Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 01:05 PM EST

PDB ID	:	4JI3
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	Demirci, H.; Wang, L.; Murphy, F.V.; Murphy, E.L.; Carr, J.; Blanchard, S.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on	:	2013-03-05
Resolution	:	3.35 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 (i) 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 (i)) were used in the production of this report:

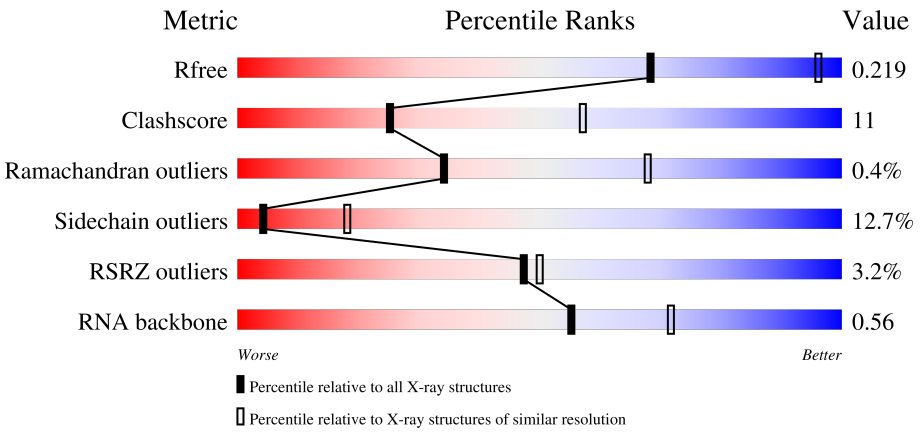
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)
RNA backbone	3102	1023 (3.80-2.92)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	.% 55% 34% 10% ••
2	B	256	.% 54% 29% 8% 9%
3	C	239	9% 44% 37% 5% 14%
4	D	209	67% 27% 6%

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Mol	Chain	Length	Quality of chain
5	E	162	54% 34% • • 7%
6	F	101	% 73% 23% •
7	G	156	8% 69% 28% • •
8	H	138	70% 28% •
9	I	128	6% 61% 36% • •
10	J	105	18% 50% 34% 9% 7%
11	K	129	63% 23% • 10%
12	L	135	% 59% 27% 7% 8%
13	M	126	6% 56% 33% 5% 6%
14	N	61	16% 59% 34% 5% •
15	O	89	% 63% 27% 8% •
16	P	88	60% 33% • 6%
17	Q	105	% 55% 37% • 6%
18	R	88	48% 31% • 20%
19	S	93	11% 51% 31% • 14%
20	T	106	% 56% 30% 8% 7%
21	U	27	33% 52% 22% 15% 11%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PSU	A	1540	-	-	-	X
1	PSU	A	1541	-	-	-	X
23	MG	A	1633	-	-	-	X
23	MG	A	1662	-	-	-	X
23	MG	A	1679	-	-	-	X
23	MG	A	1682	-	-	-	X
23	MG	A	1696	-	-	-	X
23	MG	A	1710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1723	-	-	-	X
23	MG	A	1754	-	-	-	X
23	MG	A	1755	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	A	1771	-	-	-	X
23	MG	A	1787	-	-	-	X
23	MG	A	1791	-	-	-	X
23	MG	A	1800	-	-	-	X
23	MG	A	1802	-	-	-	X
23	MG	A	1807	-	-	-	X
23	MG	A	1815	-	-	-	X
23	MG	A	1822	-	-	-	X
23	MG	A	1823	-	-	-	X
23	MG	K	201	-	-	-	X
23	MG	P	101	-	-	-	X
23	MG	P	102	-	-	-	X

2 Entry composition (i)

There are 25 unique types of molecules in this entry. The entry contains 52101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1511	32487	14468	6008	10500	1511	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called RIBOSOMAL PROTEIN S2.

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

- Molecule 3 is a protein called 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 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 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 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 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 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 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 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 RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	124	977	617	196	163	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	94	TRP	PRO	conflict	UNP F6DEQ7

- Molecule 13 is a protein called 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 RIBOSOMAL PROTEIN S14.

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 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 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 RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	Q	99	823	528	151	142	2	0	0	0

- Molecule 18 is a protein called 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 RIBOSOMAL PROTEIN S19.

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

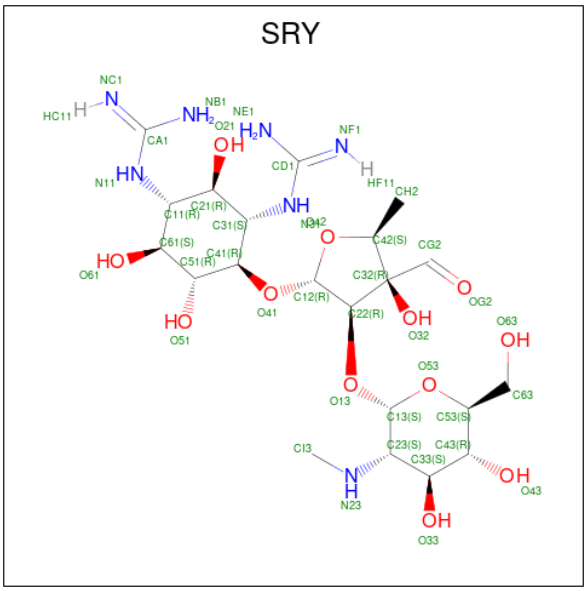
- Molecule 20 is a protein called RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN THX.

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
23	A	231	231	231	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
23	B	2	2	2	0	0
23	C	1	1	1	0	0
23	D	2	2	2	0	0
23	E	1	1	1	0	0
23	F	1	1	1	0	0
23	H	1	1	1	0	0
23	K	1	1	1	0	0
23	L	1	1	1	0	0
23	N	1	1	1	0	0
23	P	2	2	2	0	0
23	Q	2	2	2	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
25	A	223	223	223	0	0
25	D	1	1	1	0	0
25	E	4	4	4	0	0
25	L	1	1	1	0	0

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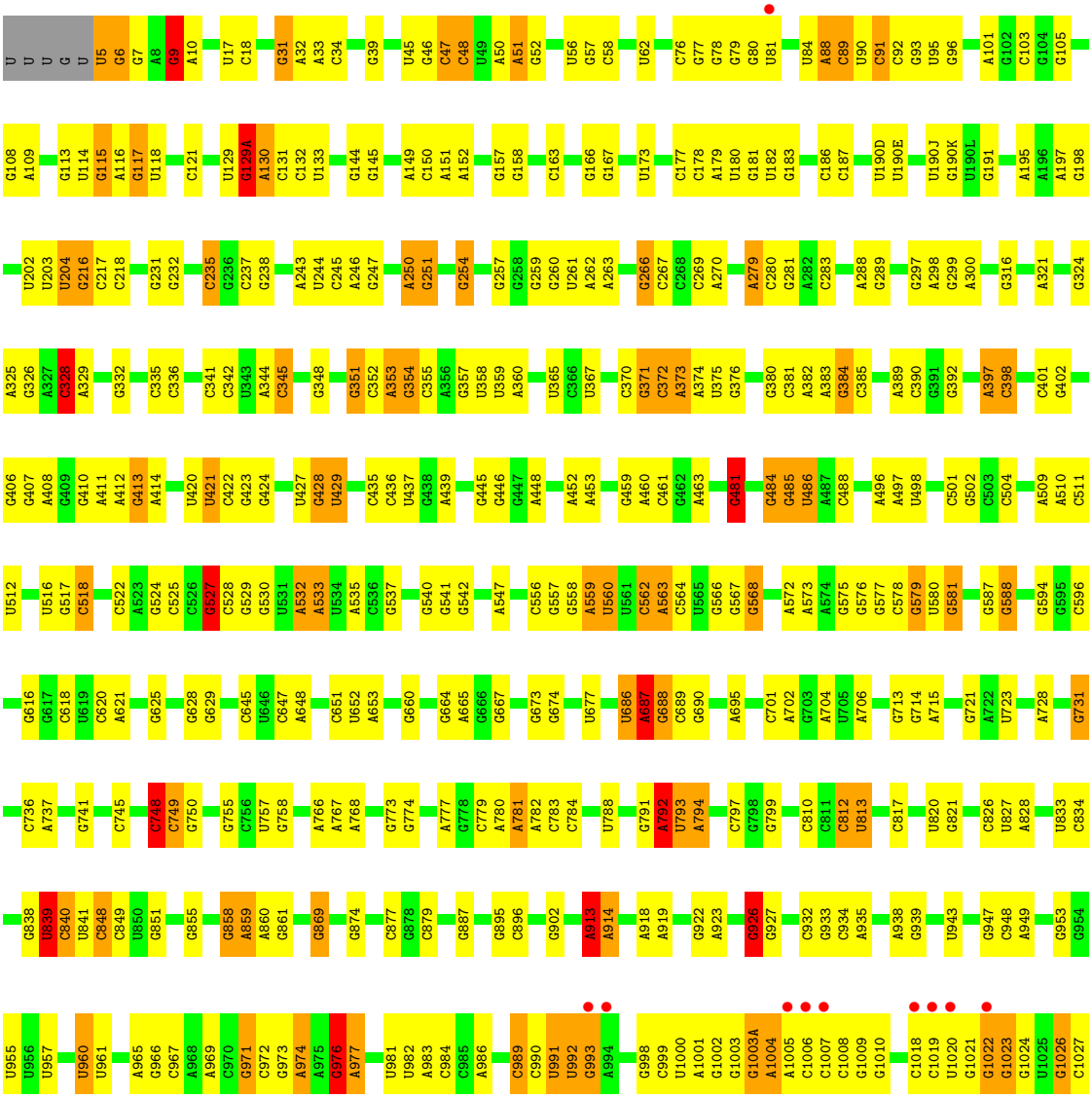
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
25	N	1	1	1	0	0
			Total	O		
25	Q	1	1	1	0	0
			Total	O		
25	T	1	1	1	0	0
			Total	O		
25	U	1	1	1	0	0

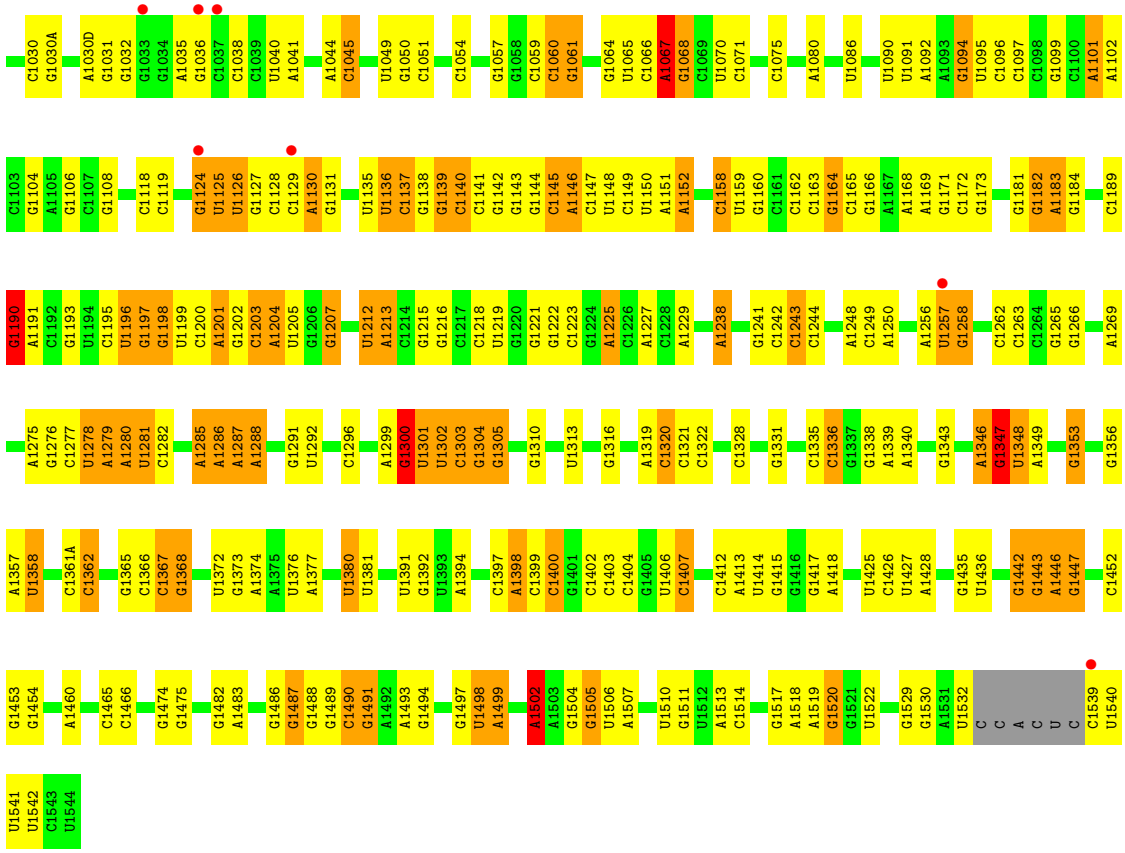
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

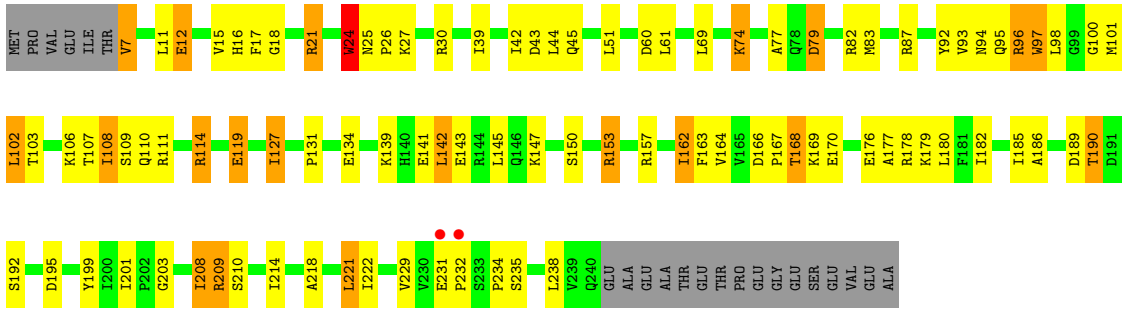
Chain A:





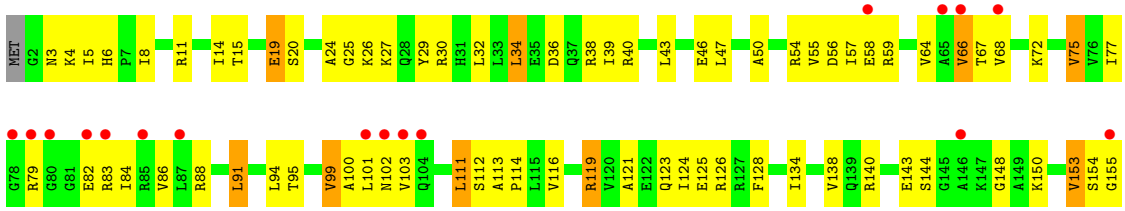
- Molecule 2: RIBOSOMAL PROTEIN S2

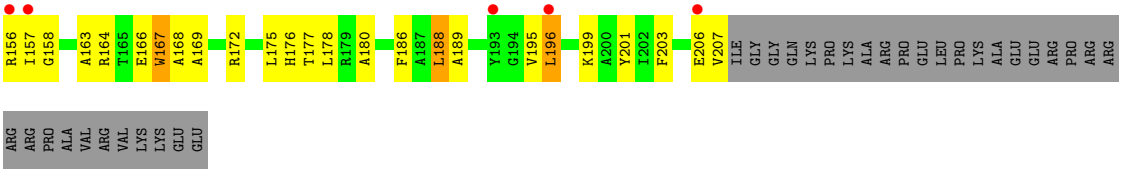
Chain B:



- Molecule 3: RIBOSOMAL PROTEIN S3

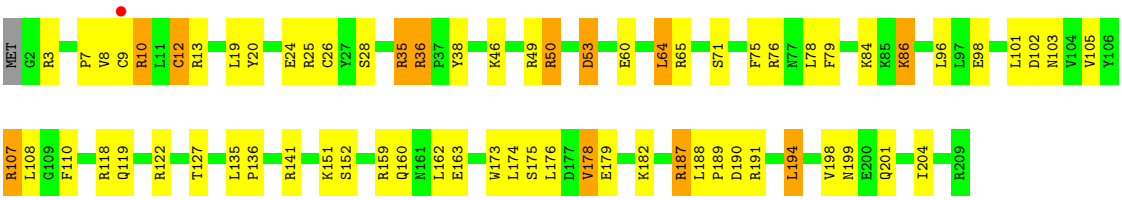
Chain C:





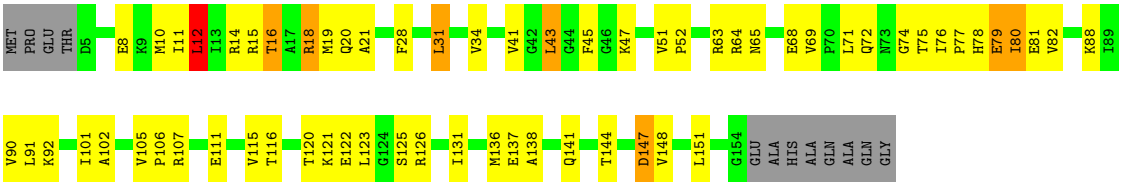
• Molecule 4: RIBOSOMAL PROTEIN S4

Chain D: 67% 27% 6%



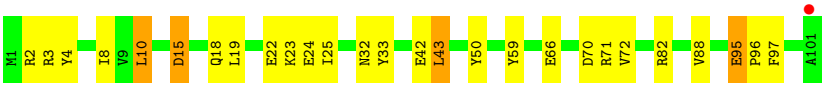
• Molecule 5: RIBOSOMAL PROTEIN S5

Chain E: 54% 34% 7%



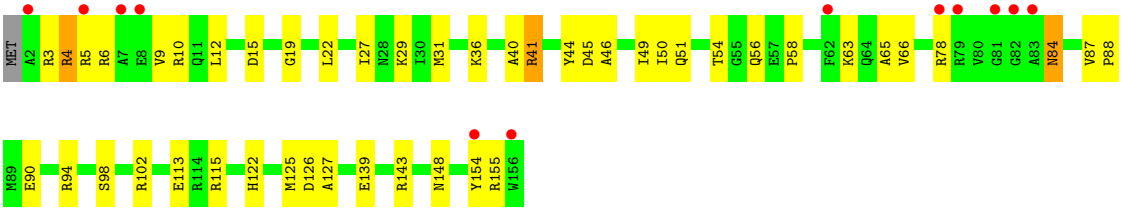
• Molecule 6: RIBOSOMAL PROTEIN S6

Chain F: % 73% 23%



• Molecule 7: RIBOSOMAL PROTEIN S7

Chain G: 8% 69% 28%

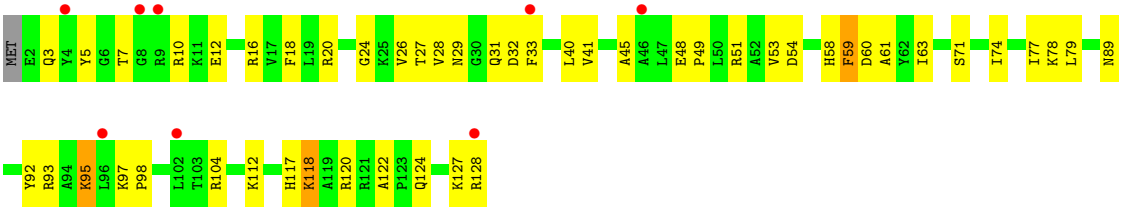


• Molecule 8: RIBOSOMAL PROTEIN S8

Chain H: 70% 28%

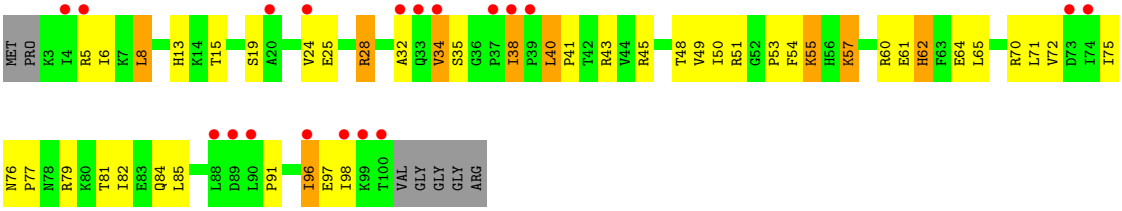
- Molecule 9: RIBOSOMAL PROTEIN S9

Chain I:



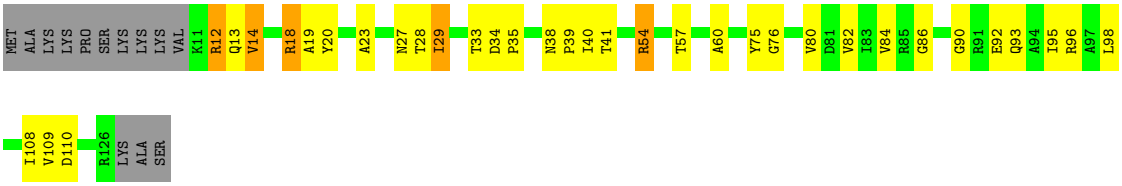
- Molecule 10: RIBOSOMAL PROTEIN S10

Chain J:



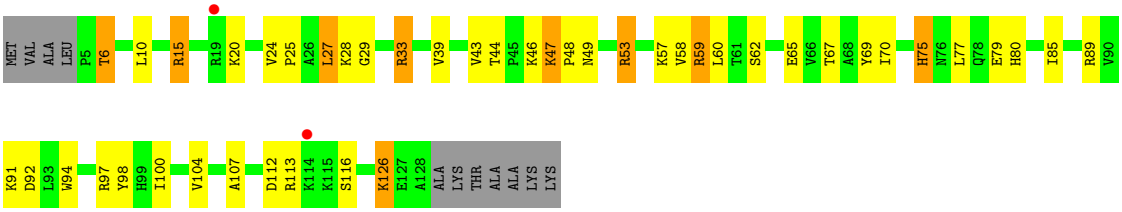
- Molecule 11: RIBOSOMAL PROTEIN S11

Chain K:



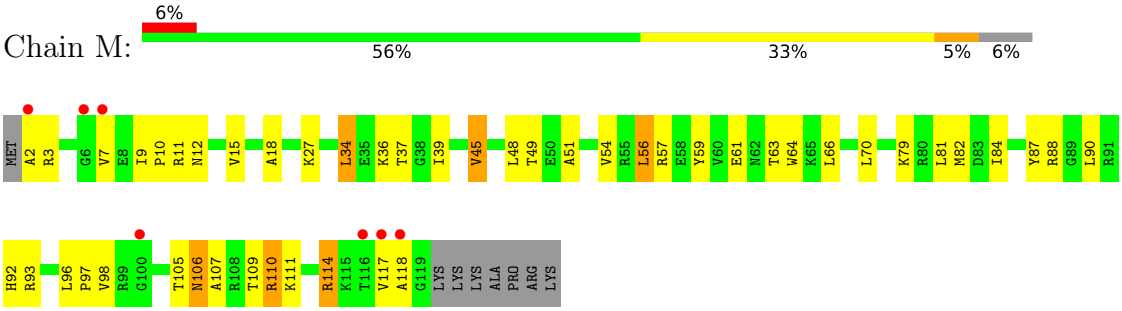
- Molecule 12: RIBOSOMAL PROTEIN S12

Chain L:



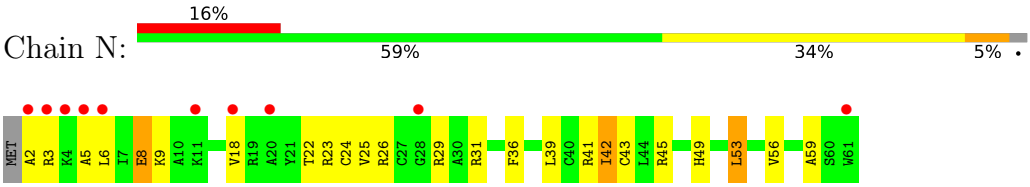
- Molecule 13: RIBOSOMAL PROTEIN S13

Chain M:



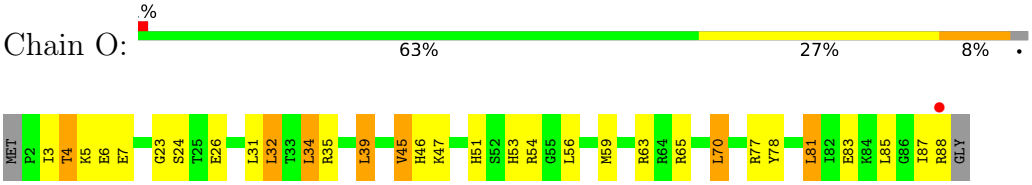
- Molecule 14: RIBOSOMAL PROTEIN S14

Chain N:



- Molecule 15: RIBOSOMAL PROTEIN S15

Chain O:

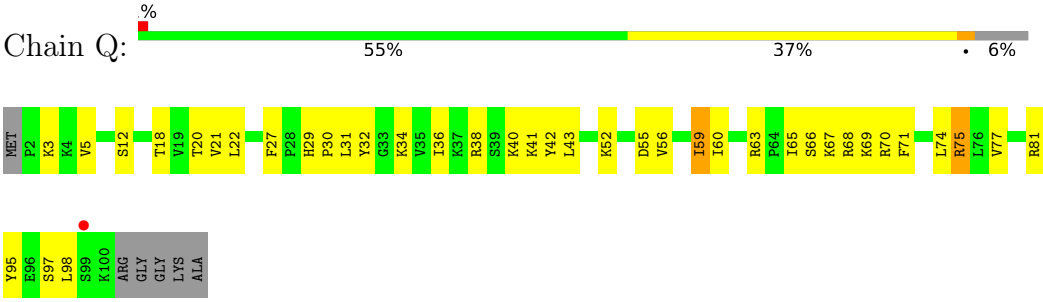


- Molecule 16: RIBOSOMAL PROTEIN S16

Chain P:

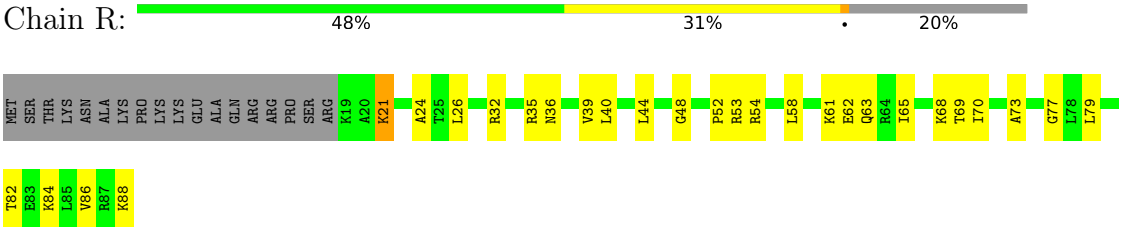
- Molecule 17: RIBOSOMAL PROTEIN S17

Chain Q:



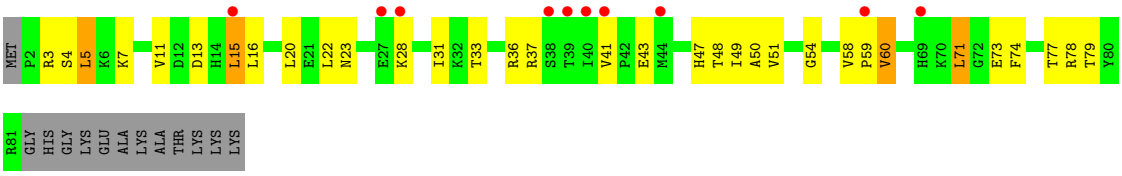
- Molecule 18: RIBOSOMAL PROTEIN S18

Chain R:



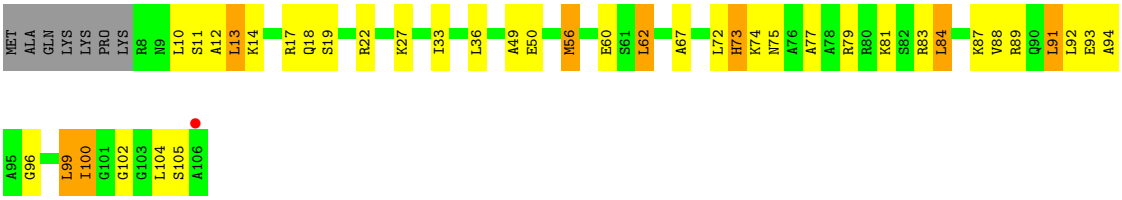
• Molecule 19: RIBOSOMAL PROTEIN S19

Chain S:



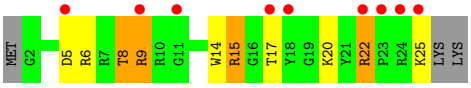
• Molecule 20: RIBOSOMAL PROTEIN S20

Chain T:



• Molecule 21: RIBOSOMAL PROTEIN THX

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	402.98Å 402.98Å 173.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.00 – 3.35 34.00 – 3.35	Depositor EDS
% Data completeness (in resolution range)	87.8 (34.00-3.35) 87.6 (34.00-3.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.32Å)	Xtriage
Refinement program	PHENIX dev_1119	Depositor
R, R_{free}	0.168 , 0.215 0.172 , 0.219	Depositor DCC
R_{free} test set	8993 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	116.5	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 105.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52101	wwPDB-VP
Average B, all atoms (Å^2)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 7MG, 2MG, MA6, 5MC, 4OC, ZN, UR3, SRY, MG, M2G, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.51	1/36018 (0.0%)	1.01	72/56209 (0.1%)
2	B	0.37	0/1935	0.59	1/2609 (0.0%)
3	C	0.32	0/1636	0.54	0/2205
4	D	0.39	1/1733 (0.1%)	0.59	1/2318 (0.0%)
5	E	0.47	0/1162	0.68	1/1564 (0.1%)
6	F	0.33	0/856	0.52	0/1154
7	G	0.30	0/1276	0.49	0/1709
8	H	0.47	0/1136	0.64	0/1527
9	I	0.33	0/1029	0.53	0/1379
10	J	0.28	0/805	0.59	0/1082
11	K	0.37	0/879	0.61	0/1187
12	L	0.41	0/994	0.67	0/1331
13	M	0.32	0/947	0.56	0/1270
14	N	0.35	0/501	0.52	0/664
15	O	0.38	0/740	0.55	0/987
16	P	0.42	0/716	0.61	0/963
17	Q	0.45	0/836	0.69	0/1117
18	R	0.34	0/579	0.55	0/768
19	S	0.27	0/661	0.56	0/890
20	T	0.39	0/765	0.65	1/1007 (0.1%)
21	U	0.30	0/212	0.45	0/277
All	All	0.47	2/55416 (0.0%)	0.90	76/82217 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1
20	T	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	869	G	N7-C5	-5.53	1.35	1.39
4	D	12	CYS	CB-SG	5.07	1.90	1.82

