Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:59 PM GMT

PDB ID	:	4DR3
Title	:	Crystal structure of the Thermus thermophilus (HB8) 30S ribosomal subunit with streptomycin bound
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-16
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

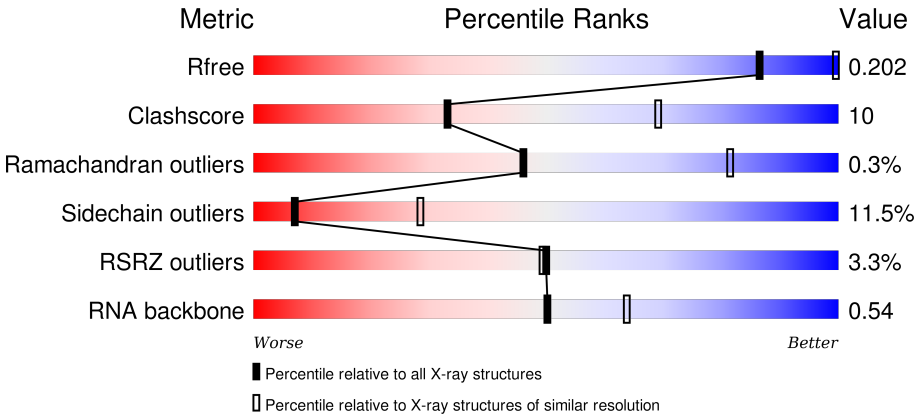
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1004 (3.40-3.28)
Clashscore	102246	1072 (3.40-3.28)
Ramachandran outliers	100387	1055 (3.40-3.28)
Sidechain outliers	100360	1054 (3.40-3.28)
RSRZ outliers	91569	1009 (3.40-3.28)
RNA backbone	2183	1007 (3.88-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	2% 56% 32% 10%
2	B	256	% 57% 30% 9%
3	C	239	7% 51% 28% 7% 14%
4	D	209	3% 71% 25%

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Mol	Chain	Length	Quality of chain
5	E	162	60% 24% 8% 7%
6	F	101	74% 23%
7	G	156	8% 71% 26%
8	H	138	67% 29%
9	I	128	5% 62% 30% 7%
10	J	105	15% 52% 36% 5% 7%
11	K	129	64% 22% 10%
12	L	135	52% 33% 7% 8%
13	M	126	4% 64% 26% 6%
14	N	61	15% 62% 33%
15	O	89	71% 24%
16	P	88	57% 34% 6%
17	Q	105	69% 22% 6%
18	R	88	51% 26% 20%
19	S	93	12% 49% 30% 6% 14%
20	T	106	% 63% 25% 5% 7%
21	U	27	33% 63% 26% 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
23	MG	A	1607	-	-	-	X
23	MG	A	1620	-	-	-	X
23	MG	A	1643	-	-	-	X
23	MG	A	1650	-	-	-	X
23	MG	A	1653	-	-	-	X
23	MG	A	1709	-	-	-	X
23	MG	A	1720	-	-	-	X
23	MG	A	1721	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	MG	A	1725	-	-	-	X
23	MG	A	1732	-	-	-	X
23	MG	A	1734	-	-	-	X
23	MG	A	1735	-	-	-	X
23	MG	A	1739	-	-	-	X
23	MG	A	1742	-	-	-	X
23	MG	A	1751	-	-	-	X
23	MG	A	1752	-	-	-	X
23	MG	A	1755	-	-	-	X
23	MG	A	1757	-	-	-	X
23	MG	A	1777	-	-	-	X
23	MG	A	1787	-	-	-	X
23	MG	A	1798	-	-	-	X
23	MG	A	1813	-	-	-	X
23	MG	A	1817	-	-	-	X
23	MG	A	1835	-	-	-	X
23	MG	A	1836	-	-	-	X
23	MG	A	1838	-	-	-	X
23	MG	A	1845	-	-	-	X
23	MG	B	301	-	-	-	X
23	MG	H	203	-	-	-	X
23	MG	N	102	-	-	-	X
23	MG	T	201	-	-	-	X

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 52164 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	1512	32507	14477	6011	10507	1512	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 30S ribosomal protein S2.

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

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

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

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

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

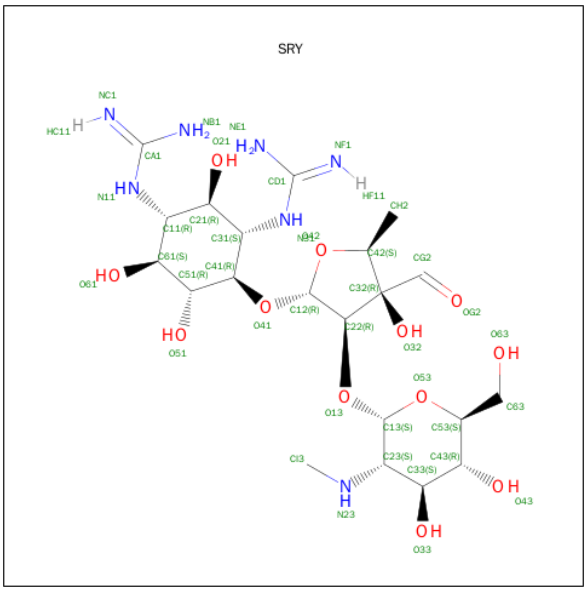
- Molecule 20 is a protein called 30S ribosomal protein S20.

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

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

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

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



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	P	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	Q	2	Total Mg 2 2	0	0
23	D	1	Total Mg 1 1	0	0
23	E	1	Total Mg 1 1	0	0
23	H	3	Total Mg 3 3	0	0
23	B	1	Total Mg 1 1	0	0
23	A	248	Total Mg 248 248	0	0
23	T	2	Total Mg 2 2	0	0
23	N	1	Total Mg 1 1	0	0
23	U	1	Total Mg 1 1	0	0
23	M	1	Total Mg 1 1	0	0

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

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

- Molecule 25 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	256	Total O 256 256	0	0
25	D	1	Total O 1 1	0	0
25	E	2	Total O 2 2	0	0
25	G	1	Total O 1 1	0	0
25	L	1	Total O 1 1	0	0

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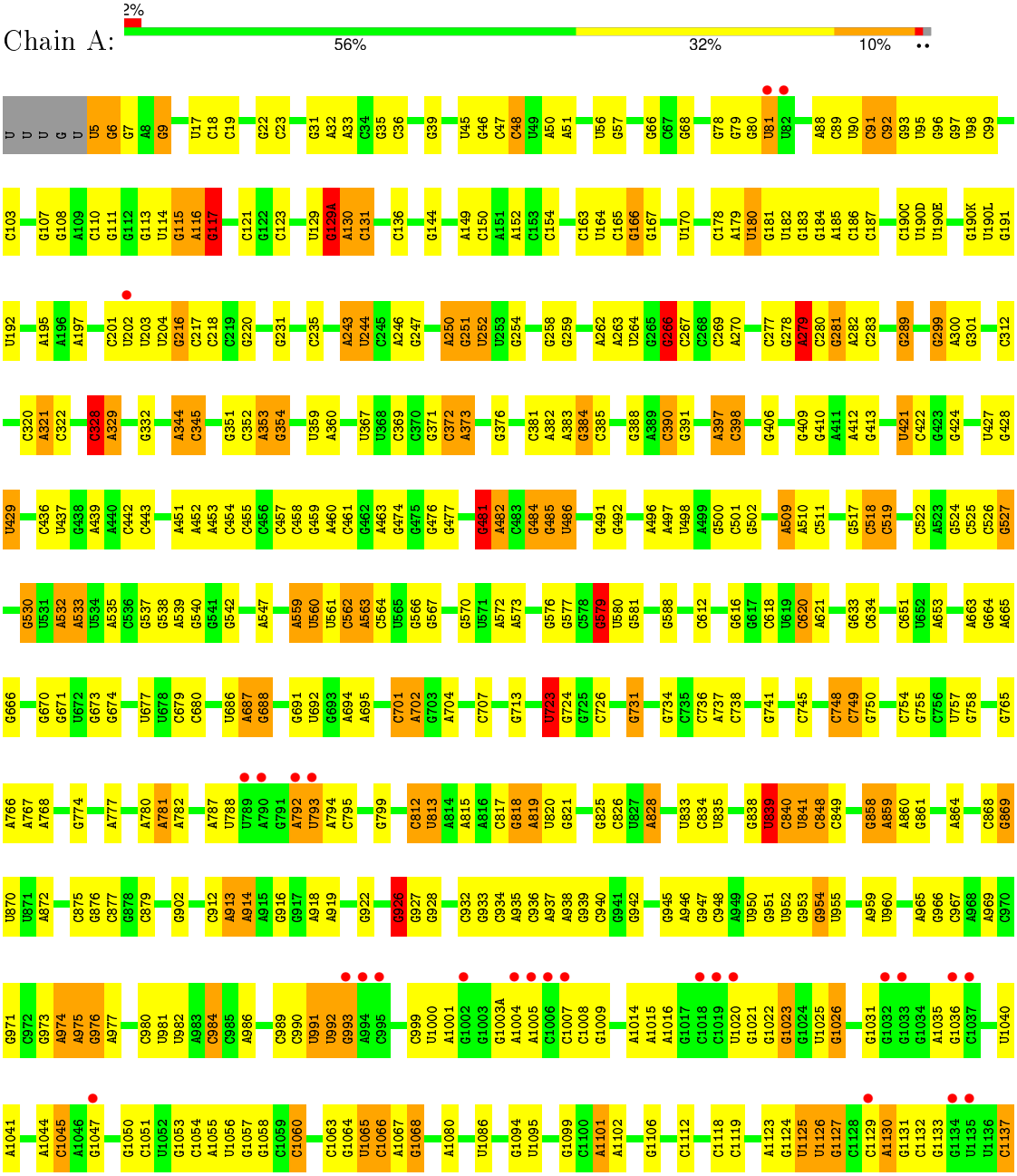
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	N	1	Total O 1 1	0	0
25	U	1	Total O 1 1	0	0

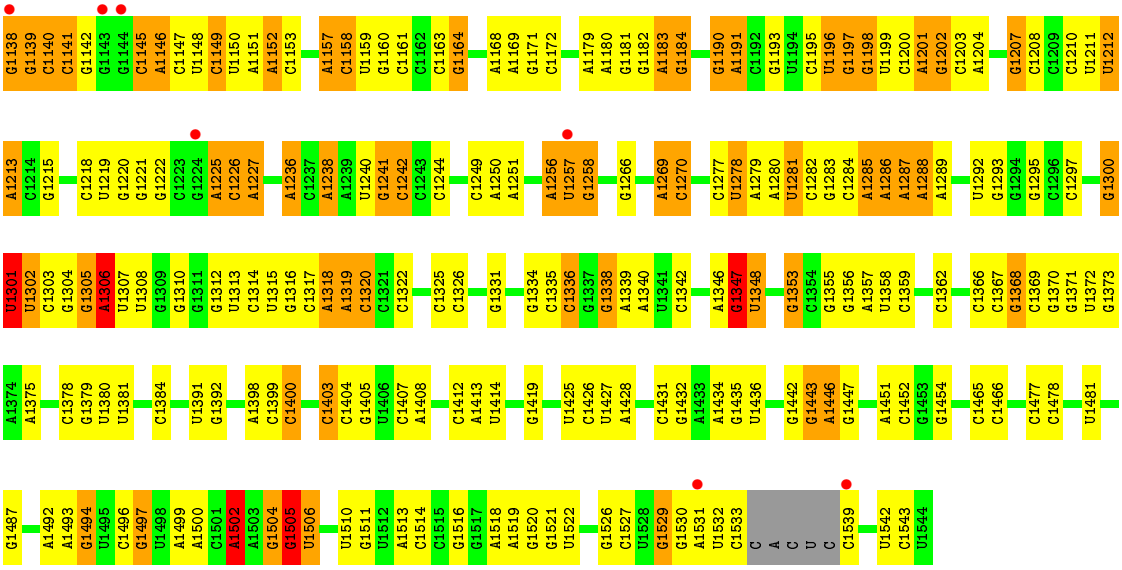
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

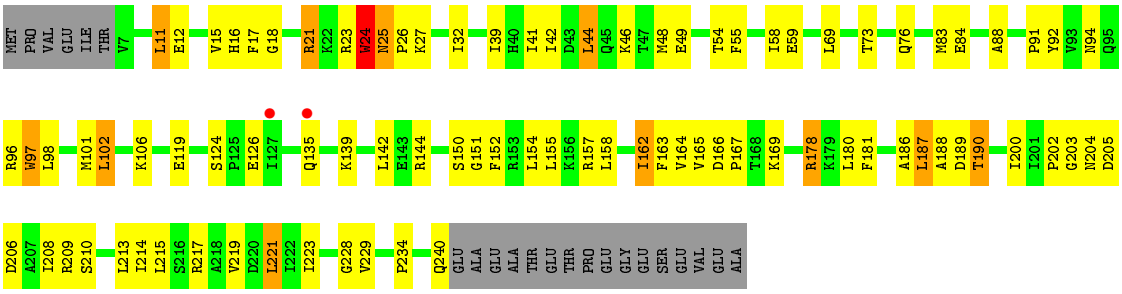
Chain A:





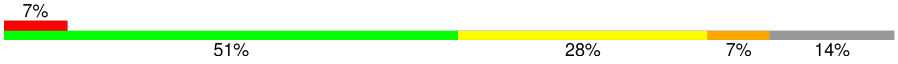
- Molecule 2: 30S ribosomal protein S2

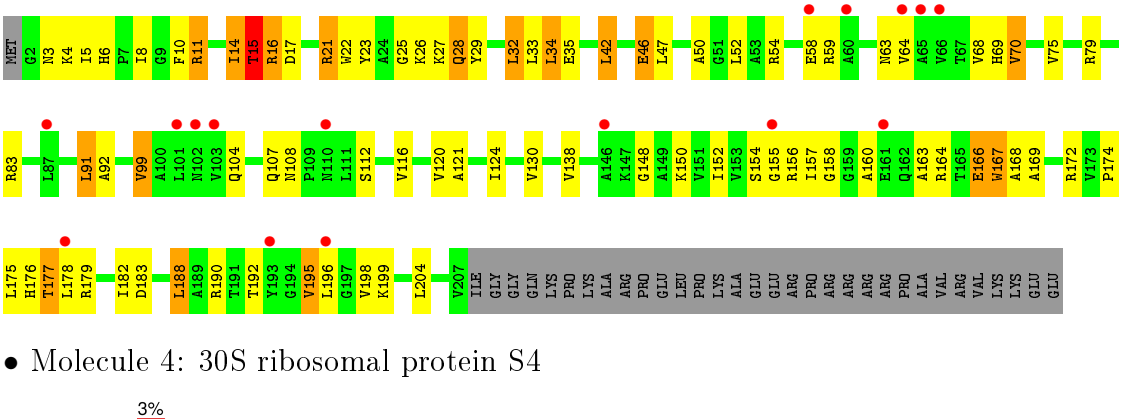
Chain B:



- Molecule 3: 30S ribosomal protein S3

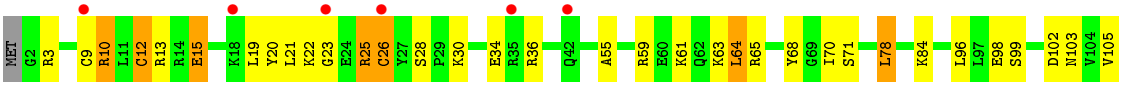
Chain C:





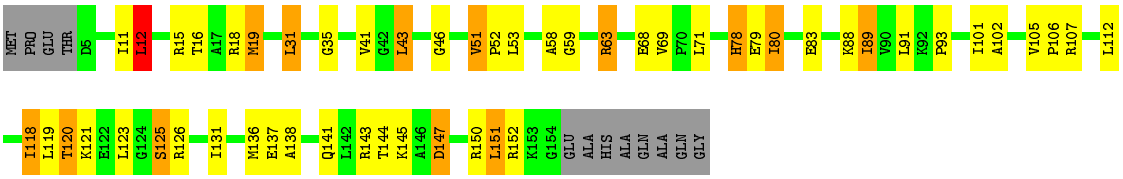
- Molecule 4: 30S ribosomal protein S4

Chain D:



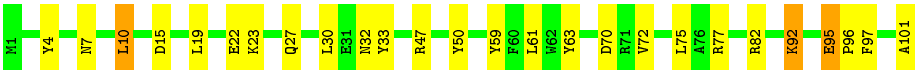
• Molecule 5: 30S ribosomal protein S5

Chain E:



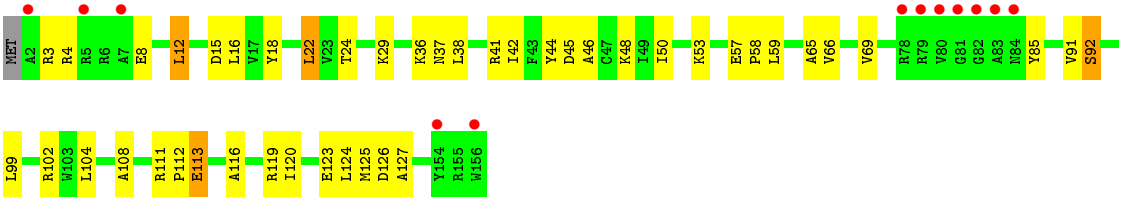
• Molecule 6: 30S ribosomal protein S6

Chain F:



• Molecule 7: 30S ribosomal protein S7

Chain G:

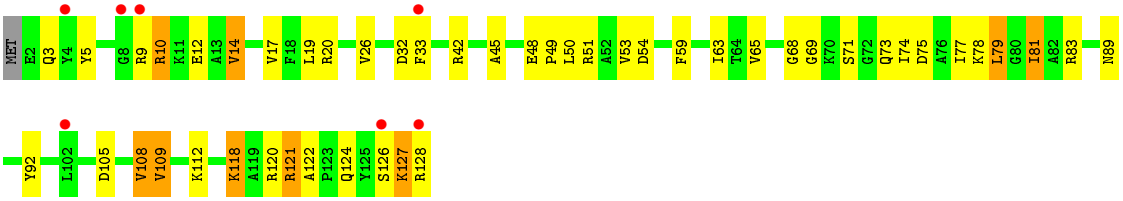


• Molecule 8: 30S ribosomal protein S8

Chain H:

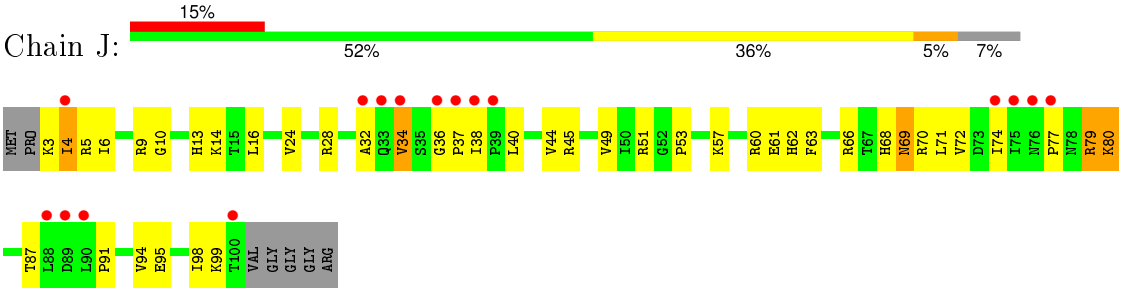
• Molecule 9: 30S ribosomal protein S9

Chain I:



