



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:10 AM UTC

PDB ID : 6CAP / pdb_00006cap
Title : Crystal Structure of 30S ribosomal subunit from *Thermus thermophilus* in complex with Sisomicin
Authors : DeMirici, H.
Deposited on : 2018-01-31
Resolution : 3.40 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

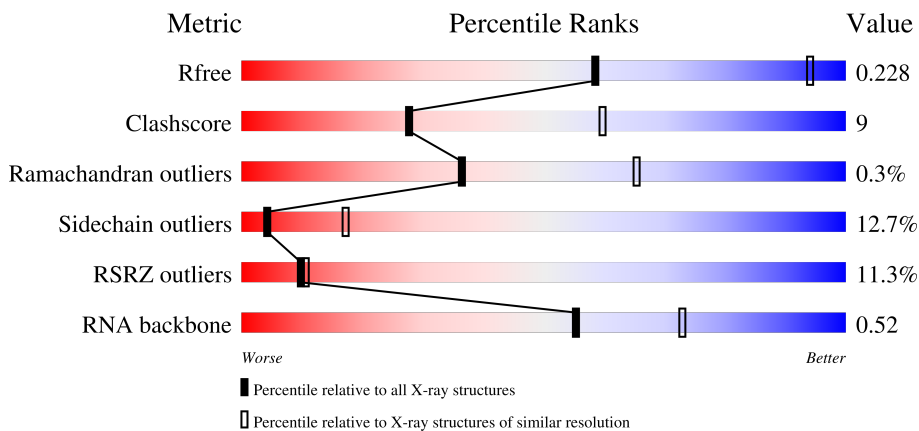
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">9% 59% 33% 8% •</p>
2	B	234	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 29%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">7% 66% 29% 5%</p>
3	C	206	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">14% 63% 33% •</p>
4	D	208	<div style="display: flex; align-items: center;"> <div style="width: 23%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="margin-left: 20px;">23% 62% 33% 5%</p>

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Mol	Chain	Length	Quality of chain			
5	E	150	9%	73%	19%	8%
6	F	101	7%	70%	27%	•
7	G	155	18%	70%	27%	•
8	H	138	4%	70%	25%	5%
9	I	127	13%	65%	29%	6%
10	J	98	9%	64%	29%	5% •
11	K	116	9%	59%	34%	6%
12	L	124	17%	65%	35%	•
13	M	118	12%	60%	36%	•
14	N	60	32%	65%	33%	•
15	O	87	7%	63%	31%	6%
16	P	83	23%	63%	36%	•
17	Q	99	18%	71%	24%	5%
18	R	70	6%	66%	31%	•
19	S	80	12%	62%	32%	5%
20	T	99	10%	64%	29%	7%
21	U	24	17%	71%	25%	•
22	Y	6		50%	50%	
23	W	15	7%	73%	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
24	MG	A	1602	-	-	-	X
24	MG	A	1677	-	-	-	X
24	MG	A	1684	-	-	-	X
24	MG	A	1733	-	-	-	X
24	MG	A	1741	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	MG	A	1786	-	-	-	X
24	MG	A	1793	-	-	-	X
24	MG	A	1796	-	-	-	X
24	MG	A	1802	-	-	-	X
24	MG	A	1808	-	-	-	X
24	MG	A	1816	-	-	-	X

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52675 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 Ribosomal RNA rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32644	14540	6040	10546	1518	0	6	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	C	U	conflict	GB 55771382

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

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

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

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	96	GLN	GLU	conflict	UNP P0DOY7

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S 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 30S ribosomal protein S20.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	Y	6	Total	C	N	O	P	0	0	0
			117	54	12	46	5			

- Molecule 23 is a RNA chain called RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	15	Total	C	N	O	P	0	0	0
			319	144	60	101	14			

- Molecule 24 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

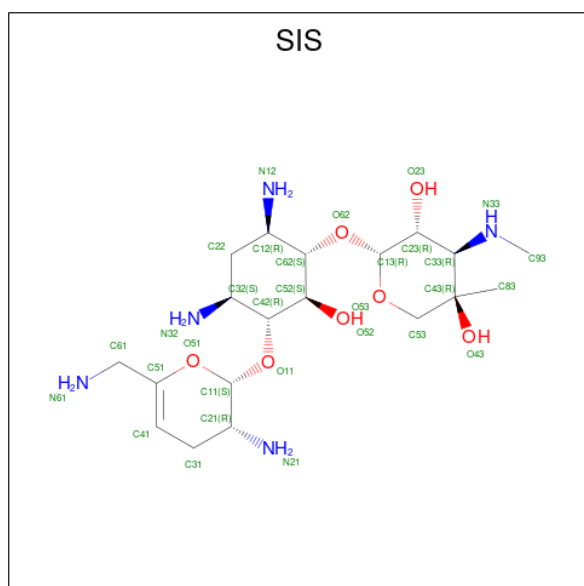
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	216	Total	Mg	0	0
			216	216		
24	B	3	Total	Mg	0	0
			3	3		
24	C	5	Total	Mg	0	0
			5	5		
24	D	3	Total	Mg	0	0
			3	3		
24	E	1	Total	Mg	0	0
			1	1		
24	F	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	H	2	Total	Mg	0	0
			2	2		
24	K	4	Total	Mg	0	0
			4	4		
24	L	3	Total	Mg	0	0
			3	3		
24	M	5	Total	Mg	0	0
			5	5		
24	P	3	Total	Mg	0	0
			3	3		
24	Q	3	Total	Mg	0	0
			3	3		
24	S	1	Total	Mg	0	0
			1	1		
24	T	1	Total	Mg	0	0
			1	1		
24	W	1	Total	Mg	0	0
			1	1		

- Molecule 25 is (1S,2S,3R,4S,6R)-4,6-diamino-3-[[[(2S,3R)-3-amino-6-(aminomethyl)-3,4-dihydro-2H-pyran-2-yl]oxy}-2-hydroxycyclohexyl 3-deoxy-4-C-methyl-3-(methylamino)-beta-L-arabinopyranoside (CCD ID: SIS) (formula: C₁₉H₃₇N₅O₇).



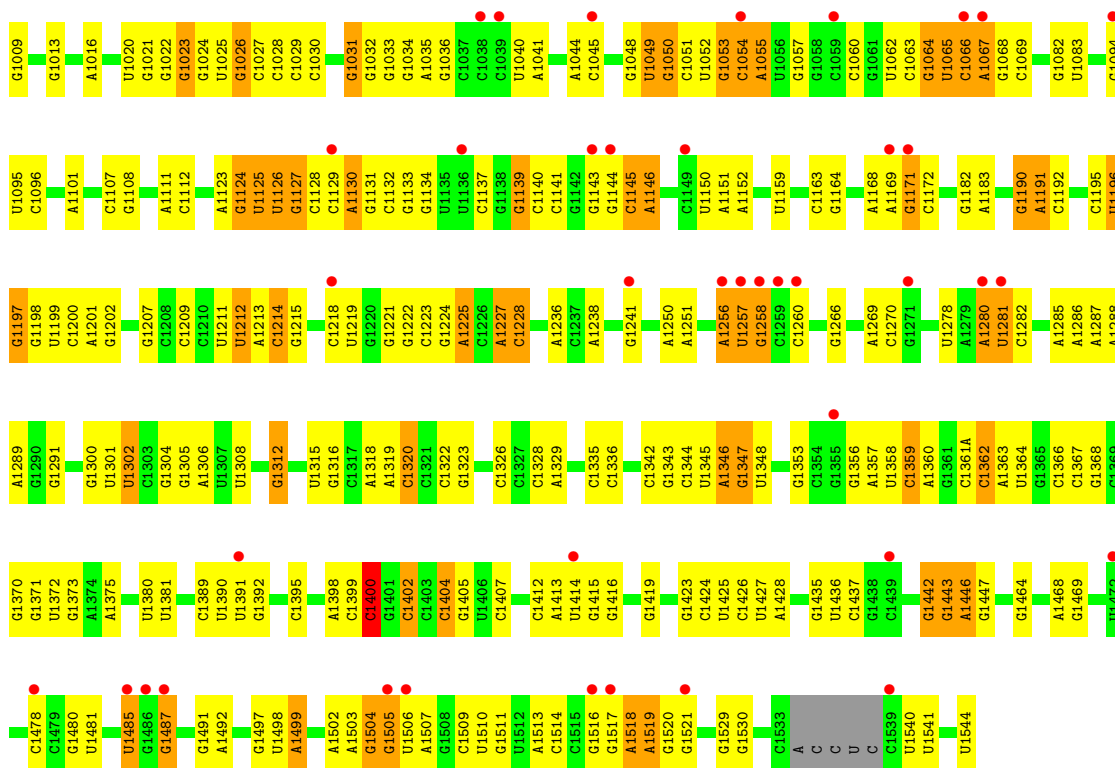
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
25	A	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

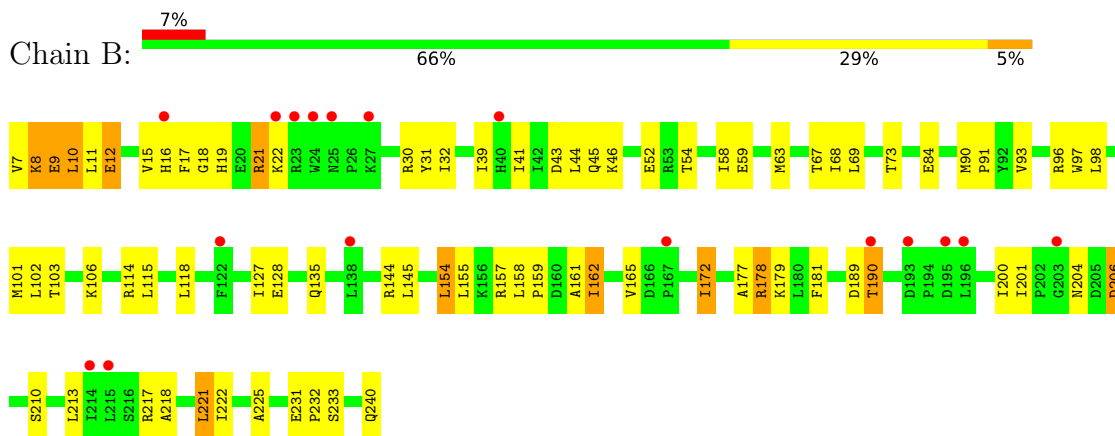
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

- Molecule 27 is water.

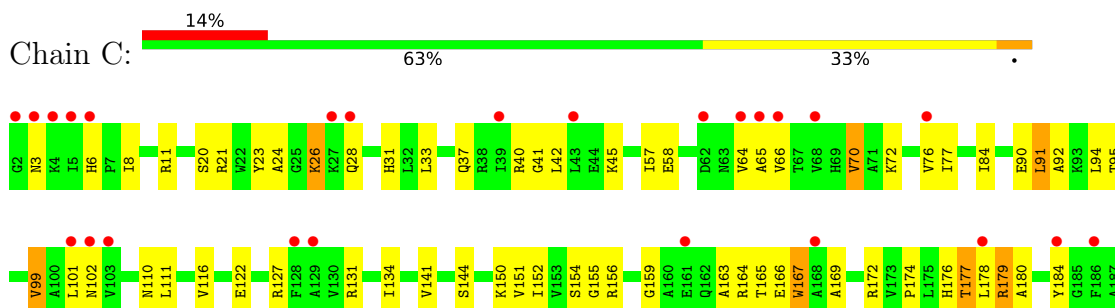
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	192	Total 192	O 192	0	0
27	C	1	Total 1	O 1	0	0
27	D	1	Total 1	O 1	0	0
27	E	6	Total 6	O 6	0	0
27	K	11	Total 11	O 11	0	0
27	L	3	Total 3	O 3	0	0
27	N	1	Total 1	O 1	0	0
27	O	1	Total 1	O 1	0	0
27	Q	2	Total 2	O 2	0	0
27	T	4	Total 4	O 4	0	0



• Molecule 2: 30S ribosomal protein S2

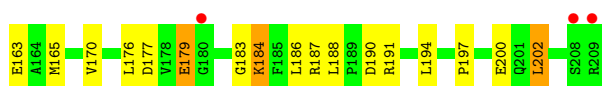
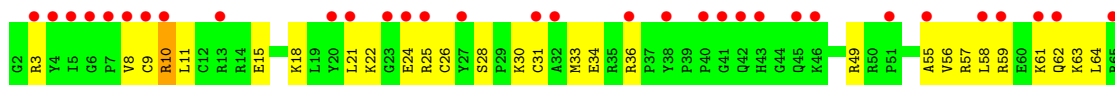


• Molecule 3: 30S ribosomal protein S3

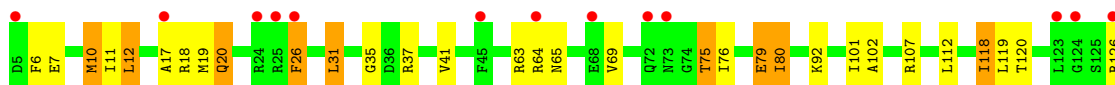




- Molecule 4: 30S ribosomal protein S4



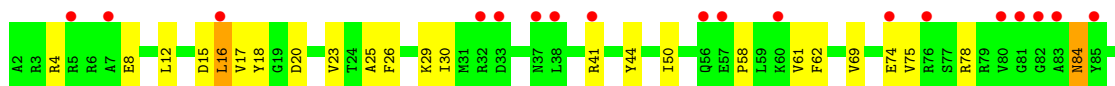
- Molecule 5: RIBOSOMAL PROTEIN S5



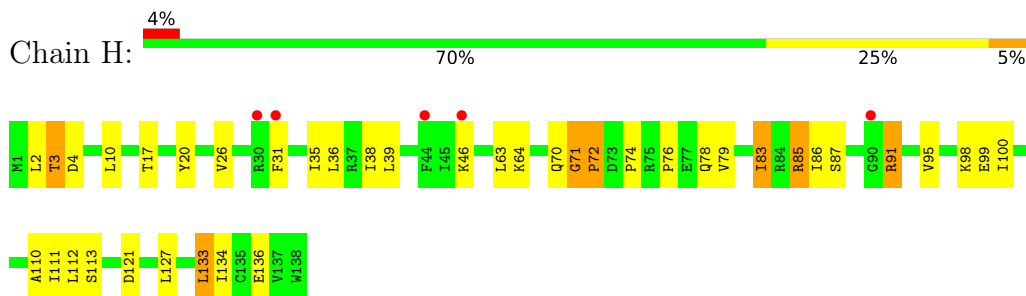
- Molecule 6: 30S ribosomal protein S6



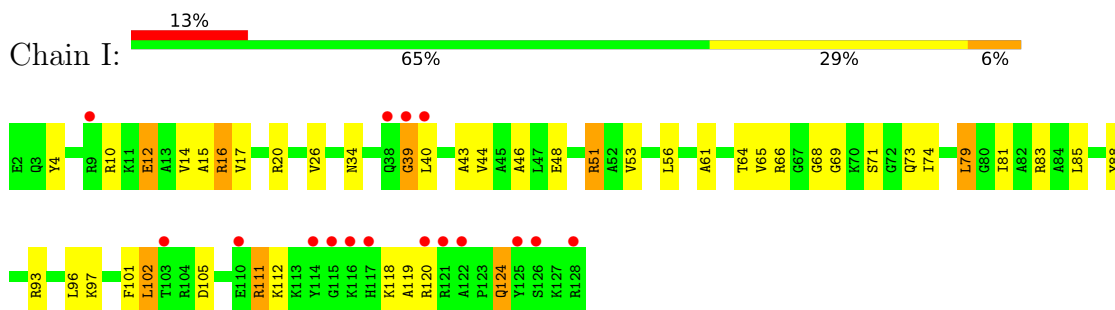
- Molecule 7: 30S ribosomal protein S7



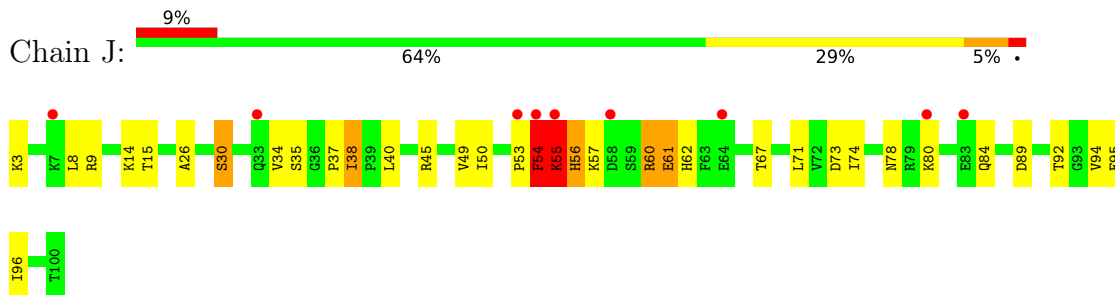
- Molecule 8: 30S ribosomal protein S8



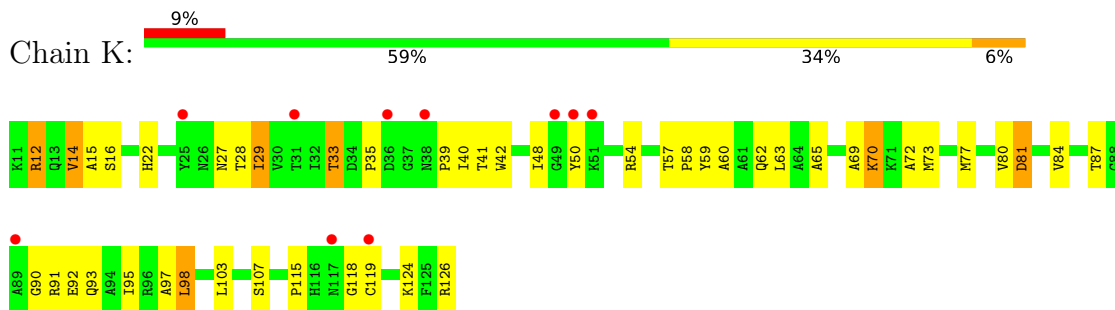
- Molecule 9: 30S ribosomal protein S9



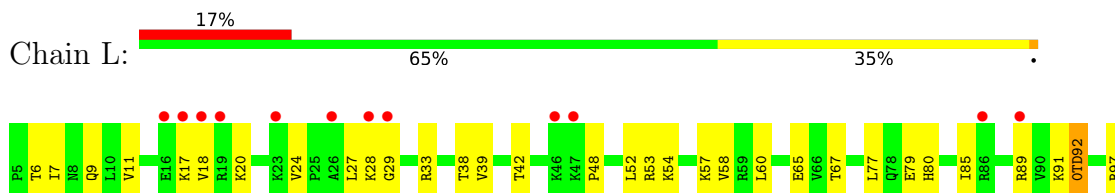
- Molecule 10: 30S ribosomal protein S10



- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12

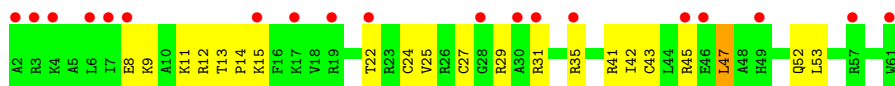




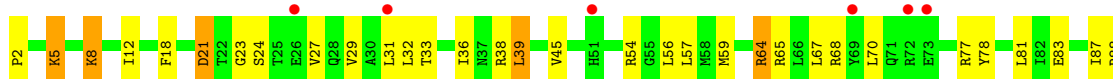
- Molecule 13: 30S ribosomal protein S13



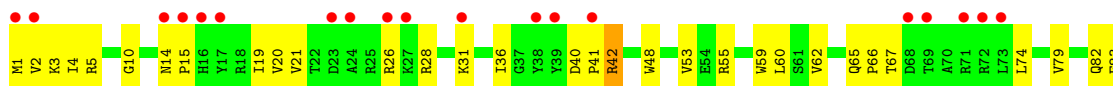
- Molecule 14: 30S ribosomal protein S14 type Z



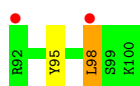
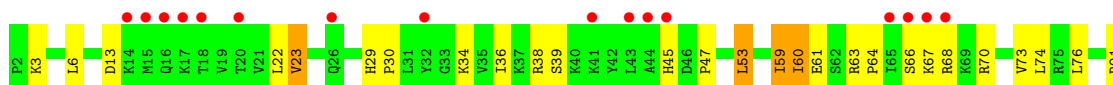
- Molecule 15: 30S ribosomal protein S15



- Molecule 16: 30S ribosomal protein S16



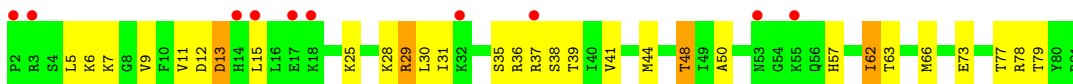
- Molecule 17: 30S ribosomal protein S17



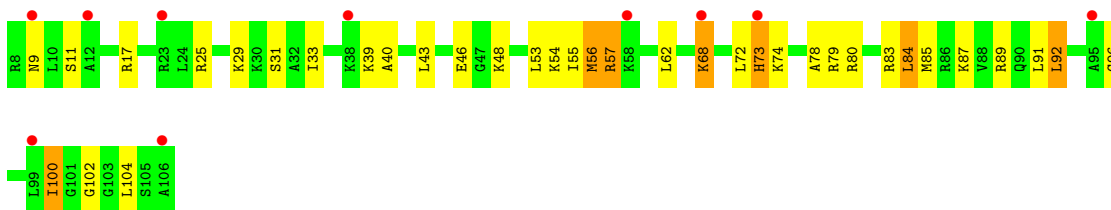
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



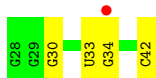
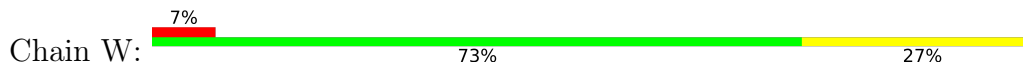
- Molecule 21: 30S ribosomal protein Thx



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



- Molecule 23: RNA (5'-R(*GP*GP*GP*AP*UP*UP*GP*AP*AP*AP*AP*UP*CP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.97Å 400.97Å 175.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.91 – 3.40 39.91 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.91-3.40) 88.4 (39.91-3.40)	Depositor EDS
R_{merge}	1.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.05 (at 3.12Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.183 , 0.230 0.185 , 0.228	Depositor DCC
R_{free} test set	2000 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	86.1	Xtrriage
Anisotropy	0.204	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 151.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52675	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 5MC, 4OC, 0TD, SIS, PSU, 2MG, G7M, M2G, ZN, UR3, MA6

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	0.21	1/36139 (0.0%)	0.43	0/56396
2	B	0.23	0/1935	0.47	0/2609
3	C	0.22	0/1636	0.44	0/2205
4	D	0.23	0/1733	0.44	0/2318
5	E	0.27	0/1162	0.48	0/1564
6	F	0.19	0/856	0.41	0/1154
7	G	0.21	0/1276	0.40	0/1709
8	H	0.25	0/1136	0.48	0/1527
9	I	0.21	0/1029	0.53	1/1379 (0.1%)
10	J	0.23	0/805	0.61	2/1082 (0.2%)
11	K	0.24	0/879	0.45	0/1187
12	L	0.24	0/977	0.48	0/1306
13	M	0.23	0/947	0.51	0/1270
14	N	0.23	0/501	0.52	0/664
15	O	0.20	0/740	0.42	0/987
16	P	0.23	0/716	0.51	0/963
17	Q	0.23	0/836	0.50	0/1117
18	R	0.21	0/579	0.43	0/768
19	S	0.20	0/661	0.52	0/890
20	T	0.22	0/765	0.46	0/1007
21	U	0.21	0/212	0.43	0/277
22	Y	0.20	0/128	0.36	0/196
23	W	0.19	0/357	0.35	0/555
All	All	0.22	1/56005 (0.0%)	0.44	3/83130 (0.0%)

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
3	C	0	2
8	H	0	1
10	J	0	2
13	M	0	2
20	T	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1498	UR3	O3'-P	5.03	1.61	1.56

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	39	GLY	N-CA-C	-6.17	98.55	113.18
10	J	54	PHE	CA-C-N	5.15	131.38	121.54
10	J	54	PHE	C-N-CA	5.15	131.38	121.54