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	N1-C6-O6	11.85	127.01	119.90
1	A	254	G	O5'-P-OP1	-9.37	97.27	105.70
1	A	117	G	C6-C5-N7	-9.03	124.98	130.40
1	A	328	C	N1-C2-O2	7.78	123.57	118.90
1	A	839	U	C2-N1-C1'	7.74	126.98	117.70
1	A	328	C	N3-C2-O2	-7.67	116.53	121.90
1	A	328	C	C2-N1-C1'	7.48	127.02	118.80
1	A	266	G	C4-C5-N7	7.46	113.79	110.80
1	A	117	G	N9-C4-C5	-7.09	102.56	105.40
1	A	1502	A	C5-N7-C8	-7.08	100.36	103.90
1	A	117	G	C5-C6-O6	-6.98	124.41	128.60
1	A	117	G	C8-N9-C1'	-6.70	118.29	127.00
1	A	839	U	N1-C2-O2	6.68	127.47	122.80
1	A	266	G	C5-N7-C8	-6.63	100.98	104.30
1	A	1502	A	C6-C5-N7	-6.54	127.72	132.30
1	A	1502	A	N1-C6-N6	6.35	122.41	118.60
1	A	1502	A	N7-C8-N9	6.30	116.95	113.80
1	A	481	G	N3-C4-N9	6.26	129.75	126.00
1	A	976	G	O5'-P-OP2	-6.23	100.09	105.70
1	A	328	C	C6-N1-C2	-6.21	117.82	120.30
1	A	1067	A	P-O3'-C3'	6.20	127.13	119.70
1	A	266	G	C6-C5-N7	-6.18	126.69	130.40
1	A	279	A	C5-N7-C8	-6.07	100.87	103.90
1	A	529	G	N1-C6-O6	6.05	123.53	119.90
1	A	129(A)	G	C4-N9-C1'	6.03	134.34	126.50
1	A	1502	A	C4-C5-N7	5.97	113.69	110.70
5	E	12	LEU	CA-CB-CG	5.96	129.01	115.30
1	A	913	A	P-O3'-C3'	5.91	126.79	119.70
1	A	9	G	N1-C6-O6	5.91	123.45	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	A	N1-C6-N6	5.89	122.14	118.60
1	A	839	U	N3-C2-O2	-5.89	118.08	122.20
1	A	1403	C	C6-N1-C2	5.89	122.66	120.30
1	A	283	C	C6-N1-C2	-5.85	117.96	120.30
1	A	1346	A	P-O3'-C3'	5.85	126.72	119.70
1	A	117	G	C4-N9-C1'	5.84	134.10	126.50
1	A	117	G	C5-C6-N1	-5.84	108.58	111.50
1	A	129(A)	G	N3-C4-N9	5.80	129.48	126.00
1	A	117	G	C4-C5-C6	5.69	122.22	118.80
1	A	748	C	P-O3'-C3'	5.67	126.50	119.70
1	A	792	A	P-O3'-C3'	5.54	126.35	119.70
20	T	94	ALA	N-CA-C	-5.54	96.05	111.00
1	A	1442	G	N3-C4-N9	5.48	129.29	126.00
1	A	687	A	P-O3'-C3'	5.47	126.26	119.70
1	A	869	G	C6-C5-N7	-5.44	127.14	130.40
1	A	1442	G	C4-N9-C1'	5.43	133.55	126.50
1	A	279	A	C2-N3-C4	-5.41	107.90	110.60
1	A	129(A)	G	C8-N9-C1'	-5.40	119.98	127.00
1	A	89	C	C6-N1-C2	-5.37	118.15	120.30
1	A	484	G	N3-C4-C5	-5.37	125.92	128.60
1	A	1158	C	N1-C2-O2	5.35	122.11	118.90
4	D	12	CYS	CA-CB-SG	5.35	123.62	114.00
1	A	324	G	N1-C6-O6	5.28	123.07	119.90
1	A	266	G	N1-C6-O6	5.25	123.05	119.90
1	A	89	C	C5-C6-N1	5.23	123.61	121.00
1	A	1502	A	C2-N3-C4	-5.23	107.99	110.60
1	A	1094	G	O4'-C1'-N9	5.22	112.37	108.20
1	A	926	G	N3-C4-N9	5.21	129.13	126.00
1	A	1190	G	P-O3'-C3'	5.21	125.95	119.70
1	A	283	C	N3-C2-O2	-5.20	118.26	121.90
1	A	1367	C	C6-N1-C2	-5.20	118.22	120.30
1	A	235	C	C6-N1-C2	5.18	122.37	120.30
1	A	5	U	P-O3'-C3'	5.14	125.87	119.70
1	A	976	G	N3-C4-C5	-5.11	126.04	128.60
1	A	328	C	P-O3'-C3'	5.09	125.81	119.70
1	A	1300	G	P-O3'-C3'	5.08	125.80	119.70
1	A	529	G	C5-C6-O6	-5.08	125.55	128.60
1	A	1380	U	P-O3'-C3'	5.08	125.79	119.70
1	A	839	U	C6-N1-C1'	-5.08	114.09	121.20
1	A	1201	A	P-O3'-C3'	5.06	125.77	119.70
1	A	115	G	P-O3'-C3'	5.05	125.76	119.70
1	A	851	G	C4-N9-C1'	5.04	133.04	126.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1347	G	OP2-P-O3'	5.04	116.28	105.20
1	A	879	C	C5-C6-N1	5.03	123.51	121.00
1	A	129(A)	G	P-O3'-C3'	5.02	125.72	119.70
2	B	12	GLU	N-CA-C	5.01	124.52	111.00
1	A	117	G	C4-C5-N7	5.00	112.80	110.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32487	0	16421	443	0
2	B	1900	0	1951	58	0
3	C	1612	0	1677	66	0
4	D	1703	0	1763	46	0
5	E	1146	0	1207	36	0
6	F	843	0	857	14	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	25	0
9	I	1010	0	1037	29	0
10	J	792	0	835	39	0
11	K	864	0	881	25	0
12	L	977	0	1060	38	0
13	M	937	0	995	28	0
14	N	492	0	529	16	0
15	O	729	0	768	20	0
16	P	700	0	720	20	0
17	Q	823	0	891	36	0
18	R	574	0	644	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	S	647	0	673	21	0
20	T	763	0	861	33	0
21	U	208	0	221	7	0
22	A	40	0	37	4	0
23	A	231	0	0	0	0
23	B	2	0	0	0	0
23	C	1	0	0	0	0
23	D	2	0	0	0	0
23	E	1	0	0	0	0
23	F	1	0	0	0	0
23	H	1	0	0	0	0
23	K	1	0	0	0	0
23	L	1	0	0	0	0
23	N	1	0	0	0	0
23	P	2	0	0	0	0
23	Q	2	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	223	0	0	3	0
25	D	1	0	0	0	0
25	E	4	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	Q	1	0	0	0	0
25	T	1	0	0	0	0
25	U	1	0	0	0	0
All	All	52101	0	36501	927	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (927) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1443:G:H5”	1:A:1446:A:H5’	1.43	0.99
1:A:279:A:OP2	17:Q:95:TYR:OH	1.88	0.89
17:Q:29:HIS:HD2	17:Q:32:TYR:H	1.11	0.89
1:A:411:A:H62	1:A:413:G:H21	1.23	0.87
1:A:298:A:N6	25:A:2054:HOH:O	2.06	0.85
3:C:180:ALA:HB3	3:C:203:PHE:HE1	1.42	0.84
1:A:235:C:N4	25:A:1986:HOH:O	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:A:OP2	1:A:190(E):U:O2'	2.00	0.80
1:A:542:G:OP1	4:D:10:ARG:NH2	2.14	0.79
1:A:1057:G:H5"	3:C:154:SER:HB2	1.65	0.79
1:A:527:7MG:OP2	22:A:1601:SRY:O32	1.99	0.79
1:A:664:G:H22	1:A:741:G:H1	1.30	0.79
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.63	0.77
4:D:3:ARG:HH21	4:D:118:ARG:HH12	1.31	0.76
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.19	0.76
1:A:1491:G:H5'	12:L:94:TRP:HZ2	1.51	0.75
1:A:412:A:O2'	4:D:35:ARG:NH2	2.19	0.75
17:Q:29:HIS:CD2	17:Q:32:TYR:H	1.99	0.74
1:A:1412:C:H2'	1:A:1413:A:C8	2.23	0.73
1:A:1266:G:N2	1:A:1269:A:OP2	2.22	0.73
1:A:427:U:OP2	4:D:36:ARG:NH2	2.22	0.73
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.70	0.73
1:A:1158:C:N3	1:A:1181:G:N2	2.37	0.72
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.55	0.72
1:A:677:U:H3	1:A:713:G:H22	1.37	0.71
1:A:838:G:H1	1:A:848:C:H42	1.36	0.71
1:A:1195:C:H3'	1:A:1196:U:H5"	1.72	0.71
1:A:92:C:H2'	1:A:93:G:H8	1.56	0.70
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.54	0.70
1:A:1373:G:H5"	7:G:36:LYS:HE2	1.73	0.70
1:A:1222:G:OP2	1:A:1322:C:N4	2.22	0.70
1:A:1200:C:O2	1:A:1205:U:N3	2.18	0.70
1:A:560:U:H5'	1:A:566:G:N2	2.06	0.70
3:C:43:LEU:HD22	3:C:47:LEU:HD22	1.74	0.70
1:A:1328:C:OP1	21:U:20:LYS:NZ	2.23	0.69
10:J:8:LEU:HB3	10:J:96:ILE:HG23	1.72	0.69
3:C:125:GLU:HG3	3:C:189:ALA:HB1	1.75	0.69
3:C:180:ALA:HB3	3:C:203:PHE:CE1	2.27	0.69
1:A:537:G:OP1	12:L:113:ARG:NH2	2.25	0.69
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.75	0.69
1:A:1414:U:H2'	1:A:1415:G:H8	1.58	0.68
4:D:107:ARG:HH21	4:D:194:LEU:HD12	1.58	0.68
7:G:51:GLN:HG2	7:G:58:PRO:HD3	1.74	0.68
1:A:972:C:H4'	10:J:57:LYS:HG2	1.75	0.68
1:A:976:G:OP2	1:A:1358:U:O2'	2.07	0.68
11:K:57:THR:HG23	11:K:60:ALA:H	1.58	0.68
20:T:49:ALA:HB3	20:T:99:LEU:HD23	1.75	0.68
1:A:1442:G:N7	1:A:1446:A:N6	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:G:N1	1:A:533:A:OP2	2.19	0.68
1:A:859:A:OP2	1:A:869:G:N1	2.23	0.68
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.12	0.68
4:D:13:ARG:NH1	4:D:38:TYR:O	2.27	0.68
1:A:1391:U:H2'	1:A:1392:G:C8	2.30	0.67
1:A:1035:A:H2'	1:A:1036:G:H8	1.60	0.67
2:B:114:ARG:NH1	2:B:141:GLU:OE1	2.27	0.67
12:L:28:LYS:HD2	12:L:33:ARG:HH12	1.59	0.67
1:A:991:U:O4	1:A:1212:U:O2'	2.12	0.67
1:A:113:G:H1'	1:A:354:G:H5'	1.76	0.67
8:H:119:LEU:HD11	8:H:127:LEU:HD12	1.76	0.67
1:A:1417:G:O2'	1:A:1483:A:N6	2.28	0.67
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.75	0.66
16:P:67:THR:HG22	16:P:69:THR:H	1.59	0.66
2:B:15:VAL:HG13	2:B:209:ARG:HG2	1.77	0.66
10:J:48:THR:HA	10:J:62:HIS:HB3	1.77	0.66
1:A:427:U:OP1	4:D:13:ARG:NH2	2.28	0.66
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.76	0.66
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.78	0.66
1:A:1412:C:H2'	1:A:1413:A:H8	1.59	0.66
1:A:1356:G:H2'	1:A:1357:A:C8	2.31	0.66
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.78	0.66
11:K:110:ASP:HB2	18:R:88:LYS:HG2	1.76	0.66
3:C:157:ILE:HD13	3:C:164:ARG:HB2	1.78	0.65
3:C:134:ILE:HD11	3:C:153:VAL:HB	1.78	0.65
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.78	0.65
1:A:250:A:H4'	1:A:251:G:O5'	1.96	0.64
1:A:579:G:H5'	1:A:728:A:H1'	1.77	0.64
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.79	0.64
1:A:144:G:H1	1:A:178:C:H42	1.45	0.64
1:A:1135:U:H4'	1:A:1136:U:H5	1.61	0.64
12:L:25:PRO:HB3	12:L:27:LEU:HD22	1.79	0.64
2:B:101:MET:HA	2:B:108:ILE:HD12	1.79	0.64
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.79	0.64
5:E:81:GLU:HG2	5:E:90:VAL:HG22	1.80	0.64
12:L:28:LYS:HE3	12:L:62:SER:HA	1.79	0.64
1:A:993:G:O6	1:A:1045:C:N4	2.31	0.64
1:A:1510:U:H2'	1:A:1511:G:C8	2.33	0.64
18:R:48:GLY:HA3	18:R:82:THR:HA	1.80	0.64
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.80	0.63
3:C:20:SER:OG	3:C:36:ASP:OD1	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:G:OP2	20:T:83:ARG:NH1	2.31	0.63
5:E:8:GLU:HB3	5:E:34:VAL:HG22	1.81	0.63
13:M:96:LEU:O	13:M:110:ARG:NH1	2.31	0.63
20:T:67:ALA:HA	20:T:73:HIS:H	1.62	0.63
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.32	0.63
3:C:88:ARG:HG3	3:C:100:ALA:HA	1.81	0.63
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.63
1:A:1305:G:N2	1:A:1331:G:H1'	2.14	0.63
9:I:54:ASP:O	9:I:58:HIS:ND1	2.32	0.62
1:A:421:U:O2	3:C:126:ARG:NH1	2.31	0.62
1:A:1493:A:HO2'	1:A:1494:G:H8	1.47	0.62
1:A:372:C:H4'	1:A:373:A:O5'	1.99	0.62
1:A:1189:C:H5"	3:C:5:ILE:HG12	1.80	0.62
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.32	0.62
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.81	0.62
3:C:188:LEU:HD21	3:C:195:VAL:HG23	1.82	0.62
11:K:27:ASN:OD1	11:K:28:THR:N	2.32	0.62
19:S:50:ALA:HA	19:S:59:PRO:HA	1.82	0.62
2:B:16:HIS:ND1	2:B:17:PHE:O	2.26	0.62
2:B:79:ASP:HB2	2:B:238:LEU:HD13	1.80	0.62
2:B:21:ARG:HA	2:B:39:ILE:HA	1.82	0.62
5:E:147:ASP:N	5:E:147:ASP:OD1	2.32	0.61
13:M:15:VAL:HG21	13:M:48:LEU:HD21	1.82	0.61
1:A:1149:C:O2'	1:A:1280:A:N1	2.27	0.61
3:C:121:ALA:HA	3:C:124:ILE:HD12	1.82	0.61
1:A:1238:A:H5'	1:A:1336:C:H41	1.64	0.61
1:A:1435:G:H2'	1:A:1436:U:C6	2.35	0.61
1:A:56:U:H2'	1:A:57:G:C8	2.36	0.61
1:A:90:U:H2'	1:A:91:C:C6	2.36	0.61
13:M:117:VAL:HG12	13:M:118:ALA:H	1.66	0.61
1:A:103:C:OP1	20:T:17:ARG:NH1	2.34	0.60
1:A:524:G:H2'	1:A:525:C:C6	2.35	0.60
1:A:76:C:H2'	1:A:77:G:C8	2.36	0.60
3:C:34:LEU:HD22	3:C:38:ARG:HE	1.65	0.60
1:A:1035:A:H2'	1:A:1036:G:C8	2.36	0.60
1:A:1491:G:H5'	12:L:94:TRP:CZ2	2.35	0.60
1:A:527:7MG:O2'	1:A:535:A:N1	2.32	0.60
1:A:1407:5MC:HN41	1:A:1494:G:H1	1.49	0.60
1:A:748:C:H4'	1:A:749:C:O5'	2.01	0.60
4:D:64:LEU:HG	4:D:198:VAL:HG11	1.83	0.60
1:A:76:C:H2'	1:A:77:G:H8	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:G:H1	1:A:89:C:H42	1.48	0.60
1:A:1229:A:OP2	13:M:114:ARG:NH1	2.34	0.60
1:A:411:A:N6	1:A:413:G:H21	1.96	0.60
1:A:1502:A:H2	1:A:1505:G:H1	1.50	0.60
22:A:1601:SRY:H61	12:L:47:LYS:HD2	1.82	0.60
5:E:43:LEU:HD22	5:E:136:MET:HG3	1.84	0.60
1:A:686:U:HO2'	1:A:687:A:H8	1.49	0.60
1:A:1442:G:N2	1:A:1447:G:N7	2.50	0.60
12:L:113:ARG:NH1	12:L:116:SER:H	2.00	0.59
1:A:736:C:H2'	1:A:737:A:C8	2.37	0.59
7:G:84:ASN:OD1	7:G:84:ASN:N	2.36	0.59
15:O:32:LEU:HD12	15:O:63:ARG:HB2	1.85	0.59
20:T:89:ARG:HG3	20:T:104:LEU:HD13	1.84	0.59
3:C:46:GLU:O	3:C:83:ARG:NH2	2.34	0.59
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.84	0.59
17:Q:5:VAL:HG22	17:Q:60:ILE:HG13	1.84	0.59
1:A:1425:U:H3	1:A:1475:G:H1	1.49	0.59
1:A:84:U:H2'	1:A:88:A:O4'	2.02	0.59
1:A:1145:C:O2'	1:A:1146:A:O5'	2.20	0.59
1:A:558:G:OP2	1:A:559:A:O2'	2.14	0.59
1:A:673:G:H2'	1:A:674:G:C8	2.37	0.59
1:A:957:U:H4'	19:S:79:THR:HB	1.85	0.59
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.84	0.59
20:T:33:ILE:HD13	20:T:62:LEU:HB3	1.85	0.59
1:A:1241:G:H2'	1:A:1242:C:C6	2.37	0.59
6:F:15:ASP:OD2	6:F:18:GLN:NE2	2.36	0.59
17:Q:43:LEU:HD12	17:Q:68:ARG:HB3	1.83	0.59
1:A:512:U:OP1	4:D:46:LYS:NZ	2.36	0.59
1:A:1068:G:H8	1:A:1068:G:OP2	1.85	0.58
7:G:27:ILE:HD12	7:G:40:ALA:HA	1.84	0.58
8:H:64:LYS:HG2	8:H:79:VAL:HG21	1.85	0.58
15:O:3:ILE:HD13	15:O:34:LEU:HD13	1.85	0.58
1:A:955:U:H1'	1:A:1227:A:N6	2.18	0.58
1:A:1064:G:H1'	1:A:1190:G:H21	1.67	0.58
1:A:1303:C:H2'	1:A:1304:G:H5'	1.86	0.58
1:A:1221:G:O3'	19:S:77:THR:HG21	2.03	0.58
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.85	0.58
15:O:87:ILE:HG22	15:O:88:ARG:H	1.68	0.58
2:B:17:PHE:HD1	2:B:18:GLY:H	1.51	0.58
5:E:101:ILE:O	5:E:120:THR:HB	2.03	0.58
11:K:13:GLN:HA	11:K:76:GLY:HA3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:C:OP2	12:L:69:TYR:OH	2.20	0.58
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.36	0.58
10:J:50:ILE:HB	14:N:41:ARG:HH21	1.69	0.58
10:J:53:PRO:HB3	14:N:42:ILE:HD12	1.85	0.58
1:A:373:A:H1'	1:A:481:G:H1'	1.86	0.57
7:G:22:LEU:HD21	7:G:66:VAL:HG11	1.85	0.57
1:A:1196:U:OP1	1:A:1197:G:H5'	2.04	0.57
10:J:84:GLN:HG3	10:J:85:LEU:HD22	1.85	0.57
13:M:34:LEU:HD12	13:M:39:ILE:HB	1.87	0.57
1:A:562:C:H1'	12:L:15:ARG:HG3	1.87	0.57
1:A:1366:C:H2'	1:A:1367:C:C6	2.39	0.57
3:C:26:LYS:NZ	10:J:45:ARG:HD2	2.20	0.57
10:J:54:PHE:O	10:J:55:LYS:HG3	2.04	0.57
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.86	0.57
1:A:407:G:O4'	4:D:119:GLN:NE2	2.38	0.57
1:A:989:C:H42	1:A:1216:G:H1	1.52	0.57
19:S:11:VAL:HG21	19:S:41:VAL:HG13	1.85	0.57
1:A:261:U:OP2	20:T:79:ARG:NH2	2.38	0.57
8:H:17:THR:OG1	8:H:18:ARG:NH1	2.38	0.57
1:A:1021:G:N2	1:A:1022:G:O2'	2.38	0.57
1:A:95:U:H2'	1:A:96:G:C8	2.40	0.57
1:A:578:C:O2'	1:A:728:A:N3	2.34	0.56
1:A:1338:G:H2'	1:A:1339:A:C8	2.40	0.56
4:D:3:ARG:HH11	4:D:71:SER:H	1.51	0.56
4:D:102:ASP:OD1	4:D:103:ASN:N	2.38	0.56
13:M:107:ALA:HB3	13:M:111:LYS:HE3	1.87	0.56
15:O:56:LEU:HA	15:O:59:MET:HE2	1.87	0.56
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.87	0.56
3:C:19:GLU:OE1	3:C:54:ARG:NE	2.37	0.56
1:A:926:G:N2	1:A:1542:U:OP1	2.38	0.56
1:A:1006:C:N4	1:A:1023:G:O6	2.38	0.56
1:A:1343:G:H4'	9:I:122:ALA:HB3	1.88	0.56
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.87	0.56
11:K:12:ARG:HB3	11:K:14:VAL:HG22	1.87	0.56
1:A:793:U:H3'	1:A:794:A:H5"	1.87	0.56
1:A:1086:U:H3	1:A:1099:G:H22	1.52	0.56
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.86	0.56
2:B:231:GLU:HG3	2:B:232:PRO:HD2	1.86	0.56
9:I:95:LYS:HE3	9:I:98:PRO:HG2	1.88	0.56
1:A:1040:U:H2'	1:A:1041:A:H8	1.71	0.56
3:C:156:ARG:H	3:C:163:ALA:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:22:LEU:HD21	19:S:28:LYS:H	1.71	0.56
1:A:1372:U:H2'	1:A:1373:G:O4'	2.06	0.56
2:B:69:LEU:HD21	2:B:93:VAL:HG23	1.88	0.56
2:B:139:LYS:NZ	2:B:143:GLU:OE2	2.37	0.56
15:O:4:THR:OG1	15:O:7:GLU:OE2	2.22	0.56
20:T:60:GLU:HG3	20:T:81:LYS:HD2	1.88	0.56
17:Q:12:SER:HB3	17:Q:20:THR:HB	1.89	0.55
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.40	0.55
10:J:32:ALA:O	10:J:34:VAL:HG23	2.07	0.55
1:A:279:A:H5'	1:A:279:A:H8	1.71	0.55
1:A:1090:U:H2'	1:A:1091:U:H6	1.72	0.55
3:C:20:SER:HB2	3:C:40:ARG:HH12	1.71	0.55
3:C:24:ALA:HB2	3:C:32:LEU:HD12	1.88	0.55
18:R:88:LYS:OXT	18:R:88:LYS:NZ	2.31	0.55
4:D:53:ASP:OD1	4:D:53:ASP:N	2.33	0.55
1:A:7:G:H5'	1:A:298:A:O4'	2.06	0.55
1:A:257:G:H1	1:A:269:C:H42	1.55	0.55
1:A:1020:U:H2'	1:A:1021:G:H8	1.70	0.55
9:I:71:SER:HA	9:I:74:ILE:HD12	1.89	0.55
1:A:1392:G:H21	1:A:1502:A:H8	1.54	0.55
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.07	0.55
1:A:1143:G:H2'	1:A:1144:G:C8	2.42	0.55
1:A:1148:U:H2'	1:A:1149:C:O4'	2.07	0.55
10:J:6:ILE:HB	10:J:72:VAL:HB	1.87	0.55
1:A:118:U:H3'	1:A:288:A:H61	1.71	0.55
1:A:990:C:H42	1:A:1215:G:H1	1.55	0.55
1:A:1313:U:O4	19:S:4:SER:OG	2.19	0.55
5:E:144:THR:O	5:E:148:VAL:HG23	2.07	0.55
16:P:68:ASP:OD1	16:P:68:ASP:N	2.37	0.55
1:A:1163:C:H2'	1:A:1164:G:C8	2.42	0.54
1:A:279:A:H5"	1:A:281:G:O4'	2.06	0.54
10:J:57:LYS:O	10:J:60:ARG:NH1	2.41	0.54
1:A:381:C:H2'	1:A:382:A:O4'	2.06	0.54
1:A:410:G:OP2	4:D:25:ARG:NE	2.29	0.54
7:G:45:ASP:O	7:G:49:ILE:HG12	2.07	0.54
3:C:20:SER:HB2	3:C:40:ARG:HH22	1.71	0.54
3:C:39:ILE:HD12	3:C:57:ILE:HD13	1.90	0.54
1:A:518:C:H2'	1:A:530:G:C8	2.43	0.54
1:A:1277:C:HO2'	1:A:1279:A:H8	1.56	0.54
7:G:9:VAL:HG13	7:G:94:ARG:HH21	1.73	0.54
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:11:ILE:HD13	5:E:105:VAL:HG13	1.89	0.54
1:A:9:G:OP2	5:E:121:LYS:NZ	2.23	0.54
2:B:87:ARG:HD3	2:B:234:PRO:HD2	1.90	0.54
4:D:65:ARG:HG3	4:D:75:PHE:CD1	2.43	0.54
3:C:167:TRP:HE3	3:C:168:ALA:N	2.06	0.54
1:A:974:A:OP2	14:N:29:ARG:NH2	2.41	0.53
1:A:108:G:H5'	1:A:109:A:H5"	1.89	0.53
1:A:736:C:H2'	1:A:737:A:H8	1.74	0.53
3:C:34:LEU:HD13	3:C:38:ARG:HH21	1.73	0.53
1:A:1010:G:H1	1:A:1019:C:H42	1.56	0.53
1:A:1225:A:H4'	19:S:78:ARG:HD3	1.89	0.53
3:C:121:ALA:HB1	3:C:189:ALA:HB2	1.89	0.53
13:M:88:ARG:HD3	19:S:3:ARG:HH21	1.73	0.53
1:A:689:C:H2'	1:A:690:G:O4'	2.09	0.53
1:A:714:G:H2'	1:A:715:A:C8	2.42	0.53
1:A:955:U:H1'	1:A:1227:A:H61	1.74	0.53
1:A:1223:C:OP2	19:S:78:ARG:NH2	2.42	0.53
1:A:974:A:OP1	1:A:974:A:H8	1.91	0.53
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.90	0.53
12:L:97:ARG:HB2	12:L:98:TYR:CE1	2.43	0.53
2:B:168:THR:HG23	2:B:192:SER:HA	1.90	0.53
1:A:179:A:H2'	1:A:180:U:C6	2.43	0.53
1:A:1303:C:C2'	1:A:1304:G:H5'	2.39	0.53
1:A:1367:C:H5'	10:J:60:ARG:HE	1.74	0.53
16:P:14:ASN:HA	16:P:42:ARG:NH1	2.24	0.53
1:A:235:C:H5'	17:Q:70:ARG:HG3	1.91	0.53
1:A:1147:C:O2	9:I:16:ARG:NH1	2.42	0.53
1:A:237:C:OP2	17:Q:40:LYS:NZ	2.42	0.53
1:A:359:U:H2'	1:A:360:A:C8	2.44	0.53
1:A:1256:A:H5'	1:A:1258:G:H1'	1.91	0.53
1:A:1296:C:H4'	1:A:1302:U:C5	2.43	0.53
3:C:167:TRP:HE3	3:C:168:ALA:H	1.56	0.53
6:F:33:TYR:HA	6:F:71:ARG:NH2	2.24	0.52
1:A:1427:U:H2'	1:A:1428:A:C8	2.44	0.52
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.91	0.52
1:A:407:G:H2'	1:A:408:A:C8	2.45	0.52
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.52
1:A:1300:G:O2'	1:A:1301:U:O5'	2.27	0.52
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.91	0.52
16:P:10:GLY:HA3	16:P:14:ASN:O	2.10	0.52
17:Q:21:VAL:HG21	17:Q:59:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:HD11	3:C:103:VAL:HG21	1.91	0.52
5:E:122:GLU:O	5:E:126:ARG:NH1	2.42	0.52
12:L:6:THR:O	12:L:10:LEU:HD12	2.09	0.52
10:J:8:LEU:HG	10:J:70:ARG:HB2	1.91	0.52
13:M:39:ILE:HD12	13:M:56:LEU:HG	1.91	0.52
1:A:1061:G:H1	1:A:1195:C:H42	1.57	0.52
1:A:1243:C:H2'	1:A:1244:C:C6	2.45	0.52
6:F:43:LEU:HD21	18:R:35:ARG:HH12	1.74	0.52
8:H:87:SER:HB2	8:H:93:VAL:H	1.75	0.52
1:A:56:U:H2'	1:A:57:G:H8	1.74	0.52
1:A:1435:G:H2'	1:A:1436:U:H6	1.74	0.52
1:A:1198:G:H2'	1:A:1199:U:C6	2.44	0.51
10:J:77:PRO:HB2	10:J:82:ILE:HD11	1.91	0.51
1:A:401:C:H2'	1:A:402:G:H8	1.75	0.51
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.92	0.51
21:U:17:THR:O	21:U:22:ARG:NH1	2.43	0.51
1:A:580:U:H2'	1:A:581:G:O4'	2.10	0.51
1:A:1007:C:O2	1:A:1023:G:N1	2.44	0.51
1:A:1499:A:H1'	1:A:1520:G:H5'	1.92	0.51
11:K:19:ALA:HB2	11:K:80:VAL:HG21	1.91	0.51
19:S:49:ILE:HG21	19:S:71:LEU:HD11	1.92	0.51
1:A:316:G:OP2	1:A:351:G:O2'	2.29	0.51
1:A:1275:A:H2'	1:A:1276:G:O4'	2.10	0.51
13:M:37:THR:HG21	13:M:56:LEU:HA	1.91	0.51
16:P:70:ALA:O	16:P:74:LEU:HG	2.10	0.51
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.41	0.51
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.41	0.51
20:T:50:GLU:HA	20:T:100:ILE:HB	1.92	0.51
6:F:18:GLN:O	6:F:22:GLU:HG2	2.10	0.51
9:I:5:TYR:HE1	9:I:7:THR:HG1	1.58	0.51
9:I:112:LYS:HE3	9:I:117:HIS:O	2.11	0.51
1:A:947:G:H2'	1:A:948:C:O4'	2.11	0.51
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.44	0.51
1:A:1221:G:OP2	19:S:37:ARG:NH2	2.43	0.51
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.44	0.51
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.93	0.51
4:D:3:ARG:NH1	4:D:71:SER:H	2.09	0.50
1:A:216:G:H2'	1:A:217:C:C6	2.46	0.50
1:A:397:A:H5'	1:A:398:C:OP1	2.11	0.50
1:A:413:G:O6	4:D:36:ARG:HD3	2.11	0.50
1:A:1080:A:O3'	5:E:16:THR:OG1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1136:U:H5"	1:A:1137:C:OP2	2.11	0.50
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.92	0.50
19:S:23:ASN:OD1	19:S:47:HIS:NE2	2.21	0.50
1:A:177:C:H2'	1:A:178:C:H6	1.75	0.50
1:A:355:C:H5'	1:A:389:A:OP2	2.12	0.50
1:A:540:G:H2'	1:A:541:G:O4'	2.11	0.50
1:A:706:A:O4'	11:K:29:ILE:HD11	2.11	0.50
1:A:335:C:H2'	1:A:336:C:C6	2.46	0.50
1:A:918:A:H2'	1:A:919:A:C8	2.46	0.50
1:A:1414:U:H2'	1:A:1415:G:C8	2.43	0.50
4:D:36:ARG:HA	4:D:38:TYR:CE2	2.45	0.50
1:A:532:A:N6	3:C:158:GLY:O	2.43	0.50
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.93	0.50
1:A:382:A:H2'	1:A:383:A:C8	2.47	0.50
1:A:1460:A:OP2	20:T:27:LYS:NZ	2.44	0.50
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.47	0.50
1:A:1145:C:HO2'	1:A:1146:A:P	2.34	0.50
1:A:1285:A:H4'	1:A:1286:A:O5'	2.10	0.50
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.93	0.50
19:S:15:LEU:HD23	19:S:33:THR:HG21	1.94	0.50
1:A:452:A:H2'	1:A:453:A:C8	2.46	0.50
1:A:686:U:O2'	1:A:687:A:H8	1.94	0.50
1:A:992:U:H4'	1:A:993:G:O5'	2.10	0.50
1:A:1124:G:H3'	1:A:1145:C:H5	1.76	0.50
1:A:1427:U:H2'	1:A:1428:A:H8	1.76	0.50
13:M:3:ARG:HH21	13:M:7:VAL:HG12	1.77	0.50
1:A:1067:A:N1	1:A:1108:G:O2'	2.43	0.49
1:A:1488:G:H2'	1:A:1489:G:C8	2.47	0.49
9:I:32:ASP:OD1	9:I:33:PHE:N	2.45	0.49
1:A:413:G:H2'	1:A:428:G:N2	2.27	0.49
1:A:1152:A:H5"	10:J:13:HIS:ND1	2.26	0.49
1:A:1172:C:H2'	1:A:1173:G:C8	2.47	0.49
3:C:54:ARG:HD3	3:C:56:ASP:OD2	2.12	0.49
20:T:50:GLU:HB2	20:T:99:LEU:HD11	1.95	0.49
1:A:279:A:C6	17:Q:98:LEU:HD13	2.48	0.49
1:A:401:C:H2'	1:A:402:G:C8	2.47	0.49
1:A:501:C:H2'	1:A:502:G:C8	2.47	0.49
3:C:55:VAL:HG22	3:C:68:VAL:HG23	1.94	0.49
3:C:150:LYS:HA	3:C:169:ALA:HA	1.94	0.49
15:O:45:VAL:HG12	15:O:46:HIS:H	1.76	0.49
1:A:943:U:H1'	9:I:124:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:U:H2'	1:A:1426:C:C6	2.48	0.49
1:A:1490:C:H5'	1:A:1491:G:OP2	2.12	0.49
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.77	0.49
7:G:139:GLU:O	7:G:143:ARG:HB2	2.12	0.49
1:A:620:C:N1	4:D:135:LEU:HD13	2.28	0.49
1:A:750:G:H1'	15:O:23:GLY:H	1.77	0.49
1:A:1021:G:C2	1:A:1022:G:H1'	2.48	0.49
10:J:50:ILE:HG12	10:J:60:ARG:HH11	1.77	0.49
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.76	0.49
1:A:833:U:H2'	1:A:834:C:C6	2.47	0.49
1:A:839:U:H5'	1:A:840:C:H5	1.78	0.49
11:K:92:GLU:HB3	11:K:96:ARG:NH2	2.28	0.49
21:U:14:TRP:CE3	21:U:15:ARG:HG2	2.48	0.49
1:A:1262:C:H2'	1:A:1263:C:C6	2.48	0.49
4:D:9:CYS:O	4:D:12:CYS:HB2	2.12	0.49
17:Q:74:LEU:HG	17:Q:75:ARG:HG2	1.94	0.49
1:A:452:A:O2'	1:A:453:A:O4'	2.20	0.49
1:A:1426:C:H42	1:A:1474:G:H1	1.60	0.49
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.95	0.49
3:C:186:PHE:HD1	3:C:199:LYS:HG2	1.77	0.49
1:A:173:U:H6	1:A:198:G:HO2'	1.56	0.49
1:A:1125:U:OP2	1:A:1145:C:N4	2.45	0.49
1:A:57:G:H2'	1:A:58:C:C6	2.48	0.49
1:A:151:A:H2'	1:A:152:A:O4'	2.13	0.49
1:A:1203:C:O2'	1:A:1204:A:OP1	2.31	0.49
1:A:269:C:H2'	1:A:270:A:C8	2.47	0.48
1:A:558:G:H3'	1:A:559:A:H3'	1.95	0.48
1:A:1218:C:H2'	1:A:1219:U:C6	2.48	0.48
3:C:186:PHE:CD1	3:C:199:LYS:HG2	2.48	0.48
14:N:8:GLU:OE2	14:N:9:LYS:N	2.45	0.48
1:A:459:G:H1'	1:A:463:A:H61	1.77	0.48
11:K:54:ARG:NH1	11:K:54:ARG:HB3	2.28	0.48
12:L:39:VAL:H	12:L:57:LYS:HB2	1.78	0.48
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.48	0.48
1:A:1139:G:O2'	1:A:1140:C:O5'	2.29	0.48
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.94	0.48
1:A:157:G:H2'	1:A:158:G:H8	1.78	0.48
1:A:1347:G:O2'	1:A:1348:U:P	2.71	0.48
2:B:189:ASP:OD1	2:B:189:ASP:N	2.46	0.48
11:K:33:THR:HA	11:K:39:PRO:HA	1.96	0.48
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:G:H2'	1:A:429:U:C5	2.48	0.48
1:A:1248:A:H2'	1:A:1249:C:C6	2.48	0.48
1:A:1488:G:H2'	1:A:1489:G:H8	1.79	0.48
5:E:69:VAL:HG12	5:E:71:LEU:HG	1.96	0.48
7:G:122:HIS:O	7:G:126:ASP:HB2	2.14	0.48
12:L:33:ARG:HG2	12:L:60:LEU:HD12	1.94	0.48
12:L:75:HIS:CD2	12:L:77:LEU:HB2	2.49	0.48