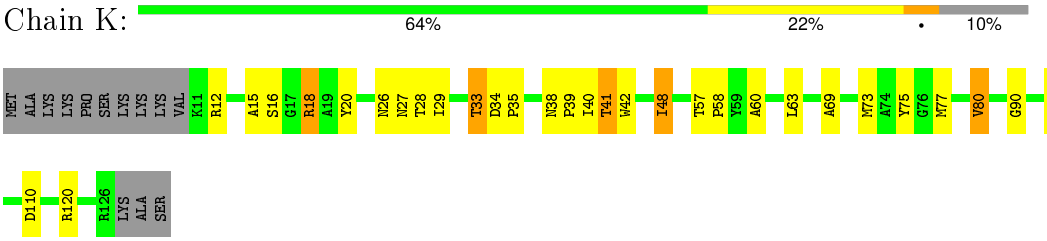
• Molecule 10: 30S ribosomal protein S10

Chain J:



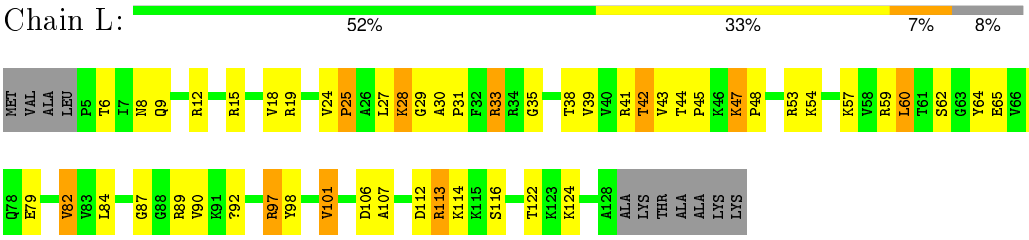
• Molecule 11: 30S ribosomal protein S11

Chain K:



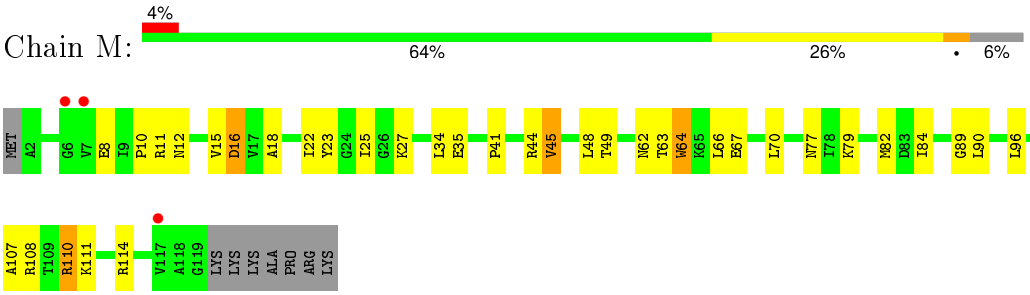
• Molecule 12: 30S ribosomal protein S12

Chain L:



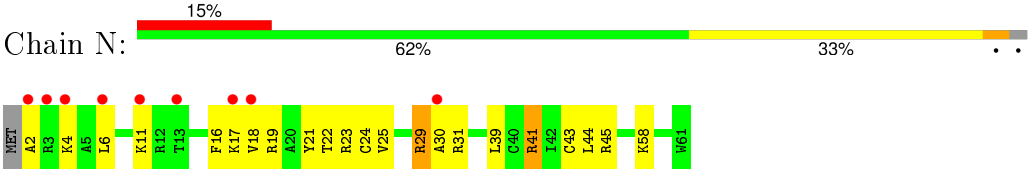
• Molecule 13: 30S ribosomal protein S13

Chain M:



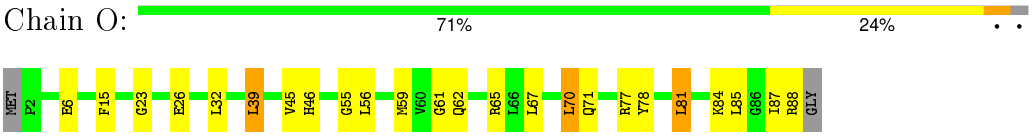
• Molecule 14: 30S ribosomal protein S14

Chain N:



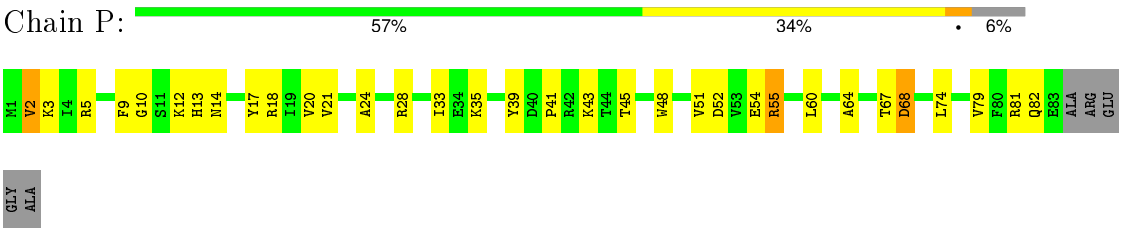
• Molecule 15: 30S ribosomal protein S15

Chain O:



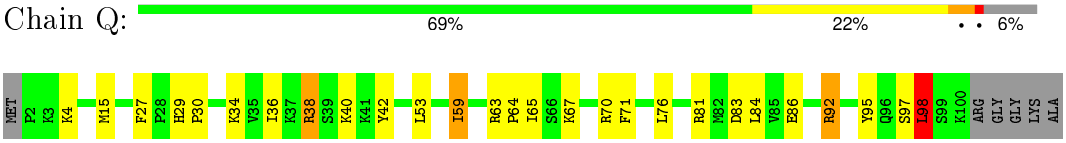
• Molecule 16: 30S ribosomal protein S16

Chain P:



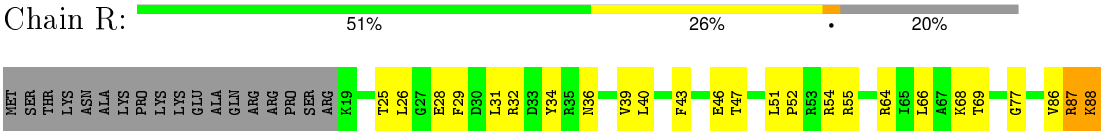
• Molecule 17: 30S ribosomal protein S17

Chain Q:



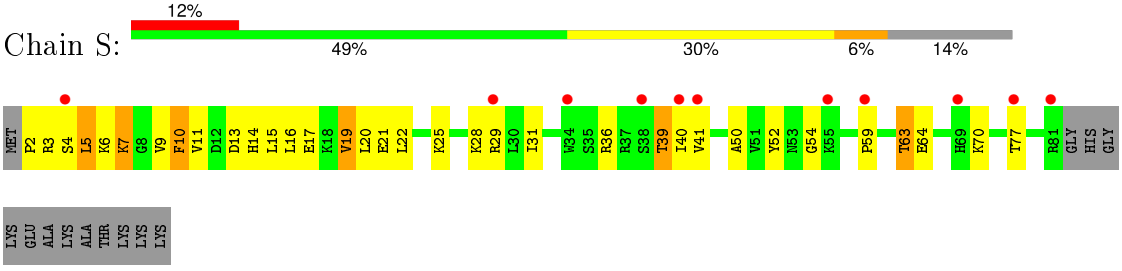
• Molecule 18: 30S ribosomal protein S18

Chain R:



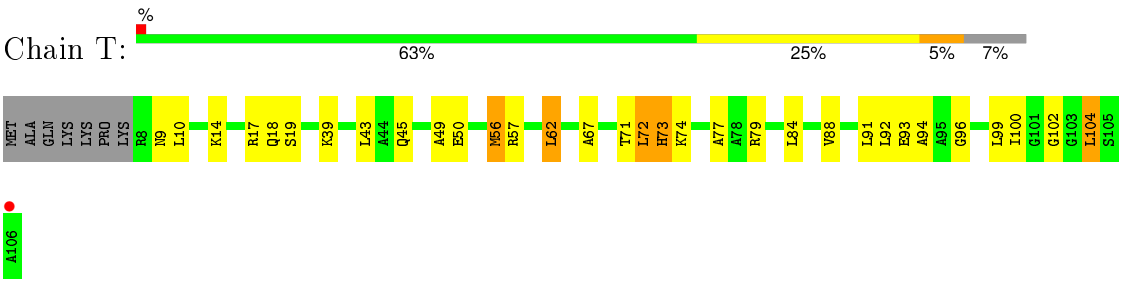
• Molecule 19: 30S ribosomal protein S19

Chain S:



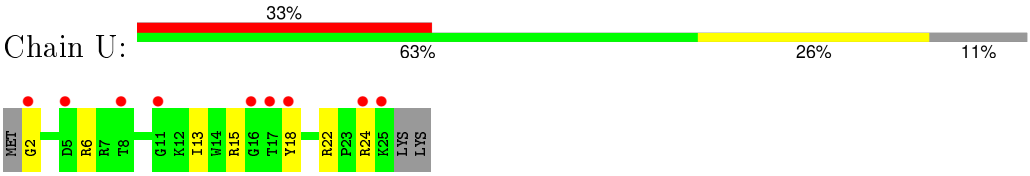
• Molecule 20: 30S ribosomal protein S20

Chain T:



• Molecule 21: 30S ribosomal protein THX

Chain U:


