



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2022 – 02:17 PM JST

PDB ID : 7DUG
Title : Crystal structure of the *Thermus thermophilus* (HB8) 30S ribosomal subunit with mRNA and cognate transfer RNA anticodon stem-loop and sisomicin derivative N1”TFMS bound
Authors : DeMirici, H.; Destan, E.
Deposited on : 2021-01-09
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.25
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.25

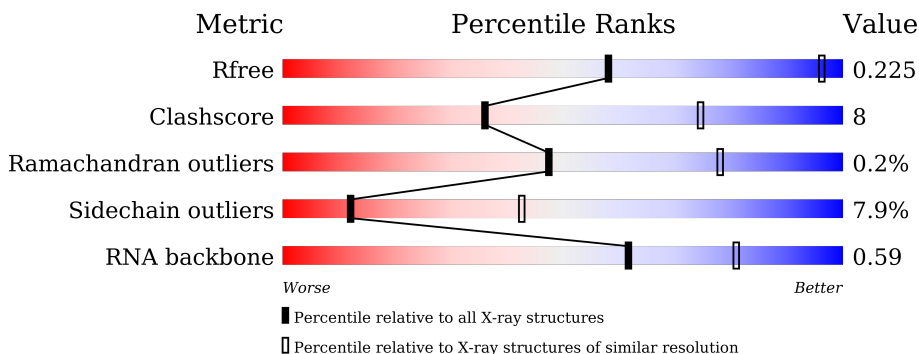
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 Å.

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











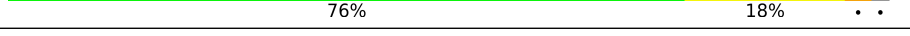

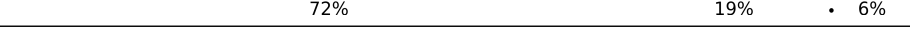
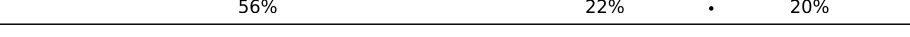

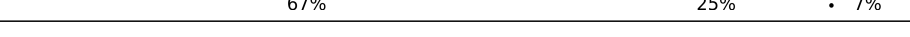



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1039 (3.94-3.58)
Clashscore	141614	1051 (3.92-3.60)
Ramachandran outliers	138981	1015 (3.92-3.60)
Sidechain outliers	138945	1011 (3.92-3.60)
RNA backbone	3102	1035 (4.52-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	57% (green), 34% (yellow), 8% (orange), 2% (red), 1% (grey)
2	B	256	66% (green), 23% (yellow), 9% (orange), 2% (red), 2% (grey)
3	C	239	62% (green), 21% (yellow), 14% (orange), 3% (red), 2% (grey)
4	D	209	74% (green), 23% (yellow), 3% (orange), 2% (red), 2% (grey)
5	E	162	72% (green), 17% (yellow), 7% (orange), 2% (red), 2% (grey)
6	F	101	83% (green), 15% (yellow), 2% (orange), 2% (red), 2% (grey)

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Mol	Chain	Length	Quality of chain
7	G	156	 79% 19% ..
8	H	138	 70% 25% .
9	I	128	 66% 31% ..
10	J	105	 59% 30% . . 7%
11	K	129	 67% 19% . 10%
12	L	135	 61% 28% . 8%
13	M	126	 71% 21% . 6%
14	N	61	 61% 36% . .
15	O	89	 76% 18% . .
16	P	88	 74% 19% . 6%
17	Q	105	 72% 19% . 6%
18	R	88	 56% 22% . 20%
19	S	93	 60% 19% 6% 14%
20	T	106	 67% 25% . 7%
21	U	27	 70% 19% 11%
22	Y	6	 50% 33% 17%
23	W	15	 80% 20%

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 52694 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 30S Ribosomal RNA rRNA.

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

- 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
			Total	C	N	O	S			
6	F	101	843	531	155	154	3	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

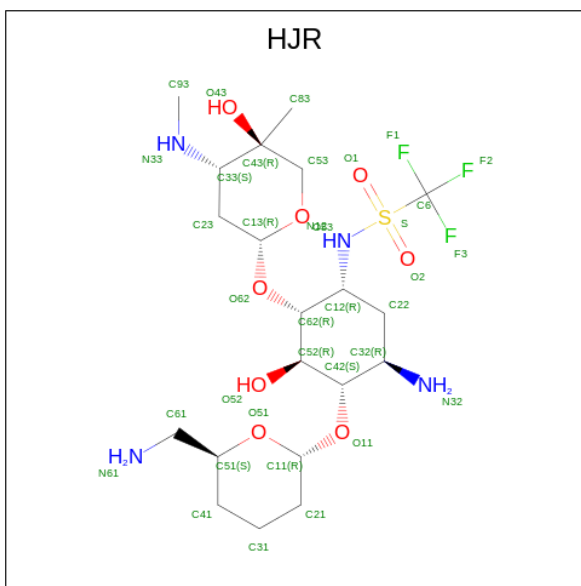
- Molecule 22 is a RNA chain called RNA (5'-R(UPUPUPUPUPU)-3').

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

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

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

- Molecule 24 is N-[(1R,2R,3R,4S,5R)-4-[(2R,6S)-6-(aminomethyl)oxan-2-yl]oxy-5-azanyl-2-[(2R,4S,5R)-5-methyl-4-(methylamino)-5-oxidanyl-oxan-2-yl]oxy-3-oxidanyl-cyclohexyl]-1,1,1-tris(fluoranyl)methanesulfonamide (three-letter code: HJR) (formula: C₂₀H₃₇F₃N₄O₈S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
24	A	1	36	20	3	4	8	1	0	0

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	231	Total Mg 231 231	0	0
25	B	3	Total Mg 3 3	0	0
25	C	3	Total Mg 3 3	0	0
25	D	3	Total Mg 3 3	0	0
25	E	1	Total Mg 1 1	0	0
25	F	1	Total Mg 1 1	0	0
25	H	1	Total Mg 1 1	0	0
25	I	1	Total Mg 1 1	0	0
25	J	1	Total Mg 1 1	0	0
25	P	2	Total Mg 2 2	0	0
25	Q	1	Total Mg 1 1	0	0
25	S	1	Total Mg 1 1	0	0

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	223	Total O 223 223	0	0
27	C	1	Total O 1 1	0	0
27	D	1	Total O 1 1	0	0
27	E	6	Total O 6 6	0	0

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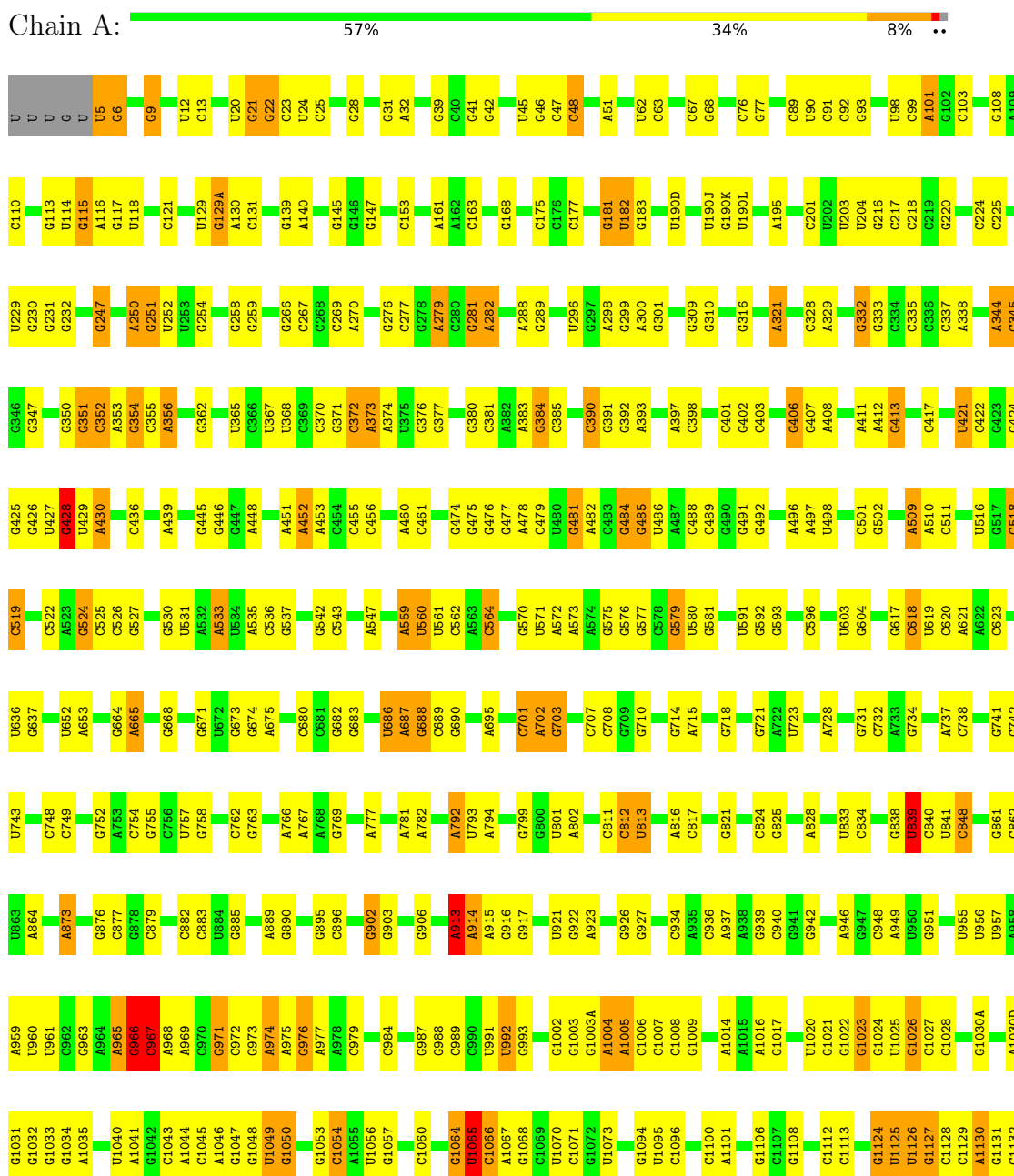
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	L	2	Total O 2 2	0	0
27	N	2	Total O 2 2	0	0
27	Q	2	Total O 2 2	0	0
27	T	2	Total O 2 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

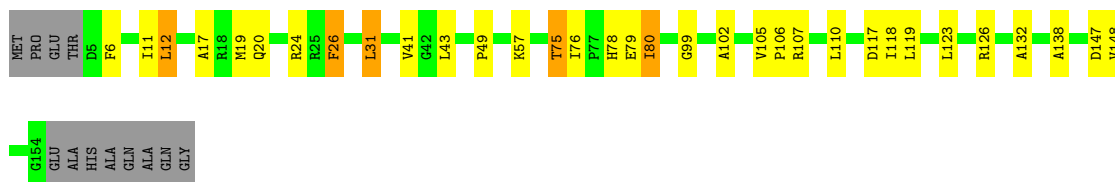
- Molecule 1: 30S Ribosomal RNA rRNA





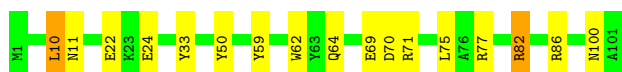
- Molecule 5: 30S ribosomal protein S5

Chain E: 72% 17% 7%



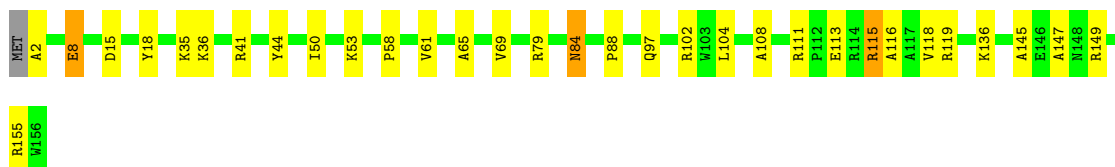
- Molecule 6: 30S ribosomal protein S6

Chain F: 83% 15%



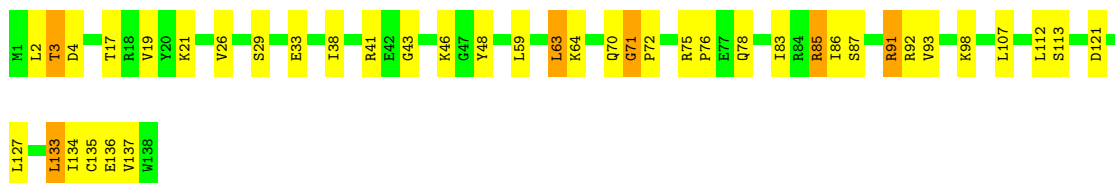
- Molecule 7: 30S ribosomal protein S7

Chain G: 79% 19%



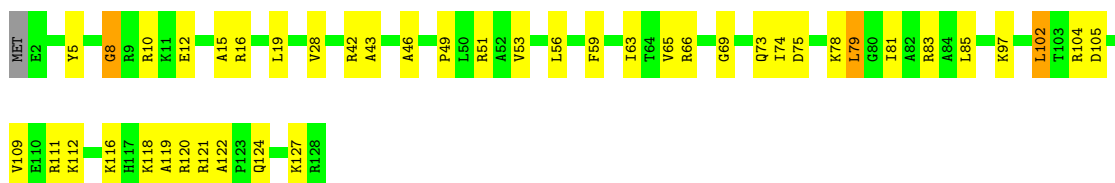
- Molecule 8: 30S ribosomal protein S8

Chain H: 70% 25%



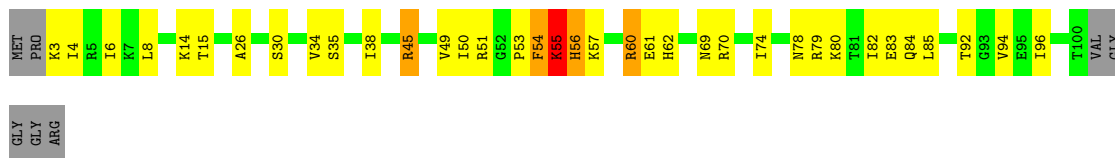
- Molecule 9: 30S ribosomal protein S9

Chain I: 66% 31%



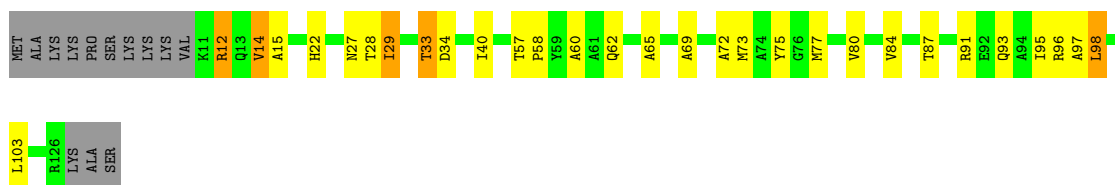
- Molecule 10: 30S ribosomal protein S10