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.79	0.48
1:A:243:A:C2	1:A:246:A:C8	3.01	0.48
1:A:254:G:OP1	17:Q:67:LYS:O	2.31	0.48
1:A:781:A:O2'	1:A:1522:U:O2	2.30	0.48
1:A:923:A:OP1	5:E:21:ALA:HB2	2.14	0.48
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.44	0.48
17:Q:29:HIS:HD2	17:Q:32:TYR:N	1.93	0.48
1:A:149:A:H2'	1:A:150:C:H6	1.78	0.48
1:A:1279:A:H2	10:J:43:ARG:HH12	1.60	0.48
1:A:1418:A:N6	1:A:1482:G:O2'	2.46	0.48
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.96	0.48
1:A:297:G:N2	1:A:300:A:OP2	2.43	0.48
1:A:376:G:H5"	16:P:5:ARG:HB2	1.96	0.48
1:A:625:G:H4'	16:P:16:HIS:CD2	2.48	0.48
9:I:45:ALA:O	9:I:78:LYS:HE2	2.14	0.48
1:A:647:C:H2'	1:A:648:A:H8	1.78	0.47
1:A:1018:C:H2'	1:A:1019:C:O4'	2.14	0.47
1:A:1300:G:O2'	1:A:1301:U:P	2.72	0.47
2:B:98:LEU:HB2	2:B:101:MET:HG3	1.95	0.47
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.48	0.47
9:I:24:GLY:HA2	9:I:59:PHE:O	2.14	0.47
1:A:31:G:N2	1:A:48:C:OP1	2.36	0.47
1:A:95:U:H2'	1:A:96:G:H8	1.79	0.47
1:A:279:A:H5'	1:A:279:A:C8	2.49	0.47
1:A:374:A:C6	1:A:375:U:C4	3.02	0.47
1:A:983:A:O5'	14:N:3:ARG:NH2	2.48	0.47
3:C:148:GLY:HA3	3:C:172:ARG:O	2.15	0.47
1:A:279:A:OP1	1:A:280:C:O2'	2.29	0.47
1:A:1090:U:H2'	1:A:1091:U:C6	2.48	0.47
2:B:162:ILE:HG23	2:B:164:VAL:HG23	1.94	0.47
12:L:25:PRO:HA	12:L:27:LEU:HB2	1.96	0.47
13:M:2:ALA:O	13:M:10:PRO:HD2	2.15	0.47
1:A:731:G:H5'	1:A:766:A:H4'	1.96	0.47
1:A:953:G:H5'	1:A:965:A:H61	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:113:ARG:HH11	12:L:116:SER:H	1.62	0.47
1:A:132:C:H2'	1:A:133:U:H6	1.79	0.47
1:A:1026:G:H5'	1:A:1027:C:OP2	2.14	0.47
1:A:1513:A:H2'	1:A:1514:C:C6	2.49	0.47
4:D:36:ARG:HD2	4:D:38:TYR:OH	2.15	0.47
1:A:244:U:H4'	1:A:245:C:H5"	1.97	0.47
4:D:79:PHE:HE1	4:D:204:ILE:HD13	1.78	0.47
9:I:118:LYS:O	9:I:120:ARG:N	2.40	0.47
10:J:6:ILE:HD13	10:J:72:VAL:HB	1.96	0.47
12:L:27:LEU:C	12:L:29:GLY:N	2.67	0.47
19:S:51:VAL:HG21	19:S:71:LEU:HD22	1.96	0.47
21:U:6:ARG:HB2	21:U:15:ARG:NH2	2.30	0.47
1:A:177:C:H2'	1:A:178:C:C6	2.50	0.47
1:A:371:G:O2'	1:A:372:C:H5'	2.15	0.47
7:G:15:ASP:HB3	7:G:19:GLY:H	1.80	0.47
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.96	0.47
1:A:1002:G:H2'	1:A:1003:G:C8	2.49	0.47
1:A:1338:G:C6	1:A:1339:A:C6	3.03	0.47
2:B:79:ASP:OD2	2:B:79:ASP:N	2.48	0.47
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.96	0.47
1:A:157:G:H2'	1:A:158:G:C8	2.50	0.47
1:A:299:G:H2'	1:A:300:A:C8	2.50	0.47
3:C:30:ARG:HB3	14:N:36:PHE:O	2.15	0.47
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.50	0.47
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.49	0.46
1:A:960:U:H1'	1:A:1223:C:H5'	1.96	0.46
1:A:972:C:P	10:J:57:LYS:HD3	2.55	0.46
1:A:1031:G:H2'	1:A:1032:G:C8	2.50	0.46
1:A:1278:U:H5'	1:A:1279:A:O4'	2.15	0.46
6:F:25:ILE:HG21	6:F:82:ARG:HD2	1.96	0.46
11:K:18:ARG:HB3	11:K:20:TYR:CE1	2.50	0.46
16:P:74:LEU:O	16:P:79:VAL:HG23	2.14	0.46
21:U:9:ARG:HD2	21:U:22:ARG:HD2	1.96	0.46
1:A:92:C:H2'	1:A:93:G:C8	2.45	0.46
1:A:556:C:H2'	1:A:557:G:O4'	2.15	0.46
3:C:180:ALA:HB2	3:C:206:GLU:O	2.15	0.46
15:O:87:ILE:HG22	15:O:88:ARG:N	2.29	0.46
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.50	0.46
1:A:384:G:H2'	1:A:385:C:C6	2.50	0.46
1:A:628:G:H2'	1:A:629:G:O4'	2.16	0.46
1:A:1486:G:H2'	1:A:1487:G:O4'	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:GLN:HG3	3:C:128:PHE:HD1	1.81	0.46
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.51	0.46
19:S:60:VAL:HG11	19:S:74:PHE:HB3	1.98	0.46
1:A:1150:U:O4	1:A:1151:A:N6	2.48	0.46
1:A:1320:C:H1'	19:S:73:GLU:HG2	1.97	0.46
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.98	0.46
8:H:17:THR:HG22	8:H:63:LEU:HG	1.97	0.46
11:K:54:ARG:H	11:K:54:ARG:HG2	1.31	0.46
12:L:28:LYS:HD2	12:L:33:ARG:NH1	2.29	0.46
1:A:992:U:H3	1:A:1044:A:H62	1.63	0.46
1:A:1051:C:H42	1:A:1207:2MG:HN1	1.62	0.46
22:A:1601:SRY:HH21	12:L:48:PRO:HG3	1.98	0.46
3:C:88:ARG:HE	3:C:101:LEU:H	1.63	0.46
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.97	0.46
17:Q:81:ARG:HB3	17:Q:84:LEU:HD12	1.98	0.46
1:A:237:C:H2'	1:A:238:G:C8	2.50	0.46
4:D:86:LYS:H	4:D:86:LYS:HD2	1.79	0.46
7:G:29:LYS:HD2	7:G:29:LYS:HA	1.68	0.46
10:J:51:ARG:NE	10:J:61:GLU:HB2	2.31	0.46
11:K:18:ARG:HD3	11:K:35:PRO:HA	1.98	0.46
16:P:34:GLU:OE1	16:P:55:ARG:NH1	2.40	0.46
1:A:269:C:H2'	1:A:270:A:H8	1.80	0.46
1:A:688:G:O2'	1:A:704:A:N1	2.45	0.46
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.97	0.46
2:B:95:GLN:HG3	2:B:147:LYS:O	2.15	0.46
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.98	0.46
1:A:933:G:OP2	7:G:3:ARG:HB3	2.16	0.46
1:A:1141:C:H2'	1:A:1142:G:C8	2.51	0.46
1:A:1392:G:N2	1:A:1502:A:H8	2.12	0.46
2:B:82:ARG:HG3	2:B:92:TYR:CZ	2.51	0.46
3:C:119:ARG:HE	3:C:140:ARG:NH2	2.14	0.46
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.40	0.46
1:A:452:A:O2'	16:P:72:ARG:HD2	2.16	0.46
1:A:1376:U:H2'	1:A:1377:A:C8	2.51	0.46
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.31	0.46
20:T:10:LEU:O	20:T:13:LEU:HD22	2.16	0.46
20:T:87:LYS:O	20:T:91:LEU:HB2	2.16	0.46
1:A:79:G:H2'	1:A:80:G:C8	2.51	0.46
1:A:791:G:N2	1:A:792:A:H62	2.13	0.46
1:A:939:G:H5"	7:G:102:ARG:HH12	1.81	0.46
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ALA:O	2:B:222:ILE:HG13	2.16	0.46
7:G:9:VAL:HG12	7:G:10:ARG:O	2.16	0.46
11:K:23:ALA:O	11:K:86:GLY:HA3	2.16	0.46
12:L:24:VAL:HG12	12:L:24:VAL:O	2.16	0.46
13:M:92:HIS:CE1	13:M:98:VAL:HG21	2.50	0.46
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.15	0.46
18:R:58:LEU:HD13	18:R:62:GLU:HB3	1.98	0.46
1:A:812:C:H4'	1:A:813:U:O5'	2.16	0.45
1:A:939:G:H5"	7:G:102:ARG:NH1	2.31	0.45
1:A:1031:G:H2'	1:A:1032:G:H8	1.80	0.45
1:A:977:A:O2'	1:A:981:U:N3	2.40	0.45
6:F:8:ILE:HD13	6:F:88:VAL:HG22	1.98	0.45
2:B:178:ARG:HH21	8:H:74:PRO:HB3	1.81	0.45
5:E:107:ARG:O	5:E:111:GLU:HB2	2.17	0.45
9:I:95:LYS:HE3	9:I:95:LYS:HA	1.97	0.45
10:J:49:VAL:HG12	10:J:50:ILE:O	2.17	0.45
14:N:5:ALA:O	14:N:8:GLU:HB3	2.16	0.45
14:N:29:ARG:HH12	14:N:41:ARG:HH11	1.65	0.45
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.31	0.45
1:A:594:G:H1	1:A:645:C:H42	1.65	0.45
1:A:667:G:H4'	15:O:51:HIS:CE1	2.51	0.45
2:B:189:ASP:HB3	2:B:203:GLY:O	2.16	0.45
4:D:190:ASP:O	4:D:194:LEU:HD22	2.17	0.45
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.99	0.45
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.97	0.45
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.99	0.45
20:T:92:LEU:O	20:T:96:GLY:HA2	2.17	0.45
1:A:660:G:H1	1:A:745:C:H42	1.65	0.45
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.98	0.45
10:J:25:GLU:HA	10:J:28:ARG:HG3	1.98	0.45
20:T:67:ALA:O	20:T:73:HIS:ND1	2.49	0.45
1:A:328:C:H2'	1:A:328:C:O2	2.17	0.45
1:A:357:G:C2	1:A:358:U:C5	3.04	0.45
1:A:382:A:H2'	1:A:383:A:H8	1.82	0.45
1:A:522:C:H41	12:L:53:ARG:HH22	1.64	0.45
1:A:1040:U:H2'	1:A:1041:A:C8	2.50	0.45
3:C:67:THR:HA	3:C:102:ASN:HB2	1.99	0.45
9:I:28:VAL:N	9:I:31:GLN:O	2.49	0.45
17:Q:29:HIS:CD2	17:Q:31:LEU:H	2.33	0.45
1:A:435:C:H2'	1:A:436:C:C6	2.52	0.45
1:A:587:G:O2'	1:A:588:G:OP2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:LEU:O	4:D:105:VAL:HG23	2.16	0.45
10:J:40:LEU:HD23	10:J:41:PRO:HD2	1.98	0.45
11:K:57:THR:CG2	11:K:60:ALA:H	2.29	0.45
12:L:25:PRO:CA	12:L:27:LEU:HB2	2.47	0.45
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.16	0.45
1:A:191:G:O2'	20:T:102:GLY:O	2.17	0.45
1:A:446:G:H1	1:A:488:C:H42	1.64	0.45
1:A:913:A:H1'	1:A:914:A:OP2	2.16	0.45
1:A:1096:C:H2'	1:A:1097:C:H6	1.81	0.45
1:A:1193:G:OP1	3:C:167:TRP:NE1	2.45	0.45
3:C:112:SER:O	3:C:116:VAL:HG23	2.16	0.45
9:I:93:ARG:HB3	9:I:93:ARG:NH1	2.31	0.45
2:B:51:LEU:HG	2:B:201:ILE:HG23	1.99	0.45
2:B:180:LEU:HA	2:B:180:LEU:HD23	1.74	0.45
3:C:77:ILE:HA	3:C:84:ILE:HB	1.99	0.45
3:C:188:LEU:HD23	3:C:196:LEU:O	2.17	0.45
4:D:60:GLU:OE2	4:D:199:ASN:N	2.31	0.45
5:E:28:PHE:CD2	5:E:51:VAL:HG22	2.52	0.45
13:M:57:ARG:O	13:M:61:GLU:HB2	2.16	0.45
1:A:838:G:H1	1:A:848:C:N4	2.09	0.45
1:A:1502:A:H2	1:A:1505:G:N1	2.12	0.45
3:C:11:ARG:NH1	3:C:177:THR:O	2.50	0.45
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.52	0.45
5:E:90:VAL:O	5:E:91:LEU:HD23	2.17	0.45
1:A:31:G:H2'	1:A:48:C:N4	2.32	0.44
1:A:390:C:O3'	16:P:28:ARG:NH2	2.50	0.44
1:A:788:U:O2'	1:A:1539:C:O2	2.34	0.44
1:A:1426:C:H2'	1:A:1427:U:C6	2.53	0.44
2:B:43:ASP:OD2	2:B:45:GLN:HG2	2.17	0.44
2:B:107:THR:O	2:B:110:GLN:HB2	2.16	0.44
3:C:14:ILE:HG22	3:C:15:THR:HG23	2.00	0.44
4:D:178:VAL:HG23	4:D:179:GLU:OE2	2.17	0.44
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.53	0.44
15:O:6:GLU:OE2	15:O:6:GLU:N	2.26	0.44
1:A:410:G:H2'	1:A:429:U:C4	2.52	0.44
1:A:858:G:O6	1:A:869:G:C8	2.71	0.44
1:A:1059:C:OP2	3:C:199:LYS:NZ	2.46	0.44
1:A:89:C:H2'	1:A:90:U:O4'	2.17	0.44
1:A:1124:G:H5'	10:J:35:SER:O	2.18	0.44
4:D:7:PRO:HG2	4:D:10:ARG:HD2	1.99	0.44
4:D:187:ARG:NH2	4:D:188:LEU:HD12	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:18:ARG:HG2	5:E:19:MET:N	2.32	0.44
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.99	0.44
18:R:61:LYS:O	18:R:65:ILE:HG13	2.17	0.44
1:A:973:G:H3'	1:A:974:A:H5"	1.99	0.44
1:A:1190:G:OP1	3:C:4:LYS:HA	2.16	0.44
3:C:134:ILE:O	3:C:138:VAL:HG23	2.18	0.44
8:H:12:ARG:NH1	8:H:25:ASP:O	2.50	0.44
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.98	0.44
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.98	0.44
1:A:972:C:OP1	10:J:57:LYS:NZ	2.26	0.44
1:A:1165:C:H2'	1:A:1166:G:C8	2.51	0.44
1:A:1181:G:O2'	1:A:1182:G:H5'	2.17	0.44
4:D:84:LYS:HD3	4:D:84:LYS:HA	1.67	0.44
14:N:26:ARG:HB3	14:N:43:CYS:SG	2.57	0.44
16:P:9:PHE:CE1	16:P:18:ARG:HD2	2.53	0.44
17:Q:75:ARG:HH22	17:Q:77:VAL:HG13	1.81	0.44
1:A:579:G:H2'	1:A:580:U:H6	1.83	0.44
1:A:1304:G:C6	1:A:1305:G:N1	2.85	0.44
1:A:1286:A:H5'	21:U:25:LYS:NZ	2.33	0.44
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.52	0.44
3:C:25:GLY:O	3:C:29:TYR:HB2	2.18	0.44
3:C:83:ARG:HA	3:C:86:VAL:HB	1.99	0.44
1:A:33:A:H2'	1:A:34:C:C6	2.53	0.44
1:A:579:G:H2'	1:A:580:U:C6	2.52	0.44
1:A:820:U:H4'	1:A:821:G:OP2	2.17	0.44
1:A:1049:U:C5	14:N:2:ALA:HA	2.53	0.44
1:A:1075:C:H5'	2:B:103:THR:HG21	2.00	0.44
8:H:120:THR:H	8:H:123:GLU:HB2	1.83	0.44
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.52	0.44
13:M:2:ALA:N	13:M:9:ILE:HG23	2.32	0.44
20:T:13:LEU:HD23	20:T:14:LYS:N	2.32	0.44
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.99	0.44
20:T:89:ARG:NH2	20:T:105:SER:O	2.46	0.44
1:A:1339:A:H2'	1:A:1340:A:O4'	2.18	0.44
4:D:24:GLU:HG2	4:D:25:ARG:N	2.32	0.44
4:D:135:LEU:HA	4:D:136:PRO:HD3	1.89	0.44
7:G:50:ILE:O	7:G:54:THR:OG1	2.26	0.44
12:L:46:LYS:N	12:L:92:ASP:O	2.50	0.44
18:R:36:ASN:O	18:R:40:LEU:HG	2.16	0.44
1:A:114:U:H1'	1:A:353:A:H1'	2.00	0.43
1:A:695:A:H61	1:A:797:C:H1'	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:A:N1	1:A:1215:G:H1'	2.33	0.43
2:B:119:GLU:HA	2:B:142:LEU:HD11	1.99	0.43
10:J:19:SER:OG	10:J:91:PRO:HG3	2.19	0.43
10:J:40:LEU:HD11	10:J:71:LEU:HB2	2.00	0.43
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.17	0.43
20:T:67:ALA:HA	20:T:73:HIS:N	2.32	0.43
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.43
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.43
1:A:1257:U:OP2	3:C:27:LYS:NZ	2.50	0.43
1:A:1265:G:H2'	1:A:1266:G:O4'	2.18	0.43
8:H:69:ARG:HG3	8:H:76:PRO:HA	1.99	0.43
18:R:53:ARG:HG2	18:R:63:GLN:OE1	2.18	0.43
1:A:563:A:H2'	1:A:567:G:C8	2.54	0.43
1:A:986:A:H1'	19:S:54:GLY:O	2.17	0.43
1:A:1286:A:C8	1:A:1287:A:H4'	2.53	0.43
1:A:1374:A:OP1	7:G:36:LYS:NZ	2.51	0.43
1:A:1465:C:H2'	1:A:1466:C:O4'	2.18	0.43
4:D:187:ARG:NH2	4:D:188:LEU:HB2	2.33	0.43
7:G:87:VAL:HA	7:G:88:PRO:HD3	1.75	0.43
20:T:91:LEU:HD13	20:T:91:LEU:HA	1.80	0.43
1:A:62:U:OP1	1:A:385:C:O2'	2.34	0.43
1:A:757:U:H2'	1:A:758:G:O4'	2.18	0.43
1:A:860:A:H2'	1:A:861:G:O4'	2.19	0.43
1:A:1163:C:H2'	1:A:1164:G:H8	1.83	0.43
2:B:131:PRO:HD2	2:B:134:GLU:OE2	2.18	0.43
2:B:166:ASP:HB3	2:B:169:LYS:HB3	1.99	0.43
4:D:50:ARG:NH2	5:E:10:MET:H	2.17	0.43
5:E:78:HIS:O	5:E:78:HIS:ND1	2.51	0.43
10:J:45:ARG:HD3	10:J:65:LEU:HD22	2.01	0.43
11:K:54:ARG:HB3	11:K:54:ARG:HH11	1.84	0.43
18:R:21:LYS:HE3	18:R:24:ALA:HB2	2.00	0.43
1:A:129:U:O3'	1:A:129(A):G:H3'	2.18	0.43
1:A:166:G:H2'	1:A:167:G:H8	1.84	0.43
1:A:976:G:OP2	1:A:1358:U:H1'	2.19	0.43
1:A:1280:A:O4'	10:J:41:PRO:HG3	2.17	0.43
1:A:1347:G:O6	9:I:10:ARG:NH2	2.50	0.43
4:D:159:ARG:O	4:D:163:GLU:HB2	2.18	0.43
5:E:65:ASN:ND2	5:E:65:ASN:O	2.51	0.43
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.19	0.43
14:N:53:LEU:HB3	14:N:56:VAL:HG21	2.01	0.43
18:R:44:LEU:HD21	18:R:70:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:C:H2'	1:A:1030(A):G:C8	2.54	0.43
1:A:1425:U:H2'	1:A:1426:C:H6	1.82	0.43
1:A:1278:U:H5"	1:A:1279:A:OP1	2.19	0.43
1:A:1287:A:H2'	1:A:1288:A:C8	2.54	0.43
2:B:179:LYS:HA	8:H:72:PRO:HD3	2.00	0.43
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.54	0.43
10:J:54:PHE:C	10:J:55:LYS:HG3	2.38	0.43
12:L:75:HIS:CD2	12:L:77:LEU:H	2.37	0.43
13:M:49:THR:HG22	13:M:51:ALA:H	1.83	0.43
13:M:64:TRP:HB2	13:M:66:LEU:HD21	2.00	0.43
1:A:260:G:H2'	1:A:261:U:C6	2.53	0.43
1:A:992:U:H1'	1:A:993:G:OP2	2.19	0.43
1:A:1092:A:H1'	1:A:1183:A:N6	2.34	0.43
8:H:108:GLY:HA3	8:H:138:TRP:HB3	2.01	0.43
10:J:24:VAL:HG13	10:J:34:VAL:HG11	2.01	0.43
1:A:129(A):G:H1'	1:A:190(E):U:H2'	2.00	0.43
1:A:528:C:H41	12:L:49:ASN:ND2	2.16	0.43
1:A:1296:C:H4'	1:A:1302:U:H5	1.82	0.43
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.77	0.43
20:T:11:SER:HA	20:T:13:LEU:HD22	2.01	0.43
1:A:436:C:H2'	1:A:437:U:H6	1.83	0.43
1:A:767:A:H2'	1:A:768:A:O4'	2.19	0.43
5:E:102:ALA:O	5:E:107:ARG:NH1	2.52	0.43
17:Q:22:LEU:HD13	17:Q:41:LYS:HG3	2.01	0.43
1:A:105:G:OP1	20:T:22:ARG:NH2	2.51	0.42
1:A:420:U:O2'	1:A:423:G:O6	2.34	0.42
1:A:1227:A:N3	13:M:117:VAL:HG21	2.34	0.42
2:B:106:LYS:HA	2:B:109:SER:HB3	2.01	0.42
5:E:137:GLU:O	5:E:141:GLN:HG3	2.19	0.42
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.22	0.42
13:M:96:LEU:HB3	13:M:97:PRO:HD2	2.01	0.42
1:A:1168:A:H2'	1:A:1169:A:C8	2.54	0.42
2:B:96:ARG:NH1	2:B:97:TRP:H	2.18	0.42
20:T:56:MET:HG2	20:T:84:LEU:HD13	2.02	0.42
1:A:10:A:OP2	5:E:126:ARG:HD2	2.19	0.42
1:A:359:U:H2'	1:A:360:A:H8	1.83	0.42
1:A:380:G:N2	1:A:382:A:H3'	2.34	0.42
1:A:1139:G:H1'	1:A:1140:C:C5	2.55	0.42
2:B:92:TYR:CE1	2:B:94:ASN:HB2	2.54	0.42
11:K:95:ILE:HD13	11:K:108:ILE:HG21	2.01	0.42
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:GLU:N	9:I:49:PRO:HD2	2.34	0.42
17:Q:56:VAL:CG2	17:Q:81:ARG:HG3	2.50	0.42
1:A:325:A:H2'	1:A:326:G:O4'	2.19	0.42
1:A:370:C:H2'	1:A:371:G:C8	2.55	0.42
1:A:412:A:H1'	4:D:35:ARG:HH22	1.85	0.42
1:A:750:G:N3	15:O:23:GLY:HA3	2.35	0.42
1:A:895:G:H2'	1:A:896:C:C6	2.54	0.42
1:A:932:C:H5'	7:G:4:ARG:HG2	2.01	0.42
1:A:186:C:H2'	1:A:187:C:C6	2.54	0.42
1:A:263:A:OP2	20:T:79:ARG:NH1	2.52	0.42
1:A:877:C:O2'	8:H:3:THR:HG23	2.20	0.42
1:A:1003(A):G:N2	1:A:1038:C:O2'	2.53	0.42
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.54	0.42
1:A:1299:A:C8	1:A:1301:U:H1'	2.53	0.42
2:B:21:ARG:HA	2:B:39:ILE:HG23	2.00	0.42
10:J:32:ALA:HB3	10:J:75:ILE:O	2.18	0.42
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.54	0.42
17:Q:59:ILE:HA	17:Q:59:ILE:HD12	1.81	0.42
1:A:839:U:H5'	1:A:840:C:C5	2.55	0.42
3:C:50:ALA:HB2	3:C:75:VAL:HB	2.02	0.42
4:D:24:GLU:O	4:D:25:ARG:HB3	2.19	0.42
7:G:155:ARG:HA	7:G:155:ARG:HD3	1.78	0.42
8:H:54:ASP:O	8:H:56:LYS:HG2	2.18	0.42
9:I:48:GLU:OE2	9:I:51:ARG:NH1	2.48	0.42
9:I:93:ARG:HH22	9:I:97:LYS:NZ	2.16	0.42
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.84	0.42
20:T:83:ARG:O	20:T:87:LYS:HB2	2.19	0.42
1:A:532:A:O2'	1:A:533:A:OP1	2.23	0.42
22:A:1601:SRY:CH2	12:L:48:PRO:HG3	2.49	0.42
10:J:38:ILE:H	10:J:38:ILE:HG13	1.55	0.42
12:L:25:PRO:C	12:L:27:LEU:HB2	2.39	0.42
19:S:16:LEU:O	19:S:20:LEU:HG	2.20	0.42
1:A:47:C:C6	1:A:365:U:H2'	2.55	0.42
1:A:949:A:OP2	13:M:106:ASN:ND2	2.53	0.42
1:A:1070:U:H2'	1:A:1071:C:H6	1.85	0.42
1:A:1135:U:H4'	1:A:1136:U:C5	2.47	0.42
1:A:1241:G:H2'	1:A:1242:C:H6	1.82	0.42
3:C:91:LEU:HD21	3:C:99:VAL:HG22	2.01	0.42
6:F:2:ARG:O	6:F:66:GLU:HA	2.19	0.42
1:A:989:C:N4	1:A:1216:G:H1	2.16	0.42
1:A:1118:C:H2'	1:A:1119:C:H6	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ASN:O	2:B:26:PRO:C	2.58	0.42
3:C:72:LYS:HE2	3:C:72:LYS:HB3	1.94	0.42
3:C:79:ARG:HG3	3:C:82:GLU:HB2	2.02	0.42
4:D:176:LEU:HD12	4:D:182:LYS:O	2.20	0.42
5:E:71:LEU:HD21	5:E:115:VAL:HG22	2.01	0.42
16:P:3:LYS:HB3	16:P:3:LYS:HE2	1.63	0.42
17:Q:12:SER:HB3	17:Q:20:THR:CB	2.48	0.42
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.55	0.42
19:S:5:LEU:H	19:S:5:LEU:HG	1.71	0.42
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.41
1:A:858:G:N7	25:A:2098:HOH:O	2.37	0.41
1:A:1000:U:H2'	1:A:1001:A:C8	2.55	0.41
1:A:1148:U:C4	1:A:1149:C:C2	3.08	0.41
1:A:1229:A:N6	13:M:105:THR:HG22	2.35	0.41
2:B:83:MET:HB2	2:B:235:SER:OG	2.20	0.41
4:D:105:VAL:HG13	4:D:110:PHE:HB2	2.01	0.41
7:G:78:ARG:NH1	7:G:154:TYR:O	2.53	0.41
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.85	0.41
17:Q:52:LYS:N	17:Q:55:ASP:OD2	2.50	0.41
2:B:221:LEU:HD23	2:B:221:LEU:HA	1.93	0.41
8:H:90:GLY:O	17:Q:34:LYS:HE2	2.20	0.41
9:I:89:ASN:HB3	9:I:92:TYR:CD1	2.55	0.41
11:K:92:GLU:HB3	11:K:96:ARG:HH22	1.84	0.41
1:A:335:C:H2'	1:A:336:C:H6	1.86	0.41
1:A:1203:C:HO2'	1:A:1204:A:P	2.43	0.41
1:A:1361(A):C:O2	1:A:1362:C:H5	2.03	0.41
2:B:210:SER:O	2:B:214:ILE:HG12	2.21	0.41
3:C:56:ASP:O	3:C:66:VAL:HA	2.19	0.41
1:A:341:C:H2'	1:A:342:C:H6	1.85	0.41
1:A:344:A:H5"	1:A:345:C:H5	1.85	0.41
1:A:1126:U:H6	1:A:1126:U:O5'	2.03	0.41
2:B:102:LEU:HD21	2:B:162:ILE:HD11	2.01	0.41
5:E:75:THR:HG23	5:E:76:ILE:O	2.20	0.41
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.56	0.41
9:I:60:ASP:OD1	9:I:61:ALA:N	2.53	0.41
10:J:81:THR:O	10:J:85:LEU:HB2	2.20	0.41
1:A:45:U:H2'	1:A:46:G:C8	2.55	0.41
1:A:216:G:H2'	1:A:217:C:H6	1.85	0.41
1:A:522:C:N4	12:L:53:ARG:HH22	2.19	0.41
1:A:1321:C:H2'	1:A:1322:C:C5	2.56	0.41
2:B:185:ILE:HA	2:B:199:TYR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:MET:SD	7:G:36:LYS:HB2	2.61	0.41
7:G:122:HIS:HA	7:G:125:MET:HG2	2.03	0.41
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.56	0.41
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.88	0.41
13:M:90:LEU:HD12	13:M:93:ARG:HH21	1.85	0.41
16:P:11:SER:H	16:P:14:ASN:HB3	1.85	0.41
17:Q:18:THR:HG23	17:Q:69:LYS:HE3	2.03	0.41
20:T:14:LYS:O	20:T:18:GLN:HG3	2.20	0.41
1:A:232:G:H1'	1:A:262:A:N1	2.36	0.41
1:A:235:C:C5'	17:Q:70:ARG:HG3	2.50	0.41
1:A:826:C:H2'	1:A:827:U:C6	2.56	0.41
1:A:938:A:N6	1:A:939:G:C6	2.88	0.41
1:A:1397:C:HO2'	1:A:1398:A:P	2.43	0.41
10:J:32:ALA:HB2	10:J:76:ASN:HB2	2.01	0.41
10:J:64:GLU:HB3	14:N:59:ALA:HB2	2.02	0.41
17:Q:3:LYS:H	17:Q:3:LYS:HG2	1.72	0.41
20:T:56:MET:HE1	20:T:104:LEU:HD21	2.02	0.41
1:A:448:A:P	1:A:485:G:H22	2.44	0.41
1:A:998:G:H2'	1:A:999:C:C6	2.56	0.41
1:A:1305:G:H22	1:A:1331:G:H1'	1.84	0.41
1:A:1406:U:O2'	1:A:1517:G:N2	2.53	0.41
8:H:17:THR:HA	8:H:65:TYR:OH	2.21	0.41
16:P:40:ASP:HA	16:P:41:PRO:HD2	1.89	0.41
1:A:78:G:C2	1:A:92:C:C2	3.09	0.41
1:A:1281:U:H3'	1:A:1282:C:H6	1.86	0.41
1:A:1366:C:H2'	1:A:1367:C:H6	1.84	0.41
2:B:25:ASN:O	2:B:27:LYS:N	2.53	0.41
2:B:195:ASP:O	8:H:74:PRO:HG3	2.20	0.41
7:G:46:ALA:O	7:G:50:ILE:HG13	2.20	0.41
7:G:88:PRO:HG3	7:G:148:ASN:CB	2.51	0.41
12:L:126:LYS:HD3	12:L:126:LYS:HA	1.82	0.41
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.21	0.41
20:T:73:HIS:HB3	20:T:74:LYS:H	1.67	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.41
1:A:651:C:O2'	1:A:652:U:H5'	2.21	0.41
1:A:1106:G:H5"	3:C:172:ARG:HD2	2.03	0.41
1:A:1291:G:H2'	1:A:1292:U:C6	2.56	0.41
1:A:1349:A:OP1	9:I:118:LYS:HD2	2.21	0.41
1:A:1376:U:OP1	7:G:98:SER:OG	2.25	0.41
2:B:24:TRP:CH2	2:B:26:PRO:HA	2.55	0.41
2:B:208:ILE:H	2:B:208:ILE:HG13	1.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.78	0.41
5:E:76:ILE:HA	5:E:77:PRO:HD3	1.90	0.41
8:H:122:ARG:NH1	8:H:122:ARG:HB2	2.36	0.41
16:P:22:THR:HA	16:P:33:ILE:HD12	2.03	0.41
18:R:52:PRO:HG3	18:R:54:ARG:HH21	1.86	0.41
1:A:485:G:O2'	1:A:486:U:P	2.77	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.41
1:A:971:G:H1'	1:A:1365:G:O2'	2.21	0.41
2:B:74:LYS:HB2	2:B:77:ALA:HB3	2.03	0.41
4:D:79:PHE:CE1	4:D:204:ILE:HD13	2.55	0.41
4:D:162:LEU:HD23	4:D:162:LEU:HA	1.86	0.41
8:H:20:TYR:HA	8:H:65:TYR:CE2	2.56	0.41
8:H:87:SER:HA	8:H:93:VAL:HG13	2.02	0.41
8:H:105:ARG:HD3	8:H:105:ARG:HA	1.83	0.41
1:A:838:G:N2	1:A:849:C:C2	2.89	0.40
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.55	0.40
1:A:1300:G:HO2'	1:A:1301:U:P	2.41	0.40
1:A:1321:C:H4'	13:M:87:TYR:CZ	2.56	0.40
4:D:98:GLU:O	4:D:103:ASN:ND2	2.54	0.40
16:P:60:LEU:HA	16:P:60:LEU:HD23	1.75	0.40
17:Q:75:ARG:NH2	17:Q:77:VAL:HG13	2.36	0.40
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.77	0.40
20:T:10:LEU:HD13	20:T:12:ALA:H	1.86	0.40
1:A:51:A:H4'	1:A:52:G:C5'	2.51	0.40
1:A:204:U:H4'	1:A:216:G:O4'	2.21	0.40
1:A:217:C:H2'	1:A:218:C:H6	1.86	0.40
1:A:411:A:N7	1:A:413:G:N3	2.69	0.40
1:A:1145:C:O2'	1:A:1146:A:H8	2.04	0.40
2:B:100:GLY:N	2:B:176:GLU:OE2	2.50	0.40
3:C:111:LEU:HD21	3:C:144:SER:O	2.21	0.40
3:C:113:ALA:N	3:C:114:PRO:HD2	2.37	0.40
5:E:72:GLN:O	5:E:75:THR:HG22	2.21	0.40
20:T:87:LYS:HB2	20:T:87:LYS:HE3	1.74	0.40
1:A:783:C:H2'	1:A:784:C:H6	1.85	0.40
1:A:1118:C:H5'	9:I:104:ARG:HG3	2.03	0.40
1:A:1276:G:H2'	1:A:1277:C:C6	2.56	0.40
2:B:145:LEU:HD23	2:B:145:LEU:HA	1.92	0.40
4:D:108:LEU:HD23	4:D:174:LEU:HD13	2.04	0.40
7:G:63:LYS:HB2	7:G:63:LYS:HE3	1.83	0.40
9:I:3:GLN:HG3	9:I:20:ARG:HG2	2.02	0.40
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:53:HIS:O	15:O:56:LEU:HB3	2.21	0.40
1:A:6:G:H4'	1:A:298:A:H4'	2.03	0.40
1:A:926:G:H3'	1:A:1505:G:H21	1.86	0.40
1:A:1139:G:HO2'	1:A:1140:C:P	2.44	0.40
1:A:1321:C:O2'	19:S:78:ARG:NH1	2.54	0.40
2:B:127:ILE:H	2:B:127:ILE:HG13	1.54	0.40
2:B:177:ALA:HB1	2:B:182:ILE:HB	2.02	0.40
6:F:33:TYR:HD2	6:F:71:ARG:HE	1.69	0.40
6:F:95:GLU:HA	6:F:96:PRO:HD3	1.90	0.40
13:M:114:ARG:H	13:M:114:ARG:HG2	1.51	0.40
17:Q:31:LEU:HD12	17:Q:31:LEU:HA	1.89	0.40
1:A:445:G:H2'	1:A:446:G:C8	2.56	0.40
1:A:579:G:H4'	15:O:54:ARG:HH21	1.87	0.40
1:A:1250:A:N1	1:A:1353:G:N2	2.64	0.40
5:E:79:GLU:HB3	5:E:92:LYS:HG2	2.04	0.40
11:K:19:ALA:HB3	11:K:82:VAL:HG22	2.03	0.40
11:K:54:ARG:O	11:K:57:THR:HG22	2.21	0.40
20:T:74:LYS:HB3	20:T:75:ASN:H	1.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/256 (91%)	210 (90%)	19 (8%)	3 (1%)	12 42
3	C	204/239 (85%)	182 (89%)	21 (10%)	1 (0%)	29 63
4	D	206/209 (99%)	198 (96%)	8 (4%)	0	100 100
5	E	148/162 (91%)	141 (95%)	6 (4%)	1 (1%)	22 56
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
7	G	153/156 (98%)	145 (95%)	8 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100	100
9	I	125/128 (98%)	113 (90%)	12 (10%)	0	100	100
10	J	96/105 (91%)	82 (85%)	13 (14%)	1 (1%)	15	49
11	K	114/129 (88%)	105 (92%)	9 (8%)	0	100	100
12	L	122/135 (90%)	109 (89%)	13 (11%)	0	100	100
13	M	116/126 (92%)	104 (90%)	12 (10%)	0	100	100
14	N	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	36
15	O	85/89 (96%)	82 (96%)	2 (2%)	1 (1%)	13	44
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	R	68/88 (77%)	64 (94%)	4 (6%)	0	100	100
19	S	78/93 (84%)	72 (92%)	5 (6%)	1 (1%)	12	42
20	T	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
21	U	22/27 (82%)	20 (91%)	2 (9%)	0	100	100
All	All	2337/2541 (92%)	2169 (93%)	159 (7%)	9 (0%)	34	68