33%
63%
26%
11%
MET
G2
D5
R6
R7
T8
G11
K12
I13
W14
R15
G16
T17
Y18
R22
P23
R24
K25
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	404.04Å 404.04Å 173.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.55 – 3.35 34.55 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (34.55-3.35) 98.1 (34.55-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_978)	Depositor
R, R_{free}	0.168 , 0.206 0.167 , 0.202	Depositor DCC
R_{free} test set	10116 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	117.9	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 130.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 200918 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52164	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M2G, MA6, 0TD, MG, 2MG, 5MC, UR3, 4OC, SRY, 7MG, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.56	3/36040 (0.0%)	0.98	71/56243 (0.1%)
2	B	0.41	0/1935	0.64	0/2609
3	C	0.32	0/1636	0.56	0/2205
4	D	0.39	0/1733	0.56	1/2318 (0.0%)
5	E	0.49	0/1162	0.70	1/1564 (0.1%)
6	F	0.32	0/856	0.52	0/1154
7	G	0.33	0/1276	0.52	0/1709
8	H	0.53	0/1136	0.69	0/1527
9	I	0.34	0/1029	0.58	0/1379
10	J	0.32	0/805	0.58	0/1082
11	K	0.38	0/879	0.60	0/1187
12	L	0.41	0/977	0.68	0/1306
13	M	0.33	0/947	0.60	0/1270
14	N	0.34	0/501	0.53	0/664
15	O	0.37	0/740	0.56	0/987
16	P	0.43	0/716	0.65	0/963
17	Q	0.49	0/836	0.74	1/1117 (0.1%)
18	R	0.34	0/579	0.57	0/768
19	S	0.27	0/661	0.53	0/890
20	T	0.39	0/765	0.64	1/1007 (0.1%)
21	U	0.32	0/212	0.53	0/277
All	All	0.51	3/55421 (0.0%)	0.88	75/82226 (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
10	J	0	1
12	L	0	1
20	T	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N9-C4	-8.65	1.32	1.37
1	A	279	A	N3-C4	-5.60	1.31	1.34
1	A	108	G	N9-C8	5.45	1.41	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117	G	N1-C6-O6	11.04	126.53	119.90
1	A	279	A	C2-N3-C4	-10.47	105.37	110.60
1	A	328	C	N1-C2-O2	8.61	124.07	118.90
1	A	117	G	C6-C5-N7	-8.21	125.47	130.40
1	A	328	C	C2-N1-C1'	8.14	127.75	118.80
1	A	328	C	N3-C2-O2	-7.85	116.41	121.90
1	A	266	G	C5-N7-C8	-7.72	100.44	104.30
1	A	279	A	C5-N7-C8	-7.61	100.09	103.90
1	A	108	G	C5-N7-C8	-7.49	100.56	104.30
1	A	839	U	N1-C2-O2	7.48	128.04	122.80
1	A	839	U	C2-N1-C1'	7.39	126.56	117.70
1	A	1502	A	C5-N7-C8	-6.91	100.44	103.90
1	A	1502	A	N7-C8-N9	6.83	117.21	113.80
1	A	266	G	C4-C5-N7	6.75	113.50	110.80
1	A	1442	G	C4-N9-C1'	6.72	135.24	126.50
1	A	279	A	N3-C4-C5	6.69	131.48	126.80
1	A	1181	G	C8-N9-C4	6.69	109.08	106.40
1	A	117	G	C5-C6-N1	-6.66	108.17	111.50
1	A	108	G	C4-C5-N7	6.64	113.45	110.80
1	A	839	U	N3-C2-O2	-6.63	117.56	122.20
1	A	651	C	C6-N1-C2	6.61	122.94	120.30
1	A	795	C	N3-C2-O2	6.56	126.49	121.90
1	A	1306	A	N7-C8-N9	6.55	117.07	113.80
1	A	723	U	C2-N1-C1'	6.51	125.52	117.70
1	A	108	G	N7-C8-N9	6.46	116.33	113.10
1	A	1502	A	C6-C5-N7	-6.45	127.78	132.30
1	A	1502	A	N1-C6-N6	6.42	122.45	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1126	U	C5-C6-N1	6.39	125.89	122.70
1	A	481	G	N3-C4-N9	6.39	129.83	126.00
1	A	1181	G	N3-C4-C5	6.37	131.78	128.60
1	A	279	A	N3-C4-N9	-6.33	122.33	127.40
1	A	579	G	N1-C6-O6	6.29	123.68	119.90
1	A	266	G	N3-C4-C5	6.28	131.74	128.60
1	A	1505	G	C8-N9-C4	-6.27	103.89	106.40
1	A	299	G	C5-C6-O6	-6.25	124.85	128.60
1	A	252	U	C5-C6-N1	-6.19	119.60	122.70
1	A	107	G	C4-C5-N7	6.13	113.25	110.80
1	A	723	U	N1-C2-O2	6.04	127.03	122.80
1	A	117	G	C4-C5-C6	6.02	122.41	118.80
1	A	328	C	C6-N1-C1'	-5.98	113.62	120.80
1	A	1181	G	C4-N9-C1'	-5.81	118.95	126.50
1	A	1442	G	C8-N9-C1'	-5.80	119.46	127.00
1	A	879	C	C5-C4-N4	-5.79	116.15	120.20
17	Q	98	LEU	CA-CB-CG	5.76	128.56	115.30
1	A	117	G	C2-N3-C4	-5.76	109.02	111.90
1	A	1442	G	N3-C4-N9	5.62	129.37	126.00
1	A	1502	A	C2-N3-C4	-5.57	107.82	110.60
1	A	266	G	N7-C8-N9	5.54	115.87	113.10
1	A	117	G	C5-C6-O6	-5.49	125.31	128.60
1	A	1347	G	C8-N9-C4	5.46	108.58	106.40
1	A	1306	A	N1-C6-N6	5.45	121.87	118.60
1	A	283	C	C6-N1-C2	-5.44	118.13	120.30
1	A	1334	G	C8-N9-C4	5.40	108.56	106.40
1	A	926	G	N3-C4-N9	5.39	129.24	126.00
1	A	1306	A	C5-N7-C8	-5.38	101.21	103.90
1	A	107	G	C6-C5-N7	-5.38	127.17	130.40
1	A	279	A	C5-C6-N1	-5.37	115.02	117.70
1	A	299	G	N9-C4-C5	-5.33	103.27	105.40
1	A	754	C	C2-N1-C1'	5.33	124.66	118.80
1	A	482	A	N7-C8-N9	5.30	116.45	113.80
1	A	948	C	C6-N1-C2	5.22	122.39	120.30
1	A	277	C	C6-N1-C2	5.18	122.37	120.30
1	A	1529	G	C8-N9-C4	-5.17	104.33	106.40
1	A	1403	C	C6-N1-C2	5.16	122.36	120.30
4	D	12	CYS	CA-CB-SG	5.16	123.28	114.00
1	A	530	G	C4-N9-C1'	5.14	133.18	126.50
1	A	879	C	N3-C4-N4	5.14	121.60	118.00
20	T	94	ALA	N-CA-C	-5.11	97.20	111.00
1	A	1502	A	C4-C5-N7	5.10	113.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129(A)	G	C4-N9-C1'	5.09	133.12	126.50
1	A	166	G	N9-C4-C5	-5.09	103.36	105.40
5	E	12	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	1301	U	P-O3'-C3'	5.06	125.77	119.70
1	A	190(C)	C	C6-N1-C2	-5.04	118.28	120.30
1	A	745	C	C6-N1-C2	5.03	122.31	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	90	GLY	Peptide
10	J	87	THR	Peptide
12	L	25	PRO	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	32507	0	16433	452	1
2	B	1900	0	1951	57	0
3	C	1612	0	1677	58	0
4	D	1703	0	1763	38	0
5	E	1146	0	1207	36	0
6	F	843	0	857	15	0
7	G	1257	0	1296	29	0
8	H	1116	0	1177	30	0
9	I	1010	0	1037	44	0
10	J	792	0	835	35	0
11	K	864	0	881	22	0
12	L	972	0	1058	40	0
13	M	937	0	995	21	0
14	N	492	0	529	23	0
15	O	729	0	768	17	0
16	P	700	0	720	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	823	0	893	21	0
18	R	574	0	644	17	0
19	S	647	0	673	26	0
20	T	763	0	861	20	0
21	U	208	0	221	6	0
22	A	40	0	36	3	0
23	A	248	0	0	0	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	1	0	0	0	0
23	H	3	0	0	0	0
23	M	1	0	0	0	0
23	N	1	0	0	0	0
23	P	3	0	0	0	0
23	Q	2	0	0	0	0
23	T	2	0	0	0	0
23	U	1	0	0	0	0
24	D	1	0	0	0	0
24	N	1	0	0	0	0
25	A	256	0	0	5	0
25	D	1	0	0	0	0
25	E	2	0	0	0	0
25	G	1	0	0	0	0
25	L	1	0	0	0	0
25	N	1	0	0	0	0
25	U	1	0	0	1	0
All	All	52164	0	36512	895	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (895) 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:235:C:H5'	17:Q:70:ARG:HG2	1.55	0.88
1:A:1443:G:H5"	1:A:1446:A:H5'	1.57	0.86
12:L:47:LYS:HD3	12:L:48:PRO:HD3	1.56	0.86
1:A:517:G:N1	1:A:533:A:OP2	2.07	0.86
1:A:103:C:OP1	20:T:17:ARG:NH1	2.09	0.85
13:M:11:ARG:HA	13:M:45:VAL:HG11	1.59	0.83
1:A:664:G:H22	1:A:741:G:H1	1.20	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:U:OP2	1:A:1145:C:N4	2.11	0.82
1:A:1125:U:H3	10:J:5:ARG:HH21	1.27	0.81
1:A:1008:C:H42	1:A:1021:G:H1	1.28	0.81
1:A:967:5MC:H4'	9:I:128:ARG:HG3	1.63	0.80
1:A:835:U:OP1	18:R:64:ARG:NH2	2.17	0.78
1:A:279:A:OP2	17:Q:95:TYR:OH	2.02	0.77
1:A:532:A:H2'	1:A:533:A:H5"	1.67	0.77
1:A:1392:G:H21	1:A:1502:A:H8	1.31	0.76
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.67	0.76
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.49	0.76
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.66	0.76
3:C:22:TRP:HB3	3:C:59:ARG:HB3	1.67	0.75
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.68	0.75
11:K:57:THR:HG23	11:K:60:ALA:H	1.52	0.74
1:A:95:U:H2'	1:A:96:G:C8	2.23	0.74
2:B:12:GLU:HG3	2:B:213:LEU:HD21	1.69	0.74
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.69	0.73
14:N:16:PHE:HD1	14:N:19:ARG:HD2	1.52	0.73
1:A:1373:G:H5"	7:G:36:LYS:HE3	1.71	0.73
1:A:959:A:HO2'	1:A:984:C:HO2'	1.32	0.72
1:A:953:G:H5'	1:A:965:A:H61	1.54	0.72
3:C:21:ARG:HE	3:C:58:GLU:HG2	1.54	0.72
1:A:974:A:OP2	14:N:29:ARG:NH2	2.23	0.72
5:E:147:ASP:OD1	5:E:147:ASP:N	2.23	0.72
1:A:263:A:OP2	20:T:79:ARG:NH1	2.23	0.71
1:A:113:G:H1'	1:A:354:G:H5'	1.72	0.71
10:J:44:VAL:HG13	10:J:66:ARG:HG2	1.71	0.71
13:M:107:ALA:HB3	13:M:111:LYS:HE2	1.72	0.71
3:C:14:ILE:HB	3:C:15:THR:HG23	1.72	0.70
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.72	0.70
1:A:1518:MA6:H93	1:A:1519:MA6:N1	2.06	0.70
1:A:788:U:O2'	1:A:1539:C:O2	2.08	0.70
1:A:1183:A:O2'	1:A:1184:G:OP1	2.09	0.70
1:A:427:U:OP1	4:D:13:ARG:NH2	2.24	0.70
1:A:1313:U:H5	19:S:4:SER:HB2	1.54	0.70
11:K:90:GLY:HA2	11:K:93:GLN:HB2	1.73	0.70
1:A:1505:G:O2'	1:A:1506:U:OP2	2.09	0.70
1:A:914:A:OP1	22:A:1601:SRY:HI33	1.92	0.70
1:A:250:A:H4'	1:A:251:G:O5'	1.92	0.70
1:A:166:G:H2'	1:A:167:G:H8	1.57	0.70
2:B:17:PHE:HD1	2:B:18:GLY:H	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:LEU:HD21	3:C:99:VAL:HG13	1.74	0.70
1:A:1305:G:HO2'	1:A:1306:A:H8	1.37	0.70
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.75	0.69
1:A:1316:G:H4'	14:N:18:VAL:HG11	1.74	0.69
1:A:372:C:H4'	1:A:373:A:O5'	1.92	0.69
3:C:46:GLU:OE1	3:C:83:ARG:NH2	2.26	0.69
1:A:560:U:H5'	1:A:566:G:N2	2.07	0.68
1:A:976:G:OP2	1:A:1358:U:H1'	1.94	0.68
1:A:1238:A:H5'	1:A:1336:C:H41	1.57	0.68
5:E:137:GLU:HG3	5:E:141:GLN:HE21	1.58	0.67
1:A:1125:U:H3	10:J:5:ARG:NH2	1.93	0.67
1:A:825:G:H21	8:H:11:THR:HG21	1.59	0.67
1:A:1008:C:N3	1:A:1021:G:N2	2.42	0.67
1:A:1510:U:H2'	1:A:1511:G:C8	2.29	0.67
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.76	0.67
1:A:1305:G:O2'	1:A:1306:A:H8	1.78	0.67
13:M:16:ASP:OD1	13:M:16:ASP:N	2.25	0.67
1:A:1285:A:H4'	1:A:1286:A:O5'	1.94	0.67
1:A:1000:U:H3	1:A:1041:A:H61	1.43	0.67
1:A:1047:G:OP1	14:N:4:LYS:NZ	2.23	0.66
1:A:144:G:H1	1:A:178:C:H42	1.43	0.66
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.30	0.66
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.61	0.66
1:A:95:U:H2'	1:A:96:G:H8	1.60	0.65
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.77	0.65
1:A:481:G:HO2'	1:A:482:A:H8	1.44	0.65
1:A:89:C:H2'	1:A:90:U:O4'	1.97	0.65
13:M:8:GLU:HG3	13:M:22:ILE:HG23	1.79	0.65
1:A:501:C:H2'	1:A:502:G:C8	2.31	0.65
1:A:1305:G:N2	1:A:1331:G:H1'	2.12	0.65
3:C:25:GLY:O	3:C:29:TYR:HB2	1.97	0.65
1:A:390:C:O3'	16:P:28:ARG:NH2	2.30	0.65
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.79	0.64
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.30	0.64
1:A:559:A:OP1	5:E:126:ARG:NH2	2.30	0.64
1:A:1119:C:OP2	9:I:9:ARG:NH2	2.31	0.64
10:J:34:VAL:HG13	10:J:74:ILE:HG12	1.79	0.64
2:B:18:GLY:HA3	2:B:41:ILE:HA	1.80	0.64
1:A:1338:G:H2'	1:A:1339:A:C8	2.33	0.64
12:L:89:ARG:HG2	12:L:97:ARG:HA	1.80	0.63
1:A:839:U:H5'	1:A:840:C:H5	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1392:G:N2	1:A:1502:A:H8	1.97	0.63
1:A:1000:U:H2'	1:A:1001:A:H8	1.63	0.63
5:E:101:ILE:O	5:E:120:THR:HB	1.98	0.63
1:A:130:A:OP2	1:A:190(E):U:O2'	2.11	0.63
1:A:421:U:H5'	1:A:422:C:H5	1.64	0.63
3:C:75:VAL:O	3:C:83:ARG:NH1	2.32	0.63
12:L:27:LEU:O	12:L:29:GLY:N	2.32	0.63
1:A:1270:C:OP2	21:U:24:ARG:NH2	2.32	0.62
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.80	0.62
9:I:10:ARG:NE	9:I:105:ASP:OD1	2.32	0.62
2:B:18:GLY:HA2	2:B:42:ILE:HG13	1.82	0.62
1:A:1195:C:H3'	1:A:1196:U:H5"	1.81	0.62
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.81	0.62
11:K:40:ILE:HG22	11:K:41:THR:HG22	1.81	0.62
1:A:1435:G:H2'	1:A:1436:U:C6	2.34	0.62
1:A:1532:U:H2'	1:A:1533:C:H3'	1.81	0.62
9:I:3:GLN:HG3	9:I:20:ARG:HG3	1.81	0.62
1:A:612:C:OP1	4:D:84:LYS:NZ	2.30	0.62
2:B:240:GLN:OE1	2:B:240:GLN:N	2.31	0.62
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.33	0.62
1:A:1493:A:H2'	1:A:1494:G:C8	2.34	0.62
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.81	0.62
5:E:137:GLU:O	5:E:141:GLN:HG3	2.00	0.62
12:L:25:PRO:HB3	12:L:27:LEU:HD13	1.81	0.62
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.18	0.62
1:A:673:G:H2'	1:A:674:G:C8	2.35	0.62
1:A:1068:G:H8	1:A:1068:G:OP2	1.82	0.62
1:A:990:C:H42	1:A:1215:G:H1	1.47	0.62
3:C:156:ARG:H	3:C:163:ALA:HA	1.64	0.62
3:C:14:ILE:O	3:C:16:ARG:N	2.32	0.61
1:A:452:A:O2'	1:A:453:A:O4'	2.19	0.61
20:T:67:ALA:HA	20:T:73:HIS:H	1.64	0.61
1:A:1195:C:H3'	1:A:1196:U:C5'	2.31	0.61
15:O:87:ILE:HG22	15:O:88:ARG:HG2	1.82	0.61
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.82	0.61
1:A:1145:C:O2'	1:A:1146:A:O5'	2.19	0.61
1:A:562:C:H1'	12:L:15:ARG:HB3	1.82	0.61
18:R:86:VAL:HG12	18:R:87:ARG:H	1.66	0.61
3:C:167:TRP:HE3	3:C:168:ALA:H	1.48	0.60
20:T:49:ALA:HB3	20:T:99:LEU:HG	1.82	0.60
1:A:80:G:H1	1:A:89:C:H42	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:G:O6	1:A:91:C:N4	2.32	0.60
20:T:45:GLN:HG2	20:T:91:LEU:HD13	1.83	0.60
1:A:1256:A:H4'	1:A:1257:U:O5'	2.01	0.60
4:D:102:ASP:OD1	4:D:103:ASN:N	2.34	0.60
1:A:928:G:O2'	1:A:1533:C:OP1	2.19	0.60
1:A:939:G:H5"	7:G:102:ARG:HH12	1.66	0.60
2:B:200:ILE:HG23	2:B:202:PRO:HD3	1.84	0.60
12:L:8:ASN:O	12:L:12:ARG:HG3	2.02	0.60
1:A:269:C:H2'	1:A:270:A:C8	2.37	0.60
11:K:27:ASN:OD1	11:K:28:THR:N	2.34	0.60
2:B:73:THR:HG21	2:B:96:ARG:HD2	1.83	0.59
1:A:1368:G:H5"	9:I:112:LYS:HB3	1.84	0.59
4:D:65:ARG:HG3	4:D:70:ILE:HG22	1.84	0.59
12:L:27:LEU:C	12:L:29:GLY:H	2.06	0.59
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.38	0.59
15:O:32:LEU:HD11	15:O:62:GLN:HB3	1.84	0.59
4:D:68:TYR:OH	4:D:98:GLU:OE1	2.17	0.59
4:D:99:SER:HB3	4:D:139:ARG:HG3	1.84	0.59
1:A:975:A:H4'	1:A:976:G:O5'	2.02	0.59
1:A:939:G:H5"	7:G:102:ARG:NH1	2.19	0.58
4:D:15:GLU:HG2	4:D:63:LYS:HG3	1.85	0.58
1:A:748:C:H4'	1:A:749:C:O5'	2.03	0.58
8:H:10:LEU:HD22	8:H:83:ILE:HG12	1.85	0.58
9:I:48:GLU:OE1	9:I:51:ARG:NH2	2.32	0.58
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.86	0.58
14:N:39:LEU:HD22	14:N:43:CYS:HB3	1.85	0.58
3:C:155:GLY:HA2	3:C:164:ARG:H	1.68	0.58
1:A:691:G:H3'	11:K:26:ASN:HD21	1.68	0.58
17:Q:95:TYR:HA	17:Q:98:LEU:HD11	1.84	0.58
1:A:1493:A:H2'	1:A:1494:G:H8	1.69	0.58
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.44	0.58
1:A:1283:G:H2'	1:A:1284:C:H6	1.69	0.58
1:A:1127:G:N1	1:A:1145:C:N3	2.52	0.58
18:R:52:PRO:HB2	18:R:54:ARG:HD3	1.86	0.58
1:A:518:C:H4'	1:A:519:C:O5'	2.03	0.58
16:P:68:ASP:OD1	16:P:68:ASP:N	2.37	0.58
1:A:926:G:N2	1:A:1542:U:OP1	2.32	0.57
1:A:353:A:H5'	1:A:353:A:H8	1.69	0.57
11:K:12:ARG:HB2	11:K:75:TYR:HD2	1.68	0.57
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.87	0.57
1:A:1007:C:O2	1:A:1023:G:N1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:C:O3'	22:A:1601:SRY:HI31	2.05	0.57
5:E:152:ARG:NH2	8:H:107:LEU:O	2.33	0.57
1:A:35:G:H2'	1:A:36:C:C6	2.40	0.57
10:J:9:ARG:HG3	10:J:95:GLU:HB2	1.87	0.57
1:A:537:G:OP1	12:L:113:ARG:NH2	2.38	0.57
1:A:1292:U:OP1	7:G:41:ARG:NH2	2.24	0.57
13:M:108:ARG:HD3	13:M:114:ARG:NH1	2.20	0.57
4:D:23:GLY:HA3	4:D:112:VAL:HG12	1.87	0.56
1:A:1203:C:OP1	14:N:2:ALA:N	2.38	0.56
20:T:71:THR:O	20:T:72:LEU:HD23	2.05	0.56
1:A:933:G:O6	7:G:3:ARG:NH2	2.38	0.56
3:C:175:LEU:HD23	3:C:182:ILE:HD12	1.87	0.56
10:J:40:LEU:HB2	10:J:69:ASN:HB2	1.87	0.56
1:A:1502:A:H2	1:A:1505:G:H1	1.54	0.56
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.69	0.56
1:A:269:C:H2'	1:A:270:A:H8	1.70	0.56
1:A:1399:C:H4'	1:A:1400:5MC:H5"	1.87	0.56
1:A:1305:G:O2'	1:A:1306:A:O5'	2.24	0.56
1:A:1047:G:H5"	14:N:4:LYS:HD3	1.85	0.56
3:C:148:GLY:HA3	3:C:172:ARG:O	2.06	0.56
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.87	0.56
11:K:48:ILE:HD13	11:K:63:LEU:HB2	1.87	0.56
3:C:26:LYS:HG2	10:J:45:ARG:HH12	1.71	0.56
1:A:973:G:H3'	1:A:974:A:H5"	1.88	0.56
10:J:16:LEU:HD23	10:J:94:VAL:HG22	1.86	0.56
1:A:1244:C:H42	1:A:1293:G:H1	1.52	0.56
5:E:102:ALA:O	5:E:107:ARG:NH1	2.39	0.56
1:A:542:G:OP1	4:D:10:ARG:NH2	2.35	0.56
1:A:129:U:O3'	1:A:129(A):G:H3'	2.06	0.56
3:C:155:GLY:O	3:C:196:LEU:HD22	2.06	0.56
6:F:97:PHE:HB2	18:R:32:ARG:NH1	2.21	0.55
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.87	0.55
1:A:299:G:H2'	1:A:300:A:C8	2.41	0.55
10:J:51:ARG:CZ	10:J:61:GLU:HB2	2.36	0.55
1:A:1356:G:H2'	1:A:1357:A:C8	2.41	0.55
1:A:1152:A:H5"	10:J:13:HIS:CD2	2.42	0.55
1:A:279:A:OP1	1:A:280:C:O2'	2.18	0.55
3:C:5:ILE:HD13	3:C:10:PHE:HB2	1.88	0.55
1:A:975:A:H5'	1:A:975:A:H8	1.72	0.55
5:E:35:GLY:HA3	5:E:41:VAL:HG12	1.87	0.55
10:J:6:ILE:HG23	10:J:98:ILE:HG12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:45:ASP:OD1	7:G:48:LYS:NZ	2.33	0.55
1:A:235:C:N4	25:A:1991:HOH:O	2.39	0.55
10:J:16:LEU:HD12	10:J:68:HIS:HB2	1.88	0.55
18:R:39:VAL:HG13	18:R:40:LEU:HD23	1.89	0.55
12:L:53:ARG:HH12	12:L:92:0TD:CG	2.19	0.55
1:A:1281:U:H5'	1:A:1282:C:H5	1.70	0.55
1:A:524:G:H2'	1:A:525:C:C6	2.42	0.54
1:A:117:G:O5'	1:A:117:G:H8	1.90	0.54
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.90	0.54
19:S:22:LEU:HD22	19:S:28:LYS:HG3	1.89	0.54
2:B:124:SER:HB2	2:B:126:GLU:HG2	1.90	0.54
1:A:481:G:O2'	1:A:482:A:H8	1.90	0.54
2:B:23:ARG:O	2:B:24:TRP:HD1	1.90	0.54
1:A:677:U:H3	1:A:713:G:H22	1.55	0.54
4:D:187:ARG:HH22	4:D:188:LEU:HD12	1.71	0.54
4:D:173:TRP:CD2	4:D:189:PRO:HB3	2.42	0.54
1:A:707:C:O2	11:K:39:PRO:HD3	2.08	0.54
12:L:59:ARG:HD3	12:L:65:GLU:HG3	1.89	0.54
11:K:15:ALA:HA	11:K:77:MET:HA	1.90	0.54
3:C:156:ARG:NH1	3:C:160:ALA:O	2.41	0.54
1:A:792:A:O2'	1:A:793:U:OP2	2.15	0.54
13:M:79:LYS:HD2	13:M:82:MET:HE3	1.89	0.54
5:E:89:ILE:HD12	5:E:91:LEU:HD21	1.90	0.54
7:G:46:ALA:O	7:G:50:ILE:HG12	2.08	0.54
1:A:166:G:H2'	1:A:167:G:C8	2.41	0.54
1:A:518:C:H2'	1:A:530:G:C8	2.43	0.54
1:A:1513:A:H2'	1:A:1514:C:C6	2.43	0.54
10:J:79:ARG:HB2	10:J:80:LYS:HD2	1.90	0.54
1:A:858:G:N7	25:A:2101:HOH:O	2.33	0.54
1:A:1124:G:H2'	1:A:1145:C:H41	1.73	0.54
1:A:1347:G:H1'	1:A:1348:U:H5	1.73	0.54
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.08	0.54
1:A:384:G:H2'	1:A:385:C:C6	2.42	0.54
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.90	0.54
10:J:32:ALA:O	10:J:34:VAL:HG23	2.08	0.54
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.43	0.53
7:G:16:LEU:HD21	9:I:42:ARG:HG3	1.90	0.53
1:A:757:U:H2'	1:A:758:G:O4'	2.08	0.53
1:A:671:G:H5'	6:F:77:ARG:HH21	1.73	0.53
2:B:16:HIS:HB3	2:B:210:SER:HB2	1.89	0.53
21:U:2:GLY:N	25:U:1401:HOH:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:ALA:O	4:D:59:ARG:HG2	2.08	0.53
2:B:21:ARG:HA	2:B:39:ILE:HA	1.89	0.53
15:O:55:GLY:O	15:O:59:MET:HG3	2.07	0.53
1:A:1419:G:H1	1:A:1481:U:H3	1.56	0.53
1:A:1318:A:H5'	19:S:10:PHE:CZ	2.44	0.53
1:A:980:C:H5'	1:A:981:U:OP2	2.09	0.53
16:P:17:TYR:HD1	16:P:39:TYR:HD2	1.55	0.53
9:I:126:SER:OG	9:I:127:LYS:N	2.42	0.53
1:A:328:C:O2	1:A:328:C:H2'	2.09	0.53
1:A:1225:A:H5'	1:A:1226:C:OP2	2.09	0.53
1:A:1372:U:H2'	1:A:1373:G:O4'	2.08	0.53
1:A:981:U:H5'	14:N:21:TYR:CZ	2.44	0.53
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.53
2:B:178:ARG:HH21	8:H:74:PRO:HB3	1.73	0.53
1:A:1301:U:O2'	1:A:1302:U:H3'	2.09	0.52
1:A:56:U:H2'	1:A:57:G:H8	1.74	0.52
1:A:1200:C:H1'	1:A:1204:A:N6	2.24	0.52
4:D:187:ARG:CZ	4:D:188:LEU:H	2.22	0.52
1:A:344:A:H5'	1:A:345:C:H5	1.75	0.52
11:K:33:THR:HB	11:K:39:PRO:HA	1.91	0.52
3:C:23:TYR:HD2	10:J:95:GLU:HG3	1.75	0.52
3:C:25:GLY:HA2	3:C:28:GLN:H	1.74	0.52
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.42	0.52
7:G:38:LEU:O	7:G:42:ILE:HG13	2.10	0.52
1:A:692:U:H1'	1:A:695:A:N7	2.25	0.52
1:A:1300:G:H4'	1:A:1301:U:O5'	2.10	0.52
1:A:1164:G:H1	1:A:1172:C:H42	1.56	0.52
1:A:258:G:H2'	1:A:259:G:H8	1.75	0.52
9:I:71:SER:HA	9:I:74:ILE:HD12	1.91	0.52
1:A:826:C:O2	8:H:15:ASN:ND2	2.43	0.52
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.10	0.52
1:A:1201:A:H4'	1:A:1202:G:O5'	2.09	0.52
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.92	0.52
2:B:16:HIS:HD2	2:B:204:ASN:HD22	1.58	0.51
1:A:838:G:H1	1:A:848:C:H42	1.58	0.51
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.92	0.51
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.91	0.51
1:A:216:G:H2'	1:A:217:C:C6	2.45	0.51
2:B:102:LEU:HB3	2:B:180:LEU:HD12	1.92	0.51
1:A:191:G:O2'	20:T:102:GLY:O	2.16	0.51
5:E:91:LEU:HB3	5:E:118:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1236:A:H4'	1:A:1304:G:H4'	1.92	0.51
4:D:78:LEU:HD21	4:D:96:LEU:HB3	1.92	0.51
1:A:371:G:O2'	1:A:372:C:H5'	2.10	0.51
1:A:694:A:N1	1:A:787:A:O2'	2.42	0.51
1:A:164:U:H2'	1:A:165:C:C6	2.46	0.51
20:T:67:ALA:HB2	20:T:77:ALA:HB2	1.92	0.51
1:A:1256:A:H5"	1:A:1258:G:H1'	1.92	0.51
1:A:184:G:H2'	1:A:185:A:H8	1.75	0.51
1:A:243:A:H4'	1:A:244:U:O5'	2.10	0.51
1:A:980:C:H5"	1:A:981:U:C5	2.46	0.51
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.10	0.51
1:A:993:G:O6	1:A:1045:C:N4	2.41	0.51
1:A:1101:A:H4'	1:A:1102:A:O5'	2.10	0.51
1:A:501:C:H2'	1:A:502:G:H8	1.76	0.51
12:L:113:ARG:NH1	12:L:116:SER:H	2.08	0.51
6:F:101:ALA:HA	18:R:28:GLU:HG3	1.93	0.51
2:B:98:LEU:O	2:B:101:MET:HG3	2.11	0.51
5:E:43:LEU:HD22	5:E:136:MET:HG3	1.93	0.51
6:F:23:LYS:O	6:F:27:GLN:HG2	2.10	0.51
17:Q:81:ARG:NH1	17:Q:84:LEU:HD11	2.25	0.51
1:A:1240:U:OP1	7:G:119:ARG:NH2	2.41	0.51
8:H:20:TYR:CE1	8:H:76:PRO:HD2	2.45	0.51
1:A:457:C:H2'	1:A:458:C:C6	2.46	0.51
1:A:1053:G:H4'	1:A:1054:C:H5'	1.92	0.51
1:A:974:A:P	14:N:41:ARG:HH12	2.34	0.50
16:P:2:VAL:O	16:P:64:ALA:HA	2.11	0.50
1:A:860:A:H2'	1:A:861:G:O4'	2.12	0.50
16:P:51:VAL:O	16:P:52:ASP:HB3	2.10	0.50
2:B:15:VAL:HG13	2:B:209:ARG:HD2	1.93	0.50
1:A:1347:G:H3'	9:I:108:VAL:O	2.11	0.50
12:L:27:LEU:C	12:L:29:GLY:N	2.64	0.50
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.44	0.50
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.44	0.50
1:A:1014:A:H4'	19:S:14:HIS:CE1	2.46	0.50
15:O:15:PHE:CE2	15:O:84:LYS:HD3	2.47	0.50
1:A:1347:G:O6	9:I:10:ARG:NH2	2.43	0.50
1:A:691:G:H2'	1:A:692:U:C6	2.45	0.50
3:C:120:VAL:O	3:C:124:ILE:HG13	2.11	0.50
1:A:1198:G:H2'	1:A:1199:U:C6	2.47	0.50
1:A:476:G:H2'	1:A:477:G:C8	2.45	0.50
1:A:476:G:H2'	1:A:477:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:3:LYS:HG3	16:P:24:ALA:HB2	1.93	0.50
1:A:1278:U:H5"	1:A:1279:A:O4'	2.11	0.50
1:A:254:G:OP1	17:Q:67:LYS:O	2.29	0.50
1:A:457:C:H2'	1:A:458:C:H6	1.77	0.50
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.92	0.50
1:A:114:U:O2'	1:A:115:G:H5'	2.12	0.50
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.77	0.50
1:A:1283:G:H2'	1:A:1284:C:C6	2.47	0.50
8:H:26:VAL:HG13	8:H:59:LEU:HB2	1.94	0.50
6:F:95:GLU:HG3	6:F:96:PRO:HD2	1.94	0.50
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.12	0.50
1:A:1147:C:O2'	9:I:5:TYR:OH	2.29	0.50
20:T:92:LEU:O	20:T:96:GLY:HA2	2.11	0.50
1:A:527:7MG:OP2	22:A:1601:SRY:O32	2.21	0.49
1:A:1305:G:O2'	1:A:1306:A:P	2.70	0.49
1:A:1434:A:H2'	1:A:1435:G:O4'	2.11	0.49
3:C:120:VAL:HB	3:C:198:VAL:HG11	1.94	0.49
1:A:992:U:H3	1:A:1044:A:N6	2.09	0.49
14:N:16:PHE:CD1	14:N:19:ARG:HD2	2.41	0.49
4:D:187:ARG:NH1	4:D:188:LEU:H	2.10	0.49
1:A:56:U:H2'	1:A:57:G:C8	2.46	0.49
1:A:243:A:C2	1:A:246:A:C8	3.00	0.49
12:L:41:ARG:HG2	12:L:42:THR:H	1.77	0.49
1:A:1266:G:N2	1:A:1269:A:OP2	2.41	0.49
1:A:918:A:H2'	1:A:919:A:C8	2.47	0.49
12:L:25:PRO:C	12:L:27:LEU:N	2.61	0.49
1:A:980:C:H3'	1:A:981:U:H6	1.76	0.49
1:A:17:U:H2'	1:A:18:C:C6	2.47	0.49
1:A:828:A:H4'	1:A:828:A:OP1	2.12	0.49
1:A:992:U:H3	1:A:1044:A:H62	1.61	0.49
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.95	0.49
1:A:580:U:H2'	1:A:581:G:O4'	2.12	0.49
1:A:93:G:C2	1:A:95:U:C2	3.00	0.49
9:I:126:SER:OG	9:I:127:LYS:HD2	2.11	0.49
1:A:1225:A:N3	1:A:1225:A:H2'	2.26	0.49
4:D:9:CYS:O	4:D:12:CYS:HB2	2.12	0.49
1:A:1035:A:H2'	1:A:1036:G:C8	2.47	0.49
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.48	0.49
1:A:975:A:H5'	1:A:975:A:C8	2.48	0.49
1:A:1055:A:H1'	3:C:156:ARG:HH21	1.77	0.49
16:P:43:LYS:HG2	16:P:48:TRP:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:118:ILE:HG12	5:E:119:LEU:N	2.28	0.49
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.95	0.49
1:A:1242:C:H42	1:A:1295:G:H1	1.59	0.49
1:A:1318:A:H5"	1:A:1319:A:OP2	2.12	0.49
6:F:7:ASN:HD21	18:R:34:TYR:HE1	1.59	0.49
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.47	0.49
1:A:191:G:H21	20:T:104:LEU:HA	1.77	0.49
1:A:1057:G:H5"	3:C:154:SER:HB2	1.94	0.49
7:G:116:ALA:O	7:G:120:ILE:HG12	2.11	0.49
2:B:189:ASP:HB3	2:B:203:GLY:O	2.12	0.49
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.47	0.49
1:A:991:U:O4	1:A:1212:U:O2'	2.24	0.49
2:B:162:ILE:HG23	2:B:164:VAL:HG23	1.94	0.49
9:I:17:VAL:HG11	9:I:81:ILE:HA	1.95	0.49
7:G:18:TYR:OH	7:G:58:PRO:HB2	2.13	0.49
17:Q:92:ARG:HH11	17:Q:92:ARG:HB3	1.78	0.49
1:A:1148:U:O3'	9:I:14:VAL:HG11	2.13	0.48
1:A:1305:G:H22	1:A:1331:G:H1'	1.76	0.48
2:B:188:ALA:O	2:B:202:PRO:HA	2.13	0.48
3:C:11:ARG:NH1	3:C:177:THR:O	2.45	0.48
3:C:174:PRO:HB2	3:C:177:THR:HG23	1.93	0.48
1:A:532:A:N6	3:C:158:GLY:O	2.43	0.48
1:A:1391:U:H2'	1:A:1392:G:C8	2.48	0.48
1:A:35:G:H2'	1:A:36:C:H6	1.77	0.48
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.78	0.48
1:A:738:C:OP2	6:F:92:LYS:HE3	2.13	0.48
13:M:96:LEU:O	13:M:110:ARG:NH1	2.45	0.48
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.46	0.48
1:A:1412:C:H2'	1:A:1413:A:C8	2.48	0.48
1:A:383:A:C5	1:A:384:G:H1'	2.49	0.48
1:A:1168:A:H2'	1:A:1169:A:C8	2.48	0.48
1:A:1366:C:H2'	1:A:1367:C:C6	2.48	0.48
2:B:44:LEU:H	2:B:44:LEU:HD12	1.77	0.48
1:A:1137:C:H4'	1:A:1138:G:C2	2.48	0.48
1:A:1250:A:H4'	9:I:68:GLY:N	2.29	0.48
1:A:967:5MC:C4'	9:I:128:ARG:HG3	2.38	0.48
3:C:22:TRP:CZ2	3:C:32:LEU:HD22	2.48	0.48
1:A:1477:C:H2'	1:A:1478:C:H6	1.79	0.48
1:A:1147:C:H4'	9:I:5:TYR:CE1	2.49	0.48
1:A:1009:G:H1	1:A:1020:U:H3	1.60	0.48
11:K:12:ARG:HB2	11:K:75:TYR:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:ARG:O	4:D:25:ARG:HG2	2.13	0.48
1:A:1126:U:H6	1:A:1126:U:O5'	1.96	0.48
16:P:74:LEU:O	16:P:79:VAL:HG23	2.14	0.48
1:A:9:G:OP2	5:E:121:LYS:NZ	2.32	0.48
7:G:91:VAL:HG12	7:G:92:SER:H	1.78	0.48
12:L:38:THR:HB	12:L:57:LYS:HB2	1.96	0.48
11:K:18:ARG:HB3	11:K:20:TYR:CE1	2.49	0.48
14:N:23:ARG:HG2	14:N:30:ALA:HB2	1.96	0.48
1:A:1403:C:H2'	1:A:1404:5MC:C6	2.49	0.48
9:I:19:LEU:HD22	9:I:59:PHE:CD2	2.49	0.48
1:A:113:G:H2'	1:A:114:U:C6	2.48	0.48
1:A:451:A:N6	1:A:481:G:C4	2.82	0.48
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.94	0.48
1:A:443:C:H42	1:A:491:G:H1	1.60	0.48
5:E:69:VAL:HG12	5:E:71:LEU:HG	1.95	0.48
1:A:731:G:OP1	1:A:766:A:H1'	2.13	0.48
1:A:1310:G:H5'	13:M:77:ASN:HD21	1.79	0.48
1:A:96:G:H2'	1:A:97:G:C8	2.49	0.48
1:A:1542:U:H2'	1:A:1543:C:C6	2.48	0.48
1:A:933:G:OP2	7:G:3:ARG:HB3	2.13	0.48
16:P:52:ASP:OD2	16:P:55:ARG:HB2	2.14	0.48
1:A:264:U:H4'	17:Q:63:ARG:HD3	1.94	0.48
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.96	0.48
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.96	0.48
9:I:26:VAL:HB	9:I:33:PHE:HB2	1.96	0.48
1:A:1207:2MG:HM23	1:A:1208:C:H1'	1.95	0.48
1:A:452:A:O2'	1:A:453:A:O5'	2.32	0.48
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.78	0.48
13:M:25:ILE:HD11	13:M:66:LEU:HD21	1.94	0.48
2:B:205:ASP:OD1	2:B:206:ASP:N	2.46	0.48
1:A:877:C:O2	8:H:3:THR:HG21	2.14	0.47
1:A:1347:G:O2'	1:A:1348:U:P	2.72	0.47
19:S:11:VAL:HG22	19:S:39:THR:HB	1.95	0.47
1:A:765:G:H5"	1:A:766:A:OP1	2.14	0.47
5:E:88:LYS:HB3	5:E:123:LEU:HB2	1.95	0.47
3:C:6:HIS:HE1	3:C:8:ILE:HD12	1.78	0.47
1:A:500:G:H5"	12:L:124:LYS:HE3	1.95	0.47
7:G:37:ASN:O	7:G:41:ARG:HG3	2.14	0.47
16:P:39:TYR:CE2	16:P:41:PRO:HB3	2.49	0.47
1:A:381:C:H2'	1:A:382:A:O4'	2.14	0.47
1:A:78:G:C2	1:A:92:C:C2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:65:ALA:HB1	7:G:127:ALA:HB3	1.96	0.47
15:O:45:VAL:HG12	15:O:46:HIS:H	1.80	0.47
1:A:825:G:N2	8:H:11:THR:HG21	2.27	0.47
1:A:481:G:O2'	1:A:482:A:C8	2.63	0.47
19:S:19:VAL:HA	19:S:22:LEU:HB2	1.96	0.47
1:A:1157:A:H4'	1:A:1158:C:O5'	2.13	0.47
1:A:359:U:H2'	1:A:360:A:C8	2.50	0.47
1:A:946:A:H2'	1:A:947:G:C8	2.49	0.47
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.50	0.47
8:H:112:LEU:HD22	8:H:133:LEU:HA	1.96	0.47
1:A:1342:C:O2'	9:I:124:GLN:HB2	2.14	0.47
21:U:13:ILE:HA	21:U:22:ARG:NH1	2.29	0.47
1:A:1443:G:H5"	1:A:1446:A:C5'	2.36	0.47
10:J:49:VAL:HG21	14:N:44:LEU:HD23	1.97	0.47
1:A:1347:G:N2	1:A:1373:G:H2'	2.30	0.47
1:A:1313:U:C5	19:S:4:SER:HB2	2.43	0.47
20:T:67:ALA:O	20:T:73:HIS:ND1	2.47	0.47
11:K:48:ILE:HG13	11:K:48:ILE:H	1.44	0.47
1:A:184:G:H2'	1:A:185:A:C8	2.50	0.47
1:A:688:G:O2'	1:A:704:A:N1	2.37	0.47
1:A:1407:5MC:O2'	1:A:1408:A:H5'	2.15	0.47
5:E:11:ILE:HG23	5:E:105:VAL:HG22	1.97	0.47
19:S:20:LEU:HD12	19:S:21:GLU:HG3	1.97	0.47
2:B:119:GLU:HG3	2:B:142:LEU:HD21	1.95	0.47
1:A:950:U:H2'	1:A:951:G:C8	2.50	0.47
9:I:89:ASN:HB3	9:I:92:TYR:CE1	2.50	0.47
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.97	0.47
20:T:73:HIS:HB3	20:T:74:LYS:H	1.50	0.47
4:D:70:ILE:HG23	4:D:71:SER:N	2.30	0.47
1:A:1281:U:H5'	1:A:1282:C:C5	2.49	0.47
15:O:71:GLN:HB2	15:O:78:TYR:CD1	2.50	0.47
11:K:16:SER:O	11:K:35:PRO:HD3	2.14	0.47
1:A:217:C:H2'	1:A:218:C:H6	1.80	0.47
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.97	0.47
17:Q:59:ILE:HG23	17:Q:71:PHE:HB3	1.96	0.47
1:A:1086:U:H3	1:A:1099:G:H22	1.62	0.47
1:A:1496:C:O2'	1:A:1497:G:O5'	2.28	0.47
10:J:91:PRO:HB2	10:J:94:VAL:HB	1.98	0.46
4:D:61:LYS:HD3	4:D:206:PHE:CE2	2.51	0.46
8:H:53:VAL:HB	8:H:58:TYR:CD1	2.50	0.46
1:A:279:A:C6	17:Q:98:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:A:O2'	1:A:1522:U:O2	2.32	0.46
1:A:1112:C:H1'	3:C:179:ARG:NH1	2.30	0.46
1:A:192:U:H4'	20:T:57:ARG:HD2	1.96	0.46
1:A:372:C:H1'	1:A:373:A:OP2	2.15	0.46
19:S:40:ILE:HG13	19:S:70:LYS:O	2.15	0.46
1:A:279:A:H5"	1:A:281:G:H5'	1.97	0.46
9:I:50:LEU:HD11	9:I:81:ILE:HD12	1.97	0.46
7:G:111:ARG:HD2	7:G:112:PRO:HD2	1.97	0.46
12:L:30:ALA:HA	12:L:31:PRO:HD3	1.77	0.46
1:A:932:C:H5'	7:G:4:ARG:HG2	1.97	0.46
1:A:750:G:N3	15:O:23:GLY:HA3	2.29	0.46
1:A:116:A:H5"	25:A:1913:HOH:O	2.14	0.46
1:A:1314:C:H2'	1:A:1315:U:C6	2.51	0.46
1:A:974:A:H4'	1:A:975:A:H3'	1.97	0.46
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.97	0.46
12:L:24:VAL:HG12	12:L:24:VAL:O	2.16	0.46
1:A:1152:A:H5"	10:J:13:HIS:CG	2.50	0.46
1:A:1241:G:H2'	1:A:1242:C:C6	2.50	0.46
1:A:45:U:H2'	1:A:46:G:C8	2.51	0.46
13:M:12:ASN:H	13:M:45:VAL:HG12	1.81	0.46
1:A:974:A:OP2	14:N:41:ARG:NH1	2.49	0.46
1:A:1281:U:H4'	1:A:1282:C:OP2	2.16	0.46
3:C:16:ARG:HH22	3:C:183:ASP:HA	1.81	0.46
1:A:1375:A:H4'	7:G:29:LYS:HE2	1.97	0.46
11:K:41:THR:OG1	11:K:42:TRP:N	2.49	0.46
6:F:33:TYR:HB2	6:F:75:LEU:HD23	1.97	0.46
1:A:455:C:H6	1:A:455:C:O5'	1.99	0.46
1:A:376:G:OP2	16:P:67:THR:HG21	2.16	0.46
9:I:121:ARG:NH1	9:I:122:ALA:O	2.49	0.46
2:B:158:LEU:HA	2:B:158:LEU:HD23	1.67	0.46
3:C:91:LEU:HD23	3:C:92:ALA:N	2.31	0.46
9:I:48:GLU:N	9:I:49:PRO:HD2	2.31	0.46
19:S:10:PHE:O	19:S:39:THR:OG1	2.18	0.46
1:A:345:C:OP2	1:A:345:C:H6	1.99	0.46
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.97	0.46
1:A:1064:G:H21	1:A:1190:G:H2'	1.81	0.46
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.30	0.46
3:C:91:LEU:HD11	3:C:99:VAL:HG22	1.98	0.46
10:J:4:ILE:HD11	10:J:74:ILE:HD12	1.97	0.46
2:B:181:PHE:CE2	8:H:70:GLN:HB3	2.50	0.46
16:P:21:VAL:HG12	16:P:33:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:103:VAL:HG12	8:H:108:GLY:HA3	1.98	0.46
1:A:1257:U:H4'	1:A:1258:G:O5'	2.17	0.45
1:A:322:C:OP2	1:A:328:C:N4	2.48	0.45
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.98	0.45
8:H:84:ARG:O	8:H:135:CYS:HB2	2.16	0.45
1:A:818:G:C3'	1:A:819:A:H5"	2.47	0.45
1:A:563:A:H2'	1:A:567:G:C8	2.52	0.45
1:A:5:U:H4'	1:A:6:G:O5'	2.15	0.45
1:A:1355:G:H2'	1:A:1356:G:H8	1.80	0.45
4:D:61:LYS:HD2	4:D:207:TYR:OH	2.15	0.45
13:M:27:LYS:HA	13:M:27:LYS:HD2	1.63	0.45
11:K:58:PRO:HA	11:K:90:GLY:HA3	1.99	0.45
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.49	0.45
1:A:986:A:H1'	19:S:54:GLY:O	2.16	0.45
2:B:152:PHE:CE1	2:B:155:LEU:HD12	2.52	0.45
2:B:215:LEU:HD23	2:B:215:LEU:HA	1.79	0.45
12:L:28:LYS:HG3	12:L:33:ARG:NH1	2.31	0.45
1:A:1366:C:H2'	1:A:1367:C:H6	1.81	0.45
12:L:38:THR:HG22	12:L:39:VAL:HG23	1.98	0.45
2:B:83:MET:HE1	2:B:234:PRO:HB2	1.99	0.45
1:A:620:C:N1	4:D:135:LEU:HD13	2.31	0.45
1:A:1118:C:H1'	1:A:1179:A:C4	2.51	0.45
1:A:1210:C:O2'	1:A:1213:A:O2'	2.22	0.45
3:C:167:TRP:HE3	3:C:168:ALA:N	2.14	0.45
19:S:11:VAL:HG21	19:S:41:VAL:HG13	1.98	0.45
11:K:34:ASP:HB2	11:K:35:PRO:HD2	1.97	0.45
1:A:436:C:H2'	1:A:437:U:H6	1.80	0.45
7:G:12:LEU:HG	7:G:12:LEU:H	1.62	0.45
3:C:59:ARG:HG3	3:C:63:ASN:O	2.17	0.45
1:A:840:C:H5"	1:A:841:U:OP1	2.17	0.45
1:A:518:C:H5"	1:A:519:C:C6	2.52	0.45
1:A:1200:C:H1'	1:A:1204:A:H62	1.81	0.45
1:A:258:G:H2'	1:A:259:G:C8	2.52	0.45
5:E:83:GLU:HG2	5:E:88:LYS:HG3	1.99	0.45
1:A:1521:G:H2'	1:A:1522:U:C6	2.52	0.45
1:A:955:U:H1'	1:A:1227:A:N6	2.31	0.45
19:S:36:ARG:NH1	19:S:52:TYR:O	2.50	0.45
1:A:936:C:H2'	1:A:937:A:O4'	2.17	0.45
12:L:82:VAL:O	12:L:106:ASP:HB2	2.17	0.45
1:A:838:G:H2'	1:A:839:U:H5"	1.98	0.45
4:D:78:LEU:CD2	4:D:96:LEU:HB3	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:108:ALA:O	7:G:119:ARG:HB3	2.17	0.45
18:R:26:LEU:HD23	18:R:29:PHE:CE2	2.52	0.45
1:A:1080:A:O3'	5:E:16:THR:OG1	2.35	0.45
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.52	0.45
1:A:1357:A:H2'	1:A:1358:U:C6	2.51	0.45
1:A:1435:G:H2'	1:A:1436:U:H6	1.82	0.45
1:A:938:A:N6	1:A:939:G:C6	2.85	0.45
1:A:679:C:H2'	1:A:680:C:C6	2.52	0.45
17:Q:38:ARG:N	17:Q:38:ARG:HD2	2.30	0.45
1:A:620:C:H2'	1:A:621:A:O4'	2.17	0.45
2:B:25:ASN:HD21	2:B:27:LYS:HE3	1.81	0.45
16:P:12:LYS:HG2	16:P:13:HIS:CD2	2.52	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.17	0.45
1:A:695:A:C2	1:A:787:A:H1'	2.52	0.45
1:A:522:C:H41	12:L:53:ARG:HH22	1.65	0.45
1:A:1123:A:H2'	1:A:1124:G:C8	2.52	0.44
1:A:1519:MA6:H8	1:A:1519:MA6:O5'	2.17	0.44
2:B:219:VAL:O	2:B:223:ILE:HG13	2.16	0.44
15:O:70:LEU:HD12	15:O:81:LEU:HD12	1.99	0.44
14:N:6:LEU:HB3	14:N:23:ARG:NH2	2.31	0.44
1:A:951:G:OP2	13:M:102:ARG:NH2	2.50	0.44
15:O:85:LEU:HD23	15:O:85:LEU:HA	1.64	0.44
1:A:980:C:H5"	1:A:981:U:H5	1.81	0.44
7:G:53:LYS:HD3	7:G:53:LYS:HA	1.82	0.44
17:Q:97:SER:O	17:Q:98:LEU:HD12	2.17	0.44
1:A:452:A:H2'	1:A:453:A:C8	2.52	0.44
16:P:39:TYR:HE2	16:P:41:PRO:HB3	1.82	0.44
1:A:579:G:H2'	1:A:580:U:C6	2.51	0.44
1:A:1058:G:H5"	3:C:199:LYS:NZ	2.33	0.44
1:A:186:C:H2'	1:A:187:C:C6	2.52	0.44
12:L:54:LYS:HD2	12:L:54:LYS:N	2.33	0.44
1:A:1022:G:N2	1:A:1023:G:O6	2.49	0.44
1:A:154:C:H42	1:A:167:G:H1	1.65	0.44
1:A:999:C:H2'	1:A:1000:U:C6	2.52	0.44
1:A:839:U:H5'	1:A:840:C:C5	2.48	0.44
1:A:1106:G:H5"	3:C:172:ARG:HG2	1.98	0.44
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.99	0.44
2:B:189:ASP:OD1	2:B:189:ASP:N	2.48	0.44
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.52	0.44
11:K:69:ALA:O	11:K:73:MET:HG2	2.18	0.44
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:LEU:HD21	3:C:59:ARG:CZ	2.48	0.44
3:C:14:ILE:C	3:C:16:ARG:H	2.21	0.44
18:R:36:ASN:O	18:R:40:LEU:HG	2.18	0.44
1:A:687:A:H4'	1:A:688:G:O5'	2.17	0.44
18:R:36:ASN:OD1	18:R:39:VAL:HG12	2.16	0.44
1:A:858:G:O2'	1:A:859:A:H5'	2.18	0.44
1:A:1179:A:H2'	1:A:1180:A:O4'	2.17	0.44
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.99	0.44
4:D:28:SER:O	4:D:30:LYS:N	2.49	0.44
1:A:539:A:H2'	1:A:540:G:C8	2.53	0.44
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.53	0.44
20:T:39:LYS:O	20:T:43:LEU:HG	2.18	0.44
16:P:10:GLY:HA3	16:P:14:ASN:O	2.18	0.44
20:T:62:LEU:HA	20:T:62:LEU:HD22	1.73	0.44
5:E:112:LEU:HA	5:E:112:LEU:HD23	1.78	0.44
4:D:64:LEU:HD23	4:D:198:VAL:HG21	1.99	0.44
21:U:6:ARG:HH11	21:U:15:ARG:HH12	1.66	0.44
3:C:42:LEU:O	3:C:46:GLU:HB2	2.18	0.44
9:I:45:ALA:HA	9:I:48:GLU:HB2	2.00	0.44
1:A:1427:U:H2'	1:A:1428:A:H8	1.83	0.44
1:A:633:G:H2'	1:A:634:C:C6	2.53	0.44
1:A:278:G:C6	17:Q:95:TYR:HD2	2.36	0.44
9:I:19:LEU:HD22	9:I:59:PHE:HD2	1.83	0.44
2:B:135:GLN:O	2:B:139:LYS:HB2	2.18	0.44
8:H:51:VAL:HG21	8:H:60:ARG:HG3	2.00	0.44
1:A:767:A:H2'	1:A:768:A:O4'	2.17	0.44
8:H:127:LEU:HA	8:H:127:LEU:HD13	1.71	0.44
10:J:10:GLY:H	10:J:16:LEU:HD11	1.82	0.44
1:A:679:C:H2'	1:A:680:C:H6	1.83	0.44
1:A:1141:C:H2'	1:A:1142:G:H8	1.82	0.44
1:A:321:A:N6	1:A:329:A:OP2	2.48	0.44
18:R:31:LEU:HD22	18:R:66:LEU:HB2	2.00	0.44
2:B:54:THR:O	2:B:58:ILE:HG13	2.18	0.44
2:B:11:LEU:HA	2:B:11:LEU:HD23	1.85	0.44
13:M:62:ASN:OD1	13:M:62:ASN:N	2.51	0.44
1:A:1427:U:H2'	1:A:1428:A:C8	2.53	0.43
10:J:5:ARG:HB3	10:J:99:LYS:HE2	2.01	0.43
12:L:27:LEU:HG	12:L:28:LYS:H	1.83	0.43
9:I:19:LEU:HD23	9:I:19:LEU:HA	1.86	0.43
19:S:63:THR:HG22	19:S:64:GLU:H	1.83	0.43
1:A:1516:G:O2'	1:A:1518:MA6:H102	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:U:OP2	4:D:36:ARG:NH2	2.52	0.43
2:B:83:MET:CE	2:B:234:PRO:HB2	2.49	0.43
10:J:3:LYS:N	10:J:77:PRO:HG3	2.33	0.43
1:A:1218:C:H2'	1:A:1219:U:C6	2.54	0.43
1:A:131:C:O2	1:A:262:A:H2	2.01	0.43
3:C:68:VAL:HG12	3:C:70:VAL:HG22	1.99	0.43
7:G:99:LEU:HD23	7:G:99:LEU:HA	1.86	0.43
1:A:1368:G:OP2	9:I:112:LYS:HD3	2.19	0.43
1:A:818:G:H3'	1:A:819:A:H5"	1.99	0.43
1:A:1015:A:H2'	1:A:1016:A:O4'	2.18	0.43
6:F:22:GLU:OE2	6:F:82:ARG:NH1	2.51	0.43
1:A:1504:G:H4'	1:A:1505:G:H5'	2.01	0.43
2:B:178:ARG:NH2	8:H:74:PRO:HB3	2.34	0.43
12:L:69:TYR:CD1	12:L:90:VAL:HG21	2.54	0.43
1:A:113:G:C1'	1:A:354:G:H5'	2.47	0.43
1:A:1257:U:O2'	1:A:1258:G:P	2.77	0.43
20:T:92:LEU:HD23	20:T:92:LEU:HA	1.80	0.43
4:D:170:VAL:CG1	4:D:174:LEU:HB2	2.49	0.43
1:A:1124:G:C8	1:A:1145:C:H5	2.36	0.43
3:C:16:ARG:NH2	3:C:183:ASP:HA	2.33	0.43
12:L:77:LEU:HD23	12:L:77:LEU:HA	1.88	0.43
1:A:670:G:O2'	6:F:77:ARG:NH2	2.52	0.43
2:B:223:ILE:HG22	2:B:228:GLY:HA3	2.00	0.43
1:A:216:G:H2'	1:A:217:C:H6	1.83	0.43
2:B:59:GLU:HB2	2:B:221:LEU:HD11	2.00	0.43
1:A:1065:U:H4'	1:A:1066:C:O5'	2.19	0.43
9:I:79:LEU:HD13	9:I:83:ARG:HD2	2.01	0.43
1:A:1526:G:H2'	1:A:1527:C:H6	1.84	0.43
1:A:1132:C:H2'	1:A:1133:G:H8	1.83	0.43
8:H:14:ARG:HG3	8:H:83:ILE:HG22	1.99	0.43
1:A:113:G:H2'	1:A:114:U:H6	1.83	0.43
1:A:1000:U:H2'	1:A:1001:A:C8	2.50	0.43
1:A:1325:C:OP1	21:U:15:ARG:HD3	2.19	0.43
9:I:75:ASP:O	9:I:78:LYS:HB3	2.18	0.43
15:O:45:VAL:HB	15:O:46:HIS:ND1	2.33	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.34	0.43
12:L:60:LEU:HD13	12:L:60:LEU:HA	1.76	0.43
4:D:152:SER:O	4:D:155:LEU:HG	2.18	0.43
2:B:46:LYS:HD3	2:B:49:GLU:OE1	2.19	0.43
10:J:36:GLY:O	10:J:38:ILE:HG22	2.19	0.43
1:A:974:A:H8	1:A:974:A:OP1	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:LEU:O	3:C:35:GLU:HB3	2.18	0.43
1:A:560:U:H4'	1:A:561:U:H5"	2.01	0.43
1:A:390:C:H2'	1:A:391:G:C8	2.54	0.43
1:A:1277:C:H1'	1:A:1282:C:O2	2.19	0.43
2:B:150:SER:OG	2:B:151:GLY:N	2.52	0.43
1:A:22:G:H2'	1:A:23:C:H6	1.84	0.43
1:A:820:U:H4'	1:A:821:G:OP2	2.19	0.43
1:A:129(A):G:H1'	1:A:190(E):U:H2'	2.01	0.42
1:A:179:A:H2'	1:A:180:U:C6	2.54	0.42
1:A:31:G:N2	1:A:48:C:OP1	2.44	0.42
1:A:833:U:H2'	1:A:834:C:C6	2.54	0.42
1:A:484:G:H4'	1:A:485:G:O5'	2.19	0.42
1:A:1123:A:H4'	10:J:37:PRO:HG2	2.01	0.42
2:B:16:HIS:CD2	2:B:204:ASN:HD22	2.36	0.42
1:A:1317:C:OP1	14:N:17:LYS:HG2	2.18	0.42
1:A:1213:A:N6	1:A:1215:G:N3	2.67	0.42
13:M:82:MET:HA	13:M:89:GLY:HA3	2.01	0.42
12:L:84:LEU:O	12:L:101:VAL:HG23	2.19	0.42
19:S:50:ALA:HA	19:S:59:PRO:HA	2.01	0.42
11:K:110:ASP:HB2	18:R:88:LYS:HG3	2.00	0.42
5:E:18:ARG:HG2	5:E:19:MET:N	2.33	0.42
1:A:1025:U:H2'	1:A:1026:G:C8	2.54	0.42
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.81	0.42
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.85	0.42
1:A:1339:A:H2'	1:A:1340:A:O4'	2.19	0.42
1:A:376:G:H5"	16:P:5:ARG:HD2	2.00	0.42
14:N:16:PHE:HB2	14:N:19:ARG:HG3	2.02	0.42
10:J:34:VAL:HG22	10:J:74:ILE:HG23	2.01	0.42
1:A:838:G:N2	1:A:849:C:C2	2.88	0.42
1:A:320:C:O2'	1:A:1435:G:H1'	2.19	0.42
13:M:63:THR:HG23	13:M:64:TRP:H	1.84	0.42
6:F:30:LEU:HD11	6:F:63:TYR:HD2	1.84	0.42
1:A:1287:A:H2	1:A:1353:G:N3	2.17	0.42
1:A:1221:G:O3'	19:S:77:THR:HG21	2.20	0.42
1:A:1320:C:H5"	19:S:3:ARG:HH22	1.85	0.42
19:S:13:ASP:O	19:S:17:GLU:HG2	2.19	0.42
2:B:24:TRP:HB2	2:B:190:THR:HG22	2.02	0.42
2:B:180:LEU:HD23	2:B:180:LEU:HA	1.89	0.42
1:A:1413:A:H2'	1:A:1414:U:O4'	2.20	0.42
6:F:30:LEU:HD23	6:F:75:LEU:HD21	2.01	0.42
7:G:108:ALA:HB2	7:G:123:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:14:LYS:O	20:T:18:GLN:HG3	2.19	0.42
1:A:459:G:H1'	1:A:463:A:H61	1.84	0.42
1:A:1222:G:OP2	1:A:1322:C:N4	2.44	0.42
15:O:61:GLY:O	15:O:65:ARG:HD2	2.20	0.42
2:B:187:LEU:HD21	2:B:214:ILE:HG13	2.01	0.42
12:L:47:LYS:H	12:L:47:LYS:HG3	1.46	0.42
12:L:25:PRO:HA	12:L:27:LEU:H	1.84	0.42
3:C:69:HIS:HA	3:C:104:GLN:O	2.19	0.42
1:A:369:C:OP2	1:A:388:G:N2	2.45	0.42
4:D:150:GLU:HA	4:D:153:ARG:HG3	2.00	0.42
1:A:1347:G:C2'	1:A:1348:U:OP2	2.68	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.75	0.42
9:I:79:LEU:HA	9:I:79:LEU:HD23	1.93	0.42
10:J:24:VAL:O	10:J:28:ARG:HG2	2.20	0.42
1:A:736:C:H2'	1:A:737:A:C8	2.55	0.42
10:J:14:LYS:HB3	10:J:14:LYS:HE2	1.82	0.42
9:I:108:VAL:HG12	9:I:109:VAL:H	1.84	0.42
1:A:1001:A:H61	1:A:1040:U:H3	1.67	0.42
1:A:1196:U:OP1	1:A:1197:G:H5'	2.20	0.42
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.45	0.42
1:A:1063:C:H2'	1:A:1064:G:C8	2.55	0.42
1:A:1425:U:H2'	1:A:1426:C:C6	2.55	0.42
5:E:51:VAL:HG23	5:E:52:PRO:HD3	2.01	0.42
2:B:166:ASP:HB3	2:B:169:LYS:HB3	2.01	0.42
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.81	0.42
19:S:7:LYS:HD3	19:S:7:LYS:H	1.83	0.42
1:A:959:A:O2'	1:A:984:C:O2'	2.13	0.41
19:S:16:LEU:O	19:S:20:LEU:HG	2.20	0.41
18:R:43:PHE:C	18:R:51:LEU:HD12	2.40	0.41
1:A:1191:A:OP1	3:C:4:LYS:NZ	2.44	0.41
1:A:869:G:H5"	1:A:870:U:OP1	2.20	0.41
1:A:1139:G:O2'	1:A:1140:C:OP2	2.30	0.41
1:A:266:G:H3'	17:Q:67:LYS:HB2	2.01	0.41
1:A:664:G:OP1	18:R:64:ARG:NH1	2.53	0.41
1:A:1007:C:H2'	1:A:1008:C:C6	2.55	0.41
1:A:1391:U:H2'	1:A:1392:G:H8	1.84	0.41
1:A:1241:G:H2'	1:A:1242:C:H6	1.85	0.41
1:A:149:A:H2'	1:A:150:C:H6	1.84	0.41
1:A:474:G:H4'	16:P:81:ARG:NH2	2.36	0.41
1:A:289:G:P	25:A:1910:HOH:O	2.78	0.41
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:34:LEU:HA	13:M:34:LEU:HD23	1.89	0.41
1:A:1318:A:H5'	19:S:10:PHE:CE1	2.56	0.41
15:O:26:GLU:OE1	15:O:77:ARG:HD2	2.20	0.41
1:A:765:G:N2	1:A:813:U:OP2	2.49	0.41
1:A:1287:A:H2'	1:A:1288:A:C8	2.55	0.41
9:I:118:LYS:O	9:I:120:ARG:N	2.49	0.41
5:E:59:GLY:O	5:E:63:ARG:HD2	2.19	0.41
1:A:509:A:H3'	1:A:509:A:C8	2.54	0.41
5:E:151:LEU:HD23	5:E:151:LEU:HA	1.71	0.41
1:A:1147:C:H4'	9:I:5:TYR:HE1	1.84	0.41
1:A:1492:A:H2'	1:A:1493:A:O4'	2.21	0.41
3:C:138:VAL:HG21	3:C:168:ALA:O	2.20	0.41
4:D:3:ARG:NH1	4:D:71:SER:HB3	2.35	0.41
6:F:4:TYR:CZ	6:F:72:VAL:HG21	2.56	0.41
13:M:15:VAL:HG21	13:M:48:LEU:HD21	2.01	0.41
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.53	0.41
8:H:109:ILE:HG13	8:H:109:ILE:O	2.20	0.41
1:A:1500:A:OP2	1:A:1505:G:OP1	2.39	0.41
1:A:1257:U:O2'	1:A:1258:G:OP2	2.27	0.41
1:A:980:C:H3'	1:A:981:U:C6	2.54	0.41
11:K:18:ARG:HB3	11:K:20:TYR:HE1	1.86	0.41
1:A:812:C:H4'	1:A:813:U:O5'	2.20	0.41
1:A:410:G:H2'	1:A:429:U:C4	2.56	0.41
4:D:190:ASP:H	4:D:193:ASP:HB2	1.86	0.41
1:A:98:U:H2'	1:A:99:C:C6	2.55	0.41
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.66	0.41
1:A:840:C:H4'	1:A:841:U:O5'	2.21	0.41
10:J:63:PHE:HE1	14:N:45:ARG:HA	1.85	0.41
3:C:47:LEU:HD23	3:C:68:VAL:HG11	2.03	0.41
12:L:35:GLY:HA3	12:L:60:LEU:HD13	2.01	0.41
9:I:118:LYS:C	9:I:120:ARG:H	2.23	0.41
7:G:22:LEU:HD21	7:G:66:VAL:HG11	2.02	0.41
4:D:184:LYS:HB2	4:D:184:LYS:HE3	1.71	0.41
15:O:67:LEU:HA	15:O:67:LEU:HD23	1.82	0.41
8:H:36:LEU:HA	8:H:36:LEU:HD23	1.83	0.41
1:A:1347:G:O2'	1:A:1348:U:OP2	2.38	0.41
1:A:35:G:C6	1:A:36:C:N4	2.88	0.41
1:A:1151:A:HO2'	1:A:1152:A:H8	1.68	0.41
12:L:59:ARG:HB2	12:L:59:ARG:HE	1.57	0.41
1:A:1310:G:N7	19:S:2:PRO:HG2	2.36	0.41
12:L:44:THR:HA	12:L:45:PRO:HD3	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1465:C:H2'	1:A:1466:C:O4'	2.21	0.41
1:A:723:U:O2	1:A:723:U:H2'	2.20	0.41
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.81	0.41
1:A:875:C:O2'	8:H:14:ARG:NH1	2.54	0.41
2:B:16:HIS:CG	2:B:17:PHE:N	2.89	0.41
5:E:46:GLY:H	5:E:58:ALA:HB2	1.86	0.41
1:A:1369:C:H2'	1:A:1370:G:C8	2.56	0.41
18:R:55:ARG:HA	18:R:55:ARG:HD2	1.93	0.41
1:A:1355:G:H2'	1:A:1356:G:C8	2.56	0.41
1:A:952:U:H2'	1:A:953:G:H8	1.86	0.41
4:D:98:GLU:HG2	4:D:189:PRO:HG3	2.03	0.41
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.56	0.41
1:A:1163:C:H2'	1:A:1164:G:C8	2.56	0.41
1:A:1367:C:H5'	10:J:60:ARG:NH1	2.36	0.41
9:I:32:ASP:OD1	9:I:33:PHE:N	2.54	0.41
11:K:34:ASP:OD2	11:K:38:ASN:HB2	2.21	0.41
1:A:1405:G:H1	1:A:1496:C:N4	2.19	0.41
1:A:815:A:N3	1:A:1527:C:O2'	2.46	0.41
1:A:701:C:H4'	1:A:702:A:O5'	2.21	0.41
13:M:23:TYR:HB3	13:M:67:GLU:H	1.85	0.41
1:A:442:C:H42	1:A:492:G:H1	1.68	0.41
19:S:25:LYS:N	19:S:25:LYS:HD2	2.36	0.41
1:A:1307:U:H2'	1:A:1308:U:C6	2.56	0.41
1:A:123:C:OP1	1:A:312:C:H5'	2.21	0.41
16:P:74:LEU:HD22	16:P:79:VAL:HG21	2.02	0.41
1:A:397:A:H5'	1:A:398:C:OP1	2.20	0.41
1:A:103:C:P	20:T:17:ARG:HH12	2.44	0.40
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.20	0.40
18:R:26:LEU:HA	18:R:26:LEU:HD12	1.97	0.40
2:B:27:LYS:HB2	2:B:27:LYS:HE3	1.88	0.40
2:B:55:PHE:CD1	2:B:58:ILE:HD12	2.56	0.40
1:A:1526:G:H2'	1:A:1527:C:C6	2.56	0.40
3:C:112:SER:O	3:C:116:VAL:HG23	2.21	0.40
1:A:912:C:O2'	1:A:913:A:H5'	2.21	0.40
1:A:663:A:H2'	1:A:664:G:O4'	2.21	0.40
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.40
1:A:1392:G:N2	1:A:1502:A:C8	2.83	0.40
14:N:17:LYS:HG3	14:N:18:VAL:HG13	2.03	0.40
10:J:51:ARG:NH2	10:J:61:GLU:HB2	2.36	0.40
10:J:79:ARG:HG2	10:J:79:ARG:H	1.68	0.40
1:A:620:C:C1'	4:D:135:LEU:HD13	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:TYR:CD1	2:B:94:ASN:HB2	2.56	0.40
2:B:217:ARG:HD3	2:B:217:ARG:HA	1.84	0.40
3:C:16:ARG:HD3	3:C:16:ARG:HA	1.94	0.40
21:U:18:TYR:CG	21:U:24:ARG:HG2	2.56	0.40
1:A:939:G:H2'	1:A:940:C:C6	2.56	0.40
5:E:93:PRO:HG2	8:H:105:ARG:HH21	1.87	0.40
1:A:1219:U:C4	1:A:1220:G:N7	2.89	0.40
15:O:6:GLU:CD	15:O:6:GLU:H	2.23	0.40
1:A:527:7MG:O2'	1:A:535:A:N1	2.41	0.40
1:A:79:G:C6	1:A:80:G:C6	3.10	0.40
1:A:1150:U:H2'	1:A:1151:A:H5'	2.03	0.40
1:A:152:A:N6	1:A:170:U:C2	2.89	0.40
1:A:19:C:OP1	5:E:125:SER:OG	2.31	0.40
3:C:33:LEU:HA	3:C:33:LEU:HD23	1.98	0.40
1:A:1020:U:H2'	1:A:1021:G:H8	1.87	0.40
3:C:16:ARG:HB2	3:C:16:ARG:HH11	1.87	0.40
1:A:1055:A:O2'	3:C:156:ARG:NH2	2.54	0.40
1:A:453:A:C6	1:A:454:C:N3	2.90	0.40
3:C:121:ALA:HB2	3:C:198:VAL:HG21	2.02	0.40
1:A:485:G:O2'	1:A:486:U:P	2.79	0.40
19:S:7:LYS:NZ	19:S:7:LYS:HB2	2.36	0.40
1:A:1431:C:H2'	1:A:1432:G:O4'	2.22	0.40
1:A:538:G:H5"	12:L:114:LYS:HB2	2.03	0.40
1:A:868:C:H3'	25:A:2103:HOH:O	2.21	0.40
11:K:80:VAL:HG22	11:K:103:LEU:HD22	2.04	0.40
5:E:144:THR:HG22	5:E:145:LYS:H	1.87	0.40
1:A:110:C:H2'	1:A:111:G:O4'	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:U:O4	1:A:1384:C:O2'[3_545]	2.19	0.01

