



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 07:19 am BST

PDB ID : 4JI1  
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus*  
Authors : Demirci, H.; Wang, L.; Murphy IV, F.; Murphy, E.; Carr, J.; Blanchard, S.;  
Jogl, G.; Dahlberg, A.E.; Gregory, S.T.  
Deposited on : 2013-03-05  
Resolution : 3.14 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

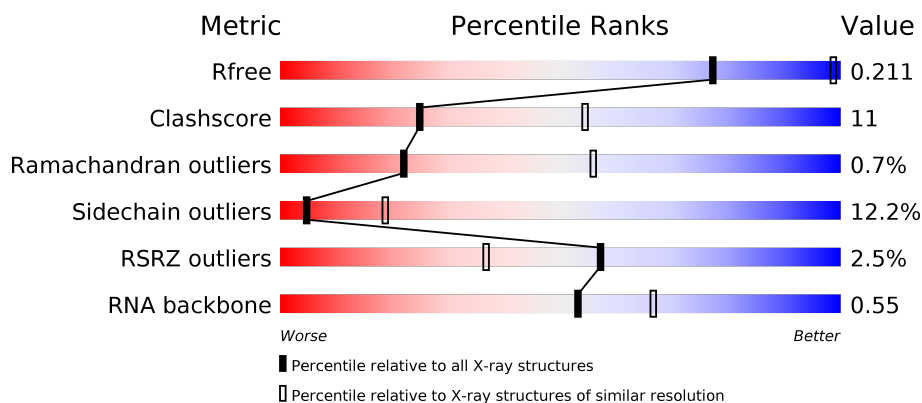
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



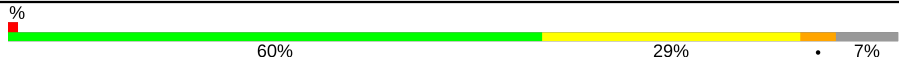
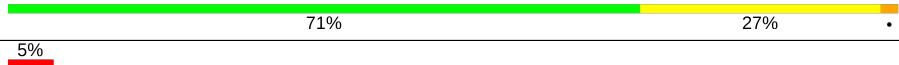
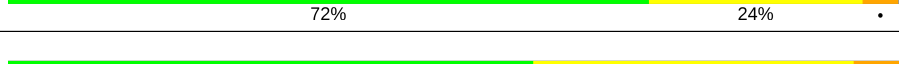
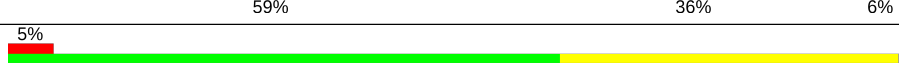
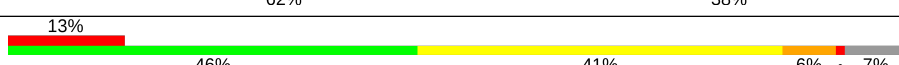


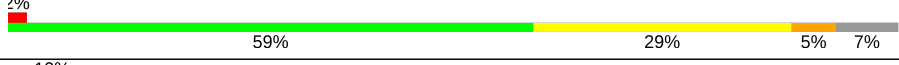
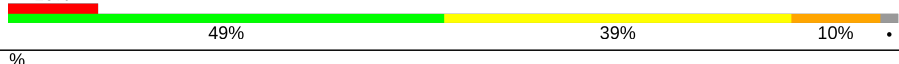





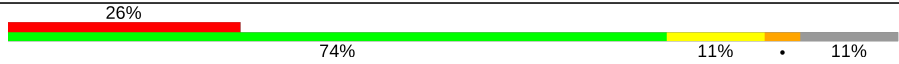

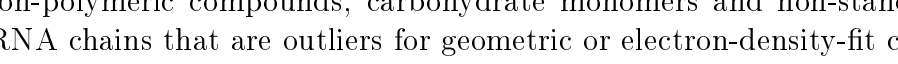
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1626 (3.18-3.10)
Clashscore	141614	1735 (3.18-3.10)
Ramachandran outliers	138981	1677 (3.18-3.10)
Sidechain outliers	138945	1677 (3.18-3.10)
RSRZ outliers	127900	1588 (3.18-3.10)
RNA backbone	3102	1000 (3.46-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>4%</div> <div>56%</div> <div>31%</div> <div>10%</div> <div>••</div> </div>
2	B	256	<div> <div>52%</div> <div>31%</div> <div>7%</div> <div>•</div> <div>9%</div> </div>
3	C	239	<div> <div>4%</div> <div>53%</div> <div>29%</div> <div>•</div> <div>14%</div> </div>
4	D	209	<div> <div>71%</div> <div>22%</div> <div>7%</div> </div>

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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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
1	PSU	A	1541	-	-	-	X
22	SRY	A	1601	X	-	-	-
23	MG	A	1634	-	-	-	X
23	MG	A	1635	-	-	-	X
23	MG	A	1666	-	-	-	X
23	MG	A	1669	-	-	-	X
23	MG	A	1680	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1681	-	-	-	X
23	MG	A	1682	-	-	-	X
23	MG	A	1684	-	-	-	X
23	MG	A	1689	-	-	-	X
23	MG	A	1694	-	-	-	X
23	MG	A	1701	-	-	-	X
23	MG	A	1703	-	-	-	X
23	MG	A	1720	-	-	-	X
23	MG	A	1761	-	-	-	X
23	MG	A	1826	-	-	-	X
23	MG	A	1834	-	-	-	X
23	MG	A	1848	-	-	-	X
23	MG	A	1850	-	-	-	X
23	MG	A	1853	-	-	-	X
23	MG	A	1855	-	-	-	X
23	MG	A	1869	-	-	-	X
23	MG	A	1873	-	-	-	X
23	MG	A	1880	-	-	-	X
23	MG	A	1891	-	-	-	X
23	MG	A	1896	-	-	-	X
23	MG	D	304	-	-	-	X
23	MG	H	203	-	-	-	X
23	MG	P	102	-	-	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52776 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
			32507	14477	6011	10507	1512			

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	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN S3.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN S10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	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	124	Total	C	N	O	S	0	0	0
			973	613	195	163	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	LEU	PRO	CONFLICT	UNP F6DEQ7

- Molecule 13 is a protein called RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	117	Total	C	N	O	S	0	0	0
			933	577	192	162	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	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 17 is a protein called RIBOSOMAL PROTEIN S17.

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

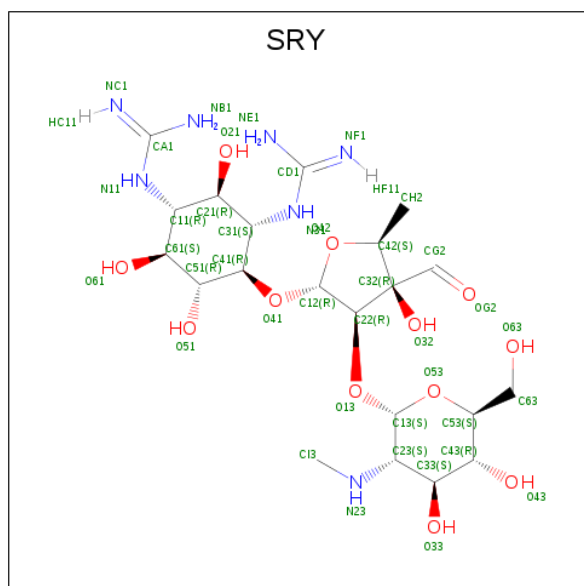
- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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





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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	J	2	Total 2	Mg 2	0	0
23	Q	4	Total 4	Mg 4	0	0
23	D	3	Total 3	Mg 3	0	0
23	K	3	Total 3	Mg 3	0	0
23	E	2	Total 2	Mg 2	0	0
23	H	4	Total 4	Mg 4	0	0
23	B	4	Total 4	Mg 4	0	0
23	I	1	Total 1	Mg 1	0	0
23	A	295	Total 295	Mg 295	0	0
23	T	1	Total 1	Mg 1	0	0
23	N	1	Total 1	Mg 1	0	0
23	S	1	Total 1	Mg 1	0	0
23	F	1	Total 1	Mg 1	0	0

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	A	702	Total 702	O 702	0	0
25	B	3	Total 3	O 3	0	0

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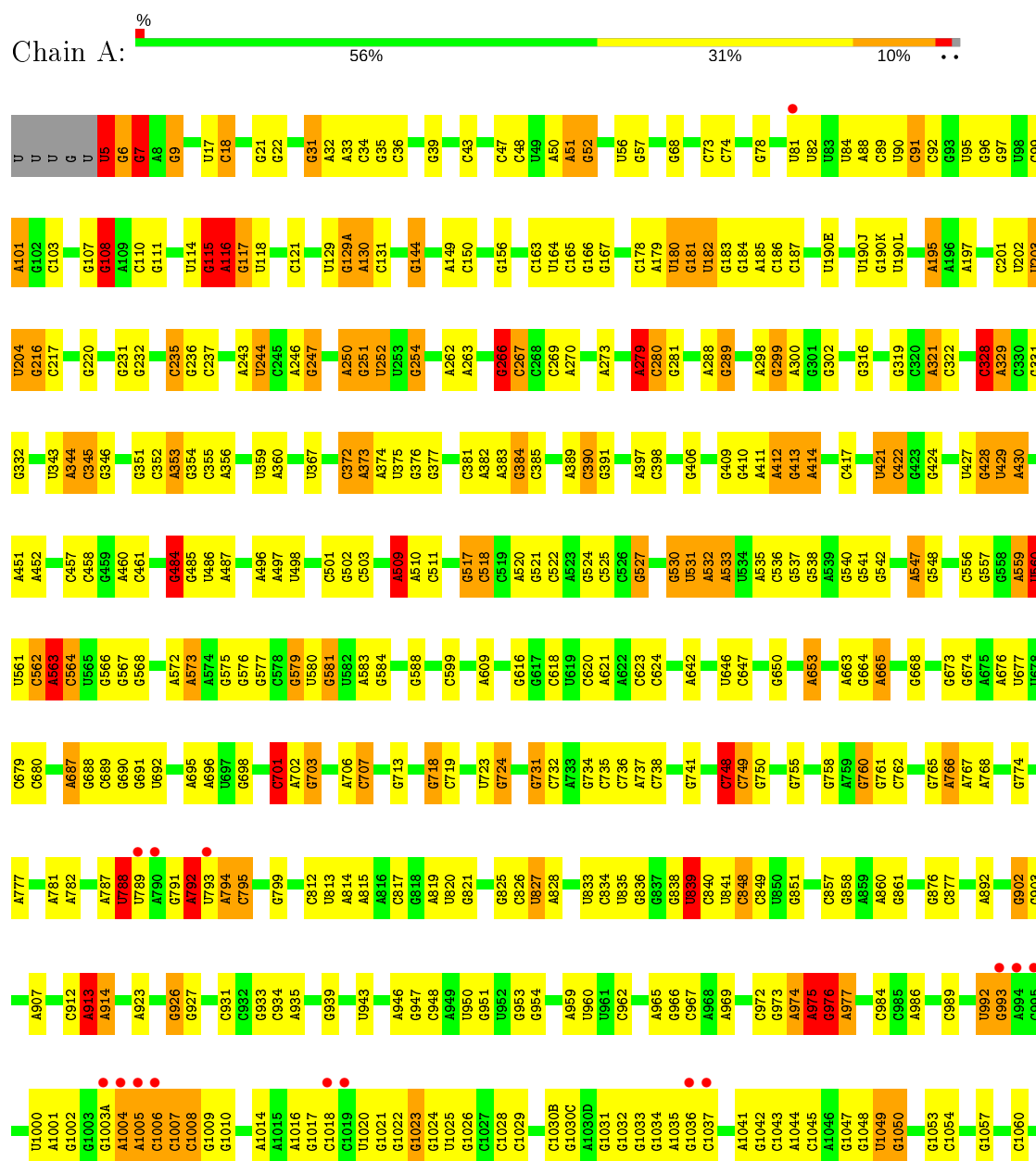
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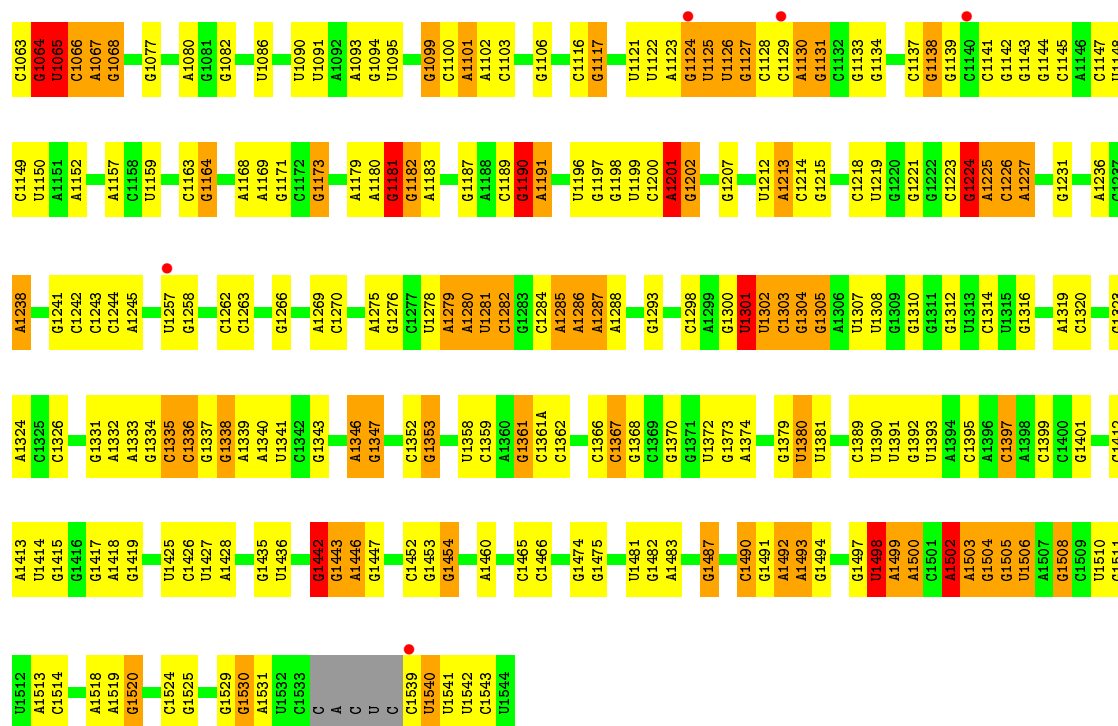
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	D	1	Total 1	O 1	0	0
25	E	8	Total 8	O 8	0	0
25	F	6	Total 6	O 6	0	0
25	H	2	Total 2	O 2	0	0
25	L	1	Total 1	O 1	0	0
25	P	1	Total 1	O 1	0	0
25	Q	6	Total 6	O 6	0	0
25	T	3	Total 3	O 3	0	0

