44
9:I:93:ARG:NH1	9:I:93:ARG:HB3	2.33	0.44
10:J:52:GLY:HA2	10:J:53:PRO:HD3	1.85	0.44
23:W:37:G:H2'	23:W:38:PSU:O4'	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:A:H2'	1:A:162:A:C8	2.53	0.44
1:A:353:A:C8	1:A:353:A:C5'	2.97	0.44
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.44
1:A:444:C:H2'	1:A:444:C:O2	2.18	0.44
1:A:559:A:H4'	1:A:560:U:O5'	2.18	0.44
1:A:926:G:N1	25:b:1:U:OP1	2.51	0.44
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.53	0.44
1:A:1162:C:H42	1:A:1174:G:H1	1.64	0.44
1:A:1245:A:C2	1:A:1293:G:C2	3.05	0.44
1:A:1511:G:H2'	1:A:1512:U:O4'	2.18	0.44
20:T:14:LYS:O	20:T:18:GLN:HG3	2.18	0.44
1:A:184:G:H2'	1:A:185:A:C8	2.53	0.43
1:A:575:G:H4'	1:A:576:G:OP1	2.16	0.43
1:A:968:A:H4'	1:A:969:A:OP2	2.18	0.43
1:A:974:A:P	14:N:41:ARG:HH12	2.39	0.43
5:E:76:ILE:CG2	5:E:77:PRO:HD2	2.48	0.43
1:A:926:G:N2	25:b:1:U:OP1	2.48	0.43
1:A:1337:G:H5''	1:A:1338:G:OP1	2.18	0.43
1:A:1369:C:H2'	1:A:1370:G:C8	2.53	0.43
1:A:1493:A:C2	23:W:37:G:O4'	2.71	0.43
27:A:1956:SRV:HI32	27:A:1956:SRV:C22	2.47	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.48	0.43
5:E:41:VAL:HG13	5:E:113:ALA:CA	2.43	0.43
9:I:51:ARG:HA	9:I:56:LEU:HG	2.00	0.43
19:S:41:VAL:HG22	19:S:44:MET:HG3	1.99	0.43
1:A:1005:A:N1	1:A:1026:G:N2	2.58	0.43
2:B:193:ASP:HB3	2:B:196:LEU:HD11	1.99	0.43
3:C:11:ARG:O	3:C:14:ILE:O	2.37	0.43
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.99	0.43
15:O:7:GLU:O	15:O:11:VAL:HG12	2.18	0.43
15:O:32:LEU:HD23	15:O:32:LEU:HA	1.73	0.43
15:O:74:ASP:OD2	15:O:77:ARG:HD3	2.17	0.43
1:A:289:G:OP2	29:A:2017:HOH:O	2.21	0.43
1:A:474:G:H5''	16:P:81:ARG:NH1	2.33	0.43
1:A:631:G:H5'	1:A:632:A:P	2.58	0.43
1:A:722:A:H4'	1:A:723:U:C5	2.53	0.43
1:A:948:C:N4	29:A:2306:HOH:O	2.50	0.43
1:A:1285:A:H4'	1:A:1286:A:O5'	2.18	0.43
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.60	0.43
7:G:113:GLU:HG3	7:G:119:ARG:HA	2.00	0.43
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:G:H2'	1:A:940:C:C6	2.53	0.43
1:A:1126:U:P	1:A:1126:U:H6	2.41	0.43
1:A:1187:G:C2	1:A:1188:A:C4	3.07	0.43
1:A:1419:G:C6	1:A:1420:C:C4	3.07	0.43
1:A:1477:C:H2'	1:A:1478:C:C6	2.53	0.43
1:A:1539:C:H2'	1:A:1540:PSU:O4'	2.18	0.43
5:E:16:THR:O	5:E:26:PHE:HA	2.18	0.43
7:G:46:ALA:O	7:G:50:ILE:HG12	2.17	0.43
1:A:84:U:C4	1:A:88:A:C2	3.07	0.43
1:A:255:G:O6	1:A:266:G:O6	2.37	0.43
1:A:345:C:OP2	1:A:345:C:H6	2.01	0.43
1:A:581:G:N1	1:A:759:A:OP2	2.35	0.43
1:A:740:U:O3'	15:O:39:LEU:HD23	2.19	0.43
1:A:1533:C:C2'	1:A:1534:C:O5'	2.66	0.43
9:I:19:LEU:HB3	9:I:59:PHE:CD2	2.54	0.43
13:M:97:PRO:HB3	13:M:101:GLN:OE1	2.18	0.43
16:P:12:LYS:O	16:P:13:HIS:HB2	2.19	0.43
18:R:85:LEU:HD23	18:R:88:LYS:HD2	2.00	0.43
1:A:187:C:N3	20:T:105:SER:HB3	2.33	0.43
1:A:510:A:H5''	1:A:511:C:OP2	2.19	0.43
1:A:1009:G:C6	1:A:1021:G:C6	3.06	0.43
1:A:1030(D):A:H2'	1:A:1031:G:H5'	2.00	0.43
3:C:34:LEU:CD2	14:N:25:VAL:HG21	2.48	0.43
5:E:147:ASP:OD1	5:E:147:ASP:N	2.52	0.43
14:N:33:VAL:HG12	14:N:40:CYS:HB3	2.00	0.43
17:Q:45:HIS:HB2	17:Q:65:ILE:HG13	2.00	0.43
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.53	0.43
20:T:37:SER:O	20:T:38:LYS:C	2.60	0.43
1:A:103:C:P	20:T:17:ARG:NH1	2.92	0.43
1:A:509:A:HO2'	1:A:510:A:P	2.38	0.43
1:A:1130:A:H3'	1:A:1130:A:OP2	2.19	0.43
1:A:1494:G:OP2	1:A:1494:G:C8	2.72	0.43
7:G:40:ALA:HB3	9:I:41:VAL:HG21	2.00	0.43
9:I:24:GLY:CA	9:I:57:GLY:HA2	2.45	0.43
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.84	0.43
11:K:50:TYR:HE2	11:K:54:ARG:NH1	2.14	0.43
12:L:92:0TD:OD1	12:L:92:0TD:C	2.66	0.43
20:T:56:MET:HE3	20:T:88:VAL:CG1	2.49	0.43
1:A:76:C:H42	1:A:93:G:H1	1.65	0.43
1:A:250:A:H4'	1:A:251:G:C5'	2.49	0.43
1:A:410:G:OP2	4:D:25:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:C8	1:A:1358:U:C2	3.06	0.43
1:A:977:A:C2'	1:A:978:A:H5'	2.48	0.43
1:A:1023:G:C6	1:A:1024:G:C5	3.07	0.43
5:E:90:VAL:C	5:E:91:LEU:HD23	2.43	0.43
6:F:91:VAL:HG13	18:R:72:ARG:NH2	2.34	0.43
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.49	0.43
15:O:87:ILE:C	15:O:89:GLY:H	2.26	0.43
20:T:63:ILE:HG22	20:T:77:ALA:HB1	2.00	0.43
1:A:29:G:O2'	1:A:30:U:H5'	2.18	0.43
1:A:328:C:O2'	1:A:329:A:P	2.77	0.43
1:A:1168:A:C6	1:A:1169:A:C6	3.07	0.43
1:A:1182:G:H1'	1:A:1183:A:OP2	2.19	0.43
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.43
1:A:1357:A:C8	1:A:1358:U:C5	3.07	0.43
3:C:179:ARG:HG3	3:C:206:GLU:HG2	1.99	0.43
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.19	0.43
4:D:62:GLN:O	4:D:66:ARG:HB2	2.18	0.43
10:J:86:MET:HG3	10:J:87:THR:H	1.84	0.43
18:R:70:ILE:O	18:R:73:ALA:HB3	2.19	0.43
20:T:74:LYS:HZ3	20:T:74:LYS:CB	2.32	0.43
1:A:28:G:C5	29:A:2696:HOH:O	2.71	0.42
1:A:235:C:N3	29:A:2119:HOH:O	2.52	0.42
1:A:323:U:H2'	1:A:324:G:O4'	2.18	0.42
1:A:947:G:H2'	1:A:948:C:O4'	2.18	0.42
1:A:1064:G:H1'	1:A:1190:G:H21	1.84	0.42
1:A:1438:G:H2'	1:A:1439:C:C6	2.53	0.42
1:A:1513:A:H2'	1:A:1514:C:C6	2.54	0.42
3:C:43:LEU:HD21	3:C:68:VAL:CG2	2.48	0.42
5:E:75:THR:HG23	5:E:76:ILE:N	2.33	0.42
7:G:16:LEU:HD22	7:G:16:LEU:N	2.34	0.42
17:Q:100:LYS:HB2	17:Q:101:ARG:NH1	2.33	0.42
20:T:65:LYS:O	20:T:68:LYS:HB2	2.19	0.42
1:A:92:C:H2'	1:A:93:G:H8	1.85	0.42
1:A:287:U:C2'	1:A:288:A:H5'	2.49	0.42
1:A:1028:C:C2	1:A:1034:G:N2	2.88	0.42
1:A:1218:C:H2'	1:A:1219:U:C6	2.54	0.42
1:A:1238:A:OP1	1:A:1336:C:H5	2.02	0.42
1:A:1368:G:OP2	9:I:114:TYR:N	2.52	0.42
5:E:138:ALA:O	5:E:139:LEU:C	2.61	0.42
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.34	0.42
9:I:51:ARG:CD	9:I:56:LEU:HD21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LEU:HB2	14:N:56:VAL:HG22	2.01	0.42
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.54	0.42
18:R:45:SER:O	18:R:47:THR:O	2.37	0.42
23:W:33:U:C5'	23:W:34:G:OP2	2.67	0.42
1:A:266:G:C5'	1:A:268:C:H41	2.32	0.42
1:A:560:U:C5'	1:A:566:G:C2	3.02	0.42
1:A:1032:G:H2'	1:A:1033:G:H8	1.84	0.42
1:A:1065:U:O2'	1:A:1066:C:OP2	2.26	0.42
1:A:1094:G:OP1	29:A:2239:HOH:O	2.21	0.42
1:A:1347:G:H1'	1:A:1348:U:H5	1.83	0.42
2:B:63:MET:HB3	2:B:225:ALA:HB1	2.00	0.42
2:B:239:VAL:O	2:B:239:VAL:HG12	2.18	0.42
4:D:150:GLU:OE1	4:D:151:LYS:HG2	2.19	0.42
4:D:194:LEU:HB3	4:D:196:LEU:HG	2.01	0.42
5:E:76:ILE:HG22	5:E:78:HIS:H	1.84	0.42
5:E:105:VAL:HG12	5:E:106:PRO:CD	2.49	0.42
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.52	0.42
8:H:112:LEU:N	8:H:112:LEU:CD2	2.83	0.42
13:M:8:GLU:HG2	13:M:22:ILE:CA	2.33	0.42
13:M:50:GLU:HG3	13:M:51:ALA:N	2.34	0.42
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.66	0.42
20:T:100:ILE:O	20:T:101:GLY:C	2.61	0.42
1:A:442:C:N4	1:A:492:G:H1	2.12	0.42
1:A:690:G:H2'	1:A:691:G:O4'	2.19	0.42
1:A:1015:A:N6	1:A:1016:A:C6	2.87	0.42
1:A:1233:G:H2'	1:A:1234:C:H6	1.84	0.42
1:A:1342:C:O2'	1:A:1343:G:H5'	2.19	0.42
2:B:178:ARG:O	8:H:71:GLY:HA2	2.20	0.42
4:D:50:ARG:HH22	5:E:9:LYS:HZ3	1.66	0.42
7:G:32:ARG:O	7:G:33:ASP:C	2.62	0.42
10:J:11:PHE:CD1	14:N:55:GLY:HA3	2.54	0.42
17:Q:9:VAL:O	17:Q:21:VAL:HA	2.18	0.42
1:A:291:C:O2'	1:A:292:G:H5'	2.20	0.42
1:A:738:C:OP2	6:F:92:LYS:NZ	2.35	0.42
1:A:1329:A:H2'	1:A:1330:U:H5'	1.99	0.42
4:D:191:ARG:HD2	4:D:200:GLU:OE2	2.19	0.42
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.34	0.42
10:J:51:ARG:HG2	10:J:61:GLU:HB2	2.01	0.42
10:J:64:GLU:N	14:N:59:ALA:HB2	2.35	0.42
11:K:50:TYR:CD2	11:K:54:ARG:HB3	2.54	0.42
15:O:54:ARG:O	15:O:58:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:31:ILE:HG23	19:S:32:LYS:N	2.34	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HG2	2.53	0.42
20:T:10:LEU:O	20:T:13:LEU:HG	2.20	0.42
1:A:232:G:H1'	1:A:262:A:N1	2.33	0.42
1:A:665:A:H2'	1:A:732:C:O2	2.19	0.42
1:A:875:C:O2'	8:H:14:ARG:NH1	2.53	0.42
1:A:1303:C:N4	1:A:1304:G:C6	2.88	0.42
2:B:25:ASN:ND2	2:B:193:ASP:HB2	2.34	0.42
2:B:43:ASP:OD2	2:B:46:LYS:HB2	2.20	0.42
2:B:61:LEU:HD22	2:B:64:ARG:HH12	1.84	0.42
2:B:134:GLU:HA	2:B:137:ARG:HG2	2.00	0.42
3:C:155:GLY:HA3	3:C:163:ALA:HB1	2.02	0.42
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.91	0.42
12:L:113:ARG:NH1	12:L:116:SER:H	2.18	0.42
15:O:66:LEU:HD23	15:O:66:LEU:HA	1.88	0.42
16:P:82:GLN:HE21	16:P:82:GLN:HB3	1.74	0.42
1:A:434:U:H2'	1:A:435:C:C6	2.55	0.42
1:A:1256:A:N6	1:A:1277:C:C6	2.86	0.42
1:A:1277:C:O2'	1:A:1279:A:H8	2.02	0.42
1:A:1279:A:C5'	1:A:1280:A:OP1	2.63	0.42
6:F:36:ARG:NH1	6:F:36:ARG:HB3	2.35	0.42
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.53	0.42
16:P:12:LYS:C	16:P:14:ASN:N	2.78	0.42
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.53	0.42
20:T:22:ARG:O	20:T:23:ARG:C	2.62	0.42
1:A:485:G:O2'	1:A:486:U:OP2	2.38	0.42
1:A:548:G:OP1	29:A:2609:HOH:O	2.22	0.42
1:A:1157:A:C1'	1:A:1181:G:N2	2.83	0.42
4:D:179:GLU:HA	4:D:179:GLU:OE2	2.19	0.42
8:H:102:ARG:H	8:H:102:ARG:NE	2.17	0.42
8:H:119:LEU:HB3	8:H:123:GLU:HB2	2.01	0.42
1:A:371:G:H2'	1:A:372:C:O4'	2.20	0.42
1:A:620:C:C1'	4:D:135:LEU:HD13	2.50	0.42
1:A:695:A:H2'	1:A:696:A:C8	2.55	0.42
1:A:1125:U:C3'	1:A:1126:U:C5	2.92	0.42
1:A:1203:C:H2'	1:A:1204:A:O4'	2.20	0.42
2:B:223:ILE:H	2:B:223:ILE:HG13	1.68	0.42
4:D:4:TYR:O	4:D:4:TYR:CG	2.71	0.42
5:E:91:LEU:HD22	5:E:120:THR:HG22	2.02	0.42
10:J:88:LEU:O	10:J:89:ASP:HB3	2.19	0.42
1:A:194:C:OP1	20:T:61:SER:OG	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:A:C8	1:A:623:C:C6	3.08	0.42
1:A:1359:C:OP1	14:N:22:THR:CG2	2.67	0.42
4:D:3:ARG:HG3	4:D:5:ILE:HD12	2.01	0.42
5:E:151:LEU:HD11	8:H:77:GLU:OE2	2.20	0.42
7:G:66:VAL:HG12	7:G:67:GLU:N	2.35	0.42
12:L:37:CYS:O	12:L:79:GLU:O	2.37	0.42
1:A:1527:C:O2'	1:A:1528:U:H5'	2.19	0.41
15:O:77:ARG:H	15:O:77:ARG:HG2	1.46	0.41
17:Q:59:ILE:HD13	17:Q:73:VAL:HA	2.02	0.41
20:T:67:ALA:HA	20:T:73:HIS:CA	2.49	0.41
20:T:105:SER:O	20:T:106:ALA:C	2.63	0.41
1:A:201:C:O2	1:A:201:C:H2'	2.19	0.41
1:A:426:G:OP1	4:D:38:TYR:OH	2.37	0.41
1:A:509:A:C8	1:A:509:A:C3'	3.02	0.41
1:A:665:A:H1'	1:A:733:A:O4'	2.20	0.41
1:A:754:C:O2	1:A:754:C:H3'	2.20	0.41
1:A:994:A:C2	1:A:995:C:C6	3.08	0.41
1:A:1130:A:OP1	1:A:1131:G:P	2.78	0.41
1:A:1144:G:C6	1:A:1145:C:N4	2.89	0.41
2:B:92:TYR:CD1	2:B:92:TYR:C	2.98	0.41
2:B:201:ILE:O	2:B:203:GLY:N	2.49	0.41
11:K:111:ASP:OD1	18:R:84:LYS:HG2	2.20	0.41
1:A:88:A:C5	1:A:89:C:C2	3.08	0.41
1:A:692:U:H1'	1:A:695:A:N7	2.35	0.41
1:A:1060:C:P	14:N:45:ARG:HH22	2.42	0.41
1:A:1408:A:H2'	1:A:1409:C:C6	2.56	0.41
2:B:10:LEU:HD23	2:B:10:LEU:HA	1.94	0.41
4:D:196:LEU:HA	4:D:197:PRO:HD2	1.89	0.41
4:D:204:ILE:N	4:D:204:ILE:HD13	2.35	0.41
6:F:74:ASP:OD2	6:F:74:ASP:N	2.53	0.41
10:J:42:THR:HG23	10:J:67:THR:O	2.20	0.41
11:K:109:VAL:HA	18:R:85:LEU:O	2.19	0.41
11:K:115:PRO:C	11:K:117:ASN:H	2.27	0.41
11:K:122:LYS:O	11:K:123:LYS:C	2.60	0.41
16:P:53:VAL:O	16:P:54:GLU:C	2.63	0.41
1:A:397:A:H3'	1:A:397:A:N3	2.35	0.41
1:A:840:C:H4'	1:A:848:C:C2	2.54	0.41
1:A:892:A:C2	1:A:907:A:C4	3.08	0.41
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.21	0.41
1:A:1034:G:H2'	1:A:1035:A:C8	2.56	0.41
4:D:11:LEU:HD22	4:D:66:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:13:ARG:NH2	4:D:40:PRO:HA	2.35	0.41
4:D:64:LEU:HD12	4:D:75:PHE:HZ	1.86	0.41
7:G:66:VAL:CG1	7:G:67:GLU:N	2.83	0.41
9:I:24:GLY:N	9:I:60:ASP:OD1	2.35	0.41
12:L:28:LYS:HB3	12:L:30:ALA:CB	2.50	0.41
15:O:48:LYS:HD3	15:O:48:LYS:HA	1.80	0.41
16:P:28:ARG:HG2	16:P:28:ARG:NH1	2.35	0.41
1:A:22:G:H2'	1:A:23:C:H6	1.84	0.41
1:A:235:C:N4	29:A:2120:HOH:O	2.54	0.41
1:A:803:G:C5	1:A:804:U:C4	3.08	0.41
1:A:993:G:H2'	1:A:993:G:N3	2.35	0.41
1:A:1003(A):G:N7	1:A:1004:A:N3	2.68	0.41
1:A:1080:A:H5''	5:E:16:THR:HG21	2.02	0.41
1:A:1371:G:C5	1:A:1372:U:C5	3.08	0.41
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.55	0.41
2:B:236:TYR:HD2	2:B:236:TYR:HA	1.69	0.41
5:E:76:ILE:HG23	5:E:77:PRO:HD2	2.02	0.41
5:E:87:SER:HB3	5:E:131:ILE:HD13	2.02	0.41
6:F:48:LEU:HG	6:F:57:GLN:HA	2.02	0.41
8:H:134:ILE:HA	8:H:134:ILE:HD13	1.80	0.41
18:R:52:PRO:O	18:R:56:THR:HG23	2.21	0.41
1:A:88:A:N7	1:A:89:C:N3	2.69	0.41
1:A:182:U:OP2	1:A:182:U:H6	2.03	0.41
1:A:196:A:OP1	20:T:68:LYS:NZ	2.48	0.41
1:A:370:C:C2	1:A:392:G:N2	2.89	0.41
1:A:421:U:OP2	1:A:422:C:N4	2.49	0.41
1:A:1081:G:C2'	1:A:1082:G:H5'	2.50	0.41
1:A:1194:U:O2	1:A:1194:U:H2'	2.20	0.41
1:A:1224:G:O2'	1:A:1322:C:OP1	2.34	0.41
1:A:1492:A:H2'	1:A:1493:A:C8	2.56	0.41
1:A:1516:G:H1'	1:A:1519:MA6:H101	2.03	0.41
2:B:135:GLN:O	2:B:139:LYS:HB2	2.21	0.41
3:C:22:TRP:CG	3:C:59:ARG:HD2	2.56	0.41
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.50	0.41
5:E:28:PHE:O	5:E:47:LYS:HA	2.21	0.41
14:N:50:LYS:HD3	14:N:50:LYS:HA	1.89	0.41
16:P:67:THR:HG22	16:P:68:ASP:N	2.35	0.41
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.46	0.41
1:A:1130:A:H5''	9:I:62:TYR:CE2	2.55	0.41
1:A:1143:G:H8	1:A:1143:G:O5'	2.04	0.41
1:A:1157:A:H4'	1:A:1158:C:C5'	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1359:C:OP1	14:N:22:THR:HG22	2.21	0.41
2:B:193:ASP:O	2:B:196:LEU:HD12	2.21	0.41
4:D:14:ARG:O	4:D:14:ARG:HD3	2.20	0.41
5:E:81:GLU:HA	5:E:89:ILE:O	2.21	0.41
8:H:17:THR:HG22	8:H:63:LEU:HG	2.01	0.41
20:T:30:LYS:O	20:T:31:SER:C	2.63	0.41
1:A:137:C:O2'	1:A:138:G:H5'	2.21	0.41
1:A:938:A:H8	1:A:938:A:O5'	2.04	0.41
1:A:1303:C:P	29:A:2278:HOH:O	2.79	0.41
2:B:40:HIS:CD2	2:B:190:THR:HG21	2.55	0.41
3:C:135:LYS:HE2	5:E:50:GLU:HG2	2.02	0.41
4:D:19:LEU:HD23	4:D:19:LEU:O	2.21	0.41
4:D:170:VAL:HG13	4:D:174:LEU:HB2	2.02	0.41
5:E:36:ASP:O	5:E:37:ARG:HB2	2.21	0.41
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.02	0.41
15:O:70:LEU:HA	15:O:70:LEU:HD23	1.84	0.41
18:R:43:PHE:C	18:R:51:LEU:HD12	2.46	0.41
20:T:67:ALA:HA	20:T:73:HIS:HA	2.02	0.41
1:A:28:G:N7	29:A:2696:HOH:O	2.53	0.41
1:A:79:G:H2'	1:A:80:G:H8	1.86	0.41
1:A:197:A:N1	1:A:220:G:O2'	2.52	0.41
1:A:553:A:O2'	12:L:29:GLY:O	2.37	0.41
1:A:577:G:H1'	1:A:816:A:N3	2.36	0.41
1:A:642:A:C6	1:A:643:C:C4	3.08	0.41
1:A:872:A:H2'	1:A:872:A:N3	2.35	0.41
1:A:1160:G:C6	1:A:1161:C:C4	3.08	0.41
1:A:1346:A:C4	7:G:10:ARG:NH2	2.88	0.41
2:B:100:GLY:O	2:B:101:MET:C	2.63	0.41
3:C:115:LEU:HD23	3:C:115:LEU:HA	1.85	0.41
5:E:36:ASP:C	5:E:38:GLN:N	2.79	0.41
12:L:46:LYS:HD3	12:L:94:PRO:HG3	2.01	0.41
12:L:124:LYS:HA	12:L:125:PRO:HD3	1.85	0.41
14:N:6:LEU:C	14:N:8:GLU:N	2.78	0.41
17:Q:56:VAL:HG12	17:Q:77:VAL:HB	2.03	0.41
18:R:18:ARG:HD3	18:R:18:ARG:HA	1.85	0.41
20:T:50:GLU:HG3	20:T:100:ILE:CG1	2.51	0.41
20:T:64:ASP:CG	20:T:81:LYS:HZ3	2.28	0.41
1:A:109:A:H4'	1:A:110:C:OP2	2.21	0.41
1:A:621:A:H2'	1:A:622:A:C8	2.56	0.41
1:A:978:A:O2'	1:A:1322:C:N3	2.51	0.41
1:A:1252:A:H2'	1:A:1253:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1330:U:H2'	1:A:1331:G:H5'	2.02	0.41
6:F:28:ARG:HG2	6:F:32:ASN:ND2	2.33	0.41
9:I:46:ALA:HB1	9:I:77:ILE:CG2	2.51	0.41
10:J:12:ASP:OD2	10:J:14:LYS:HB2	2.21	0.41
11:K:48:ILE:H	11:K:48:ILE:HG13	1.63	0.41
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.02	0.41
14:N:3:ARG:CZ	14:N:6:LEU:HD21	2.51	0.41
16:P:54:GLU:H	16:P:54:GLU:HG3	1.58	0.41
17:Q:22:LEU:HD12	17:Q:22:LEU:HA	1.88	0.41
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.89	0.41
1:A:689:C:P	11:K:46:GLY:HA3	2.60	0.40
1:A:731:G:OP1	1:A:766:A:H1'	2.21	0.40
1:A:786:G:C2	1:A:797:C:C2	3.09	0.40
1:A:862:C:O2'	1:A:863:U:H5'	2.21	0.40
1:A:1103:C:H2'	1:A:1104:G:O4'	2.21	0.40
1:A:1300:G:C6	1:A:1334:G:C5	3.09	0.40
1:A:1385:G:H2'	1:A:1386:G:O4'	2.22	0.40
2:B:40:HIS:HD2	2:B:190:THR:HG21	1.86	0.40
3:C:54:ARG:CB	3:C:54:ARG:NH1	2.84	0.40
4:D:11:LEU:O	4:D:12:CYS:C	2.63	0.40
4:D:25:ARG:C	4:D:27:TYR:H	2.27	0.40
10:J:46:ARG:HG3	10:J:46:ARG:NH1	2.36	0.40
19:S:42:PRO:O	19:S:45:VAL:HG23	2.20	0.40
1:A:513:C:H2'	1:A:514:C:C6	2.57	0.40
1:A:1124:G:H4'	10:J:38:ILE:HD11	2.02	0.40
2:B:79:ASP:HB3	2:B:238:LEU:HD13	2.04	0.40
3:C:35:GLU:O	3:C:36:ASP:C	2.64	0.40
4:D:79:PHE:HE1	4:D:204:ILE:CD1	2.34	0.40
5:E:80:ILE:HG22	8:H:104:ARG:HH12	1.85	0.40
9:I:10:ARG:O	9:I:11:LYS:C	2.63	0.40
18:R:50:ILE:HG12	18:R:70:ILE:HD13	2.03	0.40
20:T:42:GLN:OE1	20:T:46:GLU:HG3	2.22	0.40
1:A:1394:A:C5	1:A:1501:C:H4'	2.56	0.40
2:B:60:ASP:O	2:B:64:ARG:HB2	2.22	0.40
2:B:170:GLU:O	2:B:173:ALA:N	2.54	0.40
3:C:50:ALA:O	3:C:70:VAL:HG12	2.21	0.40
5:E:118:ILE:HG12	5:E:119:LEU:N	2.37	0.40
6:F:89:MET:CE	18:R:76:LEU:HG	2.50	0.40
10:J:7:LYS:CD	10:J:9:ARG:HH21	2.30	0.40
15:O:12:ILE:CD1	15:O:31:LEU:HD11	2.51	0.40
1:A:109:A:C6	1:A:327:A:C6	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:U:H2'	1:A:223:U:C6	2.56	0.40
1:A:224:C:H2'	1:A:225:C:H6	1.87	0.40
1:A:505:G:H2'	1:A:506:G:C8	2.57	0.40
1:A:1497:G:C3'	1:A:1498:UR3:H5'	2.52	0.40
2:B:16:HIS:NE2	2:B:17:PHE:HE2	2.20	0.40
2:B:69:LEU:HD23	2:B:70:PHE:N	2.36	0.40
2:B:86:GLU:HG3	2:B:92:TYR:HE2	1.87	0.40
2:B:121:LEU:HD22	2:B:127:ILE:HG23	2.03	0.40
2:B:218:ALA:O	2:B:222:ILE:HG13	2.21	0.40
5:E:83:GLU:CG	5:E:88:LYS:HD2	2.47	0.40
12:L:32:PHE:HB3	12:L:84:LEU:HD11	2.02	0.40
18:R:38:GLU:HA	18:R:41:LYS:HD3	2.03	0.40
18:R:53:ARG:O	18:R:54:ARG:C	2.65	0.40
1:A:659:U:OP2	15:O:8:LYS:NZ	2.44	0.40
1:A:738:C:H5''	6:F:69:GLU:HB3	2.04	0.40
3:C:69:HIS:HA	3:C:104:GLN:O	2.21	0.40
3:C:135:LYS:NZ	5:E:50:GLU:OE1	2.51	0.40
4:D:148:VAL:HG11	4:D:158:ILE:HG21	2.03	0.40
5:E:20:GLN:O	5:E:21:ALA:C	2.62	0.40
12:L:42:THR:HA	12:L:53:ARG:O	2.22	0.40
15:O:50:HIS:O	15:O:53:HIS:HB3	2.21	0.40
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.03	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	234/256 (91%)	213 (91%)	20 (8%)	1 (0%)	30	60
3	C	205/239 (86%)	186 (91%)	19 (9%)	0	100	100
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	135 (88%)	18 (12%)	0	100	100
8	H	136/138 (99%)	130 (96%)	6 (4%)	0	100	100
9	I	125/128 (98%)	112 (90%)	12 (10%)	1 (1%)	16	45
10	J	97/105 (92%)	78 (80%)	18 (19%)	1 (1%)	12	40
11	K	115/129 (89%)	103 (90%)	12 (10%)	0	100	100
12	L	122/135 (90%)	112 (92%)	7 (6%)	3 (2%)	4	23
13	M	116/126 (92%)	107 (92%)	8 (7%)	1 (1%)	14	43
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	P	82/88 (93%)	77 (94%)	5 (6%)	0	100	100
17	Q	98/105 (93%)	91 (93%)	7 (7%)	0	100	100
18	R	69/88 (78%)	61 (88%)	8 (12%)	0	100	100
19	S	79/93 (85%)	71 (90%)	6 (8%)	2 (2%)	4	23
20	T	97/106 (92%)	86 (89%)	10 (10%)	1 (1%)	12	40
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2349/2541 (92%)	2147 (91%)	192 (8%)	10 (0%)	30	60