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%)	15 53
3	C	204/239 (85%)	180 (88%)	23 (11%)	1 (0%)	34 73
4	D	206/209 (99%)	194 (94%)	12 (6%)	0	100 100
5	E	148/162 (91%)	140 (95%)	8 (5%)	0	100 100
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100 100
7	G	153/156 (98%)	143 (94%)	10 (6%)	0	100 100
8	H	136/138 (99%)	134 (98%)	2 (2%)	0	100 100
9	I	125/128 (98%)	114 (91%)	11 (9%)	0	100 100
10	J	96/105 (91%)	77 (80%)	17 (18%)	2 (2%)	9 43
11	K	114/129 (88%)	106 (93%)	8 (7%)	0	100 100
12	L	121/135 (90%)	112 (93%)	8 (7%)	1 (1%)	24 64
13	M	116/126 (92%)	106 (91%)	10 (9%)	0	100 100
14	N	58/61 (95%)	53 (91%)	5 (9%)	0	100 100
15	O	85/89 (96%)	83 (98%)	2 (2%)	0	100 100
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100 100
17	Q	97/105 (92%)	90 (93%)	7 (7%)	0	100 100
18	R	68/88 (77%)	63 (93%)	5 (7%)	0	100 100
19	S	78/93 (84%)	69 (88%)	8 (10%)	1 (1%)	15 53
20	T	97/106 (92%)	84 (87%)	13 (13%)	0	100 100
21	U	22/27 (82%)	21 (96%)	1 (4%)	0	100 100
All	All	2336/2541 (92%)	2153 (92%)	175 (8%)	8 (0%)	46 81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
12	L	28	LYS
19	S	31	ILE
3	C	15	THR
10	J	34	VAL
10	J	72	VAL