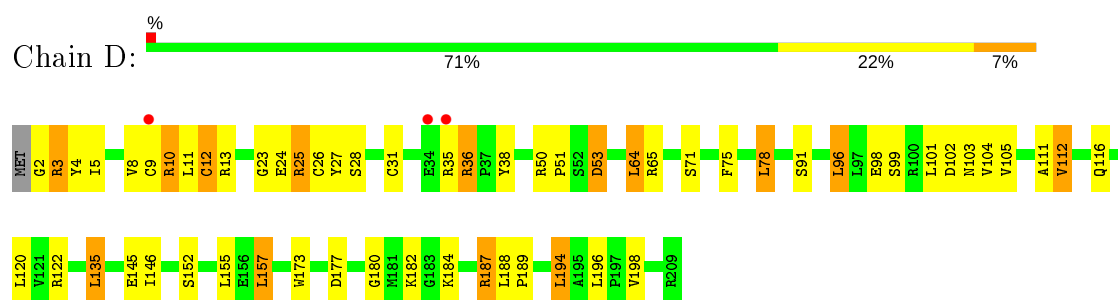
### 3 Residue-property plots

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

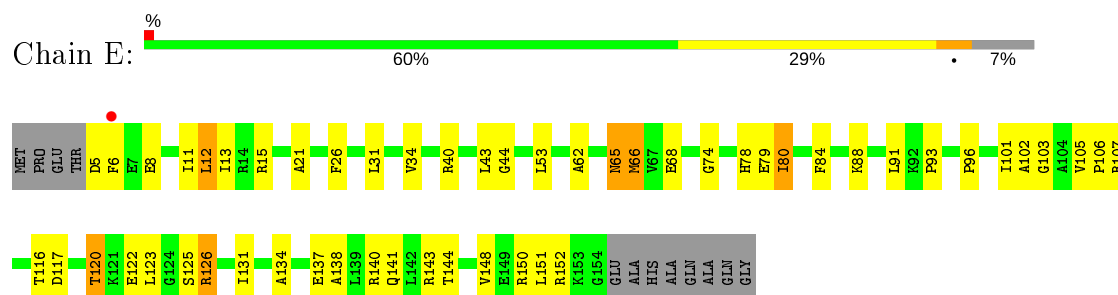
#### • Molecule 1: 16S rRNA



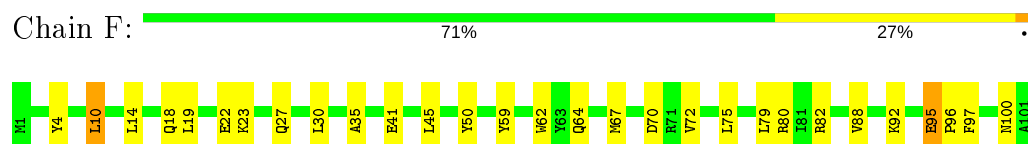




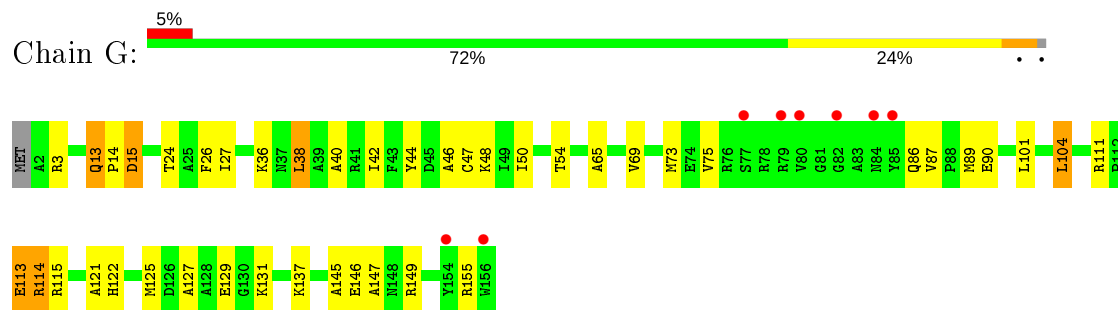
• Molecule 5: RIBOSOMAL PROTEIN S5



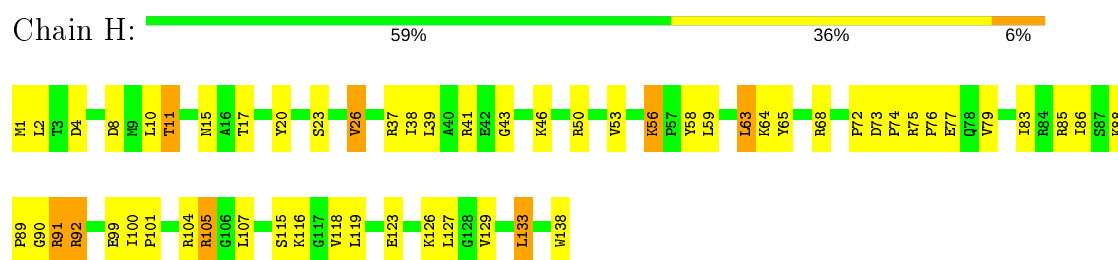
• Molecule 6: RIBOSOMAL PROTEIN S6



• Molecule 7: RIBOSOMAL PROTEIN S7

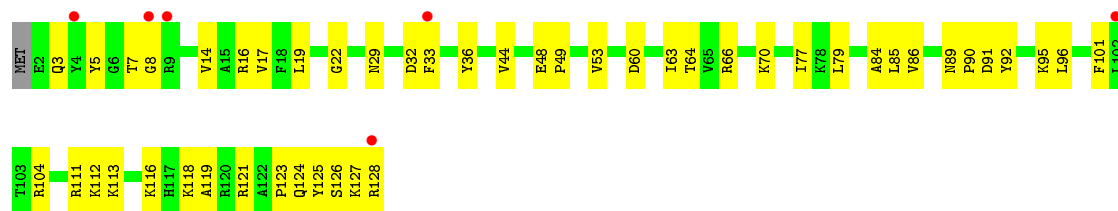


• Molecule 8: RIBOSOMAL PROTEIN S8

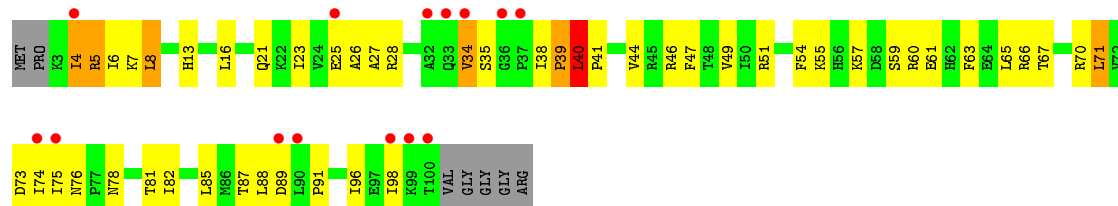


• Molecule 9: RIBOSOMAL PROTEIN S9

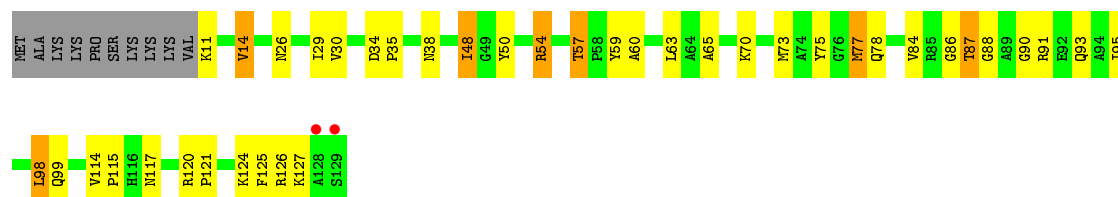




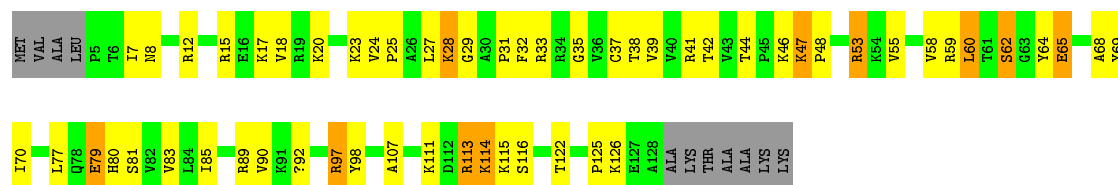
• Molecule 10: RIBOSOMAL PROTEIN S10



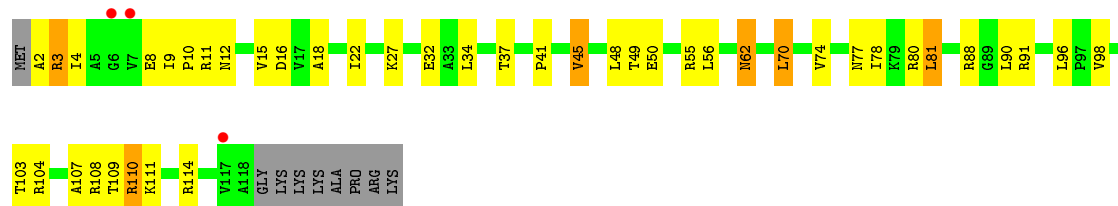
• Molecule 11: RIBOSOMAL PROTEIN S11



• Molecule 12: RIBOSOMAL PROTEIN S12



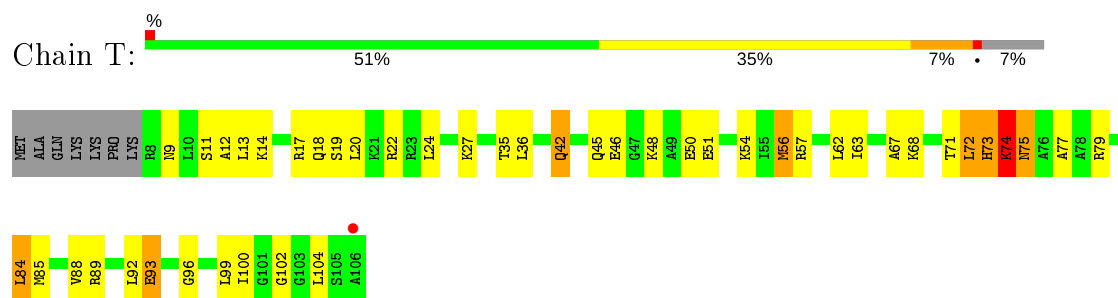
• Molecule 13: RIBOSOMAL PROTEIN S13



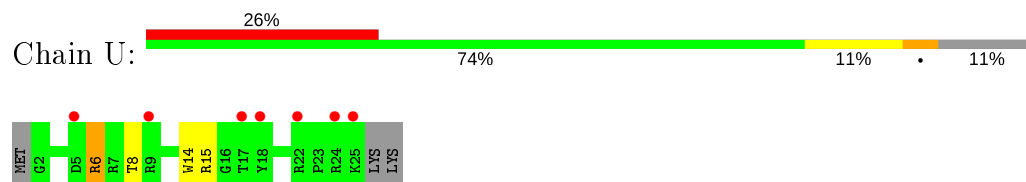
• Molecule 14: RIBOSOMAL PROTEIN S14



## • Molecule 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, $\alpha$ , $\beta$ , $\gamma$	403.17Å 403.17Å 173.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.65 – 3.14 34.65 – 3.14	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.65-3.14) 98.5 (34.65-3.14)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 3.12Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, $R_{free}$	0.165 , 0.207 0.168 , 0.211	Depositor DCC
$R_{free}$ test set	12242 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.8	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 114.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	52776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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	0.59	4/36040 (0.0%)	1.12	133/56243 (0.2%)
2	B	0.46	0/1935	0.72	1/2609 (0.0%)
3	C	0.32	0/1636	0.63	2/2205 (0.1%)
4	D	0.45	0/1733	0.65	1/2318 (0.0%)
5	E	0.53	0/1162	0.77	1/1564 (0.1%)
6	F	0.33	0/856	0.52	0/1154
7	G	0.32	0/1276	0.54	0/1709
8	H	0.54	0/1136	0.75	0/1527
9	I	0.39	0/1029	0.60	0/1379
10	J	0.32	0/805	0.64	0/1082
11	K	0.39	0/900	0.69	0/1213
12	L	0.49	0/977	0.78	2/1305 (0.2%)
13	M	0.37	0/943	0.65	0/1265
14	N	0.39	0/501	0.65	0/664
15	O	0.39	0/745	0.58	0/992
16	P	0.45	0/716	0.65	0/963
17	Q	0.50	0/870	0.80	0/1159
18	R	0.36	0/604	0.59	0/801
19	S	0.30	0/661	0.57	0/890
20	T	0.44	0/765	0.72	0/1007
21	U	0.35	0/212	0.56	0/277
All	All	0.54	4/55502 (0.0%)	1.00	140/82326 (0.2%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	2
14	N	0	1
17	Q	0	1
20	T	0	2
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-8.24	1.32	1.37
1	A	788	U	C2-N3	6.47	1.42	1.37
1	A	279	A	N3-C4	-6.29	1.31	1.34
1	A	788	U	C2-O2	5.25	1.27	1.22

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	976	G	O5'-P-OP1	-14.13	92.98	105.70
1	A	117	G	N1-C6-O6	13.79	128.18	119.90
1	A	279	A	C2-N3-C4	-11.65	104.78	110.60
1	A	117	G	C6-C5-N7	-9.87	124.48	130.40
1	A	328	C	N3-C2-O2	-9.43	115.30	121.90
1	A	328	C	N1-C2-O2	9.30	124.48	118.90
1	A	1502	A	C5-N7-C8	-9.17	99.32	103.90
1	A	108	G	C5-N7-C8	-8.92	99.84	104.30
1	A	266	G	C5-N7-C8	-8.91	99.85	104.30
1	A	279	A	C5-N7-C8	-8.72	99.54	103.90
1	A	1181	G	C4-N9-C1'	-8.60	115.32	126.50
1	A	108	G	C4-C5-N7	8.57	114.23	110.80
1	A	788	U	N3-C4-O4	8.54	125.38	119.40
1	A	1502	A	C2-N3-C4	-8.50	106.35	110.60
1	A	266	G	C4-C5-N7	8.42	114.17	110.80
1	A	117	G	C5-C6-O6	-8.12	123.73	128.60
1	A	788	U	N1-C2-N3	-8.11	110.03	114.90
1	A	1502	A	N7-C8-N9	7.89	117.75	113.80
1	A	1181	G	C8-N9-C1'	7.89	137.25	127.00
1	A	1504	G	P-O3'-C3'	7.66	128.89	119.70
1	A	108	G	N1-C6-O6	7.44	124.37	119.90
1	A	117	G	N9-C4-C5	-7.43	102.43	105.40
1	A	1502	A	N1-C6-N6	7.37	123.02	118.60
1	A	266	G	N7-C8-N9	7.33	116.76	113.10
1	A	279	A	N1-C6-N6	7.23	122.94	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	913	A	P-O3'-C3'	7.07	128.19	119.70
1	A	1502	A	C6-C5-N7	-7.04	127.37	132.30
1	A	1502	A	C4-C5-N7	7.01	114.20	110.70
1	A	1190	G	P-O3'-C3'	6.91	127.99	119.70
2	B	121	LEU	N-CA-C	-6.87	92.44	111.00
3	C	178	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	18	C	C6-N1-C2	6.84	123.04	120.30
1	A	279	A	N3-C4-N9	-6.82	121.94	127.40
1	A	117	G	C2-N3-C4	-6.81	108.49	111.90
1	A	117	G	C5-C6-N1	-6.81	108.09	111.50
1	A	266	G	C8-N9-C4	-6.81	103.68	106.40
1	A	599	C	C6-N1-C2	6.78	123.01	120.30
1	A	650	G	C8-N9-C4	6.74	109.10	106.40
1	A	328	C	C2-N1-C1'	6.71	126.19	118.80
1	A	1346	A	P-O3'-C3'	6.70	127.74	119.70
1	A	108	G	O4'-C1'-N9	6.67	113.53	108.20
1	A	839	U	N1-C2-O2	6.66	127.46	122.80
1	A	108	G	N7-C8-N9	6.63	116.42	113.10
1	A	254	G	O5'-P-OP1	-6.61	99.75	105.70
1	A	9	G	O5'-P-OP2	-6.54	99.82	105.70
1	A	788	U	C5-C6-N1	6.52	125.96	122.70
1	A	279	A	N3-C4-C5	6.51	131.36	126.80
1	A	788	U	C5-C4-O4	-6.44	122.03	125.90
1	A	1504	G	O5'-P-OP2	-6.40	99.94	105.70
1	A	975	A	O4'-C1'-N9	-6.38	103.09	108.20
1	A	1503	A	P-O3'-C3'	6.35	127.32	119.70
1	A	948	C	C6-N1-C2	6.33	122.83	120.30
1	A	795	C	N3-C2-O2	6.32	126.32	121.90
1	A	117	G	C4-C5-N7	6.28	113.31	110.80
1	A	1301	U	P-O3'-C3'	6.26	127.22	119.70
1	A	1065	U	P-O3'-C3'	6.23	127.18	119.70
1	A	1367	C	C6-N1-C2	-6.23	117.81	120.30
1	A	9	G	N1-C6-O6	6.22	123.63	119.90
1	A	788	U	C2-N3-C4	6.18	130.71	127.00
1	A	279	A	N7-C8-N9	6.17	116.89	113.80
5	E	12	LEU	CA-CB-CG	6.16	129.46	115.30
4	D	12	CYS	CA-CB-SG	6.12	125.03	114.00
1	A	108	G	N3-C4-C5	6.11	131.66	128.60
1	A	788	U	N3-C2-O2	6.10	126.47	122.20
1	A	108	G	C5-C6-O6	-6.09	124.95	128.60
1	A	1442	G	C4-N9-C1'	6.01	134.32	126.50
1	A	760	G	O5'-P-OP2	-6.01	100.30	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1067	A	P-O3'-C3'	5.97	126.87	119.70
12	L	29	GLY	N-CA-C	-5.97	98.17	113.10
1	A	1346	A	N1-C6-N6	-5.96	115.03	118.60
1	A	814	A	C2-N3-C4	-5.96	107.62	110.60
1	A	266	G	C6-C5-N7	-5.95	126.83	130.40
1	A	687	A	P-O3'-C3'	5.95	126.83	119.70
1	A	108	G	C2-N3-C4	-5.86	108.97	111.90
1	A	235	C	C6-N1-C2	5.85	122.64	120.30
1	A	839	U	C2-N1-C1'	5.81	124.67	117.70
1	A	792	A	C5-C6-N6	5.80	128.34	123.70
1	A	9	G	C5-C6-O6	-5.79	125.13	128.60
1	A	299	G	C4-C5-N7	5.76	113.10	110.80
1	A	563	A	O4'-C1'-N9	5.72	112.78	108.20
1	A	1500	A	O5'-P-OP2	-5.70	100.57	105.70
1	A	279	A	N1-C2-N3	5.69	132.15	129.30
1	A	299	G	C5-C6-O6	-5.69	125.18	128.60
1	A	117	G	C4-C5-C6	5.69	122.21	118.80
1	A	7	G	C8-N9-C4	5.67	108.67	106.40
1	A	1530	G	C8-N9-C4	5.64	108.65	106.40
1	A	1442	G	C6-C5-N7	-5.61	127.03	130.40
1	A	266	G	C2-N3-C4	-5.58	109.11	111.90
1	A	5	U	P-O3'-C3'	5.56	126.38	119.70
1	A	792	A	N1-C6-N6	-5.56	115.26	118.60
1	A	1335	C	O4'-C1'-N1	5.55	112.64	108.20
1	A	926	G	N3-C4-C5	-5.54	125.83	128.60
1	A	144	G	N1-C6-O6	5.52	123.21	119.90
1	A	1503	A	OP1-P-O3'	5.52	117.34	105.20
1	A	560	U	N1-C1'-C2'	-5.49	105.96	112.00
1	A	701	C	P-O3'-C3'	5.48	126.28	119.70
1	A	115	G	P-O3'-C3'	5.46	126.25	119.70
1	A	1442	G	N3-C4-N9	5.44	129.26	126.00
1	A	509	A	C2'-C3'-O3'	5.41	122.36	113.70
1	A	1395	C	O5'-P-OP2	-5.39	100.84	105.70
1	A	975	A	N7-C8-N9	5.39	116.49	113.80
1	A	1099	G	N3-C4-C5	5.38	131.29	128.60
1	A	975	A	C5-N7-C8	-5.37	101.22	103.90
1	A	116	A	OP2-P-O3'	5.37	117.00	105.20
1	A	7	G	N9-C4-C5	-5.35	103.26	105.40
1	A	1082	G	C8-N9-C4	5.35	108.54	106.40
1	A	1498	UR3	P-O3'-C3'	5.35	126.12	119.70
1	A	914	A	O5'-P-OP1	-5.34	100.89	105.70
1	A	748	C	P-O3'-C3'	5.34	126.11	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	724	G	C5-C6-O6	-5.32	125.41	128.60
1	A	1224	G	P-O3'-C3'	5.30	126.06	119.70
1	A	839	U	N3-C2-O2	-5.30	118.49	122.20
1	A	108	G	C5'-C4'-O4'	5.30	115.46	109.10
1	A	117	G	O5'-P-OP2	-5.26	100.97	105.70
1	A	108	G	C6-C5-N7	-5.23	127.26	130.40
1	A	279	A	C3'-C2'-C1'	5.22	105.68	101.50
1	A	575	G	O4'-C1'-N9	-5.22	104.03	108.20
1	A	1502	A	N1-C2-N3	5.22	131.91	129.30
1	A	1442	G	C8-N9-C1'	-5.21	120.22	127.00
1	A	328	C	P-O3'-C3'	5.20	125.94	119.70
1	A	1065	U	OP2-P-O3'	5.19	116.62	105.20
1	A	328	C	N3-C4-N4	-5.18	114.38	118.00
1	A	1380	U	P-O3'-C3'	5.17	125.90	119.70
1	A	1181	G	C6-C5-N7	5.15	133.49	130.40
1	A	931	C	C5-C6-N1	-5.14	118.43	121.00
1	A	560	U	C3'-C2'-C1'	5.13	105.60	101.50
1	A	1502	A	C5-C6-N1	-5.12	115.14	117.70
3	C	179	ARG	N-CA-C	-5.12	97.18	111.00
1	A	299	G	N1-C6-O6	5.11	122.97	119.90
1	A	117	G	C8-N9-C1'	-5.11	120.36	127.00
12	L	28	LYS	N-CA-C	-5.08	97.30	111.00
1	A	1064	G	OP1-P-O3'	5.05	116.31	105.20
1	A	1181	G	N3-C4-N9	-5.05	122.97	126.00
1	A	1397	C	N1-C2-O2	5.05	121.93	118.90
1	A	735	C	C6-N1-C2	5.04	122.32	120.30
1	A	484	G	P-O3'-C3'	5.04	125.75	119.70
1	A	1099	G	N3-C4-N9	-5.04	122.98	126.00
1	A	1334	G	C8-N9-C4	5.01	108.41	106.40
1	A	9	G	C8-N9-C4	5.01	108.40	106.40
1	A	1201	A	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	19	HIS	Peptide
2	B	22	LYS	Peptide
8	H	90	GLY	Peptide
12	L	115	LYS	Peptide
12	L	46	LYS	Peptide
14	N	30	ALA	Peptide

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Mol	Chain	Res	Type	Group
17	Q	13	ASP	Peptide
20	T	12	ALA	Peptide
20	T	93	GLU	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32507	0	16433	448	0
2	B	1900	0	1951	73	0
3	C	1612	0	1677	43	0
4	D	1703	0	1763	46	0
5	E	1146	0	1207	32	0
6	F	843	0	857	20	0
7	G	1257	0	1296	25	0
8	H	1116	0	1177	45	0
9	I	1010	0	1037	29	0
10	J	792	0	835	36	0
11	K	885	0	904	34	0
12	L	973	0	1062	30	0
13	M	933	0	992	26	0
14	N	492	0	529	31	0
15	O	734	0	771	15	0
16	P	700	0	720	15	0
17	Q	857	0	928	30	0
18	R	598	0	670	20	0
19	S	647	0	673	19	0
20	T	763	0	861	31	0
21	U	208	0	221	3	0
22	A	40	0	37	1	0
23	A	295	0	0	0	0
23	B	4	0	0	0	0
23	D	3	0	0	0	0
23	E	2	0	0	0	0
23	F	1	0	0	0	0
23	H	4	0	0	0	0
23	I	1	0	0	0	0
23	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K	3	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	4	0	0	0	0
23	S	1	0	0	0	0
23	T	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	702	0	0	24	0
25	B	3	0	0	0	0
25	D	1	0	0	0	0
25	E	8	0	0	0	0
25	F	6	0	0	0	0
25	H	2	0	0	0	0
25	L	1	0	0	0	0
25	P	1	0	0	0	0
25	Q	6	0	0	0	0
25	T	3	0	0	0	0
All	All	52776	0	36601	935	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 11.

