Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:29 PM GMT

PDB ID	:	4LF6
Title	:	Crystal Structure of 30S ribosomal subunit from Thermus thermophilus
Authors	:	Demirci, H.; Belardinelli, R.; Carr, J.; Murphy IV, F.; Jogl, G.; Dahlberg, A.E.; Gregory, S.T.
Deposited on	:	2013-06-26
Resolution	:	3.31 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:

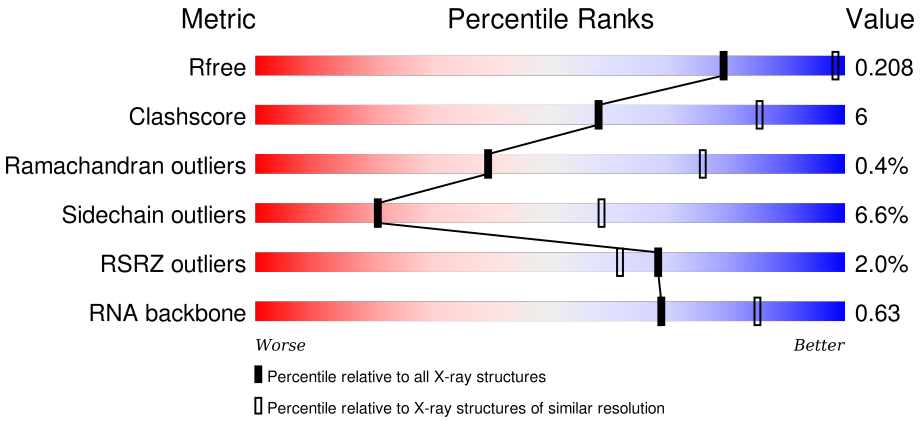
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.31 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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	70% 25%
2	B	256	72% 20% 8%
3	C	239	64% 21% 13%
4	D	209	78% 18%

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Mol	Chain	Length	Quality of chain
5	E	162	72% 19% 7%
6	F	101	84% 15%
7	G	156	73% 25%
8	H	138	71% 24% 5%
9	I	128	70% 26%
10	J	105	8% 66% 22% 7% 6%
11	K	129	70% 22% 8%
12	L	135	67% 22% 7%
13	M	126	5% 73% 18% 6%
14	N	61	3% 79% 13% 7%
15	O	89	78% 17%
16	P	88	73% 22% 5%
17	Q	105	4% 78% 19%
18	R	88	64% 19% 17%
19	S	93	69% 16% 13%
20	T	106	71% 20% 7%
21	U	27	19% 78% 11% 7%

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
22	MG	A	1615	-	-	-	X
22	MG	A	1618	-	-	-	X
22	MG	A	1624	-	-	-	X
22	MG	A	1625	-	-	-	X
22	MG	A	1629	-	-	-	X
22	MG	A	1635	-	-	-	X
22	MG	A	1637	-	-	-	X
22	MG	A	1643	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1646	-	-	-	X
22	MG	A	1651	-	-	-	X
22	MG	A	1653	-	-	-	X
22	MG	A	1654	-	-	-	X
22	MG	A	1660	-	-	-	X
22	MG	A	1670	-	-	-	X
22	MG	A	1676	-	-	-	X
22	MG	A	1685	-	-	-	X
22	MG	A	1687	-	-	-	X
22	MG	A	1688	-	-	-	X
22	MG	A	1689	-	-	-	X
22	MG	A	1690	-	-	-	X
22	MG	A	1696	-	-	-	X
22	MG	A	1702	-	-	-	X
22	MG	A	1703	-	-	-	X
22	MG	A	1705	-	-	-	X
22	MG	A	1707	-	-	-	X
22	MG	A	1708	-	-	-	X
22	MG	A	1727	-	-	-	X
22	MG	A	1815	-	-	-	X
22	MG	A	1825	-	-	-	X
22	MG	M	201	-	-	-	X
22	MG	N	102	-	-	-	X
23	K	A	1731	-	-	-	X
23	K	A	1745	-	-	-	X
23	K	A	1758	-	-	-	X
24	NMY	A	1835	-	-	-	X
24	NMY	A	1836	-	-	-	X
24	NMY	A	1837	-	-	-	X

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52131 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	1510	32462	14456	6009	10488	1509	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1533	C	A	CONFLICT	GB M26923.1
A	1534	A	C	CONFLICT	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	236	1874	1195	336	338	5	0	0	1

- Molecule 3 is a protein called ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	207	1613	1016	315	281	1	0	0	1

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	151	1147	724	218	201	4	0	0	1

- Molecule 6 is a protein called ribosomal protein S6.

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

- Molecule 7 is a protein called ribosomal protein S7.

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

- Molecule 8 is a protein called ribosomal protein S8.

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

- Molecule 9 is a protein called ribosomal protein S9.

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

- Molecule 10 is a protein called ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			973	612	196	163	2			

- Molecule 13 is a protein called ribosomal protein S13.

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

- Molecule 14 is a protein called ribosomal protein S14.

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

- Molecule 15 is a protein called ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	160	148	2			

- Molecule 18 is a protein called ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			598	381	118	99			

- Molecule 19 is a protein called ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

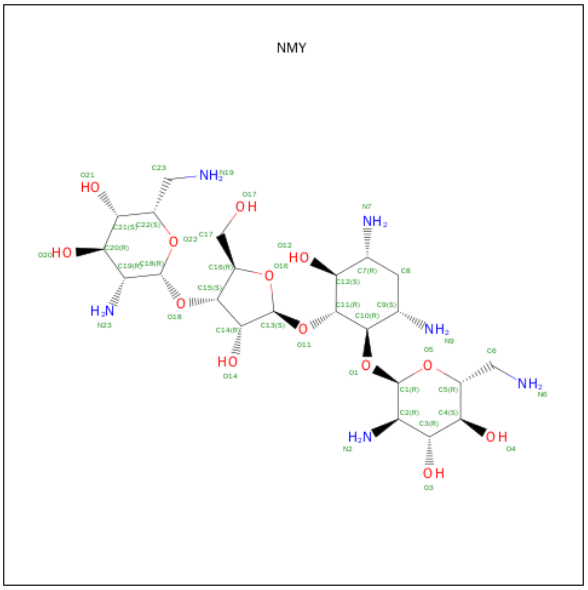
- Molecule 22 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	P	2	Total	Mg	0	0
			2	2		
22	Q	1	Total	Mg	0	0
			1	1		
22	D	2	Total	Mg	0	0
			2	2		
22	E	1	Total	Mg	0	0
			1	1		
22	H	2	Total	Mg	0	0
			2	2		
22	B	3	Total	Mg	0	0
			3	3		
22	C	2	Total	Mg	0	0
			2	2		
22	A	201	Total	Mg	0	0
			201	201		
22	N	2	Total	Mg	0	0
			2	2		
22	L	1	Total	Mg	0	0
			1	1		
22	F	1	Total	Mg	0	0
			1	1		
22	M	2	Total	Mg	0	0
			2	2		

- Molecule 23 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	30	Total	K	0	0
			30	30		

- Molecule 24 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C N O 42 23 6 13	0	0
24	A	1	Total C N O 42 23 6 13	0	0
24	A	1	Total C N O 42 23 6 13	0	0
24	A	1	Total C N O 42 23 6 13	0	0
24	A	1	Total C N O 42 23 6 13	0	0
24	A	1	Total C N O 42 23 6 13	0	0

- Molecule 25 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 26 is water.

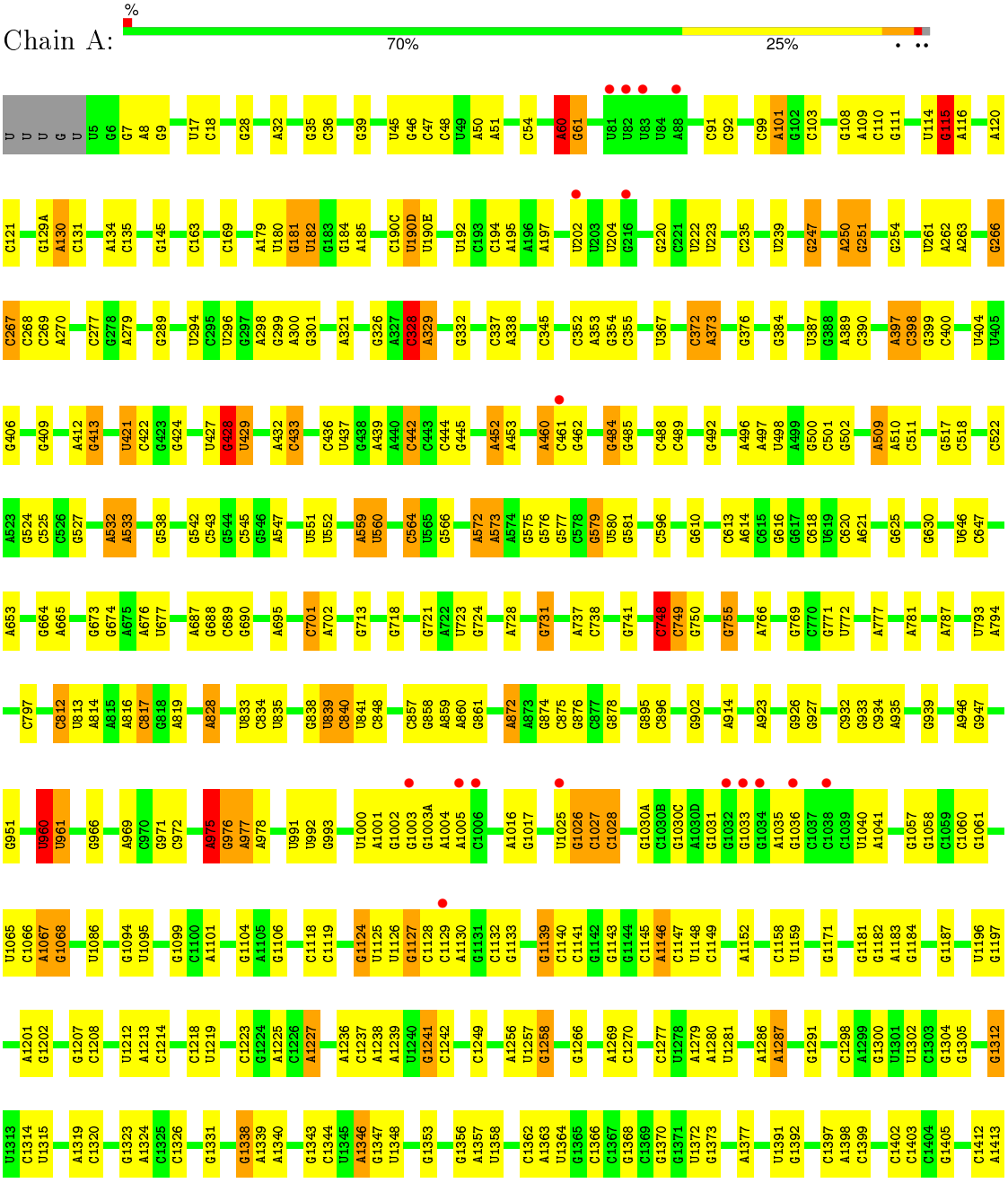
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	12	Total O 12 12	0	0

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.