Chain J:  59% 30% 7%



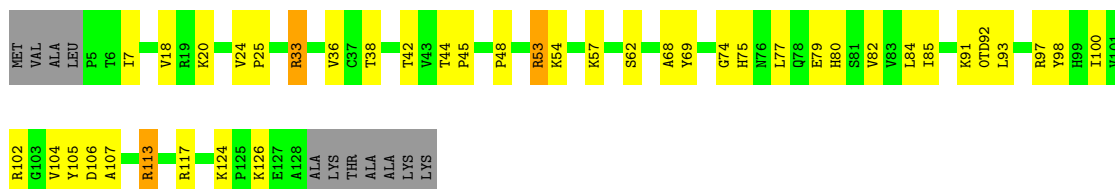
- Molecule 11: 30S ribosomal protein S11

Chain K:  67% 19% 10%



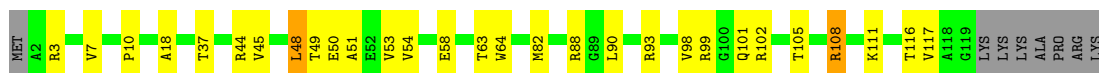
- Molecule 12: 30S ribosomal protein S12

Chain L:  61% 28% 8%



- Molecule 13: 30S ribosomal protein S13

Chain M:  71% 21% 6%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain N:  61% 36%



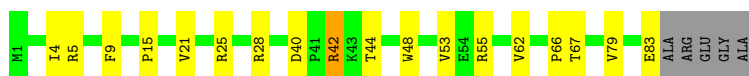
- Molecule 15: 30S ribosomal protein S15

Chain O:  76% 18%



- Molecule 16: 30S ribosomal protein S16

Chain P:  74% 19% 6%



- Molecule 17: 30S ribosomal protein S17

Chain Q:  72% 19% 6%



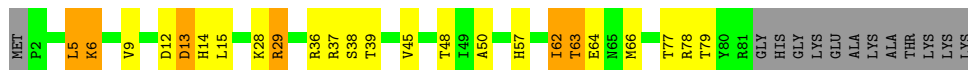
- Molecule 18: 30S ribosomal protein S18

Chain R:  56% 22% 20%



- Molecule 19: 30S ribosomal protein S19

Chain S:  60% 19% 6% 14%



- Molecule 20: 30S ribosomal protein S20

Chain T:  67% 25% 7%



- Molecule 21: 30S ribosomal protein Thx

Chain U:  70% 19% 11%




- Molecule 22: RNA (5'-R(UPUPUPUPUPU)-3')