All (935) 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)
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.49	0.92
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.60	0.84
1:A:1006:C:H42	1:A:1022:G:H1	1.24	0.83
1:A:664:G:H22	1:A:741:G:H1	1.24	0.83
20:T:67:ALA:HA	20:T:73:HIS:H	1.43	0.83
1:A:298:A:N6	25:A:1982:HOH:O	2.11	0.83
1:A:1238:A:H5'	1:A:1336:C:H41	1.43	0.83
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.44	0.82
1:A:567:G:O2'	25:A:2396:HOH:O	1.97	0.82
1:A:279:A:OP2	17:Q:95:TYR:OH	1.97	0.82
11:K:121:PRO:HG2	11:K:126:ARG:HG3	1.63	0.81
1:A:103:C:OP1	20:T:17:ARG:NH1	2.14	0.81
1:A:1163:C:H42	1:A:1173:G:H1	1.30	0.80
1:A:1057:G:H5''	3:C:154:SER:HB2	1.63	0.80
1:A:130:A:OP2	1:A:190(E):U:O2'	1.99	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:C:N4	25:A:2267:HOH:O	2.14	0.79
1:A:372:C:O2'	25:A:2575:HOH:O	2.02	0.78
4:D:3:ARG:HD2	4:D:71:SER:HB3	1.66	0.78
1:A:411:A:OP2	4:D:25:ARG:NH2	2.17	0.77
1:A:975:A:H5'	1:A:975:A:H8	1.49	0.77
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.66	0.77
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.66	0.77
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.67	0.76
10:J:44:VAL:HG13	10:J:66:ARG:HG2	1.66	0.76
1:A:1086:U:H3	1:A:1099:G:H22	1.30	0.76
12:L:47:LYS:HD2	12:L:48:PRO:HD3	1.67	0.76
1:A:517:G:N1	1:A:533:A:OP2	2.16	0.76
10:J:26:ALA:HB3	10:J:85:LEU:HD21	1.67	0.76
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.75
20:T:74:LYS:HG3	20:T:75:ASN:H	1.49	0.75
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.68	0.74
1:A:1502:A:H2	1:A:1505:G:H1	1.33	0.74
1:A:1029:C:H41	1:A:1033:G:H21	1.36	0.74
1:A:527:7MG:OP2	22:A:1601:SRY:O32	2.04	0.73
1:A:427:U:OP2	4:D:36:ARG:NH2	2.21	0.73
1:A:1008:C:N3	1:A:1021:G:N2	2.37	0.73
3:C:156:ARG:NH1	3:C:193:TYR:O	2.22	0.73
2:B:178:ARG:HH22	8:H:68:ARG:HH12	1.35	0.73
3:C:156:ARG:H	3:C:163:ALA:HA	1.54	0.73
1:A:1419:G:H1	1:A:1481:U:H3	1.37	0.72
1:A:451:A:O2'	25:A:2280:HOH:O	2.08	0.72
1:A:1305:G:N2	1:A:1331:G:H1'	2.05	0.71
3:C:154:SER:OG	3:C:155:GLY:N	2.22	0.71
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.24	0.71
1:A:1141:C:H2'	1:A:1142:G:H8	1.56	0.71
14:N:32:SER:HB3	14:N:41:ARG:H	1.56	0.70
1:A:33:A:N6	25:A:2529:HOH:O	2.24	0.70
17:Q:40:LYS:HD3	17:Q:42:TYR:CZ	2.27	0.70
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.72	0.70
1:A:503:C:OP2	12:L:116:SER:HB3	1.91	0.70
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.25	0.70
8:H:1:MET:HG2	8:H:2:LEU:H	1.57	0.70
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.73	0.69
1:A:411:A:C4	1:A:413:G:H1'	2.28	0.69
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.74	0.69
1:A:1506:U:O2'	25:A:2291:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:73:MET:HG2	7:G:90:GLU:HA	1.75	0.69
1:A:954:G:H21	1:A:1227:A:H62	1.41	0.69
10:J:4:ILE:HD12	10:J:74:ILE:HG13	1.74	0.69
1:A:563:A:N6	25:A:2394:HOH:O	2.26	0.69
1:A:673:G:H2'	1:A:674:G:C8	2.28	0.69
1:A:1163:C:N3	1:A:1173:G:N2	2.37	0.68
1:A:677:U:H3	1:A:713:G:H22	1.41	0.68
1:A:344:A:H5'	1:A:345:C:H5	1.57	0.68
9:I:32:ASP:OD1	9:I:33:PHE:N	2.25	0.68
1:A:31:G:N2	25:A:2440:HOH:O	2.26	0.68
15:O:87:ILE:HG22	15:O:88:ARG:H	1.59	0.68
10:J:6:ILE:HG22	10:J:98:ILE:HA	1.76	0.67
1:A:235:C:N4	25:A:1945:HOH:O	2.26	0.67
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.28	0.67
1:A:849:C:N4	25:A:2216:HOH:O	2.25	0.67
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.67
10:J:40:LEU:HD13	10:J:41:PRO:HD2	1.76	0.67
9:I:7:THR:HG22	9:I:8:GLY:H	1.58	0.66
1:A:1392:G:H21	1:A:1502:A:H8	1.41	0.66
5:E:8:GLU:HG3	5:E:34:VAL:HG22	1.76	0.66
1:A:835:U:OP1	18:R:64:ARG:NH2	2.29	0.66
11:K:54:ARG:HH11	11:K:54:ARG:HB3	1.60	0.66
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.77	0.66
1:A:1508:G:H5'	25:A:2293:HOH:O	1.95	0.66
3:C:3:ASN:HB2	3:C:4:LYS:HG2	1.78	0.66
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.78	0.66
1:A:1004:A:N6	1:A:1035:A:H62	1.93	0.66
2:B:178:ARG:NH2	2:B:198:ASP:OD1	2.29	0.66
1:A:975:A:H5'	1:A:975:A:C8	2.30	0.65
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.44	0.65
1:A:1148:U:H2'	1:A:1149:C:O4'	1.96	0.65
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.79	0.65
1:A:1510:U:H2'	1:A:1511:G:C8	2.31	0.65
1:A:263:A:OP2	20:T:79:ARG:NH1	2.30	0.65
1:A:144:G:H1	1:A:178:C:H42	1.43	0.65
1:A:538:G:H5''	12:L:114:LYS:HB2	1.78	0.65
2:B:16:HIS:ND1	2:B:17:PHE:O	2.27	0.65
1:A:1101:A:H61	2:B:103:THR:HG21	1.61	0.65
1:A:953:G:H5'	1:A:965:A:H61	1.61	0.65
4:D:36:ARG:HB2	4:D:38:TYR:CZ	2.32	0.65
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:G:OP1	17:Q:91:ARG:NH2	2.29	0.64
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.78	0.64
1:A:1392:G:N2	1:A:1502:A:H8	1.96	0.64
2:B:224:GLN:HA	2:B:229:VAL:HG22	1.80	0.64
14:N:30:ALA:HB1	14:N:33:VAL:HG22	1.79	0.64
1:A:1029:C:H41	1:A:1033:G:N2	1.95	0.64
2:B:130:ARG:CZ	2:B:131:PRO:HD2	2.28	0.64
1:A:1003(A):G:C2	1:A:1004:A:H1'	2.32	0.64
1:A:1314:C:N4	19:S:4:SER:OG	2.27	0.64
12:L:8:ASN:O	12:L:12:ARG:HG3	1.99	0.63
5:E:101:ILE:O	5:E:120:THR:HB	1.99	0.63
1:A:1007:C:O2	1:A:1023:G:N1	2.31	0.63
5:E:144:THR:O	5:E:148:VAL:HG23	1.97	0.63
1:A:166:G:H2'	1:A:167:G:H8	1.63	0.63
1:A:376:G:H5''	16:P:5:ARG:HD2	1.80	0.63
17:Q:86:GLU:O	17:Q:90:ILE:HG12	1.99	0.63
1:A:530:G:H5'	1:A:531:U:H5'	1.80	0.63
1:A:1143:G:H2'	1:A:1144:G:C8	2.34	0.63
1:A:1125:U:OP2	1:A:1145:C:N4	2.31	0.63
1:A:542:G:OP1	4:D:10:ARG:NH2	2.28	0.63
1:A:56:U:H2'	1:A:57:G:C8	2.34	0.63
9:I:92:TYR:O	9:I:96:LEU:HB2	1.99	0.63
13:M:37:THR:HG23	13:M:55:ARG:HB3	1.80	0.63
1:A:1031:G:H2'	1:A:1032:G:H8	1.64	0.62
3:C:43:LEU:HD22	3:C:47:LEU:HD22	1.79	0.62
6:F:41:GLU:OE1	18:R:35:ARG:NH2	2.32	0.62
1:A:562:C:H1'	12:L:15:ARG:HB3	1.82	0.62
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.33	0.62
2:B:69:LEU:HD12	2:B:155:LEU:HD11	1.80	0.62
8:H:26:VAL:HG22	8:H:59:LEU:HB2	1.82	0.62
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.33	0.61
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.82	0.61
8:H:101:PRO:HG3	8:H:133:LEU:HD11	1.81	0.61
1:A:1373:G:H5''	7:G:36:LYS:HD2	1.81	0.61
1:A:1412:C:H2'	1:A:1413:A:C8	2.36	0.61
1:A:414:A:OP2	1:A:428:G:N2	2.33	0.61
2:B:17:PHE:HD1	2:B:18:GLY:H	1.46	0.61
1:A:1366:C:H2'	1:A:1367:C:C6	2.35	0.61
1:A:269:C:H2'	1:A:270:A:C8	2.34	0.61
1:A:1443:G:H4'	1:A:1446:A:H5''	1.81	0.61
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:LEU:O	13:M:110:ARG:NH1	2.33	0.61
5:E:126:ARG:HH11	5:E:126:ARG:HG2	1.66	0.60
1:A:532:A:O2'	1:A:533:A:OP1	2.18	0.60
6:F:100:ASN:ND2	18:R:23:LYS:O	2.34	0.60
1:A:975:A:H4'	1:A:976:G:H5''	1.83	0.60
20:T:100:ILE:HG23	20:T:102:GLY:H	1.66	0.60
1:A:95:U:H2'	1:A:96:G:C8	2.36	0.60
1:A:547:A:OP2	4:D:2:GLY:N	2.34	0.60
1:A:695:A:C2	1:A:787:A:H1'	2.36	0.60
10:J:7:LYS:HG2	10:J:71:LEU:HG	1.84	0.60
9:I:126:SER:OG	9:I:127:LYS:N	2.35	0.60
16:P:14:ASN:HA	16:P:42:ARG:HH21	1.66	0.60
1:A:1505:G:H5'	25:A:2290:HOH:O	2.02	0.60
7:G:13:GLN:HG2	7:G:14:PRO:HD2	1.84	0.60
1:A:1417:G:O2'	1:A:1483:A:N6	2.35	0.59
1:A:302:G:H5''	12:L:17:LYS:HE3	1.84	0.59
1:A:1279:A:H5''	1:A:1280:A:OP1	2.02	0.59
12:L:25:PRO:C	12:L:27:LEU:H	2.04	0.59
1:A:974:A:OP2	14:N:41:ARG:NH1	2.34	0.59
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.35	0.59
19:S:12:ASP:H	19:S:38:SER:HB3	1.66	0.59
2:B:15:VAL:HG22	2:B:209:ARG:HD3	1.84	0.59
4:D:187:ARG:NE	4:D:188:LEU:H	2.01	0.59
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.85	0.59
1:A:1049:U:H6	1:A:1049:U:H5''	1.68	0.59
12:L:35:GLY:HA3	12:L:60:LEU:HD12	1.85	0.59
1:A:1047:G:H5''	14:N:4:LYS:HE2	1.85	0.59
20:T:74:LYS:HG3	20:T:75:ASN:N	2.18	0.59
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.17	0.59
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.83	0.59
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.85	0.59
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.37	0.59
1:A:518:C:H2'	1:A:530:G:C8	2.38	0.59
1:A:560:U:H5'	1:A:566:G:N2	2.18	0.58
1:A:992:U:H4'	1:A:993:G:O5'	2.03	0.58
7:G:46:ALA:O	7:G:50:ILE:HG13	2.02	0.58
1:A:1352:C:H2'	1:A:1353:G:C8	2.38	0.58
1:A:381:C:H2'	1:A:382:A:O4'	2.03	0.58
1:A:195:A:H4'	20:T:68:LYS:HE2	1.84	0.58
1:A:250:A:H4'	1:A:251:G:O5'	2.04	0.58
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:116:LYS:HD2	8:H:129:VAL:HG11	1.86	0.58
1:A:390:C:O3'	16:P:28:ARG:NH2	2.37	0.58
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.20	0.57
1:A:1427:U:H2'	1:A:1428:A:C8	2.39	0.57
1:A:299:G:N1	25:A:1982:HOH:O	2.32	0.57
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.38	0.57
1:A:344:A:H5'	1:A:345:C:C5	2.39	0.57
1:A:933:G:OP2	7:G:3:ARG:HB2	2.04	0.57
16:P:22:THR:HA	16:P:33:ILE:HG13	1.87	0.57
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.85	0.57
1:A:1063:C:OP2	1:A:1064:G:O2'	2.21	0.57
1:A:343:U:O2'	1:A:346:G:O6	2.20	0.57
7:G:47:CYS:HA	7:G:50:ILE:HD12	1.85	0.57
18:R:38:GLU:HA	18:R:41:LYS:HE2	1.87	0.57
1:A:1414:U:H2'	1:A:1415:G:H8	1.69	0.57
1:A:316:G:OP2	1:A:351:G:O2'	2.23	0.57
1:A:788:U:O2'	1:A:1539:C:N3	2.37	0.57
1:A:1068:G:H8	1:A:1068:G:OP2	1.88	0.57
1:A:953:G:N7	13:M:104:ARG:NH2	2.53	0.57
1:A:243:A:H4'	1:A:244:U:H5'	1.86	0.56
1:A:353:A:H5'	1:A:353:A:H8	1.69	0.56
3:C:14:ILE:O	3:C:16:ARG:N	2.38	0.56
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.86	0.56
1:A:1493:A:H2'	1:A:1494:G:H8	1.70	0.56
13:M:16:ASP:OD1	13:M:16:ASP:N	2.38	0.56
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.88	0.56
19:S:3:ARG:HD2	19:S:5:LEU:HD11	1.87	0.56
19:S:39:THR:HG22	19:S:70:LYS:HE2	1.88	0.56
1:A:421:U:H5'	1:A:422:C:H5	1.70	0.56
4:D:25:ARG:O	4:D:28:SER:N	2.38	0.56
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.88	0.56
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.86	0.56
14:N:26:ARG:HD2	14:N:47:LEU:HD11	1.87	0.56
1:A:692:U:OP1	11:K:124:LYS:NZ	2.32	0.56
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.36	0.56
12:L:68:ALA:HB2	12:L:85:ILE:HD11	1.88	0.56
1:A:1006:C:H2'	1:A:1007:C:C6	2.41	0.55
1:A:413:G:N2	1:A:428:G:H1'	2.21	0.55
1:A:1065:U:O2'	1:A:1066:C:OP2	2.18	0.55
1:A:1103:C:H5''	2:B:98:LEU:HD22	1.87	0.55
1:A:1305:G:H22	1:A:1331:G:H1'	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:N6	25:A:2161:HOH:O	2.39	0.55
1:A:959:A:HO2'	1:A:984:C:HO2'	1.55	0.55
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.88	0.55
2:B:240:GLN:OE1	2:B:240:GLN:N	2.40	0.55
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.88	0.55
1:A:573:A:H5'	1:A:573:A:H8	1.72	0.55
2:B:21:ARG:H	2:B:21:ARG:HE	1.53	0.55
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.42	0.55
1:A:1338:G:H2'	1:A:1339:A:C8	2.42	0.55
1:A:1502:A:H2	1:A:1505:G:N1	2.01	0.55
8:H:2:LEU:HD21	8:H:8:ASP:HB2	1.89	0.55
1:A:1303:C:H2'	1:A:1304:G:H5'	1.88	0.55
1:A:328:C:O2	1:A:328:C:H2'	2.05	0.55
1:A:646:U:H2'	1:A:647:C:C6	2.42	0.55
3:C:73:PRO:HB3	3:C:103:VAL:HG11	1.88	0.55
3:C:47:LEU:HD11	3:C:76:VAL:HG13	1.88	0.55
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.42	0.55
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.42	0.55
14:N:24:CYS:H	14:N:30:ALA:HB2	1.72	0.55
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.89	0.55
19:S:22:LEU:HD11	19:S:31:ILE:HD11	1.89	0.55
1:A:564:C:O2'	8:H:91:ARG:NH2	2.39	0.54
1:A:35:G:H2'	1:A:36:C:C6	2.41	0.54
1:A:706:A:H2'	1:A:707:C:H5'	1.90	0.54
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.89	0.54
9:I:113:LYS:HD2	9:I:119:ALA:HB1	1.89	0.54
20:T:42:GLN:O	20:T:45:GLN:HB2	2.07	0.54
1:A:1035:A:H2'	1:A:1036:G:C8	2.43	0.54
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.89	0.54
1:A:1181:G:O2'	1:A:1182:G:O5'	2.24	0.54
7:G:44:TYR:O	7:G:48:LYS:HG2	2.06	0.54
1:A:17:U:H2'	1:A:18:C:C6	2.42	0.54
8:H:92:ARG:HH11	8:H:92:ARG:CG	2.21	0.54
1:A:962:C:O2'	25:A:2249:HOH:O	2.18	0.54
2:B:230:VAL:HG22	2:B:231:GLU:H	1.72	0.54
3:C:13:GLY:HA2	14:N:57:ARG:HH22	1.71	0.54
5:E:122:GLU:HG2	5:E:131:ILE:HD12	1.89	0.54
11:K:87:THR:HG22	11:K:88:GLY:H	1.72	0.54
13:M:77:ASN:O	13:M:80:ARG:HB2	2.08	0.54
1:A:1168:A:H2'	1:A:1169:A:C8	2.43	0.54
3:C:154:SER:HB3	3:C:197:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:75:ILE:HG22	10:J:76:ASN:H	1.73	0.54
1:A:977:A:N6	1:A:1224:G:H5''	2.23	0.54
1:A:559:A:H4'	1:A:560:U:H3'	1.90	0.54
1:A:1460:A:OP2	20:T:27:LYS:NZ	2.42	0.53
1:A:5:U:H4'	1:A:6:G:O5'	2.07	0.53
1:A:820:U:H4'	1:A:821:G:OP2	2.07	0.53
8:H:38:ILE:HD13	8:H:41:ARG:HH22	1.72	0.53
15:O:30:ALA:HA	15:O:85:LEU:HD11	1.89	0.53
1:A:355:C:H5'	1:A:389:A:OP2	2.08	0.53
1:A:825:G:H21	8:H:11:THR:HG21	1.73	0.53
1:A:1101:A:H61	2:B:103:THR:CG2	2.21	0.53
1:A:1513:A:H2'	1:A:1514:C:C6	2.43	0.53
1:A:412:A:N6	4:D:35:ARG:HA	2.22	0.53
2:B:8:LYS:O	2:B:217:ARG:NH1	2.41	0.53
5:E:80:ILE:HA	8:H:104:ARG:NH2	2.24	0.53
1:A:1125:U:H3	10:J:5:ARG:HH21	1.56	0.53
1:A:1391:U:H2'	1:A:1392:G:C8	2.43	0.53
1:A:1497:G:H2'	1:A:1498:UR3:H5'	1.90	0.53
1:A:56:U:H2'	1:A:57:G:H8	1.72	0.53
8:H:17:THR:HG22	8:H:63:LEU:HG	1.91	0.53
1:A:1000:U:H2'	1:A:1001:A:C8	2.44	0.53
1:A:1064:G:N2	1:A:1191:A:OP2	2.40	0.53
1:A:1241:G:H2'	1:A:1242:C:C6	2.43	0.53
4:D:102:ASP:OD1	4:D:103:ASN:N	2.41	0.53
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.74	0.53
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.91	0.53
11:K:14:VAL:HG23	11:K:75:TYR:HB3	1.91	0.53
1:A:1116:C:H2'	1:A:1117:G:H5''	1.91	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.09	0.53
1:A:1189:C:H5''	3:C:5:ILE:HG12	1.91	0.53
9:I:118:LYS:O	9:I:119:ALA:HB3	2.08	0.53
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.08	0.53
20:T:74:LYS:CG	20:T:75:ASN:H	2.14	0.53
1:A:1031:G:H2'	1:A:1032:G:C8	2.43	0.52
2:B:178:ARG:NH2	8:H:68:ARG:HH12	2.06	0.52
20:T:73:HIS:O	20:T:74:LYS:HG2	2.09	0.52
1:A:164:U:H2'	1:A:165:C:C6	2.44	0.52
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.91	0.52
7:G:27:ILE:HD13	7:G:40:ALA:HA	1.91	0.52
14:N:11:LYS:HG2	14:N:13:THR:H	1.73	0.52
17:Q:104:LYS:NZ	17:Q:105:ALA:H	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:G:N7	12:L:53:ARG:NH2	2.56	0.52
3:C:67:THR:HA	3:C:102:ASN:HB2	1.91	0.52
4:D:101:LEU:O	4:D:105:VAL:HG23	2.10	0.52
4:D:35:ARG:O	4:D:36:ARG:HG2	2.09	0.52
1:A:1301:U:O2'	1:A:1302:U:H3'	2.10	0.52
1:A:266:G:H5''	1:A:267:C:C5	2.44	0.52
1:A:1474:G:H2'	1:A:1475:G:H8	1.74	0.52
2:B:96:ARG:NE	2:B:97:TRP:H	2.08	0.52
3:C:155:GLY:HA2	3:C:164:ARG:H	1.74	0.52
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.92	0.52
11:K:50:TYR:HB3	11:K:54:ARG:HB2	1.92	0.52
1:A:1147:C:O2	9:I:16:ARG:NH2	2.42	0.52
1:A:1303:C:C2'	1:A:1304:G:H5'	2.39	0.52
1:A:527:7MG:O2'	1:A:535:A:N1	2.31	0.52
1:A:736:C:H2'	1:A:737:A:C8	2.44	0.52
2:B:79:ASP:HB3	2:B:238:LEU:HD13	1.92	0.52
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.10	0.52
1:A:1123:A:H2	1:A:1150:U:H3	1.58	0.52
6:F:4:TYR:CE1	6:F:92:LYS:HG2	2.45	0.52
13:M:2:ALA:O	13:M:10:PRO:HD2	2.10	0.52
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.24	0.52
1:A:665:A:H2'	1:A:732:C:O2	2.09	0.52
1:A:973:G:H3'	1:A:974:A:H5''	1.92	0.52
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.92	0.52
1:A:1090:U:H2'	1:A:1091:U:H6	1.75	0.51
1:A:179:A:H2'	1:A:180:U:C6	2.45	0.51
2:B:84:GLU:OE2	2:B:235:SER:HB2	2.10	0.51
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.92	0.51
9:I:53:VAL:HA	9:I:95:LYS:HD3	1.91	0.51
1:A:1262:C:H2'	1:A:1263:C:C6	2.45	0.51
1:A:1221:G:O3'	19:S:77:THR:HG21	2.10	0.51
1:A:563:A:H2'	1:A:567:G:C8	2.46	0.51
4:D:177:ASP:OD1	4:D:180:GLY:N	2.38	0.51
8:H:46:LYS:HG2	8:H:64:LYS:HB2	1.90	0.51
1:A:1525:G:P	11:K:120:ARG:HH22	2.32	0.51
1:A:1490:C:H5'	1:A:1491:G:OP2	2.10	0.51
2:B:179:LYS:HA	8:H:72:PRO:HD3	1.91	0.51
1:A:1006:C:H2'	1:A:1007:C:H6	1.76	0.51
1:A:322:C:OP2	1:A:328:C:N4	2.43	0.51
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.51
2:B:119:GLU:HA	2:B:142:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:A:H2'	1:A:532:A:N3	2.25	0.51
1:A:946:A:H2'	1:A:947:G:C8	2.45	0.51
5:E:88:LYS:HD3	5:E:123:LEU:HD12	1.92	0.51
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.93	0.51
13:M:3:ARG:HA	13:M:8:GLU:O	2.10	0.51
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.51
1:A:1241:G:H2'	1:A:1242:C:H6	1.76	0.51
2:B:97:TRP:HZ3	2:B:176:GLU:OE2	1.93	0.51
7:G:50:ILE:O	7:G:54:THR:OG1	2.26	0.51
10:J:49:VAL:O	10:J:60:ARG:HA	2.11	0.51
12:L:27:LEU:HG	12:L:28:LYS:H	1.76	0.51
5:E:40:ARG:HB3	5:E:66:MET:HE1	1.93	0.51
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.26	0.51
10:J:71:LEU:HD22	10:J:73:ASP:HB2	1.93	0.51
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.93	0.51
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.93	0.51
3:C:54:ARG:HG3	3:C:69:HIS:HD2	1.76	0.51
1:A:1022:G:O2'	1:A:1023:G:O4'	2.22	0.51
1:A:1443:G:H5''	1:A:1446:A:H5''	1.93	0.51
1:A:1243:C:H2'	1:A:1244:C:C6	2.45	0.50
1:A:954:G:N2	1:A:1227:A:H62	2.07	0.50
2:B:195:ASP:O	8:H:74:PRO:HG3	2.11	0.50
12:L:60:LEU:HB2	12:L:64:TYR:O	2.11	0.50
20:T:46:GLU:HB2	20:T:48:LYS:HG3	1.93	0.50
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.92	0.50
16:P:68:ASP:OD1	16:P:68:ASP:N	2.28	0.50
19:S:5:LEU:C	19:S:6:LYS:HE3	2.31	0.50
1:A:269:C:H2'	1:A:270:A:H8	1.74	0.50
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.50
2:B:212:GLN:HE21	2:B:235:SER:HB3	1.76	0.50
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.93	0.50
1:A:826:C:O2	8:H:15:ASN:ND2	2.44	0.50
4:D:25:ARG:O	4:D:27:TYR:N	2.44	0.50
19:S:41:VAL:HG23	19:S:43:GLU:HG2	1.93	0.50
1:A:299:G:H2'	1:A:300:A:C8	2.45	0.50
11:K:86:GLY:O	11:K:91:ARG:HD3	2.11	0.50
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.12	0.50
1:A:359:U:H2'	1:A:360:A:C8	2.47	0.50
2:B:16:HIS:HB3	2:B:210:SER:HB3	1.94	0.50
9:I:116:LYS:HA	9:I:123:PRO:HD3	1.92	0.50
15:O:12:ILE:HG23	15:O:27:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:G:OP2	16:P:67:THR:HG21	2.11	0.50
1:A:838:G:H2'	1:A:839:U:H5''	1.93	0.50
3:C:77:ILE:HA	3:C:84:ILE:HB	1.93	0.50
14:N:22:THR:HB	14:N:33:VAL:HG21	1.93	0.50
1:A:1100:C:H3'	25:A:2418:HOH:O	2.11	0.50
1:A:1179:A:H2'	1:A:1180:A:O4'	2.12	0.50
5:E:126:ARG:HG2	5:E:126:ARG:NH1	2.27	0.50
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.45	0.50
1:A:1143:G:H2'	1:A:1144:G:H8	1.75	0.50
1:A:1524:C:N4	25:A:2000:HOH:O	2.43	0.50
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.94	0.50
1:A:731:G:OP1	1:A:766:A:H1'	2.12	0.49
10:J:54:PHE:CD2	10:J:55:LYS:HG2	2.46	0.49
10:J:54:PHE:HD2	10:J:55:LYS:HG2	1.77	0.49
20:T:92:LEU:O	20:T:96:GLY:N	2.45	0.49
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.47	0.49
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.47	0.49
1:A:156:G:H1	1:A:165:C:H42	1.60	0.49
1:A:166:G:H2'	1:A:167:G:C8	2.44	0.49
12:L:37:CYS:HB2	12:L:79:GLU:O	2.12	0.49
14:N:32:SER:HB2	14:N:40:CYS:HB2	1.95	0.49
1:A:1128:C:HO2'	1:A:1130:A:H8	1.60	0.49
3:C:22:TRP:CH2	3:C:32:LEU:HB2	2.48	0.49
12:L:27:LEU:HB2	12:L:62:SER:HB3	1.95	0.49
1:A:89:C:H2'	1:A:90:U:O4'	2.12	0.49
4:D:145:GLU:OE1	4:D:182:LYS:HD3	2.13	0.49
11:K:57:THR:CG2	11:K:60:ALA:H	2.26	0.49
18:R:38:GLU:CD	18:R:38:GLU:H	2.10	0.49
1:A:412:A:O5'	4:D:35:ARG:NH2	2.44	0.49
1:A:620:C:H2'	1:A:621:A:O4'	2.12	0.49
1:A:718:G:H5''	1:A:719:C:OP2	2.12	0.49
2:B:61:LEU:HD11	2:B:160:ASP:HB2	1.95	0.49
13:M:12:ASN:H	13:M:45:VAL:HG12	1.77	0.49
18:R:44:LEU:HD21	18:R:70:ILE:HD13	1.94	0.49
7:G:69:VAL:HG21	7:G:104:LEU:HD11	1.93	0.49
1:A:892:A:C2	1:A:907:A:C4	3.01	0.49
3:C:108:ASN:HD21	3:C:144:SER:HB3	1.78	0.49
4:D:23:GLY:HA3	4:D:112:VAL:HG13	1.93	0.49
6:F:23:LYS:O	6:F:27:GLN:HG2	2.12	0.49
10:J:89:ASP:HB3	10:J:91:PRO:HD3	1.94	0.49
2:B:23:ARG:HH11	2:B:24:TRP:N	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:G:N3	17:Q:105:ALA:HB2	2.28	0.49
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.48	0.49
1:A:1225:A:N3	1:A:1225:A:H2'	2.27	0.48
1:A:384:G:H2'	1:A:385:C:C6	2.48	0.48
4:D:24:GLU:HG2	4:D:25:ARG:H	1.78	0.48
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.76	0.48
1:A:1243:C:H2'	1:A:1244:C:H6	1.78	0.48
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.78	0.48
11:K:91:ARG:HH11	18:R:88:LYS:NZ	2.11	0.48
1:A:413:G:H2'	1:A:428:G:N2	2.29	0.48
10:J:28:ARG:HG2	10:J:34:VAL:HG11	1.95	0.48
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.47	0.48
1:A:767:A:H2'	1:A:768:A:O4'	2.12	0.48
1:A:950:U:H2'	1:A:951:G:C8	2.48	0.48
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.13	0.48
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.29	0.48
19:S:80:TYR:CE1	19:S:81:ARG:HB2	2.49	0.48
10:J:35:SER:HB2	10:J:73:ASP:O	2.14	0.48
20:T:56:MET:HE1	20:T:85:MET:HG2	1.96	0.48
1:A:1131:G:H8	1:A:1131:G:OP2	1.97	0.48
1:A:21:G:H2'	1:A:22:G:C8	2.49	0.48
1:A:374:A:C6	1:A:375:U:C4	3.01	0.48
1:A:421:U:H5'	1:A:422:C:C5	2.48	0.48
4:D:13:ARG:HD2	4:D:38:TYR:O	2.13	0.48
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.95	0.48
1:A:1359:C:O2'	1:A:1361:G:N7	2.47	0.48
1:A:737:A:H2'	1:A:738:C:C6	2.48	0.48
3:C:120:VAL:O	3:C:124:ILE:HG12	2.14	0.48
3:C:156:ARG:NE	3:C:160:ALA:O	2.46	0.48
3:C:22:TRP:HB3	3:C:59:ARG:HB2	1.96	0.48
10:J:28:ARG:HD3	10:J:34:VAL:HG21	1.95	0.48
1:A:986:A:H1'	19:S:54:GLY:O	2.14	0.48
1:A:912:C:O2'	1:A:913:A:H5'	2.13	0.48
1:A:96:G:H2'	1:A:97:G:C8	2.49	0.48
2:B:21:ARG:HA	2:B:39:ILE:HA	1.96	0.48
11:K:54:ARG:NH1	11:K:54:ARG:HB3	2.29	0.48
1:A:266:G:O3'	17:Q:67:LYS:HB2	2.14	0.48
1:A:1198:G:H2'	1:A:1199:U:C6	2.49	0.48
1:A:1286:A:C8	1:A:1287:A:H4'	2.49	0.48
1:A:1285:A:H4'	1:A:1286:A:O5'	2.13	0.48
1:A:992:U:H3	1:A:1044:A:H62	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.96	0.48
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.48	0.47
4:D:98:GLU:HG2	4:D:189:PRO:HG3	1.96	0.47
