



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:25 PM UTC

PDB ID : 4LFA / pdb_00004lfa
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*
Authors : Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on : 2013-06-26
Resolution : 3.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

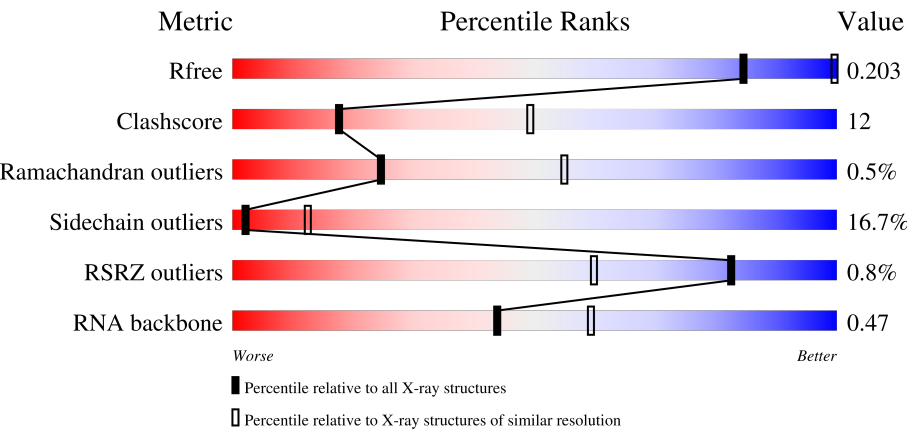
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1132 (3.76-3.52)
Clashscore	190562	1014 (3.74-3.54)
Ramachandran outliers	187476	1123 (3.76-3.52)
Sidechain outliers	187428	1121 (3.76-3.52)
RSRZ outliers	180081	1130 (3.76-3.52)
RNA backbone	3983	1026 (4.22-3.06)

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	55% 34% 9% ••
2	B	256	52% 34% 6% 8%
3	C	239	49% 33% 5% 13%
4	D	209	2% 57% 35% 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	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 51872 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1512	Total	C	N	O	P	0	0	0
			32504	14477	6011	10505	1511			

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 ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	1
			1874	1195	336	338	5			

- Molecule 3 is a protein called 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 ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 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 ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called 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 ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called 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 ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

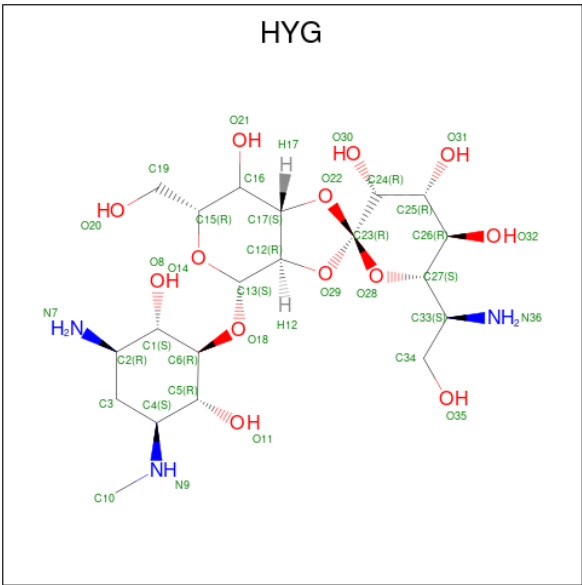
- Molecule 22 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	110	Total	Mg	0	0
			110	110		
22	B	1	Total	Mg	0	0
			1	1		
22	D	1	Total	Mg	0	0
			1	1		
22	E	2	Total	Mg	0	0
			2	2		
22	H	1	Total	Mg	0	0
			1	1		
22	J	1	Total	Mg	0	0
			1	1		
22	M	1	Total	Mg	0	0
			1	1		
22	P	1	Total	Mg	0	0
			1	1		

- Molecule 23 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	5	Total	K	0	0
			5	5		

- Molecule 24 is HYGROMYCIN B (CCD ID: HYG) (formula: C₂₀H₃₇N₃O₁₃).



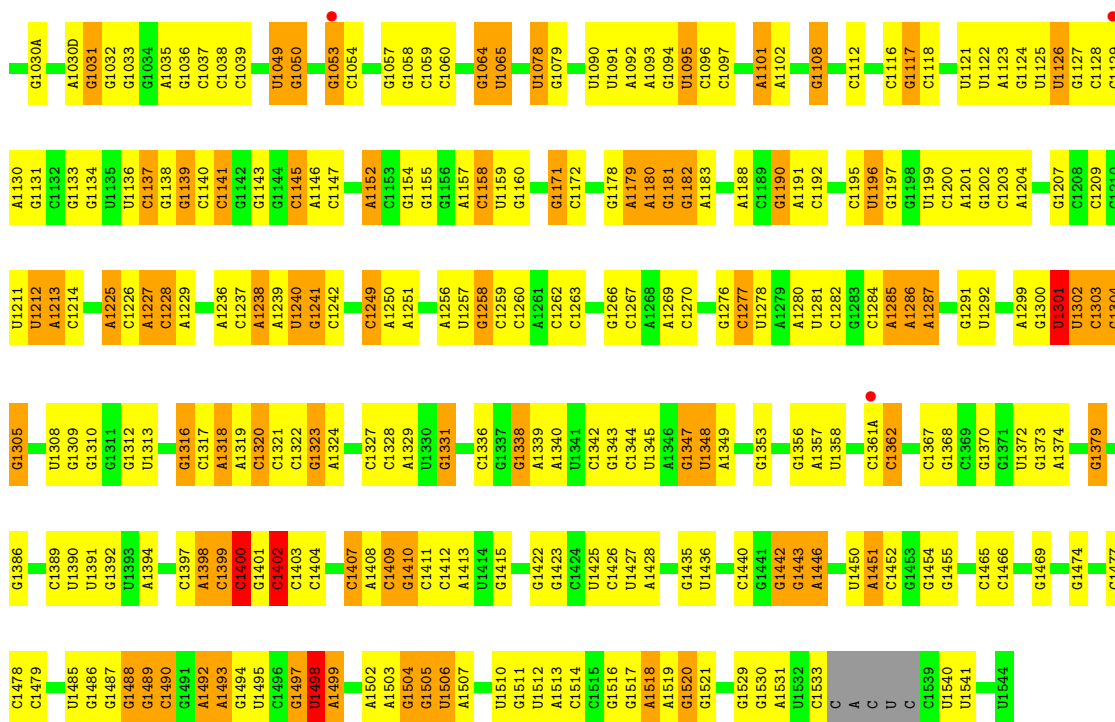
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			36	20	3	13		

- Molecule 25 is ZINC ION (CCD ID: ZN) (formula: Zn).

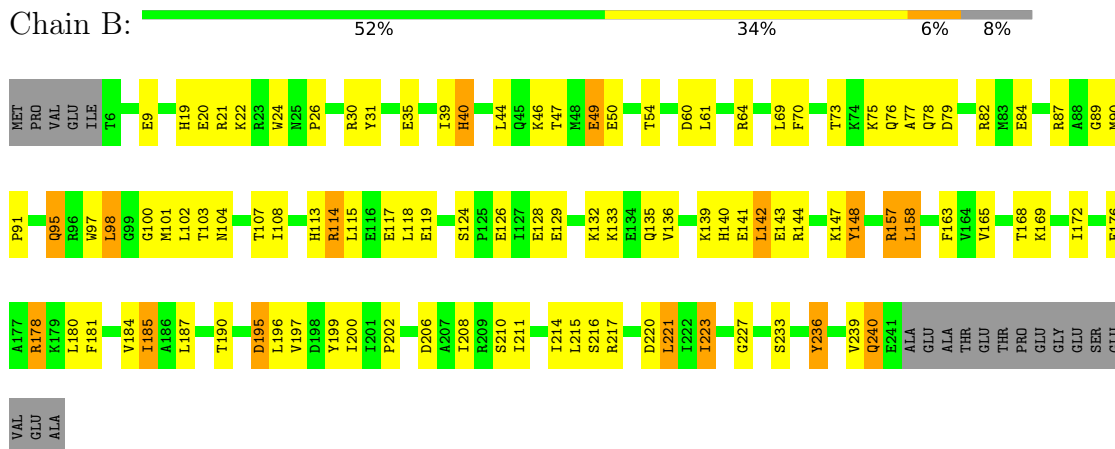
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total	Zn	0	0
			1	1		
25	N	1	Total	Zn	0	0
			1	1		

- Molecule 26 is water.

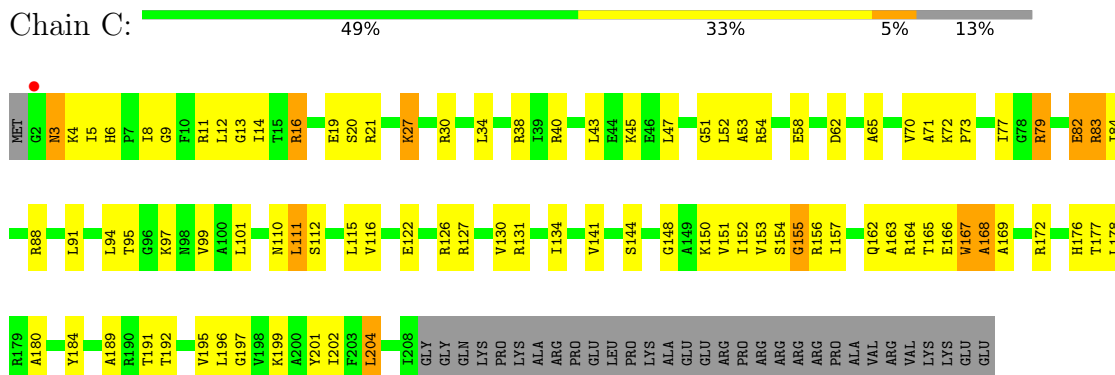
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	A	40	Total	O	0	0
			40	40		
26	H	11	Total	O	0	0
			11	11		
26	S	3	Total	O	0	0
			3	3		



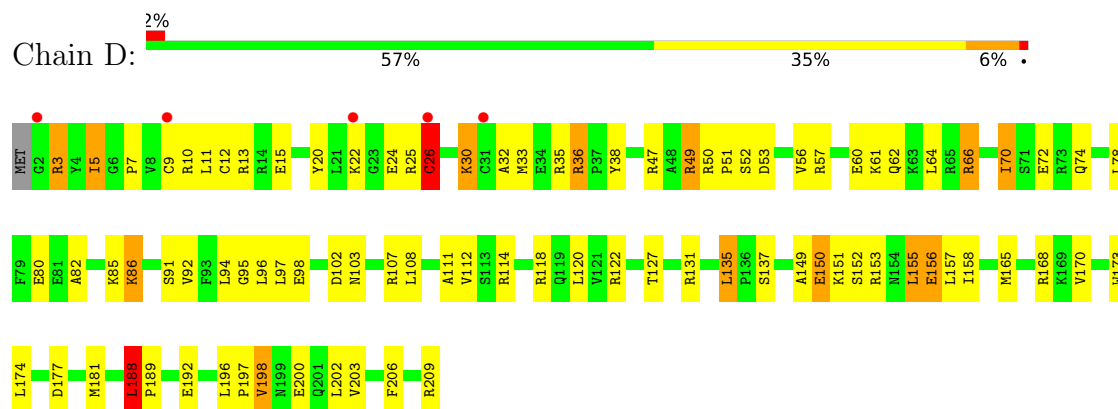
- Molecule 2: ribosomal protein S2



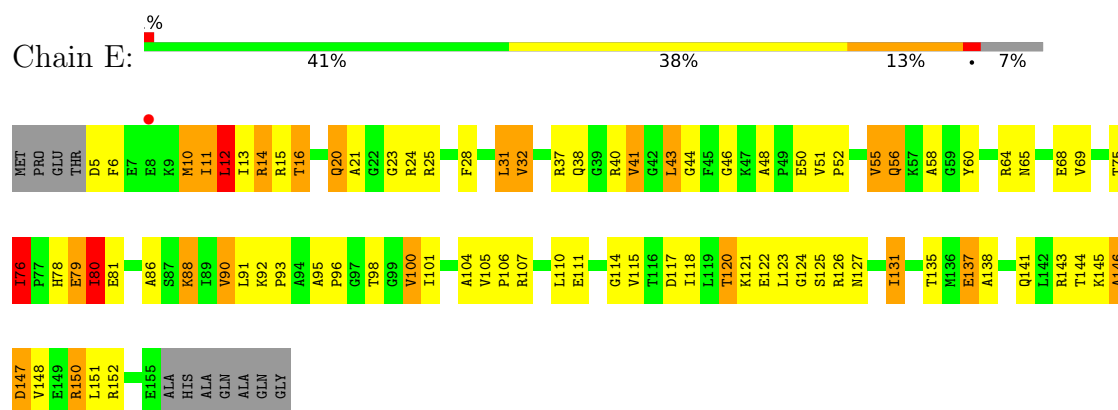
- Molecule 3: ribosomal protein S3



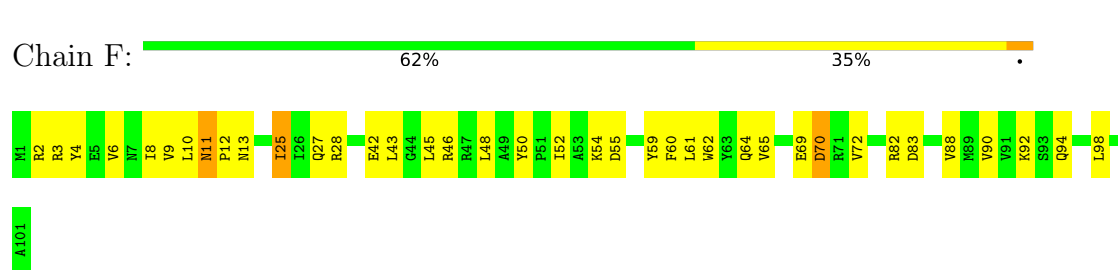
- Molecule 4: ribosomal protein S4



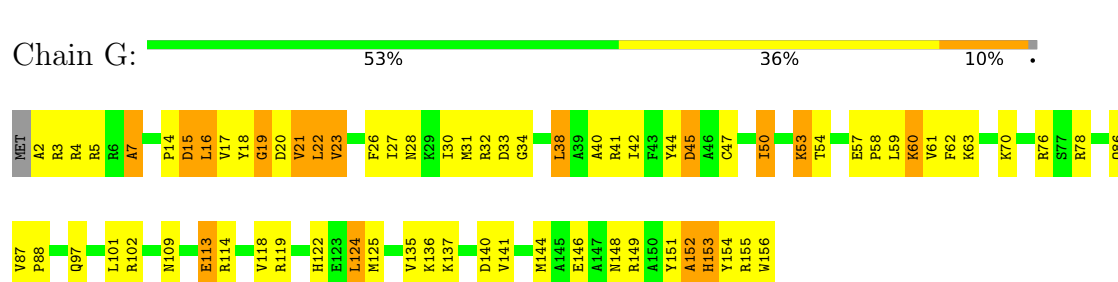
- Molecule 5: ribosomal protein S5



- Molecule 6: ribosomal protein S6



- Molecule 7: ribosomal protein S7

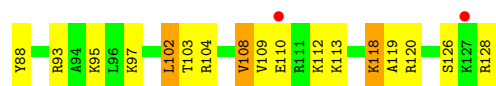
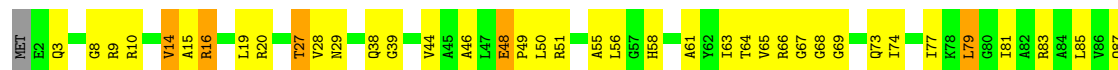


- Molecule 8: ribosomal protein S8

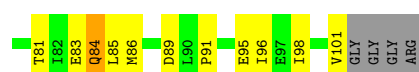
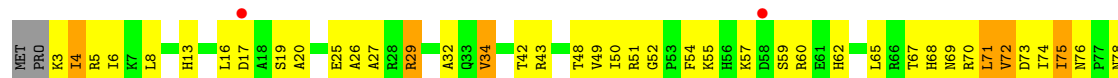
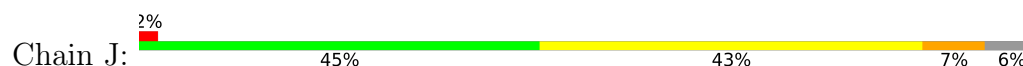