Chain Y:  50% 33% 17%



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

Chain W:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.00Å 400.00Å 173.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.78 – 3.75 39.78 – 2.91	Depositor EDS
% Data completeness (in resolution range)	98.4 (39.78-3.75) 68.9 (39.78-2.91)	Depositor EDS
R_{merge}	0.91	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.48 (at 2.90Å)	Xtrriage
Refinement program	PHENIX DEV-3318	Depositor
R, R_{free}	0.186 , 0.225 0.186 , 0.225	Depositor DCC
R_{free} test set	2000 reflections (0.70%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52694	wwPDB-VP
Average B, all atoms (Å ²)	164.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.22	0/36139	0.76	17/56396 (0.0%)
2	B	0.26	0/1935	0.42	0/2609
3	C	0.25	0/1636	0.45	0/2205
4	D	0.25	0/1733	0.41	0/2318
5	E	0.27	0/1162	0.45	0/1564
6	F	0.24	0/856	0.42	0/1154
7	G	0.25	0/1276	0.39	0/1709
8	H	0.28	0/1136	0.46	0/1527
9	I	0.27	0/1029	0.46	0/1379
10	J	0.26	0/805	0.50	0/1082
11	K	0.25	0/879	0.43	0/1187
12	L	0.26	0/977	0.48	0/1306
13	M	0.24	0/947	0.45	0/1270
14	N	0.28	0/501	0.46	0/664
15	O	0.23	0/740	0.40	0/987
16	P	0.26	0/716	0.44	0/963
17	Q	0.26	0/836	0.46	0/1117
18	R	0.27	0/579	0.44	0/768
19	S	0.25	0/661	0.48	0/890
20	T	0.25	0/765	0.42	0/1007
21	U	0.23	0/212	0.40	0/277
22	Y	0.22	0/128	0.83	0/196
23	W	0.22	0/357	0.76	0/555
All	All	0.24	0/56005	0.67	17/83130 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
8	H	0	1
10	J	0	2
13	M	0	1
All	All	0	5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	839	U	C2-N1-C1'	7.79	127.05	117.70
1	A	839	U	N1-C2-O2	7.25	127.87	122.80
1	A	839	U	N3-C2-O2	-6.71	117.50	122.20
1	A	754	C	C2-N1-C1'	5.98	125.38	118.80
1	A	754	C	N1-C2-O2	5.63	122.28	118.90
1	A	1190	G	P-O3'-C3'	5.57	126.39	119.70
1	A	1301	U	P-O3'-C3'	5.44	126.23	119.70
1	A	1305	G	P-O3'-C3'	5.37	126.15	119.70
1	A	1380	U	P-O3'-C3'	5.37	126.15	119.70
1	A	1065	U	P-O3'-C3'	5.22	125.97	119.70
1	A	1347	G	P-O3'-C3'	5.19	125.93	119.70
1	A	1346	A	P-O3'-C3'	5.17	125.90	119.70
1	A	484	G	P-O3'-C3'	5.14	125.86	119.70
1	A	1201	A	P-O3'-C3'	5.09	125.81	119.70
1	A	428	G	P-O3'-C3'	5.03	125.74	119.70
1	A	792	A	P-O3'-C3'	5.02	125.73	119.70
1	A	913	A	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	166	GLU	Peptide
8	H	71	GLY	Peptide
10	J	54	PHE	Peptide
10	J	55	LYS	Peptide
13	M	111	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32644	0	16508	385	0
2	B	1900	0	1951	35	0
3	C	1612	0	1676	35	0
4	D	1703	0	1763	34	0
5	E	1146	0	1207	21	0
6	F	843	0	857	11	0
7	G	1257	0	1296	20	0
8	H	1116	0	1177	25	0
9	I	1010	0	1037	26	0
10	J	792	0	835	29	0
11	K	864	0	881	18	0
12	L	972	0	1058	29	0
13	M	937	0	995	18	0
14	N	492	0	529	23	0
15	O	729	0	768	10	0
16	P	700	0	720	9	0
17	Q	823	0	893	12	0
18	R	574	0	644	14	0
19	S	647	0	673	16	0
20	T	763	0	861	13	0
21	U	208	0	221	3	0
22	Y	117	0	62	2	0
23	W	319	0	164	1	0
24	A	36	0	0	1	0
25	A	231	0	0	0	0
25	B	3	0	0	0	0
25	C	3	0	0	0	0
25	D	3	0	0	0	0
25	E	1	0	0	0	0
25	F	1	0	0	0	0
25	H	1	0	0	0	0
25	I	1	0	0	0	0
25	J	1	0	0	0	0
25	P	2	0	0	0	0
25	Q	1	0	0	0	0
25	S	1	0	0	0	0
26	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	N	1	0	0	0	0
27	A	223	0	0	3	0
27	C	1	0	0	0	0
27	D	1	0	0	0	0
27	E	6	0	0	0	0
27	L	2	0	0	0	0
27	N	2	0	0	0	0
27	Q	2	0	0	0	0
27	T	2	0	0	0	0
All	All	52694	0	36776	700	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (700) 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:481:G:HO2'	1:A:482:A:H8	1.01	1.01
1:A:1028:C:H42	1:A:1033:G:H1	1.23	0.82
20:T:100:ILE:HG22	20:T:102:GLY:H	1.46	0.81
8:H:86:ILE:HD11	8:H:136:GLU:HG3	1.62	0.80
1:A:1516[B]:G:N2	1:A:1519[B]:MA6:OP2	2.17	0.78
1:A:1266:G:N2	1:A:1269:A:OP2	2.17	0.77
1:A:617:G:H1	1:A:623:C:H42	1.33	0.76
1:A:1214:C:H3'	1:A:1215:G:H8	1.50	0.76
3:C:33:LEU:HD21	14:N:53:LEU:HD22	1.69	0.75
1:A:21:G:N2	1:A:885:G:O3'	2.20	0.74
1:A:664:G:H22	1:A:741:G:H1	1.35	0.74
1:A:1176:A:N6	1:A:1181:G:O6	2.20	0.73
1:A:537:G:OP1	12:L:113:ARG:NH2	2.20	0.73
19:S:12:ASP:H	19:S:38:SER:HB3	1.53	0.73
1:A:456:C:H42	1:A:476:G:H1	1.37	0.72
1:A:1128:C:O2'	1:A:1130:A:N7	2.21	0.72
1:A:1128:C:OP1	9:I:66:ARG:NH1	2.23	0.72
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.72	0.72
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.23	0.71
1:A:618:C:H5'	1:A:619:U:H5''	1.72	0.71
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.55	0.71
1:A:407:G:OP1	4:D:115:ARG:NH1	2.23	0.71
4:D:61:LYS:NZ	4:D:62:GLN:OE1	2.23	0.70
1:A:145:G:H1	1:A:177:C:H42	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:THR:O	8:H:78:GLN:NE2	2.24	0.70
1:A:1005:A:N3	1:A:1026:G:N2	2.38	0.70
1:A:1190:G:O2'	1:A:1191:A:OP2	2.05	0.70
10:J:61:GLU:OE2	14:N:58:LYS:NZ	2.22	0.69
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.75	0.69
1:A:1125:U:OP2	1:A:1145:C:N4	2.26	0.69
1:A:1316:G:N2	1:A:1319:A:OP2	2.26	0.68
5:E:11:ILE:HB	5:E:31:LEU:HB3	1.75	0.68
1:A:455:C:H42	1:A:477:G:H1	1.39	0.68
1:A:1443:G:H5''	1:A:1446:A:H5'	1.75	0.67
9:I:112:LYS:HA	9:I:119:ALA:HB2	1.76	0.67
11:K:72:ALA:HB1	11:K:77:MET:HG3	1.76	0.67
1:A:1134:G:H1	1:A:1140:C:H42	1.40	0.67
2:B:21:ARG:HA	2:B:39:ILE:HA	1.77	0.67
2:B:63:MET:HB3	2:B:225:ALA:HB1	1.77	0.66
1:A:1064:G:N2	1:A:1190:G:O2'	2.28	0.66
11:K:80:VAL:HG21	11:K:103:LEU:HD13	1.76	0.66
9:I:51:ARG:HG3	9:I:56:LEU:HD21	1.76	0.66
3:C:70:VAL:HG21	3:C:76:VAL:HG21	1.77	0.66
1:A:955:U:H1'	1:A:1227:A:H61	1.59	0.66
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.77	0.66
1:A:1100:C:OP1	2:B:96:ARG:NH1	2.29	0.65
12:L:38:THR:HB	12:L:57:LYS:HB2	1.77	0.65
14:N:50:LYS:HG2	14:N:52:GLN:HE21	1.63	0.64
1:A:976:G:OP2	1:A:1358:U:O2'	2.15	0.64
1:A:1213:A:N6	1:A:1215:G:N3	2.45	0.64
1:A:1499:A:H1'	1:A:1520[A]:G:H5'	1.78	0.64
1:A:1064:G:N2	1:A:1190:G:HO2'	1.96	0.64
1:A:1060:C:OP1	14:N:45:ARG:NH2	2.32	0.63
1:A:972:C:H4'	10:J:57:LYS:HD3	1.79	0.63
1:A:1128:C:H42	1:A:1143:G:H1	1.45	0.63
2:B:162:ILE:HD12	2:B:177:ALA:HB2	1.80	0.63
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.26	0.63
1:A:1379:G:O6	7:G:2:ALA:N	2.31	0.63
1:A:1228:C:OP1	13:M:108:ARG:NH2	2.32	0.63
1:A:1008:C:N4	1:A:1021:G:H1	1.98	0.62
1:A:1278:U:H5'	1:A:1279:A:O4'	1.99	0.62
1:A:372:C:H4'	1:A:373:A:O5'	2.00	0.62
1:A:153:C:H42	1:A:168:G:H1	1.47	0.62
1:A:501:C:OP1	12:L:117:ARG:NH2	2.33	0.62
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1020:U:H2'	1:A:1021:G:H8	1.64	0.62
1:A:1057:G:H5''	3:C:154:SER:HB2	1.82	0.62
5:E:17:ALA:HA	5:E:26:PHE:HB3	1.82	0.62
7:G:84:ASN:OD1	7:G:84:ASN:N	2.33	0.62
1:A:509:A:N3	1:A:543:C:O2'	2.31	0.61
1:A:1196:U:OP1	1:A:1197:G:H5'	2.00	0.61
1:A:916:G:H2'	1:A:917:G:H8	1.65	0.61
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.65	0.61
15:O:39:LEU:HD13	15:O:56:LEU:HB2	1.82	0.61
1:A:28:G:O2'	1:A:296:U:OP1	2.17	0.61
1:A:45:U:H2'	1:A:46:G:C8	2.35	0.61
1:A:921:U:O2'	5:E:19:MET:O	2.15	0.61
8:H:83:ILE:HG12	8:H:137:VAL:HG22	1.82	0.61
1:A:380:G:N2	1:A:383:A:OP2	2.32	0.61
1:A:1048:G:H1	1:A:1209:C:H42	1.49	0.61
1:A:1030(A):G:N2	1:A:1030(D):A:OP2	2.33	0.61
9:I:15:ALA:HB2	9:I:65:VAL:HG13	1.82	0.61
14:N:9:LYS:HD2	14:N:23:ARG:HB2	1.82	0.61
1:A:1510:U:H2'	1:A:1511:G:C8	2.36	0.61
1:A:21:G:O2'	1:A:22:G:H5'	2.01	0.60
14:N:24:CYS:H	14:N:33:VAL:HG21	1.66	0.60
1:A:417:C:H42	1:A:426:G:H1	1.50	0.60
15:O:2:PRO:O	15:O:38:ARG:NH1	2.34	0.60
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.84	0.60
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.40	0.60
10:J:61:GLU:OE1	14:N:45:ARG:NH1	2.34	0.60
3:C:20:SER:OG	3:C:40:ARG:NH2	2.31	0.59
1:A:298:A:N6	27:A:1903:HOH:O	2.35	0.59
1:A:1397:C:N4	22:Y:5:U:OP2	2.35	0.59
1:A:1419:G:H1	1:A:1481:U:H3	1.49	0.59
9:I:97:LYS:HA	9:I:102:LEU:HD11	1.82	0.59
16:P:53:VAL:HG12	16:P:79:VAL:HG22	1.84	0.59
18:R:32:ARG:HA	18:R:69:THR:HG21	1.84	0.59
1:A:1412:C:H2'	1:A:1413:A:C8	2.38	0.58
1:A:1474:G:H2'	1:A:1475:G:C8	2.38	0.58
3:C:6:HIS:HE1	3:C:8:ILE:HB	1.67	0.58
3:C:156:ARG:H	3:C:163:ALA:HA	1.68	0.58
19:S:13:ASP:OD1	19:S:13:ASP:N	2.36	0.58
10:J:69:ASN:O	10:J:70:ARG:NH1	2.31	0.58
1:A:1516[A]:G:N2	1:A:1519[A]:MA6:OP2	2.30	0.58
1:A:1113:C:H42	1:A:1187:G:H1	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:G:H4'	5:E:20:GLN:HA	1.85	0.58
1:A:1028:C:N3	1:A:1033:G:N2	2.43	0.58
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.84	0.58
1:A:113:G:H1'	1:A:354:G:H5'	1.86	0.58
1:A:448:A:OP2	1:A:485:G:N2	2.30	0.58
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.86	0.58
4:D:150:GLU:HA	4:D:153:ARG:HG3	1.86	0.58
13:M:49:THR:HG22	13:M:51:ALA:H	1.68	0.58
1:A:1126:U:O4	1:A:1127:G:N2	2.36	0.57
15:O:39:LEU:HB3	15:O:56:LEU:HD12	1.86	0.57
1:A:686:U:HO2'	1:A:687:A:H8	1.51	0.57
1:A:1003(A):G:C5	1:A:1004:A:H1'	2.39	0.57
1:A:1544:U:H4'	22:Y:1:U:H5'	1.86	0.57
7:G:50:ILE:HD11	7:G:61:VAL:HG11	1.85	0.57
3:C:11:ARG:HG2	3:C:178:LEU:HG	1.87	0.57
1:A:533:A:O2'	1:A:535:A:OP2	2.23	0.56
1:A:1139:G:H4'	1:A:1140:C:H5'	1.88	0.56
1:A:1145:C:O2'	1:A:1146:A:O5'	2.24	0.56
7:G:15:ASP:OD1	7:G:44:TYR:OH	2.23	0.56
11:K:14:VAL:HG21	11:K:40:ILE:HD13	1.87	0.56
2:B:119:GLU:OE1	2:B:153:ARG:NH2	2.38	0.56
1:A:1240:U:OP2	7:G:116:ALA:N	2.38	0.56
1:A:1404:5MC:H2'	1:A:1405:G:C8	2.41	0.56
9:I:28:VAL:HG22	9:I:63:ILE:HB	1.88	0.56
1:A:1022:G:N2	1:A:1023:G:N7	2.53	0.56
1:A:1414:U:H2'	1:A:1415:G:C8	2.41	0.56
1:A:1190:G:HO2'	1:A:1191:A:P	2.25	0.56
1:A:1064:G:N2	1:A:1191:A:OP2	2.38	0.56
7:G:113:GLU:HB2	7:G:119:ARG:HG2	1.88	0.56
1:A:1281:U:H5'	1:A:1282:C:H5	1.72	0.55
11:K:33:THR:OG1	11:K:34:ASP:N	2.38	0.55
12:L:33:ARG:HD3	12:L:62:SER:HB3	1.88	0.55
13:M:3:ARG:HE	13:M:7:VAL:HG12	1.71	0.55
1:A:1367:C:H5'	10:J:60:ARG:HE	1.70	0.55
1:A:1417:G:O2'	1:A:1483:A:N6	2.39	0.55
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.41	0.55
1:A:922:G:H1	1:A:1395:C:H42	1.53	0.55
1:A:1031:G:H2'	1:A:1032:G:C8	2.41	0.55
1:A:401:C:H2'	1:A:402:G:C8	2.42	0.55
1:A:652:U:O4	1:A:752:G:O2'	2.18	0.55
1:A:1326:C:OP2	21:U:6:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:190:ASP:OD1	4:D:191:ARG:N	2.38	0.55
5:E:75:THR:OG1	5:E:76:ILE:N	2.40	0.55
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.89	0.55
10:J:8:LEU:HD23	10:J:96:ILE:HG12	1.88	0.55
10:J:30:SER:HB3	10:J:80:LYS:HB2	1.88	0.55
1:A:1442:G:O6	1:A:1446:A:N6	2.39	0.55
1:A:390:C:O3'	16:P:28:ARG:NH2	2.40	0.54
11:K:15:ALA:HA	11:K:77:MET:HA	1.87	0.54
12:L:104:VAL:HG22	12:L:105:TYR:H	1.73	0.54
1:A:664:G:N2	1:A:741:G:H1	2.04	0.54
1:A:682:G:H2'	1:A:683:G:H8	1.73	0.54
1:A:1049:U:H4'	1:A:1050:G:O5'	2.08	0.54
1:A:1124:G:H5'	10:J:35:SER:O	2.07	0.54
1:A:1505:G:O2'	1:A:1506:U:OP2	2.17	0.54
10:J:79:ARG:O	10:J:83:GLU:N	2.40	0.54
14:N:47:LEU:HB3	14:N:53:LEU:HD21	1.89	0.54
1:A:579:G:H5'	1:A:728:A:H1'	1.90	0.54
3:C:6:HIS:CE1	3:C:8:ILE:HB	2.41	0.54
1:A:413:G:H2'	1:A:428:G:N2	2.22	0.54
1:A:603:U:H2'	1:A:604:G:C8	2.42	0.54
1:A:811:C:N4	27:A:1904:HOH:O	2.40	0.54
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.90	0.54
13:M:3:ARG:NE	13:M:7:VAL:HG12	2.23	0.54
1:A:247:G:O2'	1:A:282:A:N1	2.38	0.54
1:A:673:G:H2'	1:A:674:G:C8	2.43	0.54
1:A:250:A:H4'	1:A:251:G:O5'	2.07	0.54
1:A:939:G:H5''	7:G:102:ARG:NH1	2.23	0.53
1:A:946:A:O2'	1:A:1333:A:N3	2.37	0.53
4:D:78:LEU:HB3	4:D:93:PHE:HE1	1.73	0.53
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.90	0.53
1:A:769:G:H4'	1:A:1513:A:H4'	1.90	0.53
1:A:1112:C:O2	3:C:179:ARG:HB2	2.09	0.53
1:A:424:G:H2'	1:A:425:G:H8	1.74	0.53
1:A:518:C:H4'	1:A:519:C:O5'	2.08	0.53
4:D:162:LEU:HA	4:D:165:MET:HB2	1.91	0.53
1:A:1143:G:H2'	1:A:1144:G:C8	2.44	0.53
3:C:188:LEU:HD11	3:C:195:VAL:HG13	1.89	0.53
1:A:967:5MC:H2'	1:A:968:A:N7	2.24	0.53
1:A:1195:C:H3'	1:A:1196:U:H5''	1.90	0.53
1:A:1214:C:H3'	1:A:1215:G:C8	2.38	0.53
1:A:1391:U:H2'	1:A:1392:G:C8	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:HD11	14:N:51:GLY:HA2	1.90	0.53
1:A:1009:G:H1	1:A:1020:U:H3	1.57	0.53
1:A:559:A:OP1	5:E:126:ARG:NH1	2.42	0.53
1:A:671:G:H5'	6:F:77:ARG:HH21	1.74	0.53
20:T:75:ASN:OD1	20:T:75:ASN:N	2.40	0.53
1:A:9:G:H5''	5:E:126:ARG:HD3	1.90	0.53
1:A:13:C:H41	1:A:20:U:H3	1.57	0.53