1:A:1053:G:C3'	1:A:1054:C:H5'	2.44	0.47
1:A:1413:A:H2	1:A:1487:G:H22	1.62	0.47
1:A:359:U:H2'	1:A:360:A:H8	1.80	0.47
1:A:1032:G:N1	1:A:1033:G:N3	2.62	0.47
1:A:1372:U:H2'	1:A:1373:G:O4'	2.14	0.47
1:A:1427:U:H2'	1:A:1428:A:H8	1.78	0.47
1:A:1539:C:H3'	1:A:1540:PSU:H5'	1.96	0.47
1:A:1542:U:H2'	1:A:1543:C:C6	2.49	0.47
1:A:280:C:O2	17:Q:38:ARG:HG3	2.13	0.47
4:D:173:TRP:HB2	4:D:187:ARG:O	2.14	0.47
6:F:35:ALA:HA	6:F:67:MET:HB3	1.95	0.47
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.96	0.47
1:A:1064:G:H1'	1:A:1190:G:N2	2.29	0.47
1:A:1519:MA6:H8	1:A:1519:MA6:O5'	2.14	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.80	0.47
2:B:21:ARG:NE	2:B:21:ARG:H	2.12	0.47
8:H:126:LYS:HA	8:H:126:LYS:HD2	1.73	0.47
1:A:1064:G:H4'	1:A:1065:U:OP1	2.14	0.47
1:A:1497:G:C2'	1:A:1498:UR3:H5'	2.45	0.47
1:A:382:A:H2'	1:A:383:A:C8	2.50	0.47
1:A:581:G:N2	1:A:760:G:N7	2.62	0.47
3:C:155:GLY:HA2	3:C:164:ARG:O	2.15	0.47
9:I:48:GLU:HG3	9:I:101:PHE:HZ	1.79	0.47
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.96	0.47
2:B:24:TRP:HA	2:B:190:THR:HG22	1.96	0.47
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.96	0.47
1:A:1442:G:N7	1:A:1446:A:N6	2.62	0.47
2:B:96:ARG:CZ	2:B:97:TRP:H	2.28	0.47
5:E:15:ARG:HD3	5:E:26:PHE:CD2	2.50	0.47
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.97	0.47
19:S:22:LEU:HB3	19:S:27:GLU:O	2.15	0.47
1:A:457:C:H2'	1:A:458:C:C6	2.50	0.47
1:A:691:G:H2'	1:A:692:U:C6	2.49	0.47
3:C:139:GLN:HG2	3:C:170:GLN:HE22	1.79	0.47
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.50	0.47
13:M:70:LEU:O	13:M:74:VAL:HG23	2.13	0.47
1:A:943:U:H1'	9:I:124:GLN:HE22	1.79	0.47
2:B:80:ILE:H	2:B:80:ILE:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1442:G:C5	1:A:1446:A:N6	2.83	0.47
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.46	0.47
4:D:36:ARG:HB2	4:D:38:TYR:CE2	2.49	0.47
11:K:57:THR:HG22	11:K:60:ALA:H	1.80	0.47
20:T:18:GLN:O	20:T:22:ARG:HG3	2.15	0.47
1:A:1028:C:N3	1:A:1034:G:N2	2.64	0.46
1:A:117:G:O5'	1:A:117:G:H8	1.97	0.46
1:A:184:G:H2'	1:A:185:A:C8	2.51	0.46
1:A:51:A:H4'	1:A:52:G:O5'	2.14	0.46
1:A:838:G:N2	1:A:849:C:C2	2.83	0.46
1:A:279:A:C4	17:Q:98:LEU:HD13	2.50	0.46
1:A:540:G:H2'	1:A:541:G:O4'	2.14	0.46
1:A:765:G:H5''	1:A:766:A:OP1	2.15	0.46
1:A:1009:G:H1	1:A:1020:U:H3	1.62	0.46
1:A:679:C:H2'	1:A:680:C:H6	1.81	0.46
3:C:124:ILE:HD12	3:C:130:VAL:HG22	1.97	0.46
11:K:124:LYS:HE3	11:K:124:LYS:HB2	1.72	0.46
18:R:22:VAL:HG23	18:R:55:ARG:O	2.15	0.46
18:R:85:LEU:HD12	18:R:86:VAL:H	1.81	0.46
18:R:88:LYS:HB3	18:R:88:LYS:HE3	1.72	0.46
1:A:353:A:H5'	1:A:353:A:C8	2.50	0.46
1:A:410:G:H2'	1:A:429:U:C4	2.51	0.46
11:K:115:PRO:C	11:K:117:ASN:H	2.19	0.46
20:T:89:ARG:O	20:T:93:GLU:HG2	2.16	0.46
1:A:679:C:H2'	1:A:680:C:C6	2.51	0.46
1:A:860:A:H2'	1:A:861:G:O4'	2.14	0.46
3:C:50:ALA:HB2	3:C:75:VAL:HG23	1.98	0.46
3:C:86:VAL:HG23	3:C:87:LEU:HD23	1.97	0.46
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.74	0.46
8:H:92:ARG:HH11	8:H:92:ARG:HG2	1.81	0.46
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.96	0.46
1:A:826:C:H2'	1:A:827:U:H6	1.81	0.46
1:A:967:5MC:O2'	9:I:128:ARG:NH1	2.49	0.46
2:B:189:ASP:HB3	2:B:203:GLY:O	2.16	0.46
2:B:200:ILE:H	2:B:200:ILE:HD12	1.81	0.46
9:I:48:GLU:N	9:I:49:PRO:HD2	2.30	0.46
9:I:17:VAL:HG13	9:I:63:ILE:HG12	1.97	0.46
13:M:12:ASN:H	13:M:45:VAL:CG1	2.27	0.46
20:T:67:ALA:HA	20:T:73:HIS:N	2.22	0.46
1:A:1281:U:H3'	1:A:1282:C:H6	1.79	0.46
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:23:ARG:HD3	14:N:28:GLY:O	2.16	0.46
18:R:71:LYS:O	18:R:75:ILE:HG13	2.16	0.46
1:A:1201:A:H4'	1:A:1202:G:O5'	2.15	0.46
1:A:1231:G:H4'	9:I:126:SER:HB2	1.97	0.46
1:A:976:G:OP2	1:A:1358:U:O2'	2.31	0.46
8:H:118:VAL:O	8:H:119:LEU:HD23	2.15	0.46
9:I:16:ARG:HG3	9:I:64:THR:HB	1.98	0.46
11:K:126:ARG:O	11:K:127:LYS:HB2	2.16	0.46
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.15	0.46
17:Q:5:VAL:O	17:Q:6:LEU:HD23	2.16	0.46
2:B:100:GLY:HA2	2:B:103:THR:HG22	1.98	0.46
2:B:74:LYS:NZ	2:B:205:ASP:OD2	2.48	0.46
6:F:19:LEU:HD11	6:F:59:TYR:CZ	2.50	0.46
1:A:118:U:H3'	1:A:288:A:H61	1.80	0.46
1:A:184:G:H2'	1:A:185:A:H8	1.81	0.46
1:A:738:C:OP1	6:F:92:LYS:HD3	2.16	0.46
2:B:73:THR:N	2:B:170:GLU:OE1	2.47	0.46
15:O:74:ASP:OD2	15:O:77:ARG:HG3	2.16	0.46
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.98	0.46
1:A:1518:MA6:N6	1:A:1519:MA6:H103	2.31	0.45
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.44	0.45
20:T:74:LYS:CG	20:T:75:ASN:N	2.78	0.45
1:A:486:U:H2'	1:A:487:A:C8	2.52	0.45
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.97	0.45
8:H:20:TYR:HA	8:H:65:TYR:CZ	2.51	0.45
1:A:1004:A:H3'	1:A:1025:U:H5	1.81	0.45
1:A:1347:G:N2	1:A:1373:G:H2'	2.30	0.45
1:A:413:G:H2'	1:A:428:G:H21	1.82	0.45
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.45
3:C:202:ILE:HG22	3:C:204:LEU:HD23	1.97	0.45
5:E:65:ASN:CG	5:E:65:ASN:O	2.55	0.45
1:A:1281:U:H3'	1:A:1282:C:C6	2.51	0.45
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.52	0.45
1:A:758:G:N7	25:A:2596:HOH:O	2.48	0.45
5:E:140:ARG:O	5:E:143:ARG:NH2	2.49	0.45
11:K:57:THR:HG23	11:K:59:TYR:H	1.81	0.45
20:T:63:ILE:HG22	20:T:77:ALA:HB1	1.99	0.45
1:A:1374:A:OP1	7:G:36:LYS:NZ	2.48	0.45
1:A:838:G:H1	1:A:848:C:H42	1.64	0.45
4:D:187:ARG:HH21	4:D:188:LEU:HD12	1.81	0.45
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:HG3	9:I:101:PHE:CZ	2.51	0.45
7:G:104:LEU:HA	7:G:104:LEU:HD12	1.61	0.45
10:J:21:GLN:O	10:J:25:GLU:HG3	2.17	0.45
14:N:32:SER:CB	14:N:41:ARG:H	2.28	0.45
1:A:1426:C:H2'	1:A:1427:U:C6	2.52	0.45
1:A:556:C:H2'	1:A:557:G:O4'	2.17	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.16	0.45
2:B:139:LYS:O	2:B:143:GLU:HG3	2.17	0.45
2:B:146:GLN:O	2:B:150:SER:HB3	2.17	0.45
2:B:17:PHE:CD1	2:B:18:GLY:N	2.83	0.45
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.97	0.45
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.31	0.45
19:S:16:LEU:O	19:S:20:LEU:HG	2.17	0.45
20:T:56:MET:HG2	20:T:84:LEU:HD13	1.98	0.45
1:A:1339:A:H2'	1:A:1340:A:O4'	2.17	0.45
1:A:1392:G:N2	1:A:1502:A:C8	2.82	0.45
6:F:30:LEU:HD23	6:F:75:LEU:HD21	1.99	0.45
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.98	0.45
10:J:49:VAL:HG21	14:N:44:LEU:HD23	1.98	0.45
10:J:51:ARG:HB2	10:J:59:SER:HB2	1.97	0.45
18:R:26:LEU:HD13	18:R:26:LEU:HA	1.67	0.45
1:A:1128:C:H1'	1:A:1130:A:N7	2.32	0.45
1:A:1465:C:H2'	1:A:1466:C:O4'	2.17	0.45
1:A:668:G:O2'	15:O:46:HIS:HD2	2.00	0.45
3:C:130:VAL:HG11	3:C:157:ILE:HD13	1.99	0.45
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.99	0.45
1:A:1218:C:H2'	1:A:1219:U:C6	2.52	0.45
1:A:1425:U:H3	1:A:1475:G:H1	1.63	0.45
2:B:97:TRP:CZ2	2:B:102:LEU:HD22	2.52	0.45
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.98	0.45
2:B:9:GLU:HG2	2:B:217:ARG:NH1	2.32	0.45
3:C:121:ALA:HA	3:C:124:ILE:HG12	1.98	0.45
1:A:247:G:OP2	17:Q:99:SER:HB2	2.17	0.45
19:S:53:ASN:ND2	19:S:76:PRO:O	2.50	0.45
1:A:1141:C:H2'	1:A:1142:G:C8	2.44	0.44
1:A:181:G:H4'	1:A:182:U:H5'	2.00	0.44
1:A:6:G:O2'	1:A:7:G:H5'	2.17	0.44
5:E:5:ASP:CG	5:E:6:PHE:H	2.21	0.44
13:M:4:ILE:HB	13:M:22:ILE:HD11	2.00	0.44
16:P:39:TYR:CE2	16:P:41:PRO:HG3	2.52	0.44
1:A:107:G:H2'	1:A:108:G:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:G:C2	1:A:1134:G:C8	3.05	0.44
1:A:377:G:OP1	16:P:3:LYS:NZ	2.42	0.44
1:A:609:A:N6	25:A:2012:HOH:O	2.10	0.44
4:D:187:ARG:HE	4:D:188:LEU:H	1.66	0.44
13:M:49:THR:OG1	13:M:50:GLU:N	2.50	0.44
1:A:1426:C:H2'	1:A:1427:U:H6	1.83	0.44
12:L:59:ARG:HA	12:L:65:GLU:HG3	1.99	0.44
1:A:103:C:P	20:T:17:ARG:HH12	2.41	0.44
1:A:1499:A:H1'	1:A:1520:G:H5'	2.00	0.44
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.52	0.44
2:B:217:ARG:O	2:B:220:ASP:HB2	2.18	0.44
3:C:6:HIS:HD2	3:C:8:ILE:H	1.65	0.44
1:A:1007:C:H2'	1:A:1008:C:C6	2.53	0.44
1:A:1202:G:O2'	14:N:29:ARG:HB3	2.17	0.44
1:A:701:C:H5''	1:A:703:G:H5'	1.98	0.44
10:J:47:PHE:HB2	10:J:63:PHE:HB2	1.99	0.44
14:N:11:LYS:HD3	14:N:13:THR:O	2.18	0.44
20:T:67:ALA:O	20:T:73:HIS:ND1	2.49	0.44
1:A:1001:A:H2'	1:A:1002:G:H8	1.82	0.44
10:J:78:ASN:O	10:J:82:ILE:HG13	2.17	0.44
11:K:48:ILE:O	11:K:48:ILE:HD12	2.17	0.44
1:A:1262:C:H2'	1:A:1263:C:H6	1.81	0.44
1:A:1361:G:H5''	1:A:1361(A):C:OP2	2.17	0.44
1:A:289:G:P	25:A:1903:HOH:O	2.76	0.44
3:C:83:ARG:HA	3:C:86:VAL:HG22	2.00	0.44
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.00	0.44
18:R:37:VAL:O	18:R:41:LYS:HG3	2.18	0.44
19:S:58:VAL:HA	19:S:59:PRO:HD3	1.83	0.44
1:A:1493:A:OP1	1:A:1493:A:H4'	2.16	0.44
1:A:149:A:H2'	1:A:150:C:C6	2.53	0.44
1:A:78:G:N2	1:A:92:C:C2	2.86	0.44
2:B:164:VAL:HG11	2:B:167:PRO:HA	2.00	0.44
5:E:102:ALA:O	5:E:107:ARG:NH1	2.50	0.44
9:I:89:ASN:HA	9:I:90:PRO:HD2	1.91	0.44
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.66	0.44
1:A:1003(A):G:C6	1:A:1004:A:H8	2.36	0.44
1:A:1307:U:H2'	1:A:1308:U:C6	2.53	0.44
1:A:216:G:H2'	1:A:217:C:H6	1.83	0.44
1:A:251:G:H4'	1:A:252:U:O5'	2.16	0.44
2:B:23:ARG:HD3	2:B:23:ARG:H	1.83	0.44
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:114:LYS:HE2	12:L:125:PRO:HG2	1.99	0.44
19:S:71:LEU:HD23	19:S:71:LEU:HA	1.83	0.44
1:A:203:U:O2'	1:A:204:U:N3	2.49	0.43
2:B:116:GLU:HG2	2:B:153:ARG:HH12	1.83	0.43
1:A:1125:U:H3	10:J:5:ARG:NH2	2.15	0.43
1:A:279:A:H5''	1:A:280:C:H3'	1.99	0.43
1:A:384:G:H2'	1:A:385:C:H6	1.83	0.43
8:H:38:ILE:HD13	8:H:41:ARG:NH2	2.33	0.43
10:J:46:ARG:HD3	14:N:61:TRP:CH2	2.53	0.43
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.53	0.43
1:A:1152:A:H4'	10:J:13:HIS:CD2	2.53	0.43
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.43
1:A:1425:U:H2'	1:A:1426:C:H6	1.83	0.43
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.99	0.43
12:L:41:ARG:HG2	12:L:42:THR:N	2.33	0.43
1:A:537:G:OP1	12:L:113:ARG:NH2	2.51	0.43
1:A:623:C:H2'	1:A:624:C:O4'	2.19	0.43
1:A:1226:C:H2'	13:M:103:THR:OG1	2.18	0.43
17:Q:40:LYS:HD3	17:Q:42:TYR:CE1	2.52	0.43
11:K:91:ARG:HD2	18:R:88:LYS:NZ	2.33	0.43
1:A:1030(B):C:H2'	1:A:1030(C):G:O4'	2.19	0.43
1:A:1393:U:O4'	1:A:1502:A:H5'	2.19	0.43
1:A:321:A:N6	1:A:329:A:OP2	2.42	0.43
4:D:53:ASP:OD1	4:D:53:ASP:N	2.51	0.43
1:A:1341:U:H4'	9:I:127:LYS:HE3	2.01	0.43
10:J:16:LEU:HD23	10:J:16:LEU:HA	1.77	0.43
10:J:27:ALA:HA	10:J:81:THR:HG23	2.00	0.43
17:Q:66:SER:H	17:Q:69:LYS:HB2	1.84	0.43
1:A:1004:A:O2'	1:A:1005:A:OP1	2.30	0.43
1:A:115:G:H1'	1:A:116:A:N7	2.34	0.43
1:A:372:C:H4'	1:A:373:A:O5'	2.18	0.43
1:A:833:U:H2'	1:A:834:C:C6	2.54	0.43
1:A:972:C:OP1	10:J:57:LYS:NZ	2.24	0.43
4:D:23:GLY:HA3	4:D:112:VAL:CG1	2.49	0.43
1:A:620:C:N1	4:D:135:LEU:HD13	2.33	0.43
8:H:100:ILE:HA	8:H:101:PRO:HD2	1.83	0.43
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.49	0.43
17:Q:67:LYS:O	17:Q:68:ARG:HG2	2.19	0.43
1:A:1126:U:O4	1:A:1127:G:N2	2.51	0.43
1:A:1213:A:N1	1:A:1215:G:H1'	2.33	0.43
1:A:73:C:H2'	1:A:74:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ARG:HA	2:B:130:ARG:HD2	1.73	0.43
2:B:24:TRP:HB3	2:B:40:HIS:CE1	2.53	0.43
4:D:152:SER:O	4:D:155:LEU:HG	2.18	0.43
5:E:11:ILE:HG21	5:E:105:VAL:HG22	1.99	0.43
6:F:80:ARG:NH1	6:F:88:VAL:O	2.52	0.43
1:A:1048:G:H2'	1:A:1050:G:C8	2.53	0.43
1:A:1048:G:H2'	1:A:1050:G:H8	1.83	0.43
1:A:1474:G:H2'	1:A:1475:G:C8	2.52	0.43
1:A:748:C:H4'	1:A:749:C:O5'	2.18	0.43
1:A:826:C:H2'	1:A:827:U:C6	2.54	0.43
1:A:947:G:O3'	13:M:109:THR:OG1	2.36	0.43
3:C:23:TYR:HE1	10:J:67:THR:HG23	1.83	0.43
11:K:77:MET:HB3	11:K:77:MET:HE3	1.98	0.43
14:N:30:ALA:HB1	14:N:33:VAL:CG2	2.47	0.43
1:A:974:A:P	14:N:41:ARG:HH12	2.41	0.43
19:S:15:LEU:O	19:S:19:VAL:HG12	2.19	0.43
1:A:1137:C:HO2'	1:A:1138:G:N2	2.16	0.43
1:A:484:G:H5'	1:A:486:U:O4'	2.19	0.43
1:A:501:C:H2'	1:A:502:G:H8	1.82	0.43
7:G:26:PHE:HA	7:G:101:LEU:HD13	2.00	0.43
8:H:86:ILE:HG21	8:H:133:LEU:HD13	2.00	0.43
15:O:62:GLN:HA	15:O:65:ARG:HH11	1.83	0.43
20:T:17:ARG:HA	20:T:20:LEU:HD12	1.99	0.43
21:U:14:TRP:CE3	21:U:15:ARG:HG3	2.54	0.43
1:A:642:A:C8	8:H:115:SER:HA	2.54	0.43
4:D:116:GLN:NE2	4:D:157:LEU:HD11	2.34	0.43
6:F:22:GLU:OE2	6:F:82:ARG:NH2	2.52	0.43
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.81	0.43
20:T:75:ASN:OD1	20:T:75:ASN:N	2.52	0.43
1:A:1310:G:OP2	13:M:88:ARG:NH2	2.48	0.42
1:A:567:G:H2'	1:A:568:G:O4'	2.19	0.42
2:B:91:PRO:HB3	2:B:154:LEU:HB2	2.00	0.42
1:A:691:G:H3'	11:K:26:ASN:HD21	1.84	0.42
12:L:31:PRO:HB2	12:L:32:PHE:CD2	2.54	0.42
1:A:1009:G:H2'	1:A:1010:G:H8	1.84	0.42
1:A:1137:C:H4'	1:A:1138:G:C4	2.54	0.42
1:A:1443:G:C4'	1:A:1446:A:H5''	2.46	0.42
1:A:279:A:OP1	1:A:280:C:O2'	2.23	0.42
1:A:791:G:H2'	1:A:792:A:C8	2.54	0.42
1:A:90:U:H2'	1:A:91:C:C6	2.54	0.42
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:C:H3'	1:A:1064:G:H2'	2.02	0.42
1:A:107:G:C2'	1:A:108:G:H5'	2.49	0.42
1:A:1286:A:H2'	1:A:1287:A:H4'	2.02	0.42
1:A:1453:G:H2'	1:A:1454:G:O4'	2.19	0.42
1:A:518:C:OP2	1:A:530:G:H1'	2.19	0.42
1:A:857:C:H5''	25:A:2515:HOH:O	2.18	0.42
4:D:71:SER:O	4:D:75:PHE:HB2	2.19	0.42
1:A:421:U:H4'	1:A:422:C:OP2	2.19	0.42
1:A:923:A:OP1	5:E:21:ALA:HB2	2.20	0.42
9:I:36:TYR:CZ	9:I:70:LYS:HE2	2.55	0.42
1:A:33:A:H2'	1:A:34:C:C6	2.54	0.42
1:A:427:U:H3'	1:A:428:G:H2'	2.01	0.42
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.23	0.42
14:N:22:THR:CB	14:N:33:VAL:HG21	2.49	0.42
20:T:51:GLU:HA	20:T:54:LYS:HB3	2.02	0.42
1:A:1006:C:OP1	1:A:1037:C:O2'	2.36	0.42
1:A:1121:U:H2'	1:A:1122:U:C6	2.54	0.42
1:A:1182:G:H8	1:A:1182:G:H2'	1.72	0.42
1:A:877:C:H5''	8:H:88:LYS:HD3	2.00	0.42
2:B:74:LYS:HD2	2:B:166:ASP:HB2	2.02	0.42
6:F:75:LEU:O	6:F:79:LEU:HG	2.19	0.42
9:I:19:LEU:HD12	9:I:84:ALA:HB3	2.01	0.42
1:A:1014:A:C2	1:A:1219:U:H1'	2.55	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
1:A:78:G:C2	1:A:92:C:C2	3.08	0.42
3:C:7:PRO:HA	3:C:11:ARG:HH21	1.84	0.42
4:D:4:TYR:CE2	4:D:11:LEU:HD11	2.55	0.42
6:F:95:GLU:HG3	6:F:96:PRO:HD2	2.01	0.42
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.19	0.42
1:A:1266:G:N2	1:A:1269:A:OP2	2.36	0.42
1:A:1284:C:OP2	1:A:1285:A:O2'	2.28	0.42
1:A:1492:A:H2'	1:A:1492:A:N3	2.34	0.42
1:A:186:C:H2'	1:A:187:C:C6	2.55	0.42
1:A:243:A:C2	1:A:246:A:C8	3.07	0.42
1:A:299:G:O5'	1:A:299:G:H8	2.03	0.42
4:D:104:VAL:HG11	4:D:146:ILE:HG13	2.02	0.42
8:H:119:LEU:HB3	8:H:123:GLU:HB2	2.01	0.42
1:A:1223:C:OP1	19:S:78:ARG:NH1	2.52	0.42
2:B:21:ARG:HB2	2:B:22:LYS:H	1.66	0.42
7:G:113:GLU:HG2	7:G:113:GLU:H	1.57	0.42
13:M:91:ARG:HD2	13:M:91:ARG:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:976:G:OP1	14:N:31:ARG:O	2.38	0.42
15:O:85:LEU:HA	15:O:85:LEU:HD23	1.73	0.42
1:A:130:A:H5'	17:Q:63:ARG:HE	1.85	0.42
1:A:1493:A:H2'	1:A:1494:G:C8	2.54	0.42
1:A:51:A:H4'	1:A:52:G:C5'	2.50	0.42
2:B:59:GLU:HB2	2:B:221:LEU:HD11	2.01	0.42
10:J:88:LEU:O	10:J:89:ASP:HB2	2.19	0.42
17:Q:52:LYS:HA	17:Q:52:LYS:HD3	1.77	0.42
18:R:36:ASN:O	18:R:40:LEU:HG	2.20	0.42
1:A:1337:G:H5''	1:A:1338:G:OP1	2.20	0.41
1:A:84:U:H2'	1:A:88:A:O4'	2.20	0.41
8:H:1:MET:HG2	8:H:2:LEU:N	2.30	0.41
13:M:78:ILE:O	13:M:81:LEU:HD23	2.21	0.41
14:N:8:GLU:O	14:N:11:LYS:HB3	2.19	0.41
1:A:976:G:H5'	1:A:1358:U:O2'	2.20	0.41
1:A:236:G:H2'	1:A:237:C:O4'	2.20	0.41
1:A:653:A:O5'	8:H:56:LYS:NZ	2.53	0.41
2:B:102:LEU:HD12	2:B:102:LEU:HA	1.79	0.41
2:B:45:GLN:O	2:B:48:MET:HB2	2.20	0.41
4:D:13:ARG:NH2	4:D:36:ARG:NH2	2.69	0.41
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.55	0.41
8:H:89:PRO:HA	8:H:92:ARG:NH1	2.35	0.41
11:K:121:PRO:HB2	11:K:125:PHE:HB2	2.03	0.41
12:L:60:LEU:HA	12:L:60:LEU:HD12	1.75	0.41
1:A:750:G:N3	15:O:23:GLY:HA3	2.35	0.41
1:A:1017:G:H2'	1:A:1018:C:C6	2.56	0.41
1:A:1064:G:H21	1:A:1190:G:H1'	1.85	0.41
1:A:1091:U:O2	1:A:1093:A:C8	2.72	0.41
1:A:115:G:H5''	25:A:2550:HOH:O	2.20	0.41
1:A:1163:C:N4	1:A:1173:G:H1	2.08	0.41
1:A:1275:A:H2'	1:A:1276:G:O4'	2.19	0.41
1:A:1389:C:H2'	1:A:1390:U:O4'	2.20	0.41
1:A:547:A:H4'	1:A:548:G:O5'	2.20	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
7:G:121:ALA:O	7:G:125:MET:HG3	2.20	0.41
7:G:129:GLU:HG2	7:G:131:LYS:HG2	2.02	0.41
11:K:127:LYS:HD3	11:K:127:LYS:HA	1.87	0.41
14:N:33:VAL:H	14:N:33:VAL:HG22	1.58	0.41
16:P:9:PHE:HB2	16:P:16:HIS:O	2.21	0.41
1:A:579:G:H2'	1:A:580:U:C6	2.54	0.41
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:79:GLU:HB3	12:L:80:HIS:H	1.61	0.41
1:A:532:A:HO2'	1:A:533:A:P	2.42	0.41
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.56	0.41
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.77	0.41
11:K:48:ILE:HG13	11:K:48:ILE:H	1.54	0.41
1:A:254:G:OP1	17:Q:67:LYS:O	2.38	0.41
1:A:695:A:H2'	1:A:696:A:C8	2.56	0.41
1:A:762:C:H5'	17:Q:103:GLY:O	2.20	0.41
3:C:156:ARG:NH1	3:C:193:TYR:HB2	2.36	0.41
1:A:1326:C:OP2	21:U:6:ARG:NH1	2.54	0.41
1:A:1418:A:N6	1:A:1482:G:O2'	2.52	0.41
1:A:509:A:H3'	1:A:509:A:C8	2.56	0.41
1:A:761:G:H21	17:Q:104:LYS:HZ1	1.69	0.41
2:B:83:MET:HE1	2:B:238:LEU:HB2	2.01	0.41
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.03	0.41
4:D:3:ARG:HG2	4:D:3:ARG:H	1.60	0.41
6:F:45:LEU:H	6:F:45:LEU:HD22	1.86	0.41
1:A:1298:C:P	7:G:114:ARG:HH22	2.43	0.41
1:A:825:G:N2	8:H:11:THR:HG21	2.36	0.41
10:J:39:PRO:O	10:J:40:LEU:HB2	2.21	0.41
13:M:62:ASN:OD1	13:M:62:ASN:N	2.52	0.41
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.02	0.41
1:A:114:U:O2'	1:A:115:G:H5'	2.20	0.41
1:A:279:A:H5'	1:A:281:G:O4'	2.21	0.41
2:B:212:GLN:HG2	2:B:235:SER:OG	2.21	0.41
4:D:194:LEU:HB3	4:D:196:LEU:HG	2.03	0.41
7:G:38:LEU:O	7:G:42:ILE:HG13	2.20	0.41
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.54	0.41
13:M:88:ARG:HG3	13:M:98:VAL:CG1	2.51	0.41
17:Q:48:GLU:OE2	17:Q:50:LYS:HE3	2.21	0.41
20:T:62:LEU:HD23	20:T:62:LEU:HA	1.76	0.41
1:A:1143:G:O5'	1:A:1143:G:H8	2.04	0.41
1:A:836:G:C6	1:A:851:G:C5	3.08	0.41
3:C:134:ILE:HD11	3:C:153:VAL:HB	2.02	0.41
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.56	0.41
1:A:1245:A:C2	1:A:1293:G:C2	3.09	0.41
1:A:1236:A:O3'	1:A:1304:G:H5''	2.20	0.41
1:A:232:G:H1'	1:A:262:A:N1	2.36	0.41
1:A:390:C:H2'	1:A:391:G:C8	2.56	0.41
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.41
1:A:581:G:N7	25:A:2595:HOH:O	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:G:H2'	1:A:903:G:H8	1.86	0.41
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.21	0.41
11:K:57:THR:HG23	11:K:59:TYR:N	2.36	0.41
14:N:53:LEU:HA	14:N:54:PRO:HD2	1.95	0.41
21:U:6:ARG:HB3	21:U:15:ARG:NH1	2.35	0.41
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.41
1:A:1332:A:H2'	1:A:1333:A:C8	2.56	0.41
1:A:502:G:H2'	1:A:503:C:O4'	2.21	0.41
1:A:663:A:H2'	1:A:664:G:O4'	2.21	0.41
3:C:14:ILE:C	3:C:16:ARG:H	2.24	0.41
5:E:11:ILE:CG2	5:E:105:VAL:HG22	2.51	0.41
5:E:40:ARG:HB3	5:E:66:MET:CE	2.51	0.41
1:A:1343:G:OP1	9:I:125:TYR:HE2	2.04	0.41
18:R:47:THR:HB	18:R:49:LYS:HG3	2.03	0.41
1:A:984:C:H42	1:A:1221:G:H1	1.69	0.40
2:B:68:ILE:O	2:B:90:MET:HB3	2.21	0.40
3:C:101:LEU:HD12	3:C:101:LEU:HA	1.92	0.40
3:C:121:ALA:HB1	3:C:189:ALA:HB2	2.03	0.40
4:D:9:CYS:O	4:D:12:CYS:HB2	2.21	0.40
5:E:103:GLY:O	5:E:106:PRO:HD2	2.21	0.40
11:K:70:LYS:HA	11:K:73:MET:HE2	2.03	0.40
14:N:41:ARG:HG3	14:N:42:ILE:N	2.36	0.40
1:A:1053:G:H4'	1:A:1054:C:H5'	2.03	0.40
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.40
1:A:1399:C:C2	1:A:1401:G:C5	3.09	0.40
1:A:216:G:H2'	1:A:217:C:C6	2.56	0.40
2:B:16:HIS:O	2:B:17:PHE:CG	2.75	0.40
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.02	0.40
2:B:20:GLU:H	2:B:20:GLU:HG2	1.54	0.40
4:D:78:LEU:CD2	4:D:96:LEU:HB3	2.51	0.40
11:K:59:TYR:CZ	11:K:63:LEU:HD11	2.57	0.40
16:P:7:ALA:O	16:P:17:TYR:HA	2.21	0.40
20:T:14:LYS:O	20:T:18:GLN:HG3	2.21	0.40
1:A:273:A:H1'	17:Q:16:GLN:HE22	1.87	0.40
5:E:137:GLU:O	5:E:141:GLN:HG3	2.21	0.40
5:E:44:GLY:N	5:E:62:ALA:HB2	2.36	0.40
10:J:87:THR:O	10:J:88:LEU:HB2	2.22	0.40
10:J:8:LEU:HD22	10:J:96:ILE:HG22	2.02	0.40
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	2.03	0.40
1:A:99:C:H2'	1:A:101:A:C8	2.57	0.40
1:A:1077:G:N2	1:A:1080:A:OP2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:G:HO2'	1:A:1125:U:P	2.45	0.40
2:B:28:PHE:CZ	2:B:189:ASP:HA	2.56	0.40
4:D:173:TRP:CE2	4:D:189:PRO:HB3	2.57	0.40
4:D:31:CYS:SG	4:D:31:CYS:O	2.79	0.40
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.85	0.40
7:G:145:ALA:C	7:G:147:ALA:H	2.25	0.40
11:K:30:VAL:HG21	11:K:65:ALA:HA	2.02	0.40
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.57	0.40
19:S:31:ILE:HB	19:S:49:ILE:HD13	2.03	0.40
20:T:71:THR:O	20:T:72:LEU:HD23	2.21	0.40
1:A:520:A:N1	1:A:536:C:H1'	2.36	0.40
1:A:794:A:H3'	1:A:794:A:C8	2.56	0.40
2:B:144:ARG:HG3	2:B:145:LEU:N	2.37	0.40
2:B:92:TYR:CE1	2:B:94:ASN:HB2	2.56	0.40
5:E:152:ARG:HB3	8:H:43:GLY:HA3	2.03	0.40
11:K:73:MET:HB2	11:K:73:MET:HE2	1.88	0.40
13:M:11:ARG:HG3	13:M:12:ASN:HB2	2.03	0.40
14:N:12:ARG:O	14:N:14:PRO:HD3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	207 (89%)	22 (10%)	3 (1%)	12	41
3	C	204/239 (85%)	183 (90%)	16 (8%)	5 (2%)	5	25
4	D	206/209 (99%)	194 (94%)	9 (4%)	3 (2%)	10	37
5	E	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	142 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	115 (92%)	10 (8%)	0	100	100
10	J	96/105 (91%)	77 (80%)	16 (17%)	3 (3%)	4	21
11	K	117/129 (91%)	108 (92%)	9 (8%)	0	100	100
12	L	121/135 (90%)	110 (91%)	11 (9%)	0	100	100
13	M	115/126 (91%)	105 (91%)	10 (9%)	0	100	100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	86/89 (97%)	76 (88%)	10 (12%)	0	100	100
16	P	81/88 (92%)	79 (98%)	2 (2%)	0	100	100
17	Q	102/105 (97%)	97 (95%)	5 (5%)	0	100	100
18	R	71/88 (81%)	67 (94%)	4 (6%)	0	100	100
19	S	78/93 (84%)	69 (88%)	9 (12%)	0	100	100
20	T	97/106 (92%)	83 (86%)	12 (12%)	2 (2%)	7	28
21	U	22/27 (82%)	22 (100%)	0	0	100	100
All	All	2347/2541 (92%)	2158 (92%)	173 (7%)	16 (1%)	22	56