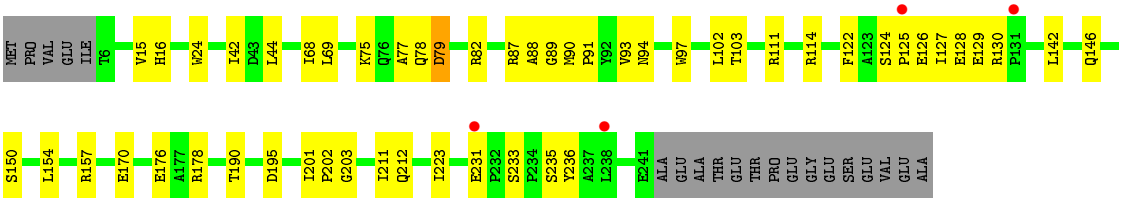
- Molecule 1: 16S rRNA

Chain A:



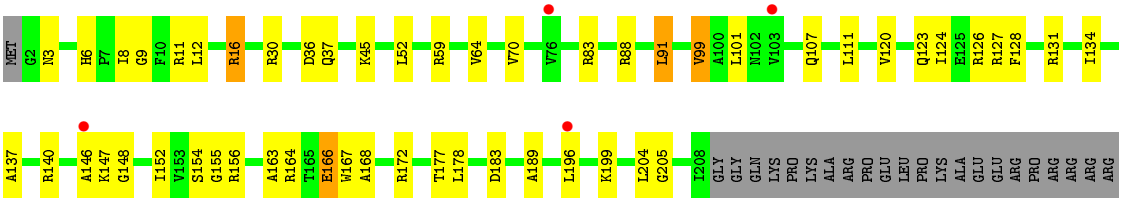
- Molecule 2: ribosomal protein S2

Chain B:



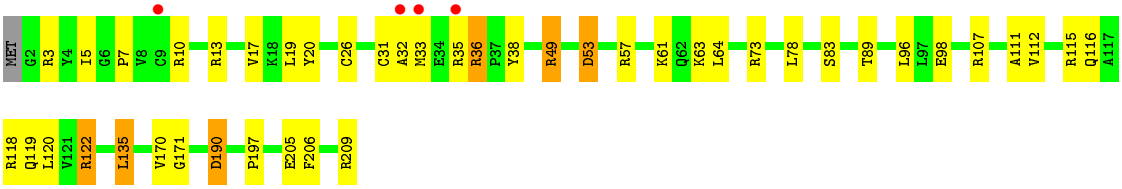
- Molecule 3: ribosomal protein S3

Chain C:



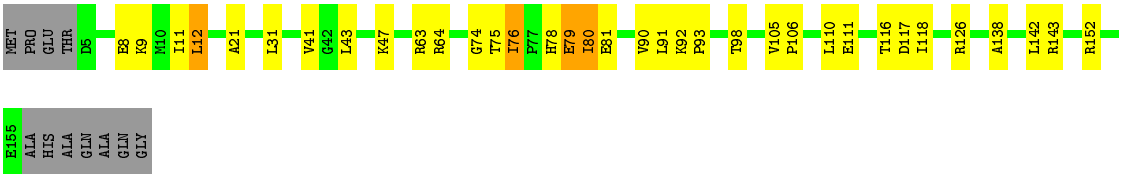
- Molecule 4: ribosomal protein S4

Chain D:



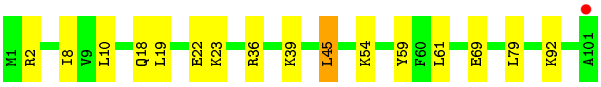
- Molecule 5: ribosomal protein S5

Chain E:



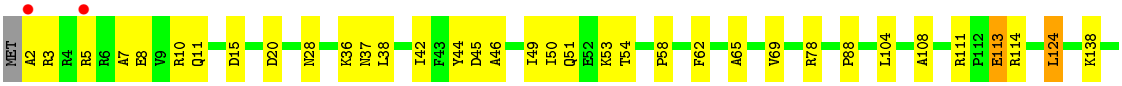
- Molecule 6: ribosomal protein S6

Chain F:



• Molecule 7: ribosomal protein S7

Chain G:

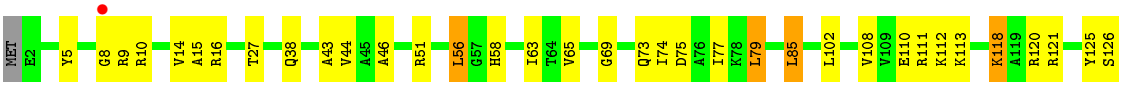


• Molecule 8: ribosomal protein S8

Chain H:

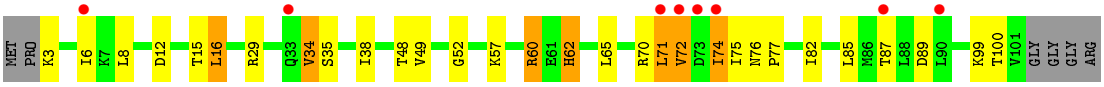
• Molecule 9: ribosomal protein S9

Chain I:



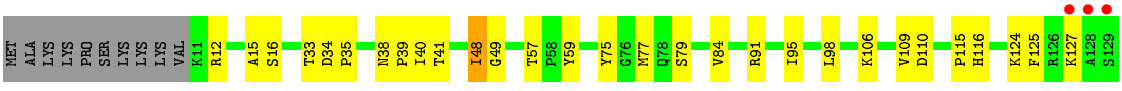
• Molecule 10: ribosomal protein S10

Chain J:



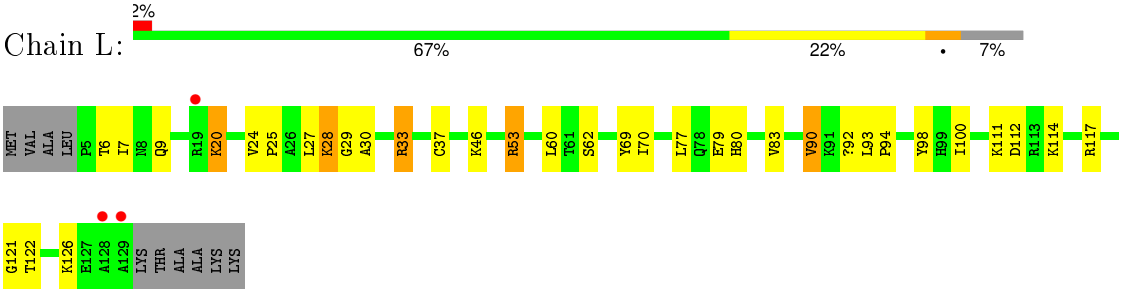
• Molecule 11: ribosomal protein S11

Chain K:



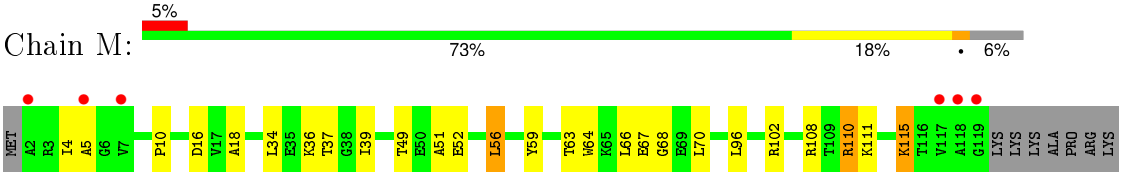
• Molecule 12: ribosomal protein S12

Chain L:



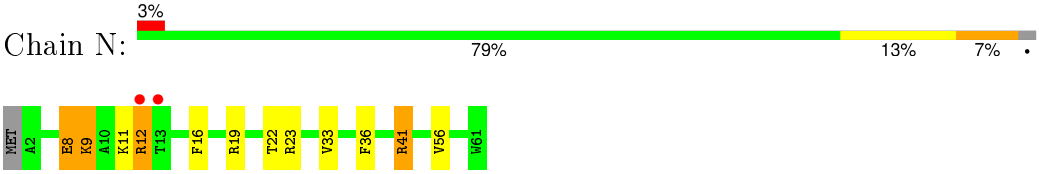
• Molecule 13: ribosomal protein S13

Chain M:



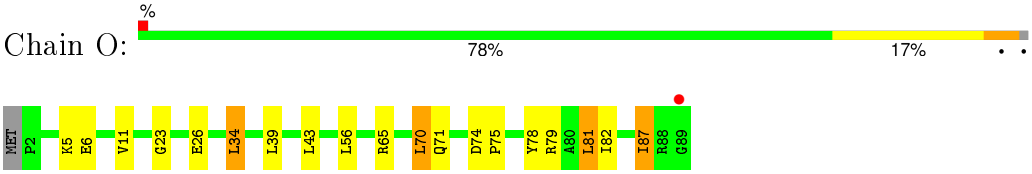
• Molecule 14: ribosomal protein S14

Chain N:



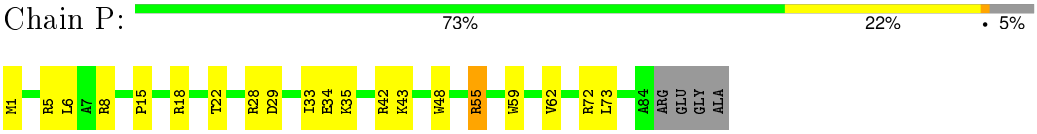
• Molecule 15: ribosomal protein S15

Chain O:



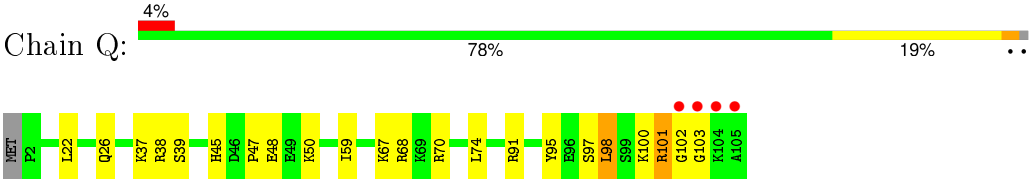
• Molecule 16: ribosomal protein S16

Chain P:



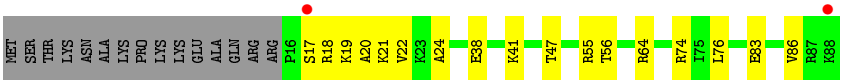
• Molecule 17: ribosomal protein S17

Chain Q:



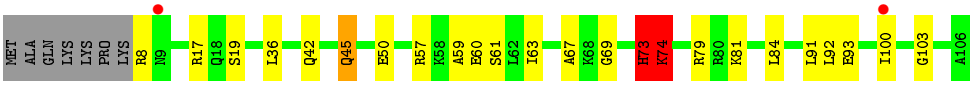
• Molecule 18: ribosomal protein S18

Chain R:

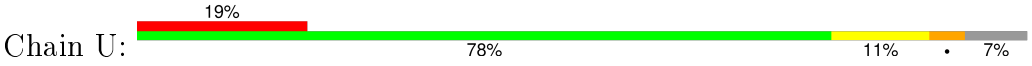


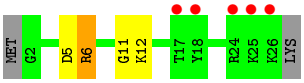
• Molecule 19: ribosomal protein S19

• Molecule 20: ribosomal protein S20



• Molecule 21: ribosomal protein THX





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	403.18Å 403.18Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.90 – 3.31 34.90 – 3.31	Depositor EDS
% Data completeness (in resolution range)	98.7 (34.90-3.31) 98.5 (34.90-3.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1119)	Depositor
R, R_{free}	0.175 , 0.210 0.176 , 0.208	Depositor DCC
R_{free} test set	10690 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	96.4	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 67.0	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 212311 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52131	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: MG, K, 0TD, ZN, NMY, 2MG, 5MC, UR3, 4OC, M2G, 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	0.35	0/36091	0.80	30/56326 (0.1%)
2	B	0.28	0/1909	0.49	0/2579
3	C	0.27	0/1637	0.47	0/2207
4	D	0.31	0/1733	0.48	0/2318
5	E	0.34	0/1163	0.56	0/1566
6	F	0.25	0/856	0.45	0/1154
7	G	0.26	0/1276	0.43	0/1709
8	H	0.34	0/1136	0.52	0/1527
9	I	0.26	0/1029	0.50	0/1379
10	J	0.28	0/806	0.54	0/1084
11	K	0.28	0/900	0.51	0/1213
12	L	0.31	0/978	0.59	0/1308
13	M	0.26	0/947	0.45	0/1270
14	N	0.29	0/501	0.48	0/664
15	O	0.28	0/745	0.46	0/992
16	P	0.29	0/717	0.52	0/965
17	Q	0.34	0/870	0.57	0/1159
18	R	0.27	0/604	0.49	0/801
19	S	0.24	0/662	0.46	0/892
20	T	0.32	0/765	0.53	0/1007
21	U	0.26	0/213	0.44	0/279
All	All	0.33	0/55538	0.72	30/82399 (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
18	R	0	1
20	T	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	3

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	C	C2-N1-C1'	8.28	127.91	118.80
1	A	328	C	N1-C2-O2	8.10	123.76	118.90
1	A	328	C	N3-C2-O2	-7.05	116.96	121.90
1	A	254	G	O5'-P-OP1	-6.99	99.41	105.70
1	A	1528	U	C2-N1-C1'	6.52	125.52	117.70
1	A	1528	U	P-O3'-C3'	6.15	127.08	119.70
1	A	1502	A	C5-N7-C8	-5.99	100.90	103.90
1	A	1502	A	N7-C8-N9	5.89	116.75	113.80
1	A	817	C	C6-N1-C2	5.74	122.60	120.30
1	A	1502	A	C6-C5-N7	-5.73	128.29	132.30
1	A	1158	C	C2-N1-C1'	5.65	125.02	118.80
1	A	328	C	C6-N1-C1'	-5.65	114.03	120.80
1	A	328	C	C6-N1-C2	-5.63	118.05	120.30
1	A	328	C	P-O3'-C3'	5.62	126.45	119.70
1	A	960	U	N1-C2-O2	5.60	126.72	122.80
1	A	60	A	P-O3'-C3'	5.40	126.18	119.70
1	A	1502	A	N1-C6-N6	5.39	121.83	118.60
1	A	428	G	P-O3'-C3'	5.33	126.10	119.70
1	A	1502	A	C4-C5-N7	5.32	113.36	110.70
1	A	1067	A	P-O3'-C3'	5.32	126.08	119.70
1	A	108	G	O4'-C1'-N9	5.28	112.42	108.20
1	A	1158	C	N1-C2-O2	5.28	122.07	118.90
1	A	812	C	P-O3'-C3'	5.20	125.94	119.70
1	A	748	C	P-O3'-C3'	5.15	125.88	119.70
1	A	484	G	P-O3'-C3'	5.07	125.79	119.70
1	A	975	A	O4'-C1'-N9	-5.06	104.15	108.20
1	A	115	G	P-O3'-C3'	5.05	125.76	119.70
1	A	1504	G	P-O3'-C3'	5.03	125.74	119.70
1	A	701	C	P-O3'-C3'	5.03	125.73	119.70
1	A	960	U	N3-C2-O2	-5.03	118.68	122.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	20	ALA	Peptide
20	T	73	HIS	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	32462	0	16406	218	0
2	B	1874	0	1887	25	0
3	C	1613	0	1677	28	0
4	D	1703	0	1763	26	0
5	E	1147	0	1207	24	0
6	F	843	0	857	10	0
7	G	1257	0	1296	25	0
8	H	1116	0	1177	27	0
9	I	1010	0	1037	24	0
10	J	793	0	835	23	0
11	K	885	0	904	19	0
12	L	973	0	1058	27	0
13	M	937	0	995	15	0
14	N	492	0	529	9	0
15	O	734	0	771	11	0
16	P	701	0	720	14	0
17	Q	857	0	928	13	0
18	R	598	0	670	11	0
19	S	648	0	673	11	0
20	T	763	0	861	19	0
21	U	209	0	221	3	0
22	A	201	0	0	0	0
22	B	3	0	0	0	0
22	C	2	0	0	0	0
22	D	2	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	H	2	0	0	0	0
22	L	1	0	0	0	0
22	M	2	0	0	0	0
22	N	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	P	2	0	0	0	0
22	Q	1	0	0	0	0
23	A	30	0	0	0	0
24	A	252	0	276	13	0
25	D	1	0	0	0	0
25	N	1	0	0	0	0
26	A	12	0	0	0	0
All	All	52131	0	36748	518	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 6.