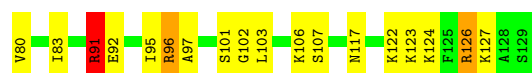
• Molecule 9: ribosomal protein S9



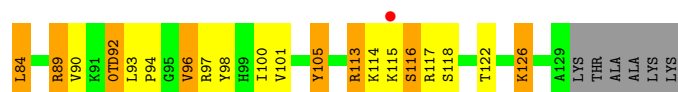
• Molecule 10: ribosomal protein S10



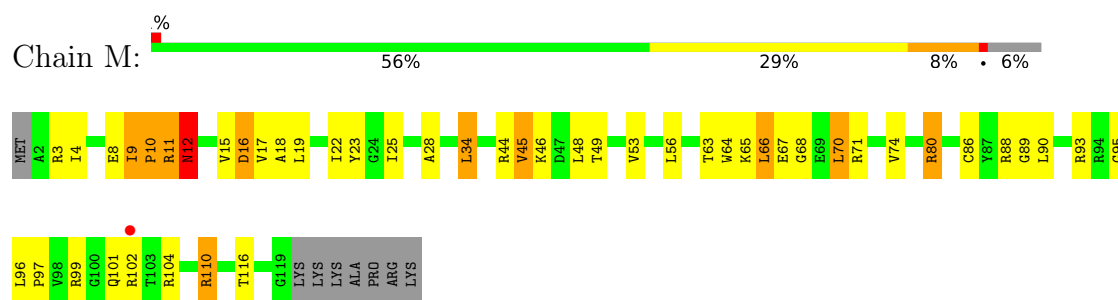
• Molecule 11: ribosomal protein S11



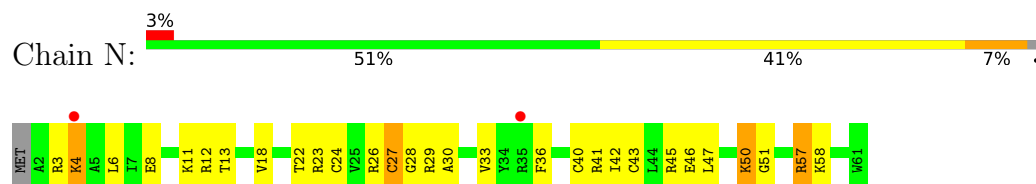
• Molecule 12: ribosomal protein S12



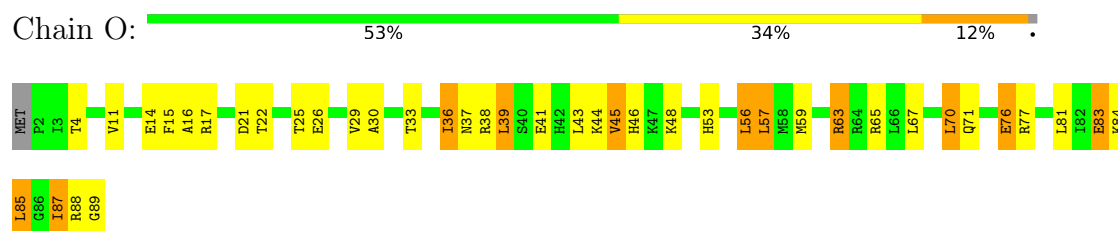
• Molecule 13: ribosomal protein S13



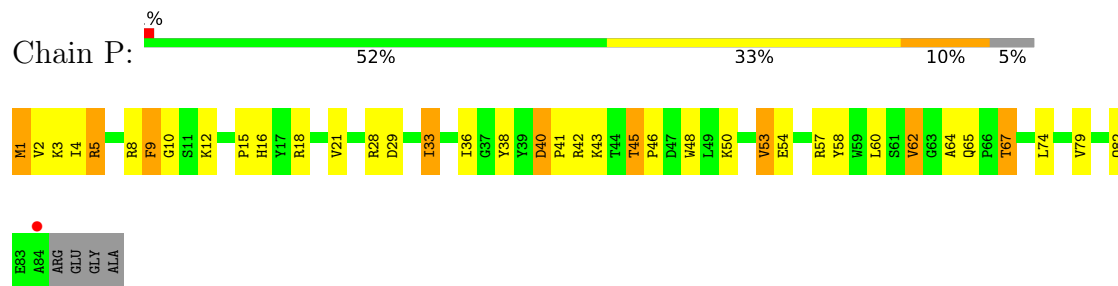
- Molecule 14: ribosomal protein S14



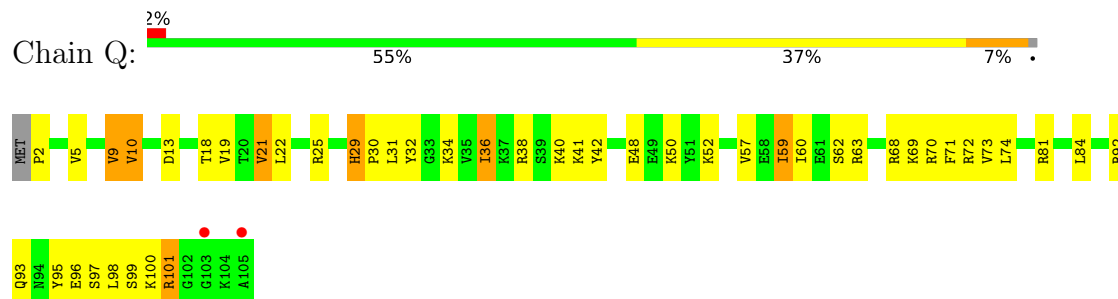
- Molecule 15: ribosomal protein S15



- Molecule 16: ribosomal protein S16

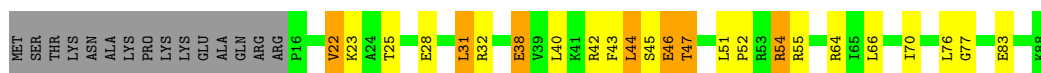


- Molecule 17: ribosomal protein S17



- Molecule 18: ribosomal protein S18

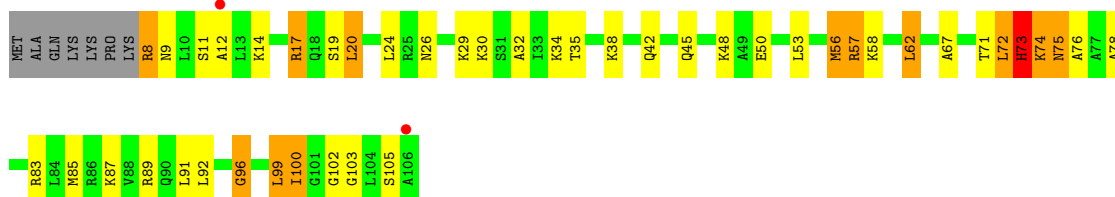




- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.31Å 402.31Å 175.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.85 – 3.65 34.85 – 3.65	Depositor EDS
% Data completeness (in resolution range)	97.1 (34.85-3.65) 96.7 (34.85-3.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.66Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.153 , 0.204 0.156 , 0.203	Depositor DCC
R_{free} test set	7729 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	147.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 110.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	51872	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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: 2MG, PSU, K, MG, 4OC, MA6, UR3, 7MG, 0TD, 5MC, HYG, M2G, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/36037	0.68	13/56239 (0.0%)
2	B	0.76	0/1909	1.14	4/2579 (0.2%)
3	C	0.62	0/1637	1.00	2/2207 (0.1%)
4	D	0.74	0/1733	1.13	11/2318 (0.5%)
5	E	0.95	0/1163	1.34	12/1566 (0.8%)
6	F	0.59	0/856	1.05	5/1154 (0.4%)
7	G	0.66	0/1276	1.09	7/1709 (0.4%)
8	H	1.03	1/1136 (0.1%)	1.33	10/1527 (0.7%)
9	I	0.64	0/1029	1.10	2/1379 (0.1%)
10	J	0.71	0/806	1.09	3/1084 (0.3%)
11	K	0.86	0/900	1.20	6/1213 (0.5%)
12	L	0.87	4/978 (0.4%)	1.34	9/1308 (0.7%)
13	M	0.68	0/947	1.03	6/1270 (0.5%)
14	N	0.66	0/501	0.95	0/664
15	O	0.83	0/745	1.07	1/992 (0.1%)
16	P	0.92	0/717	1.28	7/965 (0.7%)
17	Q	0.96	2/870 (0.2%)	1.30	3/1159 (0.3%)
18	R	0.78	0/604	1.11	1/801 (0.1%)
19	S	0.64	0/662	1.07	2/892 (0.2%)
20	T	0.85	0/765	1.18	5/1007 (0.5%)
21	U	0.57	0/213	0.93	0/279
All	All	0.61	7/55484 (0.0%)	0.86	109/82312 (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	1
7	G	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
9	I	0	1
20	T	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	109	ILE	CA-CB	-5.71	1.46	1.54
12	L	11	VAL	CA-CB	-5.63	1.47	1.54
12	L	25	PRO	CA-C	5.60	1.59	1.53
12	L	101	VAL	CA-CB	-5.53	1.47	1.54
12	L	13	LYS	CA-C	-5.24	1.49	1.52
17	Q	9	VAL	CA-CB	-5.11	1.48	1.54
17	Q	10	VAL	CA-CB	-5.09	1.48	1.53

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-13.29	96.91	114.85
12	L	26	ALA	N-CA-C	-10.53	100.62	113.15
12	L	30	ALA	CA-C-N	9.99	129.75	119.56
12	L	30	ALA	C-N-CA	9.99	129.75	119.56
2	B	9	GLU	N-CA-C	9.52	122.08	108.00
17	Q	29	HIS	CA-C-N	9.49	129.12	119.82
17	Q	29	HIS	C-N-CA	9.49	129.12	119.82
16	P	40	ASP	CA-C-N	9.23	128.91	118.85
16	P	40	ASP	C-N-CA	9.23	128.91	118.85
2	B	76	GLN	N-CA-C	-8.57	101.15	111.69
4	D	26	CYS	N-CA-C	-8.27	102.45	112.54
8	H	100	ILE	CA-C-N	7.66	127.59	119.85
8	H	100	ILE	C-N-CA	7.66	127.59	119.85
11	K	26	ASN	N-CA-C	7.32	122.39	113.17
9	I	67	GLY	N-CA-C	7.26	118.84	111.95
4	D	12	CYS	N-CA-C	-7.20	102.47	111.11
6	F	55	ASP	CA-C-N	7.19	126.83	119.56
6	F	55	ASP	C-N-CA	7.19	126.83	119.56
12	L	105	TYR	CB-CA-C	-7.12	108.37	116.63
12	L	63	GLY	N-CA-C	-7.03	105.51	115.43
11	K	91	ARG	N-CA-C	-7.01	103.39	112.23
8	H	75	ARG	CA-C-N	6.83	127.22	119.92
8	H	75	ARG	C-N-CA	6.83	127.22	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	76	ILE	CA-C-N	6.79	126.42	119.56
5	E	76	ILE	C-N-CA	6.79	126.42	119.56
6	F	11	ASN	CA-C-N	6.76	126.39	119.56
6	F	11	ASN	C-N-CA	6.76	126.39	119.56
13	M	11	ARG	N-CA-C	6.74	119.67	109.23
5	E	80	ILE	CB-CA-C	-6.73	100.12	110.95
4	D	188	LEU	CA-C-N	6.66	126.62	119.76
4	D	188	LEU	C-N-CA	6.66	126.62	119.76
5	E	104	ALA	N-CA-C	-6.65	103.96	111.14
3	C	155	GLY	N-CA-C	6.64	123.53	112.85
10	J	52	GLY	CA-C-N	6.63	126.32	119.56
10	J	52	GLY	C-N-CA	6.63	126.32	119.56
3	C	127	ARG	N-CA-C	6.62	118.66	110.91
5	E	127	ASN	CA-C-N	6.56	126.80	119.32
5	E	127	ASN	C-N-CA	6.56	126.80	119.32
17	Q	9	VAL	CB-CA-C	-6.38	101.12	110.62
5	E	12	LEU	N-CA-C	6.31	119.68	109.40
7	G	70	LYS	CA-C-N	6.30	126.79	119.99
7	G	70	LYS	C-N-CA	6.30	126.79	119.99
12	L	70	ILE	CB-CA-C	-6.28	103.96	111.18
11	K	48	ILE	CB-CA-C	-6.18	104.53	111.45
1	A	266	G	C2'-C3'-O3'	6.16	118.74	109.50
8	H	46	LYS	N-CA-C	-6.14	104.49	112.23
1	A	701	C	C4'-C3'-O3'	6.14	118.61	109.40
18	R	22	VAL	N-CA-C	6.13	116.25	110.30
20	T	76	ALA	N-CA-C	-6.07	104.66	111.28
13	M	10	PRO	CA-C-O	-5.99	114.61	121.56
13	M	9	ILE	CA-C-N	5.97	125.92	119.78
13	M	9	ILE	C-N-CA	5.97	125.92	119.78
2	B	148	TYR	N-CA-C	5.96	119.03	111.69
16	P	65	GLN	CA-C-N	5.95	126.14	120.31
16	P	65	GLN	C-N-CA	5.95	126.14	120.31
11	K	48	ILE	N-CA-C	-5.91	103.53	110.21
19	S	4	SER	N-CA-C	5.91	118.03	108.34
5	E	32	VAL	N-CA-C	5.86	117.20	108.46
4	D	33	MET	N-CA-C	-5.85	105.64	112.89
5	E	48	ALA	N-CA-C	5.85	115.04	108.25
16	P	9	PHE	N-CA-C	5.83	120.18	112.72
11	K	49	GLY	N-CA-C	5.81	121.00	113.27
10	J	71	LEU	N-CA-C	5.79	120.06	112.13
1	A	687	A	P-O3'-C3'	5.77	128.85	120.20
20	T	9	ASN	N-CA-C	5.74	119.25	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	M	17	VAL	CB-CA-C	-5.68	104.61	111.88
5	E	20	GLN	N-CA-C	-5.67	101.04	110.17
8	H	81	HIS	N-CA-C	-5.65	104.73	111.69
20	T	96	GLY	N-CA-C	5.64	118.92	111.70
7	G	118	VAL	CB-CA-C	-5.63	104.66	112.04
4	D	36	ARG	CA-C-N	5.61	125.28	119.56
4	D	36	ARG	C-N-CA	5.61	125.28	119.56
1	A	913	A	P-O3'-C3'	5.61	128.62	120.20
20	T	73	HIS	CB-CA-C	-5.59	109.14	115.79
6	F	60	PHE	N-CA-C	5.58	117.61	108.52
20	T	74	LYS	CB-CA-C	-5.57	109.16	115.79
2	B	165	VAL	N-CA-C	5.55	115.79	110.74
1	A	1301	U	P-O3'-C3'	5.52	128.49	120.20
16	P	53	VAL	N-CA-C	5.51	116.17	110.82
1	A	701	C	P-O3'-C3'	5.50	128.44	120.20
5	E	41	VAL	CB-CA-C	-5.49	100.88	110.71
7	G	16	LEU	N-CA-C	5.46	117.23	111.28
7	G	87	VAL	N-CA-C	5.45	113.94	107.73
1	A	1505	G	P-O3'-C3'	5.44	128.36	120.20
13	M	12	ASN	N-CA-C	5.43	119.07	111.90
1	A	1498	UR3	P-O3'-C3'	5.42	126.21	119.70
1	A	1182	G	C4'-C3'-O3'	5.40	117.50	109.40
8	H	134	ILE	N-CA-C	5.39	116.16	110.72
15	O	87	ILE	N-CA-C	5.38	116.28	110.21
1	A	115	G	C2'-C3'-O3'	5.37	117.56	109.50
5	E	23	GLY	N-CA-C	5.35	118.27	111.37
7	G	19	GLY	N-CA-C	-5.34	107.73	115.27
12	L	7	ILE	N-CA-C	-5.33	105.52	110.53
11	K	101	SER	N-CA-C	-5.33	106.46	113.17
7	G	7	ALA	N-CA-C	5.28	117.08	110.91
8	H	3	THR	CA-C-N	-5.26	114.43	122.42
8	H	3	THR	C-N-CA	-5.26	114.43	122.42
4	D	38	TYR	CA-C-N	5.24	125.77	120.38
4	D	38	TYR	C-N-CA	5.24	125.77	120.38
4	D	12	CYS	CA-CB-SG	5.22	126.40	114.40
19	S	30	LEU	CB-CA-C	-5.22	109.58	115.79
16	P	36	ILE	N-CA-C	5.17	117.95	112.83
12	L	115	LYS	CA-C-N	-5.15	115.15	123.23
12	L	115	LYS	C-N-CA	-5.15	115.15	123.23
1	A	266	G	P-O3'-C3'	5.14	127.91	120.20
1	A	559	A	P-O3'-C3'	5.12	127.88	120.20
1	A	115	G	P-O3'-C3'	5.12	127.87	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	ARG	N-CA-C	5.12	118.50	111.54
8	H	41	ARG	N-CA-C	-5.11	105.79	112.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	89	GLY	Peptide
7	G	152	ALA	Peptide
8	H	90	GLY	Peptide
9	I	38	GLN	Peptide
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	32504	0	16434	456	0
2	B	1874	0	1887	64	0
3	C	1613	0	1677	57	0
4	D	1703	0	1763	65	0
5	E	1147	0	1207	56	0
6	F	843	0	857	24	0
7	G	1257	0	1296	58	0
8	H	1116	0	1177	46	0
9	I	1010	0	1037	42	0
10	J	793	0	835	34	0
11	K	885	0	904	33	0
12	L	973	0	1058	44	0
13	M	937	0	995	35	0
14	N	492	0	529	21	0
15	O	734	0	771	33	0
16	P	701	0	720	30	0
17	Q	857	0	928	33	0
18	R	598	0	670	18	0
19	S	648	0	673	24	0
20	T	763	0	861	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	U	209	0	221	10	0
22	A	110	0	0	0	0
22	B	1	0	0	0	0
22	D	1	0	0	0	0
22	E	2	0	0	0	0
22	H	1	0	0	0	0
22	J	1	0	0	0	0
22	M	1	0	0	0	0
22	P	1	0	0	0	0
23	A	5	0	0	0	0
24	A	36	0	37	3	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	40	0	0	4	0
26	H	11	0	0	2	0
26	S	3	0	0	0	0
All	All	51872	0	36537	1083	0