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
20	T	73	HIS
19	S	31	ILE
12	L	115	LYS
13	M	23	TYR
9	I	119	ALA
12	L	27	LEU
19	S	6	LYS
2	B	229	VAL
10	J	34	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	201/220 (91%)	180 (90%)	21 (10%)	7	25
3	C	160/188 (85%)	132 (82%)	28 (18%)	2	9
4	D	180/181 (99%)	158 (88%)	22 (12%)	5	19
5	E	115/123 (94%)	90 (78%)	25 (22%)	1	5
6	F	90/90 (100%)	78 (87%)	12 (13%)	4	17
7	G	126/127 (99%)	112 (89%)	14 (11%)	6	22
8	H	119/119 (100%)	108 (91%)	11 (9%)	8	30
9	I	98/99 (99%)	91 (93%)	7 (7%)	13	40
10	J	87/92 (95%)	77 (88%)	10 (12%)	5	21
11	K	89/99 (90%)	81 (91%)	8 (9%)	9	31
12	L	103/110 (94%)	89 (86%)	14 (14%)	3	16
13	M	94/101 (93%)	83 (88%)	11 (12%)	5	20
14	N	49/50 (98%)	43 (88%)	6 (12%)	5	19
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	11
16	P	72/74 (97%)	65 (90%)	7 (10%)	8	28
17	Q	95/97 (98%)	83 (87%)	12 (13%)	4	18
18	R	62/77 (80%)	57 (92%)	5 (8%)	11	36
19	S	71/80 (89%)	65 (92%)	6 (8%)	10	33
20	T	76/82 (93%)	64 (84%)	12 (16%)	2	12
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	5
All	All	1985/2111 (94%)	1737 (88%)	248 (12%)	4	19