All (518) 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:1086:U:H3	1:A:1099:G:H22	1.23	0.86
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.60	0.83
1:A:664:G:H22	1:A:741:G:H1	1.27	0.81
1:A:279:A:OP2	17:Q:95:TYR:OH	1.98	0.81
19:S:33:THR:HG22	19:S:35:SER:H	1.47	0.79
18:R:38:GLU:HA	18:R:41:LYS:HD3	1.66	0.76
1:A:625:G:N7	24:A:1834:NMY:N19	2.34	0.75
12:L:53:ARG:NH1	12:L:92:0TD:OD2	2.20	0.75
2:B:103:THR:HG23	2:B:176:GLU:HG3	1.68	0.75
1:A:1057:G:H5"	3:C:154:SER:HB2	1.68	0.75
1:A:427:U:OP1	4:D:13:ARG:NH2	2.21	0.74
1:A:975:A:H4'	1:A:976:G:H5"	1.69	0.74
1:A:1405:G:O2'	1:A:1518:A:O2'	2.06	0.73
1:A:1502:A:H2	1:A:1505:G:H1	1.36	0.73
1:A:1028:C:N3	1:A:1033:G:N2	2.36	0.73
24:A:1834:NMY:O21	24:A:1834:NMY:N19	2.17	0.73
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.69	0.72
3:C:156:ARG:H	3:C:163:ALA:HA	1.53	0.72
24:A:1834:NMY:N2	24:A:1834:NMY:O16	2.22	0.72
5:E:76:ILE:HG22	5:E:93:PRO:HG3	1.72	0.70
15:O:39:LEU:HD12	15:O:56:LEU:HB2	1.74	0.70
12:L:111:LYS:HZ2	12:L:112:ASP:H	1.39	0.70
1:A:387:U:OP1	24:A:1837:NMY:N9	2.24	0.69
5:E:80:ILE:HD12	5:E:138:ALA:HB1	1.73	0.69
10:J:34:VAL:HG13	10:J:74:ILE:HA	1.74	0.69
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:G:OP1	4:D:10:ARG:NH2	2.27	0.68
7:G:146:GLU:HA	7:G:149:ARG:HB2	1.75	0.68
19:S:36:ARG:NH2	19:S:75:ALA:O	2.27	0.67
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.59	0.67
1:A:266:G:H5'	1:A:268:C:H41	1.58	0.67
10:J:49:VAL:HG13	14:N:41:ARG:HB2	1.76	0.66
1:A:266:G:H5"	1:A:267:C:C5	2.31	0.66
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.78	0.66
1:A:579:G:H5'	1:A:728:A:H1'	1.76	0.66
12:L:46:LYS:HB2	12:L:92:0TD:H8	1.77	0.65
1:A:517:G:N1	1:A:533:A:OP2	2.28	0.65
1:A:1518:A:H2'	1:A:1519:A:C8	2.31	0.65
1:A:1348:U:H4'	9:I:120:ARG:HG3	1.77	0.65
1:A:951:G:OP2	13:M:102:ARG:NH2	2.30	0.65
1:A:1392:G:H21	1:A:1502:A:H8	1.42	0.64
1:A:266:G:H5"	1:A:267:C:H5	1.61	0.64
10:J:34:VAL:HG12	10:J:35:SER:H	1.63	0.64
11:K:84:VAL:HG11	11:K:91:ARG:HE	1.63	0.64
12:L:33:ARG:HG2	12:L:62:SER:HB2	1.80	0.64
12:L:37:CYS:HB2	12:L:79:GLU:O	1.97	0.63
11:K:15:ALA:HA	11:K:77:MET:HA	1.80	0.63
1:A:413:G:N2	1:A:429:U:OP2	2.18	0.63
1:A:1145:C:H4'	1:A:1146:A:H5'	1.81	0.63
1:A:390:C:O3'	16:P:28:ARG:NH2	2.31	0.63
1:A:1392:G:N2	1:A:1502:A:H8	1.97	0.63
3:C:155:GLY:HA3	3:C:163:ALA:HB1	1.80	0.63
8:H:83:ILE:HG13	8:H:137:VAL:HG22	1.80	0.63
11:K:57:THR:HG22	11:K:59:TYR:H	1.64	0.63
9:I:10:ARG:NH1	9:I:75:ASP:OD2	2.31	0.63
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.32	0.62
1:A:1435:G:H2'	1:A:1436:U:C6	2.33	0.62
3:C:36:ASP:OD2	3:C:59:ARG:NH2	2.32	0.62
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.32	0.62
13:M:4:ILE:HG22	13:M:5:ALA:H	1.65	0.62
1:A:560:U:H5'	1:A:566:G:N2	2.14	0.61
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.83	0.61
1:A:1026:G:H3'	1:A:1027:C:H5"	1.82	0.61
24:A:1835:NMY:O21	24:A:1835:NMY:N19	2.32	0.61
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.83	0.61
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.83	0.61
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:91:ARG:NH2	11:K:110:ASP:OD1	2.33	0.61
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.64	0.60
1:A:460:A:O2'	1:A:462:G:N7	2.33	0.60
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.82	0.60
1:A:1377:A:HO2'	7:G:2:ALA:N	1.99	0.60
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.20	0.60
1:A:738:C:OP2	6:F:92:LYS:NZ	2.33	0.60
20:T:67:ALA:HA	20:T:73:HIS:H	1.66	0.60
11:K:33:THR:HG22	11:K:39:PRO:HA	1.84	0.59
1:A:1028:C:H42	1:A:1033:G:H1	1.49	0.59
1:A:372:C:H4'	1:A:373:A:O5'	2.02	0.59
2:B:87:ARG:CZ	2:B:233:SER:HB3	2.32	0.59
1:A:975:A:H5'	1:A:975:A:H8	1.66	0.59
24:A:1836:NMY:O21	16:P:29:ASP:OD1	2.20	0.59
2:B:15:VAL:HG13	2:B:203:GLY:HA2	1.85	0.58
1:A:192:U:H1'	20:T:103:GLY:HA2	1.85	0.58
17:Q:48:GLU:HG3	17:Q:50:LYS:HB2	1.85	0.58
8:H:41:ARG:NH1	8:H:123:GLU:OE2	2.37	0.58
15:O:26:GLU:HG3	15:O:81:LEU:HG	1.86	0.58
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.85	0.58
9:I:111:ARG:NH1	9:I:113:LYS:HG2	2.19	0.57
17:Q:45:HIS:CD2	17:Q:47:PRO:HG3	2.40	0.57
13:M:37:THR:HG23	13:M:39:ILE:HG13	1.87	0.57
3:C:11:ARG:NH1	3:C:177:THR:O	2.36	0.57
15:O:70:LEU:HD13	15:O:78:TYR:HA	1.86	0.57
8:H:108:GLY:HA3	8:H:138:TRP:HB3	1.85	0.57
24:A:1837:NMY:N6	24:A:1837:NMY:O11	2.36	0.57
2:B:24:TRP:HB2	2:B:190:THR:HG22	1.85	0.57
1:A:250:A:H4'	1:A:251:G:O5'	2.05	0.57
1:A:184:G:H2'	1:A:185:A:H8	1.68	0.57
16:P:43:LYS:HG2	16:P:48:TRP:CD2	2.39	0.57
3:C:155:GLY:HA2	3:C:164:ARG:H	1.70	0.56
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.88	0.56
5:E:79:GLU:HB3	5:E:92:LYS:HG2	1.88	0.56
3:C:131:ARG:NH1	3:C:166:GLU:OE2	2.38	0.56
3:C:16:ARG:NH2	3:C:183:ASP:OD2	2.39	0.56
1:A:299:G:H2'	1:A:300:A:C8	2.40	0.56
10:J:99:LYS:HG2	10:J:100:THR:H	1.70	0.56
2:B:122:PHE:HA	2:B:127:ILE:HG12	1.87	0.56
12:L:27:LEU:O	12:L:29:GLY:N	2.39	0.56
11:K:12:ARG:HB2	11:K:75:TYR:HD2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:LEU:HB2	2:B:176:GLU:HG2	1.87	0.56
5:E:11:ILE:HD13	5:E:105:VAL:HG13	1.88	0.56
1:A:328:C:H4'	1:A:329:A:H5'	1.87	0.55
1:A:1502:A:H2	1:A:1505:G:N1	2.02	0.55
1:A:239:U:O4	24:A:1835:NMY:N19	2.40	0.55
2:B:212:GLN:HE21	2:B:235:SER:HB2	1.71	0.55
1:A:1147:C:O2	9:I:16:ARG:NH1	2.40	0.55
7:G:38:LEU:O	7:G:42:ILE:HG13	2.06	0.55
24:A:1836:NMY:N19	24:A:1836:NMY:O21	2.39	0.55
1:A:45:U:H2'	1:A:46:G:C8	2.42	0.55
17:Q:68:ARG:H	17:Q:70:ARG:NH1	2.04	0.55
2:B:91:PRO:HB3	2:B:154:LEU:HB2	1.89	0.54
8:H:86:ILE:HD12	8:H:133:LEU:HD22	1.88	0.54
16:P:22:THR:HA	16:P:33:ILE:HG13	1.89	0.54
1:A:91:C:H2'	1:A:92:C:H6	1.72	0.54
13:M:49:THR:HB	13:M:52:GLU:HG2	1.90	0.54
16:P:15:PRO:HD2	16:P:42:ARG:HD2	1.89	0.54
1:A:580:U:H2'	1:A:581:G:O4'	2.06	0.54
11:K:84:VAL:HG21	11:K:95:ILE:HD11	1.90	0.54
10:J:8:LEU:HB3	10:J:16:LEU:HD21	1.89	0.54
20:T:60:GLU:HG3	20:T:81:LYS:HE3	1.89	0.54
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.40	0.54
1:A:835:U:OP1	18:R:64:ARG:NH2	2.39	0.54
8:H:116:LYS:HE3	8:H:127:LEU:HD13	1.89	0.54
5:E:105:VAL:HB	5:E:106:PRO:HD3	1.89	0.54
1:A:750:G:N3	15:O:23:GLY:HA3	2.23	0.53
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.90	0.53
6:F:8:ILE:HB	6:F:61:LEU:HB2	1.90	0.53
1:A:279:A:C5	17:Q:98:LEU:HD12	2.44	0.53
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.91	0.53
10:J:16:LEU:HD13	10:J:70:ARG:HG2	1.91	0.53
2:B:16:HIS:HB3	2:B:44:LEU:HD21	1.91	0.53
1:A:1035:A:H2'	1:A:1036:G:H8	1.74	0.53
10:J:65:LEU:HB2	14:N:56:VAL:HG22	1.90	0.53
1:A:946:A:H2'	1:A:947:G:C8	2.44	0.53
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.73	0.53
16:P:18:ARG:HD3	16:P:35:LYS:HD2	1.89	0.53
1:A:277:C:H5'	17:Q:68:ARG:HH12	1.73	0.53
1:A:718:G:C8	11:K:116:HIS:HB3	2.43	0.53
1:A:676:A:H1'	11:K:115:PRO:HB3	1.91	0.53
4:D:32:ALA:HA	4:D:35:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:A:H2'	1:A:180:U:C6	2.43	0.52
7:G:45:ASP:O	7:G:49:ILE:HG13	2.09	0.52
4:D:57:ARG:HB3	4:D:206:PHE:HB2	1.91	0.52
1:A:673:G:H2'	1:A:674:G:C8	2.44	0.52
9:I:5:TYR:HE1	9:I:16:ARG:HB3	1.75	0.52
20:T:69:GLY:O	20:T:73:HIS:ND1	2.43	0.52
9:I:65:VAL:HG11	9:I:73:GLN:HB3	1.92	0.52
3:C:137:ALA:HA	3:C:140:ARG:HE	1.75	0.52
1:A:1104:G:O5'	2:B:111:ARG:HD2	2.10	0.52
1:A:1510:U:H2'	1:A:1511:G:C8	2.44	0.51
1:A:1338:G:H2'	1:A:1339:A:C8	2.45	0.51
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.92	0.51
1:A:509:A:N3	1:A:543:C:O2'	2.33	0.51
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.91	0.51
2:B:78:GLN:O	2:B:94:ASN:ND2	2.34	0.51
1:A:559:A:OP1	5:E:126:ARG:NH2	2.32	0.51
1:A:409:G:H1	1:A:433:C:H42	1.57	0.51
1:A:17:U:H2'	1:A:18:C:C6	2.45	0.51
1:A:1339:A:H2'	1:A:1340:A:O4'	2.10	0.51
9:I:125:TYR:CD1	9:I:127:LYS:HB2	2.45	0.51
12:L:20:LYS:NZ	12:L:20:LYS:H	2.09	0.51
12:L:24:VAL:HG13	12:L:98:TYR:HE2	1.75	0.51
1:A:1218:C:H2'	1:A:1219:U:C6	2.45	0.51
9:I:9:ARG:HG2	9:I:14:VAL:HG22	1.92	0.51
7:G:51:GLN:C	7:G:53:LYS:H	2.14	0.51
12:L:24:VAL:HG13	12:L:98:TYR:CE2	2.45	0.50
1:A:564:C:O2'	8:H:91:ARG:NH2	2.43	0.50