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

All (1083) 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)
3:C:6:HIS:HD2	3:C:9:GLY:H	1.14	0.93
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.52	0.90
1:A:1128:C:H42	1:A:1143:G:H22	1.17	0.88
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.57	0.87
1:A:951:G:OP2	13:M:102:ARG:NH2	2.09	0.85
1:A:9:G:OP2	5:E:121:LYS:NZ	2.10	0.84
6:F:94:GLN:HG3	18:R:32:ARG:HD3	1.58	0.83
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.44	0.83
8:H:105:ARG:NH2	26:H:311:HOH:O	2.12	0.83
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.20	0.82
1:A:427:U:OP1	4:D:13:ARG:NH2	2.11	0.82
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.13	0.81
16:P:57:ARG:NH1	16:P:79:VAL:O	2.13	0.81
5:E:144:THR:HG22	5:E:146:ALA:H	1.44	0.81
1:A:1258:G:H1	1:A:1277:C:H42	1.28	0.81
12:L:27:LEU:O	12:L:29:GLY:N	2.13	0.81
5:E:76:ILE:HG22	5:E:93:PRO:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:16:ASP:OD1	13:M:16:ASP:N	2.13	0.81
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.14	0.81
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.48	0.78
1:A:975:A:H5''	1:A:975:A:H8	1.47	0.77
1:A:103:C:OP1	20:T:17:ARG:NH1	2.18	0.77
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.67	0.77
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.66	0.76
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.18	0.76
12:L:48:PRO:HD2	12:L:92:0TD:H3	1.65	0.76
1:A:266:G:O2'	1:A:267:C:OP2	2.05	0.74
5:E:144:THR:O	5:E:148:VAL:HG23	1.87	0.74
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.23	0.74
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.70	0.73
1:A:542:G:OP1	4:D:10:ARG:NH2	2.21	0.73
17:Q:29:HIS:HB2	17:Q:36:ILE:HD13	1.71	0.72
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.71	0.72
1:A:1487:G:H2'	1:A:1488:G:C8	2.25	0.72
2:B:157:ARG:HG2	2:B:158:LEU:HD12	1.71	0.72
1:A:279:A:OP2	17:Q:95:TYR:OH	2.06	0.72
1:A:925:G:H1	1:A:1391:U:H3	1.35	0.72
8:H:104:ARG:HH11	8:H:104:ARG:HG2	1.53	0.72
1:A:559:A:OP1	5:E:126:ARG:NH2	2.21	0.72
11:K:15:ALA:HA	11:K:77:MET:HA	1.70	0.72
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.71	0.71
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.72	0.71
5:E:147:ASP:OD1	5:E:147:ASP:N	2.15	0.71
9:I:48:GLU:OE1	9:I:51:ARG:NH2	2.24	0.71
7:G:32:ARG:O	7:G:34:GLY:N	2.24	0.70
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.72	0.70
19:S:6:LYS:HG2	19:S:7:LYS:H	1.56	0.70
1:A:1277:C:H1'	1:A:1282:C:H1'	1.74	0.69
16:P:45:THR:HG22	16:P:46:PRO:HD2	1.72	0.69
1:A:91:C:H2'	1:A:92:C:H6	1.57	0.69
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.72	0.69
6:F:25:ILE:HD12	6:F:28:ARG:HD2	1.75	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.27	0.69
12:L:25:PRO:C	12:L:27:LEU:H	1.98	0.69
12:L:20:LYS:H	12:L:20:LYS:HZ3	1.39	0.68
3:C:88:ARG:HG2	3:C:101:LEU:HD13	1.74	0.68
1:A:1180:A:OP1	9:I:103:THR:OG1	2.09	0.68
14:N:26:ARG:HH21	14:N:47:LEU:HG	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.75	0.68
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.26	0.68
1:A:1412:C:H2'	1:A:1413:A:C8	2.29	0.68
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.26	0.68
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.24	0.67
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.74	0.67
1:A:1240:U:H1'	7:G:38:LEU:HD21	1.77	0.67
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.76	0.67
10:J:25:GLU:O	10:J:29:ARG:NE	2.26	0.67
1:A:738:C:OP2	6:F:92:LYS:NZ	2.24	0.67
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.76	0.67
1:A:1338:G:H2'	1:A:1339:A:C8	2.30	0.67
15:O:15:PHE:CD2	15:O:30:ALA:HB2	2.29	0.67
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.77	0.66
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.77	0.66
2:B:114:ARG:NH1	2:B:141:GLU:OE1	2.28	0.66
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.77	0.66
12:L:27:LEU:C	12:L:29:GLY:H	2.03	0.66
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.35	0.66
17:Q:84:LEU:HD12	17:Q:84:LEU:H	1.59	0.66
1:A:501:C:H2'	1:A:502:G:H8	1.59	0.66
2:B:102:LEU:HB2	2:B:176:GLU:HG2	1.76	0.66
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.76	0.66
3:C:47:LEU:HB2	3:C:52:LEU:HD13	1.78	0.66
7:G:5:ARG:CZ	7:G:7:ALA:HA	2.26	0.66
1:A:269:C:H2'	1:A:270:A:C8	2.30	0.66
1:A:946:A:H2'	1:A:947:G:C8	2.30	0.66
1:A:1026:G:H3'	1:A:1027:C:H5''	1.78	0.66
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.77	0.66
18:R:54:ARG:H	18:R:54:ARG:HH21	1.43	0.66
4:D:3:ARG:HD2	4:D:118:ARG:HE	1.61	0.65
2:B:103:THR:N	2:B:176:GLU:OE1	2.26	0.65
19:S:6:LYS:HG2	19:S:7:LYS:HG3	1.75	0.65
1:A:191:G:H1'	20:T:105:SER:HA	1.78	0.65
3:C:131:ARG:HA	3:C:134:ILE:HD12	1.77	0.65
1:A:376:G:H2'	1:A:377:G:H8	1.61	0.65
1:A:1488:G:H2'	1:A:1489:G:C8	2.31	0.65
4:D:188:LEU:HD22	4:D:189:PRO:HD2	1.78	0.65
1:A:1427:U:H2'	1:A:1428:A:H8	1.62	0.65
3:C:6:HIS:CD2	3:C:9:GLY:H	2.05	0.65
1:A:1133:G:H1	1:A:1141:C:H42	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:149:ARG:NH2	7:G:152:ALA:HB2	2.12	0.65
1:A:266:G:H5''	1:A:268:C:H41	1.60	0.65
1:A:376:G:O3'	16:P:5:ARG:NH1	2.30	0.65
3:C:156:ARG:H	3:C:163:ALA:HA	1.62	0.64
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.78	0.64
5:E:11:ILE:HG13	5:E:31:LEU:HB3	1.78	0.64
1:A:664:G:H22	1:A:741:G:H1	1.43	0.64
2:B:79:ASP:HA	2:B:82:ARG:HG3	1.78	0.64
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.31	0.64
8:H:124:ALA:O	8:H:128:GLY:N	2.31	0.64
1:A:1435:G:H2'	1:A:1436:U:C6	2.32	0.64
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.78	0.64
13:M:88:ARG:HH11	19:S:3:ARG:HH21	1.44	0.64
20:T:56:MET:HE2	20:T:85:MET:HA	1.80	0.64
1:A:192:U:H1'	20:T:103:GLY:HA2	1.80	0.63
13:M:86:CYS:O	13:M:90:LEU:HG	1.98	0.63
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.33	0.63
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.80	0.63
20:T:89:ARG:NH2	20:T:105:SER:O	2.31	0.63
1:A:192:U:C1'	20:T:103:GLY:HA2	2.27	0.63
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.63	0.63
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.33	0.63
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.81	0.63
1:A:1236:A:H4'	1:A:1304:G:H4'	1.80	0.63
10:J:26:ALA:O	10:J:84:GLN:NE2	2.31	0.63
3:C:27:LYS:HD3	3:C:27:LYS:H	1.63	0.63
1:A:8:A:C6	4:D:209:ARG:HB2	2.34	0.63
2:B:184:VAL:HG12	2:B:197:VAL:HG13	1.80	0.63
10:J:6:ILE:HD13	10:J:72:VAL:HG11	1.81	0.63
16:P:10:GLY:H	16:P:16:HIS:HB2	1.64	0.63
17:Q:29:HIS:HD2	17:Q:32:TYR:HB2	1.63	0.62
1:A:403:C:OP1	4:D:137:SER:OG	2.16	0.62
1:A:633:G:H2'	1:A:634:C:C6	2.34	0.62
1:A:1112:C:N3	3:C:178:LEU:HB2	2.14	0.62
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.81	0.62
9:I:65:VAL:HG21	9:I:77:ILE:HD11	1.80	0.62
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.80	0.62
1:A:238:G:OP1	17:Q:25:ARG:NH2	2.33	0.62
13:M:80:ARG:HH11	13:M:80:ARG:HB3	1.63	0.62
1:A:881:G:P	12:L:12:ARG:HH22	2.22	0.62
4:D:32:ALA:O	4:D:36:ARG:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.82	0.62
1:A:620:C:H2'	1:A:621:A:O4'	1.98	0.62
2:B:113:HIS:O	2:B:117:GLU:HG3	1.98	0.62
1:A:1425:U:H2'	1:A:1426:C:C6	2.35	0.62
7:G:50:ILE:O	7:G:54:THR:HG22	1.99	0.62
8:H:21:LYS:O	8:H:65:TYR:OH	2.12	0.62
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.30	0.62
14:N:11:LYS:HG3	14:N:13:THR:H	1.64	0.62
1:A:1057:G:H5''	3:C:154:SER:HB2	1.82	0.61
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.82	0.61
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.15	0.61
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.82	0.61
1:A:677:U:H3	1:A:713:G:H22	1.47	0.61
1:A:538:G:H5''	12:L:114:LYS:HB2	1.82	0.61
1:A:1101:A:H4'	1:A:1102:A:O5'	1.99	0.61
4:D:57:ARG:HH22	5:E:107:ARG:HD3	1.65	0.61
8:H:120:THR:OG1	8:H:121:ASP:N	2.29	0.61
1:A:130:A:OP2	1:A:190(E):U:O2'	2.15	0.61
1:A:284:G:H2'	1:A:285:G:H8	1.66	0.61
18:R:46:GLU:CD	18:R:46:GLU:H	2.08	0.61
4:D:107:ARG:HH21	4:D:114:ARG:HH22	1.46	0.61
7:G:38:LEU:O	7:G:42:ILE:HG13	2.01	0.61
1:A:1415:G:C2	1:A:1486:G:C6	2.89	0.61
2:B:185:ILE:HG23	2:B:199:TYR:HB2	1.83	0.61
10:J:51:ARG:HB2	10:J:59:SER:HB3	1.82	0.61
1:A:438:G:N1	1:A:496:A:OP2	2.33	0.60
1:A:1347:G:O6	9:I:10:ARG:NH2	2.34	0.60
1:A:135:C:O2	16:P:1:MET:HB2	2.00	0.60
1:A:1157:A:H1'	1:A:1181:G:N2	2.15	0.60
1:A:1495:U:O4	24:A:1716:HYG:N9	2.35	0.60
1:A:1305:G:N2	1:A:1331:G:H2'	2.17	0.60
1:A:1520:G:H2'	1:A:1521:G:H8	1.66	0.60
5:E:147:ASP:HA	5:E:150:ARG:HB2	1.83	0.60
19:S:33:THR:HG22	19:S:35:SER:H	1.65	0.60
1:A:299:G:H2'	1:A:300:A:C8	2.35	0.60
1:A:442:C:H42	1:A:492:G:H1	1.48	0.60
1:A:1343:G:H2'	1:A:1344:C:C6	2.36	0.60
1:A:1413:A:H2	1:A:1488:G:H22	1.49	0.60
3:C:11:ARG:NH1	3:C:177:THR:O	2.35	0.60
1:A:21:G:H2'	1:A:22:G:C8	2.36	0.60
1:A:1284:C:OP2	1:A:1285:A:O2'	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ARG:HG2	3:C:94:LEU:HD21	1.83	0.60
1:A:413:G:N2	1:A:429:U:OP2	2.30	0.60
1:A:1028:C:H42	1:A:1033:G:H1	1.50	0.59
1:A:1126:U:H2'	1:A:1127:G:O4'	2.02	0.59
1:A:1227:A:OP1	19:S:80:TYR:OH	2.18	0.59
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.83	0.59
1:A:975:A:H5''	1:A:975:A:C8	2.33	0.59
17:Q:100:LYS:HB2	17:Q:101:ARG:CZ	2.32	0.59
1:A:1266:G:N2	1:A:1269:A:OP2	2.31	0.59
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.68	0.59
1:A:328:C:H4'	1:A:329:A:H5'	1.84	0.59
1:A:353:A:H5'	1:A:353:A:H8	1.68	0.59
1:A:707:C:H4'	11:K:20:TYR:CD2	2.37	0.59
1:A:976:G:OP2	1:A:1358:U:O2'	2.21	0.59
1:A:978:A:O2'	1:A:1322:C:N3	2.35	0.59
7:G:22:LEU:HB2	7:G:97:GLN:HE22	1.66	0.59
8:H:102:ARG:H	8:H:102:ARG:NE	2.00	0.59
1:A:755:G:OP2	15:O:65:ARG:HD2	2.03	0.59
1:A:1124:G:N7	1:A:1145:C:O2'	2.31	0.59
1:A:1139:G:H4'	1:A:1140:C:H5'	1.83	0.59
1:A:1178:G:N7	9:I:97:LYS:NZ	2.41	0.59
6:F:8:ILE:HG12	6:F:88:VAL:HG22	1.84	0.59
18:R:47:THR:HA	18:R:83:GLU:HB2	1.83	0.59
1:A:1238:A:H5'	1:A:1336:C:H41	1.66	0.59
11:K:57:THR:HG22	11:K:59:TYR:H	1.67	0.58
1:A:129:U:O3'	1:A:129(A):G:H3'	2.03	0.58
1:A:153:C:H42	1:A:168:G:H1	1.51	0.58
2:B:40:HIS:CD2	2:B:190:THR:HG21	2.39	0.58
1:A:1286:A:H2'	1:A:1287:A:H4'	1.85	0.58
10:J:57:LYS:O	10:J:60:ARG:NH2	2.35	0.58
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.35	0.58
2:B:98:LEU:HG	2:B:101:MET:HE3	1.86	0.58
9:I:81:ILE:O	9:I:85:LEU:HB2	2.04	0.58
15:O:15:PHE:CE2	15:O:85:LEU:HD21	2.39	0.58
1:A:266:G:C8	1:A:266:G:H5'	2.38	0.57
1:A:1487:G:C2	1:A:1488:G:C4	2.92	0.57
19:S:41:VAL:HB	19:S:42:PRO:HD2	1.85	0.57
1:A:1228:C:H2'	1:A:1229:A:H8	1.70	0.57
1:A:1392:G:H21	1:A:1502:A:H8	1.50	0.57
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.34	0.57
6:F:42:GLU:OE1	6:F:59:TYR:OH	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:78:ARG:NH1	7:G:154:TYR:O	2.37	0.57
4:D:32:ALA:HA	4:D:35:ARG:HG3	1.85	0.57
10:J:50:ILE:HG22	10:J:60:ARG:HD3	1.87	0.57
12:L:113:ARG:NH1	12:L:116:SER:H	2.01	0.57
1:A:316:G:OP2	1:A:351:G:O2'	2.21	0.57
13:M:12:ASN:H	13:M:45:VAL:HG12	1.70	0.57
1:A:1031:G:H2'	1:A:1032:G:H8	1.68	0.57
17:Q:48:GLU:HB2	17:Q:50:LYS:HG3	1.86	0.57
1:A:1313:U:O4	19:S:4:SER:OG	2.10	0.57
1:A:1321:C:H1'	19:S:77:THR:HG21	1.85	0.57
7:G:88:PRO:HG2	7:G:155:ARG:HH21	1.70	0.57
10:J:4:ILE:HD11	10:J:6:ILE:HD11	1.87	0.57
1:A:1158:C:H5'	2:B:133:LYS:HE2	1.85	0.57
4:D:11:LEU:HD13	4:D:66:ARG:HG2	1.85	0.57
6:F:6:VAL:HG13	6:F:90:VAL:HG22	1.85	0.57
20:T:53:LEU:HD12	20:T:100:ILE:HG23	1.87	0.57
20:T:75:ASN:OD1	20:T:75:ASN:N	2.37	0.57
1:A:1488:G:H2'	1:A:1489:G:H8	1.70	0.56
3:C:52:LEU:HA	3:C:70:VAL:HA	1.85	0.56
4:D:103:ASN:OD1	4:D:114:ARG:NH2	2.28	0.56
1:A:1112:C:C2	3:C:178:LEU:HB2	2.40	0.56
3:C:30:ARG:HB3	14:N:36:PHE:O	2.05	0.56
7:G:20:ASP:OD1	7:G:22:LEU:HD23	2.05	0.56
21:U:15:ARG:HH11	21:U:15:ARG:HB2	1.69	0.56
1:A:337:C:H2'	1:A:338:A:H8	1.70	0.56
1:A:491:G:H2'	1:A:492:G:H8	1.70	0.56
18:R:52:PRO:HB2	18:R:54:ARG:HD2	1.85	0.56
1:A:1285:A:H4'	1:A:1286:A:O5'	2.03	0.56
3:C:130:VAL:HG12	3:C:134:ILE:HD11	1.86	0.56
12:L:20:LYS:H	12:L:20:LYS:NZ	2.04	0.56
17:Q:29:HIS:CD2	17:Q:32:TYR:H	2.24	0.56
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.87	0.56
2:B:100:GLY:O	2:B:104:ASN:N	2.38	0.56
8:H:111:ILE:O	8:H:134:ILE:HB	2.04	0.56
1:A:429:U:H1'	1:A:430:A:H5''	1.88	0.56
1:A:560:U:H5'	1:A:566:G:N2	2.21	0.56
1:A:954:G:H21	1:A:1227:A:H62	1.54	0.56
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.41	0.56
10:J:8:LEU:HD22	10:J:20:ALA:HB2	1.88	0.56
1:A:545:C:OP2	4:D:62:GLN:NE2	2.39	0.56
1:A:553:A:O2'	12:L:29:GLY:O	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:G:OP1	1:A:1507:A:H4'	2.06	0.56
1:A:1485:U:H2'	1:A:1486:G:H8	1.71	0.55
1:A:707:C:H2'	1:A:708:C:C6	2.42	0.55
8:H:114:THR:HG22	8:H:130:GLY:O	2.06	0.55
1:A:130:A:H5'	17:Q:63:ARG:HE	1.70	0.55
1:A:932:C:H4'	7:G:4:ARG:NH2	2.22	0.55
19:S:11:VAL:HG22	19:S:39:THR:HB	1.86	0.55
1:A:953:G:N7	13:M:104:ARG:NH2	2.54	0.55
13:M:99:ARG:HB2	13:M:101:GLN:NE2	2.21	0.55
1:A:501:C:H2'	1:A:502:G:C8	2.39	0.55
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.55
2:B:195:ASP:O	8:H:68:ARG:NH2	2.38	0.55
1:A:633:G:H2'	1:A:634:C:H6	1.72	0.55
1:A:1510:U:H2'	1:A:1511:G:C8	2.41	0.55
5:E:101:ILE:O	5:E:120:THR:HG23	2.07	0.55
1:A:269:C:H2'	1:A:270:A:H8	1.71	0.55
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.14	0.55
1:A:730:G:N2	1:A:765:G:H5''	2.21	0.55
5:E:98:THR:HB	5:E:117:ASP:HB3	1.89	0.55
1:A:804:U:H5''	1:A:805:C:OP2	2.07	0.54
12:L:7:ILE:O	12:L:10:LEU:N	2.40	0.54
1:A:962:C:H2'	1:A:963:G:O4'	2.06	0.54
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.43	0.54
1:A:1239:A:H4'	1:A:1240:U:H5''	1.90	0.54
1:A:1316:G:N1	1:A:1319:A:OP2	2.37	0.54
1:A:1486:G:N1	1:A:1487:G:C2	2.75	0.54
4:D:150:GLU:CD	4:D:150:GLU:H	2.15	0.54
8:H:17:THR:HG22	8:H:63:LEU:HG	1.88	0.54
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.88	0.54
11:K:40:ILE:HG13	11:K:75:TYR:HD2	1.73	0.54
1:A:508:C:OP1	4:D:209:ARG:NH2	2.39	0.54
1:A:1347:G:O2'	1:A:1348:U:P	2.65	0.54
3:C:13:GLY:HA3	14:N:57:ARG:NH2	2.22	0.54
11:K:102:GLY:O	11:K:103:LEU:HD23	2.08	0.54
12:L:60:LEU:HB3	12:L:62:SER:H	1.73	0.54
14:N:29:ARG:NH1	14:N:40:CYS:SG	2.81	0.54
18:R:38:GLU:CD	18:R:38:GLU:H	2.14	0.54
1:A:6:G:O6	5:E:95:ALA:N	2.30	0.54
1:A:419:C:H42	1:A:424:G:H1	1.56	0.54
1:A:707:C:H2'	1:A:708:C:H6	1.72	0.54
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.43	0.54
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.89	0.54
1:A:28:G:O2'	1:A:296:U:OP1	2.25	0.54
1:A:1316:G:N2	1:A:1318:A:H3'	2.23	0.54
1:A:110:C:H2'	1:A:111:G:O4'	2.07	0.54
1:A:975:A:H4'	1:A:976:G:H5''	1.89	0.54
9:I:51:ARG:HG2	9:I:56:LEU:HD11	1.89	0.54
1:A:685:G:O2'	1:A:686:U:H5'	2.08	0.54
1:A:1329:A:P	13:M:28:ALA:HB3	2.47	0.54
2:B:87:ARG:CZ	2:B:233:SER:HB2	2.38	0.54
5:E:5:ASP:CG	5:E:6:PHE:H	2.14	0.54
1:A:537:G:H2'	1:A:538:G:H8	1.73	0.53
3:C:3:ASN:OD1	3:C:3:ASN:N	2.41	0.53
17:Q:22:LEU:HD13	17:Q:41:LYS:HG3	1.90	0.53
1:A:266:G:HO2'	1:A:267:C:P	2.31	0.53
12:L:54:LYS:HD2	12:L:54:LYS:N	2.24	0.53
12:L:93:LEU:O	12:L:96:VAL:HG23	2.08	0.53
2:B:103:THR:HG23	2:B:176:GLU:CD	2.32	0.53
1:A:372:C:H1'	1:A:373:A:OP2	2.09	0.53
1:A:1465:C:H2'	1:A:1466:C:O4'	2.09	0.53
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.16	0.53
1:A:390:C:H2'	1:A:391:G:C8	2.44	0.53
1:A:551:U:H2'	1:A:552:U:C6	2.43	0.53
1:A:1398:A:H5''	1:A:1401:G:H4'	1.91	0.53
4:D:156:GLU:OE1	4:D:157:LEU:N	2.41	0.53
12:L:84:LEU:HB2	12:L:105:TYR:CE1	2.43	0.53
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.89	0.53
19:S:5:LEU:O	19:S:6:LYS:HB2	2.09	0.53
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.91	0.53
1:A:1443:G:H5''	1:A:1443:G:N3	2.24	0.53
1:A:114:U:O2'	1:A:115:G:H5'	2.09	0.53
1:A:166:G:H2'	1:A:167:G:H8	1.74	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
1:A:1347:G:N2	1:A:1373:G:H2'	2.23	0.53
10:J:32:ALA:O	10:J:34:VAL:HG23	2.09	0.53
1:A:91:C:H2'	1:A:92:C:C6	2.42	0.53
1:A:665:A:N3	1:A:732:C:H2'	2.24	0.53
1:A:1128:C:OP1	9:I:66:ARG:NH2	2.42	0.53
7:G:17:VAL:HB	7:G:44:TYR:OH	2.09	0.53
7:G:122:HIS:HA	7:G:125:MET:HE2	1.91	0.53
14:N:24:CYS:HB3	14:N:28:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:85:LEU:N	15:O:85:LEU:HD23	2.24	0.53
1:A:8:A:N6	4:D:209:ARG:HB2	2.23	0.52
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.75	0.52
7:G:146:GLU:HA	7:G:149:ARG:HG2	1.90	0.52
9:I:3:GLN:HG3	9:I:20:ARG:HG2	1.92	0.52
13:M:19:LEU:O	13:M:22:ILE:HG12	2.09	0.52
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.89	0.52
1:A:383:A:C5	1:A:384:G:H1'	2.44	0.52
1:A:932:C:H4'	7:G:4:ARG:HH21	1.75	0.52
7:G:22:LEU:HD21	7:G:62:PHE:HE2	1.75	0.52
1:A:300:A:H8	1:A:300:A:O5'	1.93	0.52
8:H:9:MET:HG3	8:H:26:VAL:HG21	1.92	0.52
16:P:74:LEU:O	16:P:79:VAL:HG23	2.09	0.52
1:A:664:G:OP1	18:R:64:ARG:HD2	2.09	0.52
1:A:1059:C:O3'	14:N:45:ARG:NH2	2.42	0.52
1:A:1122:U:H2'	1:A:1123:A:H5'	1.92	0.52
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.90	0.52
1:A:803:G:C6	1:A:804:U:C4	2.98	0.52
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.43	0.52