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.90	0.52
9:I:5:TYR:HE1	9:I:16:ARG:HB3	1.73	0.52
18:R:48:GLY:O	18:R:74:ARG:NH2	2.42	0.52
1:A:916:G:H2'	1:A:917:G:C8	2.44	0.52
1:A:1420:C:H2'	1:A:1421:G:H8	1.73	0.52
1:A:674:G:H2'	1:A:675:A:H8	1.74	0.52
20:T:92:LEU:O	20:T:96:GLY:HA2	2.10	0.52
1:A:110:C:O2'	16:P:25:ARG:O	2.24	0.52
1:A:1106:G:H5''	3:C:172:ARG:HB3	1.91	0.52
2:B:59:GLU:HB2	2:B:221:LEU:HD11	1.92	0.52
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.91	0.52
1:A:674:G:H2'	1:A:675:A:C8	2.45	0.52
1:A:316:G:OP2	1:A:351:G:O2'	2.27	0.52
1:A:1308:U:OP1	13:M:98:VAL:N	2.43	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.92	0.52
3:C:26:LYS:HD3	10:J:45:ARG:HH21	1.75	0.52
19:S:28:LYS:HG2	19:S:29:ARG:H	1.75	0.52
20:T:14:LYS:HG3	20:T:17:ARG:HH12	1.76	0.51
1:A:914:A:H2'	1:A:915:A:H8	1.74	0.51
18:R:47:THR:HG22	18:R:83:GLU:H	1.73	0.51
1:A:738:C:H5''	6:F:69:GLU:HB3	1.91	0.51
18:R:53:ARG:HD3	18:R:63:GLN:HB2	1.92	0.51
1:A:413:G:H2'	1:A:428:G:H22	1.75	0.51
1:A:967:5MC:H2'	1:A:968:A:C8	2.45	0.51
1:A:1294:G:H2'	1:A:1295:G:H8	1.74	0.51
1:A:1198:G:H2'	1:A:1199:U:C6	2.46	0.51
1:A:1320:C:H41	19:S:37:ARG:HD3	1.76	0.51
12:L:25:PRO:HD2	12:L:97:ARG:HH12	1.75	0.51
1:A:452:A:O2'	1:A:453:A:O4'	2.29	0.51
1:A:1518[B]:MA6:H102	1:A:1519[B]:MA6:H103	1.93	0.51
10:J:50:ILE:HD12	10:J:50:ILE:H	1.74	0.51
1:A:335:C:O2'	1:A:1433:A:N3	2.40	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.44	0.51
1:A:1027:C:H42	1:A:1034:G:H1	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.75	0.51
1:A:922:G:H2'	1:A:923:A:C8	2.45	0.51
1:A:1516[A]:G:H2'	1:A:1518[A]:MA6:OP2	2.11	0.50
4:D:102:ASP:OD1	4:D:103:ASN:N	2.44	0.50
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.92	0.50
13:M:90:LEU:HD23	13:M:93:ARG:HD2	1.93	0.50
1:A:258:G:H2'	1:A:259:G:H8	1.75	0.50
6:F:10:LEU:HD12	6:F:59:TYR:HB3	1.93	0.50
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.92	0.50
1:A:356:A:N3	1:A:368:U:O2'	2.40	0.50
1:A:403:C:OP2	4:D:74:GLN:NE2	2.45	0.50
1:A:963:G:HO2'	10:J:54:PHE:HZ	1.58	0.50
2:B:204:ASN:H	2:B:204:ASN:HD22	1.59	0.50
1:A:973:G:H3'	1:A:974:A:H5''	1.94	0.50
3:C:155:GLY:HA2	3:C:164:ARG:H	1.76	0.50
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.94	0.50
14:N:50:LYS:HB3	14:N:52:GLN:HG3	1.93	0.50
1:A:269:C:H2'	1:A:270:A:C8	2.46	0.50
6:F:33:TYR:HA	6:F:71:ARG:HH21	1.76	0.50
1:A:24:U:H2'	1:A:25:C:C6	2.46	0.50
1:A:229:U:H2'	1:A:230:G:C8	2.47	0.50
1:A:1291:G:OP1	7:G:41:ARG:NH2	2.30	0.50
2:B:30:ARG:HD2	2:B:31:TYR:CZ	2.47	0.50
1:A:1175:G:H2'	1:A:1176:A:C8	2.47	0.50
1:A:1004:A:H5''	1:A:1025:U:C4	2.47	0.49
6:F:11:ASN:HD22	6:F:86:ARG:NH2	2.10	0.49
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.93	0.49
1:A:276:G:O2'	17:Q:68:ARG:NH1	2.45	0.49
1:A:718:G:O6	18:R:74:ARG:NH1	2.44	0.49
1:A:1048:G:H1	1:A:1209:C:N4	2.10	0.49
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.93	0.49
1:A:376:G:H2'	1:A:377:G:C8	2.47	0.49
1:A:1399:C:H4'	1:A:1400:5MC:H5''	1.93	0.49
11:K:27:ASN:OD1	11:K:28:THR:N	2.45	0.49
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.47	0.49
2:B:74:LYS:NZ	2:B:206:ASP:OD1	2.42	0.49
14:N:22:THR:HB	14:N:33:VAL:HB	1.95	0.49
1:A:190(J):U:H2'	1:A:190(K):G:C8	2.47	0.49
1:A:406:G:H1	1:A:436:C:H42	1.58	0.49
1:A:816:A:OP1	1:A:1526:G:O2'	2.27	0.49
12:L:74:GLY:O	12:L:102:ARG:NH1	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:47:LEU:HD12	14:N:52:GLN:HB2	1.94	0.49
1:A:1424:C:H42	1:A:1476:G:H1	1.61	0.49
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.48	0.49
21:U:13:ILE:HG22	21:U:22:ARG:CZ	2.42	0.49
1:A:1131:G:H2'	1:A:1132:C:C6	2.48	0.49
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.94	0.49
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.94	0.49
1:A:1451:A:H5''	1:A:1452:C:H5	1.77	0.49
1:A:1495:U:O4	24:A:1601:HJR:N12	2.45	0.49
4:D:31:CYS:C	4:D:33:MET:H	2.16	0.49
8:H:112:LEU:HD23	8:H:133:LEU:HA	1.94	0.49
1:A:1225:A:H2'	1:A:1225:A:N3	2.27	0.49
1:A:1228:C:H4'	13:M:116:THR:HA	1.95	0.49
9:I:104:ARG:NH1	9:I:105:ASP:O	2.45	0.49
10:J:55:LYS:HD2	10:J:56:HIS:H	1.78	0.49
1:A:1256:A:H4'	1:A:1257:U:O5'	2.13	0.48
1:A:1316:G:O6	19:S:6:LYS:NZ	2.42	0.48
2:B:43:ASP:HB3	2:B:46:LYS:HB2	1.95	0.48
18:R:40:LEU:HB3	18:R:79:LEU:HD11	1.95	0.48
1:A:190(K):G:H2'	1:A:190(L):U:C6	2.48	0.48
2:B:223:ILE:HD12	2:B:230:VAL:HG21	1.94	0.48
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.95	0.48
1:A:1420:C:H2'	1:A:1421:G:C8	2.48	0.48
1:A:1435:G:H2'	1:A:1436:U:C6	2.48	0.48
1:A:1474:G:H2'	1:A:1475:G:H8	1.77	0.48
4:D:187:ARG:CZ	4:D:188:LEU:H	2.26	0.48
17:Q:6:LEU:HB2	17:Q:59:ILE:HG22	1.95	0.48
1:A:224:C:H2'	1:A:225:C:C6	2.48	0.48
1:A:682:G:H2'	1:A:683:G:C8	2.48	0.48
3:C:8:ILE:HG13	3:C:184:TYR:HB3	1.95	0.48
11:K:87:THR:HG23	11:K:91:ARG:HH21	1.78	0.48
15:O:26:GLU:OE1	15:O:77:ARG:NH1	2.35	0.48
1:A:501:C:H2'	1:A:502:G:C8	2.48	0.48
1:A:737:A:H2'	1:A:738:C:C6	2.48	0.48
18:R:47:THR:HA	18:R:83:GLU:HB2	1.95	0.48
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.48	0.48
16:P:15:PRO:HD2	16:P:42:ARG:HD3	1.94	0.48
1:A:1308:U:OP2	13:M:99:ARG:HG2	2.14	0.48
9:I:19:LEU:HD22	9:I:59:PHE:HB3	1.96	0.48
21:U:10:ARG:O	21:U:13:ILE:HG12	2.14	0.48
19:S:5:LEU:HD12	19:S:9:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.95	0.48
12:L:117:ARG:NH2	12:L:124:LYS:HD3	2.29	0.48
1:A:801:U:H2'	1:A:802:A:C8	2.49	0.47
1:A:838:G:H1	1:A:848:C:H42	1.62	0.47
1:A:1046:A:H3'	1:A:1047:G:H8	1.79	0.47
5:E:80:ILE:HD13	5:E:138:ALA:HB1	1.96	0.47
1:A:161:A:N1	1:A:347:G:O2'	2.42	0.47
1:A:1148:U:H2'	1:A:1149:C:O4'	2.13	0.47
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.47
1:A:427:U:OP2	4:D:36:ARG:NH2	2.47	0.47
1:A:701:C:H4'	1:A:702:A:O5'	2.13	0.47
1:A:1228:C:P	13:M:108:ARG:HH22	2.37	0.47
8:H:4:ASP:OD2	8:H:85:ARG:NH1	2.47	0.47
1:A:1402:4OC:HM22	1:A:1403:C:H5'	1.95	0.47
1:A:1426:C:H42	1:A:1474:G:H1	1.63	0.47
10:J:57:LYS:O	10:J:60:ARG:NH1	2.47	0.47
11:K:22:HIS:HB3	11:K:29:ILE:HD13	1.96	0.47
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.95	0.47
1:A:390:C:H2'	1:A:391:G:C8	2.49	0.47
1:A:686:U:O2'	1:A:687:A:H8	1.97	0.47
1:A:757:U:O2'	1:A:879:C:O2	2.32	0.47
1:A:1040:U:H2'	1:A:1041:A:H8	1.79	0.47
1:A:1367:C:C5'	10:J:60:ARG:HE	2.28	0.47
1:A:1414:U:H2'	1:A:1415:G:H8	1.78	0.47
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.96	0.47
13:M:10:PRO:O	13:M:45:VAL:HG11	2.15	0.47
1:A:181:G:H4'	1:A:182:U:C5'	2.44	0.47
1:A:376:G:H5''	16:P:5:ARG:HB2	1.96	0.47
1:A:474:G:H2'	1:A:475:G:H8	1.80	0.47
1:A:701:C:H5''	1:A:703:G:H5'	1.96	0.47
1:A:707:C:H2'	1:A:708:C:C6	2.50	0.47
1:A:1319:A:OP1	19:S:5:LEU:HD22	2.15	0.47
5:E:11:ILE:HG22	5:E:12:LEU:HD12	1.96	0.47
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.96	0.47
18:R:22:VAL:HG23	18:R:56:THR:HA	1.96	0.47
1:A:401:C:H2'	1:A:402:G:H8	1.80	0.47
1:A:1189:C:OP2	10:J:51:ARG:NH2	2.48	0.47
1:A:1301:U:OP2	1:A:1303:C:N4	2.48	0.47
1:A:1405:G:O2'	1:A:1518[B]:MA6:O2'	2.33	0.47
10:J:49:VAL:HG21	14:N:44:LEU:HD23	1.97	0.47
1:A:1031:G:H2'	1:A:1032:G:H8	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:C:H2'	1:A:1329:A:H8	1.79	0.47
4:D:24:GLU:HG2	4:D:25:ARG:H	1.79	0.47
7:G:36:LYS:NZ	9:I:42:ARG:HD3	2.29	0.47
1:A:1294:G:H2'	1:A:1295:G:C8	2.50	0.47
1:A:1309:G:P	13:M:88:ARG:HH21	2.38	0.47
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.97	0.47
20:T:29:LYS:O	20:T:33:ILE:HG12	2.14	0.47
1:A:103:C:OP1	20:T:17:ARG:NH1	2.47	0.46
1:A:1222:G:H5''	19:S:78:ARG:HE	1.80	0.46
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.97	0.46
1:A:966:M2G:HM13	1:A:967:5MC:H1'	1.96	0.46
2:B:97:TRP:HZ2	2:B:102:LEU:HD22	1.80	0.46
19:S:29:ARG:HD2	19:S:29:ARG:N	2.30	0.46
1:A:281:G:H4'	1:A:282:A:O5'	2.14	0.46
1:A:1310:G:H2'	1:A:1311:G:H8	1.80	0.46
10:J:4:ILE:HG22	10:J:6:ILE:HD11	1.98	0.46
1:A:139:G:H2'	1:A:140:A:H8	1.79	0.46
1:A:1328:C:H2'	1:A:1329:A:C8	2.51	0.46
1:A:1515[A]:C:H2'	1:A:1516[A]:G:H8	1.80	0.46
4:D:18:LYS:HA	4:D:33:MET:HG3	1.96	0.46
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.97	0.46
1:A:392:G:H2'	1:A:393:A:C8	2.49	0.46
1:A:839:U:H2'	1:A:839:U:O2	2.16	0.46
1:A:1347:G:O2'	9:I:109:VAL:HA	2.16	0.46
1:A:1356:G:H2'	1:A:1357:A:C8	2.50	0.46
15:O:32:LEU:O	15:O:36:ILE:HG12	2.16	0.46
1:A:299:G:H2'	1:A:300:A:C8	2.51	0.46
1:A:1345:U:OP1	9:I:120:ARG:NH1	2.49	0.46
3:C:147:LYS:HE3	3:C:203:PHE:CE2	2.51	0.46
5:E:99:GLY:N	5:E:117:ASP:OD2	2.41	0.46
9:I:8:GLY:HA2	9:I:79:LEU:HD13	1.97	0.46
1:A:13:C:N4	1:A:20:U:H3	2.14	0.46
1:A:564:C:O2'	8:H:91:ARG:NH2	2.49	0.46
1:A:762:C:H2'	1:A:763:G:C8	2.51	0.46
1:A:1171:G:H2'	1:A:1172:C:C6	2.51	0.46
1:A:1419:G:N2	1:A:1481:U:O2	2.44	0.46
1:A:424:G:H2'	1:A:425:G:C8	2.51	0.46
1:A:1193:G:OP1	3:C:167:TRP:NE1	2.40	0.46
2:B:17:PHE:HD1	2:B:41:ILE:HD12	1.80	0.46
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.50	0.46
8:H:63:LEU:H	8:H:63:LEU:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:U:H2'	1:A:637:G:C8	2.51	0.46
9:I:116:LYS:HD2	9:I:122:ALA:HA	1.97	0.46
1:A:13:C:H42	1:A:915:A:H62	1.64	0.46
1:A:231:G:H2'	1:A:232:G:H8	1.81	0.46
1:A:762:C:H2'	1:A:763:G:H8	1.80	0.46
1:A:1197:G:H5''	27:A:1913:HOH:O	2.15	0.46
6:F:22:GLU:OE1	6:F:82:ARG:NH1	2.49	0.46
13:M:101:GLN:OE1	13:M:101:GLN:N	2.45	0.46
15:O:18:PHE:CZ	15:O:21:ASP:HB2	2.51	0.46
15:O:39:LEU:HD12	15:O:59:MET:HE2	1.97	0.46
1:A:902:G:H2'	1:A:903:G:H8	1.81	0.45
1:A:913:A:H4'	1:A:914:A:O5'	2.17	0.45
1:A:1065:U:H4'	1:A:1066:C:O5'	2.16	0.45
1:A:1427:U:H2'	1:A:1428:A:C8	2.51	0.45
20:T:40:ALA:HB2	20:T:55:ILE:HG22	1.98	0.45
1:A:5:U:H4'	1:A:6:G:O5'	2.15	0.45
1:A:445:G:H2'	1:A:446:G:C8	2.51	0.45
1:A:445:G:H2'	1:A:446:G:H8	1.81	0.45
1:A:689:C:H2'	1:A:690:G:O4'	2.16	0.45
1:A:714:G:H2'	1:A:715:A:C8	2.52	0.45
1:A:1027:C:N4	1:A:1034:G:H1	2.15	0.45
1:A:67:C:H2'	1:A:68:G:C8	2.52	0.45
1:A:384:G:H2'	1:A:385:C:C6	2.51	0.45
1:A:1300:G:H4'	1:A:1301:U:O5'	2.16	0.45
2:B:240:GLN:OE1	2:B:240:GLN:N	2.43	0.45
13:M:54:VAL:O	13:M:58:GLU:HG2	2.15	0.45
15:O:59:MET:HB2	15:O:59:MET:HE3	1.84	0.45
1:A:153:C:N4	1:A:168:G:H1	2.13	0.45
1:A:1132:C:H2'	1:A:1133:G:H8	1.81	0.45
1:A:1150:U:O4	1:A:1151:A:N6	2.49	0.45
2:B:178:ARG:O	8:H:72:PRO:HD3	2.16	0.45
14:N:24:CYS:HB3	14:N:29:ARG:HB3	1.99	0.45
1:A:1520[A]:G:H2'	1:A:1521:G:C8	2.52	0.45
1:A:430:A:P	4:D:8:VAL:H	2.40	0.45
1:A:971:G:H4'	1:A:972:C:H5''	1.98	0.45
1:A:1014:A:H4'	19:S:14:HIS:CG	2.52	0.45
1:A:1060:C:H5''	10:J:51:ARG:HB3	2.00	0.45
1:A:1437:C:H42	1:A:1464:G:H1	1.64	0.45
2:B:21:ARG:HG3	2:B:22:LYS:H	1.83	0.45
11:K:84:VAL:HG11	11:K:91:ARG:HD3	1.98	0.45
1:A:332:G:H2'	1:A:333:G:H8	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:U:H2'	1:A:1206:G:C8	2.52	0.44
2:B:179:LYS:HE3	2:B:179:LYS:HB2	1.83	0.44
12:L:54:LYS:HD2	12:L:54:LYS:N	2.32	0.44
14:N:14:PRO:C	14:N:16:PHE:H	2.20	0.44
14:N:27:CYS:HB3	14:N:43:CYS:SG	2.57	0.44
1:A:1213:A:N1	1:A:1215:G:H1'	2.30	0.44
13:M:50:GLU:HA	13:M:53:VAL:HB	1.99	0.44
16:P:42:ARG:HB2	16:P:44:THR:HG23	1.99	0.44
20:T:71:THR:HG22	20:T:72:LEU:HG	1.99	0.44
1:A:979:C:OP1	1:A:1223:C:N4	2.51	0.44
1:A:992:U:H3	1:A:1044:A:H62	1.66	0.44
1:A:1515[A]:C:H2'	1:A:1516[A]:G:C8	2.53	0.44
10:J:15:THR:HG22	10:J:94:VAL:HB	1.99	0.44
18:R:26:LEU:HD12	18:R:26:LEU:HA	1.77	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.83	0.44
1:A:1506:U:O2'	1:A:1507:A:H5'	2.17	0.44
3:C:24:ALA:HB1	3:C:28:GLN:HB2	2.00	0.44
4:D:199:ASN:ND2	4:D:202:LEU:HD23	2.33	0.44
15:O:26:GLU:HA	15:O:81:LEU:HD11	1.99	0.44
1:A:371:G:O2'	1:A:372:C:H5'	2.18	0.44
1:A:824:C:H2'	1:A:825:G:C8	2.52	0.44
1:A:877:C:O2	8:H:3:THR:HG21	2.18	0.44
7:G:108:ALA:O	7:G:111:ARG:HB2	2.18	0.44
11:K:69:ALA:O	11:K:73:MET:HG2	2.18	0.44
1:A:890:G:O2'	1:A:906:G:O6	2.28	0.44
1:A:965:A:H4'	1:A:966:M2G:OP1	2.18	0.44
3:C:180:ALA:HB1	3:C:205:GLY:O	2.17	0.44
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.98	0.44
1:A:31:G:N2	1:A:48:C:OP1	2.40	0.44
1:A:936:C:H2'	1:A:937:A:O4'	2.18	0.44
4:D:108:LEU:HD22	4:D:176:LEU:HB3	2.00	0.44
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.00	0.44
17:Q:29:HIS:CG	17:Q:30:PRO:HD2	2.53	0.44
1:A:23:C:H2'	1:A:24:U:C6	2.52	0.44
