



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 01:46 PM EST

PDB ID : 4DV7  
Title : Crystal structure of the *Thermus thermophilus* 30S ribosomal subunit with a 16S rRNA mutation, A915G, bound with streptomycin  
Authors : Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.  
Deposited on : 2012-02-22  
Resolution : 3.29 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.

The types of validation reports are described at

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

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

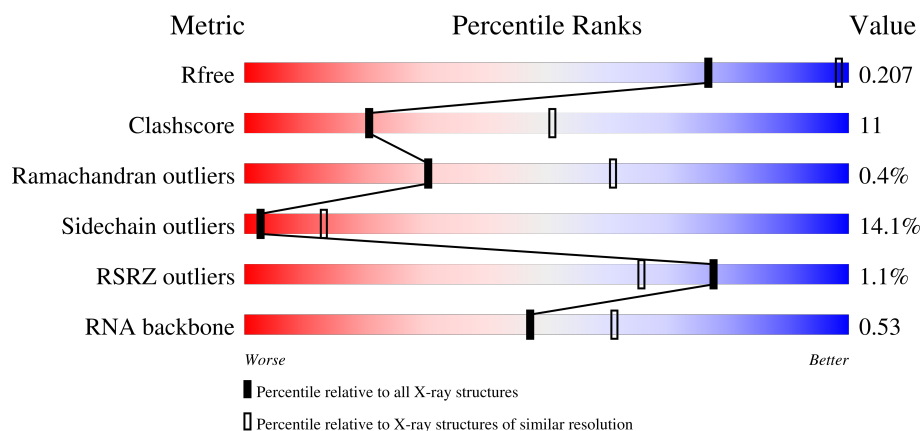
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.29 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.












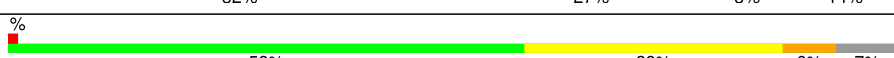

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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></div> <div>56%</div> <div>30%</div> <div>12%</div> <div>..</div> </div>
2	B	256	<div> <div>%</div> <div>58%</div> <div>30%</div> <div>..</div> <div>9%</div> </div>
3	C	239	<div> <div>%</div> <div>47%</div> <div>35%</div> <div>.</div> <div>14%</div> </div>

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1625	-	-	-	X
23	MG	A	1711	-	-	-	X
23	MG	A	1715	-	-	-	X
23	MG	A	1718	-	-	-	X
23	MG	A	1736	-	-	-	X
23	MG	A	1745	-	-	-	X
23	MG	A	1769	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1794	-	-	-	X

## 2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52337 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
			32508	14477	6011	10508	1512			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	915	G	A	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

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

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

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

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

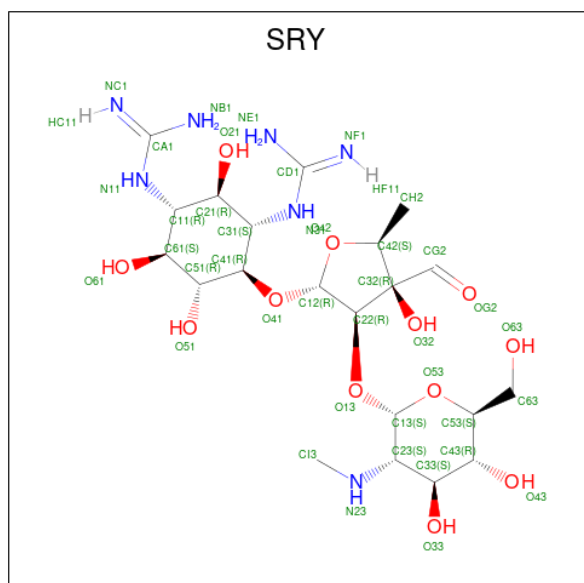
- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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



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



- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	272	Total 272	Mg 272	0	0
23	B	2	Total 2	Mg 2	0	0
23	D	1	Total 1	Mg 1	0	0
23	E	1	Total 1	Mg 1	0	0
23	H	3	Total 3	Mg 3	0	0
23	K	1	Total 1	Mg 1	0	0
23	M	2	Total 2	Mg 2	0	0
23	N	2	Total 2	Mg 2	0	0
23	P	2	Total 2	Mg 2	0	0
23	Q	2	Total 2	Mg 2	0	0
23	S	1	Total 1	Mg 1	0	0
23	T	3	Total 3	Mg 3	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	392	Total 392	O 392	0	0
25	D	1	Total 1	O 1	0	0
25	E	7	Total 7	O 7	0	0

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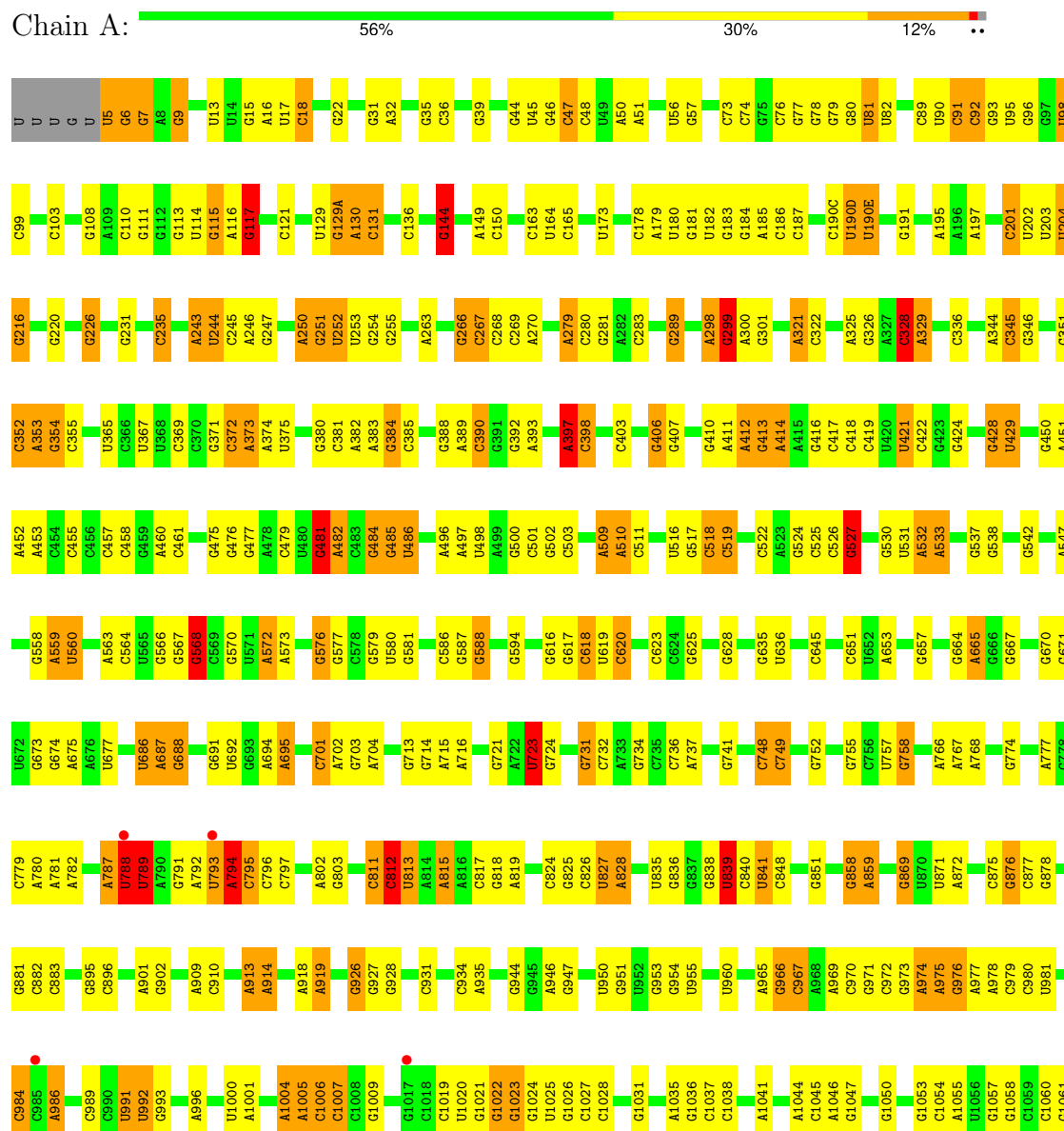
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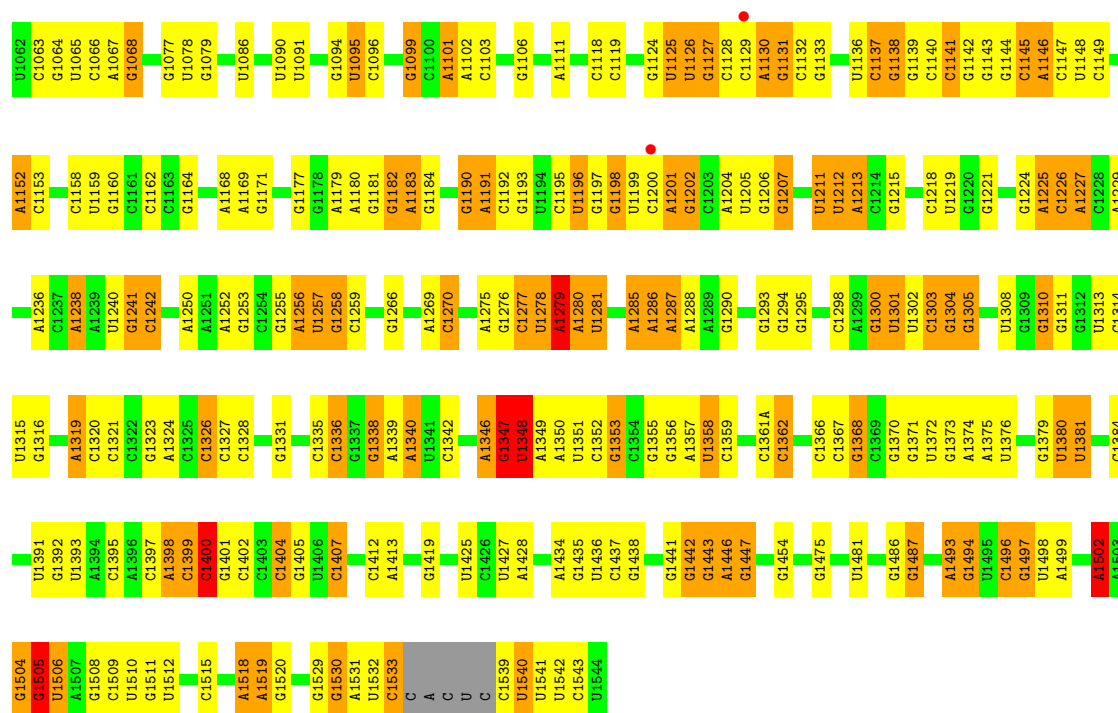
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	G	1	Total	O	0	0
			1	1		
25	L	1	Total	O	0	0
			1	1		
25	P	2	Total	O	0	0
			2	2		
25	T	2	Total	O	0	0
			2	2		
25	U	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

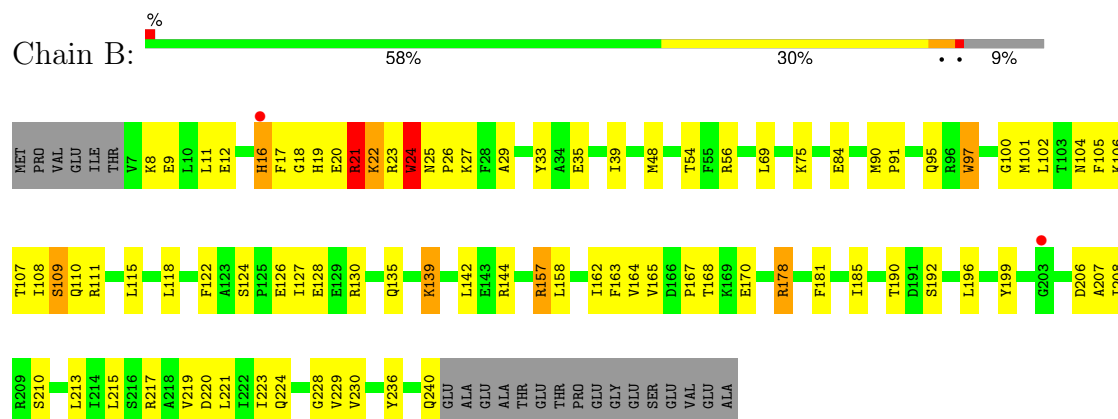
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