3:C:147:LYS:HD3	3:C:205:GLY:H	1.77	0.50
1:A:328:C:H4'	1:A:329:A:C5'	2.41	0.50
1:A:718:G:O6	18:R:74:ARG:NH1	2.45	0.50
13:M:36:LYS:HD2	13:M:59:TYR:OH	2.12	0.50
4:D:53:ASP:N	4:D:53:ASP:OD1	2.44	0.50
3:C:148:GLY:HA3	3:C:172:ARG:O	2.11	0.50
1:A:572:A:H5'	1:A:573:A:OP2	2.11	0.50
2:B:88:ALA:O	2:B:90:MET:N	2.44	0.50
1:A:103:C:OP1	20:T:17:ARG:NH1	2.45	0.50
1:A:923:A:OP1	5:E:21:ALA:HB2	2.11	0.50
1:A:1391:U:H2'	1:A:1392:G:C8	2.46	0.50
1:A:404:U:H5'	4:D:122:ARG:HD2	1.94	0.50
1:A:269:C:H2'	1:A:270:A:C8	2.47	0.50
5:E:98:THR:N	5:E:117:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:G:H5'	1:A:298:A:O4'	2.12	0.50
9:I:8:GLY:HA3	9:I:79:LEU:HB3	1.93	0.50
5:E:9:LYS:NZ	5:E:111:GLU:OE1	2.43	0.50
3:C:6:HIS:CD2	3:C:8:ILE:HB	2.46	0.49
17:Q:67:LYS:O	17:Q:68:ARG:HB2	2.12	0.49
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.94	0.49
17:Q:101:ARG:HG2	17:Q:102:GLY:H	1.78	0.49
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.92	0.49
9:I:110:GLU:OE2	9:I:113:LYS:NZ	2.41	0.49
18:R:22:VAL:HB	18:R:56:THR:HA	1.94	0.49
6:F:45:LEU:HD23	6:F:45:LEU:H	1.77	0.49
1:A:222:U:H2'	1:A:223:U:C6	2.48	0.49
10:J:82:ILE:HA	10:J:85:LEU:HB2	1.95	0.49
1:A:814:A:H2'	1:A:816:A:H5"	1.93	0.49
10:J:12:ASP:HB3	10:J:15:THR:HG22	1.93	0.49
1:A:261:U:OP2	20:T:79:ARG:NH2	2.45	0.49
1:A:1040:U:H2'	1:A:1041:A:C8	2.48	0.49
12:L:117:ARG:HB3	12:L:122:THR:HB	1.94	0.49
1:A:1495:U:H2'	1:A:1496:C:C6	2.47	0.49
1:A:976:G:H5'	1:A:1358:U:O2'	2.12	0.49
3:C:152:ILE:HB	3:C:199:LYS:HB2	1.95	0.49
7:G:138:LYS:HE2	7:G:142:GLU:OE1	2.12	0.49
1:A:109:A:H2'	1:A:326:G:N2	2.27	0.48
1:A:1225:A:N3	1:A:1225:A:H2'	2.28	0.48
10:J:6:ILE:HB	10:J:72:VAL:HB	1.94	0.48
2:B:146:GLN:O	2:B:150:SER:HB3	2.14	0.48
10:J:3:LYS:N	10:J:77:PRO:HG3	2.29	0.48
1:A:1187:G:H5'	9:I:113:LYS:HE2	1.94	0.48
1:A:247:G:OP2	17:Q:100:LYS:HG3	2.13	0.48
7:G:50:ILE:HG21	7:G:58:PRO:HA	1.96	0.48
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.29	0.48
1:A:99:C:H2'	1:A:101:A:C8	2.49	0.48
5:E:76:ILE:HG23	5:E:78:HIS:H	1.78	0.48
4:D:98:GLU:OE2	4:D:107:ARG:NE	2.35	0.48
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.95	0.48
1:A:1356:G:H2'	1:A:1357:A:C8	2.49	0.48
6:F:10:LEU:HB2	6:F:59:TYR:HB3	1.95	0.48
1:A:833:U:H2'	1:A:834:C:C6	2.50	0.47
13:M:49:THR:HG22	13:M:51:ALA:H	1.78	0.47
3:C:6:HIS:HD2	3:C:9:GLY:H	1.62	0.47
4:D:78:LEU:HA	4:D:78:LEU:HD23	1.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.47
8:H:13:ILE:O	8:H:17:THR:HG23	2.15	0.47
1:A:1326:C:H5"	21:U:12:LYS:HE3	1.96	0.47
20:T:74:LYS:H	20:T:74:LYS:HG3	1.41	0.47
8:H:17:THR:HG22	8:H:63:LEU:HG	1.96	0.47
1:A:1499:A:H1'	1:A:1520:G:H5'	1.96	0.47
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.14	0.47
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.95	0.47
12:L:90:VAL:HG21	12:L:93:LEU:HD12	1.97	0.47
1:A:192:U:H4'	20:T:57:ARG:HD3	1.97	0.47
1:A:337:C:H2'	1:A:338:A:C8	2.50	0.47
1:A:522:C:OP2	12:L:69:TYR:OH	2.24	0.47
2:B:178:ARG:O	8:H:71:GLY:HA2	2.15	0.47
19:S:80:TYR:CE1	19:S:81:ARG:HD3	2.50	0.47
1:A:192:U:C1'	20:T:103:GLY:HA2	2.45	0.47
18:R:21:LYS:HA	18:R:21:LYS:HD2	1.67	0.47
1:A:421:U:H5'	1:A:422:C:C5	2.50	0.47
18:R:47:THR:HA	18:R:83:GLU:HB2	1.95	0.47
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.97	0.47
1:A:1305:G:N2	1:A:1331:G:H1'	2.30	0.47
4:D:112:VAL:HG12	4:D:116:GLN:OE1	2.15	0.47
1:A:452:A:O3'	16:P:72:ARG:HD2	2.15	0.47
4:D:190:ASP:N	4:D:190:ASP:OD2	2.47	0.47
1:A:1504:G:OP1	1:A:1507:A:H4'	2.15	0.47
12:L:33:ARG:HA	12:L:33:ARG:HD2	1.69	0.46
1:A:1127:G:H21	1:A:1147:C:N4	2.13	0.46
3:C:126:ARG:HH21	3:C:128:PHE:HD1	1.62	0.46
7:G:46:ALA:O	7:G:50:ILE:HG12	2.15	0.46
1:A:1241:G:H2'	1:A:1242:C:C6	2.50	0.46
1:A:646:U:H2'	1:A:647:C:C6	2.50	0.46
12:L:111:LYS:NZ	12:L:112:ASP:H	2.11	0.46
2:B:68:ILE:O	2:B:90:MET:HB3	2.15	0.46
9:I:44:VAL:HG12	9:I:51:ARG:HH22	1.81	0.46
12:L:111:LYS:HA	12:L:111:LYS:HZ3	1.80	0.46
1:A:1277:C:O2'	1:A:1279:A:H1'	2.14	0.46
8:H:6:ILE:HD11	8:H:31:PHE:HD2	1.81	0.46
1:A:1236:A:H2'	1:A:1237:C:C6	2.50	0.46
13:M:64:TRP:HB3	13:M:66:LEU:HD21	1.98	0.46
11:K:98:LEU:HA	11:K:98:LEU:HD23	1.74	0.46
1:A:1518:A:H2'	1:A:1519:A:H8	1.80	0.46
18:R:21:LYS:HB3	18:R:24:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:U:H5'	1:A:840:C:H5	1.78	0.46
1:A:120:A:OP2	24:A:1835:NMY:O17	2.34	0.45
1:A:838:G:H2'	1:A:839:U:H5"	1.97	0.45
3:C:88:ARG:HA	3:C:91:LEU:HD22	1.97	0.45
1:A:677:U:H3	1:A:713:G:H22	1.63	0.45
1:A:28:G:O2'	1:A:296:U:OP1	2.25	0.45
1:A:1223:C:P	19:S:78:ARG:HH21	2.39	0.45
4:D:49:ARG:H	4:D:49:ARG:HD2	1.81	0.45
1:A:975:A:H5'	1:A:975:A:C8	2.47	0.45
5:E:78:HIS:CD2	8:H:107:LEU:HD12	2.48	0.45
1:A:960:U:H1'	1:A:1223:C:H5'	1.97	0.45
17:Q:97:SER:HA	17:Q:103:GLY:HA3	1.97	0.45
1:A:755:G:OP2	15:O:65:ARG:HD2	2.17	0.45
1:A:413:G:N2	1:A:428:G:H1'	2.31	0.45
15:O:82:ILE:HG12	15:O:87:ILE:HD12	1.98	0.45
20:T:92:LEU:HA	20:T:92:LEU:HD23	1.81	0.45
4:D:57:ARG:NH2	4:D:205:GLU:OE2	2.49	0.45
11:K:79:SER:HB2	11:K:106:LYS:HE3	1.98	0.45
1:A:35:G:H2'	1:A:36:C:C6	2.52	0.45
17:Q:26:GLN:HG2	17:Q:37:LYS:HG3	1.99	0.45
1:A:192:U:O2'	20:T:57:ARG:HG2	2.16	0.45
1:A:1016:A:H2'	1:A:1017:G:O4'	2.17	0.45
5:E:74:GLY:HA3	5:E:116:THR:HG22	1.99	0.45
1:A:427:U:OP2	4:D:36:ARG:NH2	2.50	0.45
10:J:75:ILE:HG22	10:J:76:ASN:H	1.82	0.45
14:N:16:PHE:HB2	14:N:19:ARG:HG3	1.99	0.45
1:A:1106:G:H5"	3:C:172:ARG:HG2	1.98	0.44
1:A:1057:G:H5"	3:C:154:SER:CB	2.42	0.44
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.99	0.44
1:A:748:C:H4'	1:A:749:C:O5'	2.17	0.44
5:E:75:THR:OG1	5:E:76:ILE:N	2.51	0.44
5:E:78:HIS:CE1	5:E:142:LEU:HD23	2.52	0.44
12:L:27:LEU:HG	12:L:28:LYS:H	1.83	0.44
4:D:32:ALA:HA	4:D:35:ARG:HG3	2.00	0.44
7:G:145:ALA:O	7:G:146:GLU:HB2	2.17	0.44
5:E:31:LEU:HA	5:E:31:LEU:HD23	1.81	0.44
1:A:620:C:H2'	1:A:621:A:O4'	2.17	0.44
1:A:1286:A:H2'	1:A:1287:A:H4'	1.98	0.44
11:K:57:THR:HG22	11:K:59:TYR:N	2.32	0.44
13:M:34:LEU:HA	13:M:37:THR:HG22	1.98	0.44
1:A:452:A:HO2'	1:A:453:A:H8	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:C:N1	4:D:135:LEU:HD13	2.32	0.44
7:G:78:ARG:NH1	7:G:154:TYR:O	2.41	0.44
3:C:120:VAL:O	3:C:124:ILE:HG13	2.18	0.44
1:A:194:C:OP1	20:T:61:SER:OG	2.34	0.44
1:A:399:G:H2'	1:A:400:C:C6	2.52	0.44
8:H:4:ASP:CG	8:H:85:ARG:HH11	2.20	0.44
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.98	0.44
17:Q:22:LEU:HD11	17:Q:39:SER:HB2	1.99	0.44
6:F:18:GLN:O	6:F:22:GLU:HG2	2.18	0.44
2:B:195:ASP:O	8:H:68:ARG:NH2	2.51	0.44
1:A:731:G:OP1	1:A:766:A:H1'	2.18	0.44
1:A:1000:U:H2'	1:A:1001:A:C8	2.52	0.44
1:A:1227:A:OP2	13:M:111:LYS:HE3	2.18	0.44
10:J:34:VAL:CG1	10:J:74:ILE:HA	2.45	0.44
3:C:91:LEU:HD21	3:C:99:VAL:HG22	1.99	0.44
1:A:860:A:H2'	1:A:861:G:O4'	2.17	0.44
1:A:436:C:H2'	1:A:437:U:C6	2.53	0.44
20:T:59:ALA:O	20:T:63:ILE:HG13	2.17	0.44
9:I:43:ALA:HA	9:I:74:ILE:HD13	2.00	0.44
1:A:190(C):C:H2'	1:A:190(D):U:O4'	2.17	0.44
1:A:1068:G:OP2	1:A:1068:G:H8	2.01	0.44
1:A:262:A:C6	1:A:263:A:C6	3.06	0.44
1:A:695:A:H61	1:A:797:C:H1'	1.83	0.44
9:I:125:TYR:HD1	9:I:127:LYS:HB2	1.83	0.43
10:J:87:THR:HG23	10:J:89:ASP:OD1	2.17	0.43
5:E:81:GLU:HG2	5:E:90:VAL:HG22	2.00	0.43
9:I:112:LYS:HD3	9:I:118:LYS:HA	2.00	0.43
7:G:15:ASP:HB3	7:G:20:ASP:H	1.83	0.43
24:A:1832:NMY:O11	24:A:1832:NMY:H1	2.18	0.43
11:K:16:SER:O	11:K:35:PRO:HD3	2.17	0.43
10:J:48:THR:HA	10:J:62:HIS:HB3	2.00	0.43
1:A:1128:C:H42	1:A:1143:G:H1	1.65	0.43
1:A:355:C:H5'	1:A:389:A:OP2	2.18	0.43
1:A:1266:G:N2	1:A:1269:A:OP2	2.45	0.43
3:C:30:ARG:HB3	14:N:36:PHE:O	2.19	0.43
7:G:5:ARG:HG3	7:G:7:ALA:H	1.83	0.43
7:G:108:ALA:O	7:G:111:ARG:HB2	2.18	0.43
1:A:114:U:O2'	1:A:115:G:H5'	2.18	0.43
1:A:1402:4OC:H2'	1:A:1403:C:O4'	2.18	0.43
14:N:12:ARG:H	14:N:12:ARG:HD2	1.83	0.43
13:M:115:LYS:HB2	13:M:115:LYS:NZ	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:70:ILE:HD13	12:L:77:LEU:HD12	1.99	0.43
1:A:960:U:H4'	1:A:961:U:C5'	2.49	0.43
1:A:1060:C:H2'	1:A:1061:G:H8	1.84	0.43
1:A:294:U:OP1	1:A:610:G:O2'	2.29	0.43
15:O:11:VAL:HG11	15:O:34:LEU:HD12	1.99	0.43
20:T:50:GLU:HG3	20:T:100:ILE:HD12	2.01	0.43
15:O:82:ILE:HA	15:O:87:ILE:HG13	2.01	0.43