1:A:337:C:H2'	1:A:338:A:C8	2.53	0.44
1:A:362:G:N2	1:A:365:U:OP2	2.49	0.44
1:A:956:U:H2'	1:A:957:U:O4'	2.17	0.44
1:A:1070:U:OP1	5:E:20:GLN:HG3	2.18	0.44
7:G:88:PRO:O	7:G:155:ARG:NH1	2.51	0.44
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.58	0.44
1:A:1472:U:H2'	1:A:1473:A:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:CYS:HA	4:D:31:CYS:HB2	2.00	0.44
14:N:9:LYS:NZ	14:N:12:ARG:HH21	2.16	0.44
15:O:75:PRO:O	15:O:79:ARG:HG3	2.18	0.44
1:A:89:C:H2'	1:A:90:U:O4'	2.18	0.43
1:A:92:C:H2'	1:A:93:G:H8	1.83	0.43
1:A:258:G:H2'	1:A:259:G:C8	2.53	0.43
1:A:1196:U:H3	3:C:162:GLN:NE2	2.16	0.43
1:A:1373:G:H5''	7:G:36:LYS:HE3	2.00	0.43
2:B:8:LYS:O	2:B:217:ARG:NH1	2.50	0.43
4:D:28:SER:O	4:D:30:LYS:N	2.47	0.43
14:N:23:ARG:HA	14:N:29:ARG:O	2.18	0.43
1:A:91:C:H2'	1:A:92:C:C6	2.53	0.43
1:A:118:U:H3'	1:A:288:A:H61	1.84	0.43
1:A:522:C:H41	12:L:53:ARG:NH2	2.17	0.43
1:A:812:C:H4'	1:A:813:U:O5'	2.18	0.43
1:A:1003(A):G:H2'	1:A:1004:A:H4'	2.01	0.43
2:B:118:LEU:HB2	2:B:142:LEU:HD21	1.99	0.43
11:K:65:ALA:HB1	11:K:98:LEU:HD23	1.99	0.43
12:L:54:LYS:HG2	12:L:75:HIS:CD2	2.53	0.43
12:L:69:TYR:O	12:L:100:ILE:HB	2.18	0.43
20:T:45:GLN:HA	20:T:91:LEU:HD12	2.00	0.43
1:A:12:U:H4'	1:A:526:C:O2'	2.18	0.43
1:A:592:G:H2'	1:A:593:G:H8	1.83	0.43
1:A:1054:C:N4	23:W:34:G:C8	2.86	0.43
1:A:1207:2MG:HM23	1:A:1208:C:H1'	2.00	0.43
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.54	0.43
16:P:40:ASP:HB3	16:P:48:TRP:HB2	2.01	0.43
20:T:50:GLU:HG3	20:T:100:ILE:HD11	2.00	0.43
1:A:370:C:H2'	1:A:371:G:H8	1.83	0.43
1:A:560:U:H4'	1:A:561:U:H5''	2.01	0.43
2:B:15:VAL:HG12	2:B:210:SER:HB3	1.99	0.43
3:C:11:ARG:NH1	3:C:178:LEU:HA	2.32	0.43
12:L:25:PRO:HD2	12:L:97:ARG:NH1	2.34	0.43
1:A:147:G:H1	1:A:175:C:H42	1.66	0.43
1:A:812:C:OP1	1:A:903:G:H1'	2.18	0.43
1:A:1006:C:H2'	1:A:1007:C:H6	1.84	0.43
1:A:861:G:H2'	1:A:862:C:H6	1.83	0.43
4:D:20:TYR:HD1	4:D:26:CYS:HB3	1.82	0.43
7:G:18:TYR:OH	7:G:58:PRO:HG2	2.19	0.43
8:H:33:GLU:HG3	8:H:48:TYR:CE2	2.54	0.43
10:J:26:ALA:HB1	10:J:84:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:43:LEU:HB2	20:T:52:ALA:HB2	2.01	0.43
1:A:742:G:H2'	1:A:743:U:O4'	2.19	0.43
1:A:1056:U:H5'	3:C:163:ALA:HB2	2.00	0.43
1:A:1065:U:H1'	1:A:1066:C:OP2	2.19	0.43
1:A:1073:U:OP2	5:E:57:LYS:NZ	2.36	0.43
11:K:93:GLN:HG2	11:K:96:ARG:HH21	1.82	0.43
14:N:12:ARG:HG3	14:N:13:THR:H	1.84	0.43
17:Q:59:ILE:HD12	17:Q:73:VAL:HA	2.01	0.43
19:S:63:THR:HG22	19:S:64:GLU:H	1.84	0.43
20:T:89:ARG:HH21	20:T:104:LEU:HB3	1.83	0.43
1:A:23:C:H2'	1:A:24:U:H6	1.83	0.43
1:A:279:A:C6	17:Q:98:LEU:HD13	2.54	0.43
1:A:337:C:H2'	1:A:338:A:H8	1.84	0.43
1:A:591:U:H2'	1:A:592:G:C8	2.54	0.43
1:A:603:U:H2'	1:A:604:G:H8	1.84	0.43
1:A:309:G:H2'	1:A:310:G:H8	1.84	0.43
1:A:411:A:N3	1:A:413:G:O2'	2.41	0.43
1:A:1034:G:H2'	1:A:1035:A:H8	1.84	0.43
1:A:1040:U:H2'	1:A:1041:A:C8	2.54	0.43
1:A:1163:C:H2'	1:A:1164:G:H8	1.84	0.43
5:E:105:VAL:HB	5:E:106:PRO:HD3	2.01	0.43
1:A:1108:G:H5'	3:C:176:HIS:CD2	2.54	0.43
1:A:1221:G:O3'	19:S:77:THR:HG21	2.19	0.43
5:E:147:ASP:N	5:E:147:ASP:OD1	2.52	0.43
8:H:121:ASP:N	8:H:121:ASP:OD1	2.51	0.43
12:L:48:PRO:HD2	12:L:92:OTD:H8	2.01	0.43
1:A:21:G:H4'	1:A:22:G:OP1	2.19	0.42
1:A:524:G:H2'	1:A:525:C:C6	2.54	0.42
1:A:1465:C:H2'	1:A:1466:C:O4'	2.19	0.42
3:C:179:ARG:HG2	3:C:206:GLU:O	2.19	0.42
5:E:102:ALA:O	5:E:107:ARG:NH1	2.52	0.42
11:K:98:LEU:HD22	11:K:98:LEU:HA	1.83	0.42
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.99	0.42
19:S:45:VAL:HA	19:S:62:ILE:HG13	2.01	0.42
1:A:76:C:H2'	1:A:77:G:H8	1.84	0.42
1:A:1002:G:H2'	1:A:1003:G:C8	2.54	0.42
1:A:1189:C:P	10:J:51:ARG:HH22	2.42	0.42
1:A:1512:U:H2'	1:A:1513:A:C8	2.55	0.42
3:C:202:ILE:HG22	3:C:204:LEU:HD23	2.00	0.42
5:E:43:LEU:HD21	5:E:132:ALA:HB1	2.02	0.42
1:A:62:U:H2'	1:A:63:C:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:951:G:OP2	13:M:102:ARG:NH2	2.53	0.42
1:A:1504:G:OP1	1:A:1507:A:H4'	2.18	0.42
2:B:32:ILE:HD11	2:B:190:THR:HG23	2.00	0.42
2:B:155:LEU:HD11	2:B:159:PRO:HG3	2.01	0.42
3:C:41:GLY:O	3:C:45:LYS:HG2	2.19	0.42
3:C:105:GLU:HG2	3:C:106:VAL:N	2.33	0.42
4:D:159:ARG:O	4:D:163:GLU:HB2	2.19	0.42
10:J:79:ARG:O	10:J:82:ILE:N	2.52	0.42
12:L:53:ARG:HG3	12:L:69:TYR:HE1	1.84	0.42
1:A:217:C:H2'	1:A:218:C:C6	2.55	0.42
1:A:421:U:H5'	1:A:422:C:C5	2.55	0.42
1:A:1301:U:H1'	1:A:1302:U:OP1	2.19	0.42
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.84	0.42
12:L:44:THR:HA	12:L:45:PRO:HD3	1.89	0.42
1:A:129:U:O3'	1:A:129(A):G:H3'	2.19	0.42
1:A:491:G:H2'	1:A:492:G:C8	2.54	0.42
1:A:668:G:H1	1:A:738:C:H42	1.67	0.42
3:C:64:VAL:HG12	3:C:66:VAL:HG23	2.00	0.42
9:I:53:VAL:HG21	9:I:85:LEU:HD21	2.01	0.42
13:M:48:LEU:HA	13:M:48:LEU:HD22	1.75	0.42
18:R:46:GLU:H	18:R:46:GLU:CD	2.21	0.42
1:A:895:G:H2'	1:A:896:C:C6	2.55	0.42
1:A:948:C:H2'	1:A:949:A:H8	1.85	0.42
9:I:10:ARG:HD3	9:I:105:ASP:HB3	2.02	0.42
11:K:12:ARG:HB2	11:K:75:TYR:CD2	2.55	0.42
1:A:92:C:H2'	1:A:93:G:C8	2.55	0.42
1:A:98:U:H2'	1:A:99:C:C6	2.55	0.42
1:A:1270:C:H2'	1:A:1271:G:C8	2.54	0.42
3:C:20:SER:HB3	3:C:22:TRP:HE1	1.83	0.42
1:A:254:G:OP1	17:Q:67:LYS:O	2.36	0.42
1:A:533:A:N6	1:A:536:C:C2	2.88	0.42
2:B:91:PRO:HG2	2:B:155:LEU:HG	2.01	0.42
4:D:15:GLU:HB3	4:D:63:LYS:HD3	2.01	0.42
6:F:100:ASN:O	6:F:100:ASN:ND2	2.53	0.42
8:H:26:VAL:HG13	8:H:59:LEU:HB2	2.02	0.42
18:R:53:ARG:NH1	18:R:58:LEU:O	2.52	0.42
2:B:102:LEU:HD21	2:B:162:ILE:HD11	2.02	0.42
10:J:14:LYS:HE2	10:J:14:LYS:HB3	1.89	0.42
1:A:229:U:H2'	1:A:230:G:H8	1.85	0.42
1:A:1145:C:H1'	1:A:1146:A:C8	2.54	0.42
1:A:1244:C:H42	1:A:1293:G:H1	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:70:ASP:OD1	6:F:70:ASP:N	2.53	0.42
11:K:57:THR:CG2	11:K:60:ALA:H	2.33	0.42
1:A:518:C:H2'	1:A:530:G:C8	2.55	0.41
1:A:1277:C:O2'	1:A:1279:A:H1'	2.19	0.41
8:H:19:VAL:HG23	8:H:21:LYS:HG3	2.01	0.41
8:H:87:SER:HB2	8:H:93:VAL:HB	2.02	0.41
18:R:87:ARG:O	18:R:88:LYS:HB2	2.20	0.41
1:A:478:A:H2'	1:A:479:C:C6	2.55	0.41
1:A:571:U:O4	1:A:864:A:N6	2.54	0.41
1:A:580:U:H2'	1:A:581:G:O4'	2.20	0.41
1:A:688:G:H2'	1:A:689:C:C6	2.55	0.41
1:A:833:U:H2'	1:A:834:C:C6	2.55	0.41
1:A:1218:C:H2'	1:A:1219:U:C6	2.55	0.41
5:E:118:ILE:HG12	5:E:119:LEU:N	2.35	0.41
10:J:34:VAL:HG13	10:J:74:ILE:HA	2.02	0.41
12:L:84:LEU:HB2	12:L:104:VAL:HG21	2.01	0.41
1:A:474:G:H2'	1:A:475:G:C8	2.55	0.41
4:D:15:GLU:OE1	4:D:59:ARG:NH2	2.47	0.41
7:G:115:ARG:HB2	7:G:118:VAL:HG23	2.02	0.41
8:H:38:ILE:HG13	8:H:41:ARG:HH12	1.85	0.41
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.94	0.41
14:N:50:LYS:HG2	14:N:52:GLN:NE2	2.33	0.41
1:A:665:A:H2'	1:A:732:C:O2	2.19	0.41
8:H:46:LYS:HG3	8:H:64:LYS:HB3	2.02	0.41
14:N:41:ARG:HG3	14:N:42:ILE:N	2.36	0.41
16:P:4:ILE:O	16:P:66:PRO:HA	2.19	0.41
1:A:1366:C:H2'	1:A:1367:C:C6	2.56	0.41
9:I:127:LYS:HE3	9:I:127:LYS:HB3	1.90	0.41
12:L:126:LYS:HB2	12:L:126:LYS:HE2	1.85	0.41
1:A:230:G:H2'	1:A:231:G:O4'	2.20	0.41
1:A:344:A:H5'	1:A:345:C:C5	2.56	0.41
1:A:592:G:H2'	1:A:593:G:C8	2.56	0.41
2:B:16:HIS:CG	2:B:210:SER:HB2	2.55	0.41
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.41
10:J:82:ILE:HA	10:J:85:LEU:HB2	2.02	0.41
12:L:36:VAL:HG22	12:L:82:VAL:HG12	2.02	0.41
1:A:757:U:H2'	1:A:758:G:O4'	2.20	0.41
1:A:1310:G:H2'	1:A:1311:G:C8	2.56	0.41
1:A:1384:C:H2'	1:A:1385:G:C8	2.55	0.41
2:B:16:HIS:CE1	2:B:210:SER:HB2	2.55	0.41
12:L:68:ALA:HB1	12:L:100:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:C:O2	1:A:355:C:N4	2.49	0.41
1:A:766:A:H2'	1:A:767:A:O4'	2.20	0.41
1:A:1520[A]:G:H2'	1:A:1521:G:H8	1.85	0.41
3:C:134:ILE:O	3:C:138:VAL:HG23	2.21	0.41
1:A:407:G:H2'	1:A:408:A:C8	2.56	0.41
1:A:456:C:N4	1:A:476:G:H1	2.11	0.41
1:A:488:C:H2'	1:A:489:C:C6	2.55	0.41
1:A:570:G:C6	1:A:873:A:C2	3.09	0.41
1:A:620:C:N3	4:D:135:LEU:HD22	2.36	0.41
1:A:987:G:H2'	1:A:988:G:C8	2.56	0.41
1:A:1405:G:H21	1:A:1518[A]:MA6:H1'	1.86	0.41
1:A:1480:G:H2'	1:A:1481:U:O4'	2.20	0.41
2:B:18:GLY:HA3	2:B:41:ILE:HA	2.03	0.41
3:C:131:ARG:HE	3:C:131:ARG:HB2	1.68	0.41
4:D:35:ARG:HD2	4:D:35:ARG:N	2.36	0.41
9:I:69:GLY:O	9:I:73:GLN:HG3	2.20	0.41
1:A:277:C:H5'	17:Q:68:ARG:NH1	2.36	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.20	0.41
2:B:219:VAL:O	2:B:223:ILE:HG13	2.21	0.41
6:F:33:TYR:CD1	6:F:75:LEU:HD23	2.55	0.41
8:H:86:ILE:HG13	8:H:135:CYS:HA	2.03	0.41
9:I:49:PRO:HB2	9:I:81:ILE:HG22	2.02	0.41
1:A:114:U:H2'	1:A:115:G:C8	2.56	0.40
1:A:299:G:C6	1:A:300:A:C6	3.09	0.40
1:A:321:A:H61	1:A:332:G:H1	1.68	0.40
1:A:939:G:H2'	1:A:940:C:C6	2.56	0.40
1:A:1071:C:H5''	5:E:49:PRO:HG2	2.03	0.40
1:A:1263:C:H2'	1:A:1264:C:C6	2.55	0.40
7:G:145:ALA:C	7:G:147:ALA:H	2.24	0.40
1:A:680:C:H42	1:A:710:G:H1	1.69	0.40
1:A:1016:A:H2'	1:A:1017:G:O4'	2.21	0.40
1:A:1359:C:O2'	1:A:1361:G:N7	2.53	0.40
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.02	0.40
1:A:882:C:O2'	1:A:883:C:H5'	2.21	0.40
1:A:913:A:P	12:L:91:LYS:HZ2	2.44	0.40
1:A:974:A:OP1	1:A:974:A:H8	2.05	0.40
1:A:1006:C:H2'	1:A:1007:C:C6	2.56	0.40
1:A:1241:G:OP1	7:G:35:LYS:NZ	2.54	0.40
2:B:74:LYS:O	2:B:78:GLN:HG3	2.22	0.40
4:D:24:GLU:C	4:D:26:CYS:H	2.23	0.40
4:D:177:ASP:OD1	4:D:180:GLY:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:43:GLY:O	8:H:64:LYS:HD3	2.21	0.40
12:L:82:VAL:O	12:L:106:ASP:HB2	2.20	0.40
13:M:63:THR:HG23	13:M:64:TRP:CD2	2.57	0.40
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	2.03	0.40
18:R:19:LYS:HB2	18:R:19:LYS:HE3	1.78	0.40
1:A:542:G:OP1	4:D:10:ARG:NH2	2.54	0.40
1:A:620:C:N1	4:D:135:LEU:HD13	2.36	0.40
1:A:959:A:HO2'	1:A:984:C:HO2'	1.64	0.40
1:A:1043:C:H2'	1:A:1044:A:H8	1.86	0.40
4:D:18:LYS:HB3	4:D:18:LYS:HE2	1.80	0.40
4:D:36:ARG:N	4:D:37:PRO:HD3	2.37	0.40
7:G:8:GLU:H	7:G:8:GLU:HG3	1.52	0.40
9:I:19:LEU:HD23	9:I:19:LEU:HA	1.87	0.40
12:L:53:ARG:HG2	12:L:93:LEU:HD11	2.04	0.40
1:A:475:G:H2'	1:A:476:G:H8	1.86	0.40
2:B:101:MET:HA	2:B:108:ILE:HG13	2.03	0.40
5:E:123:LEU:HD23	5:E:123:LEU:HA	1.91	0.40
7:G:53:LYS:HE3	7:G:53:LYS:HB2	1.89	0.40
9:I:79:LEU:HD22	9:I:83:ARG:HG3	2.03	0.40
19:S:36:ARG:H	19:S:36:ARG:HG2	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	232/256 (91%)	217 (94%)	15 (6%)	0	100	100
3	C	204/239 (85%)	183 (90%)	21 (10%)	0	100	100
4	D	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
5	E	148/162 (91%)	142 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	99/101 (98%)	97 (98%)	2 (2%)	0	100	100
7	G	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	H	136/138 (99%)	130 (96%)	5 (4%)	1 (1%)	22	59
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	19	56
10	J	96/105 (91%)	80 (83%)	14 (15%)	2 (2%)	7	40
11	K	114/129 (88%)	111 (97%)	3 (3%)	0	100	100
12	L	121/135 (90%)	112 (93%)	9 (7%)	0	100	100
13	M	116/126 (92%)	99 (85%)	17 (15%)	0	100	100
14	N	58/61 (95%)	50 (86%)	8 (14%)	0	100	100
15	O	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100	100
17	Q	97/105 (92%)	93 (96%)	4 (4%)	0	100	100
18	R	68/88 (77%)	65 (96%)	3 (4%)	0	100	100
19	S	78/93 (84%)	72 (92%)	6 (8%)	0	100	100
20	T	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
21	U	22/27 (82%)	22 (100%)	0	0	100	100
All	All	2336/2541 (92%)	2184 (94%)	148 (6%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	55	LYS
10	J	56	HIS
8	H	71	GLY
9	I	8	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	180 (89%)	22 (11%)	6	29
3	C	160/188 (85%)	147 (92%)	13 (8%)	11	41
4	D	180/181 (99%)	170 (94%)	10 (6%)	21	53
5	E	115/123 (94%)	105 (91%)	10 (9%)	10	39
6	F	90/90 (100%)	87 (97%)	3 (3%)	38	64
7	G	126/127 (99%)	119 (94%)	7 (6%)	21	53
8	H	119/119 (100%)	109 (92%)	10 (8%)	11	41
9	I	98/99 (99%)	91 (93%)	7 (7%)	14	46
10	J	87/92 (95%)	81 (93%)	6 (7%)	15	47
11	K	88/99 (89%)	83 (94%)	5 (6%)	20	53
12	L	103/110 (94%)	95 (92%)	8 (8%)	12	43
13	M	94/101 (93%)	87 (93%)	7 (7%)	13	44
14	N	49/50 (98%)	47 (96%)	2 (4%)	30	59
15	O	79/80 (99%)	71 (90%)	8 (10%)	7	32
16	P	72/74 (97%)	66 (92%)	6 (8%)	11	41
17	Q	94/97 (97%)	85 (90%)	9 (10%)	8	34
18	R	61/77 (79%)	57 (93%)	4 (7%)	16	48
19	S	71/80 (89%)	61 (86%)	10 (14%)	3	21
20	T	76/82 (93%)	67 (88%)	9 (12%)	5	26
21	U	19/22 (86%)	18 (95%)	1 (5%)	22	54
All	All	1983/2111 (94%)	1826 (92%)	157 (8%)	12	43