#### • Molecule 1: 16S rRNA

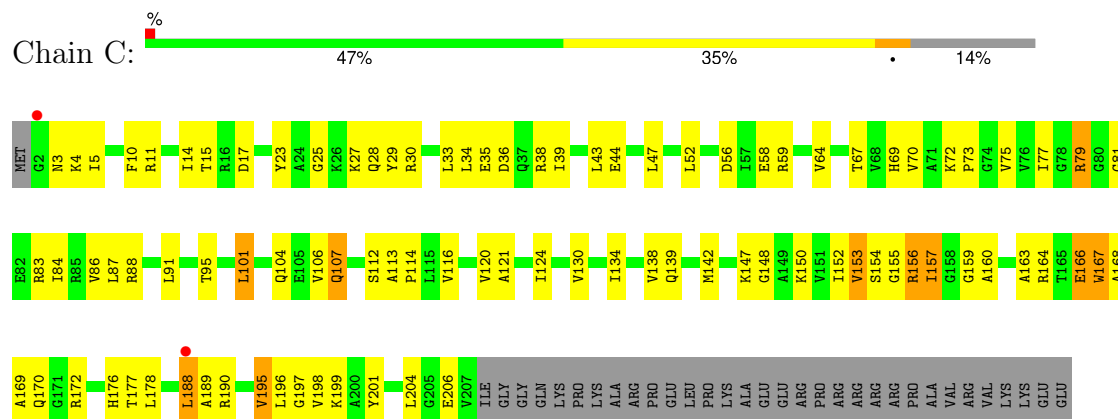




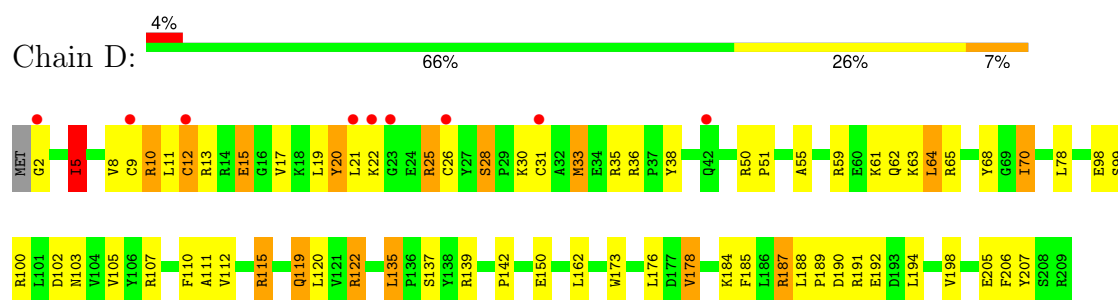
### • Molecule 2: ribosomal protein S2



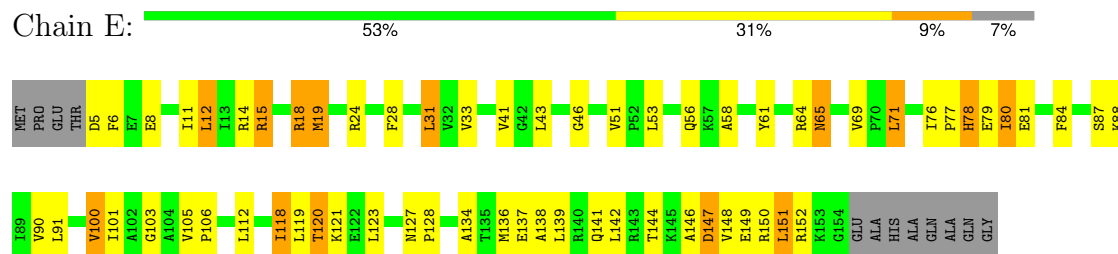
### • Molecule 3: ribosomal protein S3



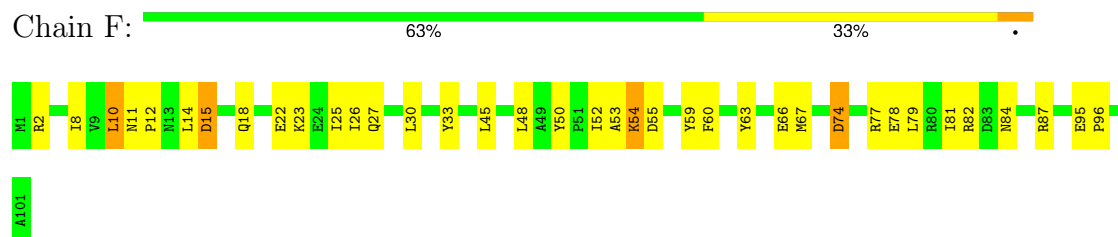
### • Molecule 4: ribosomal protein S4



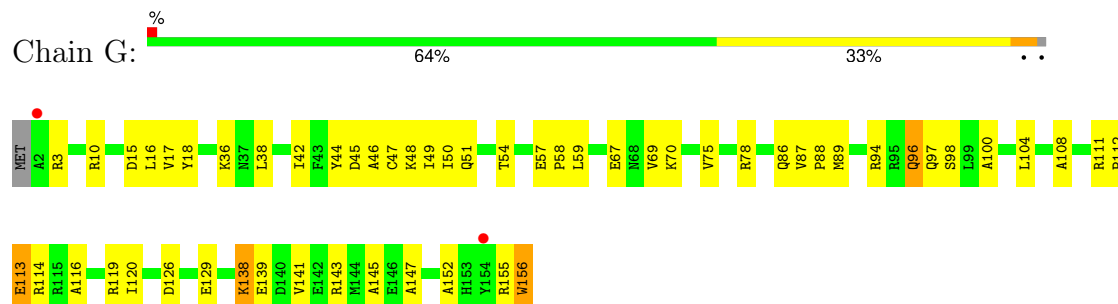
• Molecule 5: ribosomal protein S5



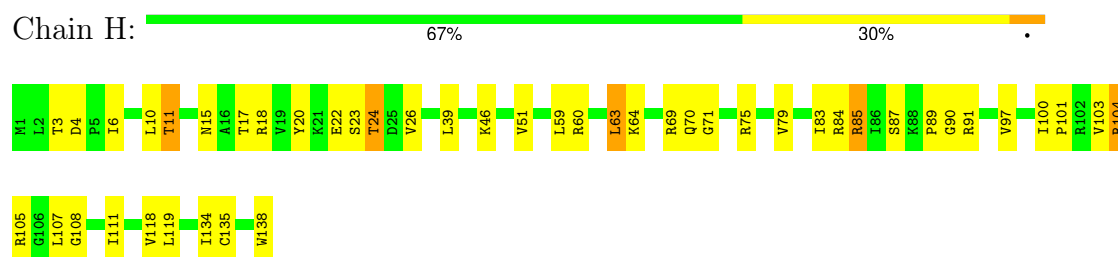
• Molecule 6: ribosomal protein S6



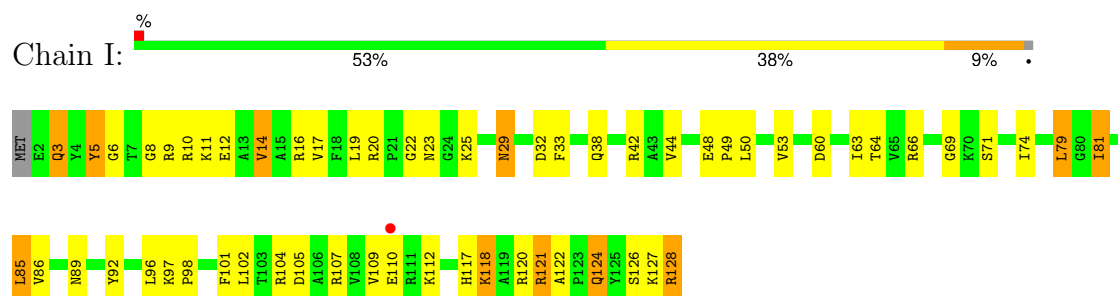
• Molecule 7: ribosomal protein S7



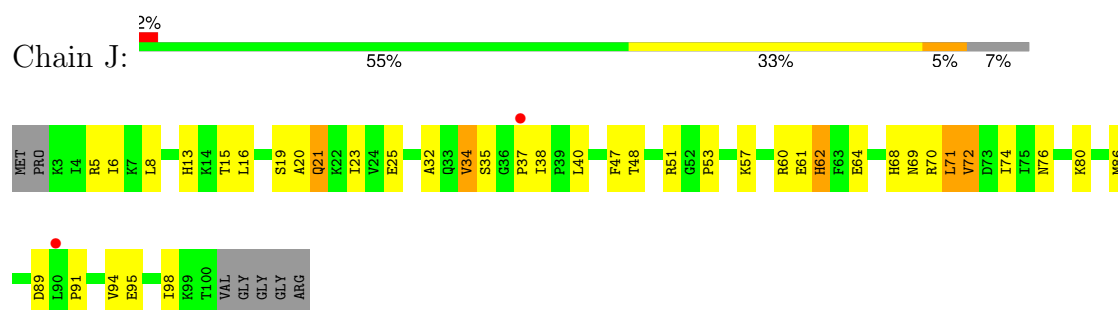
• Molecule 8: ribosomal protein S8



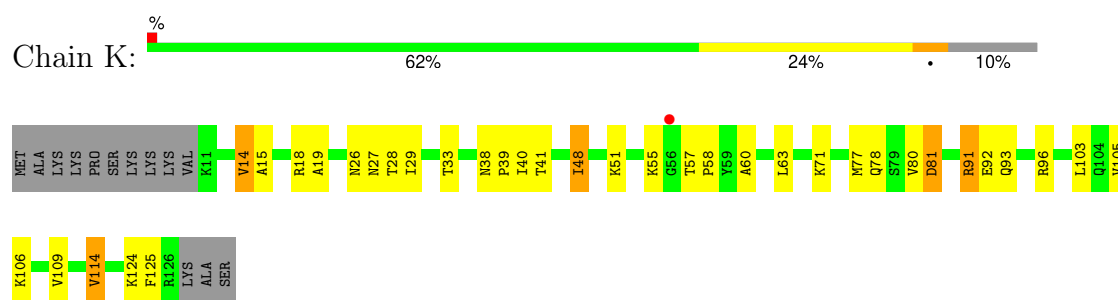
- Molecule 9: ribosomal protein S9



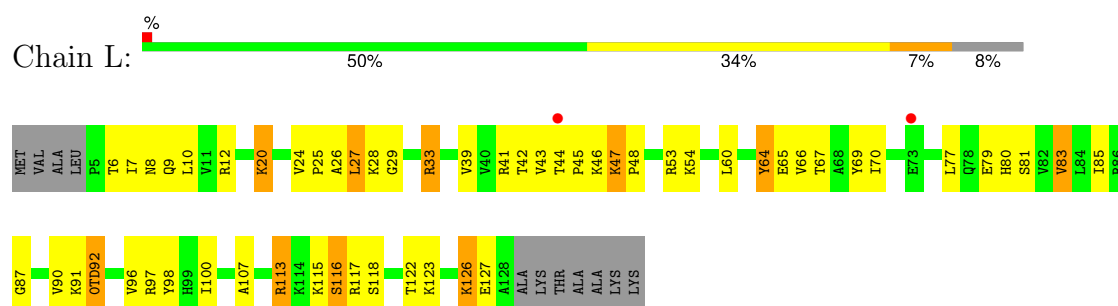
- Molecule 10: ribosomal protein S10



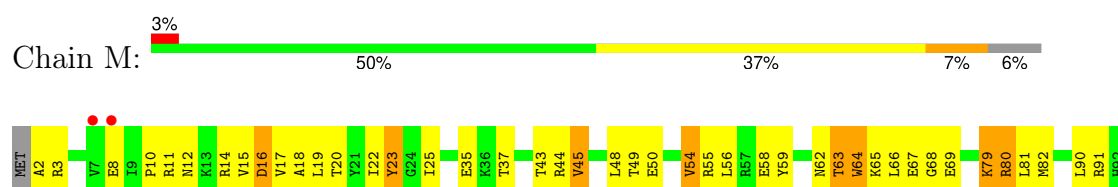
- Molecule 11: ribosomal protein S11

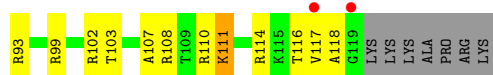


- Molecule 12: ribosomal protein S12



- Molecule 13: ribosomal protein S13





- Molecule 14: ribosomal protein S14



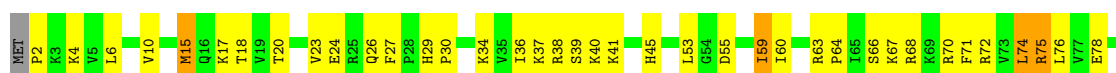
- Molecule 15: ribosomal protein S15



- Molecule 16: ribosomal protein S16



- Molecule 17: ribosomal protein S17



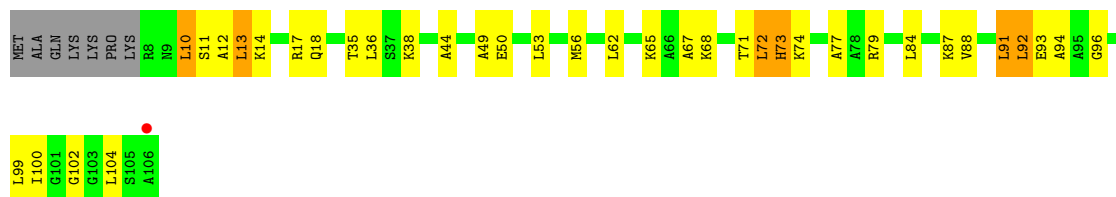
- Molecule 18: ribosomal protein S18



- Molecule 19: ribosomal protein S19



- Molecule 20: ribosomal protein S20



- Molecule 21: ribosomal protein THX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	403.37Å 403.37Å 173.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.92 – 3.29 34.92 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.6 (34.92-3.29) 98.3 (34.92-3.29)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, $R_{free}$	0.168 , 0.210 0.166 , 0.207	Depositor DCC
$R_{free}$ test set	10630 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	119.3	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 129.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	52337	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.46% 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: 2MG, 7MG, 4OC, MG, 0TD, SRY, MA6, PSU, ZN, UR3, M2G, 5MC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.65	5/36041 (0.0%)	1.06	115/56245 (0.2%)
2	B	0.44	0/1935	0.66	0/2609
3	C	0.34	0/1636	0.57	0/2205
4	D	0.45	1/1733 (0.1%)	0.61	0/2318
5	E	0.57	0/1162	0.73	0/1564
6	F	0.37	0/856	0.57	0/1154
7	G	0.36	0/1276	0.52	0/1709
8	H	0.59	1/1136 (0.1%)	0.73	0/1527
9	I	0.37	0/1029	0.60	0/1379
10	J	0.36	0/805	0.59	0/1082
11	K	0.42	0/879	0.62	0/1187
12	L	0.48	0/977	0.74	1/1306 (0.1%)
13	M	0.36	0/947	0.63	0/1270
14	N	0.34	0/501	0.57	0/664
15	O	0.42	0/740	0.60	0/987
16	P	0.47	0/716	0.68	0/963
17	Q	0.56	0/836	0.80	0/1117
18	R	0.38	0/579	0.60	0/768
19	S	0.30	0/661	0.58	0/890
20	T	0.43	0/765	0.67	1/1007 (0.1%)
21	U	0.33	0/212	0.54	0/277
All	All	0.58	7/55422 (0.0%)	0.95	117/82228 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
3	C	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
12	L	0	1
20	T	0	1
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-7.58	1.33	1.37
1	A	279	A	N3-C4	-6.22	1.31	1.34
1	A	279	A	C5-C6	-5.96	1.35	1.41
4	D	12	CYS	CB-SG	5.25	1.91	1.82
1	A	298	A	N3-C4	-5.16	1.31	1.34
1	A	1077	G	N9-C8	-5.06	1.34	1.37
8	H	135	CYS	CB-SG	-5.01	1.73	1.81

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	A	C2-N3-C4	-11.10	105.05	110.60
1	A	117	G	N1-C6-O6	10.52	126.21	119.90
1	A	117	G	C6-C5-N7	-9.13	124.92	130.40
1	A	328	C	N1-C2-O2	9.01	124.31	118.90
1	A	328	C	N3-C2-O2	-8.98	115.62	121.90
1	A	279	A	N1-C6-N6	8.90	123.94	118.60
1	A	279	A	C5-N7-C8	-8.74	99.53	103.90
1	A	108	G	C5-N7-C8	-8.40	100.10	104.30
1	A	723	U	C2-N1-C1'	8.14	127.47	117.70
1	A	144	G	N1-C6-O6	8.06	124.74	119.90
1	A	1502	A	C5-N7-C8	-8.05	99.88	103.90
1	A	869	G	N1-C6-O6	-8.03	115.08	119.90
1	A	266	G	C5-N7-C8	-7.88	100.36	104.30
1	A	235	C	C6-N1-C2	7.87	123.45	120.30
1	A	869	G	C5-C6-O6	7.87	133.32	128.60
1	A	1502	A	N7-C8-N9	7.63	117.62	113.80
1	A	824	C	C6-N1-C2	7.51	123.30	120.30
1	A	839	U	N1-C2-O2	7.50	128.05	122.80
1	A	1502	A	C6-C5-N7	-7.36	127.15	132.30
1	A	1442	G	N3-C4-N9	7.25	130.35	126.00
1	A	812	C	C6-N1-C2	-7.22	117.41	120.30
1	A	839	U	C2-N1-C1'	7.20	126.34	117.70
1	A	266	G	C4-C5-N7	7.20	113.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1442	G	C4-N9-C1'	7.19	135.85	126.50
1	A	108	G	C4-C5-N7	7.14	113.66	110.80
1	A	723	U	N1-C2-O2	7.14	127.80	122.80
1	A	1395	C	C6-N1-C2	7.05	123.12	120.30
1	A	108	G	N7-C8-N9	7.01	116.61	113.10
1	A	13	U	N1-C2-O2	6.94	127.66	122.80
1	A	572	A	N7-C8-N9	-6.68	110.46	113.80
1	A	117	G	N9-C4-C5	-6.67	102.73	105.40
1	A	876	G	C8-N9-C4	6.66	109.06	106.40
1	A	815	A	N1-C6-N6	6.63	122.58	118.60
1	A	481	G	N3-C4-N9	6.62	129.97	126.00
1	A	279	A	C6-C5-N7	-6.52	127.74	132.30
1	A	328	C	C2-N1-C1'	6.50	125.95	118.80
1	A	1502	A	N1-C6-N6	6.47	122.48	118.60
1	A	919	A	C8-N9-C4	6.40	108.36	105.80
1	A	875	C	C6-N1-C2	6.40	122.86	120.30
1	A	279	A	C4-C5-N7	6.39	113.89	110.70
1	A	795	C	N3-C2-O2	6.37	126.36	121.90
1	A	1515	C	N3-C4-C5	6.37	124.45	121.90
1	A	1442	G	C8-N9-C1'	-6.33	118.77	127.00
1	A	723	U	N3-C2-O2	-6.32	117.78	122.20
1	A	299	G	C5-C6-O6	-6.31	124.81	128.60
1	A	1502	A	C4-C5-N7	6.28	113.84	110.70
1	A	1502	A	C2-N3-C4	-6.27	107.47	110.60
1	A	117	G	C5-C6-O6	-6.25	124.85	128.60
1	A	721	G	C6-C5-N7	-6.21	126.68	130.40
1	A	1099	G	N3-C4-N9	-6.15	122.31	126.00
1	A	572	A	C8-N9-C4	6.14	108.26	105.80
1	A	635	G	N1-C6-O6	6.13	123.58	119.90
1	A	482	A	N1-C6-N6	6.09	122.25	118.60
1	A	839	U	N3-C2-O2	-6.04	117.97	122.20
1	A	815	A	C5-C6-N6	-6.03	118.88	123.70
1	A	931	C	C5-C6-N1	-6.03	117.99	121.00
1	A	1530	G	C8-N9-C4	5.95	108.78	106.40
1	A	1099	G	N3-C4-C5	5.91	131.56	128.60
1	A	235	C	N3-C4-C5	5.91	124.26	121.90
1	A	1505	G	C8-N9-C4	-5.87	104.05	106.40
1	A	266	G	N3-C4-C5	5.86	131.53	128.60
1	A	201	C	C2-N1-C1'	5.79	125.17	118.80
1	A	117	G	C4-C5-C6	5.77	122.26	118.80
1	A	117	G	C8-N9-C1'	-5.76	119.50	127.00
1	A	279	A	N3-C4-C5	5.73	130.81	126.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	628	G	N3-C4-C5	-5.67	125.77	128.60
1	A	1103	C	C5-C6-N1	-5.64	118.18	121.00
1	A	1442	G	N3-C4-C5	-5.63	125.78	128.60
1	A	279	A	N7-C8-N9	5.61	116.61	113.80
1	A	1348	U	C2-N1-C1'	5.61	124.43	117.70
1	A	1279	A	N7-C8-N9	5.59	116.60	113.80
1	A	723	U	C5-C6-N1	5.57	125.49	122.70
1	A	336	C	C6-N1-C2	5.55	122.52	120.30
1	A	1442	G	C6-C5-N7	-5.55	127.07	130.40
12	L	26	ALA	N-CA-C	-5.54	96.06	111.00
1	A	576	G	C5-C6-O6	-5.53	125.28	128.60
1	A	789	U	C5-C6-N1	5.52	125.46	122.70
1	A	131	C	N3-C2-O2	-5.52	118.04	121.90
1	A	721	G	N3-C4-N9	5.51	129.30	126.00
1	A	328	C	C6-N1-C2	-5.50	118.10	120.30
1	A	811	C	C2-N3-C4	5.48	122.64	119.90
1	A	944	G	N3-C4-C5	-5.40	125.90	128.60
1	A	190(C)	C	C2-N1-C1'	5.38	124.71	118.80
1	A	788	U	N1-C2-N3	-5.37	111.68	114.90
1	A	1279	A	C8-N9-C4	-5.35	103.66	105.80
1	A	326	G	N3-C4-C5	-5.34	125.93	128.60
1	A	397	A	C8-N9-C4	-5.34	103.67	105.80
1	A	117	G	C2-N3-C4	-5.32	109.24	111.90
1	A	758	G	N1-C6-O6	-5.31	116.71	119.90
1	A	266	G	N7-C8-N9	5.29	115.75	113.10
1	A	824	C	C5-C6-N1	-5.28	118.36	121.00
1	A	18	C	C6-N1-C2	5.25	122.40	120.30
1	A	117	G	C4-N9-C1'	5.25	133.32	126.50
1	A	797	C	C6-N1-C2	5.24	122.40	120.30
1	A	130	A	N1-C6-N6	5.22	121.73	118.60
1	A	1347	G	C8-N9-C4	5.20	108.48	106.40
1	A	481	G	N9-C4-C5	-5.20	103.32	105.40
1	A	794	A	C2-N3-C4	5.15	113.18	110.60
1	A	752	G	N1-C6-O6	5.14	122.98	119.90
1	A	913	A	P-O3'-C3'	5.14	125.87	119.70
1	A	651	C	C6-N1-C2	5.13	122.35	120.30
1	A	117	G	C5-C6-N1	-5.13	108.94	111.50
1	A	1346	A	P-O3'-C3'	5.12	125.84	119.70
1	A	568	G	C8-N9-C4	-5.11	104.36	106.40
1	A	570	G	C4-N9-C1'	5.11	133.14	126.50
1	A	108	G	C4-N9-C1'	5.11	133.14	126.50
1	A	1060	C	N3-C2-O2	-5.08	118.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	721	G	C4-N9-C1'	5.08	133.11	126.50
1	A	484	G	C4-N9-C1'	5.08	133.10	126.50
1	A	970	C	N1-C2-O2	5.07	121.94	118.90
1	A	16	A	C8-N9-C4	5.04	107.82	105.80
1	A	117	G	C4-C5-N7	5.04	112.82	110.80
1	A	839	U	C6-N1-C1'	-5.04	114.14	121.20
20	T	94	ALA	N-CA-C	-5.03	97.43	111.00
1	A	1502	A	C8-N9-C4	-5.02	103.79	105.80
1	A	1502	A	C5-C6-N1	-5.01	115.19	117.70
1	A	144	G	C5-C6-N1	-5.00	109.00	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	HIS	Peptide
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
12	L	27	LEU	Peptide
20	T	93	GLU	Peptide

## 5.2 Too-close contacts [i](#)

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	32508	0	16433	455	1
2	B	1900	0	1951	46	0
3	C	1612	0	1677	57	0
4	D	1703	0	1763	45	0
5	E	1146	0	1207	41	0
6	F	843	0	857	25	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	29	0
9	I	1010	0	1037	46	0
10	J	792	0	835	25	0
11	K	864	0	881	22	0
12	L	972	0	1058	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	937	0	995	38	0
14	N	492	0	529	15	0
15	O	729	0	768	17	0
16	P	700	0	720	17	0
17	Q	823	0	893	29	0
18	R	574	0	644	17	0
19	S	647	0	673	23	0
20	T	763	0	861	29	0
21	U	208	0	221	10	0
22	A	40	0	36	4	0
23	A	272	0	0	0	0
23	B	2	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	3	0	0	0	0
23	K	1	0	0	0	0
23	M	2	0	0	0	0
23	N	2	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
23	S	1	0	0	0	0
23	T	3	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	392	0	0	10	0
25	D	1	0	0	0	0
25	E	7	0	0	0	0
25	G	1	0	0	0	0
25	L	1	0	0	0	0
25	P	2	0	0	0	0
25	T	2	0	0	1	0
25	U	1	0	0	0	0
All	All	52337	0	36512	952	1