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Mol	Chain	Res	Type
2	B	229	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	202/220 (92%)	182 (90%)	20 (10%)	10 36
3	C	160/188 (85%)	126 (79%)	34 (21%)	1 5
4	D	180/181 (99%)	167 (93%)	13 (7%)	18 55
5	E	115/123 (94%)	96 (84%)	19 (16%)	3 13
6	F	90/90 (100%)	81 (90%)	9 (10%)	9 35
7	G	126/127 (99%)	115 (91%)	11 (9%)	13 44
8	H	119/119 (100%)	103 (87%)	16 (13%)	5 21
9	I	98/99 (99%)	87 (89%)	11 (11%)	7 30
10	J	87/92 (95%)	80 (92%)	7 (8%)	15 49
11	K	88/99 (89%)	80 (91%)	8 (9%)	12 41
12	L	103/110 (94%)	86 (84%)	17 (16%)	3 13
13	M	94/101 (93%)	84 (89%)	10 (11%)	8 33
14	N	49/50 (98%)	42 (86%)	7 (14%)	4 19
15	O	79/80 (99%)	76 (96%)	3 (4%)	40 76
16	P	72/74 (97%)	64 (89%)	8 (11%)	8 30
17	Q	94/97 (97%)	83 (88%)	11 (12%)	7 27
18	R	61/77 (79%)	54 (88%)	7 (12%)	7 28
19	S	71/80 (89%)	62 (87%)	9 (13%)	5 24
20	T	76/82 (93%)	67 (88%)	9 (12%)	6 27
21	U	19/22 (86%)	19 (100%)	0	100 100
All	All	1983/2111 (94%)	1754 (88%)	229 (12%)	7 28