1:A:689:C:H2'	1:A:690:G:O4'	2.19	0.43
1:A:1139:G:H4'	1:A:1140:C:H5'	2.00	0.43
1:A:135:C:O2	16:P:1:MET:HB2	2.18	0.43
11:K:34:ASP:HB2	11:K:35:PRO:HD2	2.00	0.43
1:A:1368:G:OP1	10:J:62:HIS:HE1	2.02	0.43
4:D:83:SER:HA	4:D:89:THR:HG23	2.00	0.43
1:A:1312:G:N7	19:S:4:SER:HB3	2.34	0.43
2:B:130:ARG:HA	2:B:130:ARG:HD3	1.71	0.43
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.99	0.43
1:A:1399:C:C2	1:A:1502:A:N6	2.87	0.43
1:A:1236:A:H4'	1:A:1304:G:H4'	2.00	0.43
21:U:5:ASP:O	21:U:11:GLY:HA3	2.19	0.43
1:A:872:A:C8	1:A:874:G:C8	3.07	0.43
5:E:92:LYS:HA	5:E:93:PRO:HD3	1.89	0.43
1:A:444:C:H2'	1:A:445:G:H8	1.83	0.43
1:A:181:G:H4'	1:A:182:U:H5'	2.01	0.43
11:K:124:LYS:HE3	11:K:125:PHE:CE2	2.54	0.43
4:D:170:VAL:HG22	4:D:171:GLY:H	1.84	0.43
1:A:1412:C:H2'	1:A:1413:A:C8	2.54	0.43
1:A:878:G:H5'	8:H:89:PRO:HG2	2.01	0.43
12:L:25:PRO:C	12:L:27:LEU:H	2.22	0.43
8:H:86:ILE:HG21	8:H:133:LEU:HD13	2.00	0.43
4:D:111:ALA:HB2	4:D:120:LEU:HD12	2.01	0.43
1:A:538:G:H5"	12:L:114:LYS:HB2	2.01	0.43
1:A:60:A:H4'	1:A:61:G:O5'	2.19	0.43
12:L:46:LYS:HG3	12:L:94:PRO:HD3	2.01	0.42
1:A:442:C:H42	1:A:492:G:H1	1.65	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.76	0.42
1:A:376:G:H5"	16:P:5:ARG:HD2	2.01	0.42
20:T:57:ARG:NH2	20:T:100:ILE:HD13	2.34	0.42
1:A:1035:A:H2'	1:A:1036:G:C8	2.54	0.42
1:A:130:A:H1'	1:A:263:A:O2'	2.19	0.42
1:A:134:A:H2'	1:A:135:C:O4'	2.19	0.42
5:E:110:LEU:HD13	5:E:118:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:69:GLU:CD	6:F:69:GLU:H	2.22	0.42
20:T:73:HIS:HB3	20:T:74:LYS:H	1.61	0.42
1:A:184:G:H2'	1:A:185:A:C8	2.53	0.42
1:A:130:A:OP2	1:A:190(E):U:O2'	2.25	0.42
4:D:3:ARG:HD2	4:D:118:ARG:NE	2.34	0.42
11:K:109:VAL:HG22	18:R:86:VAL:HG12	2.01	0.42
1:A:1002:G:H2'	1:A:1003:G:C8	2.53	0.42
1:A:110:C:H2'	1:A:111:G:O4'	2.19	0.42
2:B:79:ASP:HA	2:B:82:ARG:HG2	2.00	0.42
1:A:731:G:H5'	1:A:766:A:H4'	2.01	0.42
1:A:933:G:OP2	7:G:3:ARG:HB3	2.19	0.42
14:N:9:LYS:HE3	14:N:9:LYS:HB3	1.78	0.42
14:N:9:LYS:HE2	14:N:23:ARG:HB2	2.01	0.42
3:C:123:GLN:O	3:C:126:ARG:HG2	2.19	0.42
3:C:126:ARG:NE	3:C:128:PHE:HB2	2.34	0.42
1:A:1124:G:H4'	10:J:38:ILE:HD11	2.01	0.42
1:A:532:A:N3	1:A:532:A:H2'	2.34	0.42
1:A:875:C:O2'	8:H:14:ARG:NH1	2.52	0.42
1:A:977:A:H2'	1:A:978:A:H5"	2.01	0.42
1:A:1147:C:HO2'	9:I:5:TYR:HH	1.67	0.42
16:P:8:ARG:N	16:P:29:ASP:OD2	2.52	0.42
9:I:15:ALA:HB2	9:I:65:VAL:HG13	2.00	0.42
9:I:69:GLY:O	9:I:73:GLN:HG3	2.19	0.42
21:U:6:ARG:HG2	21:U:6:ARG:H	1.71	0.42
1:A:1314:C:C5	19:S:6:LYS:HE2	2.55	0.42
1:A:432:A:H3'	1:A:433:C:H5"	2.02	0.42
8:H:121:ASP:OD1	8:H:121:ASP:N	2.53	0.42
6:F:39:LYS:HB2	6:F:39:LYS:HE3	1.90	0.42
12:L:83:VAL:HG13	12:L:100:ILE:HG23	2.01	0.42
19:S:80:TYR:CE1	19:S:81:ARG:HB2	2.54	0.42
1:A:1343:G:H2'	1:A:1344:C:C6	2.55	0.42
18:R:17:SER:OG	18:R:55:ARG:HG2	2.20	0.42
1:A:1372:U:H2'	1:A:1373:G:O4'	2.20	0.42
1:A:1207:2MG:HM23	1:A:1208:C:H1'	2.02	0.42
16:P:59:TRP:HA	16:P:62:VAL:HG22	2.02	0.42
12:L:53:ARG:HD2	12:L:53:ARG:N	2.35	0.42
8:H:56:LYS:HA	8:H:57:PRO:HD3	1.75	0.42
9:I:85:LEU:HA	9:I:85:LEU:HD13	1.94	0.42
5:E:152:ARG:NH2	8:H:107:LEU:O	2.53	0.41
10:J:34:VAL:HG12	10:J:35:SER:N	2.33	0.41
7:G:113:GLU:H	7:G:113:GLU:HG2	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:96:LEU:O	13:M:110:ARG:NH1	2.53	0.41
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.49	0.41
1:A:1323:G:H2'	1:A:1324:A:C8	2.55	0.41
1:A:1239:A:C4	1:A:1298:C:N4	2.88	0.41
2:B:201:ILE:O	2:B:203:GLY:N	2.52	0.41
7:G:28:ASN:OD1	7:G:36:LYS:NZ	2.44	0.41
1:A:551:U:H2'	1:A:552:U:C6	2.54	0.41
1:A:1133:G:N2	1:A:1141:C:O2	2.51	0.41
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.88	0.41
1:A:1040:U:H2'	1:A:1041:A:H8	1.84	0.41
1:A:1132:C:H2'	1:A:1133:G:H8	1.84	0.41
18:R:76:LEU:HD23	18:R:76:LEU:HA	1.89	0.41
12:L:60:LEU:HB3	12:L:62:SER:HB3	2.01	0.41
10:J:57:LYS:HE2	10:J:60:ARG:NH2	2.36	0.41
1:A:109:A:C6	1:A:326:G:C6	3.09	0.41
5:E:90:VAL:O	5:E:91:LEU:HD23	2.20	0.41
1:A:8:A:N6	4:D:209:ARG:HB2	2.36	0.41
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.48	0.41
1:A:488:C:H2'	1:A:489:C:C6	2.55	0.41
1:A:857:C:H2'	1:A:858:G:O4'	2.20	0.41
1:A:737:A:H2'	1:A:738:C:C6	2.55	0.41
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.87	0.41
8:H:19:VAL:HG23	8:H:21:LYS:HD3	2.03	0.41
3:C:12:LEU:HD23	3:C:12:LEU:HA	1.88	0.41
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.48	0.41
1:A:620:C:C2	4:D:135:LEU:HD13	2.56	0.41
13:M:108:ARG:HH22	13:M:111:LYS:HE2	1.85	0.41
1:A:932:C:C5	7:G:3:ARG:HD3	2.55	0.41
15:O:74:ASP:HA	15:O:75:PRO:HD2	1.90	0.41
1:A:1425:U:H2'	1:A:1426:C:C6	2.55	0.41
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.85	0.41
2:B:42:ILE:HG21	2:B:202:PRO:O	2.20	0.41
24:A:1833:NMY:H18	24:A:1833:NMY:H16	1.27	0.41
4:D:63:LYS:NZ	4:D:197:PRO:O	2.43	0.41
10:J:52:GLY:O	14:N:41:ARG:NH2	2.54	0.41
24:A:1835:NMY:HN61	24:A:1835:NMY:H4	1.61	0.41
16:P:6:LEU:HD11	16:P:73:LEU:HD12	2.03	0.41
4:D:36:ARG:HB3	4:D:38:TYR:CZ	2.56	0.41
12:L:117:ARG:O	12:L:121:GLY:N	2.54	0.41
6:F:2:ARG:NH2	6:F:69:GLU:HG2	2.36	0.41
10:J:38:ILE:HB	10:J:71:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:C:H2'	1:A:614:A:C8	2.55	0.41
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.41
1:A:1516:G:H2'	1:A:1518:A:OP2	2.21	0.41
7:G:88:PRO:HG3	7:G:149:ARG:HA	2.02	0.41
1:A:1127:G:N2	1:A:1145:C:C2	2.89	0.41
13:M:52:GLU:O	13:M:56:LEU:HB2	2.20	0.41
1:A:1256:A:H5'	1:A:1258:G:C4	2.56	0.41
13:M:67:GLU:HB3	13:M:68:GLY:H	1.64	0.41
15:O:43:LEU:HA	15:O:43:LEU:HD23	1.87	0.41
1:A:409:G:H1	1:A:433:C:N4	2.19	0.40
1:A:1315:U:OP2	19:S:6:LYS:NZ	2.52	0.40
1:A:1030(A):G:N2	1:A:1030(C):G:H3'	2.37	0.40
1:A:771:G:H2'	1:A:772:U:C6	2.55	0.40
14:N:8:GLU:O	14:N:11:LYS:HD3	2.22	0.40
1:A:828:A:OP1	1:A:828:A:H4'	2.21	0.40
20:T:36:LEU:HA	20:T:36:LEU:HD23	1.85	0.40
7:G:65:ALA:O	7:G:69:VAL:HG23	2.20	0.40
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.53	0.40
1:A:397:A:H5'	1:A:398:C:OP1	2.20	0.40
4:D:31:CYS:C	4:D:33:MET:H	2.25	0.40
1:A:436:C:H2'	1:A:437:U:H6	1.86	0.40
3:C:52:LEU:HA	3:C:70:VAL:HA	2.03	0.40
1:A:1118:C:H2'	1:A:1119:C:C6	2.56	0.40
1:A:769:G:H4'	1:A:1513:A:H4'	2.04	0.40
1:A:1498:UR3:O5'	1:A:1498:UR3:H6	2.22	0.40
1:A:500:G:H2'	1:A:501:C:C6	2.56	0.40
2:B:126:GLU:O	2:B:129:GLU:HG2	2.20	0.40
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.21	0.40
18:R:38:GLU:H	18:R:38:GLU:CD	2.25	0.40
19:S:80:TYR:CZ	19:S:81:ARG:HB2	2.56	0.40
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.54	0.40
1:A:501:C:H2'	1:A:502:G:C8	2.57	0.40
6:F:19:LEU:O	6:F:23:LYS:HG2	2.22	0.40
9:I:126:SER:OG	9:I:128:ARG:OXT	2.40	0.40
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.57	0.40
9:I:56:LEU:O	9:I:58:HIS:N	2.54	0.40
1:A:1057:G:H2'	1:A:1058:G:O4'	2.22	0.40
1:A:328:C:O2	1:A:328:C:H2'	2.22	0.40
1:A:895:G:H2'	1:A:896:C:C6	2.57	0.40
11:K:48:ILE:HG22	11:K:49:GLY:H	1.85	0.40
8:H:102:ARG:H	8:H:102:ARG:HD2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	234/256 (91%)	208 (89%)	24 (10%)	2 (1%)	21 60
3	C	205/239 (86%)	190 (93%)	15 (7%)	0	100 100
4	D	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	34 71
5	E	149/162 (92%)	145 (97%)	4 (3%)	0	100 100
6	F	99/101 (98%)	96 (97%)	3 (3%)	0	100 100
7	G	153/156 (98%)	145 (95%)	8 (5%)	0	100 100
8	H	136/138 (99%)	133 (98%)	3 (2%)	0	100 100
9	I	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	24 62
10	J	97/105 (92%)	78 (80%)	17 (18%)	2 (2%)	9 42
11	K	117/129 (91%)	107 (92%)	10 (8%)	0	100 100
12	L	122/135 (90%)	110 (90%)	10 (8%)	2 (2%)	12 48
13	M	116/126 (92%)	109 (94%)	7 (6%)	0	100 100
14	N	58/61 (95%)	55 (95%)	3 (5%)	0	100 100
15	O	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
16	P	82/88 (93%)	80 (98%)	2 (2%)	0	100 100
17	Q	102/105 (97%)	95 (93%)	7 (7%)	0	100 100
18	R	71/88 (81%)	66 (93%)	4 (6%)	1 (1%)	14 50
19	S	79/93 (85%)	72 (91%)	7 (9%)	0	100 100
20	T	97/106 (92%)	88 (91%)	8 (8%)	1 (1%)	19 58
21	U	23/27 (85%)	22 (96%)	1 (4%)	0	100 100
All	All	2357/2541 (93%)	2189 (93%)	158 (7%)	10 (0%)	39 76