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 (952) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:ARG:HD3	2:B:22:LYS:H	1.40	0.86
1:A:664:G:H22	1:A:741:G:H1	1.20	0.86
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.58	0.85
1:A:1126:U:O4	1:A:1148:U:N3	2.11	0.84
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.60	0.83
8:H:51:VAL:HG21	8:H:60:ARG:HG3	1.61	0.83
1:A:144:G:H1	1:A:178:C:H42	1.24	0.83
1:A:1443:G:H5''	1:A:1446:A:H5'	1.61	0.82
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.62	0.82
3:C:77:ILE:HG22	3:C:81:GLY:HA2	1.60	0.81
1:A:793:U:H3'	1:A:794:A:H5''	1.62	0.80
10:J:37:PRO:HA	10:J:72:VAL:H	1.47	0.79
1:A:279:A:OP2	17:Q:95:TYR:OH	2.01	0.78
1:A:1496:C:O2'	1:A:1497:G:O5'	1.99	0.78
8:H:69:ARG:NH1	8:H:75:ARG:O	2.16	0.78
1:A:527:7MG:OP2	22:A:1601:SRV:O32	2.02	0.78
1:A:792:A:H1'	1:A:793:U:H5''	1.64	0.78
1:A:103:C:OP1	20:T:17:ARG:NH1	2.16	0.77
1:A:1238:A:H5'	1:A:1336:C:H41	1.49	0.77
7:G:70:LYS:HB3	7:G:96:GLN:HG2	1.67	0.77
13:M:16:ASP:OD1	13:M:16:ASP:N	2.18	0.77
1:A:926:G:N2	1:A:1542:U:OP1	2.16	0.77
1:A:839:U:H5'	1:A:840:C:H5	1.49	0.77
20:T:12:ALA:HA	25:T:302:HOH:O	1.85	0.76
1:A:1158:C:N3	1:A:1181:G:N2	2.34	0.76
2:B:22:LYS:O	2:B:22:LYS:NZ	2.16	0.76
5:E:64:ARG:O	5:E:65:ASN:ND2	2.17	0.76
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.69	0.74
1:A:517:G:N1	1:A:533:A:OP2	2.13	0.74
1:A:991:U:O4	1:A:1212:U:O2'	2.05	0.74
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.69	0.74
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.71	0.73
1:A:1313:U:H5	19:S:4:SER:HB3	1.54	0.72
1:A:1338:G:H2'	1:A:1339:A:C8	2.24	0.72
1:A:1493:A:H2'	1:A:1494:G:C8	2.25	0.72
1:A:1000:U:H3	1:A:1041:A:H61	1.35	0.71
1:A:1007:C:H1'	1:A:1023:G:H1	1.55	0.71
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.73	0.71
3:C:79:ARG:H	3:C:79:ARG:HD3	1.54	0.71
1:A:235:C:N4	25:A:1969:HOH:O	2.24	0.70
1:A:78:G:O6	1:A:91:C:N4	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1280:A:O2'	25:A:2110:HOH:O	2.08	0.70
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.06	0.70
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.72	0.70
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.74	0.70
1:A:1323:G:OP2	19:S:3:ARG:NH1	2.25	0.69
2:B:118:LEU:HB3	2:B:142:LEU:HD12	1.73	0.69
3:C:167:TRP:HE3	3:C:168:ALA:H	1.40	0.69
1:A:1510:U:H2'	1:A:1511:G:C8	2.27	0.69
1:A:1373:G:H5''	7:G:36:LYS:HE3	1.73	0.69
2:B:21:ARG:HA	2:B:39:ILE:HG23	1.75	0.69
16:P:68:ASP:OD1	16:P:68:ASP:N	2.17	0.69
1:A:673:G:H5''	6:F:87:ARG:NH1	2.07	0.69
1:A:953:G:H5'	1:A:965:A:H61	1.58	0.68
2:B:20:GLU:HB2	2:B:190:THR:HB	1.75	0.68
1:A:263:A:OP2	20:T:79:ARG:NH1	2.25	0.68
1:A:95:U:H2'	1:A:96:G:H8	1.58	0.68
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.34	0.68
1:A:250:A:H4'	1:A:251:G:O5'	1.94	0.68
1:A:788:U:O2'	1:A:1539:C:O2	2.11	0.68
7:G:17:VAL:HG12	7:G:18:TYR:HD1	1.59	0.67
1:A:501:C:H2'	1:A:502:G:C8	2.29	0.67
13:M:25:ILE:HD11	13:M:66:LEU:HD21	1.76	0.67
1:A:1368:G:H5''	9:I:112:LYS:HB3	1.75	0.67
1:A:1435:G:H2'	1:A:1436:U:C6	2.29	0.67
1:A:692:U:OP1	11:K:124:LYS:NZ	2.27	0.67
11:K:58:PRO:HB3	11:K:93:GLN:HG3	1.77	0.67
1:A:413:G:O2'	1:A:428:G:N2	2.28	0.67
1:A:996:A:N1	1:A:1046:A:O2'	2.24	0.67
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.76	0.67
5:E:76:ILE:HG22	5:E:78:HIS:H	1.60	0.67
1:A:113:G:H1'	1:A:354:G:H5'	1.76	0.67
1:A:1047:G:H5''	14:N:4:LYS:HD3	1.77	0.67
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.77	0.66
1:A:95:U:H2'	1:A:96:G:C8	2.30	0.66
1:A:973:G:H3'	1:A:974:A:H5''	1.77	0.66
19:S:11:VAL:HG22	19:S:39:THR:HB	1.77	0.66
1:A:858:G:N7	25:A:2236:HOH:O	2.26	0.66
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.76	0.66
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.77	0.66
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.28	0.66
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ILE:HG22	2:B:228:GLY:HA3	1.75	0.65
18:R:20:ALA:O	18:R:55:ARG:NH1	2.26	0.65
20:T:67:ALA:HA	20:T:73:HIS:H	1.61	0.65
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.30	0.65
1:A:451:A:O2'	25:A:2126:HOH:O	2.15	0.65
1:A:1305:G:N2	1:A:1331:G:H1'	2.11	0.65
1:A:1061:G:H1	1:A:1195:C:H42	1.44	0.65
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.79	0.65
4:D:102:ASP:OD1	4:D:103:ASN:N	2.29	0.65
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.78	0.65
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.79	0.65
1:A:976:G:OP2	1:A:1358:U:H1'	1.98	0.64
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.23	0.64
5:E:144:THR:OG1	5:E:147:ASP:OD1	2.12	0.64
1:A:694:A:N1	1:A:787:A:O2'	2.30	0.64
1:A:1195:C:H3'	1:A:1196:U:H5''	1.78	0.63
2:B:240:GLN:N	2:B:240:GLN:OE1	2.31	0.63
1:A:390:C:H4'	16:P:28:ARG:HH21	1.64	0.63
1:A:269:C:H2'	1:A:270:A:C8	2.33	0.63
1:A:1125:U:O4	10:J:5:ARG:NH2	2.29	0.63
1:A:1392:G:N2	1:A:1502:A:H8	1.97	0.63
11:K:15:ALA:HA	11:K:77:MET:HA	1.79	0.63
21:U:6:ARG:HG2	21:U:15:ARG:HE	1.62	0.63
1:A:691:G:H3'	11:K:26:ASN:HD21	1.64	0.63
1:A:1419:G:H1	1:A:1481:U:H3	1.47	0.63
1:A:617:G:H1	1:A:623:C:H42	1.44	0.63
5:E:101:ILE:O	5:E:120:THR:HB	1.99	0.63
1:A:372:C:H4'	1:A:373:A:O5'	1.98	0.62
1:A:1057:G:H5''	3:C:154:SER:HB2	1.81	0.62
1:A:1532:U:H2'	1:A:1533:C:H3'	1.81	0.62
2:B:124:SER:HB2	2:B:126:GLU:HG2	1.79	0.62
7:G:38:LEU:O	7:G:42:ILE:HG13	2.00	0.62
9:I:17:VAL:HG22	9:I:63:ILE:HG23	1.81	0.62
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.81	0.62
12:L:41:ARG:HG2	12:L:42:THR:H	1.64	0.62
1:A:1412:C:H2'	1:A:1413:A:C8	2.34	0.62
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.15	0.62
1:A:80:G:H1	1:A:89:C:H42	1.48	0.62
1:A:673:G:H2'	1:A:674:G:C8	2.34	0.62
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.81	0.62
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.32	0.62
18:R:36:ASN:ND2	18:R:39:VAL:HG12	2.15	0.62
1:A:1392:G:H21	1:A:1502:A:H8	1.47	0.62
3:C:156:ARG:NH1	3:C:160:ALA:O	2.31	0.62
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.81	0.62
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.82	0.62
1:A:789:U:OP1	1:A:1539:C:N4	2.30	0.61
8:H:46:LYS:NZ	8:H:63:LEU:O	2.28	0.61
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.15	0.61
3:C:147:LYS:NZ	3:C:206:GLU:OE1	2.30	0.61
1:A:835:U:OP1	18:R:64:ARG:NH2	2.31	0.61
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.82	0.61
1:A:1285:A:H4'	1:A:1286:A:O5'	2.00	0.61
1:A:1316:G:N2	1:A:1319:A:OP2	2.34	0.61
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.82	0.61
1:A:560:U:H5'	1:A:566:G:N2	2.15	0.61
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.83	0.61
1:A:1278:U:H5'	1:A:1279:A:H5'	1.83	0.60
13:M:12:ASN:H	13:M:45:VAL:HG12	1.66	0.60
17:Q:81:ARG:HH11	17:Q:84:LEU:HD11	1.67	0.60
3:C:25:GLY:O	3:C:29:TYR:HB2	2.00	0.60
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.81	0.60
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.82	0.60
1:A:452:A:O2'	1:A:453:A:O4'	2.13	0.60
1:A:1347:G:O6	9:I:10:ARG:NH2	2.34	0.60
1:A:1358:U:H5''	14:N:35:ARG:HE	1.66	0.60
1:A:881:G:OP2	12:L:12:ARG:NH2	2.34	0.60
9:I:97:LYS:HB2	9:I:102:LEU:HD12	1.82	0.60
1:A:793:U:H3'	1:A:794:A:C5'	2.32	0.60
20:T:50:GLU:H	20:T:99:LEU:HD12	1.67	0.60
1:A:1037:C:N3	1:A:1038:C:N4	2.51	0.59
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.35	0.59
19:S:3:ARG:HD3	19:S:3:ARG:H	1.67	0.59
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.83	0.59
1:A:1427:U:H2'	1:A:1428:A:C8	2.38	0.59
1:A:1355:G:H2'	1:A:1356:G:H8	1.68	0.59
2:B:19:HIS:HD2	2:B:20:GLU:HG2	1.65	0.59
20:T:87:LYS:O	20:T:91:LEU:HB2	2.01	0.59
9:I:5:TYR:HD2	9:I:6:GLY:N	2.01	0.59
9:I:50:LEU:HD11	9:I:81:ILE:HD13	1.84	0.59
11:K:57:THR:HG23	11:K:60:ALA:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H4'	1:A:976:G:O5'	2.03	0.59
1:A:1407:5MC:HN41	1:A:1494:G:H1	1.49	0.59
3:C:121:ALA:HB2	3:C:198:VAL:HG21	1.84	0.59
6:F:87:ARG:HG3	6:F:87:ARG:HH11	1.67	0.59
13:M:108:ARG:HH22	13:M:111:LYS:HD2	1.68	0.59
1:A:695:A:C2	1:A:787:A:H1'	2.38	0.59
1:A:620:C:C2	4:D:135:LEU:HD22	2.38	0.58
1:A:1009:G:H1	1:A:1020:U:H3	1.51	0.58
1:A:1168:A:H2'	1:A:1169:A:C8	2.38	0.58
3:C:56:ASP:HB2	3:C:67:THR:HB	1.84	0.58
9:I:3:GLN:HB2	9:I:20:ARG:HG2	1.84	0.58
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.84	0.58
16:P:51:VAL:O	16:P:52:ASP:HB3	2.03	0.58
1:A:537:G:OP1	12:L:113:ARG:NH2	2.37	0.58
1:A:457:C:H2'	1:A:458:C:H6	1.68	0.58
9:I:19:LEU:HD11	9:I:81:ILE:HG12	1.83	0.58
1:A:518:C:H2'	1:A:530:G:C8	2.38	0.58
8:H:17:THR:HG22	8:H:63:LEU:HG	1.85	0.58
13:M:2:ALA:O	13:M:10:PRO:HD2	2.04	0.58
19:S:53:ASN:ND2	19:S:76:PRO:O	2.33	0.58
1:A:328:C:H2'	1:A:328:C:O2	2.03	0.58
1:A:1200:C:H1'	1:A:1204:A:H62	1.69	0.58
1:A:1279:A:H4'	1:A:1280:A:OP1	2.02	0.58
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.38	0.58
1:A:992:U:H3	1:A:1044:A:N6	2.02	0.58
6:F:8:ILE:HD13	6:F:26:ILE:HD13	1.85	0.58
1:A:1201:A:H4'	1:A:1202:G:O5'	2.04	0.58
10:J:68:HIS:HB3	10:J:70:ARG:HH12	1.69	0.58
19:S:22:LEU:HD13	19:S:28:LYS:HD2	1.86	0.58
21:U:18:TYR:CD2	21:U:24:ARG:HG2	2.38	0.57
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.24	0.57
1:A:457:C:H2'	1:A:458:C:C6	2.39	0.57
9:I:126:SER:OG	9:I:127:LYS:N	2.37	0.57
1:A:411:A:H62	1:A:413:G:H21	1.51	0.57
1:A:826:C:O2	8:H:15:ASN:ND2	2.38	0.57
1:A:839:U:H5'	1:A:840:C:C5	2.36	0.57
4:D:8:VAL:O	4:D:11:LEU:N	2.37	0.57
5:E:18:ARG:HG2	5:E:19:MET:N	2.20	0.57
1:A:1111:A:H61	3:C:177:THR:HG22	1.70	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.70	0.57
1:A:677:U:H3	1:A:713:G:H22	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.87	0.57
13:M:79:LYS:HE3	13:M:82:MET:HE3	1.87	0.57
1:A:56:U:H2'	1:A:57:G:H8	1.70	0.56
1:A:1126:U:OP1	1:A:1127:G:N2	2.38	0.56
3:C:124:ILE:HG21	3:C:196:LEU:HD12	1.87	0.56
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.40	0.56
1:A:5:U:H4'	1:A:6:G:O5'	2.03	0.56
1:A:1361(A):C:HO2'	1:A:1362:C:H6	1.53	0.56
1:A:1442:G:N7	1:A:1446:A:N6	2.52	0.56
1:A:825:G:H21	8:H:11:THR:HG21	1.69	0.56
1:A:1004:A:H1'	1:A:1038:C:H42	1.70	0.56
1:A:1442:G:N2	1:A:1447:G:N7	2.54	0.56
1:A:532:A:O2'	1:A:533:A:OP1	2.16	0.56
1:A:1280:A:H3'	1:A:1281:U:H5'	1.87	0.56
1:A:129:U:O3'	1:A:129(A):G:H3'	2.06	0.56
22:A:1601:SRV:OG2	12:L:91:LYS:NZ	2.37	0.56
2:B:23:ARG:O	2:B:24:TRP:HD1	1.89	0.56
5:E:77:PRO:HD2	5:E:142:LEU:HD13	1.86	0.56
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.70	0.56
10:J:6:ILE:HD12	10:J:98:ILE:HG12	1.88	0.56
7:G:42:ILE:HG22	7:G:120:ILE:HD12	1.88	0.56
18:R:43:PHE:HD2	18:R:56:THR:HG22	1.69	0.56
18:R:43:PHE:C	18:R:51:LEU:HD12	2.27	0.56
9:I:121:ARG:NH1	9:I:122:ALA:O	2.39	0.56
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.71	0.55
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.71	0.55
13:M:54:VAL:O	13:M:58:GLU:HG2	2.06	0.55
1:A:149:A:H2'	1:A:150:C:C6	2.42	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.55
7:G:45:ASP:HA	7:G:48:LYS:HD2	1.88	0.55
1:A:9:G:OP2	5:E:121:LYS:NZ	2.21	0.55
1:A:950:U:H2'	1:A:951:G:C8	2.41	0.55
11:K:91:ARG:HH12	18:R:88:LYS:HZ3	1.54	0.55
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.22	0.55
1:A:89:C:H2'	1:A:90:U:O4'	2.06	0.55
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.55
1:A:56:U:H2'	1:A:57:G:C8	2.42	0.55
1:A:110:C:H2'	1:A:111:G:O4'	2.07	0.55
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.41	0.55
9:I:23:ASN:HB3	9:I:25:LYS:HE2	1.88	0.55
1:A:412:A:H1'	1:A:413:G:OP2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.89	0.55
1:A:731:G:OP1	1:A:766:A:H1'	2.06	0.55
1:A:1198:G:H2'	1:A:1199:U:C6	2.42	0.55
5:E:28:PHE:CD2	5:E:51:VAL:HG23	2.42	0.55
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.06	0.55
1:A:184:G:H2'	1:A:185:A:H8	1.71	0.55
1:A:542:G:OP1	4:D:10:ARG:NH2	2.40	0.54
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.19	0.54
5:E:137:GLU:O	5:E:141:GLN:HG3	2.07	0.54
12:L:8:ASN:O	12:L:12:ARG:HG3	2.07	0.54
1:A:251:G:H4'	1:A:252:U:OP1	2.07	0.54
1:A:563:A:H2'	1:A:567:G:C8	2.42	0.54
1:A:411:A:N6	1:A:413:G:H21	2.04	0.54
7:G:75:VAL:HG11	7:G:86:GLN:HB3	1.89	0.54
5:E:146:ALA:O	5:E:149:GLU:HG2	2.07	0.54
13:M:108:ARG:NH2	13:M:111:LYS:HD2	2.23	0.54
1:A:518:C:H5''	1:A:519:C:C6	2.42	0.54
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.23	0.54
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.89	0.54
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.72	0.54
1:A:411:A:C5	1:A:413:G:H1'	2.43	0.53
16:P:9:PHE:HD2	16:P:18:ARG:HG3	1.72	0.53
1:A:384:G:H2'	1:A:385:C:C6	2.43	0.53
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.39	0.53
1:A:406:G:H21	4:D:119:GLN:HE22	1.56	0.53
1:A:1391:U:H2'	1:A:1392:G:C8	2.44	0.53
3:C:155:GLY:O	3:C:196:LEU:HD22	2.07	0.53
4:D:55:ALA:O	4:D:59:ARG:HG2	2.08	0.53
9:I:32:ASP:OD1	9:I:33:PHE:N	2.42	0.53
1:A:1505:G:O2'	1:A:1506:U:OP2	2.18	0.53
1:A:518:C:H4'	1:A:519:C:O5'	2.07	0.53
1:A:881:G:P	12:L:12:ARG:HH22	2.30	0.53
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.41	0.53
15:O:22:THR:OG1	15:O:23:GLY:N	2.42	0.53
1:A:1037:C:H2'	1:A:1038:C:C6	2.44	0.53
1:A:1275:A:H2'	1:A:1276:G:O4'	2.09	0.53
13:M:117:VAL:HG12	13:M:118:ALA:H	1.74	0.53
1:A:17:U:H2'	1:A:18:C:C6	2.44	0.53
2:B:157:ARG:HG2	2:B:158:LEU:N	2.22	0.53
3:C:157:ILE:HD11	3:C:164:ARG:HB2	1.91	0.53
1:A:953:G:H2'	1:A:954:G:O4'	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1152:A:H5''	10:J:13:HIS:ND1	2.23	0.53
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.42	0.53
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.91	0.53
1:A:254:G:OP1	17:Q:67:LYS:O	2.27	0.53
13:M:19:LEU:HD21	13:M:56:LEU:HD11	1.90	0.53
1:A:321:A:N6	1:A:329:A:OP2	2.38	0.53
1:A:1314:C:C5	19:S:6:LYS:HD3	2.43	0.53
18:R:59:SER:H	18:R:62:GLU:HB2	1.74	0.53
1:A:90:U:H2'	1:A:91:C:C6	2.44	0.52
1:A:269:C:H2'	1:A:270:A:H8	1.73	0.52
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.91	0.52
1:A:47:C:C6	1:A:365:U:H2'	2.44	0.52
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.92	0.52
1:A:413:G:H22	1:A:429:U:H5''	1.74	0.52
1:A:840:C:H5''	1:A:841:U:OP1	2.09	0.52
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.91	0.52
12:L:41:ARG:HG2	12:L:42:THR:N	2.24	0.52
1:A:1303:C:H2'	1:A:1304:G:H5'	1.92	0.52
13:M:63:THR:HG23	13:M:64:TRP:H	1.74	0.52
1:A:179:A:H2'	1:A:180:U:C6	2.43	0.52
1:A:279:A:C4	17:Q:98:LEU:HD22	2.44	0.52
1:A:657:G:H4'	15:O:28:GLN:HG2	1.91	0.52
1:A:1025:U:O2	1:A:1026:G:N2	2.43	0.52
1:A:1376:U:OP1	7:G:98:SER:OG	2.18	0.52
3:C:87:LEU:HD22	3:C:101:LEU:HD11	1.92	0.52
5:E:152:ARG:O	8:H:64:LYS:NZ	2.43	0.52
19:S:28:LYS:HD3	19:S:29:ARG:H	1.74	0.52
1:A:966:M2G:HM22	1:A:967:5MC:C2	2.44	0.52
1:A:1205:U:H5''	3:C:190:ARG:HE	1.74	0.52
17:Q:75:ARG:HH11	17:Q:75:ARG:HB2	1.74	0.52
1:A:950:U:H2'	1:A:951:G:H8	1.75	0.52
1:A:1200:C:H1'	1:A:1204:A:N6	2.24	0.52
3:C:83:ARG:HA	3:C:86:VAL:HB	1.90	0.52
3:C:44:GLU:HA	3:C:52:LEU:HD13	1.92	0.52
12:L:24:VAL:HG12	12:L:24:VAL:O	2.10	0.52
1:A:914:A:OP1	22:A:1601:SRY:HI33	2.10	0.52
1:A:1079:G:O3'	5:E:14:ARG:NH2	2.43	0.52
1:A:1313:U:C5	19:S:4:SER:HB3	2.39	0.52
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.91	0.52
20:T:11:SER:HA	20:T:13:LEU:HD11	1.92	0.52
1:A:1000:U:H2'	1:A:1001:A:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:U:H4'	25:A:2111:HOH:O	2.09	0.52
18:R:25:THR:O	18:R:25:THR:OG1	2.24	0.52
1:A:538:G:P	12:L:115:LYS:HB2	2.50	0.51
11:K:91:ARG:HH22	18:R:88:LYS:HZ3	1.56	0.51
1:A:1347:G:N2	1:A:1373:G:H2'	2.25	0.51
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.91	0.51
6:F:33:TYR:HE2	6:F:74:ASP:HB3	1.75	0.51
20:T:65:LYS:HA	20:T:68:LYS:HG3	1.91	0.51
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.91	0.51
1:A:226:G:N2	25:A:2121:HOH:O	2.18	0.51
19:S:55:LYS:HG3	19:S:56:GLN:HG3	1.92	0.51
13:M:23:TYR:HB3	13:M:67:GLU:H	1.76	0.51
1:A:149:A:H2'	1:A:150:C:H6	1.75	0.51
18:R:51:LEU:HD23	18:R:52:PRO:HD2	1.92	0.51
1:A:1007:C:H1'	1:A:1023:G:N1	2.23	0.51
1:A:1047:G:OP1	14:N:4:LYS:NZ	2.28	0.51
1:A:1266:G:N2	1:A:1269:A:OP2	2.41	0.51
1:A:1366:C:H2'	1:A:1367:C:C6	2.45	0.51
5:E:147:ASP:OD1	5:E:147:ASP:N	2.29	0.51
7:G:46:ALA:HA	7:G:49:ILE:HD12	1.93	0.51
4:D:13:ARG:NH2	4:D:36:ARG:HH21	2.08	0.51
1:A:117:G:O5'	1:A:117:G:H8	1.94	0.51
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.51
5:E:84:PHE:HB3	5:E:134:ALA:HB2	1.93	0.51
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.91	0.51
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.93	0.51
1:A:558:G:H3'	1:A:559:A:H3'	1.91	0.51
5:E:151:LEU:HD23	8:H:79:VAL:HG22	1.92	0.51
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.92	0.51
1:A:191:G:O2'	20:T:102:GLY:O	2.18	0.50
1:A:701:C:H5''	1:A:703:G:H5'	1.93	0.50
1:A:955:U:H1'	1:A:1227:A:N6	2.26	0.50
4:D:187:ARG:CZ	4:D:188:LEU:H	2.24	0.50
1:A:321:A:H2'	1:A:322:C:H6	1.77	0.50
1:A:503:C:OP2	12:L:116:SER:HB3	2.12	0.50
1:A:675:A:O2'	11:K:114:VAL:O	2.24	0.50
1:A:1357:A:H2'	1:A:1358:U:C6	2.46	0.50
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.94	0.50
14:N:39:LEU:HB3	14:N:43:CYS:CB	2.41	0.50
20:T:92:LEU:O	20:T:96:GLY:HA2	2.11	0.50
1:A:352:C:H4'	1:A:354:G:OP1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:A:O2'	1:A:453:A:O5'	2.29	0.50
1:A:686:U:O2'	1:A:687:A:H8	1.94	0.50
4:D:13:ARG:NH1	4:D:38:TYR:O	2.44	0.50
16:P:14:ASN:HA	16:P:42:ARG:HH21	1.76	0.50
19:S:10:PHE:O	19:S:39:THR:OG1	2.28	0.50
1:A:965:A:OP1	1:A:1198:G:H5''	2.11	0.50
1:A:1021:G:C2	1:A:1022:G:H1'	2.47	0.50
12:L:47:LYS:N	12:L:48:PRO:HD2	2.26	0.50
20:T:35:THR:HA	20:T:38:LYS:HE3	1.93	0.50
13:M:59:TYR:O	13:M:63:THR:HG22	2.11	0.50
15:O:36:ILE:HG13	15:O:59:MET:HE2	1.93	0.50
1:A:1314:C:H2'	1:A:1315:U:C6	2.47	0.50
3:C:148:GLY:HA3	3:C:172:ARG:O	2.12	0.50
14:N:57:ARG:HG2	14:N:58:LYS:H	1.77	0.50
1:A:413:G:HO2'	1:A:414:A:P	2.35	0.50
1:A:877:C:O2'	8:H:3:THR:HG23	2.10	0.50
1:A:1308:U:OP2	13:M:99:ARG:HG3	2.11	0.50
11:K:78:GLN:O	11:K:103:LEU:HD23	2.12	0.50
1:A:1229:A:OP1	13:M:116:THR:OG1	2.29	0.50
5:E:152:ARG:NH2	8:H:107:LEU:O	2.40	0.50
6:F:22:GLU:OE2	6:F:82:ARG:NH2	2.45	0.50
1:A:451:A:N6	1:A:481:G:C4	2.80	0.49
9:I:48:GLU:N	9:I:49:PRO:HD2	2.27	0.49
12:L:25:PRO:HA	12:L:27:LEU:HB2	1.94	0.49
13:M:108:ARG:HD2	13:M:114:ARG:NH1	2.27	0.49
17:Q:26:GLN:HG2	17:Q:37:LYS:HB2	1.94	0.49
1:A:184:G:H2'	1:A:185:A:C8	2.47	0.49
1:A:411:A:H62	1:A:413:G:N2	2.11	0.49
1:A:1101:A:H4'	1:A:1102:A:O5'	2.12	0.49
3:C:43:LEU:O	3:C:47:LEU:HB2	2.11	0.49
11:K:124:LYS:HG3	11:K:125:PHE:CD2	2.47	0.49
17:Q:60:ILE:HB	17:Q:74:LEU:HG	1.94	0.49
1:A:380:G:N2	1:A:383:A:OP2	2.38	0.49
1:A:1124:G:H5'	10:J:35:SER:O	2.13	0.49
1:A:1502:A:H2	1:A:1505:G:H1	1.59	0.49
2:B:102:LEU:HD21	2:B:162:ILE:HD11	1.94	0.49
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.93	0.49
13:M:37:THR:HG23	13:M:55:ARG:HG2	1.94	0.49
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.95	0.49
1:A:667:G:H4'	15:O:51:HIS:CE1	2.48	0.49
1:A:1190:G:HO2'	1:A:1191:A:P	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1493:A:H2'	1:A:1494:G:H8	1.78	0.49
6:F:23:LYS:O	6:F:27:GLN:HG2	2.12	0.49
1:A:1145:C:H1'	1:A:1146:A:C8	2.47	0.49
1:A:1293:G:H2'	1:A:1294:G:O4'	2.12	0.49
10:J:15:THR:OG1	10:J:91:PRO:HB3	2.12	0.49
1:A:371:G:O2'	1:A:372:C:H5'	2.11	0.49
1:A:567:G:H2'	1:A:568:G:O4'	2.13	0.49
1:A:946:A:H2'	1:A:947:G:C8	2.48	0.49
1:A:1372:U:H2'	1:A:1373:G:O4'	2.13	0.49
3:C:70:VAL:O	3:C:106:VAL:N	2.45	0.49
8:H:85:ARG:NE	8:H:87:SER:O	2.46	0.49
20:T:71:THR:O	20:T:72:LEU:HD23	2.13	0.49
1:A:251:G:H4'	1:A:252:U:H5''	1.94	0.49
1:A:1443:G:H5''	1:A:1446:A:C5'	2.37	0.49
19:S:33:THR:HG22	19:S:35:SER:H	1.78	0.49
1:A:1305:G:H22	1:A:1331:G:H1'	1.76	0.49
1:A:35:G:H2'	1:A:36:C:C6	2.47	0.48
1:A:972:C:H4'	10:J:57:LYS:HD3	1.95	0.48
1:A:1190:G:OP1	3:C:4:LYS:HA	2.12	0.48
2:B:107:THR:O	2:B:110:GLN:HB2	2.13	0.48
1:A:1287:A:H2'	1:A:1288:A:C8	2.49	0.48
3:C:25:GLY:HA2	3:C:28:GLN:H	1.78	0.48
4:D:190:ASP:OD1	4:D:191:ARG:N	2.40	0.48
13:M:108:ARG:HD2	13:M:114:ARG:CZ	2.43	0.48
16:P:22:THR:HA	16:P:33:ILE:HG13	1.96	0.48
1:A:827:U:H5''	1:A:828:A:OP2	2.13	0.48
1:A:691:G:H2'	1:A:692:U:C6	2.48	0.48
1:A:984:C:H42	1:A:1221:G:H1	1.61	0.48
5:E:144:THR:O	5:E:148:VAL:HG23	2.13	0.48
1:A:321:A:H2'	1:A:322:C:C6	2.49	0.48
1:A:1441:G:H4'	1:A:1442:G:C5	2.49	0.48
2:B:135:GLN:O	2:B:139:LYS:HB2	2.14	0.48
3:C:23:TYR:HD2	10:J:95:GLU:HG3	1.78	0.48
6:F:78:GLU:HG3	6:F:81:ILE:HD12	1.95	0.48
9:I:42:ARG:HH21	9:I:71:SER:HB2	1.77	0.48
10:J:32:ALA:O	10:J:34:VAL:HG23	2.12	0.48
1:A:481:G:HO2'	1:A:482:A:H8	1.54	0.48
1:A:714:G:H2'	1:A:715:A:C8	2.48	0.48
1:A:869:G:N7	25:A:2235:HOH:O	2.35	0.48
3:C:73:PRO:O	3:C:77:ILE:HG12	2.12	0.48
6:F:14:LEU:HD22	6:F:18:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:61:LYS:O	18:R:65:ILE:HG13	2.14	0.48
1:A:594:G:H1	1:A:645:C:H42	1.62	0.48
1:A:1064:G:H1'	1:A:1190:G:H21	1.77	0.48
1:A:1258:G:H2'	1:A:1259:C:C6	2.48	0.48
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.32	0.48
15:O:6:GLU:OE1	15:O:6:GLU:N	2.22	0.48
1:A:45:U:H2'	1:A:46:G:C8	2.49	0.48
1:A:392:G:H2'	1:A:393:A:C8	2.49	0.48
1:A:688:G:O2'	1:A:704:A:N1	2.31	0.48
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.96	0.48
1:A:636:U:H5'	17:Q:2:PRO:HG3	1.96	0.48
1:A:1211:U:O2'	1:A:1213:A:N3	2.38	0.48
1:A:1303:C:C2'	1:A:1304:G:H5'	2.44	0.48
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.42	0.48
20:T:44:ALA:HB1	20:T:91:LEU:HB3	1.96	0.48
1:A:353:A:H5'	1:A:353:A:C8	2.49	0.47
1:A:838:G:H2'	1:A:839:U:H5''	1.96	0.47
1:A:1279:A:O2'	1:A:1280:A:O5'	2.31	0.47
3:C:27:LYS:O	3:C:30:ARG:NH2	2.46	0.47
5:E:76:ILE:HG23	5:E:77:PRO:HD2	1.96	0.47