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
10	J	40	LEU
3	C	168	ALA
4	D	26	CYS
3	C	169	ALA
10	J	39	PRO
2	B	24	TRP
4	D	25	ARG
20	T	73	HIS
3	C	154	SER
20	T	74	LYS
3	C	15	THR
2	B	130	ARG
4	D	5	ILE
10	J	34	VAL
3	C	66	VAL



### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	171 (85%)	31 (15%)	2	11
3	C	160/188 (85%)	136 (85%)	24 (15%)	3	12
4	D	180/181 (99%)	163 (91%)	17 (9%)	8	30
5	E	115/123 (94%)	100 (87%)	15 (13%)	4	17
6	F	90/90 (100%)	87 (97%)	3 (3%)	38	68
7	G	126/127 (99%)	113 (90%)	13 (10%)	7	25
8	H	119/119 (100%)	105 (88%)	14 (12%)	5	20
9	I	98/99 (99%)	89 (91%)	9 (9%)	9	31
10	J	87/92 (95%)	79 (91%)	8 (9%)	9	31
11	K	90/99 (91%)	78 (87%)	12 (13%)	4	16
12	L	103/110 (94%)	82 (80%)	21 (20%)	1	5
13	M	94/101 (93%)	83 (88%)	11 (12%)	5	21
14	N	49/50 (98%)	43 (88%)	6 (12%)	5	19
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	9
16	P	72/74 (97%)	66 (92%)	6 (8%)	11	36
17	Q	96/97 (99%)	87 (91%)	9 (9%)	8	30
18	R	64/77 (83%)	60 (94%)	4 (6%)	18	46
19	S	71/80 (89%)	61 (86%)	10 (14%)	3	14
20	T	76/82 (93%)	62 (82%)	14 (18%)	1	7
21	U	19/22 (86%)	17 (90%)	2 (10%)	7	24
All	All	1990/2111 (94%)	1748 (88%)	242 (12%)	5	19