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	S	31	ILE
2	B	21	ARG
2	B	24	TRP
5	E	16	THR
14	N	23	ARG
10	J	34	VAL
2	B	229	VAL
3	C	66	VAL
15	O	45	VAL

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	202/220 (92%)	173 (86%)	29 (14%)	3	14
3	C	160/188 (85%)	140 (88%)	20 (12%)	4	18
4	D	180/181 (99%)	153 (85%)	27 (15%)	3	12
5	E	115/123 (94%)	97 (84%)	18 (16%)	2	11
6	F	90/90 (100%)	81 (90%)	9 (10%)	7	29
7	G	126/127 (99%)	116 (92%)	10 (8%)	12	40
8	H	119/119 (100%)	110 (92%)	9 (8%)	13	41
9	I	98/99 (99%)	84 (86%)	14 (14%)	3	14
10	J	87/92 (95%)	74 (85%)	13 (15%)	3	13
11	K	88/99 (89%)	78 (89%)	10 (11%)	5	22
12	L	104/111 (94%)	86 (83%)	18 (17%)	2	8
13	M	94/101 (93%)	80 (85%)	14 (15%)	3	13
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	4
15	O	79/80 (99%)	66 (84%)	13 (16%)	2	10
16	P	72/74 (97%)	68 (94%)	4 (6%)	21	53
17	Q	94/97 (97%)	90 (96%)	4 (4%)	29	60
18	R	61/77 (79%)	56 (92%)	5 (8%)	11	38
19	S	71/80 (89%)	62 (87%)	9 (13%)	4	18
20	T	76/82 (93%)	65 (86%)	11 (14%)	3	14
21	U	19/22 (86%)	15 (79%)	4 (21%)	1	4
All	All	1984/2112 (94%)	1733 (87%)	251 (13%)	4	18