1:A:586:C:C2'	1:A:587:G:H5'	2.43	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.29	0.47
1:A:1126:U:C4	1:A:1149:C:H1'	2.49	0.47
3:C:153:VAL:HG12	3:C:166:GLU:HB2	1.97	0.47
4:D:15:GLU:HG3	4:D:63:LYS:NZ	2.28	0.47
5:E:46:GLY:H	5:E:58:ALA:HB2	1.80	0.47
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.34	0.47
9:I:92:TYR:O	9:I:96:LEU:HB2	2.13	0.47
12:L:7:ILE:HD13	12:L:7:ILE:HA	1.63	0.47
1:A:580:U:H2'	1:A:581:G:O4'	2.13	0.47
1:A:1195:C:H3'	1:A:1196:U:C5'	2.42	0.47
1:A:1435:G:H2'	1:A:1436:U:H6	1.79	0.47
7:G:18:TYR:HE2	7:G:59:LEU:HA	1.79	0.47
10:J:16:LEU:HD12	10:J:68:HIS:HB2	1.95	0.47
13:M:80:ARG:HH11	13:M:80:ARG:HB3	1.79	0.47
1:A:179:A:H2'	1:A:180:U:H6	1.79	0.47
1:A:532:A:H2'	1:A:533:A:H5''	1.96	0.47
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.15	0.47
2:B:178:ARG:NH1	8:H:71:GLY:O	2.47	0.47
11:K:27:ASN:OD1	11:K:28:THR:N	2.48	0.47
16:P:51:VAL:HG12	16:P:52:ASP:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:G:H8	1:A:1068:G:OP2	1.98	0.47
1:A:1391:U:H2'	1:A:1392:G:H8	1.79	0.47
2:B:17:PHE:HD1	2:B:18:GLY:H	1.63	0.47
4:D:2:GLY:HA3	4:D:5:ILE:HD11	1.97	0.47
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.50	0.47
11:K:124:LYS:HE3	11:K:124:LYS:HB2	1.66	0.47
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.97	0.47
1:A:1141:C:H2'	1:A:1142:G:H8	1.80	0.47
6:F:60:PHE:CZ	18:R:78:LEU:HD21	2.50	0.47
8:H:118:VAL:O	8:H:119:LEU:HD23	2.15	0.47
13:M:3:ARG:HA	13:M:8:GLU:O	2.15	0.47
19:S:18:LYS:O	19:S:22:LEU:HG	2.15	0.47
20:T:74:LYS:HA	20:T:74:LYS:HD3	1.67	0.47
7:G:145:ALA:C	7:G:147:ALA:H	2.18	0.47
11:K:51:LYS:O	11:K:55:LYS:HE2	2.15	0.47
1:A:243:A:H4'	1:A:244:U:O5'	2.15	0.47
1:A:1182:G:H4'	1:A:1183:A:H3'	1.97	0.47
2:B:25:ASN:O	2:B:27:LYS:N	2.47	0.47
2:B:219:VAL:O	2:B:223:ILE:HG13	2.15	0.47
5:E:90:VAL:O	5:E:91:LEU:HD23	2.14	0.47
5:E:139:LEU:HD23	5:E:139:LEU:HA	1.69	0.47
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.50	0.47
12:L:65:GLU:OE1	12:L:65:GLU:N	2.48	0.47
14:N:39:LEU:HB3	14:N:43:CYS:HB2	1.97	0.47
1:A:421:U:H5'	1:A:422:C:H5	1.81	0.46
1:A:918:A:H2'	1:A:919:A:C8	2.50	0.46
1:A:1137:C:H4'	1:A:1138:G:C4	2.51	0.46
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.97	0.46
12:L:44:THR:HA	12:L:45:PRO:HD3	1.62	0.46
1:A:1130:A:H4'	9:I:20:ARG:NH2	2.30	0.46
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.15	0.46
1:A:1357:A:H2'	1:A:1358:U:H6	1.81	0.46
1:A:1542:U:H2'	1:A:1543:C:C6	2.49	0.46
10:J:61:GLU:HG3	14:N:58:LYS:HZ3	1.79	0.46
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.96	0.46
1:A:509:A:H5''	4:D:55:ALA:HB2	1.96	0.46
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.48	0.46
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.97	0.46
14:N:21:TYR:HE2	14:N:23:ARG:HH21	1.63	0.46
1:A:93:G:C2	1:A:95:U:C2	3.03	0.46
1:A:381:C:H2'	1:A:382:A:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:G:O2'	1:A:482:A:C8	2.64	0.46
2:B:54:THR:OG1	2:B:199:TYR:HB3	2.15	0.46
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.16	0.46
17:Q:10:VAL:HG22	17:Q:55:ASP:H	1.81	0.46
1:A:687:A:H4'	1:A:688:G:O5'	2.15	0.46
1:A:1366:C:H2'	1:A:1367:C:H6	1.80	0.46
2:B:101:MET:HA	2:B:108:ILE:HG13	1.97	0.46
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.98	0.46
7:G:108:ALA:O	7:G:119:ARG:HB3	2.15	0.46
12:L:85:ILE:HD11	12:L:100:ILE:HG13	1.98	0.46
1:A:397:A:H5'	1:A:398:C:OP1	2.16	0.46
1:A:1006:C:H2'	1:A:1007:C:C6	2.50	0.46
6:F:67:MET:HE3	6:F:67:MET:HB2	1.76	0.46
1:A:1257:U:O2'	1:A:1258:G:OP2	2.28	0.46
1:A:1397:C:O2'	1:A:1398:A:OP1	2.30	0.46
16:P:8:ARG:HB3	16:P:28:ARG:NH1	2.31	0.46
1:A:670:G:O2'	6:F:77:ARG:NH2	2.49	0.46
1:A:1375:A:H2'	1:A:1376:U:O4'	2.16	0.46
3:C:112:SER:O	3:C:116:VAL:HG23	2.16	0.46
5:E:65:ASN:CG	5:E:65:ASN:O	2.55	0.46
9:I:5:TYR:CD2	9:I:6:GLY:N	2.83	0.46
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.51	0.46
19:S:7:LYS:HB2	19:S:7:LYS:NZ	2.30	0.46
20:T:73:HIS:HB3	20:T:74:LYS:H	1.60	0.46
21:U:17:THR:O	21:U:22:ARG:NH1	2.48	0.46
1:A:369:C:OP2	1:A:388:G:N2	2.43	0.46
1:A:858:G:O2'	1:A:859:A:H5'	2.16	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.16	0.46
1:A:191:G:H1'	20:T:104:LEU:O	2.16	0.46
1:A:204:U:H4'	1:A:216:G:O4'	2.16	0.46
1:A:455:C:H6	1:A:455:C:O5'	1.99	0.46
1:A:1145:C:H1'	1:A:1146:A:N7	2.30	0.46
1:A:1288:A:N1	1:A:1371:G:H1'	2.31	0.46
3:C:188:LEU:HD13	3:C:196:LEU:O	2.15	0.46
9:I:50:LEU:HD22	9:I:85:LEU:HD13	1.98	0.45
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.51	0.45
1:A:485:G:O2'	1:A:486:U:P	2.74	0.45
1:A:502:G:H2'	1:A:503:C:O4'	2.15	0.45
1:A:1179:A:H2'	1:A:1180:A:O4'	2.16	0.45
5:E:103:GLY:O	5:E:106:PRO:HD2	2.16	0.45
21:U:10:ARG:HA	21:U:13:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:C:OP2	19:S:3:ARG:NH2	2.48	0.45
4:D:25:ARG:O	4:D:25:ARG:HG2	2.16	0.45
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.98	0.45
20:T:10:LEU:HD22	20:T:10:LEU:HA	1.79	0.45
1:A:748:C:H4'	1:A:749:C:O5'	2.15	0.45
1:A:818:G:O2'	1:A:819:A:H5'	2.17	0.45
1:A:974:A:H4'	1:A:975:A:H3'	1.99	0.45
1:A:1511:G:H2'	1:A:1512:U:O4'	2.16	0.45
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.81	0.45
4:D:176:LEU:HD21	4:D:178:VAL:HG13	1.98	0.45
9:I:97:LYS:N	9:I:98:PRO:HD2	2.32	0.45
10:J:34:VAL:HG22	10:J:74:ILE:HG23	1.99	0.45
12:L:27:LEU:C	12:L:29:GLY:N	2.68	0.45
1:A:7:G:H5''	1:A:298:A:O4'	2.16	0.45
1:A:1143:G:H2'	1:A:1144:G:C8	2.52	0.45
1:A:1323:G:H2'	1:A:1324:A:C8	2.52	0.45
3:C:69:HIS:HA	3:C:104:GLN:O	2.16	0.45
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.97	0.45
4:D:31:CYS:C	4:D:33:MET:H	2.19	0.45
6:F:15:ASP:OD2	6:F:18:GLN:NE2	2.49	0.45
1:A:92:C:H2'	1:A:93:G:C8	2.51	0.45
1:A:243:A:C2	1:A:246:A:C8	3.05	0.45
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.50	0.45
1:A:1310:G:H1	1:A:1327:C:H42	1.63	0.45
3:C:142:MET:HG3	3:C:170:GLN:HB2	1.97	0.45
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.51	0.45
6:F:2:ARG:O	6:F:66:GLU:HA	2.16	0.45
6:F:87:ARG:NH1	6:F:87:ARG:HG3	2.31	0.45
11:K:14:VAL:HG23	11:K:15:ALA:H	1.81	0.45
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.98	0.45
20:T:13:LEU:O	20:T:17:ARG:HG3	2.17	0.45
1:A:1095:U:H2'	1:A:1096:C:O4'	2.16	0.45
3:C:72:LYS:HE3	3:C:75:VAL:HG21	1.99	0.45
4:D:187:ARG:HD2	4:D:187:ARG:HA	1.53	0.45
4:D:187:ARG:HH12	4:D:188:LEU:HD12	1.81	0.45
12:L:25:PRO:CA	12:L:27:LEU:HB2	2.47	0.45
1:A:384:G:H2'	1:A:385:C:H6	1.82	0.45
1:A:692:U:H1'	1:A:695:A:N7	2.32	0.45
9:I:127:LYS:HA	9:I:127:LYS:HD3	1.57	0.45
10:J:21:GLN:O	10:J:25:GLU:HG3	2.17	0.45
1:A:144:G:H1	1:A:178:C:N4	2.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:A:H3'	1:A:397:A:N3	2.32	0.44
1:A:723:U:H2'	1:A:723:U:O2	2.17	0.44
1:A:1035:A:H2'	1:A:1036:G:C8	2.52	0.44
1:A:1347:G:H1'	1:A:1348:U:H5	1.82	0.44
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.64	0.44
6:F:79:LEU:HD23	6:F:79:LEU:HA	1.74	0.44
7:G:139:GLU:O	7:G:143:ARG:HB2	2.17	0.44
10:J:40:LEU:HB2	10:J:69:ASN:HB2	2.00	0.44
1:A:413:G:N2	1:A:429:U:OP2	2.49	0.44
1:A:1252:A:H2'	1:A:1253:G:O4'	2.18	0.44
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.99	0.44
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.44
15:O:87:ILE:HG22	15:O:88:ARG:HD3	1.98	0.44
1:A:289:G:P	25:A:1908:HOH:O	2.75	0.44
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.99	0.44
1:A:1133:G:N2	1:A:1141:C:O2	2.48	0.44
2:B:122:PHE:HA	2:B:127:ILE:HG21	1.99	0.44
3:C:107:GLN:CD	3:C:107:GLN:H	2.21	0.44
4:D:20:TYR:CD1	4:D:20:TYR:N	2.86	0.44
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.17	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.52	0.44
10:J:53:PRO:HA	14:N:41:ARG:HH22	1.83	0.44
1:A:78:G:H2'	1:A:79:G:H8	1.82	0.44
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.51	0.44
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.44
1:A:1437:C:H2'	1:A:1438:G:H8	1.83	0.44
4:D:35:ARG:C	4:D:36:ARG:HG2	2.38	0.44
6:F:23:LYS:HE3	6:F:23:LYS:HB2	1.68	0.44
1:A:686:U:O2'	1:A:687:A:C8	2.66	0.44
1:A:1191:A:H2'	1:A:1192:C:C6	2.53	0.44
1:A:1339:A:H2'	1:A:1340:A:O4'	2.17	0.44
7:G:16:LEU:HD21	9:I:42:ARG:HG2	2.00	0.44
1:A:186:C:H2'	1:A:187:C:C6	2.52	0.44
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.44
3:C:120:VAL:HG12	3:C:124:ILE:HD11	2.00	0.44
9:I:42:ARG:NH2	9:I:71:SER:HB2	2.32	0.44
12:L:54:LYS:HD2	12:L:54:LYS:N	2.32	0.44
13:M:67:GLU:HB3	13:M:68:GLY:H	1.51	0.44
1:A:411:A:C4	1:A:413:G:H1'	2.52	0.44
1:A:501:C:H2'	1:A:502:G:H8	1.75	0.44
1:A:715:A:H2'	1:A:716:A:C8	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1137:C:HO2'	1:A:1138:G:N2	2.15	0.44
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.99	0.44
14:N:25:VAL:HG13	14:N:38:GLY:O	2.17	0.44
17:Q:92:ARG:HH11	17:Q:92:ARG:HB3	1.83	0.44
1:A:279:A:C8	1:A:279:A:H5'	2.53	0.44
1:A:1225:A:H5'	1:A:1226:C:OP2	2.18	0.44
1:A:1399:C:O2	1:A:1401:G:C5	2.71	0.44
3:C:134:ILE:O	3:C:138:VAL:HG23	2.18	0.44
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.47	0.44
9:I:71:SER:HA	9:I:74:ILE:HD12	1.99	0.44
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.99	0.44
13:M:117:VAL:HG12	13:M:118:ALA:N	2.32	0.44
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.75	0.44
18:R:37:VAL:HG21	18:R:78:LEU:HB3	2.00	0.44
1:A:928:G:O2'	1:A:1533:C:OP1	2.36	0.44
1:A:966:M2G:HM22	1:A:967:5MC:O2	2.18	0.44
1:A:986:A:H4'	19:S:55:LYS:HZ3	1.82	0.44
4:D:50:ARG:HA	4:D:51:PRO:HD3	1.80	0.44
5:E:112:LEU:HD23	5:E:112:LEU:HA	1.77	0.44
6:F:77:ARG:O	6:F:81:ILE:HG13	2.18	0.44
7:G:51:GLN:HG2	7:G:58:PRO:HD3	1.99	0.44
16:P:74:LEU:O	16:P:79:VAL:HG23	2.17	0.44
1:A:617:G:H1	1:A:623:C:N4	2.13	0.43
1:A:1055:A:O2'	3:C:156:ARG:NH1	2.51	0.43
4:D:99:SER:HB3	4:D:139:ARG:HG3	2.00	0.43
10:J:38:ILE:HG12	10:J:71:LEU:HG	2.00	0.43
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.99	0.43
1:A:1090:U:H2'	1:A:1091:U:H6	1.81	0.43
1:A:1126:U:N3	1:A:1149:C:H1'	2.33	0.43
1:A:1358:U:H5'	14:N:35:ARG:H	1.82	0.43
3:C:156:ARG:HD2	3:C:159:GLY:HA2	2.00	0.43
9:I:112:LYS:HE3	9:I:117:HIS:O	2.17	0.43
11:K:19:ALA:HB2	11:K:80:VAL:HG21	2.00	0.43
19:S:12:ASP:CG	19:S:38:SER:HB3	2.38	0.43
1:A:451:A:O5'	1:A:451:A:H8	2.01	0.43
1:A:665:A:H2'	1:A:732:C:O2	2.17	0.43
1:A:1132:C:H2'	1:A:1133:G:H8	1.82	0.43
8:H:18:ARG:HD3	8:H:18:ARG:HA	1.87	0.43
9:I:49:PRO:O	9:I:53:VAL:HG23	2.18	0.43
12:L:83:VAL:HG21	12:L:100:ILE:HG12	2.00	0.43
13:M:17:VAL:O	13:M:20:THR:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:53:LEU:HB2	20:T:100:ILE:HD12	1.99	0.43
1:A:413:G:O2'	1:A:414:A:OP2	2.32	0.43
1:A:538:G:OP2	12:L:115:LYS:HB2	2.18	0.43
1:A:1255:G:O2'	1:A:1258:G:H1'	2.19	0.43
11:K:48:ILE:H	11:K:48:ILE:HG13	1.48	0.43
12:L:47:LYS:NZ	12:L:47:LYS:HB2	2.31	0.43
1:A:795:C:H5'	1:A:796:C:OP2	2.19	0.43
1:A:978:A:OP2	1:A:1362:C:N4	2.49	0.43
1:A:1063:C:H2'	1:A:1064:G:C8	2.53	0.43
2:B:108:ILE:O	2:B:111:ARG:HB2	2.18	0.43
3:C:39:ILE:O	3:C:43:LEU:HB2	2.18	0.43
5:E:15:ARG:HG3	5:E:28:PHE:CE2	2.54	0.43
1:A:35:G:O2'	12:L:118:SER:O	2.30	0.43
1:A:779:C:H2'	1:A:780:A:O4'	2.19	0.43
1:A:791:G:H2'	1:A:792:A:C8	2.53	0.43
1:A:1086:U:H3	1:A:1099:G:H22	1.64	0.43
2:B:223:ILE:HG21	2:B:230:VAL:HG23	1.99	0.43
19:S:12:ASP:H	19:S:38:SER:HB2	1.82	0.43
1:A:98:U:H2'	1:A:99:C:C6	2.54	0.43
1:A:895:G:H2'	1:A:896:C:C6	2.54	0.43
1:A:1004:A:O2'	1:A:1005:A:P	2.77	0.43
1:A:1347:G:H22	1:A:1374:A:P	2.42	0.43
3:C:116:VAL:O	3:C:120:VAL:HG23	2.18	0.43
6:F:53:ALA:C	6:F:54:LYS:HD2	2.38	0.43
7:G:47:CYS:HA	7:G:50:ILE:HD12	2.01	0.43
13:M:22:ILE:HG22	13:M:23:TYR:N	2.34	0.43
1:A:788:U:H5''	1:A:789:U:OP2	2.19	0.43
1:A:828:A:H4'	1:A:828:A:OP1	2.19	0.43
1:A:1236:A:H4'	1:A:1304:G:H4'	2.01	0.43
2:B:105:PHE:O	2:B:109:SER:HB3	2.18	0.43
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.78	0.43
3:C:167:TRP:HE3	3:C:168:ALA:N	2.12	0.43
9:I:22:GLY:HA3	9:I:60:ASP:HB2	2.00	0.43
9:I:29:ASN:HB3	9:I:64:THR:HG23	1.99	0.43
12:L:46:LYS:HG3	12:L:92:OTD:O	2.19	0.43
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.18	0.43
1:A:736:C:H2'	1:A:737:A:C8	2.54	0.43
2:B:19:HIS:NE2	2:B:206:ASP:HB3	2.34	0.43
2:B:167:PRO:HG2	2:B:192:SER:HB2	2.01	0.43
3:C:35:GLU:OE2	3:C:59:ARG:NH1	2.40	0.43
7:G:138:LYS:HD3	7:G:139:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.84	0.43
12:L:113:ARG:HH11	12:L:116:SER:H	1.66	0.43
1:A:78:G:H2'	1:A:79:G:C8	2.53	0.43
1:A:92:C:H2'	1:A:93:G:H8	1.84	0.43
1:A:374:A:C6	1:A:375:U:C4	3.07	0.43
1:A:1347:G:C2'	1:A:1348:U:OP2	2.67	0.43
8:H:26:VAL:HG13	8:H:59:LEU:HB2	2.01	0.43
9:I:118:LYS:O	9:I:120:ARG:N	2.49	0.43
13:M:65:LYS:HE3	13:M:69:GLU:HG2	2.00	0.43
19:S:39:THR:HG22	19:S:40:ILE:H	1.84	0.43
1:A:329:A:H5'	25:A:2139:HOH:O	2.19	0.42
1:A:407:G:OP1	4:D:115:ARG:NH2	2.51	0.42
1:A:1200:C:O5'	1:A:1201:A:H3'	2.19	0.42
3:C:150:LYS:HB3	3:C:201:TYR:HB2	2.01	0.42
7:G:116:ALA:O	7:G:120:ILE:HG13	2.19	0.42
17:Q:6:LEU:HD13	17:Q:23:VAL:HG11	2.01	0.42
20:T:10:LEU:O	20:T:13:LEU:HG	2.19	0.42
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.78	0.42
21:U:6:ARG:O	21:U:12:LYS:HD3	2.19	0.42
1:A:1053:G:C3'	1:A:1054:C:H5'	2.49	0.42
11:K:92:GLU:O	11:K:96:ARG:HD3	2.19	0.42
12:L:7:ILE:O	12:L:10:LEU:N	2.52	0.42
12:L:7:ILE:HG21	17:Q:34:LYS:HB3	2.01	0.42
13:M:62:ASN:OD1	13:M:62:ASN:N	2.52	0.42
17:Q:84:LEU:HA	17:Q:84:LEU:HD23	1.74	0.42
20:T:67:ALA:O	20:T:73:HIS:ND1	2.52	0.42
20:T:91:LEU:HA	20:T:91:LEU:HD13	1.79	0.42
1:A:76:C:O2'	1:A:77:G:H5'	2.19	0.42
1:A:789:U:H6	1:A:789:U:O5'	2.01	0.42
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.85	0.42
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.19	0.42
1:A:788:U:H3'	1:A:789:U:O4'	2.19	0.42
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.20	0.42
1:A:1213:A:N1	1:A:1215:G:H1'	2.35	0.42
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.42
1:A:1242:C:H42	1:A:1295:G:H1	1.67	0.42
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.18	0.42
1:A:1380:U:H1'	1:A:1381:U:OP2	2.19	0.42
12:L:42:THR:HA	12:L:53:ARG:O	2.20	0.42
12:L:60:LEU:N	12:L:64:TYR:O	2.51	0.42
1:A:15:G:O2'	5:E:24:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:G:H4'	16:P:41:PRO:HB2	2.01	0.42
1:A:509:A:O2'	1:A:510:A:OP1	2.27	0.42
1:A:953:G:C2	1:A:954:G:H1'	2.54	0.42
1:A:1004:A:H5''	1:A:1025:U:O4	2.20	0.42
1:A:1064:G:H21	1:A:1190:G:H2'	1.84	0.42
5:E:127:ASN:HA	5:E:128:PRO:HD3	1.95	0.42
7:G:70:LYS:HG2	7:G:100:ALA:HB2	2.01	0.42
7:G:152:ALA:O	7:G:155:ARG:HG3	2.19	0.42
9:I:118:LYS:C	9:I:120:ARG:H	2.21	0.42
17:Q:15:MET:HB3	17:Q:18:THR:HB	2.01	0.42
1:A:36:C:H5''	12:L:123:LYS:HD3	2.00	0.42
1:A:500:G:C6	1:A:501:C:C4	3.08	0.42
4:D:28:SER:O	4:D:30:LYS:N	2.48	0.42
16:P:10:GLY:HA3	16:P:14:ASN:O	2.19	0.42
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.19	0.42
17:Q:10:VAL:HA	17:Q:20:THR:O	2.20	0.42
17:Q:78:GLU:OE2	17:Q:81:ARG:HD2	2.20	0.42
1:A:345:C:OP2	1:A:345:C:H6	2.03	0.42
1:A:355:C:H5'	1:A:389:A:OP2	2.20	0.42
1:A:581:G:C8	25:A:2230:HOH:O	2.68	0.42
1:A:1276:G:H2'	1:A:1277:C:O4'	2.19	0.42
1:A:1352:C:H2'	1:A:1353:G:C8	2.55	0.42
12:L:20:LYS:HB3	12:L:20:LYS:HE3	1.84	0.42
1:A:245:C:O2	1:A:283:C:N3	2.52	0.42
2:B:206:ASP:OD1	2:B:207:ALA:N	2.41	0.42
12:L:85:ILE:HA	12:L:85:ILE:HD13	1.65	0.42
12:L:113:ARG:NH1	12:L:116:SER:H	2.17	0.42
13:M:12:ASN:H	13:M:45:VAL:CG1	2.32	0.42
1:A:403:C:O3'	4:D:122:ARG:HD2	2.20	0.42
1:A:955:U:H1'	1:A:1227:A:H61	1.85	0.42
1:A:1298:C:C4	7:G:114:ARG:HD3	2.55	0.42
1:A:1434:A:H2'	1:A:1435:G:O4'	2.20	0.42
2:B:19:HIS:CE1	2:B:206:ASP:HB3	2.55	0.42
4:D:70:ILE:HD11	4:D:100:ARG:HD2	2.02	0.42
10:J:48:THR:OG1	10:J:62:HIS:HB3	2.20	0.42
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.55	0.42
1:A:418:C:H2'	1:A:419:C:C6	2.55	0.42
1:A:757:U:H2'	1:A:758:G:O4'	2.20	0.42
1:A:1392:G:O2'	1:A:1393:U:H5'	2.20	0.42
2:B:25:ASN:O	2:B:26:PRO:C	2.58	0.42
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:11:ASN:HA	6:F:12:PRO:HD3	1.71	0.42
9:I:105:ASP:OD1	9:I:107:ARG:HD3	2.20	0.42
17:Q:41:LYS:HB2	17:Q:41:LYS:HE2	1.77	0.42
1:A:530:G:H2'	1:A:530:G:N3	2.35	0.41
1:A:815:A:N6	1:A:1509:C:H1'	2.35	0.41
3:C:33:LEU:HD21	14:N:54:PRO:HD2	2.00	0.41
10:J:38:ILE:HG12	10:J:71:LEU:HB2	2.02	0.41
20:T:62:LEU:HA	20:T:62:LEU:HD23	1.82	0.41
1:A:625:G:H4'	16:P:16:HIS:CD2	2.54	0.41
1:A:882:C:O2'	1:A:883:C:H5'	2.20	0.41
1:A:980:C:H5'	1:A:981:U:OP2	2.20	0.41
1:A:1225:A:H2'	1:A:1225:A:N3	2.35	0.41
4:D:9:CYS:O	4:D:12:CYS:HB2	2.20	0.41
14:N:39:LEU:HB3	14:N:43:CYS:HB3	2.03	0.41
18:R:54:ARG:H	18:R:54:ARG:HG3	1.67	0.41
1:A:410:G:H2'	1:A:429:U:C4	2.55	0.41
1:A:509:A:C8	1:A:509:A:H3'	2.55	0.41
1:A:1147:C:O2'	9:I:16:ARG:HD2	2.20	0.41
1:A:1404:5MC:H2'	1:A:1405:G:O4'	2.20	0.41
1:A:1505:G:C8	1:A:1505:G:H3'	2.55	0.41
5:E:8:GLU:HA	5:E:33:VAL:O	2.20	0.41
5:E:31:LEU:HD22	5:E:43:LEU:HD11	2.03	0.41
6:F:30:LEU:HD11	6:F:63:TYR:HD2	1.85	0.41
16:P:2:VAL:O	16:P:64:ALA:HA	2.20	0.41
1:A:792:A:O2'	1:A:793:U:OP2	2.27	0.41
1:A:812:C:H4'	1:A:813:U:O5'	2.21	0.41
1:A:1347:G:H2'	1:A:1373:G:H1	1.85	0.41
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.52	0.41
3:C:188:LEU:HD11	3:C:195:VAL:HG13	2.01	0.41
4:D:8:VAL:O	4:D:10:ARG:N	2.53	0.41
15:O:68:ARG:HE	15:O:68:ARG:HB2	1.43	0.41
1:A:671:G:H5'	6:F:77:ARG:HH21	1.85	0.41
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.85	0.41
1:A:1347:G:O2'	1:A:1348:U:P	2.78	0.41
1:A:1349:A:H2'	1:A:1350:A:O4'	2.20	0.41
3:C:34:LEU:HD11	3:C:38:ARG:CZ	2.51	0.41
8:H:24:THR:HG22	8:H:63:LEU:HD21	2.03	0.41
13:M:79:LYS:HE3	13:M:79:LYS:HA	2.01	0.41
17:Q:74:LEU:HD23	17:Q:74:LEU:HA	1.85	0.41
18:R:22:VAL:HG23	18:R:56:THR:HA	2.02	0.41
1:A:1504:G:H4'	1:A:1505:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:MET:HA	2:B:91:PRO:HD3	1.97	0.41
3:C:83:ARG:O	3:C:87:LEU:HB2	2.21	0.41
7:G:89:MET:HE1	7:G:156:TRP:CD1	2.55	0.41
10:J:20:ALA:O	10:J:23:ILE:HG22	2.21	0.41
13:M:79:LYS:HA	13:M:82:MET:HE3	2.03	0.41
18:R:36:ASN:O	18:R:40:LEU:HG	2.20	0.41
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.41
1:A:811:C:O2'	1:A:901:A:N1	2.47	0.41
1:A:954:G:N2	1:A:1227:A:N6	2.68	0.41
2:B:9:GLU:HG3	2:B:213:LEU:HD11	2.02	0.41
3:C:195:VAL:C	3:C:196:LEU:HD23	2.41	0.41
1:A:392:G:H2'	1:A:393:A:H8	1.86	0.41
1:A:416:G:C5	1:A:417:C:C4	3.09	0.41
1:A:475:G:H2'	1:A:476:G:C8	2.56	0.41
1:A:501:C:OP1	12:L:117:ARG:NH2	2.53	0.41
1:A:587:G:O2'	1:A:588:G:OP2	2.30	0.41
1:A:909:A:H2'	1:A:910:C:O4'	2.20	0.41
1:A:1027:C:H2'	1:A:1028:C:C6	2.55	0.41
2:B:219:VAL:HG12	2:B:223:ILE:HD11	2.01	0.41
3:C:113:ALA:N	3:C:114:PRO:HD2	2.36	0.41
5:E:69:VAL:HG12	5:E:71:LEU:HG	2.02	0.41
11:K:81:ASP:OD2	11:K:106:LYS:HD3	2.21	0.41
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	2.02	0.41
21:U:6:ARG:HG2	21:U:15:ARG:NE	2.33	0.41
1:A:73:C:H2'	1:A:74:C:H6	1.86	0.41
1:A:383:A:C5	1:A:384:G:H1'	2.55	0.41
1:A:878:G:H5'	8:H:89:PRO:HG2	2.02	0.41
1:A:1118:C:H5'	9:I:104:ARG:HG3	2.03	0.41
1:A:1131:G:H2'	1:A:1132:C:C6	2.56	0.41
1:A:1256:A:H4'	1:A:1257:U:O5'	2.18	0.41
1:A:1300:G:H4'	1:A:1301:U:O5'	2.19	0.41
2:B:17:PHE:CD1	2:B:18:GLY:N	2.88	0.41
2:B:100:GLY:O	2:B:104:ASN:N	2.53	0.41
2:B:185:ILE:HA	2:B:199:TYR:O	2.20	0.41
4:D:61:LYS:HD3	4:D:206:PHE:CD2	2.56	0.41
5:E:18:ARG:HG2	5:E:19:MET:H	1.84	0.41
7:G:87:VAL:HA	7:G:88:PRO:HD2	1.86	0.41
8:H:100:ILE:HA	8:H:101:PRO:HD3	1.78	0.41
15:O:42:HIS:O	15:O:46:HIS:HB2	2.20	0.41
20:T:13:LEU:HG	20:T:13:LEU:H	1.51	0.41
20:T:14:LYS:O	20:T:18:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:G:C2	1:A:93:G:C2	3.09	0.41
1:A:267:C:H2'	1:A:268:C:H6	1.86	0.41
1:A:559:A:H4'	1:A:560:U:O5'	2.20	0.41
1:A:1205:U:H2'	1:A:1206:G:C8	2.55	0.41
1:A:1256:A:H5'	1:A:1258:G:C1'	2.51	0.41
2:B:21:ARG:H	2:B:21:ARG:HG3	1.64	0.41
8:H:103:VAL:HG12	8:H:108:GLY:HA3	2.03	0.41
17:Q:24:GLU:HG2	17:Q:39:SER:HB3	2.03	0.41
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	2.02	0.41
19:S:22:LEU:HD22	19:S:28:LYS:HG3	2.02	0.41
1:A:980:C:H5''	1:A:981:U:C5	2.56	0.40
5:E:118:ILE:O	5:E:119:LEU:HD23	2.21	0.40
15:O:32:LEU:HD11	15:O:62:GLN:HB3	2.03	0.40
15:O:42:HIS:O	15:O:42:HIS:CG	2.75	0.40
1:A:836:G:C6	1:A:851:G:C6	3.09	0.40
1:A:1057:G:H2'	1:A:1058:G:O4'	2.22	0.40
1:A:1241:G:H2'	1:A:1242:C:C6	2.57	0.40
2:B:217:ARG:O	2:B:220:ASP:HB2	2.21	0.40
4:D:205:GLU:OE1	5:E:100:VAL:HG23	2.21	0.40
19:S:41:VAL:O	19:S:44:MET:HG2	2.21	0.40
1:A:618:C:H5'	1:A:619:U:H5''	2.02	0.40
1:A:1531:A:O5'	1:A:1531:A:H8	2.04	0.40
3:C:84:ILE:O	3:C:88:ARG:HG3	2.21	0.40
3:C:154:SER:OG	3:C:197:GLY:N	2.54	0.40
6:F:48:LEU:HD13	6:F:52:ILE:HD12	2.02	0.40
9:I:48:GLU:HG3	9:I:101:PHE:HZ	1.86	0.40
10:J:64:GLU:O	10:J:64:GLU:HG3	2.21	0.40
11:K:40:ILE:HD13	11:K:40:ILE:HA	1.90	0.40
12:L:126:LYS:HD2	12:L:126:LYS:O	2.22	0.40
13:M:15:VAL:HG23	13:M:43:THR:O	2.21	0.40
1:A:114:U:O2'	1:A:115:G:H5'	2.22	0.40
1:A:164:U:H2'	1:A:165:C:C6	2.56	0.40
1:A:802:A:H2'	1:A:803:G:O4'	2.22	0.40
1:A:1141:C:H2'	1:A:1142:G:C8	2.57	0.40
4:D:36:ARG:HB3	4:D:38:TYR:CZ	2.56	0.40
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.85	0.40
7:G:111:ARG:HA	7:G:112:PRO:HD3	1.85	0.40
9:I:10:ARG:HE	9:I:11:LYS:HB2	1.86	0.40
16:P:82:GLN:HE21	16:P:82:GLN:HB3	1.78	0.40
1:A:79:G:C6	1:A:80:G:C6	3.10	0.40
1:A:255:G:O3'	17:Q:17:LYS:NZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:C:H4'	1:A:281:G:OP2	2.21	0.40
1:A:500:G:C6	1:A:501:C:N4	2.90	0.40
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.56	0.40
9:I:8:GLY:HA2	9:I:79:LEU:HD12	2.04	0.40
9:I:17:VAL:HG11	9:I:81:ILE:HG13	2.02	0.40
13:M:91:ARG:HA	13:M:91:ARG:HD2	1.84	0.40
15:O:85:LEU:HA	15:O:85:LEU:HD23	1.77	0.40
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:U:O4	1:A:1384:C:O2'[3_545]	2.17	0.03