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	28	LYS
10	J	34	VAL
18	R	19	LYS
10	J	72	VAL
20	T	74	LYS
2	B	128	GLU
9	I	56	LEU
2	B	89	GLY
12	L	30	ALA
4	D	5	ILE

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	194/220 (88%)	185 (95%)	9 (5%)	33	71
3	C	160/188 (85%)	145 (91%)	15 (9%)	11	39
4	D	180/181 (99%)	166 (92%)	14 (8%)	16	50
5	E	115/123 (94%)	107 (93%)	8 (7%)	19	56
6	F	90/90 (100%)	87 (97%)	3 (3%)	45	78
7	G	126/127 (99%)	119 (94%)	7 (6%)	26	65
8	H	119/119 (100%)	109 (92%)	10 (8%)	14	46
9	I	98/99 (99%)	90 (92%)	8 (8%)	14	48
10	J	87/92 (95%)	81 (93%)	6 (7%)	19	57
11	K	90/99 (91%)	88 (98%)	2 (2%)	60	84
12	L	103/110 (94%)	97 (94%)	6 (6%)	25	64
13	M	94/101 (93%)	88 (94%)	6 (6%)	22	60
14	N	49/50 (98%)	43 (88%)	6 (12%)	6	26
15	O	79/80 (99%)	71 (90%)	8 (10%)	9	35
16	P	72/74 (97%)	71 (99%)	1 (1%)	74	88
17	Q	96/97 (99%)	90 (94%)	6 (6%)	22	60
18	R	64/77 (83%)	63 (98%)	1 (2%)	70	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	S	71/80 (89%)	65 (92%)	6 (8%)	13 46
20	T	76/82 (93%)	69 (91%)	7 (9%)	11 40
21	U	19/22 (86%)	18 (95%)	1 (5%)	28 66
All	All	1982/2111 (94%)	1852 (93%)	130 (7%)	21 59