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	11	LEU

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Mol	Chain	Res	Type
2	B	69	LEU
2	B	80	ILE
2	B	97	TRP
2	B	102	LEU
2	B	121	LEU
2	B	127	ILE
2	B	128	GLU
2	B	132	LYS
2	B	139	LYS
2	B	172	ILE
2	B	187	LEU
2	B	196	LEU
2	B	204	ASN
2	B	208	ILE
2	B	221	LEU
2	B	223	ILE
2	B	226	ARG
2	B	236	TYR
3	C	3	ASN
3	C	4	LYS
3	C	5	ILE
3	C	14	ILE
3	C	15	THR
3	C	45	LYS
3	C	62	ASP
3	C	64	VAL
3	C	70	VAL
3	C	91	LEU
3	C	98	ASN
3	C	99	VAL
3	C	108	ASN
3	C	111	LEU
3	C	118	GLN
3	C	126	ARG
3	C	127	ARG
3	C	130	VAL
3	C	144	SER
3	C	156	ARG
3	C	167	TRP
3	C	188	LEU
3	C	192	THR
3	C	195	VAL

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Mol	Chain	Res	Type
3	C	196	LEU
3	C	204	LEU
3	C	206	GLU
3	C	207	VAL
4	D	15	GLU
4	D	19	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	50	ARG
4	D	58	LEU
4	D	64	LEU
4	D	96	LEU
4	D	115	ARG
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	135	LEU
4	D	150	GLU
4	D	170	VAL
4	D	187	ARG
4	D	191	ARG
4	D	192	GLU
4	D	194	LEU
4	D	201	GLN
4	D	202	LEU
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	16	THR
5	E	19	MET
5	E	24	ARG
5	E	31	LEU
5	E	43	LEU
5	E	47	LYS
5	E	50	GLU
5	E	51	VAL
5	E	53	LEU
5	E	63	ARG
5	E	64	ARG
5	E	65	ASN
5	E	68	GLU

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Mol	Chain	Res	Type
5	E	75	THR
5	E	78	HIS
5	E	79	GLU
5	E	82	VAL
5	E	105	VAL
5	E	116	THR
5	E	125	SER
5	E	126	ARG
5	E	135	THR
6	F	15	ASP
6	F	17	SER
6	F	28	ARG
6	F	37	VAL
6	F	43	LEU
6	F	45	LEU
6	F	55	ASP
6	F	65	VAL
6	F	75	LEU
6	F	83	ASP
6	F	86	ARG
6	F	93	SER
7	G	10	ARG
7	G	12	LEU
7	G	15	ASP
7	G	27	ILE
7	G	36	LYS
7	G	52	GLU
7	G	66	VAL
7	G	75	VAL
7	G	89	MET
7	G	113	GLU
7	G	114	ARG
7	G	136	LYS
7	G	140	ASP
7	G	148	ASN
8	H	1	MET
8	H	11	THR
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG