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	210 (90%)	18 (8%)	4 (2%)	7	31
3	C	204/239 (85%)	176 (86%)	28 (14%)	0	100	100
4	D	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	25	56
5	E	148/162 (91%)	141 (95%)	7 (5%)	0	100	100
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	146 (95%)	7 (5%)	0	100	100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100	100
9	I	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
10	J	96/105 (91%)	78 (81%)	15 (16%)	3 (3%)	3	21
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	121/135 (90%)	113 (93%)	8 (7%)	0	100	100
13	M	116/126 (92%)	105 (90%)	10 (9%)	1 (1%)	14	44
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100	100
15	O	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	P	81/88 (92%)	78 (96%)	3 (4%)	0	100	100
17	Q	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	R	68/88 (77%)	61 (90%)	7 (10%)	0	100	100
19	S	78/93 (84%)	68 (87%)	9 (12%)	1 (1%)	10	36
20	T	97/106 (92%)	82 (84%)	15 (16%)	0	100	100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100	100
All	All	2336/2541 (92%)	2150 (92%)	176 (8%)	10 (0%)	30	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
2	B	24	TRP
10	J	86	MET
2	B	95	GLN
13	M	23	TYR
2	B	229	VAL
10	J	34	VAL
4	D	5	ILE
10	J	72	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%)	169 (84%)	33 (16%)	2	9
3	C	160/188 (85%)	137 (86%)	23 (14%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	180/181 (99%)	153 (85%)	27 (15%)	2	11
5	E	115/123 (94%)	91 (79%)	24 (21%)	1	4
6	F	90/90 (100%)	82 (91%)	8 (9%)	8	28
7	G	126/127 (99%)	111 (88%)	15 (12%)	4	17
8	H	119/119 (100%)	107 (90%)	12 (10%)	6	23
9	I	98/99 (99%)	80 (82%)	18 (18%)	1	6
10	J	87/92 (95%)	79 (91%)	8 (9%)	7	26
11	K	88/99 (89%)	78 (89%)	10 (11%)	4	18
12	L	103/110 (94%)	84 (82%)	19 (18%)	1	6
13	M	94/101 (93%)	77 (82%)	17 (18%)	1	6
14	N	49/50 (98%)	44 (90%)	5 (10%)	6	23
15	O	79/80 (99%)	73 (92%)	6 (8%)	11	34
16	P	72/74 (97%)	63 (88%)	9 (12%)	3	16
17	Q	94/97 (97%)	79 (84%)	15 (16%)	2	9
18	R	61/77 (79%)	53 (87%)	8 (13%)	3	14
19	S	71/80 (89%)	58 (82%)	13 (18%)	1	6
20	T	76/82 (93%)	68 (90%)	8 (10%)	5	21
21	U	19/22 (86%)	18 (95%)	1 (5%)	19	47
All	All	1983/2111 (94%)	1704 (86%)	279 (14%)	3	13