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

Mol	Chain	Res	Type
2	B	7	VAL
2	B	11	LEU
2	B	12	GLU
2	B	24	TRP
2	B	30	ARG
2	B	44	LEU
2	B	60	ASP
2	B	61	LEU
2	B	74	LYS
2	B	79	ASP
2	B	96	ARG

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Mol	Chain	Res	Type
2	B	97	TRP
2	B	102	LEU
2	B	108	ILE
2	B	114	ARG
2	B	119	GLU
2	B	127	ILE
2	B	142	LEU
2	B	150	SER
2	B	153	ARG
2	B	157	ARG
2	B	162	ILE
2	B	163	PHE
2	B	168	THR
2	B	170	GLU
2	B	190	THR
2	B	208	ILE
2	B	209	ARG
2	B	221	LEU
3	C	3	ASN
3	C	19	GLU
3	C	34	LEU
3	C	58	GLU
3	C	64	VAL
3	C	75	VAL
3	C	91	LEU
3	C	94	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	119	ARG
3	C	143	GLU
3	C	153	VAL
3	C	167	TRP
3	C	175	LEU
3	C	178	LEU
3	C	188	LEU
3	C	196	LEU
3	C	207	VAL
4	D	8	VAL
4	D	10	ARG
4	D	19	LEU
4	D	28	SER

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Mol	Chain	Res	Type
4	D	35	ARG
4	D	36	ARG
4	D	49	ARG
4	D	50	ARG
4	D	53	ASP
4	D	64	LEU
4	D	76	ARG
4	D	78	LEU
4	D	86	LYS
4	D	96	LEU
4	D	107	ARG
4	D	122	ARG
4	D	127	THR
4	D	141	ARG
4	D	151	LYS
4	D	152	SER
4	D	160	GLN
4	D	175	SER
4	D	178	VAL
4	D	187	ARG
4	D	191	ARG
4	D	194	LEU
4	D	201	GLN
5	E	12	LEU
5	E	14	ARG
5	E	15	ARG
5	E	18	ARG
5	E	20	GLN
5	E	31	LEU
5	E	41	VAL
5	E	43	LEU
5	E	63	ARG
5	E	64	ARG
5	E	68	GLU
5	E	79	GLU
5	E	80	ILE
5	E	82	VAL
5	E	125	SER
5	E	131	ILE
5	E	147	ASP
5	E	151	LEU
6	F	3	ARG

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Mol	Chain	Res	Type
6	F	10	LEU
6	F	15	ASP
6	F	19	LEU
6	F	24	GLU
6	F	32	ASN
6	F	43	LEU
6	F	70	ASP
6	F	95	GLU
7	G	4	ARG
7	G	5	ARG
7	G	6	ARG
7	G	12	LEU
7	G	41	ARG
7	G	56	GLN
7	G	84	ASN
7	G	90	GLU
7	G	113	GLU
7	G	115	ARG
8	H	11	THR
8	H	23	SER
8	H	63	LEU
8	H	68	ARG
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	93	VAL
8	H	98	LYS
9	I	12	GLU
9	I	18	PHE
9	I	26	VAL
9	I	27	THR
9	I	29	ASN
9	I	40	LEU
9	I	41	VAL
9	I	53	VAL
9	I	59	PHE
9	I	79	LEU
9	I	95	LYS
9	I	118	LYS
9	I	127	LYS
9	I	128	ARG
10	J	5	ARG

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Mol	Chain	Res	Type
10	J	8	LEU
10	J	15	THR
10	J	28	ARG
10	J	38	ILE
10	J	40	LEU
10	J	55	LYS
10	J	57	LYS
10	J	62	HIS
10	J	79	ARG
10	J	96	ILE
10	J	97	GLU
10	J	98	ILE
11	K	12	ARG
11	K	14	VAL
11	K	18	ARG
11	K	29	ILE
11	K	40	ILE
11	K	41	THR
11	K	54	ARG
11	K	75	TYR
11	K	98	LEU
11	K	109	VAL
12	L	6	THR
12	L	15	ARG
12	L	20	LYS
12	L	33	ARG
12	L	43	VAL
12	L	44	THR
12	L	47	LYS
12	L	53	ARG
12	L	58	VAL
12	L	59	ARG
12	L	67	THR
12	L	75	HIS
12	L	79	GLU
12	L	80	HIS
12	L	91	LYS
12	L	104	VAL
12	L	112	ASP
12	L	126	LYS
13	M	12	ASN
13	M	34	LEU

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Mol	Chain	Res	Type
13	M	45	VAL
13	M	54	VAL
13	M	56	LEU
13	M	70	LEU
13	M	79	LYS
13	M	81	LEU
13	M	82	MET
13	M	84	ILE
13	M	106	ASN
13	M	109	THR
13	M	110	ARG
13	M	114	ARG
14	N	6	LEU
14	N	8	GLU
14	N	22	THR
14	N	24	CYS
14	N	25	VAL
14	N	31	ARG
14	N	39	LEU
14	N	42	ILE
14	N	49	HIS
14	N	53	LEU
15	O	4	THR
15	O	5	LYS
15	O	24	SER
15	O	31	LEU
15	O	32	LEU
15	O	34	LEU
15	O	35	ARG
15	O	39	LEU
15	O	47	LYS
15	O	65	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
16	P	1	MET
16	P	61	SER
16	P	68	ASP
16	P	82	GLN
17	Q	38	ARG
17	Q	59	ILE
17	Q	75	ARG

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Mol	Chain	Res	Type
17	Q	85	VAL
18	R	21	LYS
18	R	68	LYS
18	R	69	THR
18	R	84	LYS
18	R	86	VAL
19	S	5	LEU
19	S	7	LYS
19	S	15	LEU
19	S	36	ARG
19	S	43	GLU
19	S	48	THR
19	S	58	VAL
19	S	60	VAL
19	S	71	LEU
20	T	13	LEU
20	T	19	SER
20	T	36	LEU
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	84	LEU
20	T	91	LEU
20	T	99	LEU
20	T	100	ILE
21	U	8	THR
21	U	9	ARG
21	U	15	ARG
21	U	22	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	204	ASN
9	I	73	GLN
9	I	124	GLN
12	L	75	HIS
16	P	16	HIS
17	Q	29	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	259 (17%)	38 (2%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	81	U
1	A	88	A
1	A	91	C
1	A	101	A
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	145	G
1	A	163	C
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	231	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C

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Mol	Chain	Res	Type
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	345	C
1	A	348	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	371	G
1	A	372	C
1	A	373	A
1	A	384	G
1	A	392	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	424	G
1	A	429	U
1	A	439	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	496	A
1	A	497	A
1	A	498	U
1	A	504	C
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	7MG
1	A	532	A

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Mol	Chain	Res	Type
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	563	A
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	581	G
1	A	588	G
1	A	596	C
1	A	616	G
1	A	618	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	721	G
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	773	G
1	A	774	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	810	C
1	A	813	U
1	A	817	C

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Mol	Chain	Res	Type
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	855	G
1	A	858	G
1	A	859	A
1	A	874	G
1	A	887	G
1	A	902	G
1	A	913	A
1	A	914	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	969	A
1	A	971	G
1	A	974	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1008	C
1	A	1009	G
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1045	C
1	A	1050	G

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Mol	Chain	Res	Type
1	A	1054	C
1	A	1060	C
1	A	1061	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1164	G
1	A	1171	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A
1	A	1202	G
1	A	1204	A
1	A	1212	U

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Mol	Chain	Res	Type
1	A	1213	A
1	A	1225	A
1	A	1238	A
1	A	1243	C
1	A	1257	U
1	A	1258	G
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G
1	A	1305	G
1	A	1310	G
1	A	1319	A
1	A	1320	C
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	1358	U
1	A	1362	C
1	A	1368	G
1	A	1381	U
1	A	1394	A
1	A	1398	A
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1487	G
1	A	1490	C

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Mol	Chain	Res	Type
1	A	1491	G
1	A	1497	G
1	A	1498	UR3
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1532	U

All (38) 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	250	A
1	A	328	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	532	A
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	960	U
1	A	992	U
1	A	1065	U

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Mol	Chain	Res	Type
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1203	C
1	A	1285	A
1	A	1300	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

14 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	MA6	A	1518	1	19,26,27	1.28	2 (10%)	18,38,41	1.21	2 (11%)
1	7MG	A	527	1	22,26,27	4.91	4 (18%)	29,39,42	2.11	9 (31%)
1	MA6	A	1519	1	19,26,27	1.38	4 (21%)	18,38,41	0.59	0
1	UR3	A	1498	1	19,22,23	0.79	1 (5%)	26,32,35	1.00	1 (3%)
1	5MC	A	1407	1	18,22,23	1.17	2 (11%)	26,32,35	1.14	3 (11%)
1	PSU	A	516	23,1	18,21,22	1.04	1 (5%)	22,30,33	1.83	6 (27%)
1	2MG	A	1207	1	18,26,27	1.54	3 (16%)	16,38,41	1.43	2 (12%)
1	4OC	A	1402	1	20,23,24	0.89	1 (5%)	26,32,35	0.87	1 (3%)
1	M2G	A	966	1	20,27,28	1.22	3 (15%)	22,40,43	1.30	3 (13%)
1	PSU	A	1540	1	18,21,22	1.11	1 (5%)	22,30,33	1.69	4 (18%)
1	PSU	A	1541	1	18,21,22	1.10	1 (5%)	22,30,33	1.67	3 (13%)
1	5MC	A	967	1	18,22,23	0.89	1 (5%)	26,32,35	0.86	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	1400	1	18,22,23	1.15	3 (16%)	26,32,35	1.04	2 (7%)
1	5MC	A	1404	1	18,22,23	0.95	2 (11%)	26,32,35	0.96	2 (7%)