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	VAL
2	B	8	LYS
2	B	11	LEU
2	B	21	ARG
2	B	33	TYR
2	B	44	LEU
2	B	69	LEU
2	B	73	THR
2	B	102	LEU
2	B	103	THR
2	B	106	LYS

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Mol	Chain	Res	Type
2	B	122	PHE
2	B	127	ILE
2	B	153	ARG
2	B	154	LEU
2	B	157	ARG
2	B	163	PHE
2	B	178	ARG
2	B	190	THR
2	B	200	ILE
2	B	206	ASP
2	B	213	LEU
3	C	3	ASN
3	C	26	LYS
3	C	31	HIS
3	C	34	LEU
3	C	70	VAL
3	C	90	GLU
3	C	91	LEU
3	C	95	THR
3	C	99	VAL
3	C	111	LEU
3	C	131	ARG
3	C	167	TRP
3	C	196	LEU
4	D	35	ARG
4	D	49	ARG
4	D	67	ILE
4	D	115	ARG
4	D	122	ARG
4	D	135	LEU
4	D	150	GLU
4	D	155	LEU
4	D	193	ASP
4	D	202	LEU
5	E	6	PHE
5	E	12	LEU
5	E	24	ARG
5	E	26	PHE
5	E	31	LEU
5	E	41	VAL
5	E	75	THR
5	E	79	GLU