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	11	LEU
2	B	16	HIS
2	B	21	ARG
2	B	22	LYS
2	B	24	TRP
2	B	33	TYR
2	B	35	GLU
2	B	48	MET
2	B	56	ARG
2	B	69	LEU
2	B	75	LYS
2	B	97	TRP

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Mol	Chain	Res	Type
2	B	106	LYS
2	B	109	SER
2	B	115	LEU
2	B	128	GLU
2	B	130	ARG
2	B	139	LYS
2	B	144	ARG
2	B	157	ARG
2	B	163	PHE
2	B	164	VAL
2	B	165	VAL
2	B	168	THR
2	B	170	GLU
2	B	178	ARG
2	B	196	LEU
2	B	208	ILE
2	B	210	SER
2	B	221	LEU
2	B	224	GLN
2	B	236	TYR
3	C	3	ASN
3	C	11	ARG
3	C	14	ILE
3	C	15	THR
3	C	17	ASP
3	C	58	GLU
3	C	64	VAL
3	C	79	ARG
3	C	91	LEU
3	C	95	THR
3	C	101	LEU
3	C	107	GLN
3	C	130	VAL
3	C	139	GLN
3	C	153	VAL
3	C	156	ARG
3	C	157	ILE
3	C	167	TRP
3	C	176	HIS
3	C	178	LEU
3	C	188	LEU
3	C	195	VAL

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Mol	Chain	Res	Type
3	C	204	LEU
4	D	5	ILE
4	D	10	ARG
4	D	15	GLU
4	D	17	VAL
4	D	19	LEU
4	D	20	TYR
4	D	21	LEU
4	D	25	ARG
4	D	28	SER
4	D	33	MET
4	D	64	LEU
4	D	65	ARG
4	D	70	ILE
4	D	78	LEU
4	D	112	VAL
4	D	115	ARG
4	D	119	GLN
4	D	122	ARG
4	D	135	LEU
4	D	137	SER
4	D	150	GLU
4	D	162	LEU
4	D	178	VAL
4	D	184	LYS
4	D	187	ARG
4	D	192	GLU
4	D	194	LEU
5	E	5	ASP
5	E	6	PHE
5	E	12	LEU
5	E	15	ARG
5	E	18	ARG
5	E	19	MET
5	E	31	LEU
5	E	41	VAL
5	E	53	LEU
5	E	56	GLN
5	E	61	TYR
5	E	65	ASN
5	E	71	LEU
5	E	78	HIS

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Mol	Chain	Res	Type
5	E	79	GLU
5	E	80	ILE
5	E	87	SER
5	E	100	VAL
5	E	118	ILE
5	E	120	THR
5	E	136	MET
5	E	147	ASP
5	E	150	ARG
5	E	151	LEU
6	F	10	LEU
6	F	15	ASP
6	F	25	ILE
6	F	45	LEU
6	F	54	LYS
6	F	55	ASP
6	F	74	ASP
6	F	84	ASN
7	G	3	ARG
7	G	10	ARG
7	G	54	THR
7	G	57	GLU
7	G	67	GLU
7	G	78	ARG
7	G	94	ARG
7	G	96	GLN
7	G	97	GLN
7	G	113	GLU
7	G	126	ASP
7	G	129	GLU
7	G	138	LYS
7	G	141	VAL
7	G	156	TRP
8	H	11	THR
8	H	22	GLU
8	H	23	SER
8	H	24	THR
8	H	39	LEU
8	H	63	LEU
8	H	84	ARG
8	H	85	ARG
8	H	91	ARG

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Mol	Chain	Res	Type
8	H	97	VAL
8	H	104	ARG
8	H	105	ARG
9	I	3	GLN
9	I	5	TYR
9	I	12	GLU
9	I	14	VAL
9	I	29	ASN
9	I	38	GLN
9	I	44	VAL
9	I	66	ARG
9	I	79	LEU
9	I	81	ILE
9	I	85	LEU
9	I	86	VAL
9	I	109	VAL
9	I	110	GLU
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
9	I	128	ARG
10	J	19	SER
10	J	21	GLN
10	J	47	PHE
10	J	62	HIS
10	J	71	LEU
10	J	76	ASN
10	J	80	LYS
10	J	89	ASP
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	33	THR
11	K	48	ILE
11	K	81	ASP
11	K	91	ARG
11	K	105	VAL
11	K	109	VAL
11	K	114	VAL
12	L	20	LYS
12	L	33	ARG
12	L	39	VAL

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Mol	Chain	Res	Type
12	L	43	VAL
12	L	47	LYS
12	L	64	TYR
12	L	66	VAL
12	L	67	THR
12	L	79	GLU
12	L	80	HIS
12	L	81	SER
12	L	83	VAL
12	L	96	VAL
12	L	97	ARG
12	L	113	ARG
12	L	116	SER
12	L	122	THR
12	L	126	LYS
12	L	127	GLU
13	M	14	ARG
13	M	16	ASP
13	M	35	GLU
13	M	44	ARG
13	M	45	VAL
13	M	49	THR
13	M	50	GLU
13	M	54	VAL
13	M	63	THR
13	M	64	TRP
13	M	79	LYS
13	M	80	ARG
13	M	81	LEU
13	M	102	ARG
13	M	103	THR
13	M	110	ARG
13	M	111	LYS
14	N	22	THR
14	N	24	CYS
14	N	31	ARG
14	N	36	PHE
14	N	41	ARG
15	O	32	LEU
15	O	33	THR
15	O	39	LEU
15	O	45	VAL

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Mol	Chain	Res	Type
15	O	81	LEU
15	O	88	ARG
16	P	1	MET
16	P	27	LYS
16	P	31	LYS
16	P	54	GLU
16	P	55	ARG
16	P	61	SER
16	P	62	VAL
16	P	68	ASP
16	P	82	GLN
17	Q	4	LYS
17	Q	15	MET
17	Q	38	ARG
17	Q	40	LYS
17	Q	53	LEU
17	Q	59	ILE
17	Q	68	ARG
17	Q	74	LEU
17	Q	75	ARG
17	Q	76	LEU
17	Q	81	ARG
17	Q	83	ASP
17	Q	91	ARG
17	Q	92	ARG
17	Q	97	SER
18	R	19	LYS
18	R	26	LEU
18	R	28	GLU
18	R	31	LEU
18	R	36	ASN
18	R	47	THR
18	R	53	ARG
18	R	84	LYS
19	S	3	ARG
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	13	ASP
19	S	15	LEU
19	S	29	ARG
19	S	33	THR

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Mol	Chain	Res	Type
19	S	39	THR
19	S	43	GLU
19	S	63	THR
19	S	71	LEU
19	S	78	ARG
20	T	10	LEU
20	T	13	LEU
20	T	36	LEU
20	T	72	LEU
20	T	73	HIS
20	T	84	LEU
20	T	91	LEU
20	T	92	LEU
21	U	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	119	GLN
6	F	11	ASN
11	K	26	ASN
18	R	36	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	290 (19%)	45 (2%)

All (290) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	44	G
1	A	47	C

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Mol	Chain	Res	Type
1	A	48	C
1	A	50	A
1	A	51	A
1	A	81	U
1	A	82	U
1	A	91	C
1	A	92	C
1	A	98	U
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	136	C
1	A	144	G
1	A	163	C
1	A	173	U
1	A	181	G
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	190(E)	U
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
1	A	220	G
1	A	226	G
1	A	231	G
1	A	244	U
1	A	247	G
1	A	251	G
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	289	G

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Mol	Chain	Res	Type
1	A	299	G
1	A	301	G
1	A	321	A
1	A	325	A
1	A	328	C
1	A	329	A
1	A	344	A
1	A	345	C
1	A	346	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	424	G
1	A	429	U
1	A	460	A
1	A	461	C
1	A	477	G
1	A	479	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	522	C

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Mol	Chain	Res	Type
1	A	527	7MG
1	A	531	U
1	A	532	A
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	616	G
1	A	618	C
1	A	620	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	787	A
1	A	788	U
1	A	789	U
1	A	793	U
1	A	794	A
1	A	812	C

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Mol	Chain	Res	Type
1	A	813	U
1	A	817	C
1	A	827	U
1	A	828	A
1	A	839	U
1	A	841	U
1	A	848	C
1	A	858	G
1	A	859	A
1	A	871	U
1	A	872	A
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	960	U
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	979	C
1	A	984	C
1	A	986	A
1	A	989	C
1	A	991	U
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	1019	C
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1031	G

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Mol	Chain	Res	Type
1	A	1045	C
1	A	1050	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1078	U
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1146	A
1	A	1152	A
1	A	1153	C
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1177	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A
1	A	1202	G
1	A	1207	2MG
1	A	1211	U

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Mol	Chain	Res	Type
1	A	1212	U
1	A	1213	A
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1250	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1277	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1310	G
1	A	1311	G
1	A	1319	A
1	A	1320	C
1	A	1326	C
1	A	1335	C
1	A	1336	C
1	A	1338	G
1	A	1340	A
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1358	U

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Mol	Chain	Res	Type
1	A	1359	C
1	A	1362	C
1	A	1368	G
1	A	1370	G
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1399	C
1	A	1400	5MC
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1454	G
1	A	1487	G
1	A	1493	A
1	A	1494	G
1	A	1496	C
1	A	1497	G
1	A	1499	A
1	A	1502	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	1533	C
1	A	1540	PSU

All (45) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	243	A
1	A	250	A
1	A	328	C

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Mol	Chain	Res	Type
1	A	372	C
1	A	412	A
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	975	A
1	A	992	U
1	A	1004	A
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1279	A
1	A	1285	A
1	A	1300	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and



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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	5MC	A	1404	1	19,22,23	0.98	1 (5%)	26,32,35	0.89	0
1	MA6	A	1518	1	19,26,27	1.32	3 (15%)	18,38,41	0.80	0
1	7MG	A	527	1	23,26,27	4.00	4 (17%)	27,39,42	2.32	9 (33%)
1	5MC	A	1400	1	19,22,23	1.27	3 (15%)	26,32,35	0.94	2 (7%)
1	5MC	A	1407	1	19,22,23	1.14	2 (10%)	26,32,35	1.20	5 (19%)
1	2MG	A	1207	1	18,26,27	1.62	4 (22%)	16,38,41	1.40	2 (12%)
1	UR3	A	1498	1	19,22,23	0.96	1 (5%)	26,32,35	1.03	1 (3%)
1	MA6	A	1519	1	19,26,27	1.67	5 (26%)	18,38,41	0.65	0
1	5MC	A	967	1	19,22,23	0.91	1 (5%)	26,32,35	0.77	1 (3%)
1	M2G	A	966	1	20,27,28	1.28	3 (15%)	19,40,43	1.20	2 (10%)
1	4OC	A	1402	1	20,23,24	0.98	2 (10%)	25,32,35	0.73	0
1	PSU	A	516	1,23	18,21,22	1.12	1 (5%)	21,30,33	1.84	5 (23%)
1	PSU	A	1540	1,23	18,21,22	1.22	1 (5%)	21,30,33	1.72	4 (19%)
1	PSU	A	1541	1	18,21,22	1.16	1 (5%)	21,30,33	1.81	5 (23%)
12	0TD	L	92	12	8,9,10	2.19	1 (12%)	6,11,13	3.13	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	2/7/29/30	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	2/5/27/28	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1519	1	-	6/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3