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
8	H	71	GLY	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
13	M	111	LYS	Peptide
13	M	113	PRO	Peptide
20	T	11	SER	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	32644	0	16507	374	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1900	0	1951	48	0
3	C	1612	0	1676	40	0
4	D	1703	0	1763	46	0
5	E	1146	0	1207	26	0
6	F	843	0	857	16	0
7	G	1257	0	1296	33	0
8	H	1116	0	1177	29	0
9	I	1010	0	1037	29	0
10	J	792	0	835	25	0
11	K	864	0	881	30	0
12	L	972	0	1058	25	0
13	M	937	0	995	30	0
14	N	492	0	529	20	0
15	O	729	0	768	16	0
16	P	700	0	720	18	0
17	Q	823	0	893	20	0
18	R	574	0	644	17	0
19	S	647	0	673	21	0
20	T	763	0	861	24	0
21	U	208	0	221	5	0
22	Y	117	0	62	1	0
23	W	319	0	164	0	0
24	A	216	0	0	0	0
24	B	3	0	0	0	0
24	C	5	0	0	0	0
24	D	3	0	0	0	0
24	E	1	0	0	0	0
24	F	1	0	0	0	0
24	H	2	0	0	0	0
24	K	4	0	0	0	0
24	L	3	0	0	0	0
24	M	5	0	0	0	0
24	P	3	0	0	0	0
24	Q	3	0	0	0	0
24	S	1	0	0	0	0
24	T	1	0	0	0	0
24	W	1	0	0	0	0
25	A	31	0	37	2	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
27	A	192	0	0	2	0
27	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	D	1	0	0	0	0
27	E	6	0	0	0	0
27	K	11	0	0	1	0
27	L	3	0	0	0	0
27	N	1	0	0	0	0
27	O	1	0	0	0	0
27	Q	2	0	0	0	0
27	T	4	0	0	0	0
All	All	52675	0	36812	790	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (790) 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)
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.50	0.91
20:T:100:ILE:HG22	20:T:102:GLY:H	1.41	0.86
14:N:8:GLU:HB2	14:N:11:LYS:HE3	1.58	0.84
1:A:456:C:H42	1:A:476:G:H1	1.30	0.80
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.65	0.78
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.16	0.78
1:A:537:G:OP1	12:L:113:ARG:NH2	2.16	0.78
1:A:972:C:H4'	10:J:57:LYS:HD3	1.65	0.77
1:A:407:G:OP1	4:D:115:ARG:NH1	2.18	0.77
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.18	0.76
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.67	0.76
1:A:1005:A:N3	1:A:1026:G:N2	2.34	0.75
13:M:3:ARG:HE	13:M:7:VAL:HG12	1.49	0.75
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.68	0.75
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.52	0.74
1:A:1022:G:N2	1:A:1023:G:N7	2.36	0.74
1:A:664:G:H22	1:A:741:G:H1	1.36	0.74
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.69	0.73
1:A:1214:C:H3'	1:A:1215:G:H8	1.53	0.73
1:A:1028:C:H42	1:A:1033:G:H1	1.34	0.73
1:A:1266:G:N2	1:A:1269:A:OP2	2.20	0.73
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.71	0.73
1:A:1111:A:N1	3:C:177:THR:HB	2.03	0.72
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.55	0.72
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:13:ASP:HB2	17:Q:53:LEU:HD12	1.70	0.71
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.23	0.71
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.72	0.71
1:A:1443:G:H5''	1:A:1446:A:H5'	1.72	0.71
1:A:1145:C:O2'	1:A:1146:A:O5'	2.10	0.70
1:A:1057:G:H5''	3:C:154:SER:HB2	1.73	0.69
1:A:103:C:OP1	20:T:17:ARG:NH1	2.26	0.69
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.73	0.69
2:B:8:LYS:O	2:B:217:ARG:NH1	2.24	0.69
1:A:509:A:N3	1:A:543:C:O2'	2.26	0.68
1:A:1502:A:H2	1:A:1505:G:H1	1.42	0.68
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.27	0.68
4:D:78:LEU:HB3	4:D:93:PHE:HE1	1.59	0.68
1:A:1128:C:H42	1:A:1143:G:H1	1.40	0.68
1:A:877:C:O2	8:H:3:THR:HG21	1.94	0.67
19:S:41:VAL:HG22	19:S:44:MET:HE3	1.76	0.67
19:S:12:ASP:H	19:S:38:SER:HB3	1.60	0.67
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.30	0.66
1:A:533:A:O2'	1:A:535:A:OP2	2.13	0.66
1:A:955:U:H1'	1:A:1227:A:H61	1.59	0.66
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.29	0.66
1:A:976:G:OP2	1:A:1358:U:O2'	2.15	0.65
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.79	0.65
15:O:36:ILE:HD13	15:O:59:MET:HE3	1.79	0.65
1:A:1510:U:H2'	1:A:1511:G:C8	2.31	0.65
13:M:49:THR:HG22	13:M:51:ALA:H	1.61	0.65
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.78	0.65
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.78	0.65
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.32	0.64
1:A:921:U:O2'	5:E:19:MET:O	2.13	0.64
7:G:84:ASN:OD1	7:G:84:ASN:N	2.30	0.64
6:F:6:VAL:HG22	6:F:90:VAL:HG22	1.79	0.64
1:A:481:G:O2'	1:A:482:A:H8	1.80	0.64
1:A:250:A:H4'	1:A:251:G:O5'	1.97	0.64
1:A:1126:U:O4	1:A:1127:G:N2	2.29	0.64
1:A:1504:G:OP1	1:A:1507:A:H4'	1.98	0.64
8:H:17:THR:O	8:H:78:GLN:NE2	2.30	0.64
1:A:1196:U:OP1	1:A:1197:G:H5'	1.98	0.64
5:E:75:THR:OG1	5:E:76:ILE:N	2.29	0.64
1:A:1064:G:N2	1:A:1190:G:O2'	2.32	0.63
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:H5'	1:A:975:A:H8	1.63	0.63
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.63	0.63
15:O:56:LEU:HA	15:O:59:MET:HE2	1.81	0.63
1:A:413:G:H2'	1:A:428:G:H22	1.63	0.63
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.80	0.62
15:O:2:PRO:O	15:O:38:ARG:NH1	2.32	0.62
2:B:240:GLN:N	2:B:240:GLN:OE1	2.30	0.62
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.81	0.62
9:I:16:ARG:HD2	9:I:64:THR:HB	1.81	0.62
10:J:57:LYS:O	10:J:60:ARG:NH1	2.32	0.62
1:A:686:U:HO2'	1:A:687:A:H8	1.43	0.62
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.80	0.62
1:A:401:C:O2'	1:A:621:A:N3	2.32	0.62
1:A:922:G:H2'	1:A:923:A:C8	2.34	0.62
1:A:1128:C:O2'	1:A:1130:A:N7	2.32	0.62
18:R:47:THR:HA	18:R:83:GLU:HB2	1.82	0.62
2:B:21:ARG:HA	2:B:39:ILE:HA	1.81	0.62
1:A:1143:G:H2'	1:A:1144:G:C8	2.34	0.62
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.33	0.62
14:N:47:LEU:HD12	14:N:52:GLN:HB2	1.82	0.61
20:T:46:GLU:OE1	20:T:48:LYS:NZ	2.32	0.61
1:A:45:U:H2'	1:A:46:G:C8	2.35	0.61
1:A:406:G:H1	1:A:436:C:H42	1.46	0.61
1:A:1367:C:H5'	10:J:60:ARG:HE	1.65	0.61
3:C:156:ARG:H	3:C:163:ALA:HA	1.65	0.61
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.82	0.61
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.40	0.61
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.81	0.61
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.83	0.61
1:A:1195:C:H3'	1:A:1196:U:H5''	1.83	0.60
12:L:27:LEU:HG	12:L:28:LYS:H	1.66	0.60
1:A:7:G:O2'	5:E:120:THR:O	2.19	0.60
1:A:617:G:H1	1:A:623:C:H42	1.47	0.60
1:A:692:U:OP1	11:K:124:LYS:NZ	2.31	0.60
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.36	0.60
3:C:20:SER:OG	3:C:40:ARG:NH2	2.35	0.60
10:J:30:SER:HB3	10:J:80:LYS:HB2	1.83	0.60
20:T:92:LEU:O	20:T:96:GLY:HA2	2.02	0.60
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.82	0.60
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.84	0.60
1:A:413:G:H2'	1:A:428:G:N2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:VAL:HG12	2:B:210:SER:HB3	1.84	0.59
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.84	0.59
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.82	0.59
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.59
3:C:180:ALA:HB1	3:C:205:GLY:O	2.02	0.59
7:G:50:ILE:HD11	7:G:61:VAL:HG11	1.84	0.59
1:A:1006:C:H2'	1:A:1007:C:H6	1.65	0.59
1:A:1223:C:OP2	19:S:78:ARG:NH2	2.35	0.59
2:B:32:ILE:HD11	2:B:190:THR:HG23	1.84	0.59
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.00	0.59
4:D:187:ARG:NH1	4:D:188:LEU:H	2.00	0.59
18:R:32:ARG:HA	18:R:69:THR:HG21	1.84	0.59
1:A:983:A:O2'	1:A:1050:G:OP2	2.20	0.59
1:A:1281:U:H5'	1:A:1282:C:H5	1.68	0.59
1:A:501:C:H2'	1:A:502:G:C8	2.38	0.59
13:M:96:LEU:O	13:M:110:ARG:NH1	2.36	0.59
1:A:390:C:O3'	16:P:28:ARG:NH2	2.36	0.58
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.43	0.58
1:A:1048:G:H1	1:A:1209:C:H42	1.50	0.58
1:A:1190:G:HO2'	1:A:1191:A:P	2.26	0.58
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.85	0.58
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.85	0.58
1:A:411:A:N3	1:A:413:G:O2'	2.35	0.58
1:A:1228:C:H4'	13:M:116:THR:HA	1.86	0.58
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.84	0.58
1:A:1020:U:H2'	1:A:1021:G:H8	1.68	0.58
1:A:31:G:N2	1:A:48:C:OP1	2.33	0.58
3:C:37:GLN:HE22	14:N:47:LEU:HD11	1.69	0.58
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.35	0.58
1:A:372:C:H4'	1:A:373:A:O5'	2.01	0.58
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.85	0.58
20:T:29:LYS:O	20:T:33:ILE:HG12	2.04	0.58
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.85	0.58
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.39	0.58
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.86	0.58
1:A:1008:C:N4	1:A:1021:G:H1	2.02	0.58
19:S:28:LYS:HG2	19:S:29:ARG:H	1.68	0.58
11:K:12:ARG:HD2	11:K:14:VAL:HG13	1.86	0.57
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.36	0.57
13:M:3:ARG:NE	13:M:7:VAL:HG12	2.19	0.57
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:C:H42	1:A:1464:G:H1	1.51	0.57
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.22	0.57
8:H:36:LEU:HA	8:H:39:LEU:HD12	1.86	0.57
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.87	0.57
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.85	0.57
3:C:26:LYS:HD3	10:J:45:ARG:HH21	1.68	0.57
9:I:79:LEU:HD22	9:I:83:ARG:HG3	1.86	0.57
20:T:56:MET:HE2	20:T:85:MET:HA	1.87	0.57
1:A:1124:G:H5'	10:J:35:SER:O	2.05	0.57
1:A:424:G:H2'	1:A:425:G:H8	1.70	0.57
1:A:671:G:H5'	6:F:77:ARG:HH21	1.70	0.56
1:A:1316:G:N2	1:A:1319:A:OP2	2.31	0.56
17:Q:3:LYS:HB3	17:Q:61:GLU:HB3	1.87	0.56
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.86	0.56
3:C:174:PRO:HB2	3:C:177:THR:CG2	2.35	0.56
9:I:10:ARG:HD3	9:I:105:ASP:HB3	1.87	0.56
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.45	0.56
1:A:584:G:H5'	17:Q:91:ARG:HH12	1.69	0.56
1:A:1004:A:H5''	1:A:1025:U:C4	2.40	0.56
1:A:1328:C:H2'	1:A:1329:A:H8	1.71	0.56
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.86	0.56
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.87	0.56
4:D:102:ASP:OD1	4:D:103:ASN:N	2.39	0.56
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.88	0.56
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.35	0.56
11:K:15:ALA:HA	11:K:77:MET:HA	1.88	0.56
15:O:29:VAL:HG11	15:O:67:LEU:HD21	1.85	0.56
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.87	0.56
10:J:15:THR:HG22	10:J:94:VAL:HB	1.88	0.56
1:A:951:G:OP2	13:M:102:ARG:NH2	2.39	0.56
1:A:1291:G:H4'	9:I:39:GLY:HA3	1.88	0.55
1:A:166:G:H2'	1:A:167:G:H8	1.71	0.55
1:A:833:U:H2'	1:A:834:C:C6	2.41	0.55
4:D:162:LEU:HA	4:D:165:MET:HB2	1.87	0.55
1:A:1028:C:N3	1:A:1033:G:N2	2.46	0.55
1:A:1358:U:H5''	14:N:35:ARG:HG3	1.88	0.55
1:A:1419:G:H1	1:A:1481:U:H3	1.53	0.55
1:A:1007:C:H1'	1:A:1023:G:H22	1.72	0.55
1:A:1372:U:H5''	9:I:71:SER:HB3	1.89	0.55
1:A:527:G7M:H8	1:A:527:G7M:H5''	1.88	0.55
3:C:58:GLU:HB2	3:C:65:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:LEU:HD13	13:M:39:ILE:HB	1.89	0.55
7:G:12:LEU:HD13	7:G:25:ALA:HB2	1.87	0.55
13:M:54:VAL:O	13:M:58:GLU:HG2	2.07	0.55
1:A:153:C:H42	1:A:168:G:H1	1.53	0.54
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.89	0.54
7:G:16:LEU:H	7:G:16:LEU:HD22	1.72	0.54
1:A:811:C:N4	27:A:1902:HOH:O	2.39	0.54
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.07	0.54
1:A:757:U:O2'	1:A:879:C:O2	2.20	0.54
1:A:1251:A:H4'	9:I:12:GLU:HG2	1.89	0.54
5:E:35:GLY:HA3	5:E:112:LEU:HB3	1.88	0.54
1:A:686:U:O2'	1:A:687:A:H8	1.90	0.54
1:A:1029:C:H2'	1:A:1030:C:C6	2.43	0.54
1:A:1031:G:H2'	1:A:1032:G:H8	1.72	0.54
1:A:618:C:H5'	1:A:619:U:H5''	1.89	0.54
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.90	0.54
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.87	0.54
1:A:113:G:H1'	1:A:354:G:H5'	1.89	0.54
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.41	0.54
1:A:1134:G:H1	1:A:1140:C:H42	1.55	0.54
1:A:1221:G:O3'	19:S:77:THR:HG21	2.08	0.54
4:D:28:SER:O	4:D:30:LYS:N	2.37	0.54
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.88	0.54
1:A:1366:C:O3'	10:J:60:ARG:NH2	2.37	0.54
1:A:501:C:OP1	12:L:117:ARG:NH2	2.41	0.54
1:A:731:G:OP1	1:A:766:A:H1'	2.07	0.54
1:A:1139:G:H4'	1:A:1140:C:H5'	1.90	0.54
10:J:50:ILE:HD12	10:J:50:ILE:H	1.72	0.53
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	1.90	0.53
1:A:380:G:N2	1:A:383:A:OP2	2.38	0.53
1:A:455:C:H42	1:A:477:G:H1	1.55	0.53
1:A:1213:A:N6	1:A:1215:G:N3	2.55	0.53
15:O:64:ARG:HH21	15:O:68:ARG:HH21	1.56	0.53
7:G:108:ALA:O	7:G:111:ARG:HB2	2.08	0.53
8:H:111:ILE:HG22	8:H:134:ILE:HD12	1.90	0.53
10:J:49:VAL:HG13	14:N:41:ARG:HD2	1.90	0.53
1:A:344:A:H5'	1:A:345:C:C5	2.43	0.53
1:A:1190:G:O2'	1:A:1191:A:OP2	2.12	0.53
3:C:155:GLY:HA2	3:C:164:ARG:H	1.72	0.53
4:D:63:LYS:NZ	4:D:197:PRO:O	2.41	0.53
1:A:1125:U:OP2	1:A:1145:C:N4	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:24:ALA:HB1	3:C:28:GLN:HB2	1.89	0.53
1:A:371:G:O2'	1:A:372:C:H5'	2.08	0.53
1:A:437:U:H5'	4:D:155:LEU:HD21	1.90	0.53
12:L:38:THR:HB	12:L:57:LYS:HB2	1.90	0.53
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.40	0.53
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.90	0.53
1:A:452:A:O2'	1:A:453:A:O5'	2.27	0.53
2:B:16:HIS:CG	2:B:210:SER:HB2	2.44	0.53
1:A:1027:C:N4	1:A:1034:G:H1	2.07	0.53
1:A:1269:A:N1	1:A:1312:G:O2'	2.38	0.52
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.91	0.52
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.39	0.52
1:A:973:G:H3'	1:A:974:A:H5''	1.91	0.52
13:M:15:VAL:O	13:M:19:LEU:HG	2.09	0.52
1:A:316:G:OP2	1:A:351:G:O2'	2.27	0.52
1:A:337:C:H2'	1:A:338:A:H8	1.73	0.52
1:A:396:G:O2'	1:A:398:C:OP1	2.25	0.52
1:A:1425:U:H2'	1:A:1426:C:H6	1.74	0.52
4:D:15:GLU:OE1	4:D:66:ARG:NH1	2.42	0.52
5:E:101:ILE:O	5:E:120:THR:HB	2.09	0.52
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.91	0.52
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.91	0.52
12:L:7:ILE:O	12:L:11:VAL:HG23	2.10	0.52
1:A:1002:G:H2'	1:A:1003:G:C8	2.45	0.52
1:A:1328:C:H2'	1:A:1329:A:C8	2.44	0.52
1:A:142:G:O2'	1:A:195:A:N6	2.43	0.52
1:A:1356:G:H2'	1:A:1357:A:C8	2.44	0.52
1:A:258:G:H2'	1:A:259:G:H8	1.74	0.52
1:A:579:G:O3'	15:O:54:ARG:NH2	2.43	0.52
3:C:6:HIS:HE1	3:C:8:ILE:HB	1.74	0.52
6:F:33:TYR:CG	6:F:75:LEU:HD23	2.45	0.52
11:K:50:TYR:HE1	11:K:54:ARG:HH11	1.58	0.52
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.25	0.52
1:A:1320:C:H41	19:S:37:ARG:HD3	1.74	0.51
1:A:1491:G:C5	25:A:1792:SIS:H4	2.45	0.51
13:M:10:PRO:O	13:M:45:VAL:HG11	2.10	0.51
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.41	0.51
8:H:31:PHE:O	8:H:35:ILE:HG12	2.11	0.51
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.45	0.51
19:S:11:VAL:HG13	19:S:38:SER:HB2	1.93	0.51
1:A:1442:G:O6	1:A:1446:A:N6	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.51
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.92	0.51
1:A:229:U:H2'	1:A:230:G:C8	2.45	0.51
1:A:518:C:H4'	1:A:519:C:O5'	2.10	0.51
1:A:518:C:H2'	1:A:530:G:C8	2.46	0.51
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.46	0.51
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.75	0.51
1:A:299:G:H2'	1:A:300:A:C8	2.46	0.51
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.91	0.51
4:D:70:ILE:HG22	4:D:71:SER:O	2.10	0.51
1:A:1281:U:H5'	1:A:1282:C:C5	2.46	0.51
1:A:243:A:C2	1:A:246:A:C8	2.98	0.51
3:C:180:ALA:HB3	3:C:203:PHE:HE1	1.76	0.51
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.93	0.51
1:A:129:U:O3'	1:A:129(A):G:H3'	2.11	0.51
1:A:1198:G:H2'	1:A:1199:U:C6	2.46	0.51
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.92	0.51
1:A:217:C:H2'	1:A:218:C:H6	1.76	0.50
1:A:1163:C:H2'	1:A:1164:G:H8	1.76	0.50
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.94	0.50
18:R:33:ASP:OD2	18:R:36:ASN:N	2.44	0.50
1:A:532:A:N6	3:C:159:GLY:O	2.44	0.50
1:A:1035:A:H2'	1:A:1036:G:C8	2.46	0.50
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.93	0.50
10:J:80:LYS:H	10:J:80:LYS:HD2	1.75	0.50
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.30	0.50
1:A:673:G:H2'	1:A:674:G:C8	2.47	0.50
1:A:835:U:OP1	18:R:64:ARG:NH2	2.34	0.50
1:A:1064:G:N2	1:A:1190:G:HO2'	2.08	0.50
1:A:1414:U:H2'	1:A:1415:G:C8	2.46	0.50
7:G:145:ALA:C	7:G:147:ALA:H	2.18	0.50
1:A:191:G:O2'	20:T:102:GLY:O	2.27	0.50
1:A:1214:C:H3'	1:A:1215:G:C8	2.42	0.50
2:B:17:PHE:HD1	2:B:41:ILE:HD12	1.77	0.50
1:A:908:A:H2'	1:A:909:A:C8	2.47	0.50
12:L:113:ARG:HH11	12:L:116:SER:H	1.60	0.50
4:D:187:ARG:CZ	4:D:188:LEU:H	2.24	0.50
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.94	0.50
15:O:24:SER:HB2	15:O:27:VAL:HG23	1.94	0.50
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.94	0.50
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:U:H2'	1:A:604:G:C8	2.47	0.49
1:A:714:G:H2'	1:A:715:A:C8	2.46	0.49
1:A:838:G:H2'	1:A:839:U:H5''	1.94	0.49
6:F:2:ARG:CZ	6:F:69:GLU:HG2	2.42	0.49
11:K:33:THR:HA	11:K:39:PRO:HA	1.93	0.49
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.47	0.49
17:Q:3:LYS:HD3	17:Q:61:GLU:O	2.12	0.49
1:A:542:G:OP1	4:D:10:ARG:NH2	2.45	0.49
9:I:26:VAL:HG13	9:I:61:ALA:HB3	1.94	0.49
1:A:35:G:H2'	1:A:36:C:C6	2.46	0.49
1:A:401:C:H2'	1:A:402:G:C8	2.47	0.49
1:A:424:G:H2'	1:A:425:G:C8	2.47	0.49
15:O:70:LEU:HD22	15:O:78:TYR:HB2	1.94	0.49
19:S:13:ASP:OD1	19:S:13:ASP:N	2.45	0.49
1:A:21:G:H2'	1:A:22:G:C8	2.47	0.49
1:A:974:A:OP2	14:N:29:ARG:NH2	2.46	0.49
1:A:261:U:OP2	20:T:79:ARG:NH2	2.45	0.49
1:A:1049:U:H4'	1:A:1050:G:O5'	2.11	0.49
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.94	0.49
1:A:932:C:H5'	7:G:4:ARG:HG2	1.93	0.49
5:E:102:ALA:O	5:E:107:ARG:NH1	2.45	0.49
12:L:104:VAL:HG22	12:L:105:TYR:H	1.77	0.49
18:R:52:PRO:HB2	18:R:54:ARG:HG3	1.94	0.49
1:A:280:C:C2	17:Q:38:ARG:HD3	2.48	0.49
1:A:376:G:H5''	16:P:5:ARG:HB2	1.95	0.49
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.48	0.49
1:A:217:C:H2'	1:A:218:C:C6	2.48	0.49
1:A:1225:A:H2'	1:A:1225:A:N3	2.28	0.49
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.93	0.49
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.95	0.49
17:Q:60:ILE:HB	17:Q:74:LEU:HD13	1.94	0.49
1:A:1143:G:H2'	1:A:1144:G:H8	1.78	0.49
2:B:21:ARG:HG3	2:B:22:LYS:H	1.78	0.49
7:G:15:ASP:HB3	7:G:20:ASP:H	1.78	0.49
15:O:5:LYS:HA	15:O:8:LYS:HB2	1.95	0.49
17:Q:22:LEU:HD11	17:Q:39:SER:HB3	1.94	0.49
1:A:1020:U:H2'	1:A:1021:G:C8	2.45	0.48
1:A:1133:G:H1	1:A:1141:C:H42	1.61	0.48
1:A:1347:G:O6	9:I:10:ARG:NH2	2.46	0.48
1:A:1391:U:H2'	1:A:1392:G:C8	2.47	0.48
10:J:55:LYS:HD2	10:J:56:HIS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:G:H1	1:A:178:C:H42	1.59	0.48
1:A:918:A:H2'	1:A:919:A:C8	2.48	0.48
10:J:38:ILE:HG23	10:J:71:LEU:HB3	1.95	0.48
1:A:922:G:H4'	5:E:20:GLN:HA	1.94	0.48
1:A:1544:U:H4'	22:Y:1:U:H5'	1.95	0.48
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.95	0.48
10:J:26:ALA:HB1	10:J:84:GLN:HB2	1.95	0.48
1:A:1112:C:O2	3:C:179:ARG:HB2	2.14	0.48
3:C:41:GLY:O	3:C:45:LYS:HG2	2.13	0.48
3:C:57:ILE:HG23	3:C:66:VAL:HG22	1.95	0.48
5:E:144:THR:HG22	5:E:146:ALA:H	1.78	0.48
8:H:95:VAL:HB	8:H:99:GLU:HB2	1.94	0.48
20:T:72:LEU:O	20:T:74:LYS:N	2.47	0.48
1:A:262:A:H5'	20:T:74:LYS:HG3	1.96	0.48
1:A:421:U:H5'	1:A:422:C:C5	2.49	0.48
6:F:82:ARG:HA	6:F:82:ARG:HE	1.79	0.48
1:A:1066:C:O2'	1:A:1067:A:H5'	2.13	0.48
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.43	0.48
1:A:1392:G:H21	1:A:1502:A:H8	1.60	0.48
1:A:1413:A:H2	1:A:1487:G:H22	1.61	0.48
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.48	0.48
4:D:190:ASP:OD1	4:D:191:ARG:N	2.44	0.48
18:R:47:THR:HG22	18:R:48:GLY:H	1.78	0.48
1:A:258:G:H2'	1:A:259:G:C8	2.48	0.48
16:P:4:ILE:O	16:P:66:PRO:HA	2.14	0.48
19:S:29:ARG:HD2	19:S:29:ARG:N	2.29	0.48
1:A:481:G:HO2'	1:A:482:A:H8	1.61	0.48
1:A:1517[B]:G:N7	1:A:1518[B]:MA6:H103	2.29	0.48