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Mol	Chain	Res	Type
8	H	97	VAL
8	H	102	ARG
8	H	112	LEU
8	H	133	LEU
9	I	16	ARG
9	I	27	THR
9	I	48	GLU
9	I	65	VAL
9	I	79	LEU
9	I	109	VAL
9	I	118	LYS
10	J	4	ILE
10	J	6	ILE
10	J	46	ARG
10	J	57	LYS
10	J	63	PHE
10	J	65	LEU
10	J	66	ARG
10	J	67	THR
10	J	79	ARG
10	J	85	LEU
11	K	29	ILE
11	K	47	VAL
11	K	48	ILE
11	K	75	TYR
11	K	87	THR
11	K	109	VAL
11	K	114	VAL
11	K	127	LYS
12	L	12	ARG
12	L	18	VAL
12	L	20	LYS
12	L	21	LYS
12	L	39	VAL
12	L	42	THR
12	L	43	VAL
12	L	44	THR
12	L	60	LEU
12	L	67	THR
12	L	100	ILE
12	L	116	SER
12	L	118	SER

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Mol	Chain	Res	Type
12	L	127	GLU
13	M	8	GLU
13	M	17	VAL
13	M	27	LYS
13	M	44	ARG
13	M	45	VAL
13	M	50	GLU
13	M	58	GLU
13	M	69	GLU
13	M	70	LEU
13	M	78	ILE
13	M	99	ARG
14	N	9	LYS
14	N	12	ARG
14	N	26	ARG
14	N	35	ARG
14	N	44	LEU
14	N	50	LYS
15	O	4	THR
15	O	5	LYS
15	O	11	VAL
15	O	22	THR
15	O	31	LEU
15	O	34	LEU
15	O	44	LYS
15	O	70	LEU
15	O	71	GLN
15	O	73	GLU
15	O	77	ARG
15	O	81	LEU
15	O	83	GLU
16	P	11	SER
16	P	12	LYS
16	P	45	THR
16	P	47	ASP
16	P	53	VAL
16	P	54	GLU
16	P	82	GLN
17	Q	3	LYS
17	Q	11	VAL
17	Q	34	LYS
17	Q	36	ILE

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Mol	Chain	Res	Type
17	Q	37	LYS
17	Q	38	ARG
17	Q	59	ILE
17	Q	68	ARG
17	Q	74	LEU
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
18	R	39	VAL
18	R	46	GLU
18	R	82	THR
18	R	86	VAL
18	R	88	LYS
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	31	ILE
19	S	58	VAL
19	S	71	LEU
20	T	10	LEU
20	T	11	SER
20	T	13	LEU
20	T	20	LEU
20	T	41	ILE
20	T	56	MET
20	T	62	LEU
20	T	73	HIS
20	T	74	LYS
20	T	84	LEU
20	T	99	LEU
20	T	100	ILE
21	U	6	ARG
21	U	10	ARG
21	U	15	ARG
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	37	ASN
2	B	40	HIS
2	B	135	GLN

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Mol	Chain	Res	Type
2	B	212	GLN
2	B	224	GLN
3	C	6	HIS
3	C	104	GLN
3	C	108	ASN
3	C	170	GLN
4	D	45	GLN
5	E	78	HIS
6	F	7	ASN
6	F	13	ASN
6	F	32	ASN
6	F	57	GLN
6	F	84	ASN
9	I	3	GLN
9	I	73	GLN
9	I	124	GLN
11	K	99	GLN
11	K	116	HIS
12	L	80	HIS
13	M	101	GLN
20	T	18	GLN
20	T	75	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1513/1522 (99%)	239 (15%)	38 (2%)
22	V	3/4 (75%)	0	0
23	W	8/9 (88%)	1 (12%)	0
24	a	10/11 (90%)	3 (30%)	0
25	b	1/3 (33%)	1 (100%)	0
All	All	1535/1549 (99%)	244 (15%)	38 (2%)

All (244) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	50	A
1	A	51	A
1	A	81	U
1	A	82	U
1	A	88	A
1	A	90	U
1	A	101	A
1	A	108	G
1	A	115	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(E)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	204	U
1	A	216	G
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	280	C
1	A	289	G
1	A	301	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	345	C

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Mol	Chain	Res	Type
1	A	346	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	442	C
1	A	443	C
1	A	452	A
1	A	460	A
1	A	481	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	500	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A

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Mol	Chain	Res	Type
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	607	A
1	A	629	G
1	A	631	G
1	A	632	A
1	A	653	A
1	A	665	A
1	A	671	G
1	A	687	A
1	A	688	G
1	A	698	G
1	A	702	A
1	A	723	U
1	A	731	G
1	A	734	G
1	A	755	G
1	A	770	C
1	A	777	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	812	C
1	A	813	U
1	A	816	A
1	A	817	C
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	851	G
1	A	873	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	916	G
1	A	926	G

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Mol	Chain	Res	Type
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1020	U
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1126	U
1	A	1130	A
1	A	1131	G
1	A	1135	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1157	A

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Mol	Chain	Res	Type
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1191	A
1	A	1196	U
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
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
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1332	A
1	A	1338	G
1	A	1348	U
1	A	1349	A
1	A	1353	G
1	A	1362	C
1	A	1364	U

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Mol	Chain	Res	Type
1	A	1368	G
1	A	1370	G
1	A	1398	A
1	A	1400	5MC
1	A	1402	4OC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1494	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1534	C
23	W	34	G
24	a	32	U
24	a	34	G
24	a	41	U
25	b	2	U

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	266	G
1	A	328	C
1	A	428	G

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Mol	Chain	Res	Type
1	A	429	U
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	812	C
1	A	913	A
1	A	960	U
1	A	991	U
1	A	1004	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1212	U
1	A	1256	A
1	A	1281	U
1	A	1300	G
1	A	1331	G
1	A	1347	G
1	A	1397	C
1	A	1493	A
1	A	1528	U
1	A	1533	C

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

17 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	4OC	A	1402	1	20,23,24	0.98	1 (5%)	25,32,35	0.72	0
1	PSU	A	516	1	18,21,22	1.12	1 (5%)	21,30,33	1.68	4 (19%)
1	PSU	A	1541	1	18,21,22	1.19	1 (5%)	21,30,33	1.83	5 (23%)
1	5MC	A	1404	1	19,22,23	1.01	1 (5%)	26,32,35	0.96	3 (11%)
12	0TD	L	92	12	8,9,10	1.46	1 (12%)	6,11,13	2.94	3 (50%)
24	PSU	a	38	24	18,21,22	1.15	1 (5%)	21,30,33	1.99	5 (23%)
1	5MC	A	967	1	19,22,23	1.14	2 (10%)	26,32,35	0.82	0
1	M2G	A	966	1	24,27,28	1.00	2 (8%)	33,40,43	0.98	1 (3%)
1	5MC	A	1400	1	19,22,23	1.45	4 (21%)	26,32,35	0.89	1 (3%)
1	2MG	A	1207	1	23,26,27	1.63	6 (26%)	33,38,41	1.12	6 (18%)
1	PSU	A	1540	1	18,21,22	1.18	1 (5%)	21,30,33	1.76	4 (19%)
1	MA6	A	1519	1	23,26,27	1.60	5 (21%)	33,38,41	0.97	1 (3%)
1	7MG	A	527	1	23,26,27	3.83	4 (17%)	27,39,42	2.44	9 (33%)
23	PSU	W	38	23	18,21,22	1.14	1 (5%)	21,30,33	1.79	4 (19%)
1	MA6	A	1518	1	23,26,27	1.17	3 (13%)	33,38,41	0.91	0
1	UR3	A	1498	1	19,22,23	0.81	0	26,32,35	0.97	1 (3%)
1	5MC	A	1407	1	19,22,23	1.15	3 (15%)	26,32,35	1.24	4 (15%)

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	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	PSU	A	516	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
12	0TD	L	92	12	-	2/7/12/14	-
24	PSU	a	38	24	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	1/11/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/9/27/28	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	3/11/29/30	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	W	38	23	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.08	1.34	1.45
1	A	1540	PSU	C6-C5	4.07	1.39	1.35
1	A	1541	PSU	C6-C5	4.06	1.39	1.35
1	A	1207	2MG	C2-N2	3.98	1.41	1.33
23	W	38	PSU	C6-C5	3.81	1.39	1.35
24	a	38	PSU	C6-C5	3.80	1.39	1.35
1	A	1207	2MG	C2-N1	3.72	1.42	1.36
1	A	516	PSU	C6-C5	3.70	1.39	1.35
1	A	527	7MG	C5-N7	3.62	1.40	1.35
1	A	527	7MG	C2-N2	3.55	1.42	1.34
1	A	1400	5MC	C2-N1	3.26	1.46	1.40
1	A	1519	MA6	C5-C4	3.21	1.44	1.39
1	A	1519	MA6	C4-N3	3.12	1.40	1.34
1	A	1400	5MC	C6-C5	3.07	1.39	1.34
1	A	1519	MA6	C2-N1	3.05	1.39	1.33
1	A	1400	5MC	C2-N3	3.04	1.42	1.36
1	A	1404	5MC	C2-N3	2.96	1.42	1.36
1	A	1519	MA6	C6-N1	2.89	1.39	1.34
1	A	1518	MA6	C8-N9	2.89	1.42	1.37
1	A	1519	MA6	C8-N9	2.87	1.42	1.37
1	A	967	5MC	C2-N3	2.82	1.41	1.36
1	A	1407	5MC	C2-N1	2.72	1.45	1.40
12	L	92	0TD	CB-CA	-2.71	1.53	1.54
1	A	527	7MG	C4-N3	2.67	1.40	1.34
1	A	1402	4OC	C2-N3	2.65	1.41	1.36
1	A	1207	2MG	C8-N9	2.48	1.43	1.37
1	A	1207	2MG	C4-N3	2.43	1.39	1.34
1	A	1207	2MG	C6-N1	2.43	1.43	1.38
1	A	966	M2G	C2-N2	2.37	1.39	1.35
1	A	967	5MC	C4-N4	2.29	1.39	1.34
1	A	1407	5MC	C5-C4	2.18	1.45	1.44
1	A	1518	MA6	C6-N1	2.15	1.38	1.34
1	A	1407	5MC	C2-N3	2.14	1.40	1.36
1	A	1518	MA6	C5-N7	2.11	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	966	M2G	C4-N3	2.09	1.39	1.34
1	A	1207	2MG	C2-N3	2.04	1.35	1.32
1	A	1400	5MC	C4-N4	2.02	1.39	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-5.51	92.46	102.36
1	A	527	7MG	C5-C6-N1	5.38	120.41	110.94
1	A	527	7MG	N9-C4-N3	5.18	133.05	125.46
1	A	527	7MG	C2-N3-C4	5.07	121.03	112.30
24	a	38	PSU	N1-C2-N3	4.85	120.29	115.17
24	a	38	PSU	C4-N3-C2	-4.74	119.83	126.37
1	A	527	7MG	C5-C4-N3	-4.74	119.24	128.13
23	W	38	PSU	C4-N3-C2	-4.60	120.03	126.37
1	A	516	PSU	C4-N3-C2	-4.55	120.10	126.37
1	A	1541	PSU	C4-N3-C2	-4.54	120.12	126.37
1	A	1541	PSU	N1-C2-N3	4.48	119.89	115.17
1	A	1540	PSU	N1-C2-N3	4.35	119.76	115.17
1	A	1540	PSU	C4-N3-C2	-4.24	120.53	126.37
23	W	38	PSU	N1-C2-N3	4.21	119.61	115.17
1	A	516	PSU	N1-C2-N3	3.96	119.34	115.17
1	A	527	7MG	N9-C8-N7	3.73	108.66	103.37
1	A	527	7MG	C2-N1-C6	-3.46	118.83	125.11
1	A	1407	5MC	N4-C4-N3	-3.24	112.64	118.51
1	A	1540	PSU	O2-C2-N1	-3.14	119.55	122.79
12	L	92	0TD	CB-CA-N	-3.06	102.90	109.10
24	a	38	PSU	O2-C2-N1	-3.01	119.69	122.79
1	A	527	7MG	O6-C6-C5	-2.97	120.34	127.62
1	A	1407	5MC	C5-C4-N3	2.93	124.76	121.75
1	A	1540	PSU	C6-N1-C2	-2.88	120.02	122.69
1	A	1541	PSU	O2-C2-N1	-2.80	119.90	122.79
24	a	38	PSU	C6-C5-C4	2.79	120.06	118.17
1	A	527	7MG	C6-C5-C4	-2.69	117.67	122.40
23	W	38	PSU	O2-C2-N1	-2.68	120.02	122.79
1	A	1207	2MG	C5-C4-N3	-2.68	124.13	128.39
1	A	966	M2G	C5-C4-N3	-2.59	124.26	128.39
1	A	1541	PSU	C6-N1-C2	-2.53	120.35	122.69
1	A	1519	MA6	C5-C6-N6	-2.52	121.34	125.33
24	a	38	PSU	C6-N1-C2	-2.50	120.37	122.69
12	L	92	0TD	OD1-CG-CB	-2.46	117.29	122.44
1	A	527	7MG	C6-C5-N7	2.38	135.62	131.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1207	2MG	O6-C6-N1	-2.36	115.67	120.11
1	A	1207	2MG	N9-C4-N3	2.35	130.65	125.95
1	A	1407	5MC	C5-C6-N1	-2.31	120.80	123.31
1	A	1407	5MC	C4-N3-C2	-2.30	117.61	120.81
1	A	1498	UR3	C6-N1-C2	-2.26	119.95	121.80
1	A	1404	5MC	C5-C4-N3	2.24	124.06	121.75
1	A	516	PSU	O2-C2-N1	-2.21	120.51	122.79
1	A	1404	5MC	C4-N3-C2	-2.19	117.77	120.81
1	A	516	PSU	O4'-C1'-C2'	2.11	108.08	105.15
1	A	1207	2MG	O6-C6-C5	2.09	132.04	126.53
23	W	38	PSU	C6-N1-C2	-2.05	120.79	122.69
1	A	1207	2MG	C6-C5-C4	2.04	121.90	118.83
1	A	1400	5MC	N4-C4-N3	-2.04	114.82	118.51
1	A	1207	2MG	C6-C5-N7	-2.02	126.61	130.29
1	A	1404	5MC	C1'-N1-C6	-2.01	117.84	121.15
1	A	1541	PSU	O4'-C1'-C2'	2.00	107.92	105.15