All (229) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11	LEU
2	B	24	TRP
2	B	25	ASN
2	B	32	ILE
2	B	44	LEU
2	B	48	MET
2	B	69	LEU
2	B	76	GLN
2	B	97	TRP
2	B	102	LEU
2	B	106	LYS
2	B	144	ARG
2	B	162	ILE
2	B	163	PHE
2	B	165	VAL
2	B	178	ARG
2	B	187	LEU
2	B	190	THR
2	B	208	ILE
2	B	221	LEU
3	C	3	ASN
3	C	11	ARG
3	C	14	ILE
3	C	15	THR
3	C	16	ARG
3	C	17	ASP
3	C	21	ARG
3	C	27	LYS
3	C	28	GLN
3	C	32	LEU
3	C	34	LEU
3	C	42	LEU
3	C	46	GLU
3	C	52	LEU
3	C	54	ARG
3	C	64	VAL
3	C	70	VAL
3	C	79	ARG
3	C	91	LEU
3	C	99	VAL
3	C	107	GLN
3	C	108	ASN
3	C	130	VAL

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Mol	Chain	Res	Type
3	C	157	ILE
3	C	166	GLU
3	C	167	TRP
3	C	176	HIS
3	C	177	THR
3	C	178	LEU
3	C	188	LEU
3	C	190	ARG
3	C	192	THR
3	C	195	VAL
3	C	204	LEU
4	D	10	ARG
4	D	15	GLU
4	D	19	LEU
4	D	21	LEU
4	D	25	ARG
4	D	26	CYS
4	D	34	GLU
4	D	64	LEU
4	D	78	LEU
4	D	122	ARG
4	D	135	LEU
4	D	145	GLU
4	D	192	GLU
5	E	12	LEU
5	E	15	ARG
5	E	19	MET
5	E	31	LEU
5	E	43	LEU
5	E	51	VAL
5	E	53	LEU
5	E	63	ARG
5	E	68	GLU
5	E	78	HIS
5	E	79	GLU
5	E	80	ILE
5	E	89	ILE
5	E	118	ILE
5	E	120	THR
5	E	125	SER
5	E	147	ASP
5	E	150	ARG

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Mol	Chain	Res	Type
5	E	151	LEU
6	F	10	LEU
6	F	15	ASP
6	F	19	LEU
6	F	32	ASN
6	F	47	ARG
6	F	61	LEU
6	F	70	ASP
6	F	92	LYS
6	F	95	GLU
7	G	8	GLU
7	G	12	LEU
7	G	22	LEU
7	G	24	THR
7	G	57	GLU
7	G	59	LEU
7	G	85	TYR
7	G	92	SER
7	G	113	GLU
7	G	125	MET
7	G	126	ASP
8	H	11	THR
8	H	18	ARG
8	H	23	SER
8	H	24	THR
8	H	26	VAL
8	H	29	SER
8	H	39	LEU
8	H	50	ARG
8	H	56	LYS
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	98	LYS
8	H	105	ARG
8	H	120	THR
8	H	127	LEU
9	I	10	ARG
9	I	14	VAL
9	I	53	VAL
9	I	54	ASP
9	I	79	LEU

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Mol	Chain	Res	Type
9	I	81	ILE
9	I	108	VAL
9	I	109	VAL
9	I	118	LYS
9	I	121	ARG
9	I	127	LYS
10	J	4	ILE
10	J	57	LYS
10	J	62	HIS
10	J	69	ASN
10	J	71	LEU
10	J	79	ARG
10	J	80	LYS
11	K	18	ARG
11	K	29	ILE
11	K	33	THR
11	K	41	THR
11	K	48	ILE
11	K	80	VAL
11	K	104	GLN
11	K	120	ARG
12	L	18	VAL
12	L	19	ARG
12	L	33	ARG
12	L	42	THR
12	L	43	VAL
12	L	47	LYS
12	L	60	LEU
12	L	62	SER
12	L	64	TYR
12	L	67	THR
12	L	79	GLU
12	L	82	VAL
12	L	97	ARG
12	L	101	VAL
12	L	112	ASP
12	L	113	ARG
12	L	122	THR
13	M	16	ASP
13	M	35	GLU
13	M	44	ARG
13	M	45	VAL

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Mol	Chain	Res	Type
13	M	49	THR
13	M	64	TRP
13	M	70	LEU
13	M	84	ILE
13	M	90	LEU
13	M	110	ARG
14	N	11	LYS
14	N	22	THR
14	N	24	CYS
14	N	29	ARG
14	N	31	ARG
14	N	41	ARG
14	N	58	LYS
15	O	39	LEU
15	O	70	LEU
15	O	81	LEU
16	P	2	VAL
16	P	9	PHE
16	P	20	VAL
16	P	45	THR
16	P	54	GLU
16	P	55	ARG
16	P	68	ASP
16	P	82	GLN
17	Q	4	LYS
17	Q	15	MET
17	Q	34	LYS
17	Q	38	ARG
17	Q	53	LEU
17	Q	59	ILE
17	Q	76	LEU
17	Q	83	ASP
17	Q	86	GLU
17	Q	92	ARG
17	Q	98	LEU
18	R	25	THR
18	R	46	GLU
18	R	47	THR
18	R	68	LYS
18	R	69	THR
18	R	87	ARG
18	R	88	LYS

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Mol	Chain	Res	Type
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	10	PHE
19	S	15	LEU
19	S	19	VAL
19	S	29	ARG
19	S	39	THR
19	S	63	THR
20	T	9	ASN
20	T	10	LEU
20	T	19	SER
20	T	56	MET
20	T	62	LEU
20	T	72	LEU
20	T	73	HIS
20	T	84	LEU
20	T	104	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	16	HIS
2	B	25	ASN
3	C	108	ASN
5	E	78	HIS
5	E	141	GLN
6	F	11	ASN
9	I	3	GLN
10	J	13	HIS
11	K	26	ASN
13	M	77	ASN
19	S	23	ASN
19	S	47	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	282 (18%)	47 (3%)

All (282) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	9	G
1	A	32	A
1	A	33	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	66	G
1	A	68	G
1	A	81	U
1	A	88	A
1	A	91	C
1	A	92	C
1	A	115	G
1	A	116	A
1	A	117	G
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	136	C
1	A	163	C
1	A	180	U
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	195	A
1	A	197	A
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	231	G
1	A	243	A
1	A	244	U
1	A	247	G
1	A	251	G

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Mol	Chain	Res	Type
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	281	G
1	A	282	A
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	367	U
1	A	373	A
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
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	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C

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Mol	Chain	Res	Type
1	A	518	C
1	A	519	C
1	A	527	7MG
1	A	532	A
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	570	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	588	G
1	A	616	G
1	A	618	C
1	A	620	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	774	G
1	A	777	A
1	A	780	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A

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Mol	Chain	Res	Type
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	818	G
1	A	819	A
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	858	G
1	A	859	A
1	A	864	A
1	A	869	G
1	A	872	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	916	G
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	942	G
1	A	945	G
1	A	954	G
1	A	960	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	982	U
1	A	984	C
1	A	989	C
1	A	991	U
1	A	992	U
1	A	993	G

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Mol	Chain	Res	Type
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1026	G
1	A	1031	G
1	A	1045	C
1	A	1050	G
1	A	1051	C
1	A	1060	C
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1125	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1145	C
1	A	1146	A
1	A	1149	C
1	A	1152	A
1	A	1153	C
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1161	C
1	A	1164	G
1	A	1171	G
1	A	1183	A
1	A	1184	G
1	A	1191	A
1	A	1193	G