10:J:26:ALA:O	10:J:84:GLN:NE2	2.46	0.48
13:M:3:ARG:HA	13:M:8:GLU:O	2.14	0.48
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.49	0.48
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.48
1:A:1006:C:H2'	1:A:1007:C:C6	2.49	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.49	0.48
12:L:58:VAL:O	12:L:65:GLU:HA	2.14	0.48
16:P:19:ILE:HG22	16:P:36:ILE:HG13	1.96	0.48
1:A:1040:U:H2'	1:A:1041:A:H8	1.78	0.47
1:A:1256:A:H4'	1:A:1257:U:O5'	2.13	0.47
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.47
14:N:9:LYS:NZ	14:N:12:ARG:HH21	2.11	0.47
2:B:43:ASP:HB3	2:B:46:LYS:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:GLU:HG2	5:E:92:LYS:HG3	1.95	0.47
7:G:151:TYR:HB3	7:G:154:TYR:HD2	1.79	0.47
8:H:100:ILE:HG12	8:H:112:LEU:HD11	1.96	0.47
1:A:62:U:O2'	1:A:379:C:O2	2.29	0.47
1:A:161:A:N1	1:A:347:G:O2'	2.41	0.47
11:K:81:ASP:OD1	11:K:107:SER:OG	2.32	0.47
13:M:96:LEU:C	13:M:110:ARG:HG2	2.40	0.47
1:A:791:G:H2'	1:A:792:A:H5'	1.97	0.47
1:A:1343:G:H2'	1:A:1344:C:C6	2.50	0.47
3:C:150:LYS:HE2	3:C:167:TRP:HZ3	1.80	0.47
8:H:85:ARG:NE	8:H:87:SER:O	2.47	0.47
1:A:538:G:H5''	12:L:114:LYS:HB2	1.96	0.47
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.96	0.47
3:C:77:ILE:HD13	3:C:84:ILE:HD12	1.97	0.47
5:E:147:ASP:N	5:E:147:ASP:OD1	2.48	0.47
7:G:15:ASP:HB2	7:G:23:VAL:HB	1.96	0.47
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.95	0.47
20:T:56:MET:HE1	20:T:104:LEU:HD21	1.96	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.50	0.47
1:A:401:C:H2'	1:A:402:G:H8	1.80	0.47
1:A:922:G:H2'	1:A:923:A:H8	1.79	0.47
1:A:975:A:H5'	1:A:975:A:C8	2.46	0.47
2:B:178:ARG:HB3	8:H:72:PRO:HG3	1.96	0.47
1:A:244:U:H4'	1:A:245:C:H5''	1.95	0.47
1:A:533:A:N6	1:A:536:C:C2	2.83	0.47
1:A:676:A:H1'	11:K:115:PRO:HB3	1.97	0.47
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.97	0.47
7:G:17:VAL:HG12	7:G:18:TYR:CD1	2.50	0.47
7:G:100:ALA:O	7:G:104:LEU:HG	2.15	0.47
1:A:302:G:H5''	12:L:17:LYS:NZ	2.30	0.47
1:A:1048:G:H1	1:A:1209:C:N4	2.13	0.47
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.48	0.47
1:A:1250:A:H4'	9:I:68:GLY:N	2.30	0.47
15:O:64:ARG:HH21	15:O:68:ARG:NH2	2.12	0.47
1:A:427:U:OP2	4:D:36:ARG:NH2	2.44	0.46
1:A:475:G:H2'	1:A:476:G:C8	2.50	0.46
1:A:526:C:OP1	12:L:91:LYS:NZ	2.48	0.46
4:D:24:GLU:HG2	4:D:25:ARG:H	1.79	0.46
9:I:111:ARG:HG2	9:I:112:LYS:N	2.30	0.46
12:L:48:PRO:HD2	12:L:92:OTD:H3	1.96	0.46
12:L:110:VAL:HG23	12:L:120:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:11:ARG:HG3	13:M:12:ASN:HB2	1.97	0.46
1:A:865:A:H2'	1:A:866:C:C6	2.49	0.46
1:A:1131:G:H2'	1:A:1132:C:C6	2.50	0.46
1:A:1222:G:H5''	19:S:78:ARG:HE	1.79	0.46
1:A:1513:A:H2'	1:A:1514:C:C6	2.51	0.46
12:L:113:ARG:NH1	12:L:116:SER:H	2.13	0.46
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.96	0.46
1:A:17:U:H2'	1:A:18:C:C6	2.50	0.46
1:A:186:C:H5'	20:T:78:ALA:HB1	1.98	0.46
19:S:7:LYS:HB3	19:S:7:LYS:HE3	1.61	0.46
1:A:216:G:H2'	1:A:217:C:C6	2.50	0.46
2:B:9:GLU:OE1	2:B:10:LEU:N	2.48	0.46
2:B:16:HIS:CD2	2:B:204:ASN:H	2.34	0.46
11:K:57:THR:CG2	11:K:60:ALA:H	2.28	0.46
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.97	0.46
1:A:109:A:H5'	1:A:110:C:H5	1.81	0.46
14:N:9:LYS:HZ3	14:N:12:ARG:HH21	1.64	0.46
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.97	0.46
1:A:769:G:H4'	1:A:1513:A:H4'	1.97	0.46
19:S:30:LEU:HD23	19:S:48:THR:HB	1.96	0.46
1:A:701:C:H5''	1:A:703:G:H5'	1.97	0.46
1:A:1065:U:H4'	1:A:1066:C:O5'	2.16	0.46
4:D:18:LYS:HA	4:D:33:MET:HG3	1.98	0.46
7:G:113:GLU:H	7:G:113:GLU:HG2	1.52	0.46
17:Q:6:LEU:HB3	17:Q:23:VAL:HG11	1.96	0.46
21:U:10:ARG:O	21:U:13:ILE:HG12	2.16	0.46
1:A:279:A:C6	17:Q:98:LEU:HD13	2.51	0.46
1:A:767:A:H2'	1:A:768:A:O4'	2.15	0.46
1:A:1427:U:H2'	1:A:1428:A:C8	2.51	0.46
7:G:139:GLU:O	7:G:143:ARG:HG3	2.16	0.46
2:B:158:LEU:HD12	2:B:158:LEU:H	1.80	0.46
11:K:22:HIS:HB3	11:K:29:ILE:HD13	1.98	0.46
1:A:636:U:H2'	1:A:637:G:C8	2.51	0.45
1:A:1419:G:N2	1:A:1481:U:O2	2.47	0.45
14:N:12:ARG:HG3	14:N:13:THR:H	1.81	0.45
1:A:254:G:OP1	17:Q:67:LYS:O	2.34	0.45
1:A:1031:G:H2'	1:A:1032:G:C8	2.50	0.45
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.98	0.45
3:C:110:ASN:O	3:C:141:VAL:HG22	2.15	0.45
8:H:36:LEU:HD23	8:H:39:LEU:HD12	1.97	0.45
9:I:69:GLY:O	9:I:73:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.83	0.45
1:A:1318:A:O2'	19:S:37:ARG:HB3	2.15	0.45
2:B:155:LEU:HD11	2:B:159:PRO:HG3	1.98	0.45
3:C:8:ILE:HG13	3:C:184:TYR:HB3	1.98	0.45
8:H:121:ASP:OD1	8:H:121:ASP:N	2.45	0.45
1:A:478:A:H2'	1:A:479:C:C6	2.51	0.45
1:A:1150:U:O4	1:A:1151:A:N6	2.50	0.45
16:P:1:MET:HE2	16:P:1:MET:HB3	1.78	0.45
16:P:1:MET:HE3	16:P:3:LYS:HD2	1.98	0.45
1:A:376:G:H5''	16:P:5:ARG:HD2	1.98	0.45
5:E:65:ASN:ND2	5:E:65:ASN:O	2.49	0.45
5:E:69:VAL:HG22	5:E:139:LEU:HB3	1.99	0.45
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.80	0.45
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.50	0.45
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.81	0.45
9:I:4:TYR:CE2	9:I:88:TYR:HD1	2.34	0.45
11:K:16:SER:O	11:K:35:PRO:HD3	2.17	0.45
13:M:22:ILE:HB	13:M:25:ILE:HB	1.98	0.45
1:A:118:U:H3'	1:A:288:A:H61	1.79	0.45
1:A:689:C:H2'	1:A:690:G:O4'	2.17	0.45
1:A:1213:A:N1	1:A:1215:G:H1'	2.31	0.45
4:D:129:ASN:HD21	4:D:144:ASP:HA	1.80	0.45
4:D:186:LEU:O	4:D:187:ARG:HG2	2.16	0.45
13:M:87:TYR:N	19:S:73:GLU:O	2.50	0.45
1:A:564:C:O2'	8:H:91:ARG:NH2	2.49	0.45
1:A:946:A:H2'	1:A:947:G:C8	2.52	0.45
1:A:970:C:OP1	10:J:57:LYS:HE2	2.16	0.45
2:B:16:HIS:ND1	2:B:210:SER:HB2	2.32	0.45
13:M:90:LEU:HD23	13:M:90:LEU:HA	1.85	0.45
16:P:26:ARG:HD2	16:P:31:LYS:O	2.17	0.45
1:A:812:C:OP1	1:A:903:G:H1'	2.16	0.45
5:E:7:GLU:OE1	5:E:37:ARG:NH2	2.50	0.45
8:H:10:LEU:HD22	8:H:83:ILE:HD13	1.98	0.45
12:L:54:LYS:HD2	12:L:54:LYS:N	2.32	0.45
15:O:12:ILE:HG12	15:O:31:LEU:HD11	1.99	0.45
1:A:181:G:H4'	1:A:182:U:C5'	2.47	0.45
1:A:922:G:H1	1:A:1395:C:H42	1.64	0.45
1:A:974:A:OP1	1:A:974:A:H8	2.00	0.45
1:A:1027:C:H42	1:A:1034:G:H1	1.64	0.45
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.52	0.45
6:F:100:ASN:O	6:F:100:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:59:ILE:HD12	17:Q:59:ILE:HA	1.78	0.45
1:A:716:A:N3	11:K:118:GLY:HA2	2.32	0.45
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.99	0.45
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.98	0.45
11:K:126:ARG:HA	27:K:303:HOH:O	2.17	0.45
1:A:109:A:H5'	1:A:110:C:C5	2.52	0.44
13:M:62:ASN:OD1	13:M:62:ASN:N	2.50	0.44
16:P:40:ASP:HB3	16:P:48:TRP:HB2	1.99	0.44
1:A:790:A:O5'	1:A:790:A:H8	2.00	0.44
1:A:1366:C:H2'	1:A:1367:C:C6	2.53	0.44
4:D:57:ARG:HG3	4:D:202:LEU:HD13	1.98	0.44
5:E:10:MET:HB3	5:E:10:MET:HE3	1.60	0.44
11:K:69:ALA:O	11:K:73:MET:HG2	2.17	0.44
1:A:1007:C:C2	1:A:1023:G:N1	2.85	0.44
1:A:1308:U:OP1	13:M:98:VAL:N	2.47	0.44
1:A:160:A:H2'	1:A:161:A:O4'	2.17	0.44
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.99	0.44
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.53	0.44
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.82	0.44
1:A:353:A:H5'	1:A:353:A:H8	1.83	0.44
1:A:665:A:H3'	1:A:725:G:H21	1.82	0.44
1:A:1502:A:H2	1:A:1505:G:N1	2.12	0.44
2:B:16:HIS:NE2	2:B:204:ASN:N	2.65	0.44
3:C:11:ARG:HG2	3:C:178:LEU:HG	2.00	0.44
3:C:91:LEU:HD23	3:C:92:ALA:N	2.32	0.44
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.16	0.44
1:A:475:G:H2'	1:A:476:G:H8	1.82	0.44
1:A:579:G:H5'	1:A:728:A:H1'	1.99	0.44
1:A:1288:A:H2'	1:A:1289:A:C8	2.53	0.44
2:B:204:ASN:H	2:B:204:ASN:HD22	1.65	0.44
1:A:269:C:H2'	1:A:270:A:C8	2.52	0.44
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.33	0.44
1:A:1320:C:O2	19:S:36:ARG:NH2	2.47	0.44
1:A:1375:A:O2'	7:G:29:LYS:NZ	2.43	0.44
2:B:30:ARG:HG3	2:B:31:TYR:CD1	2.53	0.44
2:B:178:ARG:NH2	8:H:74:PRO:HB3	2.32	0.44
7:G:78:ARG:NH1	7:G:154:TYR:O	2.51	0.44
12:L:89:ARG:NH2	12:L:97:ARG:HE	2.16	0.44
16:P:3:LYS:HA	16:P:65:GLN:H	1.81	0.44
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.99	0.44
4:D:3:ARG:HA	4:D:3:ARG:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:11:LEU:HD13	4:D:66:ARG:HD3	1.99	0.44
13:M:4:ILE:O	13:M:57:ARG:HG3	2.18	0.44
1:A:89:C:H2'	1:A:90:U:O4'	2.17	0.44
1:A:166:G:H2'	1:A:167:G:C8	2.50	0.44
1:A:701:C:H4'	1:A:702:A:O5'	2.17	0.44
1:A:1163:C:H2'	1:A:1164:G:C8	2.53	0.44
2:B:179:LYS:HA	8:H:72:PRO:HD3	2.00	0.44
4:D:191:ARG:NH1	4:D:200:GLU:OE1	2.51	0.44
6:F:24:GLU:OE2	6:F:28:ARG:NH2	2.51	0.44
7:G:149:ARG:HB3	11:K:59:TYR:CE2	2.52	0.44
2:B:68:ILE:O	2:B:90:MET:HB3	2.18	0.43
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.53	0.43
5:E:118:ILE:HG12	5:E:119:LEU:N	2.33	0.43
18:R:53:ARG:NH1	18:R:58:LEU:O	2.48	0.43
4:D:184:LYS:HE3	4:D:184:LYS:HB2	1.73	0.43
5:E:151:LEU:HD13	8:H:79:VAL:HA	1.99	0.43
1:A:106:C:O2	1:A:379:C:H4'	2.19	0.43
1:A:130:A:H5'	17:Q:63:ARG:HE	1.83	0.43
1:A:620:C:H2'	1:A:621:A:O4'	2.18	0.43
1:A:1130:A:OP1	1:A:1130:A:H3'	2.18	0.43
1:A:1423:G:H2'	1:A:1424:C:C6	2.53	0.43
6:F:46:ARG:HH22	18:R:37:VAL:HG21	1.82	0.43
1:A:501:C:H2'	1:A:502:G:H8	1.83	0.43
1:A:567:G:H2'	1:A:568:G:O4'	2.18	0.43
2:B:91:PRO:HG3	2:B:154:LEU:HG	2.01	0.43
3:C:179:ARG:HG2	3:C:206:GLU:O	2.17	0.43
11:K:50:TYR:CE1	11:K:54:ARG:HD3	2.54	0.43
20:T:54:LYS:HA	20:T:57:ARG:NH1	2.33	0.43
1:A:67:C:H2'	1:A:68:G:C8	2.53	0.43
1:A:1026:G:O6	1:A:1035:A:N6	2.40	0.43
1:A:1034:G:H2'	1:A:1035:A:H8	1.83	0.43
1:A:1133:G:H1	1:A:1141:C:N4	2.17	0.43
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.19	0.43
3:C:101:LEU:HD23	3:C:102:ASN:N	2.33	0.43
4:D:18:LYS:NZ	4:D:26:CYS:O	2.41	0.43
4:D:59:ARG:HH22	4:D:66:ARG:HH12	1.66	0.43
4:D:150:GLU:OE2	4:D:150:GLU:N	2.50	0.43
2:B:84:GLU:OE2	2:B:233:SER:OG	2.30	0.43
13:M:19:LEU:HB3	13:M:25:ILE:HG21	2.00	0.43
18:R:50:ILE:HG13	18:R:74:ARG:NH2	2.33	0.43
1:A:404:U:H5'	4:D:122:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1416:G:N1	1:A:1485:U:O2	2.52	0.43
4:D:24:GLU:HG2	4:D:25:ARG:N	2.34	0.43
16:P:74:LEU:O	16:P:79:VAL:HG23	2.18	0.43
1:A:337:C:H2'	1:A:338:A:C8	2.52	0.43
1:A:1009:G:H1	1:A:1020:U:H3	1.66	0.43
2:B:172:ILE:H	2:B:172:ILE:HG13	1.48	0.43
6:F:26:ILE:O	6:F:30:LEU:HG	2.18	0.43
8:H:46:LYS:HG2	8:H:64:LYS:HB3	2.01	0.43
14:N:14:PRO:O	14:N:15:LYS:HB3	2.19	0.43
1:A:580:U:H2'	1:A:581:G:O4'	2.19	0.43
1:A:976:G:N2	1:A:1362:C:OP2	2.42	0.43
1:A:1052:U:O2'	1:A:1055:A:OP2	2.35	0.43
1:A:1280:A:H5'	10:J:40:LEU:HD22	2.01	0.43
1:A:1392:G:N2	1:A:1502:A:H8	2.17	0.43
2:B:98:LEU:HD12	2:B:101:MET:HE3	2.00	0.43
4:D:150:GLU:CD	4:D:150:GLU:H	2.25	0.43
7:G:50:ILE:HG23	7:G:58:PRO:HB3	2.00	0.43
10:J:14:LYS:HE2	10:J:14:LYS:HB3	1.62	0.43
16:P:10:GLY:HA3	16:P:14:ASN:O	2.19	0.43
1:A:686:U:O2	11:K:42:TRP:HZ2	2.02	0.43
1:A:235:C:H5'	17:Q:70:ARG:HG2	2.01	0.42
1:A:812:C:H4'	1:A:813:U:O5'	2.19	0.42
1:A:1003(A):G:C6	1:A:1004:A:H1'	2.53	0.42
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.00	0.42
1:A:1107:C:C4	1:A:1108:G:C8	3.07	0.42
1:A:1213:A:C5	1:A:1215:G:C4	3.06	0.42
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.82	0.42
13:M:15:VAL:HG23	13:M:43:THR:O	2.19	0.42
13:M:24:GLY:O	13:M:29:ARG:HD2	2.19	0.42
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.84	0.42
1:A:488:C:H2'	1:A:489:C:C6	2.53	0.42
1:A:560:U:H5'	1:A:566:G:C2	2.54	0.42
1:A:560:U:H5'	1:A:566:G:N2	2.34	0.42
1:A:1213:A:C6	1:A:1215:G:H1'	2.55	0.42
2:B:128:GLU:HG3	2:B:135:GLN:HE22	1.84	0.42
4:D:61:LYS:NZ	4:D:72:GLU:OE2	2.51	0.42
1:A:677:U:H3	1:A:713:G:H22	1.66	0.42
1:A:936:C:H2'	1:A:937:A:O4'	2.19	0.42
1:A:1342:C:H2'	1:A:1343:G:C8	2.55	0.42
11:K:98:LEU:HD22	11:K:98:LEU:HA	1.78	0.42
13:M:48:LEU:HA	13:M:48:LEU:HD22	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:41:ARG:HG3	14:N:42:ILE:N	2.35	0.42
1:A:551:U:H2'	1:A:552:U:C6	2.55	0.42
1:A:779:C:H42	1:A:803:G:H1	1.68	0.42
2:B:19:HIS:ND1	2:B:189:ASP:OD2	2.26	0.42
4:D:31:CYS:C	4:D:33:MET:H	2.28	0.42
7:G:50:ILE:HD11	7:G:61:VAL:CG1	2.49	0.42
1:A:229:U:H2'	1:A:230:G:H8	1.83	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.42
1:A:662:G:H1	1:A:743:U:H3	1.67	0.42
1:A:815:A:N6	1:A:1509:C:H1'	2.34	0.42
1:A:911:U:H2'	1:A:912:C:C6	2.54	0.42
1:A:1013:G:N2	1:A:1016:A:OP2	2.51	0.42
1:A:1057:G:H5''	3:C:154:SER:CB	2.45	0.42
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.42
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.55	0.42
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.02	0.42
11:K:27:ASN:OD1	11:K:28:THR:N	2.52	0.42
16:P:74:LEU:HD22	16:P:79:VAL:HG21	2.01	0.42
1:A:750:G:N3	15:O:23:GLY:HA3	2.33	0.42
1:A:939:G:H5''	7:G:102:ARG:NH1	2.34	0.42
1:A:1145:C:H1'	1:A:1146:A:C8	2.55	0.42
8:H:103:VAL:CG2	8:H:110:ALA:HB2	2.49	0.42
12:L:42:THR:HA	12:L:53:ARG:O	2.19	0.42
13:M:60:VAL:HG12	13:M:66:LEU:HD11	2.00	0.42
15:O:87:ILE:HG22	15:O:88:ARG:HG2	2.01	0.42
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.81	0.42
1:A:295:C:H2'	1:A:296:U:O4'	2.19	0.42
1:A:956:U:H2'	1:A:957:U:O4'	2.19	0.42
1:A:1288:A:H2'	1:A:1289:A:H8	1.84	0.42
2:B:54:THR:O	2:B:58:ILE:HG13	2.20	0.42
11:K:57:THR:OG1	11:K:58:PRO:HD2	2.19	0.42
1:A:452:A:O2'	1:A:453:A:O4'	2.21	0.42
1:A:965:A:H4'	1:A:966:M2G:OP1	2.19	0.42
1:A:1315:U:O2'	1:A:1360:A:N3	2.53	0.42
1:A:1468:A:H2'	1:A:1469:G:O4'	2.20	0.42
19:S:25:LYS:HD2	19:S:25:LYS:N	2.34	0.42
1:A:298:A:H2'	1:A:299:G:O4'	2.20	0.42
1:A:488:C:H2'	1:A:489:C:H6	1.85	0.42
1:A:664:G:OP1	18:R:64:ARG:NH1	2.42	0.42
1:A:824:C:H2'	1:A:825:G:C8	2.54	0.42
1:A:1404:5MC:HN41	1:A:1497:G:H1	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:LEU:HA	4:D:183:GLY:HA2	2.00	0.42
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.71	0.42
13:M:65:LYS:O	13:M:66:LEU:HD23	2.20	0.42
20:T:92:LEU:HD13	20:T:92:LEU:HA	1.78	0.42
1:A:164:U:H2'	1:A:165:C:C6	2.55	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.42
1:A:820:U:H4'	1:A:821:G:OP2	2.19	0.42
2:B:114:ARG:HH11	2:B:118:LEU:HD21	1.84	0.42
4:D:55:ALA:O	4:D:59:ARG:HG2	2.20	0.42
9:I:17:VAL:HG11	9:I:81:ILE:HA	2.01	0.42
18:R:40:LEU:HB3	18:R:79:LEU:HD11	2.01	0.42
1:A:1236:A:O2'	1:A:1304:G:H4'	2.20	0.41
1:A:1257:U:O2'	1:A:1258:G:P	2.78	0.41
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.19	0.41
4:D:101:LEU:O	4:D:105:VAL:HG23	2.19	0.41
21:U:5:ASP:O	21:U:11:GLY:HA3	2.19	0.41
1:A:153:C:N4	1:A:168:G:H1	2.17	0.41
1:A:300:A:H8	1:A:300:A:O5'	2.03	0.41
1:A:1405:G:N7	25:A:1792:SIS:N33	2.68	0.41
2:B:218:ALA:O	2:B:222:ILE:HG13	2.20	0.41
19:S:12:ASP:OD2	19:S:35:SER:HB2	2.20	0.41
1:A:437:U:H4'	4:D:155:LEU:HD11	2.02	0.41
1:A:939:G:H2'	1:A:940:C:C6	2.55	0.41
1:A:1302:U:C6	13:M:17:VAL:HG21	2.55	0.41
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.84	0.41
1:A:1145:C:O2'	1:A:1146:A:P	2.78	0.41
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.20	0.41
8:H:64:LYS:HG3	8:H:79:VAL:HG21	2.02	0.41
9:I:85:LEU:HD12	9:I:85:LEU:HA	1.94	0.41
20:T:79:ARG:HE	20:T:83:ARG:HH12	1.68	0.41
1:A:76:C:H2'	1:A:77:G:H8	1.85	0.41
1:A:768:A:OP1	1:A:804:U:H4'	2.20	0.41
1:A:939:G:H5'	7:G:102:ARG:NH2	2.35	0.41
1:A:1168:A:C6	1:A:1169:A:C6	3.09	0.41
1:A:1212:U:H6	1:A:1212:U:H2'	1.69	0.41
13:M:19:LEU:HD22	13:M:22:ILE:HD11	2.02	0.41
1:A:109:A:C6	1:A:326:G:C6	3.09	0.41
1:A:570:G:C6	1:A:873:A:C2	3.09	0.41
1:A:757:U:H2'	1:A:758:G:O4'	2.20	0.41
1:A:1069:C:O2'	1:A:1192:C:H1'	2.20	0.41
2:B:155:LEU:HD23	2:B:155:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:LYS:HB2	2:B:179:LYS:HE3	1.78	0.41
1:A:992:U:H3	1:A:1044:A:H62	1.69	0.41
1:A:1082:G:H2'	1:A:1083:U:O4'	2.20	0.41
7:G:26:PHE:CD1	7:G:101:LEU:HD22	2.49	0.41
7:G:41:ARG:HH11	7:G:41:ARG:HB3	1.86	0.41
7:G:138:LYS:HE2	7:G:142:GLU:OE1	2.20	0.41
1:A:299:G:C6	1:A:300:A:C6	3.09	0.41
1:A:1435:G:H2'	1:A:1436:U:C6	2.55	0.41
1:A:11:G:O5'	1:A:11:G:H8	2.04	0.41
1:A:390:C:H2'	1:A:391:G:C8	2.56	0.41
1:A:967:5MC:H2'	1:A:968:A:N7	2.35	0.41
1:A:1347:G:N2	1:A:1373:G:H2'	2.36	0.41
1:A:1389:C:H2'	1:A:1390:U:O4'	2.21	0.41
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.36	0.41
4:D:8:VAL:HG11	4:D:21:LEU:HB2	2.03	0.41
4:D:121:VAL:O	4:D:134:ASP:HA	2.20	0.41
4:D:127:THR:HG23	4:D:130:GLY:H	1.85	0.41
4:D:179:GLU:CD	4:D:179:GLU:H	2.28	0.41
8:H:112:LEU:HD23	8:H:133:LEU:HA	2.03	0.41
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.35	0.41
11:K:48:ILE:HD13	11:K:63:LEU:HB2	2.03	0.41
11:K:70:LYS:NZ	11:K:70:LYS:HB3	2.35	0.41
14:N:8:GLU:O	14:N:11:LYS:HG3	2.21	0.41
16:P:15:PRO:HG2	16:P:41:PRO:HG2	2.03	0.41
18:R:53:ARG:HD3	18:R:63:GLN:CB	2.51	0.41
19:S:36:ARG:H	19:S:36:ARG:HG2	1.63	0.41
20:T:39:LYS:O	20:T:43:LEU:HG	2.21	0.41
20:T:56:MET:HG3	20:T:84:LEU:CD1	2.51	0.41
20:T:68:LYS:HE3	20:T:68:LYS:HA	2.03	0.41
1:A:9:G:H5''	5:E:126:ARG:HD3	2.03	0.41
1:A:880:C:H2'	1:A:881:G:H8	1.86	0.41
2:B:97:TRP:CZ2	2:B:101:MET:HB2	2.56	0.41
13:M:8:GLU:OE2	13:M:22:ILE:HA	2.21	0.41
1:A:696:A:H8	1:A:696:A:O5'	2.04	0.40
1:A:1171:G:H2'	1:A:1172:C:C6	2.56	0.40
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.03	0.40
9:I:48:GLU:HB3	9:I:101:PHE:CZ	2.56	0.40
1:A:456:C:N4	1:A:476:G:H1	2.08	0.40
1:A:1053:G:H4'	1:A:1054:C:H5'	2.04	0.40
1:A:1062:U:H2'	1:A:1063:C:C6	2.57	0.40
1:A:1424:C:H2'	1:A:1425:U:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:G:H4'	1:A:429:U:O5'	2.22	0.40
1:A:828:A:OP1	1:A:828:A:H4'	2.21	0.40
5:E:150:ARG:HE	5:E:150:ARG:HB2	1.64	0.40
1:A:176:C:OP1	20:T:29:LYS:NZ	2.38	0.40
1:A:235:C:N4	27:A:1908:HOH:O	2.54	0.40
1:A:1359:C:H1'	1:A:1361(A):C:H41	1.86	0.40
1:A:1518[B]:MA6:H93	1:A:1519[B]:MA6:N1	2.36	0.40
2:B:12:GLU:HG3	2:B:213:LEU:HD11	2.02	0.40
4:D:81:GLU:O	4:D:85:LYS:HG3	2.22	0.40
5:E:142:LEU:HD23	5:E:142:LEU:HA	1.93	0.40
6:F:48:LEU:HD13	6:F:52:ILE:HD12	2.02	0.40
7:G:62:PHE:HA	7:G:124:LEU:CD2	2.51	0.40
11:K:40:ILE:HG22	11:K:41:THR:HG23	2.03	0.40
12:L:27:LEU:C	12:L:29:GLY:N	2.78	0.40
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.57	0.40
20:T:54:LYS:HA	20:T:57:ARG:HH11	1.87	0.40
1:A:520:A:OP1	12:L:52:LEU:HB2	2.22	0.40
1:A:737:A:H2'	1:A:738:C:C6	2.56	0.40
1:A:766:A:H2'	1:A:767:A:O4'	2.22	0.40
1:A:977:A:H2'	1:A:978:A:H5''	2.03	0.40
3:C:127:ARG:HB2	3:C:127:ARG:NH1	2.37	0.40
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.87	0.40
7:G:144:MET:O	7:G:147:ALA:HB3	2.22	0.40
8:H:3:THR:H	8:H:3:THR:HG22	1.57	0.40
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.57	0.40
20:T:87:LYS:O	20:T:91:LEU:HB2	2.22	0.40
21:U:6:ARG:H	21:U:6:ARG:HG2	1.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/234 (99%)	216 (93%)	16 (7%)	0	100	100
3	C	204/206 (99%)	182 (89%)	22 (11%)	0	100	100
4	D	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
5	E	148/150 (99%)	140 (95%)	8 (5%)	0	100	100
6	F	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
7	G	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
8	H	136/138 (99%)	129 (95%)	5 (4%)	2 (2%)	8	30
9	I	125/127 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/98 (98%)	80 (83%)	13 (14%)	3 (3%)	3	18
11	K	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
12	L	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
13	M	116/118 (98%)	99 (85%)	16 (14%)	1 (1%)	14	42
14	N	58/60 (97%)	49 (84%)	9 (16%)	0	100	100
15	O	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
16	P	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
17	Q	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
18	R	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
19	S	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
20	T	97/99 (98%)	88 (91%)	8 (8%)	1 (1%)	12	40
21	U	22/24 (92%)	20 (91%)	2 (9%)	0	100	100
All	All	2336/2377 (98%)	2162 (93%)	167 (7%)	7 (0%)	36	65