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	N1-C2-N2-CM2
1	A	1207	2MG	N3-C2-N2-CM2
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C9
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
12	L	92	0TD	CG-CB-SB-CSB
12	L	92	0TD	SB-CB-CG-OD1
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1519	MA6	C5-C6-N6-C10

There are no ring outliers.

15 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0
1	A	1541	PSU	1	0
1	A	1404	5MC	1	0
12	L	92	0TD	2	0
1	A	967	5MC	1	0
1	A	966	M2G	2	0
1	A	1400	5MC	1	0
1	A	1207	2MG	2	0
1	A	1540	PSU	3	0
1	A	1519	MA6	2	0
1	A	527	7MG	2	0
23	W	38	PSU	1	0
1	A	1518	MA6	1	0
1	A	1498	UR3	4	0
1	A	1407	5MC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 380 ligands modelled in this entry, 379 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	$\# Z > 2$
27	SRY	A	1956	-	40,42,42	2.44	10 (25%)	49,63,63	2.19	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
27	SRY	A	1956	-	-	2/20/87/87	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	1956	SRY	CD1-N31	9.86	1.50	1.33
27	A	1956	SRY	CA1-N11	6.75	1.44	1.33
27	A	1956	SRY	O53-C53	-3.29	1.36	1.44
27	A	1956	SRY	C23-N23	-3.05	1.42	1.47
27	A	1956	SRY	C21-C11	-2.99	1.47	1.53
27	A	1956	SRY	CD1-NE1	2.87	1.44	1.34
27	A	1956	SRY	CA1-NB1	2.86	1.44	1.34
27	A	1956	SRY	O32-C32	-2.41	1.40	1.44
27	A	1956	SRY	C32-CG2	-2.20	1.48	1.52
27	A	1956	SRY	O51-C51	-2.19	1.37	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	1956	SRY	C12-O42-C42	-7.26	96.75	108.48
27	A	1956	SRY	C13-O13-C22	-5.67	106.61	116.26
27	A	1956	SRY	O41-C12-O42	-5.10	106.16	111.37
27	A	1956	SRY	O13-C13-C23	4.42	115.25	108.07
27	A	1956	SRY	CI3-N23-C23	-4.05	109.00	114.23
27	A	1956	SRY	O42-C12-C22	-3.89	103.14	107.31
27	A	1956	SRY	C61-C11-N11	-3.56	104.06	110.62
27	A	1956	SRY	C43-C33-C23	-2.97	106.08	110.40
27	A	1956	SRY	C13-O53-C53	-2.55	108.73	113.72
27	A	1956	SRY	C41-C31-N31	2.53	114.95	110.91
27	A	1956	SRY	C12-O41-C41	-2.02	113.20	117.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

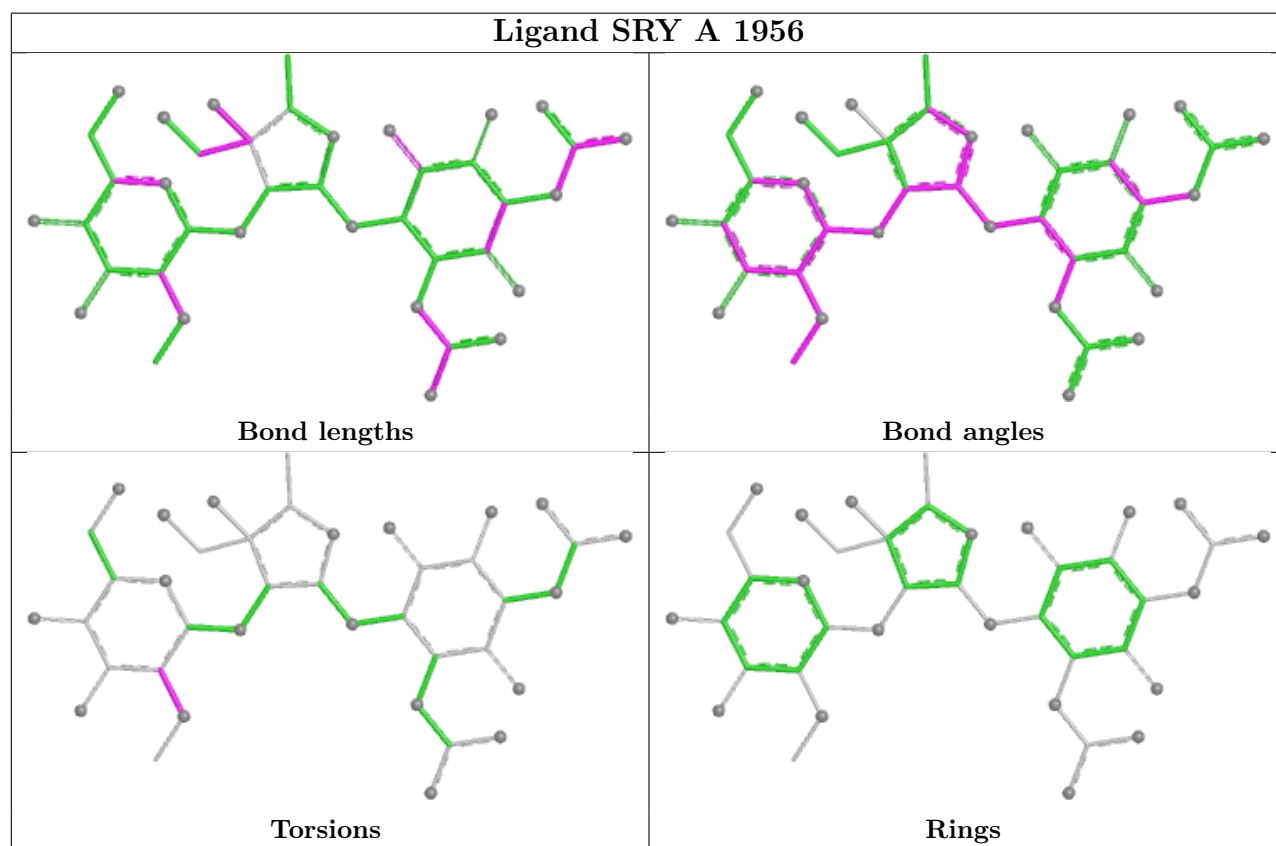
Mol	Chain	Res	Type	Atoms
27	A	1956	SRY	C13-C23-N23-CI3
27	A	1956	SRY	C33-C23-N23-CI3