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	12	GLU
2	B	19	HIS
2	B	20	GLU

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Mol	Chain	Res	Type
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	39	ILE
2	B	61	LEU
2	B	82	ARG
2	B	96	ARG
2	B	97	TRP
2	B	102	LEU
2	B	121	LEU
2	B	127	ILE
2	B	128	GLU
2	B	130	ARG
2	B	144	ARG
2	B	153	ARG
2	B	156	LYS
2	B	178	ARG
2	B	187	LEU
2	B	196	LEU
2	B	200	ILE
2	B	204	ASN
2	B	205	ASP
2	B	213	LEU
2	B	221	LEU
2	B	226	ARG
2	B	229	VAL
2	B	236	TYR
2	B	238	LEU
3	C	5	ILE
3	C	14	ILE
3	C	15	THR
3	C	26	LYS
3	C	28	GLN
3	C	34	LEU
3	C	58	GLU
3	C	64	VAL
3	C	68	VAL
3	C	75	VAL
3	C	79	ARG
3	C	87	LEU
3	C	91	LEU
3	C	99	VAL

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Mol	Chain	Res	Type
3	C	105	GLU
3	C	107	GLN
3	C	131	ARG
3	C	156	ARG
3	C	166	GLU
3	C	178	LEU
3	C	188	LEU
3	C	196	LEU
3	C	199	LYS
3	C	204	LEU
4	D	3	ARG
4	D	8	VAL
4	D	10	ARG
4	D	36	ARG
4	D	53	ASP
4	D	64	LEU
4	D	78	LEU
4	D	91	SER
4	D	96	LEU
4	D	99	SER
4	D	112	VAL
4	D	122	ARG
4	D	135	LEU
4	D	157	LEU
4	D	184	LYS
4	D	187	ARG
4	D	194	LEU
5	E	12	LEU
5	E	13	ILE
5	E	31	LEU
5	E	43	LEU
5	E	53	LEU
5	E	65	ASN
5	E	66	MET
5	E	68	GLU
5	E	79	GLU
5	E	80	ILE
5	E	120	THR
5	E	125	SER
5	E	126	ARG
5	E	150	ARG
5	E	151	LEU

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Mol	Chain	Res	Type
6	F	10	LEU
6	F	70	ASP
6	F	95	GLU
7	G	13	GLN
7	G	15	ASP
7	G	24	THR
7	G	38	LEU
7	G	87	VAL
7	G	89	MET
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	115	ARG
7	G	122	HIS
7	G	137	LYS
7	G	155	ARG
8	H	11	THR
8	H	23	SER
8	H	26	VAL
8	H	37	ARG
8	H	39	LEU
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	91	ARG
8	H	92	ARG
8	H	99	GLU
8	H	105	ARG
8	H	127	LEU
8	H	133	LEU
9	I	29	ASN
9	I	44	VAL
9	I	66	ARG
9	I	79	LEU
9	I	86	VAL
9	I	91	ASP
9	I	104	ARG
9	I	111	ARG
9	I	121	ARG
10	J	4	ILE
10	J	5	ARG
10	J	8	LEU

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Mol	Chain	Res	Type
10	J	23	ILE
10	J	38	ILE
10	J	40	LEU
10	J	65	LEU
10	J	71	LEU
11	K	11	LYS
11	K	14	VAL
11	K	29	ILE
11	K	48	ILE
11	K	54	ARG
11	K	57	THR
11	K	77	MET
11	K	78	GLN
11	K	87	THR
11	K	98	LEU
11	K	99	GLN
11	K	114	VAL
12	L	18	VAL
12	L	20	LYS
12	L	23	LYS
12	L	33	ARG
12	L	44	THR
12	L	47	LYS
12	L	53	ARG
12	L	55	VAL
12	L	58	VAL
12	L	60	LEU
12	L	62	SER
12	L	65	GLU
12	L	79	GLU
12	L	81	SER
12	L	83	VAL
12	L	97	ARG
12	L	111	LYS
12	L	113	ARG
12	L	114	LYS
12	L	122	THR
12	L	126	LYS
13	M	3	ARG
13	M	9	ILE
13	M	27	LYS
13	M	32	GLU

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Mol	Chain	Res	Type
13	M	45	VAL
13	M	56	LEU
13	M	62	ASN
13	M	70	LEU
13	M	81	LEU
13	M	90	LEU
13	M	110	ARG
14	N	6	LEU
14	N	12	ARG
14	N	24	CYS
14	N	29	ARG
14	N	33	VAL
14	N	41	ARG
15	O	4	THR
15	O	5	LYS
15	O	13	GLN
15	O	31	LEU
15	O	34	LEU
15	O	39	LEU
15	O	45	VAL
15	O	57	LEU
15	O	60	VAL
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	81	LEU
16	P	1	MET
16	P	53	VAL
16	P	54	GLU
16	P	55	ARG
16	P	68	ASP
16	P	82	GLN
17	Q	4	LYS
17	Q	13	ASP
17	Q	34	LYS
17	Q	38	ARG
17	Q	59	ILE
17	Q	67	LYS
17	Q	86	GLU
17	Q	92	ARG
17	Q	101	ARG
18	R	19	LYS

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Mol	Chain	Res	Type
18	R	47	THR
18	R	84	LYS
18	R	88	LYS
19	S	7	LYS
19	S	9	VAL
19	S	12	ASP
19	S	15	LEU
19	S	25	LYS
19	S	29	ARG
19	S	30	LEU
19	S	36	ARG
19	S	65	ASN
19	S	78	ARG
20	T	9	ASN
20	T	11	SER
20	T	13	LEU
20	T	19	SER
20	T	24	LEU
20	T	35	THR
20	T	36	LEU
20	T	42	GLN
20	T	56	MET
20	T	57	ARG
20	T	72	LEU
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	U	6	ARG
21	U	8	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
2	B	212	GLN
3	C	69	HIS
3	C	104	GLN
3	C	162	GLN
3	C	170	GLN
6	F	73	ASN
15	O	46	HIS

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	280 (18%)	44 (2%)

All (280) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	43	C
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	52	G
1	A	68	G
1	A	81	U
1	A	82	U
1	A	91	C
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	180	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G

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Mol	Chain	Res	Type
1	A	220	G
1	A	231	G
1	A	244	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	289	G
1	A	319	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	331	G
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	430	A
1	A	452	A
1	A	460	A

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Mol	Chain	Res	Type
1	A	461	C
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	517	G
1	A	518	C
1	A	522	C
1	A	527	7MG
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	588	G
1	A	616	G
1	A	618	C
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	698	G
1	A	701	C
1	A	702	A
1	A	703	G
1	A	707	C
1	A	718	G
1	A	723	U

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Mol	Chain	Res	Type
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	766	A
1	A	774	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	788	U
1	A	789	U
1	A	792	A
1	A	793	U
1	A	794	A
1	A	795	C
1	A	799	G
1	A	812	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	819	A
1	A	827	U
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	876	G
1	A	902	G
1	A	913	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	960	U
1	A	966	M2G
1	A	969	A
1	A	974	A

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Mol	Chain	Res	Type
1	A	975	A
1	A	976	G
1	A	977	A
1	A	989	C
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1007	C
1	A	1008	C
1	A	1016	A
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1041	A
1	A	1042	G
1	A	1043	C
1	A	1045	C
1	A	1049	U
1	A	1050	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1138	G
1	A	1139	G
1	A	1157	A
1	A	1159	U
1	A	1164	G
1	A	1171	G
1	A	1173	G

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Mol	Chain	Res	Type
1	A	1182	G
1	A	1183	A
1	A	1187	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1207	2MG
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1288	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	1312	G
1	A	1319	A
1	A	1320	C
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1346	A

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Mol	Chain	Res	Type
1	A	1347	G
1	A	1353	G
1	A	1361	G
1	A	1362	C
1	A	1368	G
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1397	C
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1454	G
1	A	1487	G
1	A	1490	C
1	A	1492	A
1	A	1493	A
1	A	1498	UR3
1	A	1499	A
1	A	1500	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1508	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1540	PSU
1	A	1541	PSU

All (44) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	51	A
1	A	108	G
1	A	115	G

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Mol	Chain	Res	Type
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	328	C
1	A	353	A
1	A	372	C
1	A	413	G
1	A	428	G
1	A	429	U
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A
1	A	560	U
1	A	573	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	812	C
1	A	913	A
1	A	992	U
1	A	1004	A
1	A	1064	G
1	A	1065	U
1	A	1067	A
1	A	1181	G
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1224	G
1	A	1257	U
1	A	1285	A
1	A	1301	U
1	A	1346	A
1	A	1380	U
1	A	1503	A
1	A	1504	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	M2G	A	966	1	20,27,28	1.71	4 (20%)	22,40,43	2.34	4 (18%)
1	5MC	A	1407	1	15,22,23	0.91	1 (6%)	19,32,35	1.15	1 (5%)
1	2MG	A	1207	1	19,26,27	2.56	4 (21%)	21,38,41	2.06	2 (9%)
1	UR3	A	1498	1	14,22,23	0.75	0	15,32,35	1.39	3 (20%)
1	7MG	A	527	1	22,26,27	2.27	6 (27%)	28,39,42	1.78	7 (25%)
1	5MC	A	1400	1	15,22,23	0.75	0	19,32,35	1.37	3 (15%)
1	PSU	A	1541	1,23	17,21,22	1.05	1 (5%)	20,30,33	3.14	6 (30%)
1	5MC	A	967	1	15,22,23	0.99	1 (6%)	19,32,35	0.98	1 (5%)
1	MA6	A	1519	1	19,26,27	1.18	1 (5%)	18,38,41	0.68	0
12	0TD	L	92	12	4,9,10	1.04	0	3,11,13	2.99	1 (33%)
1	PSU	A	1540	1,23	17,21,22	0.94	1 (5%)	20,30,33	3.65	9 (45%)
1	PSU	A	516	1,23	17,21,22	1.27	3 (17%)	20,30,33	2.89	6 (30%)
1	5MC	A	1404	1	15,22,23	0.75	0	19,32,35	1.22	2 (10%)
1	MA6	A	1518	1	19,26,27	1.07	2 (10%)	18,38,41	0.74	0
1	4OC	A	1402	1	16,23,24	0.86	0	17,32,35	0.92	1 (5%)

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	M2G	A	966	1	-	6/7/29/30	0/3/3/3
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	1/5/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1400	1	-	1/5/25/26	0/2/2/2
1	PSU	A	1541	1,23	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
12	0TD	L	92	12	-	2/3/12/14	-
1	PSU	A	1540	1,23	-	2/7/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1518	1	-	5/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.89	1.40	1.34
1	A	1207	2MG	C6-N1	6.30	1.44	1.33
1	A	527	7MG	C4-N3	5.97	1.41	1.34
1	A	527	7MG	C2-N2	5.34	1.44	1.33
1	A	966	M2G	C6-N1	5.21	1.42	1.33
1	A	527	7MG	C8-N9	-4.63	1.34	1.45
1	A	516	PSU	C5-C1'	-3.54	1.49	1.52
1	A	1541	PSU	C4-N3	3.34	1.38	1.33
1	A	966	M2G	C4-N3	3.20	1.40	1.35
1	A	966	M2G	C2-N1	3.12	1.40	1.34
1	A	1519	MA6	C6-N1	3.06	1.37	1.33
1	A	527	7MG	C6-N1	2.95	1.38	1.33
1	A	1540	PSU	C4-N3	2.84	1.38	1.33
1	A	527	7MG	CM7-N7	-2.79	1.41	1.46
1	A	1207	2MG	C2-N1	2.71	1.43	1.34
1	A	1518	MA6	C6-N1	2.70	1.37	1.33
1	A	516	PSU	C4-N3	2.57	1.37	1.33
1	A	527	7MG	C6-C5	2.49	1.44	1.41
1	A	967	5MC	C2-N3	2.29	1.42	1.38
1	A	1407	5MC	C5-C4	2.26	1.44	1.41
1	A	1207	2MG	C4-N3	2.24	1.39	1.35
1	A	1518	MA6	C2-N3	2.17	1.35	1.32
1	A	516	PSU	O4'-C1'	-2.10	1.41	1.44
1	A	966	M2G	C2-N2	2.08	1.38	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N1-C2-N3	-10.27	120.26	128.43
1	A	1540	PSU	N1-C2-N3	-10.07	120.43	128.43
1	A	516	PSU	N1-C2-N3	-9.37	120.98	128.43
1	A	1207	2MG	C5-C6-N1	-7.93	112.59	123.43
1	A	966	M2G	C5-C6-N1	-7.87	112.66	123.43
1	A	1540	PSU	C5-C1'-C2'	-7.61	101.75	115.32
1	A	1541	PSU	C4-N3-C2	6.30	120.46	115.14
1	A	966	M2G	C6-N1-C2	5.64	122.90	116.18
1	A	1540	PSU	C4-N3-C2	5.20	119.53	115.14
1	A	527	7MG	N3-C4-N9	4.88	133.18	126.91
1	A	516	PSU	C4-N3-C2	4.71	119.12	115.14
1	A	1541	PSU	C5-C4-N3	-4.69	119.32	125.36
12	L	92	0TD	CSB-SB-CB	-4.54	92.93	101.85
1	A	516	PSU	C5-C4-N3	-4.52	119.54	125.36
1	A	516	PSU	C5-C6-N1	-4.19	119.28	124.44
1	A	527	7MG	C5-C4-N3	-4.04	119.90	126.49
1	A	1540	PSU	C5-C4-N3	-3.91	120.32	125.36
1	A	1540	PSU	O4'-C1'-C5	3.90	115.97	109.93
1	A	1207	2MG	C6-N1-C2	3.86	122.09	115.18
1	A	1400	5MC	CM5-C5-C4	-3.76	117.91	121.72
1	A	527	7MG	N7-C8-N9	3.63	108.57	103.38
1	A	1540	PSU	C5-C6-N1	-3.22	120.48	124.44
1	A	1540	PSU	C6-N1-C2	3.20	120.65	115.36
1	A	516	PSU	C6-N1-C2	2.97	120.26	115.36
1	A	1541	PSU	C5-C1'-C2'	-2.94	110.08	115.32
1	A	1540	PSU	C3'-C2'-C1'	-2.92	98.57	101.93
1	A	1404	5MC	CM5-C5-C4	-2.91	118.77	121.72
1	A	1400	5MC	CM5-C5-C6	2.76	124.50	118.68
1	A	527	7MG	C6-N1-C2	2.70	120.22	115.93
1	A	527	7MG	C6-C5-C4	2.67	118.07	115.20
1	A	966	M2G	C2-N3-C4	-2.63	112.29	115.28
1	A	1541	PSU	C6-N1-C2	2.57	119.60	115.36
1	A	1402	4OC	CM4-N4-C4	-2.55	120.78	122.97
1	A	1404	5MC	CM5-C5-C6	2.49	123.94	118.68
1	A	1498	UR3	C3'-C2'-C1'	2.31	104.46	100.98
1	A	1540	PSU	O2'-C2'-C1'	-2.29	106.50	111.94
1	A	1407	5MC	N4-C4-N3	-2.26	113.83	117.03
1	A	527	7MG	C2-N3-C4	2.25	120.12	113.89
1	A	966	M2G	N1-C2-N2	-2.24	114.92	117.19
1	A	1541	PSU	C5-C6-N1	-2.23	121.70	124.44
1	A	527	7MG	N1-C2-N3	-2.21	121.95	125.42
1	A	967	5MC	CM5-C5-C6	2.13	123.18	118.68
1	A	1498	UR3	O3'-C3'-C2'	2.12	118.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	PSU	O4'-C1'-C2'	2.12	108.09	104.66
1	A	1498	UR3	C3U-N3-C4	2.12	120.92	118.12
1	A	1400	5MC	C2-N3-C4	2.06	118.51	116.02