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
10	J	56	HIS
10	J	54	PHE
8	H	72	PRO
8	H	71	GLY
20	T	73	HIS
13	M	112	GLY

5.3.2 Protein sidechains [i](#)

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	202/202 (100%)	173 (86%)	29 (14%)	3 13
3	C	160/160 (100%)	131 (82%)	29 (18%)	2 7
4	D	180/180 (100%)	154 (86%)	26 (14%)	3 13
5	E	115/115 (100%)	97 (84%)	18 (16%)	2 10
6	F	90/90 (100%)	82 (91%)	8 (9%)	9 31
7	G	126/126 (100%)	116 (92%)	10 (8%)	11 36
8	H	119/119 (100%)	108 (91%)	11 (9%)	8 29
9	I	98/98 (100%)	84 (86%)	14 (14%)	3 13
10	J	87/88 (99%)	75 (86%)	12 (14%)	3 14
11	K	88/88 (100%)	78 (89%)	10 (11%)	5 21
12	L	103/103 (100%)	93 (90%)	10 (10%)	8 28
13	M	94/94 (100%)	82 (87%)	12 (13%)	4 17
14	N	49/49 (100%)	45 (92%)	4 (8%)	10 35
15	O	79/79 (100%)	66 (84%)	13 (16%)	2 10
16	P	72/72 (100%)	64 (89%)	8 (11%)	6 21
17	Q	94/94 (100%)	86 (92%)	8 (8%)	10 33
18	R	61/61 (100%)	57 (93%)	4 (7%)	15 41
19	S	71/71 (100%)	61 (86%)	10 (14%)	3 13
20	T	76/76 (100%)	63 (83%)	13 (17%)	2 9
21	U	19/19 (100%)	17 (90%)	2 (10%)	6 23
All	All	1983/1984 (100%)	1732 (87%)	251 (13%)	4 17

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	9	GLU

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Mol	Chain	Res	Type
2	B	10	LEU
2	B	11	LEU
2	B	12	GLU
2	B	21	ARG
2	B	44	LEU
2	B	45	GLN
2	B	52	GLU
2	B	67	THR
2	B	69	LEU
2	B	73	THR
2	B	96	ARG
2	B	102	LEU
2	B	103	THR
2	B	106	LYS
2	B	127	ILE
2	B	144	ARG
2	B	154	LEU
2	B	157	ARG
2	B	162	ILE
2	B	165	VAL
2	B	172	ILE
2	B	178	ARG
2	B	190	THR
2	B	200	ILE
2	B	206	ASP
2	B	221	LEU
3	C	3	ASN
3	C	21	ARG
3	C	26	LYS
3	C	31	HIS
3	C	42	LEU
3	C	64	VAL
3	C	70	VAL
3	C	72	LYS
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	122	GLU
3	C	131	ARG

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Mol	Chain	Res	Type
3	C	144	SER
3	C	152	ILE
3	C	165	THR
3	C	167	TRP
3	C	172	ARG
3	C	176	HIS
3	C	177	THR
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	193	TYR
3	C	196	LEU
3	C	204	LEU
4	D	9	CYS
4	D	10	ARG
4	D	34	GLU
4	D	49	ARG
4	D	56	VAL
4	D	58	LEU
4	D	64	LEU
4	D	67	ILE
4	D	78	LEU
4	D	83	SER
4	D	115	ARG
4	D	122	ARG
4	D	127	THR
4	D	135	LEU
4	D	145	GLU
4	D	150	GLU
4	D	152	SER
4	D	154	ASN
4	D	155	LEU
4	D	163	GLU
4	D	170	VAL
4	D	177	ASP
4	D	179	GLU
4	D	184	LYS
4	D	194	LEU
4	D	202	LEU
5	E	6	PHE
5	E	10	MET
5	E	12	LEU

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Mol	Chain	Res	Type
5	E	18	ARG
5	E	20	GLN
5	E	26	PHE
5	E	31	LEU
5	E	41	VAL
5	E	63	ARG
5	E	64	ARG
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	118	ILE
5	E	131	ILE
5	E	147	ASP
5	E	148	VAL
5	E	151	LEU
6	F	10	LEU
6	F	24	GLU
6	F	25	ILE
6	F	32	ASN
6	F	37	VAL
6	F	55	ASP
6	F	82	ARG
6	F	92	LYS
7	G	8	GLU
7	G	16	LEU
7	G	75	VAL
7	G	84	ASN
7	G	92	SER
7	G	113	GLU
7	G	120	ILE
7	G	124	LEU
7	G	136	LYS
7	G	149	ARG
8	H	2	LEU
8	H	3	THR
8	H	26	VAL
8	H	38	ILE
8	H	63	LEU
8	H	83	ILE
8	H	85	ARG
8	H	91	ARG
8	H	98	LYS

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Mol	Chain	Res	Type
8	H	127	LEU
8	H	133	LEU
9	I	12	GLU
9	I	14	VAL
9	I	16	ARG
9	I	20	ARG
9	I	34	ASN
9	I	40	LEU
9	I	44	VAL
9	I	51	ARG
9	I	79	LEU
9	I	96	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	124	GLN
10	J	3	LYS
10	J	30	SER
10	J	38	ILE
10	J	55	LYS
10	J	60	ARG
10	J	61	GLU
10	J	62	HIS
10	J	67	THR
10	J	73	ASP
10	J	78	ASN
10	J	89	ASP
10	J	95	GLU
11	K	12	ARG
11	K	14	VAL
11	K	29	ILE
11	K	33	THR
11	K	70	LYS
11	K	81	ASP
11	K	87	THR
11	K	92	GLU
11	K	98	LEU
11	K	119	CYS
12	L	18	VAL
12	L	20	LYS
12	L	33	ARG
12	L	39	VAL

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Mol	Chain	Res	Type
12	L	60	LEU
12	L	67	THR
12	L	79	GLU
12	L	80	HIS
12	L	85	ILE
12	L	100	ILE
13	M	8	GLU
13	M	17	VAL
13	M	20	THR
13	M	25	ILE
13	M	44	ARG
13	M	48	LEU
13	M	56	LEU
13	M	82	MET
13	M	105	THR
13	M	108	ARG
13	M	109	THR
13	M	117	VAL
14	N	22	THR
14	N	25	VAL
14	N	31	ARG
14	N	47	LEU
15	O	5	LYS
15	O	8	LYS
15	O	21	ASP
15	O	32	LEU
15	O	33	THR
15	O	39	LEU
15	O	45	VAL
15	O	57	LEU
15	O	64	ARG
15	O	65	ARG
15	O	77	ARG
15	O	81	LEU
15	O	83	GLU
16	P	2	VAL
16	P	20	VAL
16	P	42	ARG
16	P	55	ARG
16	P	62	VAL
16	P	67	THR
16	P	82	GLN

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Mol	Chain	Res	Type
16	P	83	GLU
17	Q	23	VAL
17	Q	34	LYS
17	Q	36	ILE
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	98	LEU
18	R	31	LEU
18	R	42	ARG
18	R	54	ARG
18	R	87	ARG
19	S	6	LYS
19	S	13	ASP
19	S	15	LEU
19	S	29	ARG
19	S	31	ILE
19	S	39	THR
19	S	48	THR
19	S	62	ILE
19	S	63	THR
19	S	79	THR
20	T	9	ASN
20	T	25	ARG
20	T	31	SER
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	73	HIS
20	T	80	ARG
20	T	84	LEU
20	T	92	LEU
20	T	100	ILE
21	U	6	ARG
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	135	GLN
2	B	204	ASN
3	C	37	GLN
3	C	123	GLN
4	D	129	ASN
4	D	199	ASN
6	F	11	ASN
6	F	13	ASN
6	F	64	GLN
6	F	94	GLN
7	G	37	ASN
7	G	148	ASN
8	H	78	GLN
9	I	3	GLN
9	I	23	ASN
12	L	49	ASN
15	O	53	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1505/1522 (98%)	247 (16%)	46 (3%)
22	Y	5/6 (83%)	2 (40%)	0
23	W	14/15 (93%)	4 (28%)	0
All	All	1524/1543 (98%)	253 (16%)	46 (3%)

All (253) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	75	G
1	A	101	A
1	A	108	G
1	A	116	A

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Mol	Chain	Res	Type
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	183	G
1	A	195	A
1	A	201	C
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	245	C
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	282	A
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	371	G
1	A	373	A
1	A	374	A
1	A	381	C
1	A	384	G
1	A	390	C

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Mol	Chain	Res	Type
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	440	A
1	A	460	A
1	A	461	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	524	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	596	C
1	A	607	A
1	A	618	C
1	A	653	A
1	A	665	A

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Mol	Chain	Res	Type
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	703	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	873	A
1	A	889	A
1	A	902	G
1	A	914	A
1	A	916	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
1	A	968	A

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Mol	Chain	Res	Type
1	A	969	A
1	A	971	G
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	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	1023	G
1	A	1024	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U

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Mol	Chain	Res	Type
1	A	1171	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1306	A
1	A	1312	G
1	A	1320	C
1	A	1322	C
1	A	1323	G
1	A	1335	C
1	A	1336	C
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C

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Mol	Chain	Res	Type
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1368	G
1	A	1370	G
1	A	1381	U
1	A	1398	A
1	A	1400	5MC
1	A	1402	4OC
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1478	C
1	A	1480	G
1	A	1485	U
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
22	Y	5	U
22	Y	6	U
23	W	30	G
23	W	33	U
23	W	34	G
23	W	42	C