8:H:104:ARG:HG2	8:H:104:ARG:NH1	2.22	0.52
1:A:1531:A:N6	26:A:1830:HOH:O	2.43	0.52
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.90	0.52
1:A:9:G:OP1	5:E:122:GLU:HG3	2.10	0.52
1:A:1116:C:H2'	1:A:1117:G:H5''	1.92	0.52
1:A:1391:U:H2'	1:A:1392:G:C8	2.45	0.52
11:K:34:ASP:OD1	11:K:38:ASN:N	2.42	0.52
14:N:23:ARG:HG2	14:N:30:ALA:HB2	1.91	0.52
17:Q:21:VAL:HG23	17:Q:42:TYR:HB2	1.90	0.52
17:Q:81:ARG:NE	17:Q:84:LEU:HD11	2.24	0.52
18:R:31:LEU:HD21	18:R:66:LEU:HB2	1.92	0.52
1:A:1188:A:O3'	14:N:58:LYS:NZ	2.42	0.52
1:A:1262:C:H2'	1:A:1263:C:C6	2.45	0.52
1:A:1427:U:H2'	1:A:1428:A:C8	2.44	0.52
3:C:6:HIS:HD2	3:C:9:GLY:N	1.96	0.52
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.92	0.52
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.44	0.51
11:K:66:LEU:HD12	11:K:97:ALA:HB1	1.92	0.51
18:R:44:LEU:HD23	18:R:44:LEU:N	2.26	0.51
18:R:54:ARG:H	18:R:54:ARG:NH2	2.08	0.51
1:A:1477:C:H2'	1:A:1478:C:C6	2.45	0.51
7:G:28:ASN:O	7:G:31:MET:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:49:VAL:O	10:J:60:ARG:HA	2.11	0.51
1:A:443:C:H2'	1:A:444:C:H6	1.74	0.51
1:A:707:C:H4'	11:K:20:TYR:HD2	1.74	0.51
1:A:1126:U:H5''	26:A:1835:HOH:O	2.10	0.51
1:A:1422:G:H2'	1:A:1423:G:C8	2.45	0.51
4:D:30:LYS:HA	4:D:35:ARG:HH21	1.74	0.51
21:U:6:ARG:HD3	21:U:15:ARG:CZ	2.40	0.51
1:A:858:G:O2'	1:A:859:A:H5'	2.10	0.51
1:A:1498:UR3:O2'	1:A:1499:A:OP2	2.23	0.51
5:E:40:ARG:HG2	5:E:40:ARG:HH11	1.74	0.51
17:Q:70:ARG:HD2	17:Q:70:ARG:N	2.25	0.51
1:A:1318:A:H4'	19:S:10:PHE:CE2	2.45	0.51
1:A:376:G:H2'	1:A:377:G:C8	2.44	0.51
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.11	0.51
2:B:178:ARG:NH1	8:H:71:GLY:O	2.44	0.51
1:A:302:G:H5''	12:L:17:LYS:HE2	1.92	0.51
1:A:1516:G:H2'	1:A:1518:MA6:OP2	2.11	0.51
3:C:111:LEU:HD21	3:C:144:SER:O	2.11	0.51
15:O:84:LYS:C	15:O:85:LEU:HD23	2.35	0.51
17:Q:21:VAL:HG21	17:Q:59:ILE:HG12	1.93	0.51
12:L:27:LEU:C	12:L:29:GLY:N	2.66	0.51
1:A:284:G:H2'	1:A:285:G:C8	2.46	0.51
1:A:656:C:H42	1:A:750:G:H1	1.58	0.51
12:L:12:ARG:HH21	12:L:13:LYS:HE3	1.76	0.51
1:A:434:U:H2'	1:A:435:C:C6	2.46	0.51
5:E:55:VAL:HG12	5:E:56:GLN:N	2.26	0.51
15:O:25:THR:CG2	15:O:70:LEU:HD12	2.41	0.51
1:A:250:A:H4'	1:A:251:G:O5'	2.11	0.50
1:A:1489:G:H2'	1:A:1490:C:C6	2.46	0.50
15:O:56:LEU:HA	15:O:59:MET:HE2	1.93	0.50
19:S:6:LYS:HG2	19:S:7:LYS:N	2.25	0.50
1:A:946:A:H2'	1:A:947:G:H8	1.76	0.50
1:A:1485:U:H2'	1:A:1486:G:C8	2.47	0.50
2:B:35:GLU:HB3	2:B:40:HIS:HB3	1.93	0.50
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.94	0.50
13:M:88:ARG:HH11	19:S:3:ARG:NH2	2.06	0.50
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	1.93	0.50
1:A:1037:C:N3	1:A:1038:C:N4	2.59	0.50
5:E:152:ARG:HB3	8:H:43:GLY:HA3	1.93	0.50
20:T:71:THR:O	20:T:72:LEU:HD23	2.12	0.50
1:A:939:G:H2'	1:A:940:C:C6	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:33:THR:OG1	15:O:63:ARG:NH1	2.37	0.50
17:Q:69:LYS:C	17:Q:70:ARG:HD2	2.37	0.50
1:A:737:A:H2'	1:A:738:C:C6	2.46	0.50
10:J:76:ASN:O	10:J:78:ASN:N	2.45	0.50
15:O:14:GLU:HB3	15:O:15:PHE:HD1	1.77	0.50
1:A:376:G:OP2	16:P:67:THR:HG21	2.12	0.50
1:A:390:C:H2'	1:A:391:G:H8	1.77	0.50
1:A:539:A:H2'	1:A:540:G:C8	2.46	0.50
2:B:84:GLU:OE1	2:B:216:SER:HA	2.12	0.50
7:G:22:LEU:HB2	7:G:97:GLN:NE2	2.26	0.50
5:E:105:VAL:HG11	5:E:131:ILE:HG22	1.94	0.50
13:M:12:ASN:O	13:M:12:ASN:ND2	2.32	0.50
16:P:43:LYS:HG2	16:P:48:TRP:CE2	2.47	0.50
1:A:814:A:H2'	1:A:816:A:H5''	1.93	0.49
2:B:139:LYS:O	2:B:139:LYS:HD3	2.11	0.49
5:E:137:GLU:O	5:E:141:GLN:HG2	2.11	0.49
1:A:1301:U:O2'	1:A:1302:U:H3'	2.12	0.49
5:E:144:THR:HB	5:E:147:ASP:OD1	2.11	0.49
11:K:33:THR:HB	11:K:38:ASN:C	2.37	0.49
4:D:149:ALA:O	4:D:152:SER:N	2.45	0.49
15:O:76:GLU:CD	15:O:76:GLU:H	2.19	0.49
1:A:99:C:H2'	1:A:101:A:C8	2.48	0.49
1:A:338:A:H2'	1:A:339:C:C6	2.47	0.49
1:A:1236:A:H2'	1:A:1237:C:C6	2.47	0.49
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.49
2:B:217:ARG:O	2:B:220:ASP:HB2	2.12	0.49
12:L:28:LYS:C	12:L:30:ALA:H	2.19	0.49
1:A:735:C:O2'	1:A:736:C:H5'	2.13	0.49
3:C:6:HIS:NE2	3:C:8:ILE:HB	2.27	0.49
3:C:19:GLU:HG2	3:C:54:ARG:HH12	1.77	0.49
4:D:24:GLU:HB2	4:D:112:VAL:HG21	1.93	0.49
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.28	0.49
2:B:195:ASP:OD1	2:B:195:ASP:N	2.45	0.49
7:G:136:LYS:O	7:G:140:ASP:HB2	2.11	0.49
9:I:28:VAL:HG12	9:I:29:ASN:HB2	1.95	0.49
11:K:30:VAL:HG21	11:K:65:ALA:HA	1.94	0.49
19:S:80:TYR:CE1	19:S:81:ARG:HB2	2.48	0.49
3:C:51:GLY:O	3:C:71:ALA:N	2.45	0.49
5:E:122:GLU:O	5:E:123:LEU:HD23	2.13	0.49
11:K:19:ALA:HB2	11:K:80:VAL:HG21	1.94	0.49
13:M:68:GLY:HA2	13:M:71:ARG:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:G:H2'	1:A:779:C:O4'	2.12	0.49
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.42	0.49
16:P:58:TYR:O	16:P:62:VAL:HG22	2.12	0.49
20:T:8:ARG:N	20:T:8:ARG:HH11	2.11	0.49
1:A:1178:G:N2	1:A:1180:A:H3'	2.28	0.49
1:A:1486:G:H2'	1:A:1487:G:O4'	2.12	0.49
4:D:52:SER:O	4:D:56:VAL:HG23	2.12	0.49
18:R:43:PHE:C	18:R:51:LEU:HD12	2.37	0.49
1:A:370:C:O2'	1:A:371:G:H5'	2.13	0.49
1:A:1154:G:H2'	1:A:1155:G:H8	1.78	0.49
1:A:1309:G:OP2	13:M:99:ARG:NH1	2.46	0.49
9:I:55:ALA:O	9:I:58:HIS:ND1	2.33	0.49
2:B:70:PHE:CE2	2:B:163:PHE:HD1	2.30	0.48
10:J:50:ILE:HG22	10:J:60:ARG:CD	2.43	0.48
16:P:54:GLU:OE1	16:P:54:GLU:N	2.37	0.48
18:R:25:THR:OG1	18:R:42:ARG:NH1	2.46	0.48
1:A:617:G:H1	1:A:623:C:H42	1.59	0.48
1:A:909:A:H2'	1:A:910:C:O4'	2.13	0.48
2:B:60:ASP:O	2:B:64:ARG:HG3	2.12	0.48
7:G:109:ASN:OD1	7:G:119:ARG:NH2	2.39	0.48
11:K:33:THR:HB	11:K:38:ASN:O	2.13	0.48
1:A:872:A:O2'	1:A:873:A:H3'	2.13	0.48
1:A:1225:A:H2'	1:A:1225:A:N3	2.28	0.48
9:I:16:ARG:HD3	9:I:64:THR:HB	1.95	0.48
14:N:4:LYS:H	14:N:4:LYS:HD2	1.78	0.48
17:Q:81:ARG:HE	17:Q:84:LEU:HD11	1.77	0.48
1:A:17:U:H2'	1:A:18:C:C6	2.47	0.48
5:E:76:ILE:HG23	5:E:78:HIS:H	1.77	0.48
17:Q:93:GLN:O	17:Q:96:GLU:HG2	2.13	0.48
20:T:53:LEU:HB2	20:T:100:ILE:HG21	1.95	0.48
1:A:560:U:H4'	1:A:561:U:H5''	1.94	0.48
1:A:1492:A:O2'	1:A:1493:A:O5'	2.31	0.48
7:G:14:PRO:HB3	7:G:19:GLY:O	2.13	0.48
7:G:32:ARG:HG2	7:G:33:ASP:OD2	2.14	0.48
12:L:46:LYS:HG2	12:L:47:LYS:H	1.77	0.48
1:A:144:G:H1	1:A:178:C:H42	1.61	0.48
4:D:165:MET:SD	4:D:168:ARG:HD3	2.54	0.48
15:O:17:ARG:HD3	15:O:26:GLU:OE2	2.13	0.48
1:A:103:C:P	20:T:17:ARG:HH12	2.36	0.48
1:A:432:A:H2'	1:A:433:C:O4'	2.13	0.48
1:A:661:G:H8	1:A:661:G:H5''	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:G:H2'	1:A:954:G:O4'	2.13	0.48
1:A:1413:A:H2	1:A:1488:G:N2	2.11	0.48
1:A:1511:G:H2'	1:A:1512:U:O4'	2.14	0.48
3:C:73:PRO:O	3:C:77:ILE:HG12	2.14	0.48
4:D:70:ILE:HD12	4:D:74:GLN:HB2	1.94	0.48
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.96	0.48
1:A:267:C:H2'	1:A:268:C:H6	1.78	0.48
20:T:34:LYS:O	20:T:38:LYS:HG3	2.14	0.48
1:A:42:G:H2'	1:A:43:C:O4'	2.14	0.48
1:A:1328:C:OP1	21:U:21:TYR:OH	2.29	0.48
4:D:78:LEU:HD12	4:D:96:LEU:HB3	1.96	0.48
9:I:126:SER:C	9:I:128:ARG:H	2.22	0.48
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.12	0.48
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.96	0.48
1:A:298:A:H2'	1:A:299:G:O4'	2.14	0.48
1:A:397:A:H5'	1:A:398:C:OP1	2.14	0.48
2:B:95:GLN:NE2	2:B:147:LYS:O	2.45	0.48
3:C:154:SER:OG	3:C:197:GLY:N	2.42	0.48
15:O:85:LEU:HB2	15:O:87:ILE:HG13	1.96	0.48
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.96	0.48
1:A:337:C:H2'	1:A:338:A:C8	2.48	0.47
1:A:524:G:H2'	1:A:525:C:C6	2.49	0.47
1:A:532:A:O2'	1:A:533:A:OP1	2.28	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.97	0.47
2:B:157:ARG:HG2	2:B:158:LEU:N	2.28	0.47
5:E:10:MET:HB2	5:E:32:VAL:HG12	1.95	0.47
1:A:642:A:N7	8:H:115:SER:HA	2.28	0.47
1:A:1065:U:C5	1:A:1190:G:H1'	2.49	0.47
1:A:1488:G:C6	1:A:1489:G:C6	3.02	0.47
1:A:164:U:H2'	1:A:165:C:C6	2.49	0.47
1:A:731:G:OP1	1:A:766:A:H1'	2.14	0.47
1:A:976:G:H5'	1:A:1358:U:O2'	2.14	0.47
1:A:1262:C:H2'	1:A:1263:C:H6	1.80	0.47
1:A:1409:C:N4	1:A:1410:G:O6	2.47	0.47
11:K:16:SER:OG	11:K:106:LYS:NZ	2.47	0.47
1:A:1241:G:H2'	1:A:1242:C:H6	1.80	0.47
7:G:21:VAL:HG23	7:G:22:LEU:H	1.79	0.47
4:D:108:LEU:HD23	4:D:174:LEU:HD13	1.96	0.47
13:M:96:LEU:C	13:M:110:ARG:HG2	2.39	0.47
16:P:9:PHE:CD1	16:P:18:ARG:HG3	2.49	0.47
1:A:652:U:O4	1:A:752:G:O2'	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:G:H3'	9:I:108:VAL:O	2.14	0.47
10:J:69:ASN:O	10:J:70:ARG:NE	2.46	0.47
11:K:44:SER:H	11:K:47:VAL:HB	1.79	0.47
18:R:47:THR:HG22	18:R:83:GLU:H	1.79	0.47
1:A:109:A:H2'	1:A:326:G:N2	2.29	0.47
1:A:836:G:C6	1:A:851:G:C6	3.02	0.47
1:A:1053:G:O2'	1:A:1199:U:H5	1.97	0.47
1:A:1117:G:N2	1:A:1180:A:H1'	2.29	0.47
1:A:1250:A:H2'	1:A:1251:A:C8	2.50	0.47
2:B:101:MET:HA	2:B:108:ILE:HG13	1.95	0.47
3:C:82:GLU:OE1	3:C:83:ARG:N	2.48	0.47
20:T:45:GLN:HG3	20:T:91:LEU:HD13	1.97	0.47
13:M:3:ARG:HH21	13:M:9:ILE:HD11	1.80	0.47
13:M:96:LEU:HB3	13:M:97:PRO:HD2	1.96	0.47
16:P:8:ARG:O	16:P:9:PHE:HD2	1.97	0.47
1:A:644:G:C5	1:A:645:C:C5	3.03	0.47
1:A:1195:C:H5''	1:A:1196:U:OP2	2.15	0.47
2:B:128:GLU:O	2:B:135:GLN:NE2	2.48	0.47
3:C:131:ARG:NE	3:C:166:GLU:OE2	2.44	0.47
7:G:16:LEU:H	7:G:16:LEU:HD22	1.80	0.47
1:A:148:G:H2'	1:A:149:A:H8	1.80	0.47
1:A:679:C:H2'	1:A:680:C:H6	1.79	0.47
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.47
1:A:1442:G:C2	1:A:1446:A:N7	2.82	0.47
24:A:1716:HYG:O21	24:A:1716:HYG:O20	2.21	0.47
6:F:50:TYR:HE1	18:R:77:GLY:HA2	1.78	0.47
7:G:149:ARG:NH2	7:G:149:ARG:O	2.47	0.47
1:A:77:G:O2'	1:A:78:G:H5'	2.15	0.46
1:A:103:C:OP2	20:T:14:LYS:HD2	2.14	0.46
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.97	0.46
1:A:1035:A:H2'	1:A:1036:G:C8	2.49	0.46
1:A:1152:A:OP1	10:J:13:HIS:HB2	2.16	0.46
5:E:37:ARG:O	5:E:114:GLY:HA3	2.15	0.46
10:J:74:ILE:HG22	10:J:75:ILE:O	2.15	0.46
14:N:23:ARG:HA	14:N:30:ALA:HA	1.95	0.46
1:A:309:G:H2'	1:A:310:G:H8	1.80	0.46
1:A:1154:G:H2'	1:A:1155:G:C8	2.51	0.46
1:A:1487:G:C6	1:A:1488:G:C6	3.03	0.46
5:E:110:LEU:O	5:E:115:VAL:HB	2.16	0.46
13:M:63:THR:HG23	13:M:64:TRP:H	1.79	0.46
1:A:35:G:H2'	1:A:36:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:U:H6	1:A:1126:U:O5'	1.98	0.46
7:G:47:CYS:HB3	7:G:58:PRO:HG2	1.97	0.46
8:H:25:ASP:OD1	8:H:25:ASP:N	2.48	0.46
9:I:27:THR:OG1	9:I:28:VAL:N	2.48	0.46
9:I:118:LYS:H	9:I:118:LYS:HG3	1.54	0.46
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.50	0.46
13:M:10:PRO:HB3	13:M:18:ALA:O	2.15	0.46
14:N:24:CYS:HB3	14:N:28:GLY:N	2.31	0.46
20:T:20:LEU:HD13	20:T:20:LEU:HA	1.77	0.46
1:A:679:C:H2'	1:A:680:C:C6	2.50	0.46
3:C:43:LEU:HB3	3:C:47:LEU:HD13	1.96	0.46
12:L:15:ARG:HG3	12:L:15:ARG:HH11	1.80	0.46
1:A:406:G:H1	1:A:436:C:H42	1.62	0.46
1:A:826:C:O2	8:H:15:ASN:ND2	2.49	0.46
1:A:923:A:OP1	5:E:21:ALA:HB2	2.15	0.46
2:B:118:LEU:HB3	2:B:142:LEU:HG	1.98	0.46
3:C:20:SER:HB3	3:C:40:ARG:HH22	1.80	0.46
4:D:85:LYS:HA	4:D:86:LYS:HE2	1.97	0.46
8:H:54:ASP:OD1	8:H:55:GLY:N	2.49	0.46
1:A:109:A:C4	1:A:327:A:C2	3.03	0.46
1:A:434:U:H2'	1:A:435:C:H6	1.80	0.46
1:A:1126:U:H5''	26:A:1837:HOH:O	2.15	0.46
1:A:1281:U:H4'	26:A:1839:HOH:O	2.15	0.46
4:D:188:LEU:HA	4:D:189:PRO:HD2	1.75	0.46
5:E:43:LEU:HD22	5:E:44:GLY:N	2.31	0.46
11:K:41:THR:OG1	11:K:42:TRP:N	2.49	0.46
1:A:35:G:O2'	12:L:118:SER:O	2.26	0.46
1:A:141:A:H1'	1:A:182:U:O2	2.15	0.46
9:I:9:ARG:HG3	9:I:14:VAL:HG13	1.97	0.46
10:J:19:SER:CB	10:J:91:PRO:HG3	2.46	0.46
1:A:243:A:C2	1:A:246:A:C8	3.04	0.46
1:A:771:G:H2'	1:A:772:U:C6	2.51	0.46
1:A:864:A:H2'	1:A:865:A:C8	2.50	0.46
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.63	0.46
4:D:82:ALA:HB2	4:D:96:LEU:HD22	1.98	0.46
15:O:15:PHE:HE2	15:O:85:LEU:HD21	1.80	0.46
16:P:40:ASP:HA	16:P:41:PRO:HD3	1.64	0.46
1:A:1499:A:H1'	1:A:1520:G:H5'	1.98	0.46
2:B:139:LYS:O	2:B:143:GLU:HG3	2.16	0.46
5:E:14:ARG:HD2	5:E:16:THR:HG22	1.96	0.46
5:E:46:GLY:H	5:E:58:ALA:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:2:VAL:O	16:P:64:ALA:HA	2.15	0.46
1:A:539:A:H2'	1:A:540:G:H8	1.81	0.46
1:A:1299:A:C5	1:A:1301:U:O2	2.69	0.46
1:A:1304:G:C6	1:A:1305:G:N1	2.84	0.46
2:B:210:SER:O	2:B:214:ILE:HG12	2.15	0.46
4:D:49:ARG:H	4:D:49:ARG:HD2	1.81	0.46
4:D:102:ASP:OD1	4:D:103:ASN:N	2.48	0.46
1:A:1006:C:H2'	1:A:1007:C:C6	2.51	0.45
1:A:1192:C:O2	5:E:25:ARG:NH2	2.48	0.45
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.56	0.45
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.97	0.45
3:C:6:HIS:HE2	3:C:8:ILE:HB	1.81	0.45
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.99	0.45
6:F:48:LEU:HD13	6:F:52:ILE:HG13	1.98	0.45
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.80	0.45
10:J:3:LYS:HD2	10:J:101:VAL:N	2.31	0.45
14:N:22:THR:HG23	14:N:33:VAL:HG21	1.98	0.45
3:C:126:ARG:HE	3:C:126:ARG:HB3	1.62	0.45
3:C:177:THR:HB	3:C:180:ALA:HB2	1.97	0.45
4:D:57:ARG:HA	4:D:57:ARG:HD3	1.79	0.45
5:E:144:THR:HG22	5:E:145:LYS:N	2.30	0.45
10:J:16:LEU:HD12	10:J:68:HIS:HB2	1.98	0.45
11:K:14:VAL:HG21	11:K:40:ILE:HG12	1.98	0.45
13:M:95:GLY:O	13:M:96:LEU:HD23	2.16	0.45
1:A:1408:A:H2'	1:A:1409:C:O4'	2.16	0.45
1:A:1426:C:H2'	1:A:1427:U:C6	2.51	0.45
1:A:1488:G:O2'	1:A:1489:G:H5'	2.17	0.45
2:B:196:LEU:HD23	2:B:196:LEU:HA	1.55	0.45
3:C:53:ALA:HB2	3:C:115:LEU:HD23	1.97	0.45
4:D:196:LEU:HA	4:D:197:PRO:HD3	1.72	0.45
7:G:16:LEU:HD12	9:I:44:VAL:HG23	1.98	0.45
1:A:1349:A:C2	1:A:1374:A:C4	3.04	0.45
1:A:1372:U:H2'	1:A:1373:G:O4'	2.17	0.45
5:E:135:THR:O	5:E:138:ALA:HB3	2.17	0.45
14:N:42:ILE:O	14:N:46:GLU:HG3	2.16	0.45
19:S:31:ILE:HG22	19:S:49:ILE:HG23	1.99	0.45
1:A:1090:U:H2'	1:A:1091:U:H6	1.80	0.45
1:A:1121:U:H2'	1:A:1122:U:H6	1.80	0.45
1:A:1284:C:H3'	1:A:1285:A:H2'	1.99	0.45
1:A:1422:G:H2'	1:A:1423:G:H8	1.82	0.45
3:C:153:VAL:HG12	3:C:196:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:MET:HG3	8:H:26:VAL:HG11	1.99	0.45
12:L:126:LYS:H	12:L:126:LYS:HD2	1.82	0.45
14:N:6:LEU:HA	14:N:8:GLU:HG3	1.99	0.45
18:R:45:SER:HB2	18:R:46:GLU:OE2	2.17	0.45
1:A:109:A:C6	1:A:326:G:C6	3.05	0.45
1:A:148:G:H2'	1:A:149:A:C8	2.52	0.45
1:A:1212:U:H4'	1:A:1213:A:O5'	2.16	0.45
5:E:5:ASP:CG	5:E:6:PHE:N	2.75	0.45
7:G:153:HIS:CE1	11:K:58:PRO:HD2	2.52	0.45
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.32	0.45
20:T:8:ARG:N	20:T:8:ARG:HD2	2.31	0.45
1:A:542:G:H2'	1:A:543:C:H6	1.82	0.45
1:A:1338:G:C6	1:A:1339:A:C6	3.05	0.45
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.98	0.45
7:G:41:ARG:O	7:G:45:ASP:HB2	2.16	0.45
9:I:85:LEU:O	9:I:88:TYR:HB3	2.17	0.45
10:J:27:ALA:HA	10:J:81:THR:HG23	1.99	0.45
17:Q:29:HIS:HA	17:Q:30:PRO:HD3	1.59	0.45
20:T:67:ALA:HA	20:T:73:HIS:H	1.81	0.45
1:A:663:A:H2'	1:A:664:G:O4'	2.17	0.45
1:A:1397:C:O2'	1:A:1398:A:OP1	2.24	0.45
5:E:90:VAL:C	5:E:91:LEU:HD23	2.42	0.45
6:F:61:LEU:HA	6:F:61:LEU:HD23	1.71	0.45
7:G:20:ASP:OD1	7:G:23:VAL:N	2.40	0.45
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.99	0.45
16:P:9:PHE:N	16:P:16:HIS:O	2.48	0.45
20:T:58:LYS:O	20:T:62:LEU:HB2	2.17	0.45
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.16	0.45
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.48	0.45
8:H:104:ARG:HG3	8:H:138:TRP:CD2	2.52	0.45
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.99	0.45
10:J:50:ILE:HG22	10:J:60:ARG:NE	2.31	0.45
12:L:76:ASN:OD1	12:L:76:ASN:N	2.47	0.45
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.32	0.45
1:A:186:C:H5'	20:T:78:ALA:HB1	1.98	0.44
1:A:455:C:H6	1:A:455:C:O5'	2.00	0.44
1:A:1031:G:H2'	1:A:1032:G:C8	2.50	0.44
1:A:1096:C:H2'	1:A:1097:C:H6	1.82	0.44
1:A:1399:C:C2	1:A:1502:A:N6	2.85	0.44
1:A:1415:G:H1	1:A:1485:U:H3	1.65	0.44
1:A:1450:U:O2'	1:A:1451:A:H8	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:188:LEU:HD22	4:D:188:LEU:HA	1.85	0.44
6:F:4:TYR:CD1	6:F:92:LYS:HG2	2.53	0.44
16:P:38:TYR:HE2	16:P:50:LYS:HE2	1.82	0.44
17:Q:29:HIS:ND1	17:Q:30:PRO:HD2	2.32	0.44
21:U:23:PRO:C	21:U:25:LYS:H	2.25	0.44
1:A:794:A:H2'	1:A:795:C:C6	2.52	0.44
1:A:1091:U:O2	1:A:1093:A:C8	2.70	0.44
2:B:84:GLU:OE2	2:B:233:SER:OG	2.29	0.44
6:F:11:ASN:HA	6:F:12:PRO:HD3	1.72	0.44
7:G:151:TYR:HD2	7:G:154:TYR:HE1	1.65	0.44
8:H:23:SER:N	26:H:302:HOH:O	2.48	0.44
15:O:48:LYS:HD3	15:O:48:LYS:HA	1.74	0.44
1:A:46:G:H2'	1:A:366:C:C5	2.52	0.44
1:A:484:G:H5'	1:A:486:U:O4'	2.17	0.44
1:A:1049:U:H4'	1:A:1050:G:O5'	2.16	0.44
1:A:1506:U:O2'	1:A:1507:A:H5'	2.17	0.44
1:A:1065:U:H5''	1:A:1190:G:N2	2.33	0.44
2:B:104:ASN:O	2:B:107:THR:N	2.49	0.44
6:F:11:ASN:HD21	6:F:13:ASN:HB2	1.82	0.44
7:G:17:VAL:HG12	7:G:18:TYR:CD2	2.53	0.44
1:A:437:U:H2'	1:A:438:G:H5'	1.99	0.44
1:A:1454:G:H2'	1:A:1455:G:H8	1.82	0.44
8:H:13:ILE:O	8:H:17:THR:HG23	2.17	0.44
15:O:15:PHE:CZ	15:O:85:LEU:HD21	2.53	0.44
20:T:26:ASN:O	20:T:29:LYS:HB2	2.17	0.44
20:T:30:LYS:HB3	20:T:30:LYS:HE2	1.88	0.44
1:A:1191:A:OP1	3:C:4:LYS:HE2	2.18	0.44
6:F:46:ARG:HB3	6:F:46:ARG:CZ	2.47	0.44
1:A:390:C:O3'	16:P:28:ARG:NH2	2.51	0.44
1:A:684:A:N3	11:K:39:PRO:HD2	2.33	0.44
1:A:707:C:O3'	11:K:20:TYR:HE2	2.00	0.44
1:A:1425:U:H2'	1:A:1426:C:H6	1.80	0.44
2:B:147:LYS:HE2	2:B:148:TYR:HE2	1.83	0.44
12:L:79:GLU:OE1	12:L:80:HIS:N	2.51	0.44