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Mol	Chain	Res	Type
1	A	1196	U
1	A	1197	G
1	A	1198	G
1	A	1201	A
1	A	1202	G
1	A	1207	2MG
1	A	1211	U
1	A	1212	U
1	A	1213	A
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1236	A
1	A	1238	A
1	A	1241	G
1	A	1242	C
1	A	1257	U
1	A	1258	G
1	A	1269	A
1	A	1270	C
1	A	1278	U
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1288	A
1	A	1289	A
1	A	1297	C
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1306	A
1	A	1312	G
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1326	C
1	A	1335	C
1	A	1336	C
1	A	1338	G

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Mol	Chain	Res	Type
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1368	G
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1398	A
1	A	1400	5MC
1	A	1443	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1452	C
1	A	1454	G
1	A	1487	G
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (47) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	7	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	251	G

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Mol	Chain	Res	Type
1	A	281	G
1	A	328	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	532	A
1	A	559	A
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	840	C
1	A	913	A
1	A	975	A
1	A	991	U
1	A	992	U
1	A	1065	U
1	A	1067	A
1	A	1139	G
1	A	1145	C
1	A	1182	G
1	A	1183	A
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	2MG	A	1207	1	17,26,27	2.17	4 (23%)	21,38,41	2.14	3 (14%)
1	5MC	A	1400	1	13,22,23	0.94	0	15,32,35	0.96	1 (6%)
1	4OC	A	1402	1	13,23,24	0.47	0	18,32,35	0.69	0
1	5MC	A	1404	1	13,22,23	0.80	0	15,32,35	0.77	0
1	5MC	A	1407	1	13,22,23	0.91	0	15,32,35	1.12	3 (20%)
1	UR3	A	1498	1	12,22,23	0.63	0	16,32,35	1.25	2 (12%)
1	MA6	A	1518	1	16,26,27	1.16	4 (25%)	18,38,41	1.14	2 (11%)
1	MA6	A	1519	1	16,26,27	1.39	4 (25%)	18,38,41	1.04	2 (11%)
1	PSU	A	1540	1,23	13,21,22	1.13	1 (7%)	18,30,33	3.91	6 (33%)
1	PSU	A	1541	1	13,21,22	1.01	1 (7%)	18,30,33	3.58	5 (27%)
1	PSU	A	516	1,23	13,21,22	1.18	3 (23%)	18,30,33	3.65	5 (27%)
1	7MG	A	527	1	19,26,27	2.45	5 (26%)	24,39,42	1.96	5 (20%)
1	M2G	A	966	1	17,27,28	1.96	4 (23%)	22,40,43	1.93	1 (4%)
1	5MC	A	967	1	13,22,23	0.78	0	15,32,35	0.83	1 (6%)
12	0TD	L	92	12	4,9,10	0.96	0	4,11,13	3.19	4 (100%)

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	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	5MC	A	1400	1	-	0/3/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/7/29/30	0/2/2/2
1	5MC	A	1404	1	-	0/3/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1540	1,23	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	1,23	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	0/7/37/38	0/3/3/3
1	M2G	A	966	1	-	0/7/29/30	0/3/3/3
1	5MC	A	967	1	-	0/3/25/26	0/2/2/2
12	0TD	L	92	12	-	0/2/12/14	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-7.25	1.34	1.45
1	A	527	7MG	CM7-N7	-2.69	1.41	1.46
1	A	516	PSU	C5-C1'	-2.26	1.50	1.52
1	A	516	PSU	O4'-C1'	-2.13	1.41	1.44
1	A	527	7MG	C6-N1	2.01	1.36	1.33
1	A	1518	MA6	C2-N3	2.04	1.35	1.32
1	A	1518	MA6	C5-C4	2.05	1.45	1.40
1	A	1207	2MG	C2-N1	2.06	1.42	1.34
1	A	1519	MA6	C2-N1	2.08	1.37	1.33
1	A	1519	MA6	C2-N3	2.15	1.36	1.32
1	A	1518	MA6	C2-N1	2.30	1.38	1.33
1	A	1519	MA6	C4-N3	2.32	1.39	1.35
1	A	1518	MA6	C6-N1	2.37	1.37	1.34
1	A	516	PSU	C4-N3	2.62	1.38	1.33
1	A	1207	2MG	C4-N3	2.83	1.40	1.35
1	A	1541	PSU	C4-N3	2.99	1.38	1.33
1	A	1519	MA6	C6-N1	3.04	1.38	1.34
1	A	966	M2G	C2-N1	3.15	1.40	1.34
1	A	1540	PSU	C4-N3	3.22	1.39	1.33
1	A	966	M2G	C2-N2	3.25	1.40	1.34
1	A	966	M2G	C4-N3	3.35	1.41	1.35
1	A	527	7MG	C4-N3	4.34	1.39	1.34
1	A	527	7MG	C2-N2	4.65	1.43	1.34
1	A	966	M2G	C6-N1	5.39	1.43	1.33
1	A	1207	2MG	C6-N1	5.52	1.43	1.33
1	A	1207	2MG	C2-N2	5.73	1.40	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1540	PSU	N1-C2-N3	-13.96	119.43	128.33
1	A	516	PSU	N1-C2-N3	-13.16	119.94	128.33
1	A	1541	PSU	N1-C2-N3	-12.88	120.11	128.33
1	A	966	M2G	C5-C6-N1	-8.09	112.52	123.59
1	A	1207	2MG	C5-C6-N1	-7.54	113.29	123.59
1	A	527	7MG	C5-C4-N3	-7.13	119.88	126.82
12	L	92	0TD	CSB-SB-CB	-4.81	92.47	101.54
1	A	1540	PSU	C5-C1'-C2'	-4.09	108.26	115.52
1	A	516	PSU	C5-C6-N1	-3.16	119.93	124.39
12	L	92	0TD	C-CA-N	-2.64	104.32	109.83
12	L	92	0TD	CB-CA-N	-2.54	104.16	109.66
1	A	1407	5MC	N4-C4-N3	-2.21	113.75	116.95
1	A	1541	PSU	C5-C6-N1	-2.20	121.28	124.39
1	A	1540	PSU	C5-C6-N1	-2.15	121.36	124.39
1	A	527	7MG	C5-C6-N1	-2.07	120.28	123.46
12	L	92	0TD	O-C-CA	-2.04	120.06	125.44
1	A	1498	UR3	C4'-O4'-C1'	2.01	111.93	109.72
1	A	1519	MA6	N3-C2-N1	2.03	130.45	128.89
1	A	1407	5MC	C5-C4-N3	2.07	124.72	121.27
1	A	527	7MG	C2-N3-C4	2.08	120.59	114.53
1	A	1407	5MC	CM5-C5-C6	2.18	123.01	118.62
1	A	967	5MC	CM5-C5-C6	2.29	123.22	118.62
1	A	1518	MA6	C2-N1-C6	2.32	116.37	111.43
1	A	1519	MA6	C2-N1-C6	2.46	116.66	111.43
1	A	527	7MG	C6-N1-C2	2.49	119.39	115.94
1	A	1400	5MC	CM5-C5-C6	2.54	123.74	118.62
1	A	1207	2MG	C4-C5-N7	2.57	111.85	109.48
1	A	1498	UR3	C6-C5-C4	2.73	122.39	117.28
1	A	1518	MA6	N3-C2-N1	2.84	131.07	128.89
1	A	1541	PSU	C6-N1-C2	2.88	120.09	115.47
1	A	1540	PSU	O4'-C1'-C2'	3.04	107.83	104.73
1	A	1540	PSU	C6-N1-C2	3.09	120.44	115.47
1	A	516	PSU	C6-N1-C2	3.15	120.54	115.47
1	A	1541	PSU	O4'-C1'-C2'	3.35	108.14	104.73
1	A	516	PSU	O4'-C1'-C2'	3.50	108.29	104.73
1	A	527	7MG	N3-C4-N9	3.74	132.37	126.75
1	A	1207	2MG	C6-N1-C2	4.77	122.24	115.31
1	A	516	PSU	C4-N3-C2	5.37	119.89	115.25
1	A	1540	PSU	C4-N3-C2	5.85	120.30	115.25
1	A	1541	PSU	C4-N3-C2	5.92	120.37	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1400	5MC	1	0
1	A	1404	5MC	1	0
1	A	1407	5MC	1	0
1	A	1518	MA6	2	0
1	A	1519	MA6	2	0
1	A	527	7MG	2	0
1	A	967	5MC	2	0
12	L	92	0TD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 267 ligands modelled in this entry, 266 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	-	33,42,42	1.37	5 (15%)	36,63,63	1.58	3 (8%)