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G

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Mol	Chain	Res	Type
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	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	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	991	U
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1404	1	19,22,23	1.09	2 (10%)	26,32,35	1.07	2 (7%)
1	PSU	A	1541	1	18,21,22	1.13	1 (5%)	21,30,33	1.75	4 (19%)
1	5MC	A	1400	1	19,22,23	1.12	2 (10%)	26,32,35	1.04	2 (7%)
1	G7M	A	527	1	23,26,27	1.28	3 (13%)	34,39,42	1.69	7 (20%)
1	MA6	A	1519[B]	1	23,26,27	1.35	5 (21%)	33,38,41	0.89	0
1	M2G	A	966	1	24,27,28	1.10	3 (12%)	33,40,43	0.88	1 (3%)
1	PSU	A	516	24,1	18,21,22	1.22	1 (5%)	21,30,33	1.72	5 (23%)
1	MA6	A	1518[A]	1	23,26,27	0.92	2 (8%)	33,38,41	0.82	1 (3%)
12	0TD	L	92	12	8,9,10	0.95	0	6,11,13	1.77	2 (33%)
1	5MC	A	1407	1	19,22,23	1.11	2 (10%)	26,32,35	0.99	2 (7%)
1	5MC	A	967	1	19,22,23	1.05	2 (10%)	26,32,35	0.94	1 (3%)
1	UR3	A	1498	1	19,22,23	1.26	2 (10%)	26,32,35	1.18	1 (3%)
1	PSU	A	1540	1	18,21,22	1.18	1 (5%)	21,30,33	1.67	4 (19%)
1	MA6	A	1518[B]	1	23,26,27	1.40	5 (21%)	33,38,41	0.95	1 (3%)
1	2MG	A	1207	1	23,26,27	1.40	5 (21%)	33,38,41	1.09	3 (9%)
1	4OC	A	1402	1	20,23,24	1.14	3 (15%)	25,32,35	0.76	0
1	MA6	A	1519[A]	1	23,26,27	0.96	2 (8%)	33,38,41	0.89	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	1/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
1	MA6	A	1519[B]	1	-	4/11/29/30	0/3/3/3
1	M2G	A	966	1	-	3/11/29/30	0/3/3/3
1	PSU	A	516	24,1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	2/11/29/30	0/3/3/3
12	0TD	L	92	12	-	2/7/12/14	-
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	2/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	2/7/25/26	0/2/2/2
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[B]	1	-	1/11/29/30	0/3/3/3
1	2MG	A	1207	1	-	0/9/27/28	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	MA6	A	1519[A]	1	-	3/11/29/30	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1540	PSU	C6-C5	4.17	1.39	1.35
1	A	516	PSU	C6-C5	4.16	1.39	1.35
1	A	527	G7M	C2-N2	4.14	1.43	1.34
1	A	1498	UR3	C2-N1	4.09	1.44	1.38
1	A	1541	PSU	C6-C5	3.77	1.39	1.35
1	A	1207	2MG	C2-N1	3.23	1.41	1.36
1	A	1400	5MC	C2-N1	3.22	1.46	1.40
1	A	1518[B]	MA6	C5-C4	3.09	1.44	1.39
1	A	1207	2MG	C2-N2	3.04	1.39	1.33
1	A	1519[B]	MA6	C5-C4	3.01	1.44	1.39
1	A	1404	5MC	C2-N1	3.00	1.46	1.40
1	A	1498	UR3	C2-N3	2.88	1.44	1.39
1	A	966	M2G	C2-N2	2.84	1.40	1.35
1	A	1407	5MC	C2-N1	2.77	1.45	1.40
1	A	1519[B]	MA6	C8-N9	2.72	1.42	1.37
1	A	1402	4OC	C2-N1	2.72	1.45	1.40
1	A	527	G7M	C4-N3	2.59	1.40	1.34
1	A	1407	5MC	C2-N3	2.59	1.41	1.36
1	A	527	G7M	CN7-N7	-2.57	1.42	1.46
1	A	1207	2MG	C8-N9	2.55	1.43	1.37
1	A	1519[B]	MA6	C2-N1	2.53	1.38	1.33
1	A	966	M2G	C4-N3	2.48	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C2-N3	2.47	1.41	1.36
1	A	1519[A]	MA6	C5-C4	2.43	1.43	1.39
1	A	1518[B]	MA6	C8-N9	2.42	1.41	1.37
1	A	967	5MC	C2-N1	2.39	1.45	1.40
1	A	1207	2MG	C6-N1	2.38	1.43	1.38
1	A	1404	5MC	C2-N3	2.38	1.41	1.36
1	A	1518[A]	MA6	C5-C4	2.36	1.43	1.39
1	A	967	5MC	C2-N3	2.34	1.41	1.36
1	A	1402	4OC	C2-N3	2.29	1.40	1.36
1	A	1518[B]	MA6	C2-N1	2.27	1.38	1.33
1	A	1519[A]	MA6	C8-N9	2.12	1.41	1.37
1	A	966	M2G	C6-N1	2.10	1.42	1.38
1	A	1518[A]	MA6	C8-N9	2.10	1.41	1.37
1	A	1518[B]	MA6	C6-N1	2.09	1.38	1.34
1	A	1402	4OC	C4-N4	2.07	1.40	1.36
1	A	1207	2MG	C4-N3	2.06	1.39	1.34
1	A	1519[B]	MA6	C4-N3	2.04	1.38	1.34
1	A	1518[B]	MA6	C4-N3	2.03	1.38	1.34
1	A	1519[B]	MA6	C6-N1	2.02	1.38	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	527	G7M	C2-N3-C4	4.68	120.36	112.30
1	A	1541	PSU	C4-N3-C2	-4.58	120.06	126.37
1	A	516	PSU	C4-N3-C2	-4.43	120.27	126.37
1	A	1540	PSU	C4-N3-C2	-4.27	120.49	126.37
1	A	1541	PSU	N1-C2-N3	4.22	119.62	115.17
1	A	516	PSU	N1-C2-N3	4.15	119.55	115.17
1	A	1540	PSU	N1-C2-N3	4.12	119.52	115.17
1	A	527	G7M	C5-C4-N3	-4.11	120.38	128.15
1	A	1498	UR3	C6-N1-C2	-3.67	118.80	121.80
1	A	527	G7M	C5-C6-N1	3.63	119.35	111.84
1	A	527	G7M	O6-C6-C5	-3.12	121.06	128.01
1	A	527	G7M	N9-C4-N3	2.97	131.89	125.95
1	A	1404	5MC	N4-C4-N3	-2.94	113.19	118.51
1	A	527	G7M	C6-C5-N7	2.89	135.80	132.17
1	A	1541	PSU	O2-C2-N1	-2.76	119.94	122.79
1	A	527	G7M	C2-N1-C6	-2.70	120.21	125.11
1	A	1407	5MC	N4-C4-N3	-2.68	113.65	118.51
12	L	92	0TD	CSB-SB-CB	-2.52	97.84	102.36
1	A	1207	2MG	C5-C4-N3	-2.47	124.45	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1540	PSU	O2-C2-N1	-2.43	120.28	122.79
1	A	1404	5MC	C5-C4-N3	2.37	124.18	121.75
1	A	1400	5MC	N4-C4-N3	-2.30	114.33	118.51
1	A	1540	PSU	C6-N1-C2	-2.29	120.57	122.69
12	L	92	0TD	OD1-CG-CB	-2.28	117.67	122.44
1	A	967	5MC	N4-C4-N3	-2.26	114.42	118.51
1	A	1207	2MG	N9-C4-N3	2.21	130.38	125.95
1	A	516	PSU	O4'-C1'-C2'	2.20	108.19	105.15
1	A	1541	PSU	C6-N1-C2	-2.19	120.66	122.69
1	A	516	PSU	O2-C2-N1	-2.19	120.53	122.79
1	A	1400	5MC	C5-C4-N3	2.19	124.00	121.75
1	A	1518[A]	MA6	C2-N1-C6	2.18	117.15	111.83
1	A	516	PSU	C6-N1-C2	-2.16	120.69	122.69
1	A	966	M2G	C5-C4-N3	-2.13	125.00	128.39
1	A	1518[B]	MA6	C2-N1-C6	2.08	116.91	111.83
1	A	1407	5MC	C5-C4-N3	2.07	123.88	121.75
1	A	1207	2MG	C6-C5-N7	-2.06	126.54	130.29
1	A	1519[A]	MA6	C2-N1-C6	2.06	116.86	111.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	966	M2G	C4'-C5'-O5'-P
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1519[B]	MA6	C5-C6-N6-C10
12	L	92	0TD	CG-CB-SB-CSB
1	A	1498	UR3	O4'-C4'-C5'-O5'
12	L	92	0TD	SB-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1518[A]	MA6	C3'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	1518[A]	MA6	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	1519[B]	MA6	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	1	0
1	A	1400	5MC	1	0
1	A	527	G7M	1	0
1	A	1519[B]	MA6	3	0
1	A	966	M2G	1	0
1	A	1518[A]	MA6	1	0
12	L	92	0TD	2	0
1	A	967	5MC	1	0
1	A	1518[B]	MA6	3	0
1	A	1519[A]	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 255 ligands modelled in this entry, 254 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
25	SIS	A	1792	-	31,33,33	1.61	3 (9%)	28,49,49	1.10	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	SIS	A	1792	-	-	2/9/65/65	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1792	SIS	C41-C51	5.54	1.40	1.32
25	A	1792	SIS	C31-C41	-4.98	1.40	1.50
25	A	1792	SIS	C61-C51	-3.92	1.39	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	1792	SIS	C93-N33-C33	-3.36	109.84	114.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	A	1792	SIS	C23-C33-N33-C93
25	A	1792	SIS	C52-C42-O11-C11

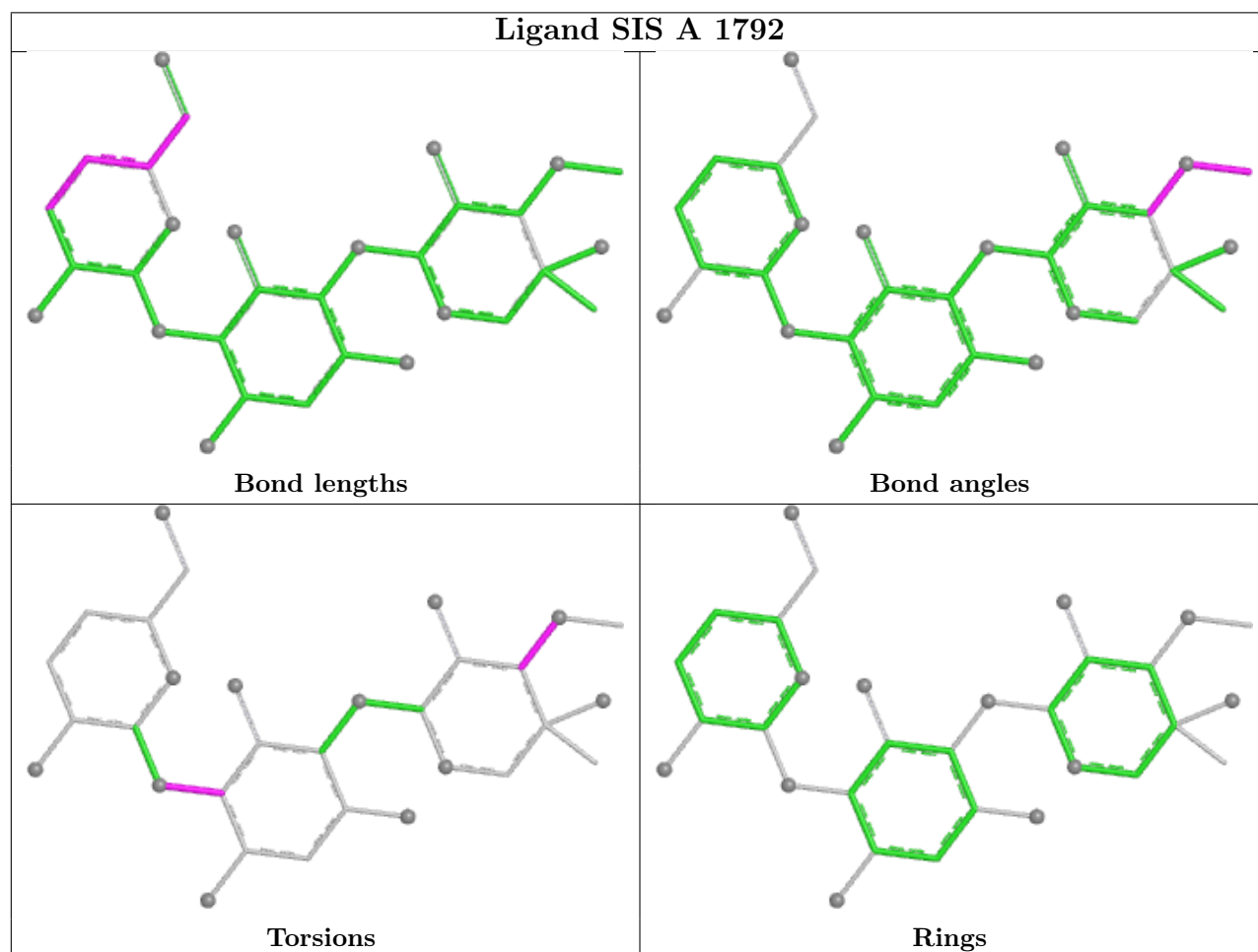
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	1792	SIS	2	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1498/1522 (98%)	0.36	132 (8%) 15 14	53, 129, 208, 321	4 (0%)
2	B	234/234 (100%)	0.29	17 (7%) 21 18	110, 156, 242, 273	0
3	C	206/206 (100%)	0.70	29 (14%) 6 8	127, 161, 211, 242	0
4	D	208/208 (100%)	1.08	48 (23%) 2 3	98, 140, 186, 241	0
5	E	150/150 (100%)	0.42	14 (9%) 14 14	92, 118, 155, 215	0
6	F	101/101 (100%)	0.35	7 (6%) 23 18	113, 155, 188, 220	0
7	G	155/155 (100%)	0.79	28 (18%) 3 5	111, 143, 198, 255	0
8	H	138/138 (100%)	0.07	6 (4%) 40 29	87, 114, 150, 162	0
9	I	127/127 (100%)	0.54	16 (12%) 8 9	123, 154, 204, 230	0
10	J	98/98 (100%)	0.74	9 (9%) 14 14	125, 185, 259, 314	0
11	K	116/116 (100%)	0.56	10 (8%) 16 15	90, 126, 172, 188	0
12	L	123/124 (99%)	0.94	21 (17%) 4 5	83, 129, 183, 252	0
13	M	118/118 (100%)	0.45	14 (11%) 9 10	116, 150, 198, 288	0
14	N	60/60 (100%)	1.50	19 (31%) 1 1	117, 150, 207, 269	0
15	O	87/87 (100%)	0.36	6 (6%) 23 18	100, 132, 175, 210	0
16	P	83/83 (100%)	0.91	19 (22%) 2 4	97, 129, 169, 222	0
17	Q	99/99 (100%)	0.85	18 (18%) 3 5	88, 116, 156, 172	0
18	R	70/70 (100%)	0.46	4 (5%) 29 22	97, 138, 204, 227	0
19	S	80/80 (100%)	0.80	10 (12%) 8 9	136, 171, 226, 273	0
20	T	99/99 (100%)	0.50	10 (10%) 12 12	101, 128, 175, 216	0
21	U	24/24 (100%)	0.84	4 (16%) 4 6	113, 146, 189, 199	0
22	Y	6/6 (100%)	0.31	0 100 100	161, 167, 236, 265	0
23	W	15/15 (100%)	0.89	1 (6%) 24 19	146, 159, 244, 247	0
All	All	3895/3920 (99%)	0.53	442 (11%) 10 10	53, 138, 208, 321	4 (0%)

All (442) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	S	3	ARG	15.2
3	C	161	GLU	12.6
1	A	532	A	11.6
4	D	42	GLN	10.4
12	L	19	ARG	9.9
17	Q	68	ARG	9.7
19	S	2	PRO	9.1
1	A	1258	G	8.7
1	A	353	A	8.3
14	N	31	ARG	7.3
3	C	4	LYS	7.2
13	M	8	GLU	7.1
4	D	7	PRO	6.8
7	G	95	ARG	6.5
13	M	21	TYR	6.4
16	P	39	TYR	6.4
3	C	199	LYS	6.4
7	G	99	LEU	6.1
12	L	47	LYS	6.1
7	G	56	GLN	6.0
1	A	64	G	6.0
3	C	184	TYR	5.9
7	G	76	ARG	5.9
14	N	46	GLU	5.8
1	A	982	U	5.8
1	A	1003(A)	G	5.7
13	M	9	ILE	5.7
17	Q	16	GLN	5.6
3	C	201	TYR	5.6
11	K	49	GLY	5.5
17	Q	67	LYS	5.4
4	D	27	TYR	5.4
17	Q	43	LEU	5.3
16	P	41	PRO	5.1
7	G	156	TRP	5.1
1	A	1257	U	5.1
7	G	74	GLU	5.0
7	G	81	GLY	5.0
12	L	18	VAL	5.0
12	L	120	TYR	5.0
1	A	105	G	5.0
20	T	9	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	760	G	4.9
10	J	83	GLU	4.9
7	G	83	ALA	4.9
11	K	51	LYS	4.9
3	C	2	GLY	4.9
15	O	72	ARG	4.9
1	A	373	A	4.9
7	G	85	TYR	4.8
1	A	114	U	4.8
14	N	61	TRP	4.8
4	D	84	LYS	4.8
12	L	119	LYS	4.8
9	I	117	HIS	4.8
17	Q	15	MET	4.7
12	L	26	ALA	4.7
1	A	428	G	4.7
1	A	1038	C	4.7
14	N	8	GLU	4.7
16	P	72	ARG	4.6
1	A	769	G	4.6
4	D	41	GLY	4.6
12	L	17	LYS	4.6
1	A	216	G	4.6
1	A	926	G	4.6
1	A	564	C	4.5
1	A	1487	G	4.5
4	D	122	ARG	4.5
6	F	88	VAL	4.5
1	A	63	C	4.4
4	D	6	GLY	4.4
1	A	1505	G	4.4
4	D	45	GLN	4.4
1	A	458	C	4.4
1	A	983	A	4.4
17	Q	14	LYS	4.4
9	I	121	ARG	4.4
12	L	105	TYR	4.4
4	D	43	HIS	4.3
9	I	115	GLY	4.3
1	A	1039	C	4.3
5	E	126	ARG	4.3
1	A	68	G	4.3