21:U:5:ASP:O	21:U:11:GLY:HA3	2.17	0.44
1:A:75:G:C6	1:A:76:C:C4	3.06	0.44
1:A:1003:G:N2	1:A:1039:C:O2	2.49	0.44
4:D:53:ASP:O	4:D:57:ARG:HG2	2.17	0.44
8:H:134:ILE:HD13	8:H:134:ILE:HA	1.72	0.44
11:K:16:SER:HA	11:K:79:SER:O	2.18	0.44
12:L:76:ASN:O	12:L:77:LEU:HD23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:22:VAL:HG23	18:R:55:ARG:O	2.18	0.44
1:A:782:A:H2'	1:A:783:C:O4'	2.18	0.44
1:A:1259:C:H42	1:A:1276:G:H1	1.66	0.44
1:A:1277:C:H5''	1:A:1278:U:OP2	2.18	0.44
2:B:114:ARG:HD2	2:B:141:GLU:OE2	2.18	0.44
1:A:283:C:C2	1:A:284:G:C8	3.06	0.43
1:A:537:G:OP1	12:L:113:ARG:NH2	2.51	0.43
1:A:793:U:H5'	1:A:794:A:H5''	2.00	0.43
1:A:1308:U:H3'	13:M:99:ARG:HH12	1.83	0.43
2:B:239:VAL:O	2:B:240:GLN:HG2	2.18	0.43
5:E:100:VAL:O	5:E:101:ILE:HD13	2.17	0.43
9:I:69:GLY:O	9:I:73:GLN:HG3	2.17	0.43
11:K:33:THR:HA	11:K:40:ILE:H	1.82	0.43
15:O:83:GLU:OE2	15:O:84:LYS:N	2.50	0.43
17:Q:59:ILE:HD12	17:Q:59:ILE:HA	1.66	0.43
1:A:738:C:P	6:F:92:LYS:HD3	2.58	0.43
1:A:1426:C:H2'	1:A:1427:U:H6	1.84	0.43
3:C:151:VAL:O	3:C:167:TRP:O	2.36	0.43
7:G:27:ILE:HD12	7:G:40:ALA:HA	2.00	0.43
1:A:192:U:O4'	20:T:103:GLY:HA2	2.18	0.43
1:A:264:U:H2'	1:A:265:G:O4'	2.18	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.83	0.43
1:A:1317:C:H2'	1:A:1318:A:O4'	2.17	0.43
5:E:79:GLU:O	8:H:104:ARG:NH1	2.51	0.43
7:G:5:ARG:NH1	7:G:7:ALA:HA	2.33	0.43
8:H:110:ALA:HB3	8:H:121:ASP:HB3	2.00	0.43
9:I:9:ARG:O	9:I:104:ARG:NH1	2.52	0.43
9:I:50:LEU:HD22	9:I:55:ALA:HB3	1.99	0.43
16:P:1:MET:HE3	16:P:1:MET:HB3	1.83	0.43
1:A:1118:C:P	9:I:104:ARG:HE	2.41	0.43
4:D:196:LEU:HA	4:D:196:LEU:HD23	1.66	0.43
7:G:53:LYS:HB2	7:G:53:LYS:NZ	2.33	0.43
13:M:8:GLU:OE1	13:M:22:ILE:HA	2.17	0.43
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.68	0.43
1:A:1487:G:N1	1:A:1488:G:C6	2.86	0.43
5:E:10:MET:HE2	5:E:13:ILE:HD11	2.00	0.43
9:I:118:LYS:C	9:I:120:ARG:H	2.25	0.43
11:K:91:ARG:HG2	11:K:92:GLU:N	2.33	0.43
15:O:41:GLU:OE2	15:O:41:GLU:HA	2.19	0.43
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.53	0.43
1:A:115:G:O5'	1:A:115:G:H8	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1028:C:N4	1:A:1033:G:H1	2.15	0.43
1:A:1361(A):C:H2'	1:A:1362:C:H5''	2.01	0.43
5:E:86:ALA:O	5:E:124:GLY:HA3	2.18	0.43
8:H:112:LEU:N	8:H:112:LEU:HD23	2.34	0.43
9:I:48:GLU:N	9:I:49:PRO:HD2	2.34	0.43
9:I:65:VAL:HG11	9:I:73:GLN:HB3	2.01	0.43
1:A:806:C:O2'	1:A:807:A:H5'	2.18	0.43
1:A:881:G:OP2	12:L:12:ARG:NH2	2.51	0.43
1:A:1291:G:H2'	1:A:1292:U:C6	2.54	0.43
2:B:49:GLU:HG3	2:B:50:GLU:N	2.33	0.43
2:B:90:MET:HA	2:B:91:PRO:HD2	1.76	0.43
5:E:90:VAL:O	5:E:120:THR:HA	2.18	0.43
6:F:10:LEU:HD11	6:F:61:LEU:HD12	2.00	0.43
7:G:88:PRO:HG2	7:G:155:ARG:NH2	2.31	0.43
8:H:4:ASP:OD1	8:H:6:ILE:N	2.52	0.43
8:H:60:ARG:HG3	8:H:60:ARG:NH1	2.33	0.43
13:M:89:GLY:O	13:M:93:ARG:HG3	2.19	0.43
1:A:593:G:H1	1:A:646:U:H3	1.67	0.43
1:A:748:C:H4'	1:A:749:C:O5'	2.17	0.43
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.53	0.43
1:A:1402:4OC:HM43	1:A:1403:C:N3	2.34	0.43
2:B:180:LEU:O	2:B:181:PHE:HB2	2.19	0.43
3:C:79:ARG:NH2	3:C:82:GLU:HG2	2.34	0.43
3:C:110:ASN:O	3:C:141:VAL:HG22	2.18	0.43
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.88	0.43
4:D:74:GLN:O	4:D:78:LEU:HD23	2.19	0.43
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.51	0.43
4:D:155:LEU:HD11	4:D:157:LEU:HB3	2.00	0.43
7:G:31:MET:HG3	7:G:32:ARG:N	2.34	0.43
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.19	0.43
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.75	0.43
1:A:378:G:H2'	1:A:379:C:C6	2.54	0.43
1:A:858:G:O6	1:A:869:G:C8	2.72	0.43
1:A:1058:G:C6	1:A:1059:C:N3	2.87	0.43
1:A:1239:A:H62	1:A:1299:A:H62	1.65	0.43
1:A:1328:C:P	21:U:21:TYR:HH	2.40	0.43
1:A:1486:G:C6	1:A:1487:G:C6	3.07	0.43
2:B:30:ARG:HG3	2:B:31:TYR:CD2	2.54	0.43
2:B:223:ILE:O	2:B:227:GLY:N	2.52	0.43
4:D:149:ALA:C	4:D:151:LYS:N	2.76	0.43
7:G:153:HIS:HB3	7:G:154:TYR:H	1.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:56:LEU:HD23	13:M:56:LEU:HA	1.77	0.43
20:T:67:ALA:O	20:T:73:HIS:ND1	2.52	0.43
1:A:235:C:H5'	17:Q:70:ARG:HG2	2.01	0.43
1:A:730:G:H21	1:A:765:G:H5''	1.84	0.43
1:A:1487:G:H2'	1:A:1488:G:O4'	2.19	0.43
3:C:58:GLU:HB2	3:C:65:ALA:HB3	2.00	0.43
4:D:32:ALA:C	4:D:35:ARG:H	2.27	0.43
5:E:107:ARG:O	5:E:111:GLU:HB2	2.19	0.43
11:K:44:SER:O	11:K:48:ILE:HG12	2.19	0.43
1:A:106:C:O2	1:A:379:C:H4'	2.18	0.42
1:A:540:G:H2'	1:A:541:G:O4'	2.18	0.42
1:A:931:C:H42	1:A:1386:G:H1	1.67	0.42
1:A:933:G:OP2	7:G:3:ARG:HB3	2.19	0.42
1:A:1389:C:H2'	1:A:1390:U:O4'	2.19	0.42
2:B:129:GLU:N	2:B:129:GLU:OE2	2.52	0.42
2:B:236:TYR:CD1	2:B:239:VAL:HG21	2.54	0.42
3:C:8:ILE:HG23	3:C:16:ARG:HG3	2.00	0.42
6:F:45:LEU:O	6:F:45:LEU:HD12	2.18	0.42
9:I:93:ARG:CZ	9:I:93:ARG:HB3	2.48	0.42
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.20	0.42
1:A:1171:G:H2'	1:A:1172:C:C6	2.54	0.42
1:A:1250:A:H4'	9:I:68:GLY:N	2.34	0.42
4:D:60:GLU:HA	4:D:60:GLU:OE1	2.20	0.42
10:J:48:THR:HA	10:J:62:HIS:HB3	2.02	0.42
1:A:338:A:C6	1:A:339:C:C4	3.07	0.42
1:A:695:A:OP1	11:K:52:GLY:HA3	2.19	0.42
1:A:854:G:C2	1:A:855:G:C8	3.07	0.42
1:A:965:A:H4'	1:A:966:M2G:OP2	2.17	0.42
7:G:26:PHE:O	7:G:30:ILE:HG12	2.20	0.42
7:G:149:ARG:HD2	7:G:149:ARG:HA	1.86	0.42
12:L:42:THR:HA	12:L:53:ARG:O	2.20	0.42
13:M:34:LEU:HD22	13:M:34:LEU:HA	1.65	0.42
15:O:36:ILE:HG22	15:O:37:ASN:N	2.35	0.42
1:A:328:C:O2	1:A:328:C:H2'	2.18	0.42
1:A:741:G:H5'	15:O:39:LEU:HD21	2.00	0.42
1:A:1179:A:O2'	1:A:1180:A:OP1	2.34	0.42
1:A:1320:C:N3	19:S:36:ARG:HD3	2.34	0.42
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.42
1:A:1379:G:O6	7:G:2:ALA:N	2.52	0.42
2:B:35:GLU:HA	2:B:40:HIS:HA	2.01	0.42
3:C:45:LYS:HE3	3:C:45:LYS:HB2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:LEU:HD23	10:J:16:LEU:HA	1.88	0.42
12:L:25:PRO:C	12:L:27:LEU:N	2.69	0.42
1:A:384:G:H2'	1:A:385:C:C6	2.53	0.42
1:A:1095:U:OP1	1:A:1108:G:N1	2.47	0.42
1:A:1260:C:O5'	1:A:1284:C:H4'	2.20	0.42
1:A:1397:C:OP2	5:E:24:ARG:NH2	2.41	0.42
1:A:1450:U:H2'	1:A:1452:C:C5	2.55	0.42
1:A:1486:G:C6	1:A:1487:G:C2	3.08	0.42
2:B:163:PHE:CD2	2:B:185:ILE:HB	2.55	0.42
7:G:113:GLU:O	7:G:119:ARG:HD2	2.19	0.42
8:H:121:ASP:OD2	8:H:122:ARG:N	2.52	0.42
11:K:54:ARG:CZ	11:K:54:ARG:HB2	2.49	0.42
12:L:28:LYS:HZ2	12:L:28:LYS:HG3	1.59	0.42
13:M:101:GLN:N	13:M:101:GLN:OE1	2.52	0.42
1:A:567:G:H2'	1:A:568:G:O4'	2.19	0.42
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.42
2:B:73:THR:HB	2:B:169:LYS:HE2	2.00	0.42
3:C:112:SER:O	3:C:116:VAL:HG23	2.19	0.42
7:G:140:ASP:OD2	7:G:144:MET:HE3	2.20	0.42
10:J:85:LEU:HB3	10:J:86:MET:H	1.59	0.42
19:S:77:THR:O	19:S:77:THR:OG1	2.35	0.42
1:A:803:G:C5	1:A:804:U:C5	3.08	0.42
1:A:1118:C:H1'	1:A:1179:A:C5	2.54	0.42
1:A:1136:U:H5''	1:A:1137:C:C5	2.55	0.42
1:A:1269:A:N1	1:A:1312:G:O2'	2.50	0.42
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.67	0.42
10:J:5:ARG:HA	10:J:73:ASP:OD2	2.20	0.42
1:A:878:G:C5'	8:H:89:PRO:HG2	2.50	0.42
1:A:912:C:OP1	12:L:94:PRO:HB3	2.20	0.42
1:A:939:G:H5''	7:G:102:ARG:NH1	2.35	0.42
1:A:1092:A:H5''	7:G:4:ARG:NH1	2.34	0.42
1:A:1228:C:H2'	1:A:1229:A:C8	2.53	0.42
3:C:62:ASP:O	3:C:97:LYS:HG3	2.20	0.42
8:H:4:ASP:CG	8:H:85:ARG:NH1	2.76	0.42
10:J:16:LEU:HD13	10:J:70:ARG:HG2	2.02	0.42
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.47	0.42
1:A:620:C:C2	4:D:135:LEU:HD13	2.55	0.42
9:I:19:LEU:HD23	9:I:61:ALA:HB2	2.01	0.42
13:M:70:LEU:HD23	13:M:70:LEU:HA	1.77	0.42
1:A:938:A:H5'	7:G:76:ARG:HH22	1.85	0.42
24:A:1716:HYG:H103	24:A:1716:HYG:H32A	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:151:VAL:HG12	3:C:152:ILE:N	2.34	0.42
3:C:155:GLY:HA2	3:C:164:ARG:H	1.85	0.42
5:E:151:LEU:HB3	8:H:79:VAL:HG22	2.00	0.42
7:G:124:LEU:HD13	7:G:124:LEU:HA	1.82	0.42
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.35	0.42
11:K:73:MET:HB2	11:K:73:MET:HE2	1.69	0.42
15:O:41:GLU:OE2	15:O:44:LYS:HD3	2.19	0.42
1:A:190(L):U:O2	20:T:105:SER:HB2	2.20	0.41
1:A:786:G:C2	1:A:797:C:C2	3.08	0.41
1:A:791:G:C6	1:A:792:A:N7	2.88	0.41
1:A:866:C:H2'	1:A:867:G:O4'	2.20	0.41
7:G:54:THR:HG21	7:G:61:VAL:HG21	2.02	0.41
8:H:9:MET:HB3	8:H:9:MET:HE2	1.81	0.41
10:J:42:THR:HG23	10:J:67:THR:O	2.20	0.41
11:K:123:LYS:HA	11:K:126:ARG:HG3	2.02	0.41
1:A:122:G:C2	1:A:123:C:C2	3.08	0.41
1:A:491:G:H2'	1:A:492:G:C8	2.51	0.41
1:A:630:G:H5'	1:A:631:G:OP2	2.19	0.41
1:A:892:A:C2	1:A:907:A:C4	3.08	0.41
1:A:986:A:H1'	19:S:54:GLY:O	2.21	0.41
4:D:94:LEU:HD23	4:D:94:LEU:HA	1.81	0.41
5:E:92:LYS:O	5:E:118:ILE:HG13	2.20	0.41
15:O:87:ILE:C	15:O:89:GLY:H	2.27	0.41
1:A:908:A:C2	1:A:909:A:C4	3.08	0.41
1:A:1006:C:H2'	1:A:1007:C:H6	1.84	0.41
1:A:1203:C:H2'	1:A:1204:A:O4'	2.19	0.41
2:B:118:LEU:HD23	2:B:118:LEU:HA	1.73	0.41
2:B:221:LEU:HA	2:B:221:LEU:HD22	1.69	0.41
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.03	0.41
12:L:28:LYS:C	12:L:30:ALA:N	2.78	0.41
12:L:117:ARG:HB3	12:L:122:THR:O	2.20	0.41
13:M:23:TYR:HB3	13:M:67:GLU:H	1.85	0.41
14:N:50:LYS:HA	14:N:50:LYS:HE2	2.01	0.41
15:O:63:ARG:HE	15:O:63:ARG:HB3	1.79	0.41
17:Q:29:HIS:CD2	17:Q:32:TYR:HB2	2.49	0.41
1:A:135:C:C2	16:P:1:MET:HB2	2.54	0.41
1:A:443:C:H2'	1:A:444:C:C6	2.53	0.41
1:A:1134:G:H1	1:A:1140:C:H42	1.67	0.41
1:A:1478:C:H2'	1:A:1479:C:C6	2.55	0.41
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.50	0.41
5:E:32:VAL:HG22	5:E:58:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.52	0.41
11:K:95:ILE:HD13	11:K:95:ILE:HA	1.77	0.41
16:P:33:ILE:H	16:P:33:ILE:HG13	1.59	0.41
1:A:60:A:H4'	1:A:61:G:O5'	2.21	0.41
1:A:841:U:H6	1:A:841:U:OP1	2.04	0.41
1:A:986:A:O2'	19:S:55:LYS:O	2.37	0.41
1:A:1240:U:OP1	7:G:119:ARG:NH1	2.50	0.41
1:A:1410:G:H2'	1:A:1411:C:O4'	2.21	0.41
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.28	0.41
5:E:12:LEU:C	5:E:12:LEU:HD22	2.45	0.41
5:E:15:ARG:HB2	5:E:28:PHE:CE2	2.55	0.41
15:O:57:LEU:HA	15:O:57:LEU:HD12	1.77	0.41
1:A:372:C:H4'	1:A:373:A:O5'	2.21	0.41
1:A:377:G:OP1	16:P:3:LYS:HD2	2.20	0.41
1:A:976:G:N2	1:A:1362:C:OP2	2.51	0.41
1:A:1308:U:H3'	13:M:99:ARG:NH1	2.35	0.41
1:A:1327:C:H5''	21:U:20:LYS:HE3	2.03	0.41
4:D:3:ARG:HD2	4:D:118:ARG:NE	2.31	0.41
4:D:47:ARG:HB2	4:D:47:ARG:HH11	1.85	0.41
17:Q:22:LEU:HA	17:Q:22:LEU:HD12	1.72	0.41
19:S:5:LEU:HD21	19:S:70:LYS:HE2	2.03	0.41
19:S:33:THR:CG2	19:S:35:SER:H	2.31	0.41
1:A:1147:C:O2	9:I:16:ARG:NH2	2.54	0.41
2:B:19:HIS:NE2	2:B:206:ASP:OD2	2.49	0.41
3:C:8:ILE:HG13	3:C:184:TYR:HB3	2.03	0.41
4:D:78:LEU:CD1	4:D:96:LEU:HB3	2.51	0.41
4:D:92:VAL:O	4:D:95:GLY:N	2.54	0.41
4:D:153:ARG:NH1	4:D:181:MET:HB2	2.36	0.41
4:D:200:GLU:HA	4:D:203:VAL:HG23	2.02	0.41
5:E:144:THR:CG2	5:E:145:LYS:N	2.84	0.41
13:M:99:ARG:HH21	19:S:2:PRO:HD2	1.86	0.41
1:A:191:G:O2'	20:T:102:GLY:O	2.36	0.41
1:A:376:G:P	16:P:67:THR:HG21	2.61	0.41
1:A:1487:G:C2	1:A:1488:G:C5	3.09	0.41
2:B:132:LYS:O	2:B:136:VAL:HG23	2.21	0.41
4:D:3:ARG:NH2	4:D:5:ILE:HD11	2.35	0.41
6:F:25:ILE:HD12	6:F:25:ILE:HA	1.84	0.41
7:G:32:ARG:C	7:G:34:GLY:N	2.79	0.41
7:G:86:GLN:HB2	7:G:148:ASN:ND2	2.35	0.41
15:O:43:LEU:HD11	15:O:53:HIS:HA	2.02	0.41
1:A:76:C:O2'	1:A:77:G:H5'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:A:H2'	1:A:161:A:O4'	2.21	0.41
1:A:346:G:H2'	1:A:347:G:O4'	2.20	0.41
1:A:353:A:H5'	1:A:353:A:C8	2.52	0.41
1:A:355:C:C4	1:A:356:A:N7	2.89	0.41
1:A:392:G:H5'	16:P:12:LYS:HE2	2.02	0.41
1:A:736:C:H2'	1:A:737:A:C8	2.56	0.41
1:A:771:G:H2'	1:A:772:U:H6	1.86	0.41
1:A:920:U:H2'	1:A:921:U:C6	2.56	0.41
1:A:1303:C:C2'	1:A:1304:G:H5'	2.51	0.41
2:B:119:GLU:HG3	2:B:142:LEU:HD21	2.03	0.41
3:C:148:GLY:HA3	3:C:172:ARG:O	2.20	0.41
5:E:76:ILE:HA	5:E:76:ILE:HD12	1.72	0.41
6:F:70:ASP:OD2	6:F:70:ASP:N	2.53	0.41
7:G:58:PRO:O	7:G:59:LEU:C	2.63	0.41
14:N:3:ARG:HH21	14:N:6:LEU:HD21	1.86	0.41
16:P:15:PRO:HD2	16:P:42:ARG:HD3	2.01	0.41
1:A:625:G:H2'	1:A:626:U:C6	2.56	0.41
1:A:908:A:O2'	1:A:909:A:H5'	2.20	0.41
2:B:31:TYR:CD1	2:B:202:PRO:HB3	2.56	0.41
2:B:124:SER:HB2	2:B:126:GLU:HG2	2.02	0.41
7:G:32:ARG:C	7:G:34:GLY:H	2.21	0.41
7:G:60:LYS:HD3	7:G:63:LYS:HB2	2.03	0.41
8:H:104:ARG:O	8:H:105:ARG:C	2.64	0.41
1:A:79:G:N1	1:A:80:G:C5	2.90	0.40
1:A:1488:G:C5	1:A:1489:G:N7	2.89	0.40
2:B:197:VAL:HB	2:B:200:ILE:HG13	2.02	0.40
4:D:60:GLU:HG2	4:D:202:LEU:HB2	2.03	0.40
8:H:116:LYS:HG2	8:H:127:LEU:CD1	2.52	0.40
14:N:58:LYS:HE2	14:N:58:LYS:HB3	1.94	0.40
15:O:87:ILE:HG22	15:O:88:ARG:H	1.86	0.40
21:U:18:TYR:CD1	21:U:24:ARG:HG3	2.56	0.40
1:A:601:C:H42	1:A:637:G:H1	1.69	0.40
1:A:833:U:H2'	1:A:834:C:H6	1.85	0.40
1:A:854:G:H3'	1:A:871:U:O4	2.22	0.40
1:A:925:G:C2	1:A:927:G:C8	3.09	0.40
1:A:1267:C:O2'	21:U:20:LYS:HG3	2.21	0.40
2:B:236:TYR:HA	2:B:239:VAL:HG23	2.04	0.40
4:D:62:GLN:HB3	4:D:66:ARG:NH1	2.36	0.40
4:D:95:GLY:HA3	4:D:188:LEU:HD11	2.03	0.40
4:D:155:LEU:HD12	4:D:158:ILE:HG13	2.03	0.40
5:E:80:ILE:HG13	5:E:91:LEU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:LYS:HE3	5:E:123:LEU:HB2	2.04	0.40
12:L:20:LYS:HD2	12:L:20:LYS:O	2.22	0.40
16:P:74:LEU:HD23	16:P:74:LEU:HA	1.77	0.40
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.72	0.40
20:T:57:ARG:HH21	20:T:102:GLY:HA2	1.85	0.40
20:T:92:LEU:O	20:T:96:GLY:N	2.54	0.40
1:A:107:G:C2	1:A:108:G:H1'	2.57	0.40
1:A:303:A:H2'	1:A:304:U:O4'	2.21	0.40
1:A:1190:G:OP1	3:C:4:LYS:HA	2.21	0.40
9:I:50:LEU:HB3	9:I:56:LEU:H	1.86	0.40
12:L:89:ARG:HB3	12:L:97:ARG:HA	2.03	0.40
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.21	0.40
17:Q:62:SER:OG	17:Q:72:ARG:HG3	2.22	0.40
1:A:235:C:OP1	17:Q:70:ARG:NH1	2.54	0.40
1:A:832:C:H2'	1:A:833:U:O4'	2.22	0.40
1:A:1078:U:H5''	1:A:1079:G:OP2	2.21	0.40
1:A:1487:G:O2'	1:A:1488:G:H5'	2.21	0.40
3:C:12:LEU:HD11	14:N:51:GLY:HA2	2.02	0.40
4:D:192:GLU:OE2	4:D:192:GLU:N	2.54	0.40
8:H:101:PRO:HA	8:H:102:ARG:CZ	2.51	0.40
8:H:103:VAL:HG21	8:H:109:ILE:C	2.46	0.40
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.03	0.40
12:L:47:LYS:HB3	12:L:48:PRO:HD3	2.04	0.40
12:L:57:LYS:HE3	12:L:57:LYS:HB3	1.94	0.40
13:M:8:GLU:CD	13:M:22:ILE:HA	2.46	0.40
13:M:25:ILE:HD11	13:M:66:LEU:HD21	2.02	0.40
15:O:85:LEU:HD12	15:O:87:ILE:HD11	2.04	0.40
17:Q:68:ARG:HH11	17:Q:68:ARG:HD3	1.76	0.40
20:T:29:LYS:O	20:T:32:ALA:HB3	2.21	0.40
1:A:653:A:C8	8:H:56:LYS:HG2	2.56	0.40
1:A:692:U:OP1	11:K:124:LYS:NZ	2.51	0.40
1:A:803:G:C5	1:A:804:U:C4	3.10	0.40
1:A:951:G:C6	1:A:952:U:C4	3.10	0.40
1:A:1064:G:N2	1:A:1190:G:H2'	2.35	0.40
1:A:1121:U:H2'	1:A:1122:U:C6	2.56	0.40
4:D:173:TRP:CD1	4:D:189:PRO:HD3	2.57	0.40
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.57	0.40
11:K:44:SER:OG	11:K:45:GLY:N	2.53	0.40
11:K:53:SER:C	11:K:55:LYS:H	2.29	0.40
15:O:45:VAL:HG12	15:O:46:HIS:H	1.87	0.40
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	234/256 (91%)	212 (91%)	21 (9%)	1 (0%)	30	59
3	C	205/239 (86%)	190 (93%)	14 (7%)	1 (0%)	24	55
4	D	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	24	55
5	E	149/162 (92%)	142 (95%)	6 (4%)	1 (1%)	18	48
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/156 (98%)	136 (89%)	17 (11%)	0	100	100
8	H	136/138 (99%)	129 (95%)	7 (5%)	0	100	100
9	I	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	16	45
10	J	97/105 (92%)	78 (80%)	17 (18%)	2 (2%)	5	27
11	K	117/129 (91%)	105 (90%)	11 (9%)	1 (1%)	14	43
12	L	122/135 (90%)	109 (89%)	12 (10%)	1 (1%)	16	45
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
15	O	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	P	82/88 (93%)	80 (98%)	2 (2%)	0	100	100
17	Q	102/105 (97%)	93 (91%)	9 (9%)	0	100	100
18	R	71/88 (81%)	65 (92%)	6 (8%)	0	100	100
19	S	79/93 (85%)	69 (87%)	8 (10%)	2 (2%)	4	24
20	T	97/106 (92%)	85 (88%)	11 (11%)	1 (1%)	12	41
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
All	All	2357/2541 (93%)	2155 (91%)	190 (8%)	12 (0%)	24	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
19	S	31	ILE
9	I	119	ALA
10	J	72	VAL
20	T	99	LEU
2	B	21	ARG
3	C	168	ALA
5	E	146	ALA
11	K	117	ASN
19	S	6	LYS
10	J	34	VAL
4	D	5	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	194/220 (88%)	164 (84%)	30 (16%)	2	14
3	C	160/188 (85%)	135 (84%)	25 (16%)	2	14
4	D	180/181 (99%)	156 (87%)	24 (13%)	4	18
5	E	115/123 (94%)	82 (71%)	33 (29%)	0	2
6	F	90/90 (100%)	79 (88%)	11 (12%)	5	20
7	G	126/127 (99%)	108 (86%)	18 (14%)	3	16
8	H	119/119 (100%)	93 (78%)	26 (22%)	1	6
9	I	98/99 (99%)	87 (89%)	11 (11%)	6	24
10	J	87/92 (95%)	75 (86%)	12 (14%)	3	17
11	K	90/99 (91%)	76 (84%)	14 (16%)	2	14
12	L	103/110 (94%)	83 (81%)	20 (19%)	1	8
13	M	94/101 (93%)	77 (82%)	17 (18%)	2	10
14	N	49/50 (98%)	43 (88%)	6 (12%)	5	20
15	O	79/80 (99%)	64 (81%)	15 (19%)	1	9
16	P	72/74 (97%)	64 (89%)	8 (11%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Q	96/97 (99%)	78 (81%)	18 (19%)	1	9
18	R	64/77 (83%)	54 (84%)	10 (16%)	2	14
19	S	71/80 (89%)	59 (83%)	12 (17%)	2	12
20	T	76/82 (93%)	57 (75%)	19 (25%)	0	4
21	U	19/22 (86%)	17 (90%)	2 (10%)	6	26
All	All	1982/2111 (94%)	1651 (83%)	331 (17%)	2	12