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Mol	Chain	Res	Type
5	E	80	ILE
5	E	148	VAL
6	F	10	LEU
6	F	24	GLU
6	F	82	ARG
7	G	8	GLU
7	G	79	ARG
7	G	84	ASN
7	G	97	GLN
7	G	115	ARG
7	G	136	LYS
7	G	149	ARG
8	H	2	LEU
8	H	3	THR
8	H	29	SER
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	98	LYS
8	H	127	LEU
8	H	133	LEU
9	I	12	GLU
9	I	79	LEU
9	I	102	LEU
9	I	111	ARG
9	I	118	LYS
9	I	121	ARG
9	I	124	GLN
10	J	3	LYS
10	J	38	ILE
10	J	45	ARG
10	J	60	ARG
10	J	62	HIS
10	J	78	ASN
11	K	12	ARG
11	K	14	VAL
11	K	29	ILE
11	K	33	THR
11	K	98	LEU
12	L	18	VAL
12	L	20	LYS

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Mol	Chain	Res	Type
12	L	33	ARG
12	L	42	THR
12	L	53	ARG
12	L	79	GLU
12	L	80	HIS
12	L	113	ARG
13	M	37	THR
13	M	44	ARG
13	M	48	LEU
13	M	82	MET
13	M	105	THR
13	M	108	ARG
13	M	117	VAL
14	N	11	LYS
14	N	22	THR
15	O	5	LYS
15	O	32	LEU
15	O	39	LEU
15	O	45	VAL
15	O	65	ARG
15	O	70	LEU
15	O	81	LEU
15	O	83	GLU
16	P	9	PHE
16	P	42	ARG
16	P	55	ARG
16	P	62	VAL
16	P	67	THR
16	P	83	GLU
17	Q	34	LYS
17	Q	36	ILE
17	Q	39	SER
17	Q	53	LEU
17	Q	59	ILE
17	Q	60	ILE
17	Q	76	LEU
17	Q	91	ARG
17	Q	98	LEU
18	R	31	LEU
18	R	42	ARG
18	R	47	THR
18	R	87	ARG

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Mol	Chain	Res	Type
19	S	5	LEU
19	S	6	LYS
19	S	13	ASP
19	S	15	LEU
19	S	29	ARG
19	S	39	THR
19	S	48	THR
19	S	62	ILE
19	S	63	THR
19	S	79	THR
20	T	9	ASN
20	T	53	LEU
20	T	56	MET
20	T	57	ARG
20	T	62	LEU
20	T	68	LYS
20	T	73	HIS
20	T	84	LEU
20	T	92	LEU
21	U	25	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	204	ASN
3	C	37	GLN
5	E	65	ASN
12	L	99	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	234 (15%)	46 (3%)
22	Y	5/6 (83%)	2 (40%)	0
23	W	14/15 (93%)	2 (14%)	0
All	All	1523/1543 (98%)	238 (15%)	46 (3%)

All (238) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	21	G
1	A	22	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	101	A
1	A	108	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	163	C
1	A	182	U
1	A	183	G
1	A	190(D)	U
1	A	195	A
1	A	201	C
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	247	G
1	A	251	G
1	A	252	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	282	A
1	A	289	G
1	A	301	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	350	G

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Mol	Chain	Res	Type
1	A	351	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	356	A
1	A	367	U
1	A	373	A
1	A	374	A
1	A	381	C
1	A	384	G
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	429	U
1	A	430	A
1	A	439	A
1	A	451	A
1	A	452	A
1	A	460	A
1	A	461	C
1	A	481	G
1	A	485	G
1	A	486	U
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	519	C
1	A	524	G
1	A	531	U
1	A	533	A
1	A	547	A
1	A	559	A
1	A	560	U
1	A	562	C
1	A	564	C

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Mol	Chain	Res	Type
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	618	C
1	A	653	A
1	A	665	A
1	A	686	U
1	A	687	A
1	A	688	G
1	A	695	A
1	A	701	C
1	A	702	A
1	A	703	G
1	A	721	G
1	A	723	U
1	A	731	G
1	A	734	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	799	G
1	A	812	C
1	A	813	U
1	A	817	C
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	873	A
1	A	876	G
1	A	889	A
1	A	902	G

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Mol	Chain	Res	Type
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	942	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	967	5MC
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	989	C
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1005	A
1	A	1023	G
1	A	1024	G
1	A	1026	G
1	A	1045	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1096	C
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A

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Mol	Chain	Res	Type
1	A	1137	C
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1171	G
1	A	1183	A
1	A	1191	A
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1211	U
1	A	1212	U
1	A	1214	C
1	A	1224	G
1	A	1225	A
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1278	U
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1306	A
1	A	1320	C
1	A	1322	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1347	G

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Mol	Chain	Res	Type
1	A	1348	U
1	A	1353	G
1	A	1359	C
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1381	U
1	A	1398	A
1	A	1400	5MC
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1451	A
1	A	1478	C
1	A	1479	C
1	A	1485	U
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1504	G
1	A	1506	U
1	A	1529	G
1	A	1530	G
22	Y	5	U
22	Y	6	U
23	W	30	G
23	W	33	U

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	21	G
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	204	U
1	A	250	A
1	A	251	G
1	A	281	G
1	A	328	C
1	A	372	C

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Mol	Chain	Res	Type
1	A	428	G
1	A	429	U
1	A	484	G
1	A	485	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	559	A
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	792	A
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1145	C
1	A	1182	G
1	A	1190	G
1	A	1201	A
1	A	1256	A
1	A	1257	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1305	G
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1505	G

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

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	5MC	A	1404	1	15,22,23	0.94	0	19,32,35	1.01	1 (5%)
1	7MG	A	527	1	22,26,27	2.13	6 (27%)	28,39,42	1.75	6 (21%)
1	5MC	A	1400	1	15,22,23	0.91	0	19,32,35	1.05	1 (5%)
1	M2G	A	966	1	20,27,28	2.00	4 (20%)	22,40,43	2.40	4 (18%)
1	PSU	A	1540	1	17,21,22	1.05	1 (5%)	20,30,33	3.18	6 (30%)
1	PSU	A	516	25,1	17,21,22	1.06	2 (11%)	20,30,33	3.17	6 (30%)
1	PSU	A	1541	25,1	17,21,22	1.02	2 (11%)	20,30,33	3.16	6 (30%)
1	4OC	A	1402	1	16,23,24	0.86	0	17,32,35	0.85	1 (5%)
12	0TD	L	92	12	4,9,10	0.78	0	3,11,13	1.56	0
1	MA6	A	1518[B]	1	19,26,27	1.24	2 (10%)	18,38,41	0.75	0
1	UR3	A	1498	1	14,22,23	1.01	2 (14%)	15,32,35	1.07	1 (6%)
1	MA6	A	1518[A]	1	19,26,27	0.92	1 (5%)	18,38,41	0.73	0
1	MA6	A	1519[B]	1	19,26,27	1.28	3 (15%)	18,38,41	0.57	0
1	MA6	A	1519[A]	1	19,26,27	1.04	2 (10%)	18,38,41	0.58	0
1	5MC	A	967	1	15,22,23	0.89	0	19,32,35	1.08	1 (5%)
1	5MC	A	1407	1	15,22,23	0.93	0	19,32,35	1.13	2 (10%)
1	2MG	A	1207	1	19,26,27	2.27	4 (21%)	21,38,41	2.00	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1404	1	-	0/5/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	5MC	A	1400	1	-	2/5/25/26	0/2/2/2
1	M2G	A	966	1	-	3/7/29/30	0/3/3/3
1	PSU	A	1540	1	-	0/7/25/26	0/2/2/2
1	PSU	A	516	25,1	-	0/7/25/26	0/2/2/2
1	PSU	A	1541	25,1	-	1/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2
12	0TD	L	92	12	-	2/3/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1518[B]	1	-	2/7/29/30	0/3/3/3
1	UR3	A	1498	1	-	0/5/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	0/7/29/30	0/3/3/3
1	MA6	A	1519[B]	1	-	3/7/29/30	0/3/3/3
1	MA6	A	1519[A]	1	-	5/7/29/30	0/3/3/3
1	5MC	A	967	1	-	2/5/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/5/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1207	2MG	C2-N2	7.18	1.40	1.34
1	A	966	M2G	C6-N1	5.90	1.43	1.33
1	A	527	7MG	C4-N3	5.67	1.41	1.34
1	A	1207	2MG	C6-N1	5.66	1.42	1.33
1	A	527	7MG	C2-N2	4.86	1.43	1.33
1	A	527	7MG	C8-N9	-4.33	1.35	1.45
1	A	966	M2G	C2-N2	4.02	1.41	1.34
1	A	966	M2G	C2-N1	3.76	1.41	1.34
1	A	1518[B]	MA6	C6-N1	3.56	1.38	1.33
1	A	1519[B]	MA6	C6-N1	3.48	1.38	1.33
1	A	966	M2G	C4-N3	3.25	1.40	1.35
1	A	1540	PSU	C4-N3	3.18	1.38	1.33
1	A	1541	PSU	C4-N3	3.12	1.38	1.33
1	A	516	PSU	C4-N3	3.06	1.38	1.33
1	A	527	7MG	C6-N1	3.01	1.38	1.33
1	A	1498	UR3	C6-N1	2.63	1.39	1.35
1	A	527	7MG	C5-C6	2.59	1.45	1.41
1	A	1519[A]	MA6	C6-N1	2.53	1.36	1.33
1	A	1518[A]	MA6	C6-N1	2.48	1.36	1.33
1	A	1519[B]	MA6	C2-N1	2.43	1.38	1.33
1	A	527	7MG	CM7-N7	-2.31	1.42	1.46
1	A	1207	2MG	C4-N3	2.22	1.39	1.35
1	A	1207	2MG	C2-N1	2.21	1.41	1.34
1	A	1518[B]	MA6	C2-N1	2.20	1.38	1.33
1	A	1498	UR3	C4-N3	2.16	1.41	1.38
1	A	516	PSU	O4'-C1'	-2.15	1.41	1.44
1	A	1519[A]	MA6	C2-N1	2.14	1.37	1.33
1	A	1519[B]	MA6	C2-N3	2.14	1.35	1.32
1	A	1541	PSU	O4'-C1'	-2.02	1.41	1.44