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	1956	SRY	9	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1500/1522 (98%)	-0.83	6 (0%) 88 79	63, 101, 198, 295	4 (0%)
2	B	236/256 (92%)	-0.07	9 (3%) 44 30	72, 130, 193, 213	0
3	C	207/239 (86%)	-0.03	6 (2%) 53 35	79, 157, 196, 214	0
4	D	208/209 (99%)	0.07	9 (4%) 40 25	75, 114, 162, 193	0
5	E	151/162 (93%)	-0.51	1 (0%) 84 70	64, 93, 130, 174	0
6	F	101/101 (100%)	-0.28	2 (1%) 65 46	97, 134, 166, 197	0
7	G	155/156 (99%)	-0.17	7 (4%) 38 25	95, 138, 197, 213	0
8	H	138/138 (100%)	-0.42	1 (0%) 84 70	61, 84, 112, 137	0
9	I	127/128 (99%)	0.12	4 (3%) 51 35	100, 162, 201, 225	0
10	J	99/105 (94%)	0.44	5 (5%) 33 22	84, 191, 266, 285	0
11	K	117/129 (90%)	-0.16	4 (3%) 48 32	80, 106, 142, 160	0
12	L	124/135 (91%)	0.01	6 (4%) 35 24	70, 102, 139, 224	0
13	M	118/126 (93%)	-0.06	3 (2%) 58 39	99, 131, 163, 208	0
14	N	60/61 (98%)	0.21	3 (5%) 34 23	121, 142, 179, 239	0
15	O	88/89 (98%)	-0.28	0 100 100	73, 102, 145, 195	0
16	P	84/88 (95%)	-0.11	0 100 100	80, 103, 128, 221	0
17	Q	100/105 (95%)	-0.23	2 (2%) 65 46	72, 94, 131, 157	0
18	R	71/88 (80%)	-0.45	0 100 100	78, 113, 160, 215	0
19	S	81/93 (87%)	0.25	5 (6%) 26 18	72, 158, 210, 238	0
20	T	99/106 (93%)	0.05	4 (4%) 42 28	76, 106, 145, 181	0
21	U	25/27 (92%)	0.90	4 (16%) 5 4	90, 144, 162, 196	0
22	V	4/4 (100%)	1.58	1 (25%) 2 1	187, 188, 193, 201	0
23	W	8/9 (88%)	0.23	0 100 100	173, 214, 258, 287	0
24	a	10/11 (90%)	0.65	0 100 100	155, 188, 323, 325	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	b	2/3 (66%)	6.57	2 (100%) 0 0	62, 62, 62, 149	2 (100%)
All	All	3913/4090 (95%)	-0.36	84 (2%) 63 44	61, 115, 195, 325	6 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	U	12.0
1	A	83	U	8.6
25	b	2	U	7.9
4	D	2	GLY	7.9
21	U	25	LYS	6.9
19	S	3	ARG	5.8
20	T	12	ALA	5.6
14	N	12	ARG	5.5
25	b	1	U	5.2
12	L	28	LYS	4.9
11	K	127	LYS	4.9
4	D	9	CYS	4.7
12	L	19	ARG	4.7
19	S	4	SER	4.6
1	A	84	U	4.5
14	N	13	THR	4.4
3	C	196	LEU	4.4
19	S	2	PRO	4.2
22	V	4	U	4.2
12	L	25	PRO	4.1
9	I	127	LYS	4.1
9	I	9	ARG	4.0
4	D	31	CYS	3.9
12	L	26	ALA	3.7
7	G	5	ARG	3.7
9	I	105	ASP	3.6
11	K	49	GLY	3.5
10	J	57	LYS	3.5
10	J	34	VAL	3.3
7	G	33	ASP	3.3
7	G	13	GLN	3.3
3	C	188	LEU	3.1
4	D	22	LYS	3.1
7	G	8	GLU	3.0
5	E	81	GLU	2.9
4	D	3	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1129	C	2.9
2	B	240	GLN	2.9
3	C	201	TYR	2.9
7	G	80	VAL	2.8
7	G	84	ASN	2.8
4	D	21	LEU	2.8
6	F	101	ALA	2.7
4	D	26	CYS	2.7
2	B	188	ALA	2.7
21	U	6	ARG	2.7
3	C	208	ILE	2.7
1	A	982	U	2.6
4	D	12	CYS	2.5
2	B	187	LEU	2.4
10	J	77	PRO	2.4
12	L	47	LYS	2.4
20	T	9	ASN	2.4
19	S	78	ARG	2.4
6	F	95	GLU	2.4
13	M	56	LEU	2.3
13	M	8	GLU	2.3
21	U	18	TYR	2.3
2	B	160	ASP	2.3
20	T	73	HIS	2.3
13	M	119	GLY	2.3
2	B	162	ILE	2.2
2	B	203	GLY	2.2
17	Q	100	LYS	2.2
3	C	184	TYR	2.2
10	J	3	LYS	2.2
1	A	1286	A	2.2
14	N	6	LEU	2.2
12	L	128	ALA	2.1
7	G	82	GLY	2.1
2	B	164	VAL	2.1
2	B	211	ILE	2.1
19	S	10	PHE	2.1
9	I	126	SER	2.1
21	U	15	ARG	2.1
11	K	25	TYR	2.1
11	K	126	ARG	2.1
20	T	10	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	155	GLY	2.1
10	J	37	PRO	2.1
2	B	73	THR	2.0
4	D	44	GLY	2.0
8	H	99	GLU	2.0
17	Q	101	ARG	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(Å ²)	Q<0.9
1	PSU	A	1541	20/21	0.51	0.16	176,205,227,228	1
23	PSU	W	38	20/21	0.69	0.11	205,221,227,228	0
1	PSU	A	1540	20/21	0.76	0.14	152,168,179,180	2
24	PSU	a	38	20/21	0.91	0.10	158,164,169,169	0
1	2MG	A	1207	24/25	0.92	0.09	130,139,151,155	0
1	UR3	A	1498	21/22	0.93	0.13	89,97,116,118	0
1	PSU	A	516	20/21	0.95	0.06	111,121,127,131	0
1	MA6	A	1518	24/25	0.95	0.08	85,106,116,122	0
1	5MC	A	1407	21/22	0.96	0.06	109,120,126,130	0
1	MA6	A	1519	24/25	0.96	0.08	82,107,115,116	0
12	0TD	L	92	10/11	0.97	0.11	77,93,111,233	0
1	M2G	A	966	25/26	0.97	0.10	92,112,125,128	0
1	5MC	A	1400	21/22	0.97	0.09	77,102,129,132	0
1	5MC	A	967	21/22	0.98	0.07	97,105,118,120	0
1	4OC	A	1402	22/23	0.98	0.09	82,89,99,102	0
1	5MC	A	1404	21/22	0.98	0.09	89,93,103,111	0
1	7MG	A	527	24/25	0.98	0.07	70,87,95,97	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(Å ²)	Q<0.9
26	MG	A	1889	1/1	0.12	0.16	401,401,401,401	0
26	MG	A	1814	1/1	0.22	0.12	384,384,384,384	0
26	MG	A	1869	1/1	0.30	0.11	412,412,412,412	0
26	MG	A	1811	1/1	0.38	0.10	411,411,411,411	0
26	MG	A	1819	1/1	0.38	0.10	488,488,488,488	0
26	MG	A	1836	1/1	0.41	0.10	409,409,409,409	0
26	MG	A	1842	1/1	0.41	0.14	460,460,460,460	0
26	MG	A	1820	1/1	0.42	0.12	427,427,427,427	0
26	MG	A	1690	1/1	0.43	0.19	189,189,189,189	0
26	MG	A	1727	1/1	0.48	0.15	222,222,222,222	0
26	MG	A	1823	1/1	0.50	0.07	435,435,435,435	0
26	MG	A	1865	1/1	0.51	0.14	476,476,476,476	1
26	MG	A	1870	1/1	0.52	0.15	456,456,456,456	0
26	MG	A	1776	1/1	0.54	0.33	110,110,110,110	0
26	MG	A	1785	1/1	0.57	0.29	108,108,108,108	0
26	MG	A	1895	1/1	0.57	0.10	364,364,364,364	0
26	MG	A	1817	1/1	0.61	0.33	378,378,378,378	0
26	MG	A	1899	1/1	0.62	0.08	422,422,422,422	0
26	MG	A	1830	1/1	0.63	0.10	426,426,426,426	0
26	MG	A	1861	1/1	0.63	0.08	428,428,428,428	0
26	MG	G	201[A]	1/1	0.63	0.61	62,62,62,62	1
26	MG	G	201[B]	1/1	0.63	0.61	50,50,50,50	1
26	MG	A	1930	1/1	0.64	0.24	107,107,107,107	0
26	MG	A	1843	1/1	0.65	0.10	346,346,346,346	0
26	MG	A	1621	1/1	0.65	0.21	130,130,130,130	0
26	MG	A	1863	1/1	0.65	0.12	414,414,414,414	0
26	MG	A	1755	1/1	0.66	0.19	119,119,119,119	0
26	MG	A	1905	1/1	0.66	0.27	105,105,105,105	0
26	MG	A	1924	1/1	0.66	0.31	109,109,109,109	0
26	MG	A	1921	1/1	0.68	0.14	134,134,134,134	0
26	MG	A	1901	1/1	0.68	0.12	399,399,399,399	0
26	MG	A	1925	1/1	0.68	0.23	82,82,82,82	0
26	MG	A	1808	1/1	0.69	0.19	486,486,486,486	0
26	MG	A	1902	1/1	0.70	0.12	326,326,326,326	0
26	MG	A	1821	1/1	0.70	0.07	356,356,356,356	0
26	MG	A	1919	1/1	0.70	0.25	101,101,101,101	0
26	MG	A	1691	1/1	0.71	0.25	130,130,130,130	0
26	MG	A	1853	1/1	0.71	0.09	395,395,395,395	0
26	MG	A	1787	1/1	0.72	0.37	132,132,132,132	0
26	MG	A	1915	1/1	0.72	0.08	120,120,120,120	0
26	MG	A	1758	1/1	0.72	0.42	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1928	1/1	0.73	0.26	94,94,94,94	0
26	MG	A	1793	1/1	0.73	0.10	105,105,105,105	0
26	MG	A	1818	1/1	0.73	0.08	329,329,329,329	0
26	MG	A	1714	1/1	0.73	0.14	202,202,202,202	0
26	MG	P	102	1/1	0.73	0.14	117,117,117,117	0
26	MG	A	1916	1/1	0.74	0.22	121,121,121,121	0
26	MG	A	1742	1/1	0.74	0.28	102,102,102,102	0
26	MG	A	1938	1/1	0.74	0.32	100,100,100,100	0
26	MG	A	1946	1/1	0.74	0.34	111,111,111,111	0
26	MG	A	1804	1/1	0.74	0.17	130,130,130,130	0
26	MG	A	1617	1/1	0.74	0.20	111,111,111,111	0
26	MG	A	1789	1/1	0.74	0.31	124,124,124,124	0
26	MG	A	1684	1/1	0.75	0.09	137,137,137,137	0
26	MG	A	1806	1/1	0.75	0.23	100,100,100,100	0
26	MG	A	1879	1/1	0.75	0.12	406,406,406,406	0
26	MG	A	1948	1/1	0.75	0.28	115,115,115,115	0
26	MG	A	1735	1/1	0.75	0.28	116,116,116,116	0
26	MG	A	1913	1/1	0.75	0.29	102,102,102,102	0
26	MG	A	1846	1/1	0.75	0.12	390,390,390,390	0
26	MG	A	1630	1/1	0.76	0.52	105,105,105,105	0
26	MG	A	1689	1/1	0.76	0.10	273,273,273,273	0
26	MG	A	1922	1/1	0.76	0.18	104,104,104,104	0
26	MG	A	1827	1/1	0.76	0.09	376,376,376,376	0
26	MG	A	1940	1/1	0.76	0.17	102,102,102,102	0
26	MG	A	1738	1/1	0.77	0.23	85,85,85,85	0
26	MG	A	1725	1/1	0.77	0.23	119,119,119,119	0
26	MG	A	1816	1/1	0.77	0.09	495,495,495,495	0
26	MG	A	1605	1/1	0.77	0.33	100,100,100,100	0
26	MG	A	1868	1/1	0.77	0.12	435,435,435,435	0
26	MG	A	1687	1/1	0.77	0.32	155,155,155,155	0
26	MG	A	1935	1/1	0.77	0.28	108,108,108,108	0
26	MG	S	102	1/1	0.77	0.14	99,99,99,99	0
26	MG	A	1774	1/1	0.78	0.69	101,101,101,101	0
26	MG	A	1844	1/1	0.78	0.21	330,330,330,330	0
26	MG	A	1704	1/1	0.78	0.10	205,205,205,205	0
26	MG	A	1947	1/1	0.78	0.19	126,126,126,126	0
26	MG	A	1707	1/1	0.78	0.09	437,437,437,437	0
26	MG	A	1926	1/1	0.78	0.94	111,111,111,111	0
26	MG	A	1728	1/1	0.78	0.45	109,109,109,109	0
26	MG	A	1652	1/1	0.78	0.23	77,77,77,77	0
26	MG	A	1813	1/1	0.78	0.09	461,461,461,461	0
26	MG	A	1851	1/1	0.79	0.13	259,259,259,259	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	MG	A	1810	1/1	0.79	0.11	277,277,277,277	0
26	MG	A	1640	1/1	0.79	0.17	203,203,203,203	0
26	MG	A	1855	1/1	0.80	0.11	315,315,315,315	0
26	MG	A	1631	1/1	0.80	0.39	159,159,159,159	0
26	MG	A	1756	1/1	0.80	0.32	101,101,101,101	0
26	MG	A	1740	1/1	0.80	0.25	90,90,90,90	0
26	MG	A	1659	1/1	0.80	0.17	105,105,105,105	0
26	MG	A	1936	1/1	0.81	0.26	101,101,101,101	0
26	MG	A	1731	1/1	0.81	0.83	117,117,117,117	0
26	MG	A	1669	1/1	0.81	0.31	106,106,106,106	0
26	MG	A	1795	1/1	0.81	0.48	108,108,108,108	0
26	MG	A	1788	1/1	0.81	0.24	82,82,82,82	0
26	MG	A	1941	1/1	0.82	0.21	112,112,112,112	0
26	MG	A	1629	1/1	0.82	0.23	123,123,123,123	0
26	MG	D	304	1/1	0.83	0.18	467,467,467,467	0
26	MG	A	1839	1/1	0.83	0.17	375,375,375,375	0
26	MG	A	1826	1/1	0.83	0.14	382,382,382,382	0
26	MG	A	1832	1/1	0.83	0.11	421,421,421,421	0
26	MG	A	1710	1/1	0.83	0.11	247,247,247,247	0
26	MG	A	1798	1/1	0.84	0.10	96,96,96,96	0
26	MG	A	1849	1/1	0.84	0.15	301,301,301,301	0
26	MG	A	1794	1/1	0.84	0.23	87,87,87,87	0
26	MG	A	1805	1/1	0.84	0.15	79,79,79,79	0
26	MG	A	1757	1/1	0.84	0.32	91,91,91,91	0
26	MG	A	1834	1/1	0.84	0.20	364,364,364,364	0
26	MG	A	1862	1/1	0.84	0.30	463,463,463,463	1
26	MG	Q	201	1/1	0.84	0.19	91,91,91,91	0
26	MG	A	1943	1/1	0.84	0.23	92,92,92,92	0
26	MG	A	1880	1/1	0.85	0.14	402,402,402,402	0
26	MG	A	1741	1/1	0.85	0.49	119,119,119,119	0
26	MG	A	1625	1/1	0.85	0.21	89,89,89,89	0
26	MG	A	1745	1/1	0.85	0.27	89,89,89,89	0
26	MG	A	1920	1/1	0.85	0.17	113,113,113,113	0
26	MG	A	1900	1/1	0.85	0.28	409,409,409,409	0
26	MG	A	1675	1/1	0.85	0.14	153,153,153,153	0
26	MG	A	1877	1/1	0.85	0.09	430,430,430,430	0
26	MG	A	1668	1/1	0.85	0.18	122,122,122,122	0
26	MG	A	1932	1/1	0.86	0.23	102,102,102,102	0
26	MG	A	1887	1/1	0.86	0.04	365,365,365,365	0