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	GLU
2	B	22	LYS
2	B	39	ILE
2	B	40	HIS
2	B	44	LEU
2	B	46	LYS
2	B	47	THR
2	B	49	GLU
2	B	61	LEU
2	B	69	LEU
2	B	95	GLN
2	B	98	LEU
2	B	114	ARG
2	B	115	LEU
2	B	140	HIS
2	B	142	LEU
2	B	144	ARG
2	B	157	ARG
2	B	158	LEU
2	B	168	THR
2	B	172	ILE
2	B	178	ARG
2	B	185	ILE
2	B	187	LEU
2	B	195	ASP
2	B	208	ILE
2	B	221	LEU
2	B	223	ILE
2	B	236	TYR
2	B	240	GLN

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Mol	Chain	Res	Type
3	C	3	ASN
3	C	5	ILE
3	C	14	ILE
3	C	16	ARG
3	C	21	ARG
3	C	27	LYS
3	C	34	LEU
3	C	72	LYS
3	C	79	ARG
3	C	82	GLU
3	C	83	ARG
3	C	84	ILE
3	C	91	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	122	GLU
3	C	162	GLN
3	C	165	THR
3	C	167	TRP
3	C	176	HIS
3	C	191	THR
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	9	CYS
4	D	15	GLU
4	D	20	TYR
4	D	25	ARG
4	D	26	CYS
4	D	30	LYS
4	D	49	ARG
4	D	66	ARG
4	D	70	ILE
4	D	80	GLU
4	D	86	LYS
4	D	91	SER
4	D	97	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	135	LEU