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1498	UR3	O4'-C1'-N1-C6
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
12	L	92	0TD	O-C-CA-CB
12	L	92	0TD	CG-CB-SB-CSB
1	A	1540	PSU	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518	MA6	N1-C6-N6-C9
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	1519	MA6	N1-C6-N6-C10
1	A	1541	PSU	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM2
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1541	PSU	O4'-C4'-C5'-O5'
1	A	1518	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 10 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 328 ligands modelled in this entry, 327 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	SRY	A	1601	-	40,42,42	2.30	11 (27%)	49,63,63	1.95	13 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SRY	A	1601	-	1/1/17/21	2/20/87/87	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.08	1.49	1.33
22	A	1601	SRY	CA1-N11	6.35	1.44	1.33
22	A	1601	SRY	O53-C53	-3.58	1.35	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRV	C21-C11	-2.99	1.47	1.53
22	A	1601	SRV	O32-C32	-2.44	1.40	1.44
22	A	1601	SRV	CD1-NE1	2.32	1.44	1.34
22	A	1601	SRV	O51-C51	-2.31	1.37	1.43
22	A	1601	SRV	CA1-NB1	2.30	1.44	1.34
22	A	1601	SRV	O43-C43	-2.28	1.37	1.43
22	A	1601	SRV	C23-N23	-2.27	1.43	1.47
22	A	1601	SRV	C21-C31	-2.19	1.49	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRV	C13-O13-C22	-5.24	107.15	116.25
22	A	1601	SRV	C12-O42-C42	-5.16	100.27	108.38
22	A	1601	SRV	C51-C61-C11	4.22	116.52	110.34
22	A	1601	SRV	C61-C11-N11	-3.81	103.43	110.62
22	A	1601	SRV	C61-C51-C41	3.77	118.29	109.68
22	A	1601	SRV	C21-C11-N11	-3.27	104.43	110.62
22	A	1601	SRV	C63-C53-C43	-2.77	106.51	113.00
22	A	1601	SRV	O13-C22-C32	2.52	117.63	111.75
22	A	1601	SRV	C12-O41-C41	-2.43	111.94	117.96
22	A	1601	SRV	CI3-N23-C23	-2.36	110.94	114.38
22	A	1601	SRV	C33-C43-C53	2.32	114.37	110.24
22	A	1601	SRV	O41-C41-C51	2.27	113.31	107.28
22	A	1601	SRV	O21-C21-C31	2.19	114.07	109.66

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	1601	SRV	C51

All (2) torsion outliers are listed below:

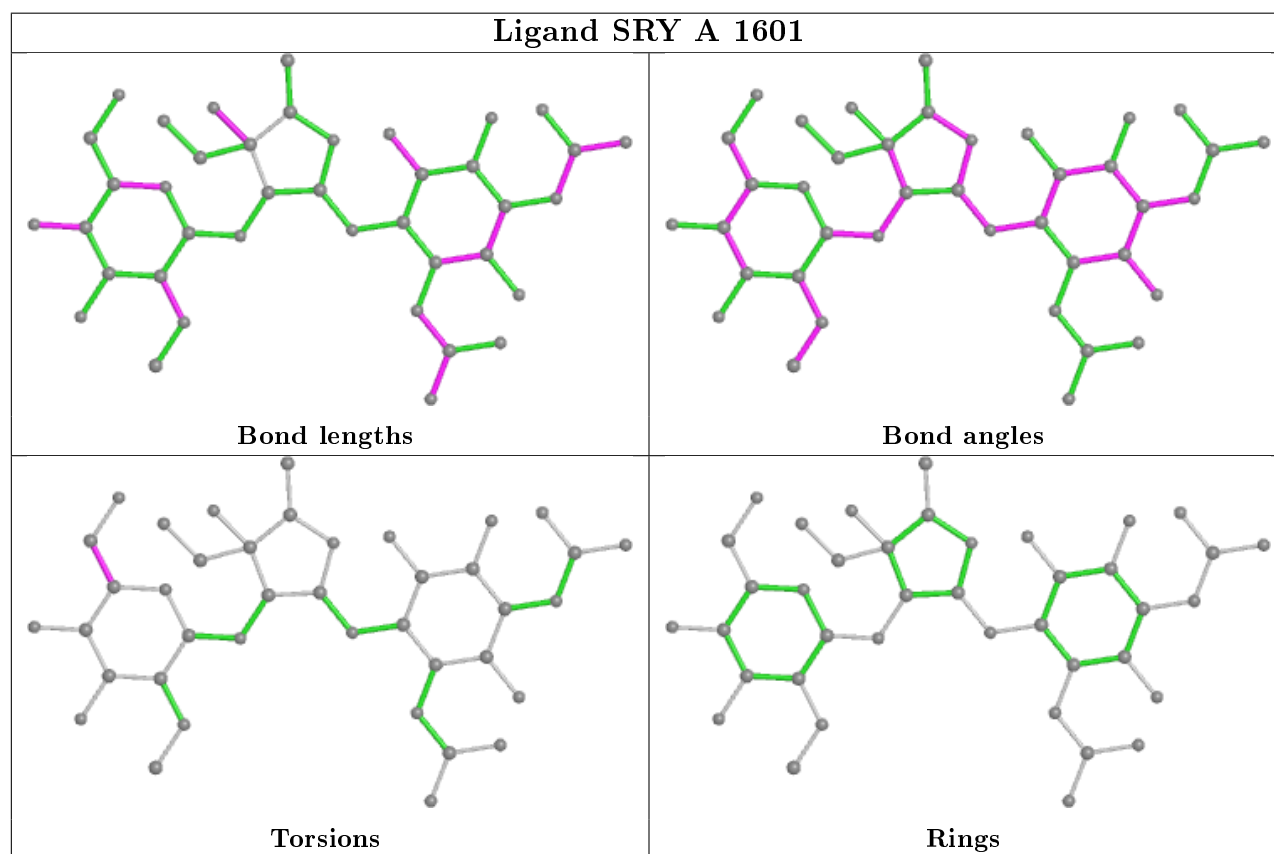
Mol	Chain	Res	Type	Atoms
22	A	1601	SRV	C43-C53-C63-O63
22	A	1601	SRV	O53-C53-C63-O63

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	1	0

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



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1498/1522 (98%)	-0.26	20 (1%) 77 61	60, 103, 221, 351	0
2	B	234/256 (91%)	-0.36	2 (0%) 84 72	72, 114, 194, 226	0
3	C	206/239 (86%)	-0.06	9 (4%) 34 17	106, 161, 215, 248	0
4	D	208/209 (99%)	-0.34	3 (1%) 75 59	73, 103, 147, 180	0
5	E	150/162 (92%)	-0.48	1 (0%) 87 77	62, 83, 119, 159	0
6	F	101/101 (100%)	-0.46	0 100 100	94, 133, 160, 185	0
7	G	155/156 (99%)	-0.03	8 (5%) 27 12	104, 152, 205, 237	0
8	H	138/138 (100%)	-0.57	0 100 100	59, 78, 109, 131	0
9	I	127/128 (99%)	0.12	6 (4%) 31 15	100, 169, 207, 221	0
10	J	98/105 (93%)	0.72	14 (14%) 2 1	108, 194, 272, 302	0
11	K	119/129 (92%)	-0.30	2 (1%) 70 51	80, 108, 162, 211	0
12	L	123/135 (91%)	-0.36	0 100 100	61, 101, 141, 188	0
13	M	117/126 (92%)	-0.16	3 (2%) 56 35	101, 132, 161, 211	0
14	N	60/61 (98%)	0.51	6 (10%) 7 2	116, 148, 200, 226	0
15	O	88/89 (98%)	-0.34	1 (1%) 80 66	73, 100, 145, 183	0
16	P	83/88 (94%)	-0.44	0 100 100	84, 100, 131, 168	0
17	Q	104/105 (99%)	-0.23	5 (4%) 30 14	59, 87, 140, 220	0
18	R	73/88 (82%)	-0.32	0 100 100	79, 112, 181, 226	0
19	S	80/93 (86%)	0.60	10 (12%) 3 1	135, 179, 226, 253	0
20	T	99/106 (93%)	-0.35	1 (1%) 82 70	81, 106, 147, 180	0
21	U	24/27 (88%)	1.09	7 (29%) 0 0	107, 128, 159, 184	0
All	All	3885/4063 (95%)	-0.21	98 (2%) 57 37	59, 113, 208, 351	0

All (98) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
17	Q	103	GLY	10.2
1	A	1129	C	7.5
1	A	793	U	7.2
11	K	129	SER	7.2
13	M	7	VAL	6.4
9	I	128	ARG	6.2
11	K	128	ALA	5.7
17	Q	102	GLY	5.4
10	J	33	GLN	5.4
17	Q	104	LYS	5.3
10	J	37	PRO	5.0
10	J	34	VAL	4.8
14	N	3	ARG	4.7
17	Q	105	ALA	4.5
10	J	32	ALA	4.4
17	Q	101	ARG	4.4
3	C	103	VAL	4.3
10	J	74	ILE	4.3
14	N	4	LYS	4.2
1	A	1005	A	4.2
21	U	25	LYS	4.1
15	O	89	GLY	4.1
7	G	79	ARG	4.1
19	S	38	SER	3.9
1	A	789	U	3.9
1	A	1539	C	3.8
10	J	89	ASP	3.7
7	G	80	VAL	3.7
10	J	90	LEU	3.7
21	U	18	TYR	3.7
19	S	3	ARG	3.6
9	I	4	TYR	3.6
3	C	65	ALA	3.5
1	A	790	A	3.5
14	N	2	ALA	3.4
7	G	154	TYR	3.4
19	S	4	SER	3.4
9	I	102	LEU	3.4
1	A	1019	C	3.4
1	A	1004	A	3.3
7	G	156	TRP	3.3
1	A	1037	C	3.3
21	U	17	THR	3.3