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Mol	Chain	Res	Type	RSRZ
4	D	36	ARG	4.3
4	D	4	TYR	4.3
1	A	632	A	4.2
2	B	193	ASP	4.2
11	K	117	ASN	4.2
23	W	34	G	4.2
12	L	115	LYS	4.2
4	D	20	TYR	4.1
1	A	633	G	4.1
1	A	1486	G	4.1
3	C	43	LEU	4.1
1	A	203	U	4.1
1	A	204	U	4.1
3	C	101	LEU	4.1
5	E	5	ASP	4.0
10	J	64	GLU	4.0
5	E	124	GLY	4.0
12	L	28	LYS	3.9
11	K	25	TYR	3.9
4	D	112	VAL	3.9
1	A	1506	U	3.9
1	A	1478	C	3.9
16	P	69	THR	3.9
3	C	66	VAL	3.8
4	D	24	GLU	3.8
15	O	51	HIS	3.8
1	A	113	G	3.8
13	M	113	PRO	3.8
4	D	209	ARG	3.8
1	A	530	G	3.8
14	N	15	LYS	3.8
14	N	3	ARG	3.8
4	D	132	ARG	3.7
12	L	103	GLY	3.7
20	T	68	LYS	3.7
14	N	30	ALA	3.7
1	A	1006	C	3.7
17	Q	98	LEU	3.7
1	A	1485	U	3.7
21	U	24	ARG	3.7
17	Q	65	ILE	3.7
4	D	32	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	214	ILE	3.6
9	I	116	LYS	3.6
10	J	58	ASP	3.6
3	C	27	LYS	3.6
19	S	14	HIS	3.6
1	A	759	A	3.6
1	A	47	C	3.6
1	A	984	C	3.6
1	A	1260	C	3.6
4	D	3	ARG	3.6
7	G	60	LYS	3.6
1	A	106	C	3.5
5	E	149	GLU	3.5
1	A	1472	U	3.5
4	D	62	GLN	3.5
20	T	73	HIS	3.5
4	D	8	VAL	3.5
10	J	54	PHE	3.5
11	K	31	THR	3.5
1	A	1169	A	3.5
1	A	795	C	3.5
1	A	1259	C	3.5
1	A	818	G	3.5
1	A	993	G	3.5
6	F	63	TYR	3.5
3	C	129	ALA	3.4
2	B	195	ASP	3.4
1	A	352	C	3.4
1	A	1129	C	3.4
1	A	794	A	3.4
16	P	17	TYR	3.4
12	L	121	GLY	3.4
1	A	1144	G	3.4
6	F	75	LEU	3.4
4	D	23	GLY	3.4
3	C	6	HIS	3.4
17	Q	66	SER	3.4
3	C	64	VAL	3.4
1	A	66	G	3.4
1	A	792	A	3.3
14	N	35	ARG	3.3
1	A	41	G	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	306	G	3.3
1	A	561	U	3.3
13	M	2	ALA	3.3
9	I	38	GLN	3.3
16	P	73	LEU	3.3
17	Q	45	HIS	3.3
4	D	61	LYS	3.3
1	A	1059	C	3.3
14	N	7	ILE	3.3
14	N	19	ARG	3.2
20	T	99	LEU	3.2
2	B	27	LYS	3.2
8	H	44	PHE	3.2
4	D	106	TYR	3.2
1	A	921	U	3.2
8	H	46	LYS	3.2
14	N	4	LYS	3.2
17	Q	17	LYS	3.2
4	D	58	LEU	3.2
3	C	103	VAL	3.2
1	A	125	U	3.2
7	G	38	LEU	3.2
17	Q	18	THR	3.2
1	A	95	U	3.1
10	J	80	LYS	3.1
4	D	9	CYS	3.1
1	A	541	G	3.1
1	A	1066	C	3.1
7	G	41	ARG	3.1
14	N	49	HIS	3.1
19	S	55	LYS	3.1
3	C	68	VAL	3.1
18	R	54	ARG	3.1
1	A	69	G	3.1
7	G	33	ASP	3.1
16	P	2	VAL	3.1
18	R	61	LYS	3.1
1	A	663	A	3.1
1	A	770	C	3.1
4	D	65	ARG	3.1
1	A	351	G	3.0
1	A	890	G	3.0

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Mol	Chain	Res	Type	RSRZ
4	D	10	ARG	3.0
9	I	39	GLY	3.0
19	S	37	ARG	3.0
1	A	426	G	3.0
12	L	86	ARG	3.0
3	C	3	ASN	3.0
5	E	26	PHE	3.0
1	A	1256	A	3.0
4	D	151	LYS	3.0
5	E	45	PHE	3.0
8	H	90	GLY	2.9
1	A	981	U	2.9
1	A	1281	U	2.9
6	F	79	LEU	2.9
11	K	50	TYR	2.9
16	P	38	TYR	2.9
3	C	65	ALA	2.9
3	C	102	ASN	2.9
7	G	32	ARG	2.9
17	Q	32	TYR	2.9
3	C	39	ILE	2.9
1	A	1218	C	2.8
10	J	53	PRO	2.8
1	A	1271	G	2.8
1	A	1517[A]	G	2.8
4	D	46	LYS	2.8
4	D	124	GLY	2.8
9	I	125	TYR	2.8
3	C	76	VAL	2.8
7	G	57	GLU	2.8
20	T	58	LYS	2.8
1	A	374	A	2.8
2	B	40	HIS	2.8
13	M	11	ARG	2.8
13	M	10	PRO	2.8
16	P	31	LYS	2.8
7	G	37	ASN	2.8
1	A	871	U	2.8
2	B	16	HIS	2.8
5	E	72	GLN	2.8
13	M	13	LYS	2.8
1	A	459	G	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	481	G	2.8
12	L	104	VAL	2.8
4	D	123	HIS	2.7
16	P	1	MET	2.7
7	G	155	ARG	2.7
12	L	89	ARG	2.7
3	C	207	VAL	2.7
4	D	31	CYS	2.7
1	A	315	A	2.7
14	N	22	THR	2.7
1	A	124	G	2.7
2	B	203	GLY	2.7
12	L	16	GLU	2.7
1	A	224	C	2.7
1	A	1539	C	2.7
1	A	1414	U	2.7
14	N	6	LEU	2.7
1	A	412	A	2.6
10	J	33	GLN	2.6
19	S	32	LYS	2.6
15	O	26	GLU	2.6
1	A	1143	G	2.6
18	R	53	ARG	2.6
1	A	559	A	2.6
1	A	787	A	2.6
2	B	24	TRP	2.6
4	D	21	LEU	2.6
9	I	122	ALA	2.6
1	A	67	C	2.6
1	A	221	C	2.6
6	F	8	ILE	2.6
1	A	1004	A	2.6
4	D	38	TYR	2.6
1	A	40	C	2.6
3	C	28	GLN	2.6
1	A	911	U	2.6
8	H	30	ARG	2.6
17	Q	20	THR	2.6
7	G	89	MET	2.6
9	I	114	TYR	2.6
2	B	196	LEU	2.6
1	A	1045	C	2.6

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Mol	Chain	Res	Type	RSRZ
13	M	88	ARG	2.6
1	A	427	U	2.5
4	D	77	ASN	2.5
16	P	68	ASP	2.5
1	A	811	C	2.5
7	G	16	LEU	2.5
7	G	106	GLN	2.5
15	O	31	LEU	2.5
21	U	10	ARG	2.5
3	C	62	ASP	2.5
1	A	1439	C	2.5
12	L	101	VAL	2.5
12	L	128	ALA	2.5
2	B	122	PHE	2.5
4	D	40	PRO	2.5
19	S	18	LYS	2.5
1	A	452	A	2.5
1	A	634	C	2.5
4	D	25	ARG	2.5
9	I	9	ARG	2.5
1	A	968	A	2.4
4	D	134	ASP	2.4
5	E	24	ARG	2.4
19	S	15	LEU	2.4
7	G	82	GLY	2.4
20	T	95	ALA	2.4
16	P	26	ARG	2.4
16	P	71	ARG	2.4
21	U	25	LYS	2.4
2	B	138	LEU	2.4
4	D	120	LEU	2.4
16	P	24	ALA	2.4
1	A	1521	G	2.4
16	P	23	ASP	2.4
1	A	889	A	2.4
1	A	1005	A	2.4
1	A	1280	A	2.4
9	I	128	ARG	2.4
14	N	17	LYS	2.4
16	P	27	LYS	2.4
3	C	178	LEU	2.4
8	H	107	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	380	G	2.4
1	A	1094	G	2.4
6	F	6	VAL	2.4
5	E	73	ASN	2.4
12	L	29	GLY	2.4
4	D	13	ARG	2.4
14	N	28	GLY	2.3
20	T	23	ARG	2.3
1	A	1171	G	2.3
3	C	5	ILE	2.3
11	K	38	ASN	2.3
4	D	75	PHE	2.3
1	A	1355	G	2.3
7	G	5	ARG	2.3
9	I	120	ARG	2.3
7	G	103	TRP	2.3
13	M	112	GLY	2.3
16	P	14	ASN	2.3
1	A	197	A	2.3
1	A	354	G	2.3
1	A	1241	G	2.3
10	J	7	LYS	2.3
12	L	23	LYS	2.3
4	D	81	GLU	2.3
9	I	110	GLU	2.3
9	I	40	LEU	2.3
15	O	69	TYR	2.3
2	B	23	ARG	2.3
14	N	45	ARG	2.3
7	G	80	VAL	2.3
11	K	36	ASP	2.3
1	A	9	G	2.2
1	A	841	U	2.2
1	A	1054	C	2.2
5	E	25	ARG	2.2
14	N	57	ARG	2.2
4	D	5	ILE	2.2
20	T	12	ALA	2.2
9	I	103	THR	2.2
20	T	38	LYS	2.2
1	A	173	U	2.2
7	G	102	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
7	G	110	GLN	2.2
3	C	128	PHE	2.2
4	D	59	ARG	2.2
13	M	87	TYR	2.2
1	A	509	A	2.2
1	A	576	G	2.2
4	D	180	GLY	2.2
16	P	15	PRO	2.2
13	M	99	ARG	2.2
17	Q	26	GLN	2.2
20	T	106	ALA	2.2
1	A	244	U	2.2
1	A	512	U	2.2
1	A	10	A	2.2
7	G	91	VAL	2.1
1	A	330	C	2.1
1	A	810	C	2.1
6	F	30	LEU	2.1
2	B	25	ASN	2.1
2	B	167	PRO	2.1
4	D	51	PRO	2.1
1	A	253	U	2.1
1	A	1136	U	2.1
3	C	195	VAL	2.1
12	L	46	LYS	2.1
5	E	64	ARG	2.1
7	G	7	ALA	2.1
17	Q	44	ALA	2.1
4	D	208	SER	2.1
5	E	68	GLU	2.1
21	U	2	GLY	2.1
1	A	796	C	2.1
13	M	7	VAL	2.1
13	M	17	VAL	2.1
1	A	1391	U	2.1
2	B	215	LEU	2.1
4	D	55	ALA	2.1
8	H	31	PHE	2.1
9	I	126	SER	2.1
19	S	53	ASN	2.1
1	A	377	G	2.1
1	A	1516[A]	G	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1149	C	2.1
17	Q	92	ARG	2.1
5	E	17	ALA	2.1
18	R	57	GLY	2.1
3	C	186	PHE	2.1
15	O	73	GLU	2.1
17	Q	41	LYS	2.1
16	P	16	HIS	2.1
1	A	314	C	2.1
1	A	254	G	2.1
3	C	168	ALA	2.1
19	S	17	GLU	2.1
2	B	22	LYS	2.0
10	J	55	LYS	2.0
2	B	190	THR	2.0
11	K	119	CYS	2.0
14	N	2	ALA	2.0
1	A	902	G	2.0
1	A	891	U	2.0
11	K	89	ALA	2.0
1	A	1067	A	2.0
5	E	123	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	A	1540	20/21	0.85	0.24	208,219,231,237	0
1	PSU	A	1541	20/21	0.89	0.20	210,228,262,308	0
1	PSU	A	516	20/21	0.91	0.10	146,154,162,165	0
1	5MC	A	967	21/22	0.94	0.15	111,125,130,136	0
1	5MC	A	1407	21/22	0.94	0.09	103,117,127,135	0
1	MA6	A	1518[B]	24/25	0.95	0.15	100,108,119,121	24
1	UR3	A	1498	21/22	0.95	0.12	101,107,122,134	0
1	MA6	A	1518[A]	24/25	0.95	0.15	100,102,108,109	24
1	M2G	A	966	25/26	0.96	0.13	129,134,151,152	0
1	G7M	A	527	24/25	0.96	0.09	105,113,126,128	0
1	5MC	A	1400	21/22	0.96	0.10	101,126,143,146	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	0TD	L	92	10/11	0.96	0.12	132,154,192,194	0
1	MA6	A	1519[B]	24/25	0.97	0.12	99,105,109,112	24
1	2MG	A	1207	24/25	0.97	0.07	127,142,156,160	0
1	4OC	A	1402	22/23	0.97	0.12	103,107,119,123	0
1	MA6	A	1519[A]	24/25	0.97	0.12	98,100,109,125	24
1	5MC	A	1404	21/22	0.98	0.07	99,108,113,115	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	1795	1/1	-0.25	0.12	395,395,395,395	0
24	MG	T	201	1/1	0.03	0.12	387,387,387,387	0
24	MG	A	1793	1/1	0.12	0.86	372,372,372,372	0
24	MG	A	1661	1/1	0.40	0.31	109,109,109,109	0
24	MG	K	202	1/1	0.41	0.22	353,353,353,353	0
24	MG	A	1717	1/1	0.44	0.35	127,127,127,127	0
24	MG	A	1802	1/1	0.44	0.46	126,126,126,126	0
24	MG	A	1602	1/1	0.46	0.77	244,244,244,244	0
24	MG	K	201	1/1	0.51	0.26	343,343,343,343	0
24	MG	A	1672	1/1	0.55	0.31	120,120,120,120	0
24	MG	A	1808	1/1	0.56	0.69	132,132,132,132	0
24	MG	A	1758	1/1	0.58	0.22	129,129,129,129	0
24	MG	A	1791	1/1	0.59	0.38	131,131,131,131	0
24	MG	A	1816	1/1	0.60	0.40	181,181,181,181	0
24	MG	A	1639	1/1	0.60	0.32	193,193,193,193	0
24	MG	A	1741	1/1	0.61	0.47	101,101,101,101	0
24	MG	M	201	1/1	0.61	0.23	123,123,123,123	0
24	MG	A	1801	1/1	0.61	0.35	124,124,124,124	0
24	MG	L	201	1/1	0.63	0.28	113,113,113,113	0
24	MG	A	1709	1/1	0.64	0.37	142,142,142,142	0
24	MG	M	202	1/1	0.64	0.09	125,125,125,125	0
24	MG	A	1719	1/1	0.64	0.25	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	1786	1/1	0.65	0.54	98,98,98,98	0
24	MG	L	203	1/1	0.66	0.10	118,118,118,118	0
24	MG	D	304	1/1	0.66	0.12	130,130,130,130	0
24	MG	B	303	1/1	0.68	0.10	126,126,126,126	0
24	MG	A	1798	1/1	0.68	0.17	107,107,107,107	0
24	MG	A	1817	1/1	0.68	0.20	146,146,146,146	0
24	MG	A	1811	1/1	0.69	0.09	137,137,137,137	0
24	MG	A	1739	1/1	0.69	0.28	111,111,111,111	0
24	MG	A	1813	1/1	0.70	0.09	112,112,112,112	0
24	MG	A	1730	1/1	0.70	0.23	101,101,101,101	0
24	MG	A	1744	1/1	0.70	0.12	121,121,121,121	0
24	MG	A	1733	1/1	0.71	0.56	120,120,120,120	0
24	MG	Q	202	1/1	0.72	0.26	133,133,133,133	0
24	MG	L	202	1/1	0.72	0.16	118,118,118,118	0
24	MG	A	1706	1/1	0.73	0.37	172,172,172,172	0
24	MG	A	1805	1/1	0.73	0.31	151,151,151,151	0
24	MG	A	1735	1/1	0.73	0.21	105,105,105,105	0
24	MG	A	1810	1/1	0.74	0.30	153,153,153,153	0
24	MG	A	1777	1/1	0.74	0.15	144,144,144,144	0
24	MG	A	1629	1/1	0.75	0.10	139,139,139,139	0
24	MG	A	1799	1/1	0.75	0.09	147,147,147,147	0
24	MG	A	1605	1/1	0.76	0.28	89,89,89,89	0
24	MG	A	1752	1/1	0.76	0.34	98,98,98,98	0
24	MG	A	1796	1/1	0.78	0.41	115,115,115,115	0
24	MG	A	1797	1/1	0.78	0.19	111,111,111,111	0
24	MG	M	204	1/1	0.78	0.13	111,111,111,111	0
24	MG	M	205	1/1	0.78	0.19	118,118,118,118	0
24	MG	A	1626	1/1	0.78	0.32	128,128,128,128	0
24	MG	A	1619	1/1	0.78	0.24	89,89,89,89	0
24	MG	A	1663	1/1	0.79	0.35	112,112,112,112	0
24	MG	D	303	1/1	0.79	0.13	157,157,157,157	0
24	MG	A	1665	1/1	0.79	0.33	75,75,75,75	0
24	MG	A	1631	1/1	0.79	0.17	108,108,108,108	0
24	MG	A	1814	1/1	0.79	0.06	116,116,116,116	0
24	MG	P	103	1/1	0.79	0.09	111,111,111,111	0
24	MG	A	1677	1/1	0.79	0.42	104,104,104,104	0
24	MG	A	1685	1/1	0.79	0.20	106,106,106,106	0
24	MG	A	1693	1/1	0.80	0.26	116,116,116,116	0
24	MG	C	302	1/1	0.80	0.21	120,120,120,120	0
24	MG	A	1701	1/1	0.80	0.28	196,196,196,196	0
24	MG	A	1684	1/1	0.80	0.47	109,109,109,109	0
24	MG	A	1687	1/1	0.81	0.16	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1729	1/1	0.81	0.17	107,107,107,107	0
24	MG	A	1759	1/1	0.81	0.14	113,113,113,113	0
24	MG	K	203	1/1	0.81	0.14	103,103,103,103	0
24	MG	C	301	1/1	0.81	0.09	104,104,104,104	0
24	MG	A	1658	1/1	0.81	0.15	108,108,108,108	0
24	MG	A	1670	1/1	0.81	0.14	112,112,112,112	0
24	MG	A	1682	1/1	0.82	0.28	131,131,131,131	0
24	MG	A	1614	1/1	0.82	0.33	110,110,110,110	0
24	MG	A	1674	1/1	0.82	0.15	117,117,117,117	0
24	MG	A	1627	1/1	0.82	0.36	88,88,88,88	0
24	MG	A	1716	1/1	0.82	0.11	101,101,101,101	0
24	MG	A	1763	1/1	0.82	0.17	110,110,110,110	0
24	MG	A	1769	1/1	0.82	0.48	122,122,122,122	0
24	MG	B	302	1/1	0.82	0.12	139,139,139,139	0
24	MG	A	1690	1/1	0.82	0.40	150,150,150,150	0
24	MG	A	1780	1/1	0.82	0.13	84,84,84,84	0
24	MG	A	1803	1/1	0.82	0.50	160,160,160,160	0
24	MG	A	1740	1/1	0.82	0.46	86,86,86,86	0
24	MG	A	1807	1/1	0.82	0.30	110,110,110,110	0
24	MG	A	1762	1/1	0.83	0.70	101,101,101,101	0
24	MG	A	1694	1/1	0.83	0.34	112,112,112,112	0
24	MG	A	1718	1/1	0.84	0.29	105,105,105,105	0
24	MG	A	1648	1/1	0.84	0.19	107,107,107,107	0
24	MG	C	305	1/1	0.84	0.06	124,124,124,124	0
24	MG	A	1669	1/1	0.84	0.29	125,125,125,125	0
24	MG	A	1712	1/1	0.84	0.33	116,116,116,116	0
24	MG	A	1774	1/1	0.84	0.20	111,111,111,111	0
24	MG	A	1806	1/1	0.84	0.21	139,139,139,139	0
24	MG	A	1630	1/1	0.84	0.53	93,93,93,93	0
24	MG	A	1679	1/1	0.84	0.27	101,101,101,101	0
24	MG	A	1673	1/1	0.85	0.29	106,106,106,106	0
24	MG	A	1761	1/1	0.85	0.64	94,94,94,94	0
24	MG	M	203	1/1	0.85	0.17	129,129,129,129	0
24	MG	A	1713	1/1	0.85	0.22	120,120,120,120	0
24	MG	A	1680	1/1	0.85	0.14	104,104,104,104	0
24	MG	P	101	1/1	0.85	0.10	112,112,112,112	0
24	MG	A	1732	1/1	0.85	0.15	104,104,104,104	0
24	MG	A	1666	1/1	0.85	0.34	93,93,93,93	0
24	MG	A	1642	1/1	0.85	0.07	101,101,101,101	0
24	MG	A	1800	1/1	0.86	0.12	109,109,109,109	0
24	MG	A	1657	1/1	0.86	0.25	85,85,85,85	0
24	MG	A	1683	1/1	0.86	0.10	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1722	1/1	0.86	0.31	94,94,94,94	0
24	MG	A	1771	1/1	0.86	0.09	116,116,116,116	0
24	MG	A	1634	1/1	0.86	0.22	149,149,149,149	0
24	MG	W	101	1/1	0.86	0.06	123,123,123,123	0
24	MG	K	204	1/1	0.87	0.12	110,110,110,110	0
24	MG	A	1787	1/1	0.87	0.24	102,102,102,102	0
24	MG	A	1809	1/1	0.87	0.12	120,120,120,120	0
24	MG	A	1728	1/1	0.87	0.20	93,93,93,93	0
24	MG	A	1779	1/1	0.87	0.22	114,114,114,114	0
24	MG	A	1601	1/1	0.87	0.21	98,98,98,98	0
24	MG	A	1764	1/1	0.87	0.20	93,93,93,93	0
24	MG	A	1650	1/1	0.88	0.24	107,107,107,107	0
24	MG	A	1675	1/1	0.88	0.26	142,142,142,142	0
24	MG	A	1781	1/1	0.88	0.11	117,117,117,117	0
24	MG	A	1702	1/1	0.88	0.18	110,110,110,110	0
24	MG	A	1668	1/1	0.88	0.24	142,142,142,142	0
24	MG	A	1691	1/1	0.88	0.30	83,83,83,83	0
24	MG	A	1633	1/1	0.88	0.24	105,105,105,105	0
24	MG	S	101	1/1	0.88	0.16	99,99,99,99	0
24	MG	A	1812	1/1	0.88	0.07	124,124,124,124	0
24	MG	A	1723	1/1	0.88	0.25	105,105,105,105	0
24	MG	A	1707	1/1	0.89	0.10	121,121,121,121	0
24	MG	H	202	1/1	0.89	0.05	106,106,106,106	0
24	MG	A	1616	1/1	0.89	0.34	85,85,85,85	0
24	MG	A	1727	1/1	0.89	0.26	109,109,109,109	0
24	MG	A	1640	1/1	0.89	0.17	138,138,138,138	0
24	MG	A	1767	1/1	0.89	0.13	93,93,93,93	0
24	MG	A	1737	1/1	0.89	0.13	112,112,112,112	0
24	MG	A	1618	1/1	0.89	0.16	135,135,135,135	0
24	MG	A	1760	1/1	0.89	0.15	80,80,80,80	0
24	MG	A	1794	1/1	0.89	0.27	215,215,215,215	0
24	MG	A	1754	1/1	0.90	0.20	87,87,87,87	0
24	MG	A	1756	1/1	0.90	0.33	120,120,120,120	0
24	MG	A	1688	1/1	0.90	0.13	138,138,138,138	0
24	MG	A	1606	1/1	0.90	0.24	122,122,122,122	0
24	MG	A	1662	1/1	0.90	0.19	102,102,102,102	0
24	MG	A	1652	1/1	0.90	0.13	96,96,96,96	0
24	MG	A	1617	1/1	0.90	0.23	80,80,80,80	0
24	MG	A	1783	1/1	0.90	0.18	114,114,114,114	0
24	MG	A	1615	1/1	0.90	0.12	134,134,134,134	0
24	MG	A	1746	1/1	0.90	0.13	95,95,95,95	0
24	MG	A	1815	1/1	0.90	0.26	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1734	1/1	0.90	0.12	94,94,94,94	0
24	MG	A	1804	1/1	0.90	0.12	150,150,150,150	0
24	MG	A	1747	1/1	0.91	0.32	92,92,92,92	0
24	MG	A	1624	1/1	0.91	0.14	106,106,106,106	0
24	MG	A	1753	1/1	0.91	0.21	110,110,110,110	0
24	MG	A	1603	1/1	0.91	0.16	116,116,116,116	0
24	MG	A	1788	1/1	0.91	0.13	114,114,114,114	0
24	MG	A	1768	1/1	0.91	0.26	107,107,107,107	0
24	MG	A	1755	1/1	0.91	0.24	99,99,99,99	0
24	MG	A	1641	1/1	0.91	0.26	104,104,104,104	0
24	MG	A	1621	1/1	0.91	0.20	109,109,109,109	0
24	MG	A	1776	1/1	0.91	0.10	144,144,144,144	0
24	MG	E	201	1/1	0.91	0.19	166,166,166,166	0
24	MG	A	1742	1/1	0.91	0.12	100,100,100,100	0
24	MG	A	1778	1/1	0.91	0.14	104,104,104,104	0
24	MG	A	1681	1/1	0.91	0.20	80,80,80,80	0
24	MG	A	1622	1/1	0.91	0.21	129,129,129,129	0
24	MG	A	1686	1/1	0.92	0.09	106,106,106,106	0
24	MG	D	302	1/1	0.92	0.06	97,97,97,97	0
24	MG	A	1653	1/1	0.92	0.24	130,130,130,130	0
24	MG	A	1710	1/1	0.92	0.38	79,79,79,79	0
24	MG	A	1696	1/1	0.92	0.40	99,99,99,99	0
24	MG	A	1655	1/1	0.92	0.28	177,177,177,177	0
24	MG	A	1715	1/1	0.92	0.09	71,71,71,71	0
24	MG	A	1651	1/1	0.92	0.17	81,81,81,81	0
24	MG	A	1703	1/1	0.92	0.15	163,163,163,163	0
24	MG	A	1772	1/1	0.92	0.16	97,97,97,97	0
24	MG	A	1644	1/1	0.92	0.10	82,82,82,82	0
24	MG	C	304	1/1	0.92	0.13	146,146,146,146	0
24	MG	A	1667	1/1	0.93	0.13	87,87,87,87	0
24	MG	A	1612	1/1	0.93	0.09	124,124,124,124	0
24	MG	A	1775	1/1	0.93	0.15	94,94,94,94	0
24	MG	A	1721	1/1	0.93	0.53	97,97,97,97	0
24	MG	A	1613	1/1	0.93	0.18	147,147,147,147	0
24	MG	A	1638	1/1	0.93	0.17	94,94,94,94	0
24	MG	A	1725	1/1	0.93	0.09	95,95,95,95	0
24	MG	A	1607	1/1	0.93	0.26	90,90,90,90	0
24	MG	A	1620	1/1	0.93	0.18	102,102,102,102	0
24	MG	A	1609	1/1	0.93	0.12	84,84,84,84	0
24	MG	A	1698	1/1	0.93	0.14	138,138,138,138	0
24	MG	A	1765	1/1	0.93	0.12	79,79,79,79	0
24	MG	A	1750	1/1	0.93	0.27	88,88,88,88	0