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	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	MA6	A	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	23,1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	A	1402	1	-	2/9/29/30	0/2/2/2
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-21.88	1.33	1.46
1	A	527	7MG	C5-N7	4.37	1.40	1.35
1	A	527	7MG	C2-N2	4.28	1.44	1.34
1	A	1207	2MG	C6-N1	4.03	1.43	1.37
1	A	1518	MA6	C6-N1	3.73	1.38	1.33
1	A	1541	PSU	C6-C5	3.69	1.39	1.35
1	A	1519	MA6	C6-N1	3.69	1.38	1.33
1	A	1540	PSU	C6-C5	3.62	1.39	1.35
1	A	1207	2MG	C2-N1	3.23	1.41	1.36
1	A	1407	5MC	C2-N1	3.16	1.46	1.40
1	A	516	PSU	C6-C5	3.07	1.38	1.35
1	A	966	M2G	C6-N1	2.98	1.42	1.37
1	A	1207	2MG	C2-N2	2.93	1.39	1.33
1	A	1402	4OC	C2-N3	2.85	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1400	5MC	C6-C5	2.77	1.39	1.34
1	A	966	M2G	C2-N3	2.62	1.33	1.30
1	A	1519	MA6	C2-N3	2.59	1.36	1.32
1	A	967	5MC	C2-N3	2.57	1.41	1.36
1	A	1518	MA6	C2-N1	2.53	1.38	1.33
1	A	527	7MG	C4-N3	2.42	1.40	1.34
1	A	1400	5MC	C2-N1	2.38	1.45	1.40
1	A	1404	5MC	C2-N3	2.38	1.41	1.36
1	A	1519	MA6	C4-N3	2.35	1.38	1.35
1	A	1400	5MC	C2-N3	2.25	1.40	1.36
1	A	1519	MA6	C2-N1	2.25	1.38	1.33
1	A	1407	5MC	C2-N3	2.08	1.40	1.36
1	A	1498	UR3	C2-N1	2.07	1.41	1.38
1	A	1404	5MC	C2-N1	2.06	1.44	1.40
1	A	966	M2G	C5-C6	-2.01	1.43	1.47

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C5-C6-N1	4.99	119.79	110.99
1	A	527	7MG	N9-C4-N3	4.86	132.73	125.47
1	A	516	PSU	C4-N3-C2	-4.67	119.61	126.34
1	A	516	PSU	N1-C2-N3	4.46	120.19	115.13
1	A	1541	PSU	C4-N3-C2	-4.44	119.94	126.34
1	A	1540	PSU	C4-N3-C2	-4.37	120.04	126.34
1	A	527	7MG	C2-N3-C4	4.32	119.99	112.30
1	A	1540	PSU	N1-C2-N3	4.26	119.96	115.13
1	A	1207	2MG	O6-C6-N1	-4.25	115.63	120.65
1	A	527	7MG	C5-C4-N3	-4.20	120.13	128.13
1	A	1541	PSU	N1-C2-N3	4.17	119.86	115.13
1	A	966	M2G	O6-C6-N1	-3.67	116.31	120.65
1	A	527	7MG	N9-C8-N7	3.49	108.37	103.38
1	A	966	M2G	O6-C6-C5	3.39	131.00	124.37
1	A	1207	2MG	O6-C6-C5	3.36	130.94	124.37
1	A	1518	MA6	C1'-N9-C4	-3.20	121.03	126.64
1	A	527	7MG	C2-N1-C6	-3.03	119.58	125.10
1	A	1407	5MC	N4-C4-N3	-2.88	113.23	118.48
1	A	516	PSU	C6-C5-C4	2.69	120.08	118.20
1	A	527	7MG	O6-C6-C5	-2.52	121.35	127.54
1	A	1540	PSU	O2-C2-N1	-2.51	120.03	122.79
1	A	516	PSU	O2-C2-N1	-2.48	120.06	122.79
1	A	966	M2G	N1-C2-N2	-2.40	115.99	118.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	527	7MG	C6-C5-N7	2.40	135.68	131.91
1	A	1541	PSU	O2-C2-N1	-2.36	120.19	122.79
1	A	1400	5MC	C5-C4-N3	2.36	124.22	121.67
1	A	1518	MA6	N1-C6-N6	-2.30	114.63	117.06
1	A	1404	5MC	N4-C4-N3	-2.30	114.28	118.48
1	A	1540	PSU	C6-N1-C2	-2.30	120.33	122.68
1	A	527	7MG	C6-C5-C4	-2.29	117.91	122.62
1	A	1400	5MC	N4-C4-N3	-2.28	114.33	118.48
1	A	1498	UR3	C6-N1-C2	-2.25	119.77	121.79
1	A	967	5MC	N4-C4-N3	-2.24	114.40	118.48
1	A	1407	5MC	C5-C4-N3	2.20	124.05	121.67
1	A	1404	5MC	C5-C4-N3	2.17	124.01	121.67
1	A	1402	4OC	C5-C4-N4	-2.15	118.23	122.61
1	A	1407	5MC	O2-C2-N3	-2.11	118.91	122.33
1	A	516	PSU	C6-N1-C2	-2.07	120.57	122.68
1	A	516	PSU	O4'-C1'-C2'	2.02	108.00	105.14
1	A	967	5MC	C5-C4-N3	2.01	123.84	121.67

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM1
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C9
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	966	M2G	N3-C2-N2-CM2
1	A	966	M2G	N1-C2-N2-CM2
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519	MA6	C5-C6-N6-C10
1	A	1402	4OC	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	527	7MG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1407	5MC	1	0
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 249 ligands modelled in this entry, 248 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
22	SRY	A	1601	-	40,42,42	2.31	9 (22%)	49,63,63	1.71	9 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	SRY	A	1601	-	-	4/20/87/87	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	CD1-N31	9.19	1.49	1.33
22	A	1601	SRY	CA1-N11	6.98	1.45	1.33
22	A	1601	SRY	O53-C53	-3.49	1.35	1.44
22	A	1601	SRY	O51-C51	-2.57	1.36	1.43
22	A	1601	SRY	CA1-NB1	2.50	1.45	1.34
22	A	1601	SRY	CD1-NE1	2.44	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	O32-C32	-2.43	1.40	1.44
22	A	1601	SRY	C23-N23	-2.42	1.43	1.47
22	A	1601	SRY	O43-C43	-2.15	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C12-O42-C42	-5.33	99.99	108.38
22	A	1601	SRY	C61-C11-N11	-4.54	102.04	110.62
22	A	1601	SRY	C13-O13-C22	-3.54	110.10	116.25
22	A	1601	SRY	O41-C12-O42	-3.26	107.90	111.43
22	A	1601	SRY	C13-O53-C53	-3.24	107.34	113.69
22	A	1601	SRY	O13-C13-C23	2.68	112.86	108.24
22	A	1601	SRY	O42-C42-C32	2.66	108.14	104.33
22	A	1601	SRY	CH2-C42-C32	-2.47	112.28	116.65
22	A	1601	SRY	O42-C12-C22	-2.05	105.08	107.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1601	SRY	C61-C11-N11-CA1
22	A	1601	SRY	C21-C11-N11-CA1
22	A	1601	SRY	C13-C23-N23-CI3
22	A	1601	SRY	C21-C31-N31-CD1

There are no ring outliers.

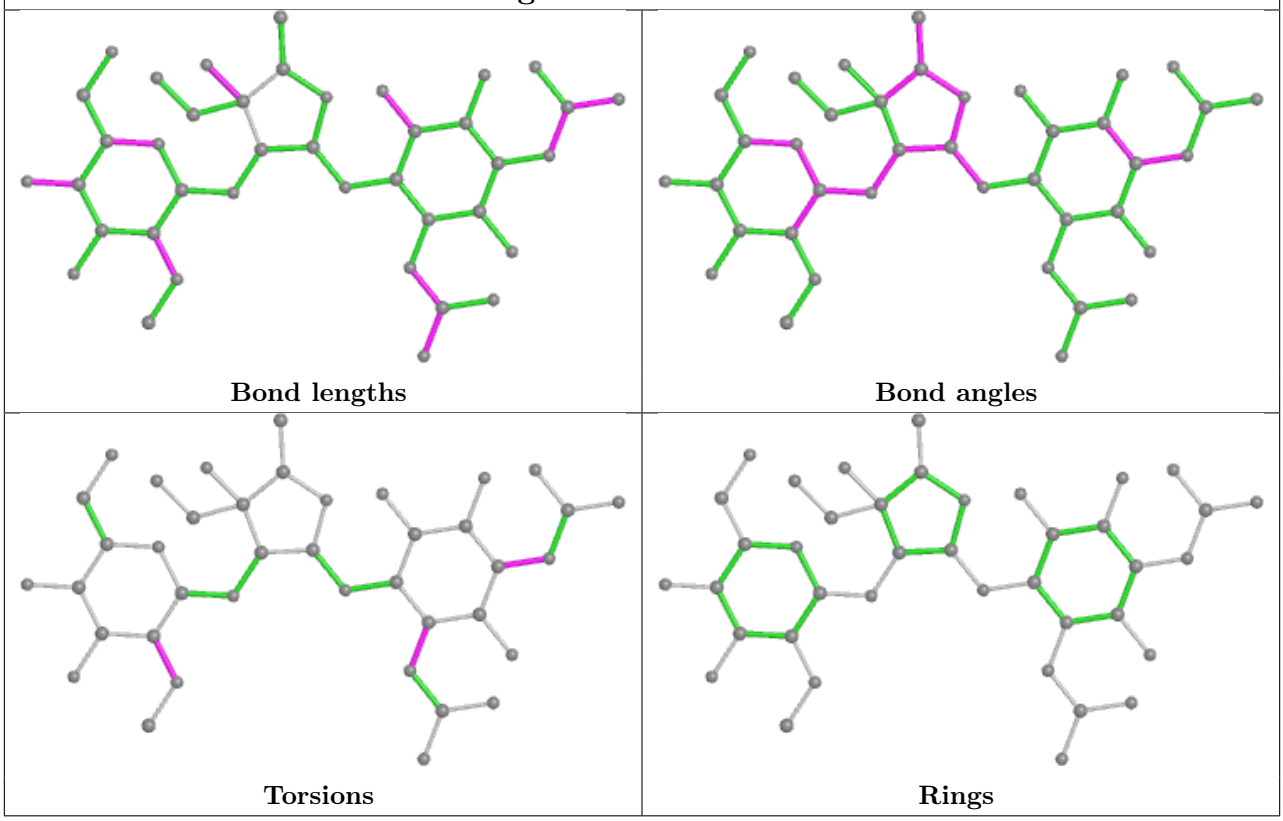
1 monomer is involved in 4 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand SRY A 1601



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	1497/1522 (98%)	-0.32	17 (1%) 80 84	75, 126, 254, 372	0
2	B	234/256 (91%)	-0.35	2 (0%) 84 87	102, 148, 210, 229	0
3	C	206/239 (86%)	0.28	22 (10%) 6 7	130, 188, 244, 266	0
4	D	208/209 (99%)	-0.23	1 (0%) 91 93	90, 129, 167, 202	0
5	E	150/162 (92%)	-0.40	0 100 100	79, 107, 143, 204	0
6	F	101/101 (100%)	-0.40	1 (0%) 82 86	111, 155, 184, 234	0
7	G	155/156 (99%)	0.04	12 (7%) 13 15	120, 170, 221, 244	0
8	H	138/138 (100%)	-0.39	0 100 100	73, 99, 132, 167	0
9	I	127/128 (99%)	0.23	8 (6%) 20 22	132, 195, 242, 259	0
10	J	98/105 (93%)	0.84	19 (19%) 1 1	126, 214, 306, 335	0
11	K	116/129 (89%)	-0.36	0 100 100	98, 130, 174, 208	0
12	L	124/135 (91%)	-0.20	2 (1%) 72 74	74, 122, 159, 213	0
13	M	118/126 (93%)	0.02	7 (5%) 22 25	119, 153, 193, 258	0
14	N	60/61 (98%)	0.68	10 (16%) 1 2	149, 175, 240, 282	0
15	O	87/89 (97%)	-0.36	1 (1%) 80 84	82, 117, 154, 175	0
16	P	83/88 (94%)	-0.32	0 100 100	92, 121, 150, 183	0
17	Q	99/105 (94%)	-0.37	1 (1%) 82 86	80, 108, 144, 168	0
18	R	70/88 (79%)	-0.33	0 100 100	100, 131, 181, 209	0
19	S	80/93 (86%)	0.73	10 (12%) 3 4	149, 204, 249, 280	0
20	T	99/106 (93%)	-0.35	1 (1%) 82 86	96, 127, 179, 211	0
21	U	24/27 (88%)	2.04	9 (37%) 0 0	131, 162, 193, 205	0
All	All	3874/4063 (95%)	-0.17	123 (3%) 47 50	73, 137, 230, 372	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	65	ALA	9.9
21	U	25	LYS	8.5
19	S	38	SER	7.4
10	J	34	VAL	7.2
21	U	18	TYR	6.8
10	J	37	PRO	6.6
3	C	66	VAL	6.1
3	C	103	VAL	5.9
1	A	1129	C	5.2
13	M	117	VAL	5.2
14	N	11	LYS	4.9
3	C	193	TYR	4.8
10	J	74	ILE	4.7
7	G	156	TRP	4.6
21	U	17	THR	4.6
19	S	39	THR	4.5
3	C	155	GLY	4.4
13	M	7	VAL	4.2
7	G	154	TYR	4.2
9	I	128	ARG	4.1
14	N	18	VAL	4.1
10	J	4	ILE	4.1
14	N	4	LYS	3.7
1	A	1037	C	3.5
10	J	24	VAL	3.5
10	J	38	ILE	3.5
13	M	116	THR	3.4
7	G	81	GLY	3.4
10	J	32	ALA	3.4
21	U	23	PRO	3.4
19	S	44	MET	3.3
1	A	1020	U	3.3
9	I	102	LEU	3.3
21	U	24	ARG	3.2
1	A	1036	G	3.2
1	A	1019	C	3.2
21	U	9	ARG	3.2
1	A	994	A	3.2
1	A	1006	C	3.1
7	G	7	ALA	3.1
10	J	100	THR	3.1
7	G	5	ARG	3.1
1	A	1257	U	3.1

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Mol	Chain	Res	Type	RSRZ
10	J	88	LEU	3.1
14	N	3	ARG	3.1
7	G	83	ALA	3.0
9	I	8	GLY	3.0
10	J	33	GLN	3.0
1	A	1007	C	3.0
14	N	6	LEU	3.0
1	A	1005	A	2.9
10	J	73	ASP	2.9
14	N	20	ALA	2.9
10	J	90	LEU	2.9
19	S	69	HIS	2.9
3	C	87	LEU	2.9
20	T	106	ALA	2.9
1	A	1539	C	2.8
14	N	2	ALA	2.8
13	M	2	ALA	2.7
21	U	22	ARG	2.7
10	J	96	ILE	2.7
7	G	82	GLY	2.7
19	S	41	VAL	2.7
7	G	2	ALA	2.7
9	I	9	ARG	2.6
10	J	5	ARG	2.6
3	C	80	GLY	2.6
1	A	81	U	2.6
3	C	83	ARG	2.6
2	B	231	GLU	2.6
10	J	99	LYS	2.6
1	A	1018	C	2.6
10	J	89	ASP	2.6
19	S	40	ILE	2.6
9	I	96	LEU	2.5
7	G	8	GLU	2.5
10	J	39	PRO	2.5
7	G	79	ARG	2.5
17	Q	99	SER	2.5
3	C	156	ARG	2.5
21	U	5	ASP	2.4
10	J	98	ILE	2.4
3	C	102	ASN	2.4
19	S	27	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	68	VAL	2.4
1	A	1124	G	2.4
13	M	6	GLY	2.4
6	F	101	ALA	2.4
14	N	61	TRP	2.4
3	C	79	ARG	2.4
3	C	104	GLN	2.3
1	A	1033	G	2.3
3	C	82	GLU	2.3
9	I	4	TYR	2.3
3	C	196	LEU	2.2
4	D	9	CYS	2.2
19	S	15	LEU	2.2
2	B	232	PRO	2.2
1	A	1022	G	2.2
21	U	11	GLY	2.2
3	C	78	GLY	2.2
3	C	206	GLU	2.2
3	C	58	GLU	2.2
1	A	993	G	2.1
13	M	118	ALA	2.1
3	C	85	ARG	2.1
15	O	88	ARG	2.1
14	N	5	ALA	2.1
12	L	19	ARG	2.1
12	L	114	LYS	2.1
19	S	28	LYS	2.1
13	M	100	GLY	2.1
9	I	46	ALA	2.1
10	J	20	ALA	2.1
14	N	28	GLY	2.1
7	G	62	PHE	2.0
7	G	78	ARG	2.0
3	C	101	LEU	2.0
3	C	157	ILE	2.0
3	C	146	ALA	2.0
9	I	33	PHE	2.0
19	S	59	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.69	0.52	307,319,331,332	0
1	PSU	A	1540	20/21	0.71	0.72	293,304,328,333	0
1	2MG	A	1207	24/25	0.86	0.27	166,200,208,210	0
1	5MC	A	1407	21/22	0.92	0.17	143,156,168,170	0
1	5MC	A	1404	21/22	0.94	0.20	112,125,133,135	0
1	M2G	A	966	25/26	0.95	0.17	128,130,135,137	0
1	5MC	A	967	21/22	0.95	0.15	117,134,142,143	0
1	UR3	A	1498	21/22	0.95	0.20	107,119,127,139	0
1	MA6	A	1518	24/25	0.95	0.16	114,128,149,156	0
1	PSU	A	516	20/21	0.95	0.11	114,120,134,135	0
1	5MC	A	1400	21/22	0.95	0.16	96,119,128,133	0
1	MA6	A	1519	24/25	0.97	0.13	109,131,137,140	0
1	7MG	A	527	24/25	0.97	0.15	102,107,117,124	0
1	4OC	A	1402	22/23	0.97	0.19	105,113,122,124	0