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Mol	Chain	Res	Type
4	D	150	GLU
4	D	155	LEU
4	D	156	GLU
4	D	170	VAL
4	D	177	ASP
4	D	188	LEU
4	D	198	VAL
5	E	10	MET
5	E	11	ILE
5	E	12	LEU
5	E	14	ARG
5	E	16	THR
5	E	20	GLN
5	E	31	LEU
5	E	38	GLN
5	E	41	VAL
5	E	43	LEU
5	E	50	GLU
5	E	55	VAL
5	E	56	GLN
5	E	60	TYR
5	E	64	ARG
5	E	65	ASN
5	E	68	GLU
5	E	69	VAL
5	E	75	THR
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
5	E	81	GLU
5	E	88	LYS
5	E	90	VAL
5	E	96	PRO
5	E	100	VAL
5	E	120	THR
5	E	125	SER
5	E	131	ILE
5	E	137	GLU
5	E	147	ASP
5	E	150	ARG
6	F	3	ARG
6	F	9	VAL

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Mol	Chain	Res	Type
6	F	25	ILE
6	F	27	GLN
6	F	43	LEU
6	F	54	LYS
6	F	65	VAL
6	F	70	ASP
6	F	82	ARG
6	F	83	ASP
6	F	98	LEU
7	G	15	ASP
7	G	21	VAL
7	G	22	LEU
7	G	23	VAL
7	G	38	LEU
7	G	45	ASP
7	G	50	ILE
7	G	53	LYS
7	G	57	GLU
7	G	60	LYS
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	135	VAL
7	G	137	LYS
7	G	141	VAL
7	G	153	HIS
7	G	156	TRP
8	H	3	THR
8	H	11	THR
8	H	18	ARG
8	H	19	VAL
8	H	24	THR
8	H	25	ASP
8	H	26	VAL
8	H	45	ILE
8	H	50	ARG
8	H	52	ASP
8	H	53	VAL
8	H	63	LEU
8	H	79	VAL
8	H	83	ILE
8	H	84	ARG

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Mol	Chain	Res	Type
8	H	85	ARG
8	H	88	LYS
8	H	95	VAL
8	H	102	ARG
8	H	104	ARG
8	H	112	LEU
8	H	116	LYS
8	H	120	THR
8	H	127	LEU
8	H	133	LEU
8	H	134	ILE
9	I	14	VAL
9	I	16	ARG
9	I	27	THR
9	I	48	GLU
9	I	79	LEU
9	I	87	GLN
9	I	95	LYS
9	I	102	LEU
9	I	108	VAL
9	I	109	VAL
9	I	118	LYS
10	J	4	ILE
10	J	17	ASP
10	J	29	ARG
10	J	43	ARG
10	J	65	LEU
10	J	71	LEU
10	J	75	ILE
10	J	83	GLU
10	J	84	GLN
10	J	95	GLU
10	J	96	ILE
10	J	98	ILE
11	K	18	ARG
11	K	33	THR
11	K	40	ILE
11	K	44	SER
11	K	51	LYS
11	K	66	LEU
11	K	73	MET
11	K	83	ILE

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Mol	Chain	Res	Type
11	K	91	ARG
11	K	96	ARG
11	K	107	SER
11	K	122	LYS
11	K	126	ARG
11	K	127	LYS
12	L	7	ILE
12	L	12	ARG
12	L	15	ARG
12	L	16	GLU
12	L	20	LYS
12	L	28	LYS
12	L	39	VAL
12	L	41	ARG
12	L	65	GLU
12	L	79	GLU
12	L	80	HIS
12	L	81	SER
12	L	84	LEU
12	L	89	ARG
12	L	90	VAL
12	L	96	VAL
12	L	100	ILE
12	L	113	ARG
12	L	116	SER
12	L	126	LYS
13	M	4	ILE
13	M	12	ASN
13	M	15	VAL
13	M	16	ASP
13	M	34	LEU
13	M	44	ARG
13	M	45	VAL
13	M	46	LYS
13	M	48	LEU
13	M	49	THR
13	M	53	VAL
13	M	65	LYS
13	M	66	LEU
13	M	70	LEU
13	M	74	VAL
13	M	80	ARG

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Mol	Chain	Res	Type
13	M	110	ARG
14	N	4	LYS
14	N	12	ARG
14	N	27	CYS
14	N	41	ARG
14	N	50	LYS
14	N	57	ARG
15	O	4	THR
15	O	11	VAL
15	O	22	THR
15	O	36	ILE
15	O	38	ARG
15	O	39	LEU
15	O	45	VAL
15	O	56	LEU
15	O	57	LEU
15	O	63	ARG
15	O	70	LEU
15	O	71	GLN
15	O	76	GLU
15	O	83	GLU
15	O	85	LEU
16	P	1	MET
16	P	5	ARG
16	P	33	ILE
16	P	45	THR
16	P	53	VAL
16	P	62	VAL
16	P	67	THR
16	P	82	GLN
17	Q	5	VAL
17	Q	9	VAL
17	Q	13	ASP
17	Q	21	VAL
17	Q	31	LEU
17	Q	34	LYS
17	Q	36	ILE
17	Q	38	ARG
17	Q	52	LYS
17	Q	57	VAL
17	Q	59	ILE
17	Q	60	ILE

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Mol	Chain	Res	Type
17	Q	74	LEU
17	Q	92	ARG
17	Q	97	SER
17	Q	98	LEU
17	Q	99	SER
17	Q	101	ARG
18	R	23	LYS
18	R	28	GLU
18	R	31	LEU
18	R	38	GLU
18	R	40	LEU
18	R	44	LEU
18	R	46	GLU
18	R	47	THR
18	R	54	ARG
18	R	70	ILE
19	S	7	LYS
19	S	15	LEU
19	S	17	GLU
19	S	18	LYS
19	S	27	GLU
19	S	31	ILE
19	S	56	GLN
19	S	58	VAL
19	S	63	THR
19	S	65	ASN
19	S	77	THR
19	S	81	ARG
20	T	8	ARG
20	T	11	SER
20	T	17	ARG
20	T	19	SER
20	T	20	LEU
20	T	24	LEU
20	T	35	THR
20	T	42	GLN
20	T	48	LYS
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS

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Mol	Chain	Res	Type
20	T	74	LYS
20	T	75	ASN
20	T	83	ARG
20	T	87	LYS
20	T	100	ILE
21	U	9	ARG
21	U	15	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	6	HIS
3	C	104	GLN
3	C	162	GLN
4	D	42	GLN
5	E	38	GLN
7	G	37	ASN
7	G	84	ASN
9	I	73	GLN
10	J	76	ASN
11	K	116	HIS
12	L	9	GLN
12	L	99	HIS
15	O	9	GLN
15	O	13	GLN
17	Q	29	HIS
19	S	69	HIS
20	T	42	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1510/1522 (99%)	279 (18%)	35 (2%)

All (279) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	32	A

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Mol	Chain	Res	Type
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	80	G
1	A	81	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	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	216	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
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	381	C
1	A	384	G

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Mol	Chain	Res	Type
1	A	390	C
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	410	G
1	A	412	A
1	A	413	G
1	A	419	C
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	432	A
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
1	A	461	C
1	A	482	A
1	A	484	G
1	A	485	G
1	A	496	A
1	A	497	A
1	A	498	U
1	A	509	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	527	7MG
1	A	530	G
1	A	532	A
1	A	533	A
1	A	540	G
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	568	G
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	596	C
1	A	630	G
1	A	631	G
1	A	632	A
1	A	641	U
1	A	653	A
1	A	656	C
1	A	658	G
1	A	661	G
1	A	665	A
1	A	672	U
1	A	687	A
1	A	688	G
1	A	702	A
1	A	717	C
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	785	G
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	828	A
1	A	829	G
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C

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Mol	Chain	Res	Type
1	A	858	G
1	A	859	A
1	A	872	A
1	A	889	A
1	A	902	G
1	A	913	A
1	A	914	A
1	A	916	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	954	G
1	A	960	U
1	A	961	U
1	A	963	G
1	A	966	M2G
1	A	967	5MC
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	980	C
1	A	982	U
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1005	A
1	A	1009	G
1	A	1025	U
1	A	1027	C
1	A	1028	C
1	A	1031	G
1	A	1050	G
1	A	1053	G
1	A	1054	C

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Mol	Chain	Res	Type
1	A	1060	C
1	A	1064	G
1	A	1065	U
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1108	G
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1141	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1171	G
1	A	1180	A
1	A	1181	G
1	A	1183	A
1	A	1190	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1209	C
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1225	A
1	A	1226	C
1	A	1227	A

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Mol	Chain	Res	Type
1	A	1228	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1249	C
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1277	C
1	A	1280	A
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1310	G
1	A	1316	G
1	A	1318	A
1	A	1320	C
1	A	1323	G
1	A	1331	G
1	A	1338	G
1	A	1340	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362	C
1	A	1370	G
1	A	1379	G
1	A	1394	A
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1402	4OC
1	A	1407	5MC
1	A	1409	C
1	A	1410	G
1	A	1440	C

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Mol	Chain	Res	Type
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1451	A
1	A	1469	G
1	A	1474	G
1	A	1488	G
1	A	1489	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1533	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	80	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	266	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	432	A
1	A	484	G
1	A	496	A

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Mol	Chain	Res	Type
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	1004	A
1	A	1049	U
1	A	1179	A
1	A	1182	G
1	A	1201	A
1	A	1212	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1347	G
1	A	1443	G
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	967	1	19,22,23	1.08	4 (21%)	26,32,35	1.07	2 (7%)
1	MA6	A	1518	1	23,26,27	1.05	1 (4%)	33,38,41	0.90	1 (3%)
1	4OC	A	1402	1	20,23,24	1.39	3 (15%)	25,32,35	0.78	0
1	7MG	A	527	1,22	23,26,27	4.01	4 (17%)	27,39,42	2.42	9 (33%)
1	5MC	A	1407	1	19,22,23	1.14	2 (10%)	26,32,35	1.21	2 (7%)
1	UR3	A	1498	1	19,22,23	1.18	3 (15%)	26,32,35	1.31	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	516	1,22	18,21,22	1.22	2 (11%)	21,30,33	1.65	3 (14%)
1	5MC	A	1404	1	19,22,23	1.48	2 (10%)	26,32,35	1.04	2 (7%)
1	PSU	A	1540	1	18,21,22	1.15	2 (11%)	21,30,33	1.64	3 (14%)
1	PSU	A	1541	1	18,21,22	1.09	1 (5%)	21,30,33	2.15	6 (28%)
1	5MC	A	1400	1	19,22,23	0.89	1 (5%)	26,32,35	0.90	1 (3%)
1	2MG	A	1207	1	23,26,27	1.41	4 (17%)	33,38,41	1.13	3 (9%)
12	0TD	L	92	12	8,9,10	1.53	1 (12%)	6,11,13	2.08	2 (33%)
1	M2G	A	966	1	24,27,28	0.81	1 (4%)	33,40,43	1.01	3 (9%)
1	MA6	A	1519	1	23,26,27	1.32	6 (26%)	33,38,41	1.02	1 (3%)

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	5MC	A	967	1	-	3/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
1	7MG	A	527	1,22	-	2/7/37/38	0/3/3/3
1	5MC	A	1407	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,22	-	1/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
12	0TD	L	92	12	-	2/7/12/14	-
1	M2G	A	966	1	-	6/11/29/30	0/3/3/3
1	MA6	A	1519	1	-	1/11/29/30	0/3/3/3

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-18.05	1.34	1.45
1	A	1404	5MC	C5-C4	-4.53	1.40	1.44
1	A	516	PSU	C6-C5	3.93	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1402	4OC	C4-N4	3.84	1.44	1.36
1	A	527	7MG	C2-N2	3.80	1.43	1.34
1	A	1540	PSU	C6-C5	3.63	1.39	1.35
1	A	1498	UR3	C4-N3	-3.45	1.33	1.40
1	A	1541	PSU	C6-C5	3.38	1.39	1.35
1	A	1407	5MC	C2-N1	3.28	1.46	1.40
12	L	92	0TD	CB-CA	3.14	1.55	1.54
1	A	1404	5MC	C2-N3	3.10	1.42	1.36
1	A	1207	2MG	C2-N1	3.00	1.41	1.36
1	A	1519	MA6	C5-C4	2.99	1.44	1.39
1	A	1402	4OC	C2-N3	2.97	1.42	1.36
1	A	1207	2MG	C4-N3	2.92	1.40	1.34
1	A	1207	2MG	C2-N2	2.89	1.39	1.33
1	A	1519	MA6	C8-N9	2.81	1.42	1.37
1	A	527	7MG	C4-N3	2.80	1.40	1.34
1	A	527	7MG	C5-N7	2.59	1.38	1.35
1	A	1407	5MC	C2-N3	2.57	1.41	1.36
1	A	1498	UR3	C6-N1	-2.45	1.32	1.38
1	A	1400	5MC	C4-N4	2.35	1.40	1.34
1	A	1402	4OC	C2-N1	2.32	1.44	1.40
1	A	967	5MC	C2-N3	2.30	1.40	1.36
1	A	967	5MC	C5-C4	2.26	1.45	1.44
1	A	1519	MA6	C2-N1	2.15	1.37	1.33
1	A	966	M2G	C4-N3	2.14	1.39	1.34
1	A	1498	UR3	C3U-N3	-2.14	1.43	1.47
1	A	1207	2MG	C8-N9	2.12	1.42	1.37
1	A	1519	MA6	C4-N3	2.12	1.38	1.34
1	A	1519	MA6	C5-N7	2.11	1.42	1.39
1	A	1518	MA6	C5-C4	2.08	1.42	1.39
1	A	516	PSU	O4'-C1'	-2.06	1.41	1.43
1	A	1540	PSU	C4-C5	-2.05	1.38	1.44
1	A	967	5MC	C2-N1	2.03	1.44	1.40
1	A	967	5MC	C4-N4	2.02	1.39	1.34
1	A	1519	MA6	C8-N7	2.02	1.35	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	C5-C6-N1	5.30	120.28	110.94
1	A	1541	PSU	N1-C2-N3	5.30	120.75	115.17
1	A	1541	PSU	C4-N3-C2	-5.24	119.16	126.37
1	A	527	7MG	C2-N3-C4	5.01	120.93	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	7MG	N9-C4-N3	4.69	132.34	125.46
1	A	527	7MG	C5-C4-N3	-4.65	119.41	128.13
1	A	1540	PSU	C4-N3-C2	-4.61	120.02	126.37
1	A	527	7MG	N9-C8-N7	4.30	109.47	103.37
1	A	516	PSU	C4-N3-C2	-3.93	120.95	126.37
12	L	92	0TD	CSB-SB-CB	-3.74	95.64	102.36
1	A	516	PSU	N1-C2-N3	3.63	119.00	115.17
1	A	1540	PSU	N1-C2-N3	3.41	118.77	115.17
1	A	1541	PSU	O2-C2-N1	-3.27	119.41	122.79
1	A	527	7MG	C2-N1-C6	-3.15	119.40	125.11
1	A	1541	PSU	C6-C5-C4	3.00	120.20	118.17
1	A	1407	5MC	N4-C4-N3	-3.00	113.08	118.51
1	A	967	5MC	N4-C4-N3	-2.95	113.17	118.51
1	A	527	7MG	C6-C5-N7	2.81	136.29	131.93
1	A	1498	UR3	C6-N1-C2	-2.74	119.56	121.80
1	A	1207	2MG	C5-C4-N3	-2.73	124.04	128.39
1	A	1407	5MC	C5-C4-N3	2.72	124.54	121.75
1	A	527	7MG	C6-C5-C4	-2.70	117.65	122.40
1	A	1207	2MG	N9-C4-N3	2.57	131.08	125.95
1	A	1207	2MG	O6-C6-N1	-2.50	115.40	120.11
1	A	1404	5MC	C5-C4-N3	2.50	124.32	121.75
1	A	1498	UR3	O3'-C3'-C2'	2.49	119.79	111.82
1	A	516	PSU	O4'-C1'-C2'	2.48	108.58	105.15
1	A	1518	MA6	C2-N1-C6	2.41	117.71	111.83
1	A	966	M2G	C5-C4-N3	-2.39	124.59	128.39
1	A	527	7MG	O6-C6-C5	-2.37	121.80	127.62
1	A	1541	PSU	O4'-C1'-C2'	2.35	108.41	105.15
1	A	1400	5MC	N4-C4-N3	-2.26	114.42	118.51
1	A	1541	PSU	C6-N1-C2	-2.25	120.61	122.69
1	A	967	5MC	C5-C4-N3	2.24	124.05	121.75
12	L	92	0TD	OD1-CG-CB	-2.23	117.77	122.44
1	A	966	M2G	O6-C6-C5	2.23	132.42	126.53
1	A	966	M2G	O6-C6-N1	-2.21	115.96	120.11
1	A	1498	UR3	O2-C2-N3	-2.17	118.34	121.33
1	A	1540	PSU	O4-C4-C5	-2.13	118.73	124.01
1	A	1519	MA6	C2-N1-C6	2.10	116.97	111.83
1	A	1404	5MC	C6-N1-C2	-2.07	118.20	120.95

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	966	M2G	N1-C2-N2-CM1
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1407	5MC	O4'-C4'-C5'-O5'
1	A	1407	5MC	C3'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	1519	MA6	C5-C6-N6-C9
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	966	M2G	N3-C2-N2-CM1
1	A	516	PSU	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM2
1	A	1541	PSU	O4'-C1'-C5-C6
1	A	1402	4OC	C3'-C2'-O2'-CM2
1	A	967	5MC	C2'-C1'-N1-C2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	967	5MC	1	0
1	A	1518	MA6	1	0
1	A	1402	4OC	2	0
1	A	1498	UR3	3	0
1	A	1400	5MC	1	0
12	L	92	0TD	2	0
1	A	966	M2G	2	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 126 ligands modelled in this entry, 125 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
24	HYG	A	1716	-	36,39,39	1.89	7 (19%)	44,60,60	2.59	16 (36%)

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
24	HYG	A	1716	-	-	8/12/87/87	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1716	HYG	C27-C33	5.64	1.59	1.52
24	A	1716	HYG	C34-C33	4.66	1.60	1.52
24	A	1716	HYG	C4-N9	3.44	1.51	1.47
24	A	1716	HYG	C16-C15	3.29	1.60	1.53
24	A	1716	HYG	C5-C4	2.95	1.58	1.52
24	A	1716	HYG	O29-C12	-2.34	1.39	1.43
24	A	1716	HYG	O28-C27	-2.04	1.40	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1716	HYG	O29-C12-C13	6.93	128.59	110.89
24	A	1716	HYG	O28-C27-C26	6.77	117.96	108.50
24	A	1716	HYG	O18-C13-C12	5.45	119.69	109.09
24	A	1716	HYG	O14-C15-C16	5.23	119.12	109.70
24	A	1716	HYG	C13-O14-C15	4.98	123.45	113.72
24	A	1716	HYG	C16-C17-C12	-4.31	103.21	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1716	HYG	C23-O28-C27	4.19	119.99	112.00
24	A	1716	HYG	C26-C25-C24	3.16	115.69	111.18
24	A	1716	HYG	O14-C13-C12	-2.81	104.02	109.49
24	A	1716	HYG	C25-C26-C27	2.79	116.01	109.68
24	A	1716	HYG	O29-C23-O22	2.79	109.07	105.90
24	A	1716	HYG	C3-C4-C5	2.49	115.02	109.89
24	A	1716	HYG	O32-C26-C27	-2.28	104.09	109.94
24	A	1716	HYG	O20-C19-C15	-2.28	103.58	111.33
24	A	1716	HYG	C6-C1-C2	2.26	115.39	109.93
24	A	1716	HYG	C13-C12-C17	-2.11	105.11	111.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