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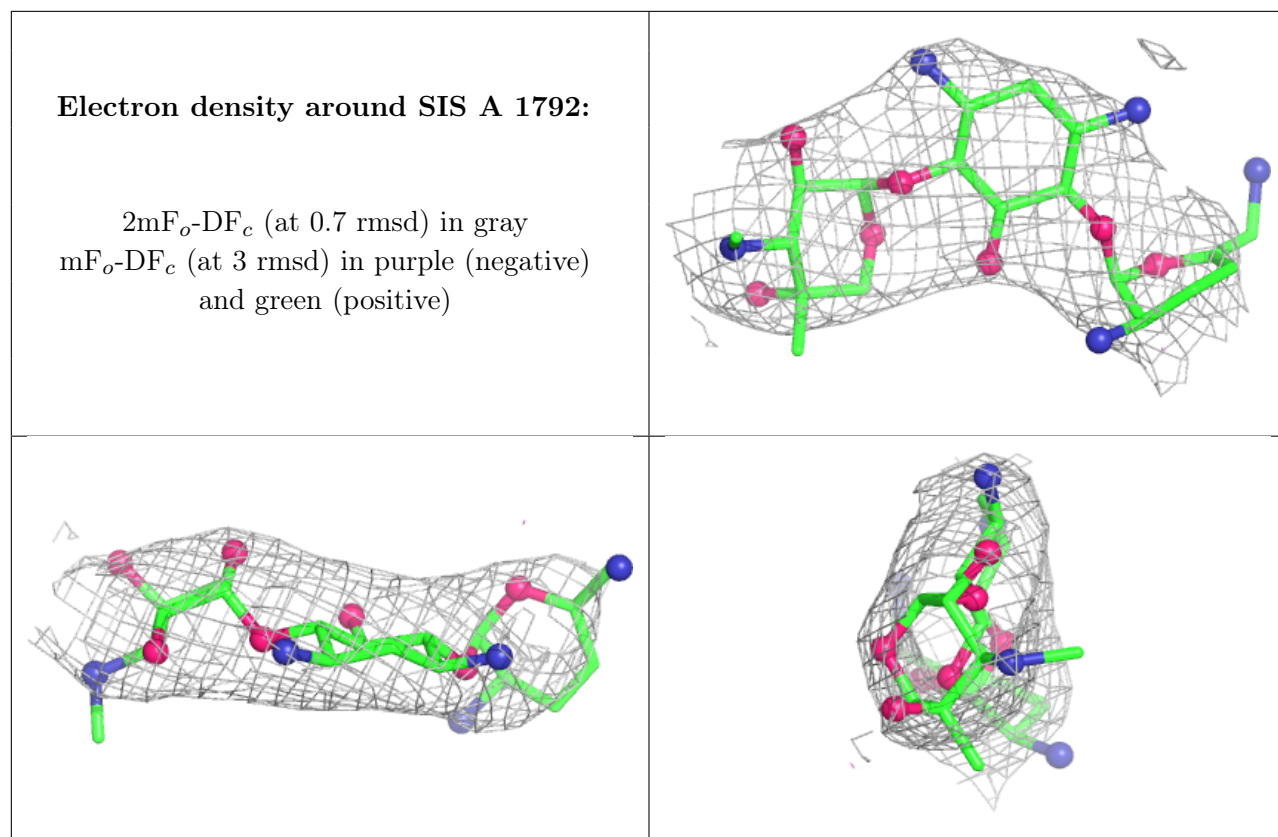
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	MG	A	1790	1/1	0.93	0.06	98,98,98,98	0
24	MG	Q	201	1/1	0.93	0.07	119,119,119,119	0
24	MG	A	1751	1/1	0.93	0.14	91,91,91,91	0
24	MG	A	1611	1/1	0.93	0.10	92,92,92,92	0
24	MG	H	201	1/1	0.93	0.25	76,76,76,76	0
24	MG	A	1676	1/1	0.93	0.12	113,113,113,113	0
24	MG	A	1785	1/1	0.94	0.25	131,131,131,131	0
24	MG	A	1646	1/1	0.94	0.10	99,99,99,99	0
24	MG	A	1704	1/1	0.94	0.16	118,118,118,118	0
24	MG	A	1678	1/1	0.94	0.16	107,107,107,107	0
24	MG	A	1789	1/1	0.94	0.16	84,84,84,84	0
24	MG	A	1749	1/1	0.94	0.13	88,88,88,88	0
24	MG	A	1647	1/1	0.94	0.21	157,157,157,157	0
24	MG	A	1757	1/1	0.94	0.14	101,101,101,101	0
24	MG	A	1610	1/1	0.94	0.11	106,106,106,106	0
24	MG	C	303	1/1	0.95	0.17	118,118,118,118	0
24	MG	A	1745	1/1	0.95	0.20	83,83,83,83	0
24	MG	A	1782	1/1	0.95	0.14	118,118,118,118	0
24	MG	A	1660	1/1	0.95	0.09	149,149,149,149	0
24	MG	A	1770	1/1	0.95	0.05	78,78,78,78	0
24	MG	A	1726	1/1	0.95	0.11	114,114,114,114	0
24	MG	A	1748	1/1	0.95	0.09	98,98,98,98	0
24	MG	A	1697	1/1	0.95	0.07	154,154,154,154	0
24	MG	A	1738	1/1	0.95	0.10	120,120,120,120	0
24	MG	A	1628	1/1	0.95	0.28	92,92,92,92	0
24	MG	A	1720	1/1	0.95	0.12	77,77,77,77	0
24	MG	Q	203	1/1	0.95	0.07	110,110,110,110	0
24	MG	A	1705	1/1	0.95	0.11	108,108,108,108	0
24	MG	A	1699	1/1	0.95	0.24	88,88,88,88	0
24	MG	A	1671	1/1	0.95	0.20	87,87,87,87	0
24	MG	A	1689	1/1	0.96	0.11	130,130,130,130	0
24	MG	A	1724	1/1	0.96	0.13	111,111,111,111	0
24	MG	A	1743	1/1	0.96	0.09	99,99,99,99	0
24	MG	A	1635	1/1	0.96	0.10	122,122,122,122	0
24	MG	A	1773	1/1	0.96	0.14	78,78,78,78	0
24	MG	A	1659	1/1	0.96	0.14	104,104,104,104	0
24	MG	A	1649	1/1	0.96	0.24	103,103,103,103	0
24	MG	A	1654	1/1	0.96	0.12	88,88,88,88	0
24	MG	A	1623	1/1	0.96	0.12	116,116,116,116	0
24	MG	A	1608	1/1	0.96	0.05	120,120,120,120	0
24	MG	A	1784	1/1	0.97	0.11	109,109,109,109	0
24	MG	A	1604	1/1	0.97	0.09	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	MG	A	1643	1/1	0.97	0.10	87,87,87,87	0
24	MG	A	1656	1/1	0.97	0.12	140,140,140,140	0
24	MG	F	201	1/1	0.97	0.04	108,108,108,108	0
24	MG	A	1766	1/1	0.97	0.13	79,79,79,79	0
24	MG	A	1637	1/1	0.97	0.21	115,115,115,115	0
24	MG	A	1695	1/1	0.97	0.13	124,124,124,124	0
24	MG	A	1645	1/1	0.97	0.22	184,184,184,184	0
25	SIS	A	1792	31/31	0.97	0.10	85,103,118,122	0
24	MG	A	1625	1/1	0.98	0.05	57,57,57,57	0
24	MG	A	1636	1/1	0.98	0.13	95,95,95,95	0
24	MG	P	102	1/1	0.98	0.33	75,75,75,75	0
24	MG	A	1700	1/1	0.98	0.05	118,118,118,118	0
24	MG	A	1692	1/1	0.98	0.17	108,108,108,108	0
24	MG	B	301	1/1	0.98	0.03	82,82,82,82	0
24	MG	A	1736	1/1	0.98	0.06	112,112,112,112	0
24	MG	A	1714	1/1	0.98	0.06	86,86,86,86	0
24	MG	A	1632	1/1	0.98	0.06	112,112,112,112	0
24	MG	A	1708	1/1	0.98	0.22	150,150,150,150	0
24	MG	A	1731	1/1	0.98	0.05	62,62,62,62	0
24	MG	A	1664	1/1	0.99	0.07	95,95,95,95	0
24	MG	A	1711	1/1	0.99	0.05	90,90,90,90	0
26	ZN	D	301	1/1	0.99	0.20	113,113,113,113	0
26	ZN	N	101	1/1	0.99	0.06	130,130,130,130	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.