26	MG	A	1673	1/1	0.86	0.28	179,179,179,179	0
26	MG	E	203	1/1	0.86	0.08	115,115,115,115	0
26	MG	A	1841	1/1	0.86	0.15	387,387,387,387	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1896	1/1	0.86	0.13	378,378,378,378	0
26	MG	A	1702	1/1	0.86	0.41	91,91,91,91	0
26	MG	A	1815	1/1	0.86	0.10	368,368,368,368	0
26	MG	A	1603	1/1	0.86	0.19	105,105,105,105	0
26	MG	A	1718	1/1	0.87	0.12	160,160,160,160	0
26	MG	A	1739	1/1	0.87	0.56	105,105,105,105	0
26	MG	A	1907	1/1	0.87	0.21	89,89,89,89	0
26	MG	A	1609	1/1	0.87	0.21	85,85,85,85	0
26	MG	L	201	1/1	0.87	0.16	86,86,86,86	0
26	MG	A	1933	1/1	0.87	0.39	94,94,94,94	0
26	MG	A	1777	1/1	0.87	0.24	81,81,81,81	0
26	MG	A	1894	1/1	0.87	0.09	340,340,340,340	0
26	MG	S	103	1/1	0.87	0.09	92,92,92,92	0
26	MG	A	1873	1/1	0.88	0.23	424,424,424,424	0
26	MG	A	1848	1/1	0.88	0.20	361,361,361,361	0
26	MG	A	1910	1/1	0.88	0.23	114,114,114,114	0
26	MG	A	1680	1/1	0.88	0.07	258,258,258,258	0
26	MG	A	1809	1/1	0.88	0.07	268,268,268,268	0
26	MG	A	1884	1/1	0.88	0.08	345,345,345,345	0
26	MG	A	1681	1/1	0.88	0.34	114,114,114,114	0
26	MG	A	1672	1/1	0.88	0.15	91,91,91,91	0
26	MG	A	1838	1/1	0.88	0.18	462,462,462,462	0
26	MG	A	1953	1/1	0.88	0.35	104,104,104,104	0
26	MG	A	1693	1/1	0.88	0.21	129,129,129,129	0
26	MG	A	1923	1/1	0.88	0.43	99,99,99,99	0
26	MG	F	202	1/1	0.88	0.18	98,98,98,98	0
26	MG	A	1822	1/1	0.88	0.09	281,281,281,281	0
26	MG	A	1676	1/1	0.88	0.07	121,121,121,121	0
26	MG	A	1760	1/1	0.88	0.33	123,123,123,123	0
26	MG	A	1762	1/1	0.88	0.26	100,100,100,100	0
26	MG	A	1829	1/1	0.88	0.35	387,387,387,387	0
26	MG	A	1903	1/1	0.88	0.09	268,268,268,268	0
26	MG	A	1904	1/1	0.88	0.13	397,397,397,397	0
26	MG	T	201	1/1	0.88	0.35	129,129,129,129	0
26	MG	A	1679	1/1	0.89	0.16	98,98,98,98	0
26	MG	A	1864	1/1	0.89	0.34	407,407,407,407	1
26	MG	A	1650	1/1	0.89	0.24	93,93,93,93	0
26	MG	A	1733	1/1	0.89	0.09	90,90,90,90	0
26	MG	A	1790	1/1	0.89	0.39	112,112,112,112	0
26	MG	A	1954	1/1	0.89	0.21	86,86,86,86	0
26	MG	A	1761	1/1	0.89	0.37	115,115,115,115	0
26	MG	A	1643	1/1	0.89	0.32	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1773	1/1	0.89	0.33	78,78,78,78	0
26	MG	A	1748	1/1	0.89	0.39	109,109,109,109	0
26	MG	A	1852	1/1	0.89	0.23	426,426,426,426	0
26	MG	A	1934	1/1	0.89	0.28	79,79,79,79	0
26	MG	N	102	1/1	0.89	0.21	87,87,87,87	0
26	MG	A	1800	1/1	0.89	0.27	87,87,87,87	0
26	MG	A	1754	1/1	0.89	0.12	92,92,92,92	0
26	MG	A	1858	1/1	0.89	0.23	255,255,255,255	1
26	MG	A	1645	1/1	0.89	0.14	84,84,84,84	0
26	MG	A	1708	1/1	0.89	0.07	284,284,284,284	0
26	MG	A	1661	1/1	0.90	0.23	158,158,158,158	0
26	MG	A	1692	1/1	0.90	0.40	128,128,128,128	0
26	MG	A	1688	1/1	0.90	0.08	130,130,130,130	0
26	MG	A	1694	1/1	0.90	0.17	113,113,113,113	0
26	MG	A	1749	1/1	0.90	0.23	105,105,105,105	0
26	MG	A	1664	1/1	0.90	0.07	167,167,167,167	0
26	MG	A	1737	1/1	0.90	0.65	104,104,104,104	0
26	MG	A	1918	1/1	0.90	0.57	114,114,114,114	0
26	MG	A	1866	1/1	0.90	0.12	425,425,425,425	1
26	MG	A	1802	1/1	0.90	0.14	118,118,118,118	0
26	MG	A	1831	1/1	0.90	0.10	438,438,438,438	0
26	MG	A	1719	1/1	0.90	0.08	141,141,141,141	0
26	MG	A	1942	1/1	0.90	0.25	92,92,92,92	0
26	MG	A	1658	1/1	0.90	0.23	115,115,115,115	0
26	MG	A	1945	1/1	0.90	0.48	129,129,129,129	0
26	MG	A	1726	1/1	0.90	0.11	293,293,293,293	0
26	MG	A	1878	1/1	0.91	0.15	389,389,389,389	0
26	MG	A	1715	1/1	0.91	0.38	176,176,176,176	0
26	MG	A	1686	1/1	0.91	0.09	210,210,210,210	0
26	MG	A	1927	1/1	0.91	0.17	100,100,100,100	0
26	MG	A	1662	1/1	0.91	0.17	122,122,122,122	0
26	MG	A	1908	1/1	0.91	0.33	117,117,117,117	0
26	MG	A	1722	1/1	0.91	0.13	100,100,100,100	0
26	MG	A	1616	1/1	0.91	0.19	76,76,76,76	0
26	MG	A	1914	1/1	0.91	0.15	118,118,118,118	0
26	MG	A	1613	1/1	0.91	0.09	170,170,170,170	0
26	MG	A	1656	1/1	0.91	0.25	94,94,94,94	0
26	MG	A	1837	1/1	0.91	0.23	429,429,429,429	0
26	MG	A	1898	1/1	0.91	0.24	370,370,370,370	0
26	MG	A	1803	1/1	0.91	0.13	91,91,91,91	0
26	MG	S	101	1/1	0.91	0.27	82,82,82,82	0
26	MG	A	1824	1/1	0.91	0.18	404,404,404,404	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1876	1/1	0.91	0.19	289,289,289,289	0
26	MG	A	1769	1/1	0.91	0.26	98,98,98,98	0
26	MG	A	1882	1/1	0.92	0.14	247,247,247,247	0
26	MG	A	1883	1/1	0.92	0.16	426,426,426,426	0
26	MG	A	1753	1/1	0.92	0.20	93,93,93,93	0
26	MG	A	1835	1/1	0.92	0.19	448,448,448,448	0
26	MG	A	1888	1/1	0.92	0.23	347,347,347,347	0
26	MG	A	1909	1/1	0.92	0.16	95,95,95,95	0
26	MG	A	1929	1/1	0.92	0.05	87,87,87,87	0
26	MG	A	1859	1/1	0.92	0.15	278,278,278,278	0
26	MG	A	1911	1/1	0.92	0.29	99,99,99,99	0
26	MG	A	1871	1/1	0.92	0.17	346,346,346,346	0
26	MG	A	1697	1/1	0.92	0.21	122,122,122,122	0
26	MG	A	1639	1/1	0.92	0.33	124,124,124,124	0
26	MG	A	1897	1/1	0.92	0.09	235,235,235,235	0
26	MG	P	101	1/1	0.92	0.36	75,75,75,75	0
26	MG	A	1792	1/1	0.92	0.14	94,94,94,94	0
26	MG	A	1786	1/1	0.92	0.21	120,120,120,120	0
26	MG	A	1744	1/1	0.92	0.17	111,111,111,111	0
26	MG	A	1833	1/1	0.92	0.37	455,455,455,455	1
26	MG	A	1881	1/1	0.92	0.26	316,316,316,316	0
26	MG	A	1944	1/1	0.92	0.28	100,100,100,100	0
26	MG	A	1717	1/1	0.93	0.14	197,197,197,197	0
26	MG	A	1847	1/1	0.93	0.12	335,335,335,335	0
26	MG	D	302	1/1	0.93	0.11	92,92,92,92	0
26	MG	A	1825	1/1	0.93	0.13	188,188,188,188	0
26	MG	A	1642	1/1	0.93	0.18	118,118,118,118	0
26	MG	A	1736	1/1	0.93	0.18	97,97,97,97	0
26	MG	A	1828	1/1	0.93	0.34	439,439,439,439	0
26	MG	A	1912	1/1	0.93	0.20	97,97,97,97	0
26	MG	A	1747	1/1	0.93	0.20	75,75,75,75	0
26	MG	A	1696	1/1	0.93	0.17	132,132,132,132	0
26	MG	A	1791	1/1	0.93	0.85	91,91,91,91	0
26	MG	A	1783	1/1	0.93	0.11	96,96,96,96	1
26	MG	A	1917	1/1	0.93	0.54	103,103,103,103	0
26	MG	A	1931	1/1	0.93	0.12	76,76,76,76	0
26	MG	A	1767	1/1	0.93	0.35	107,107,107,107	0
26	MG	A	1949	1/1	0.93	0.19	88,88,88,88	0
26	MG	A	1951	1/1	0.93	0.13	122,122,122,122	0
26	MG	A	1699	1/1	0.94	0.09	117,117,117,117	0
26	MG	A	1608	1/1	0.94	0.07	125,125,125,125	0
26	MG	A	1665	1/1	0.94	0.17	189,189,189,189	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	F	201	1/1	0.94	0.38	101,101,101,101	0
26	MG	A	1667	1/1	0.94	0.14	121,121,121,121	0
26	MG	A	1607	1/1	0.94	0.24	76,76,76,76	0
26	MG	A	1695	1/1	0.94	0.13	123,123,123,123	0
26	MG	A	1797	1/1	0.94	0.11	84,84,84,84	0
26	MG	A	1857	1/1	0.94	0.27	254,254,254,254	0
26	MG	A	1885	1/1	0.94	0.13	316,316,316,316	0
26	MG	A	1633	1/1	0.94	0.13	148,148,148,148	0
26	MG	P	103	1/1	0.94	0.17	89,89,89,89	0
26	MG	A	1634	1/1	0.94	0.26	240,240,240,240	0
26	MG	A	1730	1/1	0.94	0.47	103,103,103,103	0
26	MG	A	1952	1/1	0.94	0.23	79,79,79,79	0
26	MG	A	1890	1/1	0.94	0.22	423,423,423,423	0
26	MG	A	1893	1/1	0.94	0.13	304,304,304,304	0
26	MG	E	201	1/1	0.95	0.18	111,111,111,111	0
26	MG	A	1781	1/1	0.95	0.21	72,72,72,72	0
26	MG	A	1651	1/1	0.95	0.21	109,109,109,109	0
26	MG	A	1734	1/1	0.95	0.13	114,114,114,114	0
26	MG	A	1764	1/1	0.95	0.09	62,62,62,62	0
26	MG	A	1678	1/1	0.95	0.11	95,95,95,95	0
26	MG	H	201	1/1	0.95	0.15	73,73,73,73	0
26	MG	A	1768	1/1	0.95	0.20	115,115,115,115	0
26	MG	A	1720	1/1	0.95	0.11	126,126,126,126	0
26	MG	A	1716	1/1	0.95	0.25	111,111,111,111	1
26	MG	A	1867	1/1	0.95	0.15	170,170,170,170	1
26	MG	A	1746	1/1	0.95	0.18	120,120,120,120	0
26	MG	A	1775	1/1	0.95	0.14	84,84,84,84	0
26	MG	A	1685	1/1	0.95	0.22	335,335,335,335	0
26	MG	A	1732	1/1	0.95	0.21	95,95,95,95	0
26	MG	A	1780	1/1	0.95	0.18	116,116,116,116	0
26	MG	A	1892	1/1	0.95	0.31	354,354,354,354	0
26	MG	A	1772	1/1	0.96	0.11	116,116,116,116	0
26	MG	A	1700	1/1	0.96	0.10	167,167,167,167	0
26	MG	A	1623	1/1	0.96	0.17	85,85,85,85	0
26	MG	A	1703	1/1	0.96	0.06	117,117,117,117	0
26	MG	A	1796	1/1	0.96	0.08	74,74,74,74	0
26	MG	A	1620	1/1	0.96	0.07	81,81,81,81	0
26	MG	A	1706	1/1	0.96	0.10	99,99,99,99	0
26	MG	A	1872	1/1	0.96	0.10	287,287,287,287	0
26	MG	A	1799	1/1	0.96	0.10	100,100,100,100	1
26	MG	A	1778	1/1	0.96	0.39	83,83,83,83	0
26	MG	A	1801	1/1	0.96	0.26	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1779	1/1	0.96	0.35	65,65,65,65	0
26	MG	A	1657	1/1	0.96	0.08	131,131,131,131	0
26	MG	A	1647	1/1	0.96	0.20	133,133,133,133	0
26	MG	A	1649	1/1	0.96	0.10	93,93,93,93	0
26	MG	A	1670	1/1	0.96	0.19	189,189,189,189	0
26	MG	J	201	1/1	0.96	0.09	87,87,87,87	0
26	MG	A	1856	1/1	0.96	0.10	156,156,156,156	0
26	MG	A	1807	1/1	0.96	0.12	100,100,100,100	0
26	MG	A	1939	1/1	0.96	0.27	88,88,88,88	0
26	MG	A	1671	1/1	0.96	0.12	99,99,99,99	0
26	MG	A	1766	1/1	0.96	0.19	109,109,109,109	0
26	MG	A	1860	1/1	0.96	0.17	303,303,303,303	0
26	MG	A	1632	1/1	0.96	0.18	110,110,110,110	0
26	MG	A	1619	1/1	0.96	0.16	80,80,80,80	0
26	MG	A	1663	1/1	0.96	0.14	146,146,146,146	0
26	MG	A	1771	1/1	0.96	0.22	63,63,63,63	0
28	ZN	D	301	1/1	0.96	0.23	116,116,116,116	0
26	MG	A	1950	1/1	0.97	0.37	90,90,90,90	0
26	MG	A	1750	1/1	0.97	0.09	109,109,109,109	0
26	MG	A	1751	1/1	0.97	0.31	82,82,82,82	0
26	MG	A	1752	1/1	0.97	0.13	85,85,85,85	0
26	MG	A	1618	1/1	0.97	0.10	89,89,89,89	0
26	MG	A	1955	1/1	0.97	0.09	69,69,69,69	0
26	MG	A	1615	1/1	0.97	0.14	72,72,72,72	0
26	MG	D	303	1/1	0.97	0.10	83,83,83,83	0
26	MG	A	1906	1/1	0.97	0.19	118,118,118,118	0
26	MG	A	1729	1/1	0.97	0.12	78,78,78,78	0
26	MG	E	202	1/1	0.97	0.03	107,107,107,107	0
26	MG	A	1610	1/1	0.97	0.07	66,66,66,66	0
26	MG	A	1601	1/1	0.97	0.09	63,63,63,63	1
26	MG	A	1743	1/1	0.97	0.08	72,72,72,72	0
26	MG	A	1886	1/1	0.97	0.12	224,224,224,224	0
26	MG	A	1759	1/1	0.97	0.35	83,83,83,83	0
26	MG	A	1937	1/1	0.97	0.05	60,60,60,60	0
26	MG	A	1840	1/1	0.97	0.07	119,119,119,119	0
26	MG	A	1644	1/1	0.97	0.17	80,80,80,80	0
26	MG	A	1653	1/1	0.97	0.07	116,116,116,116	0
26	MG	A	1637	1/1	0.97	0.12	99,99,99,99	0
26	MG	A	1782	1/1	0.97	0.04	92,92,92,92	0
26	MG	A	1763	1/1	0.97	0.10	89,89,89,89	0
26	MG	A	1784	1/1	0.97	0.08	121,121,121,121	0
26	MG	A	1724	1/1	0.97	0.06	103,103,103,103	0