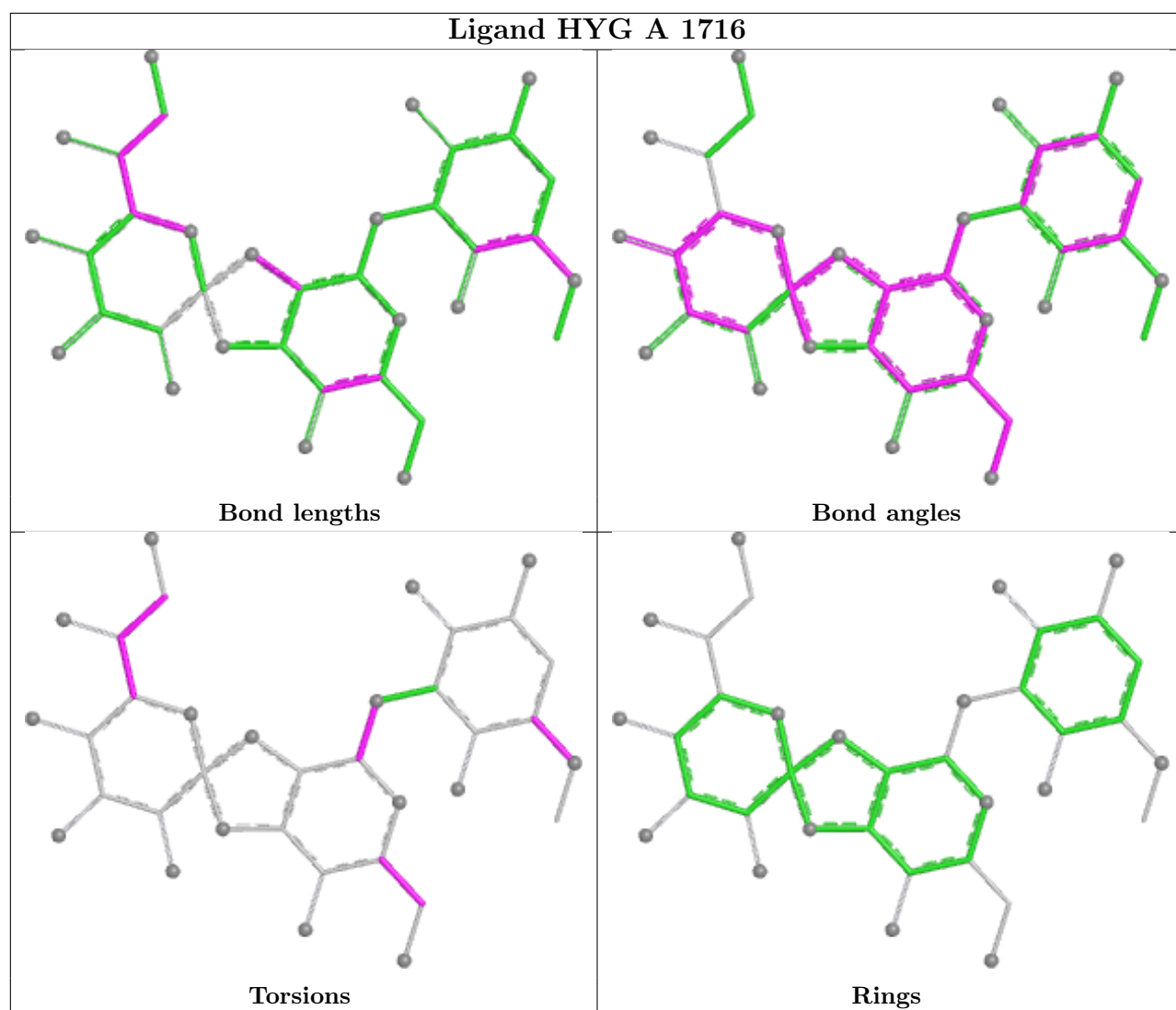
Mol	Chain	Res	Type	Atoms
24	A	1716	HYG	O28-C27-C33-C34
24	A	1716	HYG	C27-C33-C34-O35
24	A	1716	HYG	N36-C33-C34-O35
24	A	1716	HYG	O14-C13-O18-C6
24	A	1716	HYG	O14-C15-C19-O20
24	A	1716	HYG	C3-C4-N9-C10
24	A	1716	HYG	C26-C27-C33-C34
24	A	1716	HYG	C12-C13-O18-C6

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1716	HYG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	-0.63	7 (0%) 87 67	70, 126, 240, 358	0
2	B	236/256 (92%)	-0.57	0 100 100	71, 143, 231, 265	0
3	C	207/239 (86%)	-0.43	1 (0%) 87 67	86, 181, 224, 245	0
4	D	208/209 (99%)	-0.37	5 (2%) 59 35	86, 134, 184, 240	0
5	E	151/162 (93%)	-0.73	1 (0%) 84 62	72, 108, 143, 194	0
6	F	101/101 (100%)	-0.68	0 100 100	100, 150, 180, 218	0
7	G	155/156 (99%)	-0.54	0 100 100	104, 155, 208, 226	0
8	H	138/138 (100%)	-0.69	0 100 100	71, 94, 137, 163	0
9	I	127/128 (99%)	-0.35	2 (1%) 70 44	132, 177, 218, 243	0
10	J	99/105 (94%)	-0.24	2 (2%) 65 39	102, 202, 278, 346	0
11	K	119/129 (92%)	-0.60	0 100 100	88, 120, 167, 194	0
12	L	124/135 (91%)	-0.40	2 (1%) 70 44	86, 132, 163, 239	0
13	M	118/126 (93%)	-0.56	1 (0%) 82 60	127, 152, 193, 242	0
14	N	60/61 (98%)	-0.17	2 (3%) 49 29	130, 169, 205, 254	0
15	O	88/89 (98%)	-0.60	0 100 100	74, 116, 166, 207	0
16	P	84/88 (95%)	-0.48	1 (1%) 76 50	86, 124, 158, 241	0
17	Q	104/105 (99%)	-0.52	2 (1%) 66 40	78, 111, 167, 253	0
18	R	73/88 (82%)	-0.60	0 100 100	85, 130, 210, 244	0
19	S	81/93 (87%)	-0.05	3 (3%) 45 27	79, 193, 246, 257	0
20	T	99/106 (93%)	-0.38	2 (2%) 65 39	89, 123, 166, 209	0
21	U	25/27 (92%)	-0.20	0 100 100	71, 156, 193, 222	0
All	All	3895/4063 (95%)	-0.54	31 (0%) 82 60	70, 137, 224, 358	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	9.8
3	C	2	GLY	7.1
20	T	106	ALA	6.2
1	A	1129	C	5.7
4	D	31	CYS	4.9
19	S	2	PRO	4.9
4	D	2	GLY	4.7
12	L	115	LYS	3.5
4	D	26	CYS	3.3
9	I	110	GLU	3.2
19	S	4	SER	2.9
4	D	9	CYS	2.9
14	N	4	LYS	2.8
20	T	12	ALA	2.6
17	Q	103	GLY	2.6
9	I	127	LYS	2.5
17	Q	105	ALA	2.5
10	J	17	ASP	2.5
4	D	22	LYS	2.3
10	J	58	ASP	2.3
16	P	84	ALA	2.3
13	M	102	ARG	2.2
1	A	1053	G	2.2
1	A	723	U	2.1
1	A	1361(A)	C	2.1
1	A	985	C	2.1
1	A	532	A	2.0
14	N	35	ARG	2.0
1	A	1027	C	2.0
5	E	8	GLU	2.0
12	L	73	GLU	2.0

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

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	M2G	A	966	25/26	0.94	0.11	144,155,162,169	0
1	PSU	A	1540	20/21	0.94	0.17	219,245,263,265	0
1	PSU	A	1541	20/21	0.94	0.12	220,236,242,246	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	5MC	A	1400	21/22	0.95	0.09	98,114,124,126	0
1	PSU	A	516	20/21	0.96	0.08	137,149,167,170	0
1	MA6	A	1519	24/25	0.97	0.13	94,111,118,123	0
1	2MG	A	1207	24/25	0.97	0.07	176,181,195,199	0
1	5MC	A	967	21/22	0.97	0.06	128,137,161,162	0
12	0TD	L	92	10/11	0.97	0.08	130,135,159,306	0
1	MA6	A	1518	24/25	0.98	0.09	107,118,134,137	0
1	7MG	A	527	24/25	0.98	0.06	107,117,135,139	0
1	5MC	A	1404	21/22	0.98	0.06	100,110,125,127	0
1	5MC	A	1407	21/22	0.98	0.06	126,137,143,148	0
1	UR3	A	1498	21/22	0.98	0.08	95,107,114,124	0
1	4OC	A	1402	22/23	0.99	0.05	100,104,114,116	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1709	1/1	0.51	0.16	390,390,390,390	0
22	MG	A	1610	1/1	0.62	0.37	105,105,105,105	0
22	MG	A	1701	1/1	0.68	0.20	107,107,107,107	0
22	MG	A	1638	1/1	0.73	0.23	124,124,124,124	0
22	MG	A	1699	1/1	0.73	0.20	108,108,108,108	0
22	MG	A	1608	1/1	0.76	0.31	73,73,73,73	0
22	MG	A	1705	1/1	0.77	0.13	143,143,143,143	0
22	MG	A	1651	1/1	0.77	0.16	122,122,122,122	0
22	MG	A	1611	1/1	0.78	0.25	82,82,82,82	0
22	MG	A	1713	1/1	0.78	0.05	382,382,382,382	0
22	MG	A	1615	1/1	0.79	0.26	94,94,94,94	0
22	MG	A	1652	1/1	0.80	0.17	123,123,123,123	0
23	K	A	1696	1/1	0.80	0.19	167,167,167,167	0
22	MG	A	1646	1/1	0.81	0.32	68,68,68,68	0
23	K	A	1693	1/1	0.81	0.16	144,144,144,144	0
22	MG	A	1656	1/1	0.81	0.28	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1605	1/1	0.82	0.18	107,107,107,107	0
22	MG	A	1636	1/1	0.83	0.19	77,77,77,77	0
23	K	A	1697	1/1	0.83	0.16	156,156,156,156	0
22	MG	D	302	1/1	0.84	0.17	89,89,89,89	0
22	MG	A	1607	1/1	0.84	0.40	99,99,99,99	0
22	MG	A	1712	1/1	0.85	0.07	366,366,366,366	0
22	MG	A	1660	1/1	0.85	0.34	64,64,64,64	0
22	MG	A	1686	1/1	0.86	0.06	124,124,124,124	0
22	MG	A	1715	1/1	0.86	0.10	320,320,320,320	0
22	MG	A	1684	1/1	0.86	0.32	100,100,100,100	0
22	MG	A	1628	1/1	0.87	0.29	76,76,76,76	0
22	MG	A	1649	1/1	0.88	0.20	110,110,110,110	0
22	MG	A	1644	1/1	0.88	0.23	88,88,88,88	0
22	MG	A	1630	1/1	0.88	0.18	76,76,76,76	0
22	MG	A	1691	1/1	0.89	0.06	92,92,92,92	0
22	MG	A	1708	1/1	0.89	0.09	371,371,371,371	0
22	MG	A	1664	1/1	0.89	0.26	84,84,84,84	0
22	MG	A	1687	1/1	0.89	0.11	82,82,82,82	0
22	MG	A	1703	1/1	0.89	0.24	108,108,108,108	0
22	MG	A	1617	1/1	0.90	0.18	71,71,71,71	0
22	MG	A	1631	1/1	0.90	0.29	95,95,95,95	0
22	MG	A	1645	1/1	0.90	0.31	83,83,83,83	0
22	MG	A	1688	1/1	0.90	0.14	69,69,69,69	0
22	MG	A	1658	1/1	0.90	0.30	73,73,73,73	0
22	MG	A	1632	1/1	0.90	0.35	65,65,65,65	0
22	MG	A	1609	1/1	0.90	0.35	62,62,62,62	0
22	MG	A	1675	1/1	0.90	0.21	69,69,69,69	0
22	MG	A	1683	1/1	0.90	0.10	91,91,91,91	0
22	MG	A	1702	1/1	0.91	0.23	126,126,126,126	0
22	MG	A	1639	1/1	0.91	0.07	138,138,138,138	0
22	MG	A	1678	1/1	0.91	0.28	81,81,81,81	0
22	MG	A	1654	1/1	0.91	0.35	82,82,82,82	0
22	MG	A	1629	1/1	0.91	0.27	69,69,69,69	0
22	MG	A	1668	1/1	0.91	0.11	99,99,99,99	0
22	MG	A	1682	1/1	0.92	0.17	86,86,86,86	0
22	MG	A	1692	1/1	0.92	0.07	106,106,106,106	0
22	MG	A	1618	1/1	0.92	0.25	97,97,97,97	0
22	MG	A	1700	1/1	0.92	0.26	88,88,88,88	0
22	MG	A	1714	1/1	0.92	0.04	413,413,413,413	0
22	MG	A	1626	1/1	0.92	0.18	76,76,76,76	0
22	MG	A	1674	1/1	0.92	0.32	91,91,91,91	0
22	MG	A	1601	1/1	0.92	0.17	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1704	1/1	0.92	0.14	106,106,106,106	0
22	MG	A	1613	1/1	0.92	0.37	43,43,43,43	0
22	MG	A	1680	1/1	0.93	0.10	79,79,79,79	0
22	MG	A	1606	1/1	0.93	0.24	66,66,66,66	0
22	MG	A	1640	1/1	0.93	0.23	68,68,68,68	0
22	MG	H	201	1/1	0.93	0.08	402,402,402,402	0
22	MG	M	201	1/1	0.93	0.05	106,106,106,106	0
22	MG	A	1710	1/1	0.93	0.06	233,233,233,233	0
22	MG	A	1662	1/1	0.93	0.52	101,101,101,101	0
22	MG	A	1657	1/1	0.93	0.19	61,61,61,61	0
22	MG	A	1624	1/1	0.94	0.24	31,31,31,31	0
22	MG	A	1661	1/1	0.94	0.18	102,102,102,102	0
22	MG	A	1604	1/1	0.94	0.21	33,33,33,33	0
22	MG	A	1643	1/1	0.94	0.29	60,60,60,60	0
22	MG	A	1665	1/1	0.94	0.26	42,42,42,42	0
22	MG	A	1666	1/1	0.94	0.17	58,58,58,58	0
22	MG	A	1650	1/1	0.94	0.48	60,60,60,60	0
22	MG	A	1669	1/1	0.94	0.15	60,60,60,60	0
22	MG	P	101	1/1	0.94	0.06	85,85,85,85	0
22	MG	A	1707	1/1	0.94	0.04	98,98,98,98	0
22	MG	A	1670	1/1	0.94	0.14	56,56,56,56	0
22	MG	A	1619	1/1	0.94	0.17	75,75,75,75	0
22	MG	A	1637	1/1	0.95	0.19	53,53,53,53	0
22	MG	A	1616	1/1	0.95	0.32	40,40,40,40	0
22	MG	A	1676	1/1	0.95	0.17	65,65,65,65	0
22	MG	A	1690	1/1	0.95	0.08	84,84,84,84	0
22	MG	E	201	1/1	0.95	0.20	63,63,63,63	0
22	MG	A	1706	1/1	0.95	0.05	110,110,110,110	0
22	MG	A	1659	1/1	0.95	0.51	87,87,87,87	0
22	MG	A	1667	1/1	0.95	0.19	43,43,43,43	0
22	MG	A	1614	1/1	0.95	0.42	52,52,52,52	0
23	K	A	1694	1/1	0.95	0.16	122,122,122,122	0
22	MG	A	1602	1/1	0.95	0.32	74,74,74,74	0
22	MG	A	1641	1/1	0.95	0.19	69,69,69,69	0
22	MG	A	1648	1/1	0.96	0.34	81,81,81,81	0
22	MG	A	1620	1/1	0.96	0.26	46,46,46,46	0
22	MG	A	1663	1/1	0.96	0.14	87,87,87,87	0
22	MG	A	1635	1/1	0.96	0.12	56,56,56,56	0
22	MG	A	1627	1/1	0.96	0.22	66,66,66,66	0
22	MG	A	1625	1/1	0.96	0.07	71,71,71,71	0
22	MG	A	1653	1/1	0.96	0.13	69,69,69,69	0
22	MG	A	1689	1/1	0.96	0.14	63,63,63,63	0

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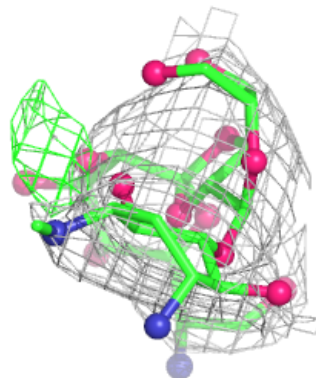
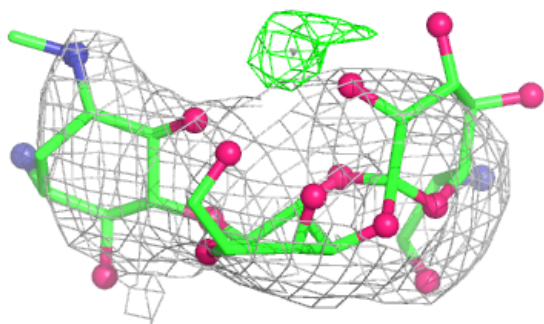
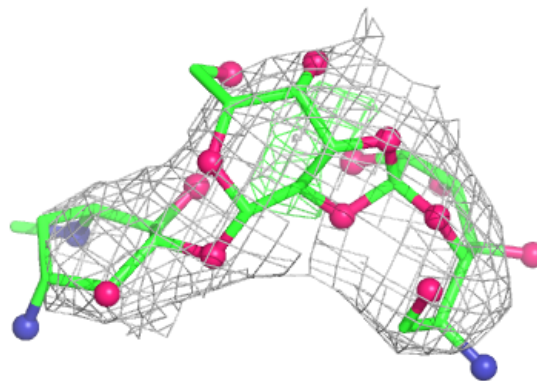
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
22	MG	A	1679	1/1	0.96	0.24	81,81,81,81	0
24	HYG	A	1716	36/36	0.96	0.10	91,158,184,193	0
22	MG	A	1647	1/1	0.97	0.04	55,55,55,55	0
22	MG	E	202	1/1	0.97	0.17	91,91,91,91	0
22	MG	A	1642	1/1	0.97	0.14	87,87,87,87	0
22	MG	J	201	1/1	0.97	0.13	84,84,84,84	0
22	MG	A	1634	1/1	0.97	0.30	60,60,60,60	0
22	MG	A	1711	1/1	0.97	0.06	165,165,165,165	0
22	MG	A	1621	1/1	0.97	0.20	70,70,70,70	0
22	MG	A	1622	1/1	0.97	0.09	82,82,82,82	0
22	MG	A	1672	1/1	0.97	0.13	91,91,91,91	0
22	MG	A	1673	1/1	0.97	0.13	74,74,74,74	0
22	MG	A	1623	1/1	0.97	0.04	78,78,78,78	0
22	MG	A	1603	1/1	0.98	0.43	38,38,38,38	0
22	MG	A	1612	1/1	0.98	0.35	74,74,74,74	0
22	MG	A	1698	1/1	0.98	0.28	70,70,70,70	0
23	K	A	1695	1/1	0.98	0.19	168,168,168,168	0
22	MG	A	1685	1/1	0.98	0.07	64,64,64,64	0
22	MG	A	1633	1/1	0.98	0.21	65,65,65,65	0
22	MG	B	301	1/1	0.98	0.04	96,96,96,96	0
22	MG	A	1681	1/1	0.99	0.07	103,103,103,103	0
22	MG	A	1671	1/1	0.99	0.12	64,64,64,64	0
22	MG	A	1655	1/1	0.99	0.10	62,62,62,62	0
22	MG	A	1677	1/1	0.99	0.09	111,111,111,111	0
25	ZN	D	301	1/1	0.99	0.19	97,97,97,97	0
25	ZN	N	101	1/1	0.99	0.04	214,214,214,214	0

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

Electron density around HYG A 1716:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.