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Mol	Chain	Res	Type	RSRZ
21	U	24	ARG	3.3
4	D	35	ARG	3.2
9	I	8	GLY	3.1
19	S	41	VAL	3.1
10	J	75	ILE	3.1
19	S	59	PRO	3.0
1	A	993	G	3.0
2	B	231	GLU	2.9
3	C	102	ASN	2.9
1	A	995	C	2.9
1	A	81	U	2.9
14	N	12	ARG	2.9
7	G	84	ASN	2.8
19	S	28	LYS	2.8
10	J	36	GLY	2.7
10	J	4	ILE	2.7
3	C	66	VAL	2.7
19	S	27	GLU	2.7
1	A	1006	C	2.6
19	S	40	ILE	2.6
10	J	99	LYS	2.5
13	M	6	GLY	2.5
14	N	13	THR	2.5
1	A	1124	G	2.5
3	C	161	GLU	2.5
10	J	100	THR	2.5
4	D	9	CYS	2.4
14	N	18	VAL	2.4
19	S	44	MET	2.4
2	B	127	ILE	2.4
4	D	34	GLU	2.4
1	A	1036	G	2.4
9	I	9	ARG	2.4
21	U	22	ARG	2.3
1	A	1257	U	2.3
3	C	104	GLN	2.3
1	A	1140	C	2.3
7	G	82	GLY	2.2
3	C	85	ARG	2.2
19	S	69	HIS	2.2
3	C	80	GLY	2.2
21	U	5	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	193	TYR	2.2
1	A	1018	C	2.2
20	T	106	ALA	2.2
1	A	1003(A)	G	2.2
10	J	25	GLU	2.2
7	G	85	TYR	2.1
1	A	994	A	2.1
9	I	33	PHE	2.1
7	G	77	SER	2.1
21	U	9	ARG	2.0
13	M	117	VAL	2.0
10	J	98	ILE	2.0
5	E	6	PHE	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PSU	A	1541	20/21	0.42	0.95	234,276,292,296	0
1	PSU	A	1540	20/21	0.63	0.44	231,237,297,298	0
1	2MG	A	1207	24/25	0.90	0.25	139,148,169,171	0
1	5MC	A	1407	21/22	0.92	0.20	119,132,142,148	0
1	5MC	A	967	21/22	0.95	0.16	87,104,113,124	0
1	UR3	A	1498	21/22	0.96	0.19	77,99,105,117	0
1	M2G	A	966	25/26	0.96	0.19	80,104,113,124	0
1	5MC	A	1400	21/22	0.97	0.14	73,105,120,123	0
1	5MC	A	1404	21/22	0.97	0.16	84,89,96,99	0
1	MA6	A	1518	24/25	0.97	0.14	74,99,119,126	0
1	7MG	A	527	24/25	0.98	0.15	67,83,96,100	0
1	PSU	A	516	20/21	0.98	0.11	86,101,114,115	0
1	MA6	A	1519	24/25	0.98	0.13	73,94,106,114	0
12	0TD	L	92	10/11	0.98	0.22	82,101,112,282	0
1	4OC	A	1402	22/23	0.98	0.17	75,86,94,100	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
23	MG	A	1696	1/1	0.18	0.28	97,97,97,97	0
23	MG	A	1826	1/1	0.42	0.44	132,132,132,132	0
23	MG	A	1891	1/1	0.45	0.45	111,111,111,111	0
23	MG	A	1715	1/1	0.47	0.13	153,153,153,153	0
23	MG	A	1682	1/1	0.47	0.68	122,122,122,122	0
23	MG	A	1680	1/1	0.48	0.43	123,123,123,123	0
23	MG	A	1694	1/1	0.53	0.46	117,117,117,117	0
23	MG	A	1850	1/1	0.58	0.58	95,95,95,95	0
23	MG	A	1634	1/1	0.58	0.86	101,101,101,101	0
23	MG	A	1843	1/1	0.58	0.14	91,91,91,91	0
23	MG	A	1701	1/1	0.60	1.02	137,137,137,137	0
23	MG	Q	204	1/1	0.62	0.32	114,114,114,114	0
23	MG	A	1828	1/1	0.62	0.34	103,103,103,103	0
23	MG	A	1681	1/1	0.65	0.47	105,105,105,105	0
23	MG	N	102	1/1	0.65	0.36	111,111,111,111	0
23	MG	A	1848	1/1	0.66	0.48	109,109,109,109	0
23	MG	A	1869	1/1	0.66	0.53	112,112,112,112	0
23	MG	A	1703	1/1	0.67	0.47	113,113,113,113	0
23	MG	A	1635	1/1	0.67	0.67	96,96,96,96	0
23	MG	S	101	1/1	0.67	0.20	107,107,107,107	0
23	MG	A	1716	1/1	0.68	0.35	109,109,109,109	0
23	MG	A	1890	1/1	0.69	0.26	120,120,120,120	0
23	MG	A	1647	1/1	0.71	0.19	96,96,96,96	0
23	MG	A	1831	1/1	0.72	0.34	113,113,113,113	0
23	MG	A	1761	1/1	0.72	0.45	405,405,405,405	0
23	MG	A	1689	1/1	0.72	1.28	107,107,107,107	0
23	MG	A	1733	1/1	0.72	0.31	507,507,507,507	0
23	MG	A	1895	1/1	0.73	0.32	89,89,89,89	0
23	MG	H	203	1/1	0.73	0.46	97,97,97,97	0
23	MG	A	1894	1/1	0.73	0.27	120,120,120,120	0
23	MG	A	1825	1/1	0.74	0.29	110,110,110,110	0
23	MG	A	1884	1/1	0.74	0.18	111,111,111,111	0
23	MG	P	102	1/1	0.74	0.42	81,81,81,81	0
23	MG	B	301	1/1	0.74	0.29	106,106,106,106	0
23	MG	D	304	1/1	0.74	0.63	90,90,90,90	0
23	MG	A	1720	1/1	0.74	0.62	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1873	1/1	0.75	0.67	99,99,99,99	0
23	MG	A	1669	1/1	0.76	0.68	108,108,108,108	0
23	MG	A	1854	1/1	0.76	0.25	101,101,101,101	0
23	MG	A	1867	1/1	0.77	0.19	112,112,112,112	0
23	MG	A	1880	1/1	0.77	0.66	109,109,109,109	0
23	MG	A	1834	1/1	0.77	0.74	115,115,115,115	0
23	MG	A	1684	1/1	0.77	0.49	108,108,108,108	0
23	MG	A	1666	1/1	0.77	0.53	100,100,100,100	0
23	MG	A	1729	1/1	0.78	0.29	462,462,462,462	0
23	MG	A	1617	1/1	0.78	0.28	96,96,96,96	0
23	MG	A	1853	1/1	0.78	0.76	109,109,109,109	0
23	MG	A	1888	1/1	0.78	0.33	108,108,108,108	0
23	MG	A	1702	1/1	0.78	0.12	99,99,99,99	0
23	MG	A	1874	1/1	0.78	0.38	104,104,104,104	0
23	MG	A	1896	1/1	0.78	0.59	100,100,100,100	0
23	MG	A	1740	1/1	0.79	0.39	436,436,436,436	0
23	MG	A	1855	1/1	0.79	0.41	103,103,103,103	0
23	MG	H	201	1/1	0.79	0.32	112,112,112,112	0
23	MG	H	204	1/1	0.79	0.39	93,93,93,93	0
23	MG	A	1763	1/1	0.80	0.24	245,245,245,245	0
23	MG	A	1833	1/1	0.80	0.72	102,102,102,102	0
23	MG	A	1693	1/1	0.81	0.76	95,95,95,95	0
23	MG	D	302	1/1	0.81	0.71	96,96,96,96	0
23	MG	A	1882	1/1	0.81	0.45	115,115,115,115	0
23	MG	A	1747	1/1	0.81	0.31	388,388,388,388	0
23	MG	A	1643	1/1	0.81	0.14	118,118,118,118	0
23	MG	A	1883	1/1	0.81	0.34	99,99,99,99	0
23	MG	A	1815	1/1	0.81	0.56	106,106,106,106	0
23	MG	A	1620	1/1	0.81	0.23	101,101,101,101	0
23	MG	A	1698	1/1	0.81	0.50	111,111,111,111	0
23	MG	A	1844	1/1	0.82	0.17	142,142,142,142	0
23	MG	J	201	1/1	0.82	0.29	84,84,84,84	0
23	MG	A	1653	1/1	0.83	0.47	108,108,108,108	0
23	MG	A	1615	1/1	0.83	0.44	93,93,93,93	0
23	MG	A	1652	1/1	0.83	0.28	76,76,76,76	0
23	MG	A	1691	1/1	0.83	0.28	110,110,110,110	0
23	MG	Q	203	1/1	0.83	0.42	94,94,94,94	0
23	MG	A	1640	1/1	0.83	0.12	140,140,140,140	0
23	MG	A	1881	1/1	0.83	1.10	100,100,100,100	0
23	MG	Q	202	1/1	0.83	0.14	372,372,372,372	0
23	MG	A	1862	1/1	0.84	0.74	98,98,98,98	0
23	MG	A	1806	1/1	0.84	0.42	342,342,342,342	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1835	1/1	0.84	0.40	102,102,102,102	0
23	MG	A	1868	1/1	0.84	0.12	102,102,102,102	0
23	MG	A	1837	1/1	0.85	0.30	100,100,100,100	0
23	MG	A	1859	1/1	0.85	0.57	107,107,107,107	0
23	MG	A	1885	1/1	0.85	0.27	86,86,86,86	0
23	MG	A	1742	1/1	0.85	0.54	436,436,436,436	0
23	MG	A	1638	1/1	0.85	0.30	89,89,89,89	0
23	MG	A	1858	1/1	0.85	0.30	76,76,76,76	0
23	MG	A	1864	1/1	0.85	1.66	108,108,108,108	0
23	MG	A	1866	1/1	0.85	0.83	100,100,100,100	0
23	MG	A	1875	1/1	0.85	0.17	125,125,125,125	0
23	MG	A	1830	1/1	0.85	0.39	94,94,94,94	0
23	MG	A	1646	1/1	0.85	0.45	114,114,114,114	0
23	MG	J	202	1/1	0.86	0.42	89,89,89,89	0
23	MG	A	1728	1/1	0.86	0.31	511,511,511,511	0
23	MG	A	1852	1/1	0.86	0.33	98,98,98,98	0
23	MG	A	1726	1/1	0.86	0.11	233,233,233,233	0
23	MG	A	1662	1/1	0.86	0.30	108,108,108,108	0
23	MG	A	1737	1/1	0.87	0.11	245,245,245,245	0
23	MG	A	1876	1/1	0.87	0.28	100,100,100,100	0
23	MG	A	1889	1/1	0.87	0.28	102,102,102,102	0
23	MG	A	1675	1/1	0.87	0.38	95,95,95,95	0
23	MG	A	1792	1/1	0.87	0.76	518,518,518,518	0
23	MG	A	1841	1/1	0.87	0.29	101,101,101,101	0
23	MG	A	1738	1/1	0.87	0.58	506,506,506,506	0
23	MG	A	1612	1/1	0.87	0.62	82,82,82,82	0
23	MG	K	202	1/1	0.88	0.25	111,111,111,111	0
23	MG	A	1709	1/1	0.88	0.17	119,119,119,119	0
23	MG	A	1829	1/1	0.88	0.23	116,116,116,116	0
23	MG	A	1872	1/1	0.88	0.33	92,92,92,92	0
23	MG	A	1672	1/1	0.88	0.28	89,89,89,89	0
23	MG	A	1695	1/1	0.88	0.17	128,128,128,128	0
23	MG	A	1692	1/1	0.88	0.26	88,88,88,88	0
23	MG	A	1827	1/1	0.88	0.20	106,106,106,106	0
23	MG	A	1604	1/1	0.88	0.28	97,97,97,97	0
23	MG	D	303	1/1	0.88	0.09	81,81,81,81	0
23	MG	A	1700	1/1	0.88	0.22	122,122,122,122	0
23	MG	B	302	1/1	0.89	0.28	95,95,95,95	0
23	MG	A	1665	1/1	0.89	0.11	123,123,123,123	0
23	MG	A	1668	1/1	0.89	0.35	89,89,89,89	0
23	MG	A	1856	1/1	0.89	0.21	98,98,98,98	0
23	MG	A	1877	1/1	0.89	0.30	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1796	1/1	0.89	0.12	131,131,131,131	0
23	MG	A	1667	1/1	0.89	0.25	83,83,83,83	0
23	MG	A	1832	1/1	0.89	0.14	103,103,103,103	0
23	MG	A	1845	1/1	0.89	0.33	96,96,96,96	0
23	MG	A	1741	1/1	0.89	0.65	388,388,388,388	0
23	MG	A	1752	1/1	0.89	0.47	447,447,447,447	0
23	MG	A	1734	1/1	0.89	0.15	362,362,362,362	0
23	MG	A	1857	1/1	0.89	0.53	91,91,91,91	0
23	MG	A	1687	1/1	0.90	0.42	103,103,103,103	0
23	MG	A	1679	1/1	0.90	0.17	95,95,95,95	0
23	MG	A	1863	1/1	0.90	0.39	92,92,92,92	0
23	MG	A	1892	1/1	0.90	0.59	99,99,99,99	0
23	MG	A	1839	1/1	0.90	0.26	90,90,90,90	0
23	MG	A	1637	1/1	0.90	0.13	103,103,103,103	0
23	MG	A	1677	1/1	0.90	0.26	126,126,126,126	0
23	MG	A	1870	1/1	0.90	0.35	112,112,112,112	0
23	MG	B	304	1/1	0.90	0.13	89,89,89,89	0
23	MG	A	1759	1/1	0.90	0.31	504,504,504,504	0
23	MG	A	1611	1/1	0.90	0.56	99,99,99,99	0
23	MG	A	1838	1/1	0.90	0.37	103,103,103,103	0
23	MG	A	1699	1/1	0.90	0.59	104,104,104,104	0
23	MG	A	1712	1/1	0.90	0.09	243,243,243,243	0
23	MG	A	1821	1/1	0.90	0.32	400,400,400,400	0
23	MG	A	1714	1/1	0.90	0.18	373,373,373,373	0
23	MG	A	1847	1/1	0.91	0.61	98,98,98,98	0
23	MG	A	1671	1/1	0.91	0.11	80,80,80,80	0
23	MG	E	201	1/1	0.91	0.11	94,94,94,94	0
23	MG	A	1893	1/1	0.91	0.07	102,102,102,102	0
23	MG	A	1654	1/1	0.91	0.07	145,145,145,145	0
23	MG	P	101	1/1	0.91	0.24	105,105,105,105	0
23	MG	A	1849	1/1	0.91	0.34	80,80,80,80	0
23	MG	A	1706	1/1	0.91	0.27	81,81,81,81	0
23	MG	A	1808	1/1	0.91	0.34	437,437,437,437	0
23	MG	A	1736	1/1	0.91	0.09	344,344,344,344	0
23	MG	A	1721	1/1	0.91	0.13	248,248,248,248	0
23	MG	A	1717	1/1	0.91	0.21	120,120,120,120	0
23	MG	A	1718	1/1	0.91	0.45	94,94,94,94	0
23	MG	A	1722	1/1	0.91	0.12	442,442,442,442	0
23	MG	A	1878	1/1	0.92	0.26	116,116,116,116	0
23	MG	A	1777	1/1	0.92	0.20	422,422,422,422	0
23	MG	A	1871	1/1	0.92	0.17	129,129,129,129	0
23	MG	A	1664	1/1	0.92	0.44	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1836	1/1	0.92	0.29	77,77,77,77	0
23	MG	A	1719	1/1	0.92	0.22	94,94,94,94	0
23	MG	P	103	1/1	0.92	0.46	108,108,108,108	0
23	MG	A	1686	1/1	0.92	0.30	88,88,88,88	0
23	MG	A	1865	1/1	0.92	0.38	74,74,74,74	0
23	MG	K	203	1/1	0.92	0.24	79,79,79,79	0
23	MG	A	1791	1/1	0.92	0.36	294,294,294,294	0
23	MG	A	1846	1/1	0.92	0.15	101,101,101,101	0
23	MG	K	201	1/1	0.92	0.41	107,107,107,107	0
23	MG	A	1708	1/1	0.92	0.48	111,111,111,111	0
23	MG	A	1801	1/1	0.92	0.15	243,243,243,243	0
23	MG	A	1685	1/1	0.93	0.22	84,84,84,84	0
23	MG	H	202	1/1	0.93	0.06	225,225,225,225	0
23	MG	A	1775	1/1	0.93	0.41	478,478,478,478	0
23	MG	A	1879	1/1	0.93	0.11	89,89,89,89	0
23	MG	A	1805	1/1	0.93	0.12	123,123,123,123	0
23	MG	A	1670	1/1	0.93	0.42	106,106,106,106	0
23	MG	A	1840	1/1	0.93	0.33	95,95,95,95	0
23	MG	A	1690	1/1	0.93	0.46	96,96,96,96	0
23	MG	A	1711	1/1	0.93	0.27	89,89,89,89	0
23	MG	A	1648	1/1	0.93	0.42	159,159,159,159	0
23	MG	A	1613	1/1	0.93	0.35	92,92,92,92	0
23	MG	A	1773	1/1	0.93	0.53	262,262,262,262	0
23	MG	I	201	1/1	0.94	0.26	89,89,89,89	0
23	MG	A	1798	1/1	0.94	0.45	406,406,406,406	0
23	MG	A	1817	1/1	0.94	0.21	97,97,97,97	0
23	MG	A	1625	1/1	0.94	0.77	79,79,79,79	0
23	MG	A	1851	1/1	0.94	0.30	70,70,70,70	0
23	MG	A	1765	1/1	0.94	0.65	519,519,519,519	0
23	MG	A	1778	1/1	0.94	0.19	377,377,377,377	0
23	MG	A	1607	1/1	0.94	0.11	70,70,70,70	0
23	MG	A	1774	1/1	0.94	0.24	343,343,343,343	0
23	MG	A	1787	1/1	0.94	0.38	391,391,391,391	0
23	MG	A	1794	1/1	0.94	0.24	484,484,484,484	0
23	MG	A	1788	1/1	0.94	0.17	247,247,247,247	0
23	MG	A	1764	1/1	0.94	0.17	329,329,329,329	0
23	MG	A	1861	1/1	0.94	0.16	112,112,112,112	0
23	MG	A	1673	1/1	0.94	0.18	100,100,100,100	0
23	MG	A	1731	1/1	0.94	0.06	115,115,115,115	0
23	MG	T	201	1/1	0.94	0.26	81,81,81,81	0
23	MG	A	1812	1/1	0.94	0.09	334,334,334,334	0
23	MG	A	1824	1/1	0.94	0.23	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1697	1/1	0.94	0.10	140,140,140,140	0
23	MG	A	1822	1/1	0.94	0.18	101,101,101,101	0
23	MG	A	1749	1/1	0.94	0.19	358,358,358,358	0
23	MG	A	1608	1/1	0.94	0.17	50,50,50,50	0
23	MG	A	1744	1/1	0.94	0.30	519,519,519,519	0
23	MG	A	1660	1/1	0.95	0.11	70,70,70,70	0
23	MG	A	1623	1/1	0.95	0.39	69,69,69,69	0
23	MG	A	1800	1/1	0.95	0.34	317,317,317,317	0
23	MG	A	1674	1/1	0.95	0.15	71,71,71,71	0
23	MG	A	1724	1/1	0.95	0.12	441,441,441,441	0
23	MG	A	1757	1/1	0.95	0.32	290,290,290,290	0
23	MG	A	1739	1/1	0.95	0.45	514,514,514,514	0
23	MG	A	1616	1/1	0.95	0.23	126,126,126,126	0
23	MG	A	1750	1/1	0.95	0.39	396,396,396,396	0
23	MG	A	1887	1/1	0.95	0.25	106,106,106,106	0
23	MG	A	1786	1/1	0.95	0.18	473,473,473,473	0
23	MG	A	1622	1/1	0.95	0.17	63,63,63,63	0
23	MG	A	1605	1/1	0.95	0.10	148,148,148,148	0
23	MG	A	1758	1/1	0.95	0.39	295,295,295,295	0
23	MG	A	1688	1/1	0.95	0.22	109,109,109,109	0
23	MG	A	1710	1/1	0.95	0.08	89,89,89,89	0
23	MG	E	202	1/1	0.95	0.24	91,91,91,91	0
23	MG	A	1707	1/1	0.95	0.44	89,89,89,89	0
23	MG	A	1768	1/1	0.95	0.06	102,102,102,102	0
23	MG	A	1642	1/1	0.95	0.31	112,112,112,112	0
23	MG	A	1656	1/1	0.95	0.19	109,109,109,109	0
23	MG	A	1799	1/1	0.95	0.23	351,351,351,351	0
23	MG	A	1705	1/1	0.96	0.10	86,86,86,86	0
23	MG	A	1771	1/1	0.96	0.05	91,91,91,91	0
23	MG	A	1676	1/1	0.96	0.12	113,113,113,113	0
23	MG	A	1776	1/1	0.96	0.17	241,241,241,241	0
23	MG	A	1813	1/1	0.96	0.09	128,128,128,128	0
23	MG	A	1602	1/1	0.96	0.29	117,117,117,117	0
23	MG	A	1627	1/1	0.96	0.22	59,59,59,59	0
23	MG	A	1797	1/1	0.96	0.07	129,129,129,129	0
23	MG	A	1809	1/1	0.96	0.04	99,99,99,99	0
23	MG	A	1769	1/1	0.96	0.30	292,292,292,292	0
23	MG	Q	201	1/1	0.96	0.19	76,76,76,76	0
23	MG	A	1730	1/1	0.96	0.04	125,125,125,125	0
23	MG	A	1860	1/1	0.96	0.14	62,62,62,62	0
23	MG	A	1802	1/1	0.96	0.30	274,274,274,274	0
23	MG	A	1789	1/1	0.96	0.07	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1618	1/1	0.96	0.18	96,96,96,96	0
23	MG	A	1725	1/1	0.96	0.04	459,459,459,459	0
23	MG	A	1751	1/1	0.96	0.09	130,130,130,130	0
23	MG	A	1790	1/1	0.97	0.09	202,202,202,202	0
23	MG	A	1636	1/1	0.97	0.11	77,77,77,77	0
23	MG	A	1639	1/1	0.97	0.19	89,89,89,89	0
23	MG	A	1811	1/1	0.97	0.31	278,278,278,278	0
23	MG	A	1807	1/1	0.97	0.32	336,336,336,336	0
23	MG	A	1633	1/1	0.97	0.15	95,95,95,95	0
23	MG	A	1683	1/1	0.97	0.25	66,66,66,66	0
23	MG	A	1645	1/1	0.97	0.34	147,147,147,147	0
23	MG	A	1628	1/1	0.97	0.23	67,67,67,67	0
23	MG	A	1819	1/1	0.97	0.11	120,120,120,120	0
23	MG	A	1644	1/1	0.97	0.15	81,81,81,81	0
23	MG	A	1793	1/1	0.97	0.09	317,317,317,317	0
23	MG	A	1606	1/1	0.97	0.08	92,92,92,92	0
23	MG	A	1784	1/1	0.97	0.15	87,87,87,87	0
23	MG	A	1704	1/1	0.97	0.54	89,89,89,89	0
23	MG	A	1743	1/1	0.97	0.30	418,418,418,418	0
23	MG	A	1723	1/1	0.97	0.12	172,172,172,172	0
23	MG	A	1814	1/1	0.97	0.44	329,329,329,329	0
22	SRY	A	1601	40/40	0.97	0.17	61,91,106,116	0
23	MG	B	303	1/1	0.97	0.39	533,533,533,533	0
23	MG	A	1783	1/1	0.97	0.29	379,379,379,379	0
23	MG	A	1785	1/1	0.97	0.16	430,430,430,430	0
23	MG	A	1630	1/1	0.97	0.27	49,49,49,49	0
23	MG	A	1649	1/1	0.97	0.08	82,82,82,82	0
23	MG	A	1760	1/1	0.97	0.27	152,152,152,152	0
23	MG	A	1782	1/1	0.97	0.23	285,285,285,285	0
23	MG	A	1614	1/1	0.97	0.07	114,114,114,114	0
23	MG	A	1762	1/1	0.97	0.35	183,183,183,183	0
23	MG	A	1810	1/1	0.97	0.17	173,173,173,173	0
23	MG	A	1754	1/1	0.97	0.36	406,406,406,406	0
23	MG	A	1629	1/1	0.98	0.13	76,76,76,76	0
23	MG	A	1663	1/1	0.98	0.07	81,81,81,81	0
23	MG	A	1610	1/1	0.98	0.17	68,68,68,68	0
24	ZN	N	101	1/1	0.98	0.16	139,139,139,139	0
23	MG	A	1624	1/1	0.98	0.11	49,49,49,49	0
23	MG	A	1745	1/1	0.98	0.36	461,461,461,461	0
23	MG	A	1770	1/1	0.98	0.11	98,98,98,98	0
23	MG	A	1657	1/1	0.98	0.10	98,98,98,98	0
23	MG	A	1803	1/1	0.98	0.63	518,518,518,518	0

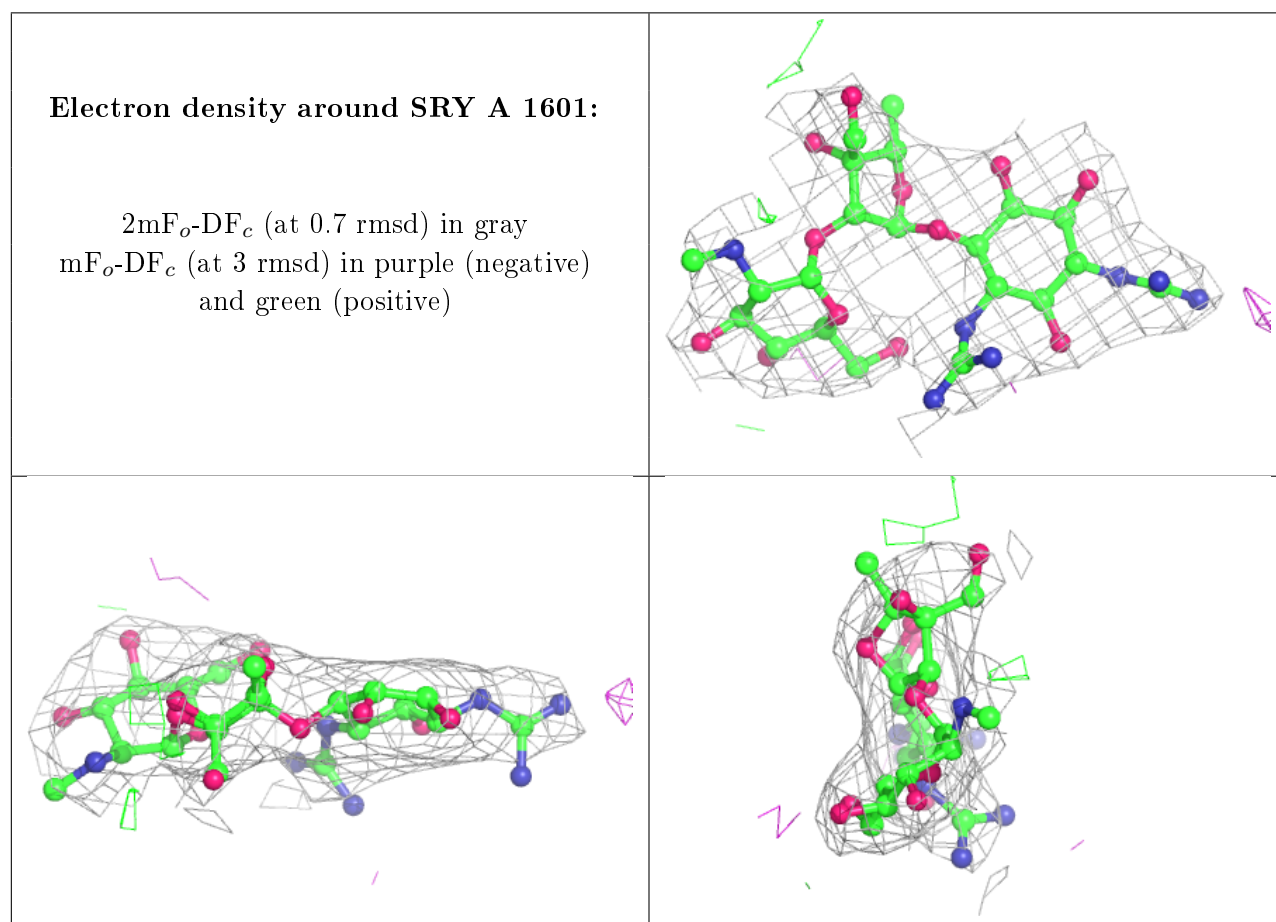
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1753	1/1	0.98	0.41	396,396,396,396	0
23	MG	A	1823	1/1	0.98	0.12	108,108,108,108	0
23	MG	A	1621	1/1	0.98	0.23	134,134,134,134	0
23	MG	A	1661	1/1	0.98	0.33	199,199,199,199	0
23	MG	A	1842	1/1	0.98	0.25	77,77,77,77	0
23	MG	A	1609	1/1	0.98	0.30	77,77,77,77	0
23	MG	A	1746	1/1	0.98	0.19	255,255,255,255	0
23	MG	A	1772	1/1	0.98	0.29	381,381,381,381	0
23	MG	A	1727	1/1	0.98	0.07	130,130,130,130	0
23	MG	A	1658	1/1	0.98	0.19	122,122,122,122	0
23	MG	A	1781	1/1	0.98	0.18	177,177,177,177	0
23	MG	A	1659	1/1	0.98	0.34	84,84,84,84	0
23	MG	A	1820	1/1	0.98	0.21	50,50,50,50	0
23	MG	A	1641	1/1	0.98	0.14	95,95,95,95	0
23	MG	A	1816	1/1	0.98	0.51	120,120,120,120	0
23	MG	A	1651	1/1	0.98	0.20	152,152,152,152	0
23	MG	A	1626	1/1	0.98	0.25	93,93,93,93	0
23	MG	A	1655	1/1	0.98	0.11	97,97,97,97	0
23	MG	A	1780	1/1	0.98	0.17	313,313,313,313	0
23	MG	A	1713	1/1	0.98	0.22	212,212,212,212	0
23	MG	A	1678	1/1	0.98	0.09	76,76,76,76	0
23	MG	A	1755	1/1	0.98	0.62	550,550,550,550	0
24	ZN	D	301	1/1	0.99	0.36	88,88,88,88	0
23	MG	A	1631	1/1	0.99	0.22	79,79,79,79	0
23	MG	A	1818	1/1	0.99	0.09	89,89,89,89	0
23	MG	A	1767	1/1	0.99	0.09	75,75,75,75	0
23	MG	A	1804	1/1	0.99	0.28	338,338,338,338	0
23	MG	A	1735	1/1	0.99	0.06	106,106,106,106	0
23	MG	A	1766	1/1	0.99	0.29	178,178,178,178	0
23	MG	A	1886	1/1	0.99	0.10	118,118,118,118	0
23	MG	A	1748	1/1	0.99	0.09	86,86,86,86	0
23	MG	F	201	1/1	0.99	0.16	363,363,363,363	0
23	MG	A	1603	1/1	0.99	0.11	81,81,81,81	0
23	MG	A	1779	1/1	0.99	0.17	354,354,354,354	0
23	MG	A	1619	1/1	0.99	0.13	69,69,69,69	0
23	MG	A	1732	1/1	0.99	0.09	84,84,84,84	0
23	MG	A	1650	1/1	0.99	0.15	104,104,104,104	0
23	MG	A	1632	1/1	0.99	0.24	107,107,107,107	0
23	MG	A	1795	1/1	0.99	0.10	94,94,94,94	0
23	MG	A	1756	1/1	0.99	0.14	111,111,111,111	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.