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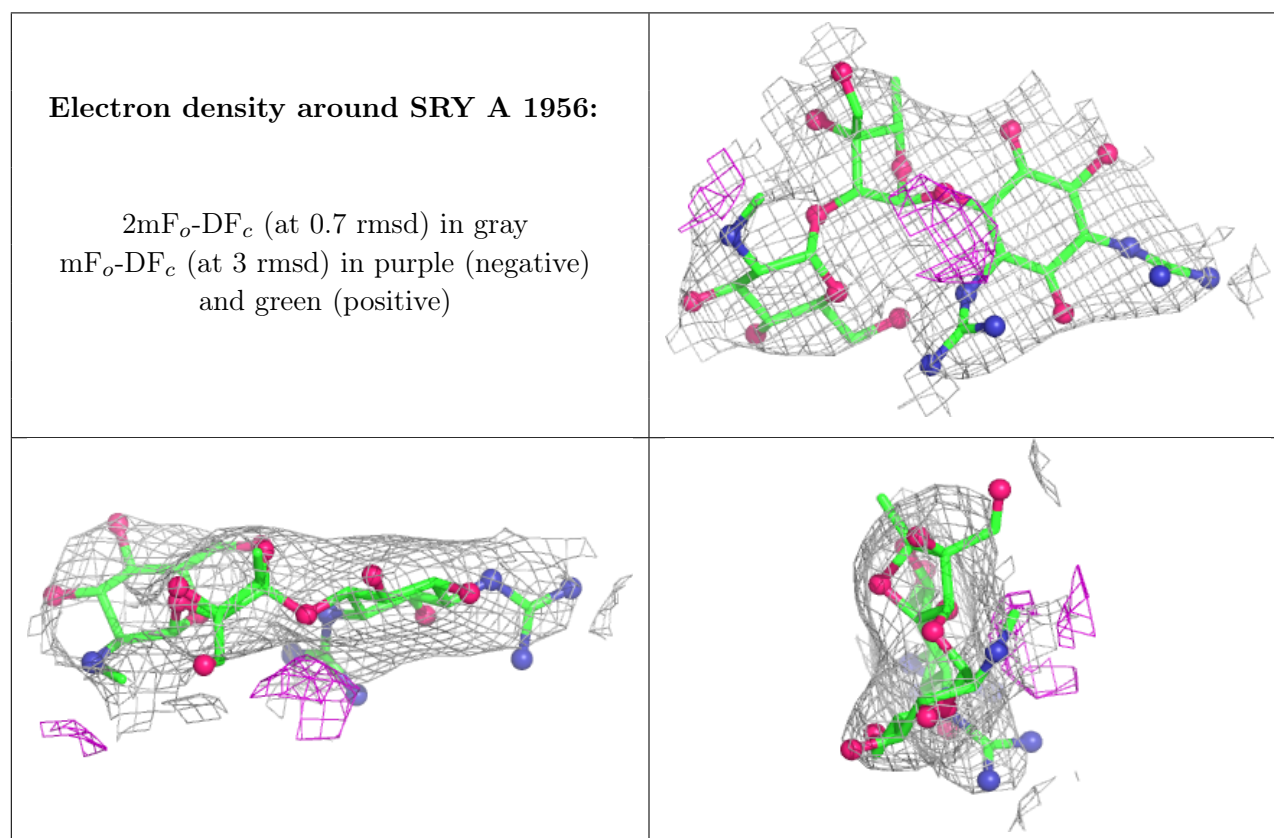
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	MG	A	1765	1/1	0.97	0.13	77,77,77,77	0
26	MG	A	1711	1/1	0.97	0.07	86,86,86,86	0
26	MG	A	1874	1/1	0.97	0.06	197,197,197,197	0
26	MG	A	1682	1/1	0.97	0.15	133,133,133,133	0
26	MG	A	1683	1/1	0.98	0.09	113,113,113,113	0
26	MG	A	1641	1/1	0.98	0.05	70,70,70,70	0
26	MG	A	1721	1/1	0.98	0.06	175,175,175,175	0
26	MG	A	1701	1/1	0.98	0.10	83,83,83,83	0
26	MG	A	1875	1/1	0.98	0.06	151,151,151,151	0
26	MG	A	1850	1/1	0.98	0.04	199,199,199,199	0
26	MG	A	1723	1/1	0.98	0.06	116,116,116,116	0
26	MG	A	1654	1/1	0.98	0.06	78,78,78,78	0
26	MG	A	1622	1/1	0.98	0.05	112,112,112,112	0
26	MG	A	1854	1/1	0.98	0.08	134,134,134,134	1
26	MG	A	1614	1/1	0.98	0.05	92,92,92,92	0
26	MG	A	1606	1/1	0.98	0.04	75,75,75,75	0
26	MG	A	1626	1/1	0.98	0.09	94,94,94,94	0
26	MG	A	1660	1/1	0.98	0.09	118,118,118,118	0
26	MG	A	1812	1/1	0.98	0.08	180,180,180,180	0
26	MG	A	1770	1/1	0.98	0.17	79,79,79,79	0
26	MG	A	1709	1/1	0.98	0.10	93,93,93,93	0
26	MG	A	1635	1/1	0.98	0.04	73,73,73,73	0
26	MG	A	1677	1/1	0.98	0.10	99,99,99,99	0
26	MG	A	1713	1/1	0.98	0.11	116,116,116,116	0
26	MG	A	1891	1/1	0.98	0.20	398,398,398,398	1
26	MG	A	1648	1/1	0.98	0.13	139,139,139,139	0
26	MG	A	1627	1/1	0.98	0.15	229,229,229,229	0
26	MG	A	1638	1/1	0.98	0.10	72,72,72,72	0
26	MG	A	1611	1/1	0.98	0.07	131,131,131,131	0
26	MG	A	1604	1/1	0.98	0.05	134,134,134,134	0
27	SRY	A	1956	40/40	0.98	0.06	55,83,98,109	0
26	MG	A	1845	1/1	0.98	0.05	98,98,98,98	0
26	MG	A	1705	1/1	0.99	0.08	98,98,98,98	0
26	MG	A	1602	1/1	0.99	0.06	124,124,124,124	0
26	MG	A	1624	1/1	0.99	0.09	79,79,79,79	0
26	MG	A	1698	1/1	0.99	0.04	108,108,108,108	0
26	MG	A	1674	1/1	0.99	0.06	98,98,98,98	0
26	MG	A	1646	1/1	0.99	0.04	47,47,47,47	0
26	MG	A	1636	1/1	0.99	0.07	94,94,94,94	0
26	MG	A	1712	1/1	0.99	0.05	109,109,109,109	0
26	MG	A	1628	1/1	0.99	0.06	89,89,89,89	0
26	MG	A	1655	1/1	0.99	0.03	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
26	MG	A	1612	1/1	0.99	0.05	112,112,112,112	0
28	ZN	N	101	1/1	0.99	0.04	138,138,138,138	0
26	MG	A	1666	1/1	1.00	0.02	80,80,80,80	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.