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	-	-	0/16/87/87	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	1601	SRY	O53-C53	-3.27	1.36	1.44
22	A	1601	SRY	O51-C51	-2.63	1.36	1.43
22	A	1601	SRY	C23-N23	-2.59	1.43	1.47
22	A	1601	SRY	C11-N11	-2.30	1.43	1.47
22	A	1601	SRY	O32-C32	-2.14	1.40	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	1601	SRY	C13-O13-C22	-5.67	106.12	116.30
22	A	1601	SRY	O42-C12-C22	-3.84	103.65	107.42
22	A	1601	SRY	C13-C23-N23	2.04	115.01	111.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1601	SRY	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1498/1522 (98%)	-0.12	33 (2%) 65 65	70, 129, 260, 393	0
2	B	234/256 (91%)	-0.27	2 (0%) 85 86	95, 139, 218, 251	0
3	C	206/239 (86%)	0.23	16 (7%) 16 16	129, 201, 262, 285	0
4	D	208/209 (99%)	-0.06	6 (2%) 55 55	87, 136, 183, 219	0
5	E	150/162 (92%)	-0.32	0 100 100	72, 103, 137, 175	0
6	F	101/101 (100%)	-0.40	0 100 100	120, 154, 180, 209	0
7	G	155/156 (99%)	0.08	12 (7%) 16 16	132, 181, 235, 243	0
8	H	138/138 (100%)	-0.43	0 100 100	65, 93, 130, 146	0
9	I	127/128 (99%)	0.21	7 (5%) 29 28	136, 204, 254, 268	0
10	J	98/105 (93%)	0.77	16 (16%) 2 2	152, 218, 293, 338	0
11	K	116/129 (89%)	-0.28	0 100 100	100, 130, 166, 195	0
12	L	123/135 (91%)	-0.20	0 100 100	71, 124, 164, 204	0
13	M	118/126 (93%)	0.01	5 (4%) 40 38	131, 161, 192, 300	0
14	N	60/61 (98%)	0.83	9 (15%) 3 3	146, 184, 244, 276	0
15	O	87/89 (97%)	-0.21	0 100 100	83, 116, 157, 169	0
16	P	83/88 (94%)	-0.19	0 100 100	97, 129, 169, 193	0
17	Q	99/105 (94%)	-0.35	0 100 100	78, 106, 146, 159	0
18	R	70/88 (79%)	-0.31	0 100 100	92, 127, 183, 213	0
19	S	80/93 (86%)	0.84	11 (13%) 4 3	176, 226, 259, 274	0
20	T	99/106 (93%)	-0.22	1 (1%) 84 85	99, 131, 178, 198	0
21	U	24/27 (88%)	1.77	9 (37%) 0 1	139, 164, 207, 223	0
All	All	3874/4063 (95%)	-0.06	127 (3%) 50 49	65, 140, 243, 393	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	103	VAL	8.7
14	N	2	ALA	7.9
3	C	65	ALA	7.3
19	S	40	ILE	7.2
10	J	33	GLN	6.8
10	J	34	VAL	6.7
7	G	2	ALA	6.4
19	S	38	SER	6.3
21	U	25	LYS	6.2
10	J	37	PRO	6.2
1	A	793	U	6.1
9	I	128	ARG	5.9
1	A	1129	C	5.4
10	J	32	ALA	5.3
21	U	24	ARG	5.3
20	T	106	ALA	5.2
7	G	156	TRP	5.1
10	J	90	LEU	5.0
14	N	3	ARG	5.0
14	N	4	LYS	4.9
3	C	102	ASN	4.7
1	A	1019	C	4.6
21	U	18	TYR	4.4
9	I	9	ARG	4.3
10	J	4	ILE	4.3
10	J	74	ILE	4.3
1	A	1037	C	4.2
1	A	1018	C	4.1
21	U	11	GLY	4.1
10	J	76	ASN	4.1
1	A	1006	C	4.1
21	U	17	THR	4.0
13	M	7	VAL	4.0
1	A	1036	G	3.8
19	S	4	SER	3.8
13	M	117	VAL	3.7
4	D	35	ARG	3.7
14	N	18	VAL	3.7
9	I	102	LEU	3.6
3	C	64	VAL	3.6
21	U	5	ASP	3.6
19	S	69	HIS	3.5
3	C	193	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	789	U	3.5
7	G	154	TYR	3.4
10	J	89	ASP	3.4
1	A	1004	A	3.4
3	C	66	VAL	3.4
1	A	993	G	3.3
1	A	994	A	3.3
10	J	77	PRO	3.3
1	A	1005	A	3.3
10	J	36	GLY	3.3
14	N	6	LEU	3.3
19	S	41	VAL	3.2
9	I	4	TYR	3.2
3	C	161	GLU	3.2
10	J	75	ILE	3.2
7	G	83	ALA	3.2
7	G	82	GLY	3.1
13	M	100	GLY	3.1
19	S	59	PRO	3.1
9	I	8	GLY	3.0
1	A	1007	C	3.0
1	A	1539	C	3.0
4	D	9	CYS	2.9
7	G	84	ASN	2.9
1	A	1032	G	2.9
3	C	87	LEU	2.8
1	A	995	C	2.8
3	C	101	LEU	2.8
1	A	81	U	2.7
1	A	1257	U	2.7
1	A	1135	U	2.7
2	B	127	ILE	2.7
7	G	80	VAL	2.7
13	M	6	GLY	2.7
1	A	792	A	2.7
10	J	38	ILE	2.7
7	G	7	ALA	2.6
14	N	13	THR	2.6
7	G	79	ARG	2.5
3	C	146	ALA	2.5
14	N	11	LYS	2.5
14	N	17	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1047	G	2.4
1	A	1531	A	2.4
14	N	30	ALA	2.4
21	U	16	GLY	2.4
7	G	78	ARG	2.4
7	G	81	GLY	2.4
1	A	82	U	2.4
10	J	39	PRO	2.4
10	J	100	THR	2.3
4	D	42	GLN	2.3
3	C	196	LEU	2.3
19	S	81	ARG	2.3
3	C	178	LEU	2.3
4	D	18	LYS	2.3
1	A	1224	G	2.3
4	D	23	GLY	2.2
9	I	126	SER	2.2
1	A	1033	G	2.2
3	C	155	GLY	2.2
1	A	1143	G	2.2
19	S	29	ARG	2.2
1	A	202	U	2.1
2	B	135	GLN	2.1
4	D	26	CYS	2.1
1	A	1020	U	2.1
1	A	1134	G	2.1
9	I	33	PHE	2.1
1	A	790	A	2.1
21	U	2	GLY	2.1
3	C	58	GLU	2.1
19	S	77	THR	2.1
19	S	34	TRP	2.1
10	J	88	LEU	2.1
7	G	5	ARG	2.1
19	S	55	LYS	2.1
3	C	60	ALA	2.1
1	A	1002	G	2.0
13	M	101	GLN	2.0
1	A	1144	G	2.0
1	A	1138	G	2.0
3	C	110	ASN	2.0
21	U	8	THR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
1	UR3	A	1498	21/22	0.96	0.16	-	106,117,127,143	0
1	PSU	A	516	20/21	0.94	0.14	-	121,133,147,153	0
1	M2G	A	966	25/26	0.94	0.18	-	117,136,146,153	0
1	MA6	A	1518	24/25	0.97	0.14	-	110,123,144,146	0
1	4OC	A	1402	22/23	0.98	0.18	-	104,109,121,128	0
12	0TD	L	92	10/11	0.97	0.35	-	103,124,136,321	0
1	5MC	A	1400	21/22	0.94	0.18	-	98,130,139,140	0
1	PSU	A	1541	20/21	0.65	0.58	-	272,282,296,297	0
1	PSU	A	1540	20/21	0.64	0.59	-	182,221,301,301	0
1	5MC	A	1407	21/22	0.94	0.15	-	118,141,154,159	0
1	5MC	A	1404	21/22	0.96	0.15	-	103,108,121,123	0
1	5MC	A	967	21/22	0.95	0.16	-	121,129,139,144	0
1	7MG	A	527	24/25	0.97	0.16	-	94,105,118,125	0
1	MA6	A	1519	24/25	0.96	0.16	-	101,119,127,132	0
1	2MG	A	1207	24/25	0.84	0.26	-	175,197,217,222	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1725	1/1	0.85	0.96	26.90	133,133,133,133	0
23	MG	A	1734	1/1	0.79	0.94	24.45	102,102,102,102	0
23	MG	A	1836	1/1	0.81	0.42	22.29	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	B	301	1/1	0.90	0.44	20.07	131,131,131,131	0
23	MG	H	203	1/1	0.94	0.68	15.37	120,120,120,120	0
23	MG	A	1835	1/1	0.92	0.83	12.65	132,132,132,132	0
23	MG	A	1813	1/1	0.85	0.49	9.97	139,139,139,139	0
23	MG	A	1607	1/1	0.99	0.39	9.39	91,91,91,91	0
23	MG	A	1620	1/1	0.79	0.57	9.36	111,111,111,111	0
23	MG	A	1720	1/1	0.86	0.27	8.38	97,97,97,97	0
23	MG	A	1751	1/1	0.72	0.41	7.87	104,104,104,104	0
23	MG	A	1838	1/1	0.89	0.31	7.20	82,82,82,82	0
23	MG	A	1732	1/1	0.89	0.48	7.19	126,126,126,126	0
23	MG	A	1777	1/1	0.74	0.27	4.91	102,102,102,102	0
23	MG	A	1650	1/1	0.97	0.28	4.20	109,109,109,109	0
23	MG	A	1798	1/1	0.85	0.20	4.07	117,117,117,117	0
23	MG	A	1755	1/1	0.96	0.21	4.01	81,81,81,81	0
23	MG	A	1653	1/1	0.98	0.23	3.89	86,86,86,86	0
23	MG	A	1735	1/1	0.91	0.29	3.74	83,83,83,83	0
23	MG	A	1739	1/1	0.91	0.27	3.60	127,127,127,127	0
23	MG	A	1817	1/1	0.93	0.67	3.32	119,119,119,119	0
23	MG	A	1709	1/1	0.92	0.32	3.20	138,138,138,138	0
23	MG	A	1845	1/1	0.84	0.36	3.17	128,128,128,128	0
23	MG	A	1643	1/1	0.76	0.26	3.14	123,123,123,123	0
23	MG	A	1742	1/1	0.97	0.27	2.87	126,126,126,126	0
23	MG	A	1757	1/1	0.97	0.20	2.82	78,78,78,78	0
23	MG	A	1721	1/1	0.90	0.24	2.46	99,99,99,99	0
23	MG	T	201	1/1	0.96	0.38	2.21	70,70,70,70	0
23	MG	A	1759	1/1	0.93	0.29	1.78	112,112,112,112	0
23	MG	N	102	1/1	0.59	0.49	1.67	139,139,139,139	0
23	MG	A	1762	1/1	0.94	0.24	1.63	102,102,102,102	0
23	MG	A	1625	1/1	0.94	0.23	1.62	83,83,83,83	0
23	MG	A	1611	1/1	0.93	0.24	1.58	74,74,74,74	0
23	MG	A	1752	1/1	0.76	0.46	1.27	146,146,146,146	0
23	MG	A	1637	1/1	0.94	0.19	1.16	118,118,118,118	0
23	MG	A	1810	1/1	0.84	0.20	1.03	151,151,151,151	0
23	MG	A	1658	1/1	0.87	0.20	0.92	134,134,134,134	0
23	MG	A	1787	1/1	0.81	0.41	0.91	140,140,140,140	0
23	MG	A	1692	1/1	0.99	0.20	0.89	92,92,92,92	0
23	MG	A	1642	1/1	0.97	0.19	0.64	65,65,65,65	0
24	ZN	D	301	1/1	0.97	0.35	0.58	113,113,113,113	0
23	MG	A	1617	1/1	0.93	0.21	0.55	75,75,75,75	0
23	MG	A	1626	1/1	0.97	0.15	0.25	87,87,87,87	0
23	MG	U	1300	1/1	0.97	0.30	0.18	166,166,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1616	1/1	0.98	0.17	0.18	80,80,80,80	0
23	MG	A	1708	1/1	0.84	0.15	0.17	170,170,170,170	0
23	MG	A	1689	1/1	0.99	0.15	0.10	149,149,149,149	0
22	SRY	A	1601	40/40	0.96	0.20	0.04	86,111,131,138	0
23	MG	A	1803	1/1	0.92	0.17	-0.10	96,96,96,96	0
23	MG	A	1793	1/1	0.95	0.20	-0.12	139,139,139,139	0
23	MG	A	1659	1/1	0.98	0.16	-0.22	102,102,102,102	0
23	MG	A	1710	1/1	0.95	0.15	-0.49	173,173,173,173	0
23	MG	A	1797	1/1	0.97	0.18	-0.58	129,129,129,129	0
23	MG	A	1785	1/1	0.95	0.13	-0.71	99,99,99,99	0
23	MG	A	1700	1/1	0.94	0.19	-0.78	121,121,121,121	0
23	MG	A	1795	1/1	0.94	0.11	-0.78	75,75,75,75	0
24	ZN	N	101	1/1	0.97	0.16	-0.91	163,163,163,163	0
23	MG	D	302	1/1	0.98	0.11	-1.00	111,111,111,111	0
23	MG	A	1806	1/1	0.95	0.12	-1.04	87,87,87,87	0
23	MG	A	1662	1/1	0.99	0.16	-1.04	105,105,105,105	0
23	MG	A	1827	1/1	0.96	0.08	-1.20	189,189,189,189	0
23	MG	A	1802	1/1	0.97	0.13	-1.30	171,171,171,171	0
23	MG	A	1822	1/1	0.85	0.08	-1.82	80,80,80,80	0
23	MG	A	1635	1/1	0.97	0.13	-1.83	109,109,109,109	0
23	MG	Q	201	1/1	0.90	0.10	-2.64	114,114,114,114	0
23	MG	A	1847	1/1	0.94	0.09	-2.95	81,81,81,81	0
23	MG	A	1646	1/1	0.98	0.09	-2.97	69,69,69,69	0
23	MG	A	1704	1/1	0.94	0.09	-3.27	98,98,98,98	0
23	MG	A	1706	1/1	0.94	0.11	-4.87	94,94,94,94	0
23	MG	A	1825	1/1	0.86	0.11	-	282,282,282,282	0
23	MG	A	1794	1/1	0.73	0.27	-	129,129,129,129	0
23	MG	A	1645	1/1	0.92	0.58	-	89,89,89,89	0
23	MG	A	1707	1/1	0.98	0.25	-	288,288,288,288	0
23	MG	A	1718	1/1	0.95	0.10	-	213,213,213,213	0
23	MG	A	1753	1/1	0.87	0.52	-	133,133,133,133	0
23	MG	A	1674	1/1	0.77	0.17	-	116,116,116,116	0
23	MG	A	1652	1/1	0.88	0.78	-	97,97,97,97	0
23	MG	A	1648	1/1	0.97	0.25	-	156,156,156,156	0
23	MG	A	1792	1/1	0.79	0.37	-	110,110,110,110	0
23	MG	H	202	1/1	0.58	0.22	-	88,88,88,88	0
23	MG	A	1765	1/1	0.85	0.61	-	119,119,119,119	0
23	MG	A	1633	1/1	0.97	0.20	-	111,111,111,111	0
23	MG	A	1829	1/1	0.97	0.17	-	101,101,101,101	0
23	MG	A	1833	1/1	0.77	0.16	-	113,113,113,113	0
23	MG	A	1605	1/1	0.89	0.27	-	115,115,115,115	0
23	MG	A	1789	1/1	0.58	0.46	-	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1743	1/1	0.82	0.19	-	94,94,94,94	0
23	MG	A	1654	1/1	0.97	0.16	-	93,93,93,93	0
23	MG	A	1634	1/1	0.93	0.37	-	102,102,102,102	0
23	MG	A	1622	1/1	0.97	0.27	-	90,90,90,90	0
23	MG	A	1723	1/1	0.91	0.18	-	115,115,115,115	0
23	MG	A	1749	1/1	0.85	0.27	-	123,123,123,123	0
23	MG	A	1629	1/1	0.97	0.14	-	93,93,93,93	0
23	MG	A	1618	1/1	0.98	0.36	-	109,109,109,109	0
23	MG	A	1831	1/1	0.91	0.14	-	122,122,122,122	0
23	MG	A	1711	1/1	0.95	0.31	-	123,123,123,123	0
23	MG	A	1730	1/1	0.91	0.31	-	102,102,102,102	0
23	MG	T	202	1/1	0.74	0.16	-	106,106,106,106	0
23	MG	A	1664	1/1	0.82	0.80	-	105,105,105,105	0
23	MG	A	1712	1/1	0.91	0.42	-	117,117,117,117	0
23	MG	A	1834	1/1	0.83	0.16	-	143,143,143,143	0
23	MG	A	1657	1/1	0.98	0.24	-	155,155,155,155	0
23	MG	A	1767	1/1	0.89	1.09	-	91,91,91,91	0
23	MG	A	1695	1/1	0.94	0.19	-	150,150,150,150	0
23	MG	A	1814	1/1	0.79	0.43	-	118,118,118,118	0
23	MG	A	1610	1/1	0.46	0.53	-	122,122,122,122	0
23	MG	A	1826	1/1	0.97	0.08	-	237,237,237,237	0
23	MG	A	1740	1/1	0.83	0.23	-	107,107,107,107	0
23	MG	A	1714	1/1	0.97	0.19	-	181,181,181,181	0
23	MG	A	1744	1/1	0.59	1.03	-	118,118,118,118	0
23	MG	A	1690	1/1	0.79	0.32	-	102,102,102,102	0
23	MG	A	1717	1/1	0.86	0.21	-	140,140,140,140	0
23	MG	A	1703	1/1	0.91	0.11	-	259,259,259,259	0
23	MG	A	1731	1/1	0.88	0.29	-	121,121,121,121	0
23	MG	A	1655	1/1	0.96	0.20	-	69,69,69,69	0
23	MG	A	1832	1/1	0.91	1.02	-	110,110,110,110	0
23	MG	A	1726	1/1	0.90	0.52	-	93,93,93,93	0
23	MG	Q	202	1/1	0.82	0.34	-	89,89,89,89	0
23	MG	A	1768	1/1	0.80	0.28	-	136,136,136,136	0
23	MG	A	1688	1/1	0.78	1.22	-	111,111,111,111	0
23	MG	A	1606	1/1	0.99	0.10	-	97,97,97,97	0
23	MG	A	1736	1/1	0.97	0.40	-	119,119,119,119	0
23	MG	A	1679	1/1	0.93	0.26	-	120,120,120,120	0
23	MG	A	1821	1/1	0.94	0.21	-	116,116,116,116	0
23	MG	A	1728	1/1	0.94	0.21	-	113,113,113,113	0
23	MG	A	1819	1/1	0.63	0.59	-	117,117,117,117	0
23	MG	A	1639	1/1	0.99	0.35	-	65,65,65,65	0
23	MG	A	1621	1/1	0.98	0.09	-	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1696	1/1	0.97	0.09	-	116,116,116,116	0
23	MG	A	1716	1/1	0.92	0.10	-	135,135,135,135	0
23	MG	A	1698	1/1	0.85	0.10	-	194,194,194,194	0
23	MG	A	1677	1/1	0.97	0.23	-	130,130,130,130	0
23	MG	A	1790	1/1	0.89	0.34	-	112,112,112,112	0
23	MG	A	1701	1/1	0.97	0.13	-	136,136,136,136	0
23	MG	A	1780	1/1	0.38	0.59	-	110,110,110,110	0
23	MG	A	1680	1/1	0.70	0.23	-	151,151,151,151	0
23	MG	A	1724	1/1	0.97	0.08	-	111,111,111,111	0
23	MG	A	1849	1/1	0.82	0.52	-	126,126,126,126	0
23	MG	A	1623	1/1	0.94	0.35	-	136,136,136,136	0
23	MG	A	1823	1/1	0.80	0.47	-	138,138,138,138	0
23	MG	A	1812	1/1	0.95	0.47	-	128,128,128,128	0
23	MG	A	1670	1/1	0.95	0.24	-	133,133,133,133	0
23	MG	A	1840	1/1	0.81	0.35	-	105,105,105,105	0
23	MG	A	1624	1/1	0.95	0.25	-	126,126,126,126	0
23	MG	A	1604	1/1	0.94	0.22	-	113,113,113,113	0
23	MG	A	1776	1/1	0.61	0.37	-	122,122,122,122	0
23	MG	A	1748	1/1	0.75	1.08	-	106,106,106,106	0
23	MG	A	1660	1/1	0.92	0.26	-	103,103,103,103	0
23	MG	A	1837	1/1	0.90	0.37	-	89,89,89,89	0
23	MG	A	1636	1/1	0.95	0.36	-	162,162,162,162	0
23	MG	A	1848	1/1	0.96	0.22	-	116,116,116,116	0
23	MG	A	1727	1/1	0.96	0.15	-	99,99,99,99	0
23	MG	A	1756	1/1	0.90	0.30	-	115,115,115,115	0
23	MG	A	1702	1/1	0.90	0.26	-	343,343,343,343	0
23	MG	A	1788	1/1	0.84	0.18	-	114,114,114,114	0
23	MG	A	1684	1/1	0.71	0.42	-	152,152,152,152	0
23	MG	A	1786	1/1	0.97	0.25	-	96,96,96,96	0
23	MG	A	1808	1/1	0.86	0.36	-	147,147,147,147	0
23	MG	A	1846	1/1	0.88	0.19	-	156,156,156,156	0
23	MG	A	1603	1/1	0.88	0.18	-	113,113,113,113	0
23	MG	A	1811	1/1	0.98	1.09	-	93,93,93,93	0
23	MG	A	1773	1/1	0.79	0.54	-	75,75,75,75	0
23	MG	A	1632	1/1	0.96	0.16	-	192,192,192,192	0
23	MG	A	1705	1/1	0.97	0.16	-	208,208,208,208	0
23	MG	A	1661	1/1	0.92	0.14	-	214,214,214,214	0
23	MG	A	1758	1/1	0.57	1.56	-	132,132,132,132	0
23	MG	A	1631	1/1	0.74	1.24	-	128,128,128,128	0
23	MG	A	1686	1/1	0.97	0.41	-	142,142,142,142	0
23	MG	A	1761	1/1	0.95	0.43	-	105,105,105,105	0
23	MG	P	101	1/1	0.79	0.35	-	92,92,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1775	1/1	0.73	0.09	-	142,142,142,142	0
23	MG	A	1763	1/1	0.74	0.61	-	121,121,121,121	0
23	MG	A	1750	1/1	0.74	0.58	-	97,97,97,97	0
23	MG	A	1782	1/1	0.95	0.20	-	120,120,120,120	0
23	MG	A	1774	1/1	0.87	0.44	-	150,150,150,150	0
23	MG	A	1741	1/1	0.91	0.20	-	117,117,117,117	0
23	MG	A	1613	1/1	0.99	0.11	-	112,112,112,112	0
23	MG	A	1630	1/1	0.93	0.11	-	142,142,142,142	0
23	MG	A	1678	1/1	0.97	0.14	-	124,124,124,124	0
23	MG	A	1841	1/1	0.89	0.11	-	107,107,107,107	0
23	MG	A	1807	1/1	0.80	0.36	-	106,106,106,106	0
23	MG	A	1737	1/1	0.79	0.58	-	114,114,114,114	0
23	MG	A	1746	1/1	0.35	0.54	-	116,116,116,116	0
23	MG	A	1729	1/1	0.74	0.51	-	121,121,121,121	0
23	MG	A	1602	1/1	0.97	0.26	-	133,133,133,133	0
23	MG	A	1666	1/1	0.98	0.23	-	113,113,113,113	0
23	MG	A	1772	1/1	0.88	0.23	-	105,105,105,105	0
23	MG	P	103	1/1	0.59	0.24	-	120,120,120,120	0
23	MG	A	1818	1/1	0.65	0.41	-	111,111,111,111	0
23	MG	A	1697	1/1	0.85	0.65	-	110,110,110,110	0
23	MG	A	1719	1/1	0.68	0.10	-	206,206,206,206	0
23	MG	A	1804	1/1	0.90	0.49	-	116,116,116,116	0
23	MG	A	1799	1/1	0.78	0.21	-	144,144,144,144	0
23	MG	A	1805	1/1	0.88	0.24	-	104,104,104,104	0
23	MG	A	1673	1/1	0.78	0.49	-	143,143,143,143	0
23	MG	A	1672	1/1	0.96	0.19	-	136,136,136,136	0
23	MG	A	1651	1/1	0.91	0.24	-	111,111,111,111	0
23	MG	A	1779	1/1	0.94	0.15	-	97,97,97,97	0
23	MG	A	1644	1/1	0.94	0.20	-	164,164,164,164	0
23	MG	A	1809	1/1	0.91	0.24	-	115,115,115,115	0
23	MG	A	1691	1/1	0.53	0.32	-	123,123,123,123	0
23	MG	A	1842	1/1	0.89	0.98	-	108,108,108,108	0
23	MG	A	1671	1/1	0.96	0.12	-	173,173,173,173	0
23	MG	A	1843	1/1	0.88	0.14	-	139,139,139,139	0
23	MG	A	1682	1/1	0.97	0.13	-	154,154,154,154	0
23	MG	A	1830	1/1	0.54	0.53	-	103,103,103,103	0
23	MG	A	1665	1/1	0.86	0.55	-	116,116,116,116	0
23	MG	A	1609	1/1	0.99	0.33	-	101,101,101,101	0
23	MG	A	1766	1/1	0.92	0.17	-	125,125,125,125	0
23	MG	A	1615	1/1	0.97	0.18	-	79,79,79,79	0
23	MG	A	1656	1/1	0.99	0.24	-	90,90,90,90	0
23	MG	A	1800	1/1	0.94	0.14	-	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1669	1/1	0.99	0.11	-	124,124,124,124	0
23	MG	A	1820	1/1	0.93	0.15	-	163,163,163,163	0
23	MG	A	1627	1/1	0.94	0.26	-	147,147,147,147	0
23	MG	A	1685	1/1	0.80	0.52	-	197,197,197,197	0
23	MG	A	1769	1/1	0.94	0.76	-	96,96,96,96	0
23	MG	A	1828	1/1	0.88	0.13	-	436,436,436,436	0
23	MG	E	201	1/1	0.94	0.25	-	129,129,129,129	0
23	MG	A	1649	1/1	0.98	0.46	-	121,121,121,121	0
23	MG	H	201	1/1	0.79	0.39	-	85,85,85,85	0
23	MG	A	1676	1/1	0.80	0.41	-	108,108,108,108	0
23	MG	A	1638	1/1	0.99	0.15	-	69,69,69,69	0
23	MG	A	1771	1/1	0.82	0.65	-	101,101,101,101	0
23	MG	A	1675	1/1	0.92	0.22	-	187,187,187,187	0
23	MG	A	1683	1/1	0.91	0.19	-	111,111,111,111	0
23	MG	M	201	1/1	0.83	0.47	-	136,136,136,136	0
23	MG	A	1784	1/1	0.91	0.21	-	132,132,132,132	0
23	MG	A	1745	1/1	0.99	0.09	-	85,85,85,85	0
23	MG	A	1693	1/1	0.92	0.21	-	95,95,95,95	0
23	MG	A	1844	1/1	0.86	0.56	-	118,118,118,118	0
23	MG	A	1738	1/1	0.87	0.60	-	98,98,98,98	0
23	MG	A	1715	1/1	0.78	0.30	-	131,131,131,131	0
23	MG	A	1783	1/1	0.82	0.14	-	118,118,118,118	0
23	MG	A	1614	1/1	0.96	0.12	-	108,108,108,108	0
23	MG	A	1816	1/1	0.35	1.01	-	95,95,95,95	0
23	MG	A	1681	1/1	0.97	0.07	-	149,149,149,149	0
23	MG	A	1640	1/1	0.95	0.23	-	110,110,110,110	0
23	MG	A	1764	1/1	0.89	0.83	-	118,118,118,118	0
23	MG	A	1747	1/1	0.99	0.31	-	124,124,124,124	0
23	MG	A	1815	1/1	0.57	0.75	-	110,110,110,110	0
23	MG	A	1839	1/1	0.62	0.35	-	111,111,111,111	0
23	MG	A	1668	1/1	0.98	0.10	-	153,153,153,153	0
23	MG	A	1801	1/1	0.97	0.09	-	274,274,274,274	0
23	MG	A	1791	1/1	0.83	0.41	-	100,100,100,100	0
23	MG	A	1647	1/1	0.87	0.28	-	135,135,135,135	0
23	MG	A	1713	1/1	0.99	0.32	-	389,389,389,389	0
23	MG	A	1628	1/1	0.99	0.24	-	123,123,123,123	0
23	MG	A	1663	1/1	0.91	0.26	-	121,121,121,121	0
23	MG	A	1619	1/1	0.81	0.34	-	109,109,109,109	0
23	MG	A	1667	1/1	0.66	0.16	-	110,110,110,110	0
23	MG	A	1778	1/1	0.62	1.10	-	129,129,129,129	0
23	MG	A	1770	1/1	0.96	0.25	-	119,119,119,119	0
23	MG	A	1781	1/1	0.89	0.25	-	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
23	MG	A	1754	1/1	0.97	0.14	-	100,100,100,100	0
23	MG	A	1699	1/1	0.76	0.24	-	227,227,227,227	0
23	MG	A	1612	1/1	0.93	0.30	-	120,120,120,120	0
23	MG	P	102	1/1	0.79	0.34	-	128,128,128,128	0
23	MG	A	1760	1/1	0.86	0.67	-	105,105,105,105	0
23	MG	A	1687	1/1	0.93	0.57	-	113,113,113,113	0
23	MG	A	1641	1/1	0.98	0.26	-	169,169,169,169	0
23	MG	A	1694	1/1	0.95	0.25	-	114,114,114,114	0
23	MG	A	1608	1/1	0.89	0.10	-	137,137,137,137	0
23	MG	A	1722	1/1	0.89	0.38	-	127,127,127,127	0
23	MG	A	1733	1/1	0.70	0.36	-	125,125,125,125	0
23	MG	A	1796	1/1	0.79	0.88	-	132,132,132,132	0
23	MG	A	1824	1/1	0.96	0.14	-	300,300,300,300	0

6.5 Other polymers

There are no such residues in this entry.