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

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-17.81	1.34	1.45
12	L	92	0TD	CB-CA	-5.41	1.53	1.54
1	A	1519	MA6	C6-N1	4.60	1.38	1.32
1	A	527	7MG	C2-N2	4.56	1.44	1.34
1	A	1540	PSU	C6-C5	4.27	1.40	1.35
1	A	1541	PSU	C6-C5	4.16	1.39	1.35
1	A	1518	MA6	C6-N1	3.95	1.38	1.32
1	A	1207	2MG	C6-N1	3.72	1.43	1.37
1	A	966	M2G	C6-N1	3.64	1.43	1.37
1	A	1207	2MG	C2-N2	3.57	1.40	1.33
1	A	1519	MA6	C4-N3	3.51	1.40	1.35
1	A	527	7MG	C5-N7	3.49	1.40	1.35
1	A	516	PSU	C6-C5	3.44	1.39	1.35
1	A	1207	2MG	C2-N1	3.38	1.42	1.36
1	A	1404	5MC	C2-N3	3.07	1.42	1.36
1	A	1407	5MC	C2-N1	2.83	1.46	1.40
1	A	1402	4OC	C2-N3	2.82	1.41	1.36
1	A	967	5MC	C2-N3	2.74	1.41	1.36
1	A	1498	UR3	C2-N1	2.65	1.42	1.38
1	A	1400	5MC	C6-C5	2.59	1.38	1.34
1	A	966	M2G	C2-N2	2.49	1.39	1.35
1	A	1400	5MC	C2-N1	2.46	1.45	1.40
1	A	1518	MA6	C2-N1	2.45	1.38	1.33
1	A	1400	5MC	C2-N3	2.44	1.41	1.36
1	A	1519	MA6	C2-N3	2.32	1.35	1.32
1	A	1519	MA6	C2-N1	2.29	1.38	1.33
1	A	1518	MA6	C2-N3	2.25	1.35	1.32
1	A	1207	2MG	C5-C6	-2.22	1.43	1.47
1	A	1402	4OC	O2-C2	-2.22	1.19	1.23
1	A	1407	5MC	C6-C5	2.17	1.38	1.34
1	A	1519	MA6	C9-N6	2.15	1.50	1.45
1	A	527	7MG	C4-N3	2.13	1.39	1.34
1	A	966	M2G	C5-C6	-2.03	1.43	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	92	0TD	CSB-SB-CB	-6.70	90.31	102.36
1	A	527	7MG	C5-C6-N1	5.30	120.27	110.94
1	A	527	7MG	C2-N3-C4	4.88	120.71	112.30
1	A	516	PSU	C4-N3-C2	-4.73	119.86	126.37
1	A	527	7MG	N9-C4-N3	4.55	132.13	125.46
1	A	1541	PSU	N1-C2-N3	4.55	119.96	115.17
1	A	527	7MG	C5-C4-N3	-4.54	119.60	128.13
1	A	516	PSU	N1-C2-N3	4.45	119.86	115.17
1	A	1540	PSU	C4-N3-C2	-4.35	120.38	126.37
1	A	1540	PSU	N1-C2-N3	4.03	119.41	115.17
1	A	1541	PSU	C4-N3-C2	-4.00	120.87	126.37
1	A	1207	2MG	O6-C6-N1	-3.95	115.93	120.62
1	A	527	7MG	C2-N1-C6	-3.46	118.83	125.11
1	A	1207	2MG	O6-C6-C5	3.40	131.06	124.32
1	A	1541	PSU	O2-C2-N1	-3.35	119.33	122.79
1	A	527	7MG	N9-C8-N7	3.31	108.06	103.37
1	A	966	M2G	O6-C6-C5	3.28	130.83	124.32
1	A	966	M2G	O6-C6-N1	-3.22	116.80	120.62
1	A	1541	PSU	C6-N1-C2	-3.08	119.83	122.69
1	A	527	7MG	C6-C5-N7	2.68	136.08	131.93
1	A	1498	UR3	C6-N1-C2	-2.66	119.63	121.80
1	A	1540	PSU	O2-C2-N1	-2.65	120.05	122.79
1	A	1407	5MC	C5-C4-N3	2.63	124.45	121.75
1	A	1407	5MC	N4-C4-N3	-2.54	113.90	118.51
1	A	527	7MG	C6-C5-C4	-2.48	118.04	122.40
1	A	1540	PSU	C6-N1-C2	-2.43	120.43	122.69
1	A	527	7MG	O6-C6-C5	-2.39	121.75	127.62
1	A	1407	5MC	C4-N3-C2	-2.35	117.54	120.81
12	L	92	0TD	OD1-CG-CB	-2.24	117.75	122.44
1	A	1407	5MC	O2-C2-N3	-2.23	118.82	122.33
1	A	1541	PSU	O4'-C1'-C2'	2.21	108.21	105.15
1	A	516	PSU	C6-N1-C2	-2.18	120.67	122.69
1	A	1400	5MC	C5-C4-N3	2.16	123.97	121.75
1	A	516	PSU	C6-C5-C4	2.12	119.61	118.17
1	A	1407	5MC	C5-C6-N1	-2.10	121.03	123.31
1	A	516	PSU	O4'-C1'-C2'	2.08	108.03	105.15
1	A	1400	5MC	N4-C4-N3	-2.05	114.80	118.51
1	A	967	5MC	N4-C4-N3	-2.02	114.85	118.51

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2
1	A	1207	2MG	O4'-C4'-C5'-O5'
1	A	1207	2MG	C3'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
1	A	1541	PSU	C2'-C1'-C5-C4
1	A	1541	PSU	C2'-C1'-C5-C6
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1518	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	O4'-C4'-C5'-O5'
1	A	1519	MA6	N1-C6-N6-C10
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM2
12	L	92	0TD	CG-CB-SB-CSB
1	A	1519	MA6	C5-C6-N6-C9
12	L	92	0TD	SB-CB-CG-OD1
1	A	1519	MA6	C3'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C1'-C5-C4
1	A	1518	MA6	C3'-C4'-C5'-O5'
1	A	1540	PSU	O4'-C4'-C5'-O5'
1	A	1402	4OC	C2'-C1'-N1-C2

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	1	0
1	A	1518	MA6	1	0
1	A	527	7MG	1	0
1	A	1400	5MC	1	0
1	A	1407	5MC	1	0
1	A	1519	MA6	1	0
1	A	967	5MC	3	0
1	A	966	M2G	2	0
12	L	92	0TD	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 295 ligands modelled in this entry, 294 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	2.37	12 (30%)	49,63,63	2.00	12 (24%)

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	-	-	2/20/87/87	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.08	1.48	1.33
22	A	1601	SRY	CA1-N11	6.77	1.44	1.33
22	A	1601	SRY	O53-C53	-3.42	1.36	1.44
22	A	1601	SRY	CA1-NB1	3.04	1.45	1.34
22	A	1601	SRY	CD1-NE1	2.85	1.44	1.34
22	A	1601	SRY	C23-N23	-2.68	1.43	1.47
22	A	1601	SRY	O51-C51	-2.61	1.36	1.43
22	A	1601	SRY	C21-C11	-2.45	1.48	1.53
22	A	1601	SRY	O32-C32	-2.42	1.40	1.44
22	A	1601	SRY	C32-CG2	-2.16	1.48	1.52
22	A	1601	SRY	O43-C43	-2.16	1.37	1.43
22	A	1601	SRY	C21-C31	-2.01	1.49	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	1601	SRY	O41-C12-O42	-6.11	105.12	111.37
22	A	1601	SRY	C12-O42-C42	-4.72	100.86	108.48
22	A	1601	SRY	CI3-N23-C23	-4.57	108.33	114.23
22	A	1601	SRY	C13-O13-C22	-3.98	109.50	116.26
22	A	1601	SRY	O13-C13-C23	3.71	114.09	108.07
22	A	1601	SRY	C43-C33-C23	-3.65	105.09	110.40
22	A	1601	SRY	C61-C11-N11	-3.07	104.96	110.62
22	A	1601	SRY	C13-O53-C53	-2.89	108.07	113.72
22	A	1601	SRY	C31-N31-CD1	-2.76	117.92	123.39
22	A	1601	SRY	C11-N11-CA1	-2.47	118.50	123.39
22	A	1601	SRY	C13-C23-N23	2.19	114.75	110.92
22	A	1601	SRY	C12-O41-C41	-2.07	113.08	117.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

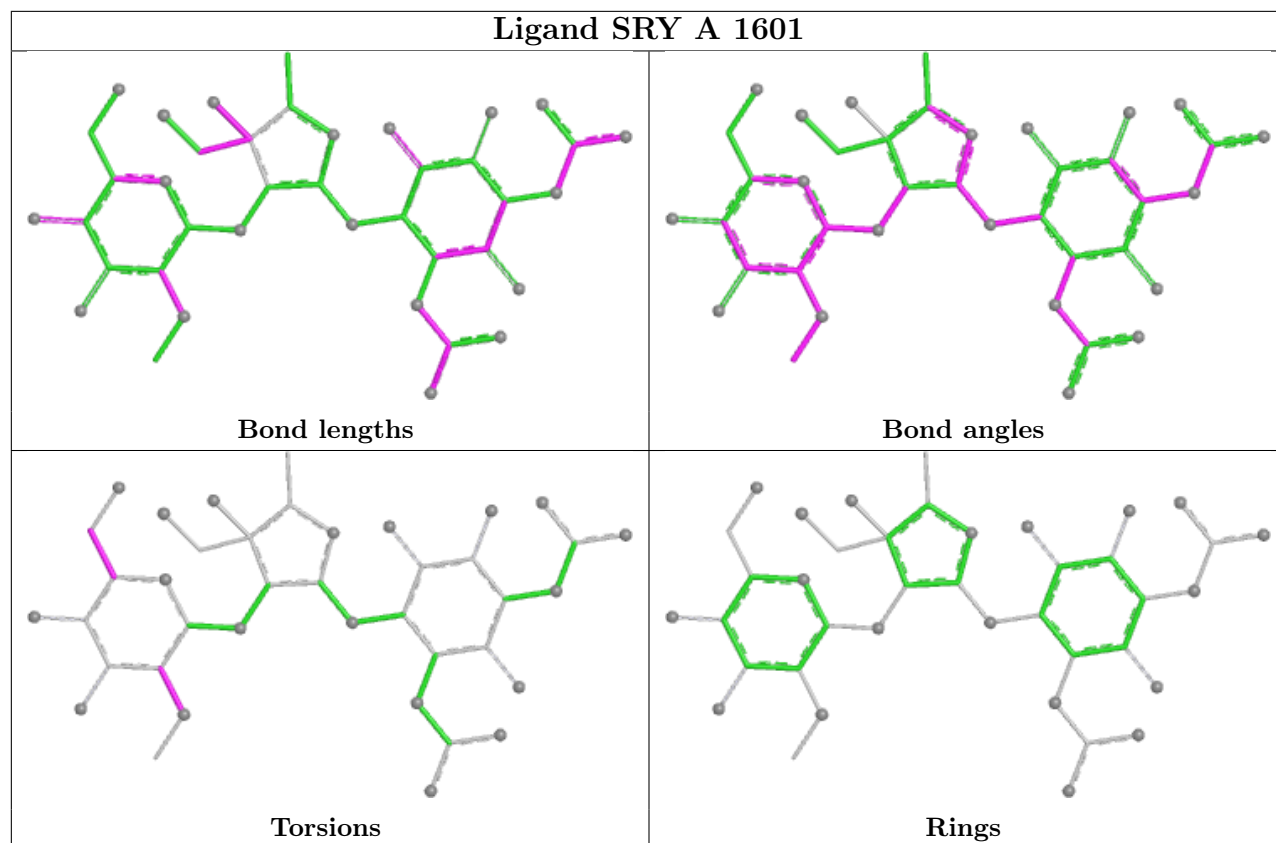
Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C43-C53-C63-O63

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	4	0

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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%)	-0.63	6 (0%) 89 83	84, 140, 292, 377	0
2	B	234/256 (91%)	-0.48	2 (0%) 81 70	104, 155, 237, 275	0
3	C	206/239 (86%)	-0.20	2 (0%) 79 68	154, 222, 279, 297	0
4	D	208/209 (99%)	-0.19	9 (4%) 40 30	95, 146, 196, 234	0
5	E	150/162 (92%)	-0.60	0 100 100	87, 116, 150, 189	0
6	F	101/101 (100%)	-0.54	0 100 100	128, 171, 203, 245	0
7	G	155/156 (99%)	-0.36	2 (1%) 74 61	134, 194, 249, 267	0
8	H	138/138 (100%)	-0.73	0 100 100	82, 104, 147, 176	0
9	I	127/128 (99%)	-0.16	1 (0%) 82 72	139, 225, 270, 296	0
10	J	98/105 (93%)	0.09	2 (2%) 64 50	169, 249, 317, 359	0
11	K	116/129 (89%)	-0.34	1 (0%) 81 70	114, 140, 200, 247	0
12	L	123/135 (91%)	-0.34	2 (1%) 70 57	81, 136, 177, 242	0
13	M	118/126 (93%)	-0.28	4 (3%) 48 35	132, 174, 213, 263	0
14	N	60/61 (98%)	0.58	5 (8%) 19 17	170, 213, 261, 270	0
15	O	87/89 (97%)	-0.61	0 100 100	87, 129, 171, 196	0
16	P	83/88 (94%)	-0.40	0 100 100	107, 135, 170, 216	0
17	Q	99/105 (94%)	-0.59	0 100 100	82, 115, 153, 171	0
18	R	70/88 (79%)	-0.57	0 100 100	102, 145, 197, 210	0
19	S	80/93 (86%)	0.25	6 (7%) 22 19	187, 240, 280, 318	0
20	T	99/106 (93%)	-0.24	1 (1%) 79 68	103, 143, 194, 220	0
21	U	24/27 (88%)	0.06	0 100 100	151, 181, 217, 225	0
All	All	3874/4063 (95%)	-0.44	43 (1%) 77 66	81, 153, 264, 377	0

All (43) RSRZ outliers are listed below:



Mol	Chain	Res	Type	RSRZ
14	N	2	ALA	11.6
20	T	106	ALA	8.6
1	A	1129	C	5.3
10	J	37	PRO	5.0
19	S	4	SER	4.5
4	D	31	CYS	4.2
4	D	2	GLY	4.2
4	D	9	CYS	3.9
4	D	26	CYS	3.9
14	N	3	ARG	3.8
11	K	56	GLY	3.7
4	D	23	GLY	3.6
13	M	8	GLU	3.5
4	D	22	LYS	3.5
1	A	793	U	3.4
2	B	203	GLY	3.4
19	S	2	PRO	3.3
19	S	3	ARG	2.9
4	D	21	LEU	2.8
10	J	90	LEU	2.8
14	N	4	LYS	2.8
13	M	117	VAL	2.8
14	N	5	ALA	2.7
1	A	788	U	2.7
3	C	2	GLY	2.6
9	I	110	GLU	2.6
12	L	44	THR	2.6
12	L	73	GLU	2.5
19	S	53	ASN	2.5
1	A	1017	G	2.5
3	C	188	LEU	2.5
19	S	37	ARG	2.4
2	B	16	HIS	2.4
7	G	154	TYR	2.3
4	D	42	GLN	2.3
13	M	119	GLY	2.2
4	D	12	CYS	2.2
13	M	7	VAL	2.2
1	A	1200	C	2.1
19	S	35	SER	2.1
1	A	985	C	2.1
7	G	2	ALA	2.1
14	N	6	LEU	2.1