6.3 Carbohydrates (i)

There are no monosaccharides 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
23	MG	A	1767	1/1	0.38	0.38	119,119,119,119	0
23	MG	A	1723	1/1	0.42	0.66	111,111,111,111	0
23	MG	A	1801	1/1	0.48	0.31	114,114,114,114	0
23	MG	A	1831	1/1	0.51	0.34	130,130,130,130	0
23	MG	A	1807	1/1	0.59	0.81	120,120,120,120	0
23	MG	A	1633	1/1	0.59	0.59	122,122,122,122	0
23	MG	A	1682	1/1	0.60	0.46	106,106,106,106	0
23	MG	A	1787	1/1	0.61	0.58	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1815	1/1	0.62	0.55	113,113,113,113	0
23	MG	A	1666	1/1	0.63	0.24	133,133,133,133	0
23	MG	A	1638	1/1	0.65	0.35	101,101,101,101	0
23	MG	A	1823	1/1	0.66	2.07	143,143,143,143	0
23	MG	A	1652	1/1	0.66	0.33	118,118,118,118	0
23	MG	A	1731	1/1	0.67	0.30	126,126,126,126	0
23	MG	A	1777	1/1	0.67	0.20	135,135,135,135	0
23	MG	L	201	1/1	0.67	0.23	123,123,123,123	0
23	MG	P	102	1/1	0.67	0.54	125,125,125,125	0
23	MG	Q	202	1/1	0.68	0.36	89,89,89,89	0
23	MG	A	1771	1/1	0.69	0.43	111,111,111,111	0
23	MG	A	1785	1/1	0.70	0.18	154,154,154,154	0
23	MG	A	1679	1/1	0.70	0.41	112,112,112,112	0
23	MG	A	1743	1/1	0.72	0.37	110,110,110,110	0
23	MG	A	1822	1/1	0.73	0.45	97,97,97,97	0
23	MG	A	1792	1/1	0.73	0.26	120,120,120,120	0
23	MG	A	1757	1/1	0.73	1.11	123,123,123,123	0
23	MG	A	1748	1/1	0.74	0.29	117,117,117,117	0
23	MG	P	101	1/1	0.74	0.42	97,97,97,97	0
23	MG	A	1802	1/1	0.75	0.59	125,125,125,125	0
23	MG	A	1662	1/1	0.75	0.46	126,126,126,126	0
23	MG	A	1800	1/1	0.76	1.05	128,128,128,128	0
23	MG	A	1696	1/1	0.76	0.45	104,104,104,104	0
23	MG	D	303	1/1	0.76	0.15	104,104,104,104	0
23	MG	Q	201	1/1	0.76	0.24	119,119,119,119	0
23	MG	F	201	1/1	0.76	0.16	112,112,112,112	0
23	MG	K	201	1/1	0.77	0.41	100,100,100,100	0
23	MG	A	1710	1/1	0.77	0.53	115,115,115,115	0
23	MG	A	1755	1/1	0.78	0.93	116,116,116,116	0
23	MG	A	1709	1/1	0.78	0.21	253,253,253,253	0
23	MG	A	1816	1/1	0.79	0.29	100,100,100,100	0
23	MG	A	1631	1/1	0.80	0.52	107,107,107,107	0
23	MG	A	1809	1/1	0.80	0.50	132,132,132,132	0
23	MG	A	1754	1/1	0.80	0.46	118,118,118,118	0
23	MG	A	1747	1/1	0.80	0.28	136,136,136,136	0
23	MG	A	1791	1/1	0.80	0.68	155,155,155,155	0
23	MG	A	1827	1/1	0.81	0.26	116,116,116,116	0
23	MG	A	1659	1/1	0.81	0.25	158,158,158,158	0
23	MG	A	1625	1/1	0.81	0.34	134,134,134,134	0
23	MG	A	1717	1/1	0.81	0.33	107,107,107,107	0
23	MG	A	1721	1/1	0.81	0.28	77,77,77,77	0
23	MG	A	1719	1/1	0.82	0.72	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1730	1/1	0.82	0.17	92,92,92,92	0
23	MG	A	1828	1/1	0.82	0.38	122,122,122,122	0
23	MG	A	1644	1/1	0.83	0.33	95,95,95,95	0
23	MG	A	1768	1/1	0.83	0.29	149,149,149,149	0
23	MG	A	1674	1/1	0.83	0.27	128,128,128,128	0
23	MG	A	1683	1/1	0.83	0.64	117,117,117,117	0
23	MG	A	1776	1/1	0.84	0.27	137,137,137,137	0
23	MG	A	1664	1/1	0.84	0.88	96,96,96,96	0
23	MG	A	1762	1/1	0.84	0.14	119,119,119,119	0
23	MG	A	1639	1/1	0.84	0.24	160,160,160,160	0
23	MG	A	1697	1/1	0.84	0.08	166,166,166,166	0
23	MG	A	1814	1/1	0.84	0.34	108,108,108,108	0
23	MG	A	1667	1/1	0.84	0.44	97,97,97,97	0
23	MG	A	1763	1/1	0.85	0.28	146,146,146,146	0
23	MG	A	1733	1/1	0.85	0.14	120,120,120,120	0
23	MG	A	1621	1/1	0.85	0.70	127,127,127,127	0
23	MG	A	1812	1/1	0.85	0.29	117,117,117,117	0
23	MG	A	1778	1/1	0.86	0.16	90,90,90,90	0
23	MG	A	1766	1/1	0.86	0.69	73,73,73,73	0
23	MG	A	1825	1/1	0.86	0.28	126,126,126,126	0
23	MG	A	1813	1/1	0.86	0.42	130,130,130,130	0
23	MG	A	1623	1/1	0.86	0.89	120,120,120,120	0
23	MG	A	1788	1/1	0.86	0.29	124,124,124,124	0
23	MG	A	1760	1/1	0.86	0.97	116,116,116,116	0
23	MG	A	1806	1/1	0.87	0.73	96,96,96,96	0
23	MG	A	1661	1/1	0.87	0.35	110,110,110,110	0
23	MG	A	1669	1/1	0.87	0.18	133,133,133,133	0
23	MG	A	1810	1/1	0.87	0.50	106,106,106,106	0
23	MG	N	102	1/1	0.87	0.40	130,130,130,130	0
23	MG	A	1811	1/1	0.87	0.73	105,105,105,105	0
23	MG	A	1729	1/1	0.87	0.25	110,110,110,110	0
23	MG	A	1774	1/1	0.87	0.31	106,106,106,106	0
23	MG	A	1627	1/1	0.87	0.36	108,108,108,108	0
23	MG	A	1765	1/1	0.88	0.21	126,126,126,126	0
23	MG	A	1779	1/1	0.88	0.14	122,122,122,122	0
23	MG	A	1799	1/1	0.88	0.17	361,361,361,361	0
23	MG	A	1722	1/1	0.88	0.24	106,106,106,106	0
23	MG	D	302	1/1	0.88	0.88	105,105,105,105	0
23	MG	A	1618	1/1	0.88	0.27	109,109,109,109	0
23	MG	A	1678	1/1	0.88	0.19	104,104,104,104	0
23	MG	A	1713	1/1	0.89	0.32	109,109,109,109	0
23	MG	C	301	1/1	0.89	0.05	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1805	1/1	0.89	0.98	123,123,123,123	0
23	MG	A	1753	1/1	0.89	0.25	112,112,112,112	0
23	MG	A	1728	1/1	0.89	0.31	120,120,120,120	0
23	MG	A	1817	1/1	0.89	0.17	113,113,113,113	0
23	MG	A	1819	1/1	0.89	0.27	123,123,123,123	0
23	MG	A	1808	1/1	0.89	0.42	95,95,95,95	0
23	MG	A	1741	1/1	0.89	0.25	125,125,125,125	0
23	MG	A	1628	1/1	0.89	0.10	165,165,165,165	0
23	MG	A	1718	1/1	0.89	0.16	144,144,144,144	0
23	MG	A	1770	1/1	0.89	0.30	114,114,114,114	0
23	MG	A	1675	1/1	0.90	0.35	129,129,129,129	0
23	MG	A	1794	1/1	0.90	0.30	120,120,120,120	0
23	MG	A	1681	1/1	0.90	0.30	146,146,146,146	0
23	MG	A	1734	1/1	0.90	0.51	112,112,112,112	0
23	MG	A	1736	1/1	0.90	0.40	114,114,114,114	0
23	MG	A	1629	1/1	0.90	0.29	103,103,103,103	0
23	MG	H	201	1/1	0.90	0.17	107,107,107,107	0
23	MG	A	1761	1/1	0.91	0.18	117,117,117,117	0
23	MG	A	1665	1/1	0.91	0.40	117,117,117,117	0
23	MG	A	1698	1/1	0.91	0.12	136,136,136,136	0
23	MG	A	1705	1/1	0.91	0.10	82,82,82,82	0
23	MG	A	1673	1/1	0.91	0.26	148,148,148,148	0
23	MG	A	1797	1/1	0.91	0.34	126,126,126,126	0
23	MG	A	1605	1/1	0.92	0.51	118,118,118,118	0
23	MG	A	1720	1/1	0.92	0.11	165,165,165,165	0
23	MG	A	1660	1/1	0.92	0.14	154,154,154,154	0
23	MG	A	1783	1/1	0.92	0.29	319,319,319,319	0
23	MG	A	1824	1/1	0.92	0.85	118,118,118,118	0
23	MG	A	1737	1/1	0.92	0.20	128,128,128,128	0
23	MG	A	1804	1/1	0.92	1.12	116,116,116,116	0
23	MG	A	1781	1/1	0.93	0.17	200,200,200,200	0
23	MG	B	302	1/1	0.93	0.27	168,168,168,168	0
23	MG	A	1782	1/1	0.93	0.20	264,264,264,264	0
23	MG	A	1650	1/1	0.93	0.21	107,107,107,107	0
23	MG	A	1769	1/1	0.93	0.21	115,115,115,115	0
23	MG	E	201	1/1	0.93	0.07	140,140,140,140	0
23	MG	A	1746	1/1	0.93	0.17	85,85,85,85	0
23	MG	A	1640	1/1	0.93	0.12	67,67,67,67	0
23	MG	A	1677	1/1	0.93	0.18	244,244,244,244	0
23	MG	A	1751	1/1	0.93	0.10	89,89,89,89	0
23	MG	A	1603	1/1	0.93	0.13	126,126,126,126	0
23	MG	A	1707	1/1	0.93	0.23	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1798	1/1	0.93	0.28	129,129,129,129	0
23	MG	A	1685	1/1	0.93	0.31	173,173,173,173	0
23	MG	A	1830	1/1	0.93	0.42	107,107,107,107	0
23	MG	A	1727	1/1	0.94	0.41	91,91,91,91	0
23	MG	A	1663	1/1	0.94	0.14	113,113,113,113	0
23	MG	A	1773	1/1	0.94	0.12	109,109,109,109	0
23	MG	A	1786	1/1	0.94	0.26	115,115,115,115	0
23	MG	A	1764	1/1	0.94	0.10	123,123,123,123	0
23	MG	A	1630	1/1	0.94	0.54	102,102,102,102	0
23	MG	A	1657	1/1	0.94	0.20	88,88,88,88	0
23	MG	A	1642	1/1	0.94	0.17	113,113,113,113	0
23	MG	A	1694	1/1	0.94	0.29	116,116,116,116	0
23	MG	A	1725	1/1	0.94	0.71	120,120,120,120	0
23	MG	A	1820	1/1	0.94	0.38	92,92,92,92	0
23	MG	A	1832	1/1	0.95	0.17	132,132,132,132	0
23	MG	A	1711	1/1	0.95	0.15	103,103,103,103	0
23	MG	A	1790	1/1	0.95	0.24	142,142,142,142	0
23	MG	A	1818	1/1	0.95	0.13	134,134,134,134	0
23	MG	A	1671	1/1	0.95	0.28	115,115,115,115	0
23	MG	A	1622	1/1	0.95	0.16	94,94,94,94	0
23	MG	A	1643	1/1	0.95	0.28	77,77,77,77	0
23	MG	A	1742	1/1	0.95	0.27	94,94,94,94	0
23	MG	A	1758	1/1	0.95	0.17	111,111,111,111	0
23	MG	A	1706	1/1	0.95	0.30	159,159,159,159	0
23	MG	A	1688	1/1	0.95	0.20	120,120,120,120	0
23	MG	A	1680	1/1	0.95	0.14	125,125,125,125	0
23	MG	A	1829	1/1	0.95	0.52	114,114,114,114	0
23	MG	A	1651	1/1	0.95	0.25	76,76,76,76	0
23	MG	A	1803	1/1	0.95	0.39	110,110,110,110	0
23	MG	A	1744	1/1	0.96	0.30	99,99,99,99	0
23	MG	B	301	1/1	0.96	0.29	125,125,125,125	0
23	MG	A	1672	1/1	0.96	0.08	134,134,134,134	0
23	MG	A	1732	1/1	0.96	0.35	87,87,87,87	0
23	MG	A	1789	1/1	0.96	0.10	125,125,125,125	0
23	MG	A	1649	1/1	0.96	0.16	106,106,106,106	0
23	MG	A	1821	1/1	0.96	0.44	135,135,135,135	0
23	MG	A	1687	1/1	0.96	0.59	179,179,179,179	0
23	MG	A	1752	1/1	0.96	0.20	87,87,87,87	0
23	MG	A	1726	1/1	0.96	0.24	120,120,120,120	0
23	MG	A	1795	1/1	0.96	0.64	79,79,79,79	0
23	MG	A	1612	1/1	0.96	0.14	127,127,127,127	0
23	MG	A	1690	1/1	0.96	0.33	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1604	1/1	0.96	0.21	107,107,107,107	0
23	MG	A	1784	1/1	0.96	0.13	119,119,119,119	0
23	MG	A	1646	1/1	0.96	0.27	103,103,103,103	0
24	ZN	N	101	1/1	0.96	0.19	166,166,166,166	0
23	MG	A	1796	1/1	0.97	0.25	98,98,98,98	0
23	MG	A	1645	1/1	0.97	0.09	88,88,88,88	0
23	MG	A	1745	1/1	0.97	0.19	100,100,100,100	0
23	MG	A	1676	1/1	0.97	0.17	106,106,106,106	0
23	MG	A	1826	1/1	0.97	0.21	82,82,82,82	0
23	MG	A	1772	1/1	0.97	0.40	101,101,101,101	0
23	MG	A	1617	1/1	0.97	0.31	112,112,112,112	0
23	MG	A	1647	1/1	0.97	0.24	143,143,143,143	0
23	MG	A	1724	1/1	0.97	0.10	140,140,140,140	0
23	MG	A	1699	1/1	0.97	0.10	108,108,108,108	0
23	MG	A	1701	1/1	0.97	0.15	113,113,113,113	0
23	MG	A	1702	1/1	0.97	0.10	138,138,138,138	0
23	MG	A	1780	1/1	0.97	0.06	122,122,122,122	0
23	MG	A	1648	1/1	0.97	0.36	117,117,117,117	0
23	MG	A	1756	1/1	0.97	0.08	153,153,153,153	0
23	MG	A	1635	1/1	0.97	0.15	119,119,119,119	0
23	MG	A	1626	1/1	0.97	0.90	75,75,75,75	0
23	MG	A	1759	1/1	0.97	0.51	88,88,88,88	0
23	MG	A	1609	1/1	0.97	0.14	106,106,106,106	0
23	MG	A	1610	1/1	0.97	0.13	85,85,85,85	0
23	MG	A	1684	1/1	0.97	0.10	114,114,114,114	0
23	MG	A	1712	1/1	0.97	0.15	194,194,194,194	0
23	MG	A	1656	1/1	0.97	0.14	174,174,174,174	0
23	MG	A	1715	1/1	0.97	0.16	116,116,116,116	0
22	SRY	A	1601	40/40	0.97	0.22	93,111,127,129	0
23	MG	A	1613	1/1	0.97	0.11	105,105,105,105	0
23	MG	A	1624	1/1	0.97	0.59	64,64,64,64	0
23	MG	A	1703	1/1	0.98	0.17	141,141,141,141	0
23	MG	A	1616	1/1	0.98	0.19	61,61,61,61	0
23	MG	A	1749	1/1	0.98	0.27	127,127,127,127	0
23	MG	A	1750	1/1	0.98	0.24	120,120,120,120	0
23	MG	A	1775	1/1	0.98	0.14	108,108,108,108	0
23	MG	A	1686	1/1	0.98	0.18	146,146,146,146	0
23	MG	A	1611	1/1	0.98	0.10	179,179,179,179	0
23	MG	A	1708	1/1	0.98	0.26	325,325,325,325	0
23	MG	A	1607	1/1	0.98	0.45	111,111,111,111	0
23	MG	A	1689	1/1	0.98	0.22	202,202,202,202	0
23	MG	A	1653	1/1	0.98	0.10	99,99,99,99	0

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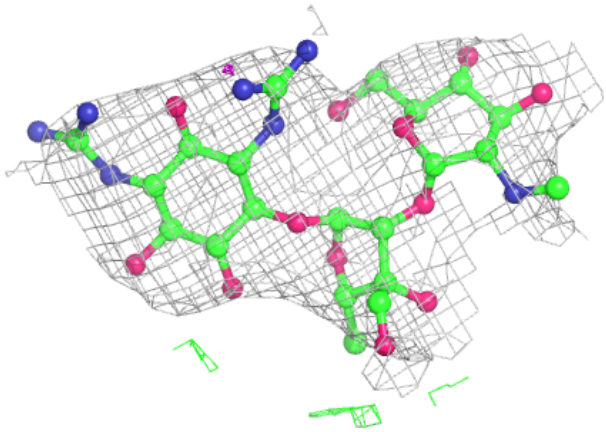
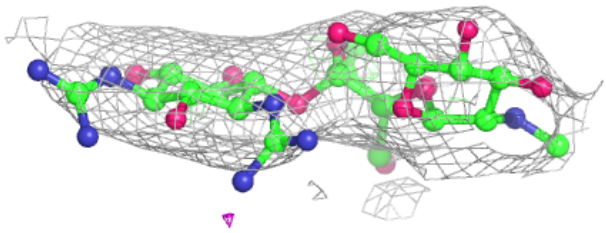
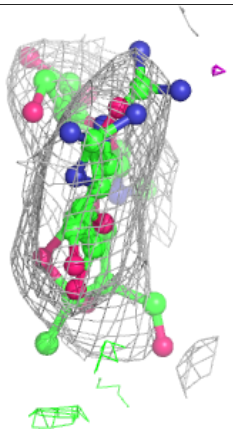
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	MG	A	1693	1/1	0.98	0.12	108,108,108,108	0
23	MG	A	1654	1/1	0.98	0.27	71,71,71,71	0
23	MG	A	1695	1/1	0.98	0.12	144,144,144,144	0
23	MG	A	1735	1/1	0.98	0.11	110,110,110,110	0
23	MG	A	1716	1/1	0.98	0.11	102,102,102,102	0
23	MG	A	1619	1/1	0.98	0.39	117,117,117,117	0
23	MG	A	1738	1/1	0.98	0.11	91,91,91,91	0
23	MG	A	1739	1/1	0.98	0.17	106,106,106,106	0
23	MG	A	1668	1/1	0.98	0.16	116,116,116,116	0
23	MG	A	1620	1/1	0.98	0.20	128,128,128,128	0
23	MG	A	1608	1/1	0.98	0.06	114,114,114,114	0
23	MG	A	1793	1/1	0.98	0.27	92,92,92,92	0
23	MG	A	1700	1/1	0.98	0.16	226,226,226,226	0
23	MG	A	1615	1/1	0.98	0.21	83,83,83,83	0
24	ZN	D	301	1/1	0.98	0.34	102,102,102,102	0
23	MG	A	1641	1/1	0.98	0.11	101,101,101,101	0
23	MG	A	1632	1/1	0.99	0.12	85,85,85,85	0
23	MG	A	1614	1/1	0.99	0.10	98,98,98,98	0
23	MG	A	1740	1/1	0.99	0.14	126,126,126,126	0
23	MG	A	1714	1/1	0.99	0.20	54,54,54,54	0
23	MG	A	1691	1/1	0.99	0.14	136,136,136,136	0
23	MG	A	1692	1/1	0.99	0.21	112,112,112,112	0
23	MG	A	1704	1/1	0.99	0.37	112,112,112,112	0
23	MG	A	1634	1/1	0.99	0.33	133,133,133,133	0
23	MG	A	1606	1/1	0.99	0.09	89,89,89,89	0
23	MG	A	1658	1/1	0.99	0.14	98,98,98,98	0
23	MG	A	1636	1/1	0.99	0.12	97,97,97,97	0
23	MG	A	1637	1/1	0.99	0.28	99,99,99,99	0
23	MG	A	1602	1/1	0.99	0.21	109,109,109,109	0
23	MG	A	1670	1/1	0.99	0.11	105,105,105,105	0
23	MG	A	1655	1/1	1.00	0.09	93,93,93,93	0

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

Electron density around SRY A 1601: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.