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1541	PSU	N3-C2-N1	-10.95	119.72	128.43
1	A	516	PSU	N3-C2-N1	-10.86	119.80	128.43
1	A	1540	PSU	N3-C2-N1	-10.74	119.89	128.43
1	A	966	M2G	C5-C6-N1	-8.10	112.36	123.43
1	A	1207	2MG	C5-C6-N1	-7.56	113.09	123.43
1	A	966	M2G	C2-N1-C6	5.93	123.24	116.18
1	A	516	PSU	C2-N3-C4	5.73	119.98	115.14
1	A	1541	PSU	C2-N3-C4	5.72	119.97	115.14
1	A	1540	PSU	C2-N3-C4	5.68	119.93	115.14
1	A	527	7MG	N3-C4-N9	4.71	132.96	126.91
1	A	1540	PSU	C5-C4-N3	-4.24	119.90	125.36
1	A	516	PSU	C5-C4-N3	-4.17	119.98	125.36
1	A	527	7MG	N9-C8-N7	4.14	109.29	103.38
1	A	527	7MG	C5-C4-N3	-4.11	119.79	126.49
1	A	1541	PSU	C5-C4-N3	-4.09	120.09	125.36
1	A	1207	2MG	C2-N1-C6	3.76	121.92	115.18
1	A	516	PSU	C5-C6-N1	-3.35	120.32	124.44
1	A	1541	PSU	C6-N1-C2	3.29	120.78	115.36
1	A	516	PSU	C6-N1-C2	3.25	120.72	115.36
1	A	1540	PSU	C6-N1-C2	3.21	120.66	115.36
1	A	1540	PSU	C5-C6-N1	-3.21	120.49	124.44
1	A	1541	PSU	C5-C6-N1	-3.20	120.51	124.44
1	A	1540	PSU	C5-C1'-C2'	-2.81	110.30	115.32
1	A	966	M2G	N3-C2-N2	2.55	119.77	117.18
1	A	527	7MG	C2-N1-C6	2.54	119.97	115.93
1	A	527	7MG	C2-N3-C4	2.33	120.34	113.89
1	A	527	7MG	C4-C5-C6	2.32	117.69	115.20
1	A	1404	5MC	C4-N3-C2	2.29	118.78	116.02
1	A	967	5MC	C4-N3-C2	2.27	118.75	116.02
1	A	1400	5MC	C4-N3-C2	2.24	118.72	116.02
1	A	1402	4OC	CM4-N4-C4	-2.23	121.06	122.97
1	A	966	M2G	C2-N3-C4	-2.16	112.82	115.28
1	A	1407	5MC	C4-N3-C2	2.15	118.61	116.02
1	A	516	PSU	O4'-C1'-C2'	2.14	108.13	104.66
1	A	1498	UR3	C3'-C2'-C1'	2.10	104.14	100.98
1	A	1407	5MC	CM5-C5-C6	2.09	123.09	118.68
1	A	1207	2MG	C4-C5-N7	2.07	111.55	109.40
1	A	1541	PSU	O4'-C1'-C2'	2.01	107.92	104.66

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	L	92	0TD	O-C-CA-CB
12	L	92	0TD	CG-CB-SB-CSB
1	A	966	M2G	C4'-C5'-O5'-P
1	A	967	5MC	O4'-C4'-C5'-O5'
1	A	1400	5MC	O4'-C4'-C5'-O5'
1	A	1402	4OC	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	C5-C6-N6-C9
1	A	1519[A]	MA6	C5-C6-N6-C10
1	A	1519[B]	MA6	C5-C6-N6-C9
1	A	527	7MG	C3'-C4'-C5'-O5'
1	A	967	5MC	C3'-C4'-C5'-O5'
1	A	1400	5MC	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C4'-C5'-O5'
1	A	1519[A]	MA6	O4'-C4'-C5'-O5'
1	A	1519[A]	MA6	N1-C6-N6-C9
1	A	1519[B]	MA6	N1-C6-N6-C9
1	A	1519[B]	MA6	C5-C6-N6-C10
1	A	966	M2G	O4'-C4'-C5'-O5'
1	A	1518[B]	MA6	O4'-C4'-C5'-O5'
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	C3'-C4'-C5'-O5'
1	A	1541	PSU	O4'-C1'-C5-C4
1	A	1518[B]	MA6	C3'-C4'-C5'-O5'
1	A	1402	4OC	C3'-C2'-O2'-CM2

There are no ring outliers.

11 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1404	5MC	1	0
1	A	1400	5MC	1	0
1	A	966	M2G	2	0
1	A	1402	4OC	1	0
12	L	92	0TD	2	0
1	A	1518[B]	MA6	2	0
1	A	1518[A]	MA6	2	0
1	A	1519[B]	MA6	2	0
1	A	1519[A]	MA6	1	0
1	A	967	5MC	3	0
1	A	1207	2MG	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 252 ligands modelled in this entry, 251 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
24	HJR	A	1601	-	34,38,38	3.24	8 (23%)	42,58,58	2.66	15 (35%)

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
24	HJR	A	1601	-	-	7/26/72/72	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1601	HJR	O1-S	11.81	1.65	1.43
24	A	1601	HJR	O2-S	11.70	1.65	1.43
24	A	1601	HJR	S-N12	4.59	1.71	1.60
24	A	1601	HJR	O53-C53	3.63	1.48	1.43
24	A	1601	HJR	C23-C33	-2.84	1.49	1.53
24	A	1601	HJR	C62-C12	2.54	1.56	1.52
24	A	1601	HJR	O53-C13	2.34	1.48	1.41
24	A	1601	HJR	C31-C21	-2.24	1.47	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	HJR	O43-C43-C83	-10.75	84.57	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1601	HJR	C12-N12-S	-6.16	111.18	122.84
24	A	1601	HJR	O2-S-O1	-5.38	109.65	120.57
24	A	1601	HJR	O11-C42-C52	4.02	117.98	107.28
24	A	1601	HJR	C93-N33-C33	-3.20	110.58	114.53
24	A	1601	HJR	O2-S-C6	3.20	109.50	103.90
24	A	1601	HJR	O51-C51-C41	3.11	113.21	109.86
24	A	1601	HJR	O62-C62-C12	3.08	116.08	108.85
24	A	1601	HJR	O1-S-C6	2.61	108.47	103.90
24	A	1601	HJR	C11-O51-C51	-2.35	109.58	113.35
24	A	1601	HJR	O62-C62-C52	2.30	113.40	107.28
24	A	1601	HJR	C13-O62-C62	2.27	119.26	114.66
24	A	1601	HJR	C6-S-N12	2.16	109.63	104.69
24	A	1601	HJR	C22-C12-C62	2.06	113.30	109.47
24	A	1601	HJR	C31-C41-C51	2.03	115.49	110.62

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	1601	HJR	C41-C51-C61-N61
24	A	1601	HJR	O51-C51-C61-N61
24	A	1601	HJR	C52-C42-O11-C11
24	A	1601	HJR	C52-C62-O62-C13
24	A	1601	HJR	C12-N12-S-O2
24	A	1601	HJR	C21-C11-O11-C42
24	A	1601	HJR	O51-C11-O11-C42

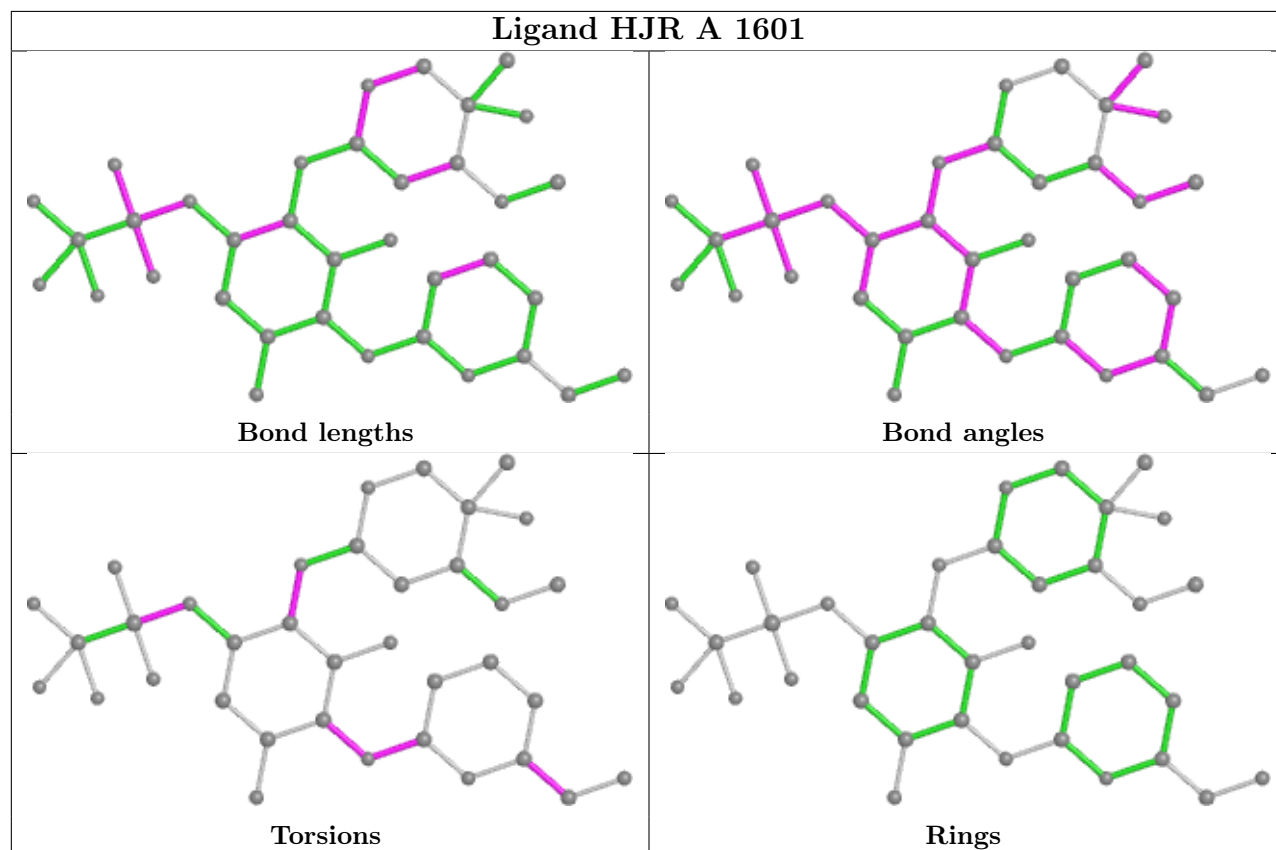
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1601	HJR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

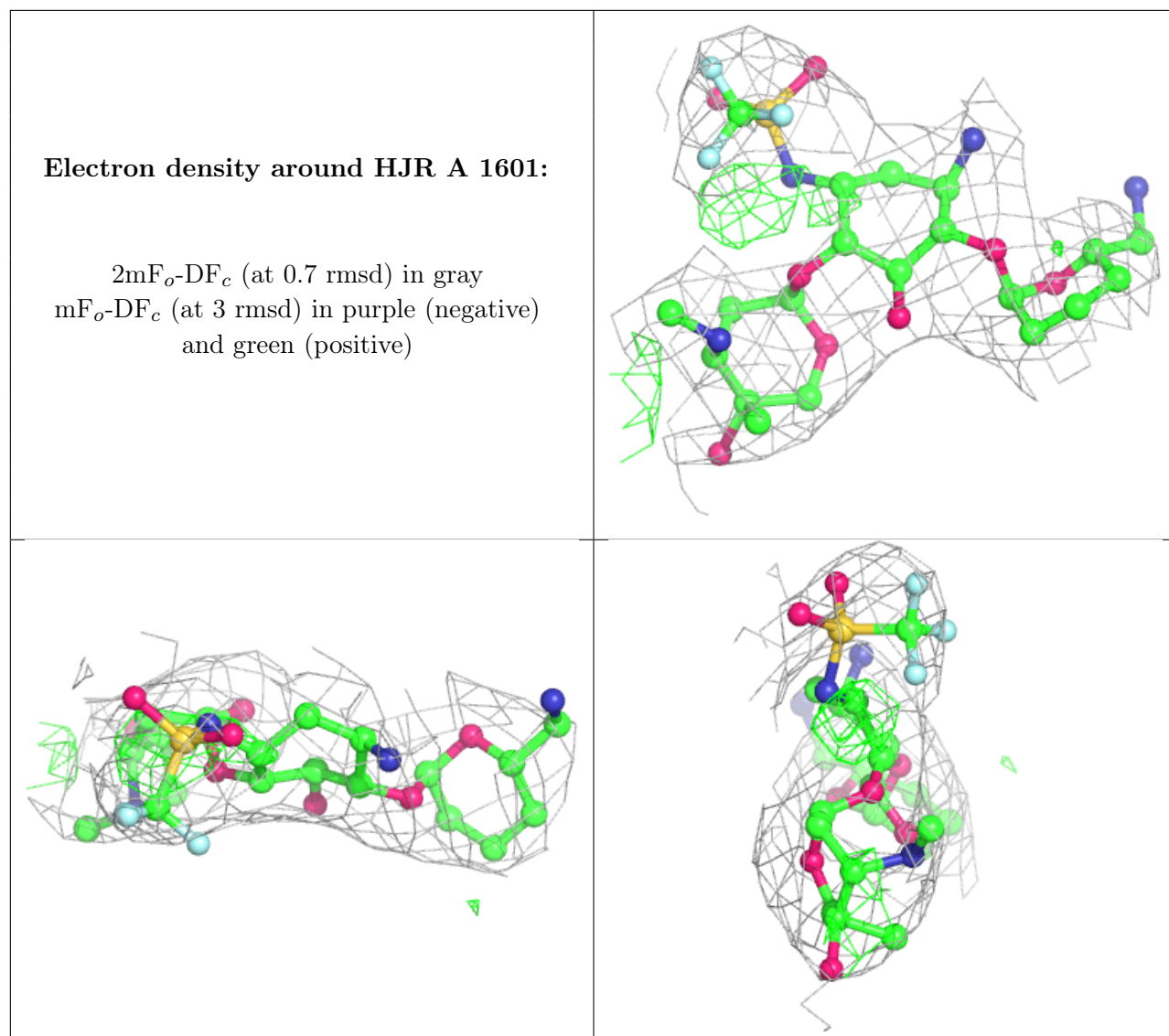
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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



6.5 Other polymers [\(i\)](#)

Unable to reproduce the depositors R factor - this section is therefore empty.