## 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	0.52	0.18	259,271,323,325	0
1	PSU	A	1540	20/21	0.80	0.19	215,251,324,324	0
1	5MC	A	1404	21/22	0.92	0.12	119,127,141,150	0
1	2MG	A	1207	24/25	0.94	0.13	204,240,247,253	0
1	MA6	A	1519	24/25	0.95	0.09	111,125,136,142	0
1	PSU	A	516	20/21	0.95	0.09	129,146,157,158	0
1	MA6	A	1518	24/25	0.95	0.08	120,140,152,155	0
1	5MC	A	1400	21/22	0.96	0.08	106,137,150,154	0
1	UR3	A	1498	21/22	0.96	0.10	115,129,150,155	0
1	M2G	A	966	25/26	0.97	0.07	133,146,154,159	0
1	5MC	A	967	21/22	0.97	0.07	137,145,156,160	0
1	5MC	A	1407	21/22	0.97	0.08	141,152,168,173	0
1	7MG	A	527	24/25	0.97	0.09	105,116,135,140	0
1	4OC	A	1402	22/23	0.98	0.08	116,120,139,144	0
12	0TD	L	92	10/11	0.98	0.09	107,131,154,325	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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	1769	1/1	0.50	0.42	130,130,130,130	0
23	MG	A	1781	1/1	0.53	0.34	151,151,151,151	0
23	MG	A	1794	1/1	0.56	0.48	128,128,128,128	0
23	MG	A	1686	1/1	0.59	0.12	375,375,375,375	0
23	MG	A	1821	1/1	0.65	0.18	156,156,156,156	0
23	MG	A	1809	1/1	0.66	0.26	141,141,141,141	0
23	MG	A	1736	1/1	0.66	0.54	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	K	201	1/1	0.66	0.15	168,168,168,168	0
23	MG	A	1625	1/1	0.68	0.49	152,152,152,152	0
23	MG	A	1786	1/1	0.70	0.11	495,495,495,495	0
23	MG	A	1807	1/1	0.71	0.35	145,145,145,145	0
23	MG	A	1773	1/1	0.72	0.39	150,150,150,150	0
23	MG	A	1673	1/1	0.73	0.31	143,143,143,143	0
23	MG	A	1796	1/1	0.73	0.27	134,134,134,134	0
23	MG	A	1718	1/1	0.75	0.45	142,142,142,142	0
23	MG	A	1816	1/1	0.75	0.38	136,136,136,136	0
23	MG	A	1802	1/1	0.76	0.18	140,140,140,140	0
23	MG	A	1812	1/1	0.77	0.25	160,160,160,160	0
23	MG	A	1660	1/1	0.77	0.35	127,127,127,127	0
23	MG	A	1669	1/1	0.77	0.37	122,122,122,122	0
23	MG	A	1798	1/1	0.77	0.22	139,139,139,139	0
23	MG	A	1738	1/1	0.78	0.25	150,150,150,150	0
23	MG	A	1745	1/1	0.78	0.70	114,114,114,114	0
23	MG	A	1711	1/1	0.78	0.75	145,145,145,145	0
23	MG	A	1715	1/1	0.78	0.48	129,129,129,129	0
23	MG	A	1784	1/1	0.79	0.13	198,198,198,198	0
23	MG	A	1662	1/1	0.79	0.39	124,124,124,124	0
23	MG	A	1731	1/1	0.79	0.31	117,117,117,117	0
23	MG	M	201	1/1	0.79	0.29	160,160,160,160	0
23	MG	S	101	1/1	0.79	0.28	132,132,132,132	0
23	MG	A	1722	1/1	0.80	0.24	126,126,126,126	0
23	MG	A	1797	1/1	0.80	0.22	157,157,157,157	0
23	MG	A	1725	1/1	0.80	0.42	142,142,142,142	0
23	MG	A	1838	1/1	0.81	0.17	386,386,386,386	0
23	MG	H	203	1/1	0.81	0.27	132,132,132,132	0
23	MG	A	1697	1/1	0.81	0.20	147,147,147,147	0
23	MG	A	1775	1/1	0.81	0.36	128,128,128,128	0
23	MG	A	1723	1/1	0.81	0.74	155,155,155,155	0
23	MG	A	1851	1/1	0.82	0.35	151,151,151,151	0
23	MG	A	1814	1/1	0.82	0.13	129,129,129,129	0
23	MG	A	1751	1/1	0.82	0.27	123,123,123,123	0
23	MG	A	1684	1/1	0.82	0.13	191,191,191,191	0
23	MG	Q	201	1/1	0.82	0.13	119,119,119,119	0
23	MG	A	1700	1/1	0.82	0.10	246,246,246,246	0
23	MG	A	1748	1/1	0.83	0.73	129,129,129,129	0
23	MG	A	1806	1/1	0.83	0.17	145,145,145,145	0
23	MG	A	1813	1/1	0.83	0.59	135,135,135,135	0
23	MG	A	1845	1/1	0.83	0.09	267,267,267,267	0
23	MG	A	1680	1/1	0.83	0.21	141,141,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1818	1/1	0.84	0.61	121,121,121,121	0
23	MG	A	1778	1/1	0.84	0.16	124,124,124,124	0
23	MG	A	1734	1/1	0.84	0.75	127,127,127,127	0
23	MG	A	1661	1/1	0.84	0.12	192,192,192,192	0
23	MG	A	1757	1/1	0.84	0.17	147,147,147,147	0
23	MG	B	301	1/1	0.84	0.17	141,141,141,141	0
23	MG	A	1787	1/1	0.84	0.15	130,130,130,130	0
23	MG	A	1789	1/1	0.84	0.22	124,124,124,124	0
23	MG	A	1737	1/1	0.84	0.29	126,126,126,126	0
23	MG	A	1726	1/1	0.84	0.26	133,133,133,133	0
23	MG	A	1627	1/1	0.84	0.13	126,126,126,126	0
23	MG	A	1752	1/1	0.85	0.71	124,124,124,124	0
23	MG	A	1682	1/1	0.85	0.31	128,128,128,128	0
23	MG	A	1792	1/1	0.85	0.22	93,93,93,93	0
23	MG	A	1768	1/1	0.85	0.31	111,111,111,111	0
23	MG	A	1850	1/1	0.85	0.29	122,122,122,122	0
23	MG	A	1777	1/1	0.85	0.17	155,155,155,155	0
23	MG	T	202	1/1	0.85	0.25	135,135,135,135	0
23	MG	A	1855	1/1	0.86	0.28	138,138,138,138	0
23	MG	A	1873	1/1	0.86	0.07	423,423,423,423	0
23	MG	A	1772	1/1	0.86	0.19	131,131,131,131	0
23	MG	H	201	1/1	0.86	0.14	106,106,106,106	0
23	MG	A	1603	1/1	0.86	0.25	133,133,133,133	0
23	MG	A	1808	1/1	0.86	0.61	118,118,118,118	0
23	MG	A	1724	1/1	0.86	0.49	171,171,171,171	0
23	MG	A	1624	1/1	0.86	0.17	162,162,162,162	0
23	MG	A	1658	1/1	0.86	0.16	175,175,175,175	0
23	MG	A	1791	1/1	0.86	0.53	127,127,127,127	0
23	MG	A	1694	1/1	0.87	0.21	137,137,137,137	0
23	MG	A	1810	1/1	0.87	0.13	149,149,149,149	0
23	MG	A	1854	1/1	0.87	0.11	194,194,194,194	0
23	MG	A	1602	1/1	0.87	0.16	158,158,158,158	0
23	MG	A	1856	1/1	0.87	0.11	161,161,161,161	0
23	MG	A	1857	1/1	0.87	0.26	121,121,121,121	0
23	MG	A	1859	1/1	0.87	0.10	144,144,144,144	0
23	MG	A	1717	1/1	0.87	0.12	132,132,132,132	0
23	MG	A	1641	1/1	0.87	0.23	105,105,105,105	0
23	MG	A	1815	1/1	0.87	0.22	146,146,146,146	0
23	MG	A	1803	1/1	0.87	0.34	142,142,142,142	0
23	MG	A	1817	1/1	0.87	0.21	119,119,119,119	0
23	MG	A	1805	1/1	0.87	0.34	132,132,132,132	0
23	MG	N	103	1/1	0.87	0.18	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
23	MG	A	1763	1/1	0.87	0.05	183,183,183,183	0
23	MG	A	1766	1/1	0.87	0.24	130,130,130,130	0
23	MG	A	1710	1/1	0.87	0.23	128,128,128,128	0
23	MG	A	1849	1/1	0.88	0.18	126,126,126,126	0
23	MG	B	302	1/1	0.88	0.12	111,111,111,111	0
23	MG	A	1696	1/1	0.88	0.66	140,140,140,140	0
23	MG	A	1705	1/1	0.88	0.10	112,112,112,112	0
23	MG	A	1776	1/1	0.88	0.35	126,126,126,126	0
23	MG	A	1645	1/1	0.88	0.13	139,139,139,139	0
23	MG	A	1747	1/1	0.88	0.19	131,131,131,131	0
23	MG	A	1822	1/1	0.88	0.10	101,101,101,101	0
23	MG	A	1759	1/1	0.88	0.39	145,145,145,145	0
23	MG	A	1782	1/1	0.88	0.11	214,214,214,214	0
23	MG	A	1654	1/1	0.89	0.14	129,129,129,129	0
23	MG	A	1788	1/1	0.89	0.61	121,121,121,121	0
23	MG	A	1864	1/1	0.89	0.18	333,333,333,333	0
23	MG	A	1872	1/1	0.89	0.14	209,209,209,209	0
23	MG	A	1755	1/1	0.89	0.42	132,132,132,132	0
23	MG	A	1790	1/1	0.89	0.08	140,140,140,140	0
23	MG	A	1837	1/1	0.89	0.17	306,306,306,306	0
23	MG	A	1663	1/1	0.89	0.37	148,148,148,148	0
23	MG	A	1665	1/1	0.89	0.31	126,126,126,126	0
23	MG	A	1640	1/1	0.89	0.17	129,129,129,129	0
23	MG	A	1714	1/1	0.89	0.28	116,116,116,116	0
23	MG	N	102	1/1	0.89	0.11	182,182,182,182	0
23	MG	A	1616	1/1	0.89	0.28	115,115,115,115	0
23	MG	A	1730	1/1	0.89	0.59	147,147,147,147	0
23	MG	A	1801	1/1	0.89	0.21	100,100,100,100	0
23	MG	A	1615	1/1	0.89	0.11	114,114,114,114	0
23	MG	A	1830	1/1	0.90	0.20	199,199,199,199	0
23	MG	A	1728	1/1	0.90	0.25	134,134,134,134	0
23	MG	A	1672	1/1	0.90	0.21	122,122,122,122	0
23	MG	A	1690	1/1	0.90	0.13	111,111,111,111	0
23	MG	A	1799	1/1	0.90	0.32	152,152,152,152	0
23	MG	A	1732	1/1	0.90	0.18	111,111,111,111	0
23	MG	A	1618	1/1	0.90	0.12	115,115,115,115	0
23	MG	A	1754	1/1	0.90	0.43	126,126,126,126	0
23	MG	A	1604	1/1	0.90	0.40	133,133,133,133	0
23	MG	A	1628	1/1	0.90	0.42	112,112,112,112	0
23	MG	A	1820	1/1	0.90	0.52	113,113,113,113	0
23	MG	A	1653	1/1	0.90	0.29	114,114,114,114	0
23	MG	A	1741	1/1	0.90	0.17	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1704	1/1	0.91	0.10	121,121,121,121	0
23	MG	A	1779	1/1	0.91	0.22	131,131,131,131	0
23	MG	H	202	1/1	0.91	0.11	125,125,125,125	0
23	MG	A	1670	1/1	0.91	0.39	197,197,197,197	0
23	MG	A	1811	1/1	0.91	0.09	138,138,138,138	0
23	MG	A	1761	1/1	0.91	0.21	134,134,134,134	0
23	MG	A	1744	1/1	0.91	0.14	128,128,128,128	0
23	MG	A	1793	1/1	0.91	0.33	107,107,107,107	0
23	MG	P	102	1/1	0.91	0.12	135,135,135,135	0
23	MG	A	1610	1/1	0.91	0.14	141,141,141,141	0
23	MG	A	1795	1/1	0.91	0.30	108,108,108,108	0
23	MG	A	1635	1/1	0.91	0.16	98,98,98,98	0
23	MG	A	1630	1/1	0.92	0.14	128,128,128,128	0
23	MG	A	1666	1/1	0.92	0.15	161,161,161,161	0
23	MG	A	1606	1/1	0.92	0.41	130,130,130,130	0
23	MG	A	1804	1/1	0.92	0.29	126,126,126,126	0
23	MG	A	1869	1/1	0.92	0.11	278,278,278,278	0
23	MG	A	1679	1/1	0.92	0.23	132,132,132,132	0
23	MG	P	101	1/1	0.92	0.20	98,98,98,98	0
23	MG	A	1735	1/1	0.92	0.58	129,129,129,129	0
23	MG	A	1698	1/1	0.92	0.15	155,155,155,155	0
23	MG	A	1823	1/1	0.92	0.15	90,90,90,90	0
23	MG	A	1825	1/1	0.92	0.24	147,147,147,147	0
23	MG	A	1623	1/1	0.93	0.14	114,114,114,114	0
23	MG	A	1819	1/1	0.93	0.12	150,150,150,150	0
23	MG	A	1852	1/1	0.93	0.30	126,126,126,126	0
23	MG	A	1643	1/1	0.93	0.12	130,130,130,130	0
23	MG	A	1743	1/1	0.93	0.44	146,146,146,146	0
23	MG	A	1720	1/1	0.93	0.23	116,116,116,116	0
23	MG	A	1800	1/1	0.93	0.40	159,159,159,159	0
23	MG	A	1709	1/1	0.93	0.12	109,109,109,109	0
23	MG	A	1637	1/1	0.93	0.13	170,170,170,170	0
23	MG	A	1622	1/1	0.93	0.15	163,163,163,163	0
23	MG	A	1676	1/1	0.93	0.30	124,124,124,124	0
23	MG	A	1687	1/1	0.93	0.15	118,118,118,118	0
23	MG	A	1771	1/1	0.93	0.36	119,119,119,119	0
23	MG	A	1695	1/1	0.94	0.07	139,139,139,139	0
23	MG	A	1758	1/1	0.94	0.25	99,99,99,99	0
23	MG	A	1860	1/1	0.94	0.17	362,362,362,362	0
23	MG	A	1780	1/1	0.94	0.13	90,90,90,90	0
23	MG	A	1740	1/1	0.94	0.22	119,119,119,119	0
23	MG	A	1760	1/1	0.94	0.09	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1783	1/1	0.94	0.12	284,284,284,284	0
23	MG	A	1667	1/1	0.94	0.07	176,176,176,176	0
23	MG	A	1727	1/1	0.94	0.14	94,94,94,94	0
23	MG	A	1828	1/1	0.94	0.13	114,114,114,114	0
23	MG	A	1626	1/1	0.94	0.10	208,208,208,208	0
23	MG	A	1767	1/1	0.94	0.39	121,121,121,121	0
23	MG	A	1611	1/1	0.94	0.11	139,139,139,139	0
23	MG	A	1699	1/1	0.94	0.33	201,201,201,201	0
23	MG	A	1655	1/1	0.94	0.16	131,131,131,131	0
23	MG	A	1749	1/1	0.94	0.25	113,113,113,113	0
23	MG	A	1703	1/1	0.94	0.07	137,137,137,137	0
23	MG	A	1774	1/1	0.94	0.13	190,190,190,190	0
23	MG	A	1664	1/1	0.94	0.17	137,137,137,137	0
23	MG	A	1648	1/1	0.94	0.11	115,115,115,115	0
23	MG	A	1652	1/1	0.94	0.17	131,131,131,131	0
23	MG	A	1858	1/1	0.95	0.25	167,167,167,167	0
23	MG	A	1675	1/1	0.95	0.30	103,103,103,103	0
23	MG	A	1689	1/1	0.95	0.05	90,90,90,90	0
23	MG	A	1824	1/1	0.95	0.32	123,123,123,123	0
23	MG	A	1756	1/1	0.95	0.10	152,152,152,152	0
23	MG	A	1870	1/1	0.95	0.15	245,245,245,245	0
23	MG	A	1609	1/1	0.95	0.10	76,76,76,76	0
23	MG	A	1706	1/1	0.95	0.07	115,115,115,115	0
23	MG	A	1835	1/1	0.95	0.12	172,172,172,172	0
23	MG	A	1708	1/1	0.95	0.17	117,117,117,117	0
23	MG	A	1742	1/1	0.95	0.28	107,107,107,107	0
23	MG	A	1840	1/1	0.95	0.13	222,222,222,222	0
23	MG	A	1677	1/1	0.95	0.18	111,111,111,111	0
23	MG	A	1847	1/1	0.95	0.12	380,380,380,380	0
23	MG	A	1678	1/1	0.95	0.41	114,114,114,114	0
23	MG	M	202	1/1	0.95	0.19	139,139,139,139	0
23	MG	A	1765	1/1	0.95	0.08	120,120,120,120	0
23	MG	A	1612	1/1	0.95	0.10	94,94,94,94	0
23	MG	A	1650	1/1	0.95	0.09	222,222,222,222	0
23	MG	A	1619	1/1	0.95	0.15	140,140,140,140	0
23	MG	A	1716	1/1	0.95	0.24	123,123,123,123	0
23	MG	A	1608	1/1	0.95	0.23	96,96,96,96	0
23	MG	T	201	1/1	0.95	0.14	87,87,87,87	0
23	MG	A	1674	1/1	0.95	0.21	154,154,154,154	0
23	MG	A	1861	1/1	0.96	0.21	339,339,339,339	0
23	MG	A	1863	1/1	0.96	0.17	99,99,99,99	0
23	MG	A	1831	1/1	0.96	0.13	346,346,346,346	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1832	1/1	0.96	0.11	290,290,290,290	0
23	MG	A	1633	1/1	0.96	0.24	125,125,125,125	0
23	MG	A	1871	1/1	0.96	0.06	211,211,211,211	0
23	MG	A	1836	1/1	0.96	0.26	236,236,236,236	0
23	MG	A	1702	1/1	0.96	0.28	119,119,119,119	0
23	MG	A	1729	1/1	0.96	0.20	91,91,91,91	0
23	MG	A	1634	1/1	0.96	0.10	85,85,85,85	0
23	MG	D	302	1/1	0.96	0.13	111,111,111,111	0
23	MG	A	1841	1/1	0.96	0.06	161,161,161,161	0
23	MG	A	1692	1/1	0.96	0.29	158,158,158,158	0
23	MG	A	1746	1/1	0.96	0.10	146,146,146,146	0
23	MG	A	1607	1/1	0.96	0.09	140,140,140,140	0
23	MG	A	1733	1/1	0.96	0.18	119,119,119,119	0
23	MG	A	1681	1/1	0.96	0.09	127,127,127,127	0
23	MG	A	1750	1/1	0.96	0.20	122,122,122,122	0
23	MG	A	1707	1/1	0.96	0.14	129,129,129,129	0
23	MG	A	1770	1/1	0.96	0.27	147,147,147,147	0
22	SRY	A	1601	40/40	0.96	0.10	97,126,151,158	0
23	MG	A	1753	1/1	0.96	0.12	119,119,119,119	0
23	MG	Q	202	1/1	0.96	0.07	104,104,104,104	0
23	MG	A	1647	1/1	0.96	0.23	159,159,159,159	0
23	MG	A	1638	1/1	0.96	0.10	131,131,131,131	0
23	MG	A	1639	1/1	0.96	0.25	119,119,119,119	0
23	MG	A	1868	1/1	0.97	0.14	262,262,262,262	0
23	MG	A	1629	1/1	0.97	0.15	124,124,124,124	0
23	MG	A	1839	1/1	0.97	0.10	137,137,137,137	0
23	MG	A	1671	1/1	0.97	0.17	110,110,110,110	0
23	MG	A	1712	1/1	0.97	0.43	106,106,106,106	0
23	MG	A	1843	1/1	0.97	0.20	309,309,309,309	0
23	MG	A	1644	1/1	0.97	0.07	80,80,80,80	0
23	MG	A	1683	1/1	0.97	0.28	301,301,301,301	0
23	MG	A	1649	1/1	0.97	0.08	127,127,127,127	0
23	MG	A	1685	1/1	0.97	0.10	138,138,138,138	0
23	MG	A	1656	1/1	0.97	0.20	135,135,135,135	0
23	MG	A	1719	1/1	0.97	0.20	155,155,155,155	0
23	MG	A	1853	1/1	0.97	0.19	143,143,143,143	0
23	MG	A	1657	1/1	0.97	0.18	147,147,147,147	0
23	MG	A	1826	1/1	0.97	0.07	113,113,113,113	0
23	MG	A	1688	1/1	0.97	0.16	204,204,204,204	0
23	MG	A	1739	1/1	0.97	0.25	131,131,131,131	0
23	MG	A	1620	1/1	0.97	0.15	139,139,139,139	0
23	MG	A	1659	1/1	0.97	0.40	142,142,142,142	0

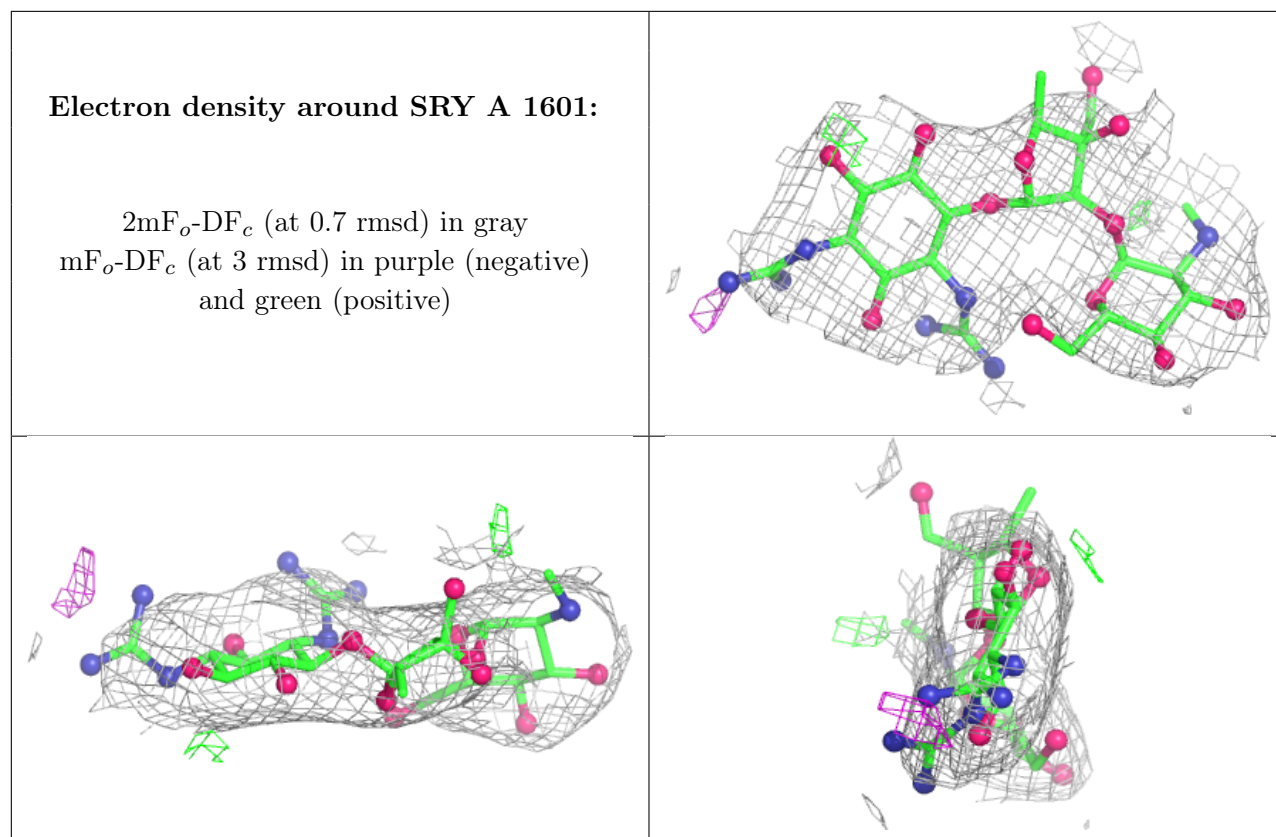
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	MG	A	1833	1/1	0.97	0.16	320,320,320,320	0
23	MG	A	1668	1/1	0.97	0.23	163,163,163,163	0
23	MG	A	1693	1/1	0.97	0.13	166,166,166,166	0
23	MG	A	1646	1/1	0.97	0.20	177,177,177,177	0
23	MG	A	1865	1/1	0.97	0.07	173,173,173,173	0
23	MG	T	203	1/1	0.97	0.20	350,350,350,350	0
24	ZN	D	301	1/1	0.97	0.21	114,114,114,114	0
23	MG	A	1834	1/1	0.98	0.07	282,282,282,282	0
23	MG	A	1721	1/1	0.98	0.05	98,98,98,98	0
23	MG	A	1785	1/1	0.98	0.09	214,214,214,214	0
23	MG	A	1762	1/1	0.98	0.12	157,157,157,157	0
23	MG	A	1621	1/1	0.98	0.11	96,96,96,96	0
23	MG	A	1713	1/1	0.98	0.12	94,94,94,94	0
23	MG	A	1613	1/1	0.98	0.13	101,101,101,101	0
23	MG	A	1691	1/1	0.98	0.15	309,309,309,309	0
23	MG	A	1842	1/1	0.98	0.14	233,233,233,233	0
23	MG	A	1827	1/1	0.98	0.28	153,153,153,153	0
23	MG	A	1844	1/1	0.98	0.10	239,239,239,239	0
23	MG	A	1632	1/1	0.98	0.17	100,100,100,100	0
23	MG	A	1866	1/1	0.98	0.12	396,396,396,396	0
23	MG	A	1867	1/1	0.98	0.06	212,212,212,212	0
23	MG	A	1829	1/1	0.98	0.05	170,170,170,170	0
23	MG	A	1848	1/1	0.98	0.07	168,168,168,168	0
23	MG	A	1614	1/1	0.98	0.12	79,79,79,79	0
23	MG	A	1701	1/1	0.98	0.11	111,111,111,111	0
23	MG	A	1651	1/1	0.98	0.04	111,111,111,111	0
23	MG	A	1617	1/1	0.98	0.06	86,86,86,86	0
24	ZN	N	101	1/1	0.98	0.05	201,201,201,201	0
23	MG	A	1764	1/1	0.99	0.09	181,181,181,181	0
23	MG	A	1605	1/1	0.99	0.07	114,114,114,114	0
23	MG	E	201	1/1	0.99	0.02	177,177,177,177	0
23	MG	A	1846	1/1	0.99	0.07	98,98,98,98	0
23	MG	A	1631	1/1	0.99	0.08	130,130,130,130	0
23	MG	A	1642	1/1	0.99	0.14	104,104,104,104	0
23	MG	A	1636	1/1	0.99	0.03	80,80,80,80	0
23	MG	A	1862	1/1	1.00	0.07	69,69,69,69	0

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.