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	69	LEU
2	B	79	ASP
2	B	114	ARG
2	B	142	LEU
2	B	157	ARG
2	B	170	GLU
2	B	223	ILE
2	B	231	GLU
2	B	236	TYR
3	C	3	ASN
3	C	16	ARG
3	C	37	GLN
3	C	45	LYS
3	C	64	VAL
3	C	83	ARG
3	C	91	LEU
3	C	99	VAL
3	C	101	LEU
3	C	107	GLN
3	C	127	ARG
3	C	166	GLU
3	C	167	TRP
3	C	178	LEU
3	C	204	LEU
4	D	17	VAL
4	D	19	LEU
4	D	36	ARG
4	D	49	ARG
4	D	53	ASP
4	D	61	LYS
4	D	64	LEU
4	D	73	ARG
4	D	96	LEU

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Mol	Chain	Res	Type
4	D	115	ARG
4	D	119	GLN
4	D	122	ARG
4	D	135	LEU
4	D	190	ASP
5	E	12	LEU
5	E	41	VAL
5	E	43	LEU
5	E	47	LYS
5	E	64	ARG
5	E	76	ILE
5	E	79	GLU
5	E	80	ILE
6	F	36	ARG
6	F	45	LEU
6	F	54	LYS
7	G	8	GLU
7	G	11	GLN
7	G	54	THR
7	G	113	GLU
7	G	114	ARG
7	G	124	LEU
7	G	156	TRP
8	H	19	VAL
8	H	26	VAL
8	H	39	LEU
8	H	63	LEU
8	H	68	ARG
8	H	85	ARG
8	H	91	ARG
8	H	92	ARG
8	H	102	ARG
8	H	133	LEU
9	I	27	THR
9	I	38	GLN
9	I	79	LEU
9	I	85	LEU
9	I	102	LEU
9	I	108	VAL
9	I	118	LYS
9	I	121	ARG
10	J	16	LEU

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Mol	Chain	Res	Type
10	J	29	ARG
10	J	60	ARG
10	J	62	HIS
10	J	71	LEU
10	J	74	ILE
11	K	48	ILE
11	K	127	LYS
12	L	20	LYS
12	L	33	ARG
12	L	53	ARG
12	L	80	HIS
12	L	90	VAL
12	L	126	LYS
13	M	16	ASP
13	M	56	LEU
13	M	63	THR
13	M	70	LEU
13	M	110	ARG
13	M	115	LYS
14	N	8	GLU
14	N	9	LYS
14	N	12	ARG
14	N	22	THR
14	N	33	VAL
14	N	41	ARG
15	O	5	LYS
15	O	6	GLU
15	O	34	LEU
15	O	70	LEU
15	O	71	GLN
15	O	79	ARG
15	O	81	LEU
15	O	87	ILE
16	P	55	ARG
17	Q	38	ARG
17	Q	59	ILE
17	Q	74	LEU
17	Q	91	ARG
17	Q	98	LEU
17	Q	101	ARG
18	R	18	ARG
19	S	7	LYS

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Mol	Chain	Res	Type
19	S	15	LEU
19	S	27	GLU
19	S	61	TYR
19	S	65	ASN
19	S	81	ARG
20	T	8	ARG
20	T	19	SER
20	T	42	GLN
20	T	45	GLN
20	T	73	HIS
20	T	74	LYS
20	T	84	LEU
21	U	6	ARG

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

Mol	Chain	Res	Type
2	B	212	GLN
3	C	6	HIS
7	G	51	GLN
9	I	73	GLN
13	M	106	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1507/1522 (99%)	201 (13%)	28 (1%)

All (201) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	50	A
1	A	51	A
1	A	54	C
1	A	60	A

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Mol	Chain	Res	Type
1	A	61	G
1	A	101	A
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	145	G
1	A	163	C
1	A	169	C
1	A	182	U
1	A	190(D)	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	220	G
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
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	345	C
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	397	A
1	A	398	C
1	A	406	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	424	G
1	A	429	U

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Mol	Chain	Res	Type
1	A	433	C
1	A	439	A
1	A	442	C
1	A	452	A
1	A	460	A
1	A	461	C
1	A	485	G
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	527	7MG
1	A	532	A
1	A	533	A
1	A	545	C
1	A	547	A
1	A	559	A
1	A	560	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	616	G
1	A	618	C
1	A	630	G
1	A	653	A
1	A	665	A
1	A	687	A
1	A	688	G
1	A	702	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A

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Mol	Chain	Res	Type
1	A	781	A
1	A	787	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
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	859	A
1	A	872	A
1	A	876	G
1	A	902	G
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	939	G
1	A	960	U
1	A	961	U
1	A	966	M2G
1	A	969	A
1	A	971	G
1	A	972	C
1	A	975	A
1	A	976	G
1	A	977	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	1003(A)	G
1	A	1004	A
1	A	1005	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1028	C
1	A	1031	G

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Mol	Chain	Res	Type
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	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1129	C
1	A	1130	A
1	A	1139	G
1	A	1146	A
1	A	1152	A
1	A	1159	U
1	A	1171	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1196	U
1	A	1197	G
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1238	A
1	A	1241	G
1	A	1257	U
1	A	1258	G
1	A	1270	C
1	A	1280	A
1	A	1281	U
1	A	1287	A
1	A	1300	G
1	A	1302	U
1	A	1312	G
1	A	1319	A
1	A	1320	C

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Mol	Chain	Res	Type
1	A	1338	G
1	A	1346	A
1	A	1347	G
1	A	1353	G
1	A	1362	C
1	A	1363	A
1	A	1364	U
1	A	1370	G
1	A	1398	A
1	A	1442	G
1	A	1443	G
1	A	1446	A
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1502	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1529	G
1	A	1530	G
1	A	1531	A

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	60	A
1	A	115	G
1	A	129(A)	G
1	A	181	G
1	A	250	A
1	A	266	G
1	A	328	C
1	A	352	C
1	A	372	C
1	A	428	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	559	A

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Mol	Chain	Res	Type
1	A	575	G
1	A	687	A
1	A	701	C
1	A	723	U
1	A	748	C
1	A	812	C
1	A	960	U
1	A	1065	U
1	A	1067	A
1	A	1182	G
1	A	1201	A
1	A	1397	C
1	A	1504	G
1	A	1528	U

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

11 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	1.89	3 (17%)	21,38,41	2.16	3 (14%)
1	5MC	A	1400	1	13,22,23	0.95	0	15,32,35	0.90	1 (6%)
1	4OC	A	1402	1	13,23,24	0.65	0	18,32,35	0.75	0
1	5MC	A	1404	1	13,22,23	0.81	0	15,32,35	0.98	1 (6%)
1	5MC	A	1407	1	13,22,23	1.07	1 (7%)	15,32,35	1.06	1 (6%)
1	UR3	A	1498	1	12,22,23	0.79	0	16,32,35	1.25	1 (6%)
1	PSU	A	516	1,22	13,21,22	1.08	1 (7%)	18,30,33	3.69	5 (27%)
1	7MG	A	527	1	19,26,27	2.60	5 (26%)	24,39,42	2.13	6 (25%)
1	M2G	A	966	1	17,27,28	1.96	4 (23%)	22,40,43	1.98	2 (9%)
1	5MC	A	967	1	13,22,23	0.93	0	15,32,35	0.81	0
12	0TD	L	92	12	4,9,10	0.84	0	4,11,13	1.85	2 (50%)

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
1	PSU	A	516	1,22	-	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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-6.98	1.35	1.45
1	A	527	7MG	CM7-N7	-2.09	1.42	1.46
1	A	1407	5MC	C5-C4	2.43	1.45	1.41
1	A	1207	2MG	C4-N3	2.46	1.39	1.35
1	A	527	7MG	C6-N1	2.84	1.38	1.33
1	A	966	M2G	C4-N3	2.92	1.40	1.35
1	A	516	PSU	C4-N3	2.95	1.38	1.33
1	A	966	M2G	C2-N2	3.38	1.40	1.34
1	A	966	M2G	C2-N1	3.55	1.41	1.34
1	A	1207	2MG	C2-N2	4.66	1.39	1.34
1	A	527	7MG	C2-N2	4.83	1.43	1.34
1	A	1207	2MG	C6-N1	5.25	1.42	1.33
1	A	966	M2G	C6-N1	5.36	1.43	1.33
1	A	527	7MG	C4-N3	5.96	1.42	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	N1-C2-N3	-13.44	119.76	128.33
1	A	966	M2G	C5-C6-N1	-8.29	112.25	123.59
1	A	1207	2MG	C5-C6-N1	-7.58	113.23	123.59
1	A	527	7MG	C5-C4-N3	-7.48	119.53	126.82
12	L	92	0TD	CSB-SB-CB	-2.44	96.94	101.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	516	PSU	C5-C6-N1	-2.42	120.98	124.39
12	L	92	0TD	O-C-CA	-2.38	119.15	125.44
1	A	527	7MG	C5-C6-N1	-2.28	119.95	123.46
1	A	527	7MG	N1-C2-N3	-2.25	121.85	125.53
1	A	1407	5MC	N4-C4-N3	-2.17	113.80	116.95
1	A	966	M2G	N3-C2-N2	2.02	119.45	117.16
1	A	527	7MG	C2-N3-C4	2.12	120.71	114.53
1	A	1404	5MC	CM5-C5-C6	2.15	122.94	118.62
1	A	1400	5MC	CM5-C5-C6	2.15	122.94	118.62
1	A	1498	UR3	C6-C5-C4	2.54	122.02	117.28
1	A	1207	2MG	C4-C5-N7	2.57	111.85	109.48
1	A	516	PSU	C6-N1-C2	3.04	120.35	115.47
1	A	516	PSU	O4'-C1'-C2'	3.05	107.83	104.73
1	A	527	7MG	C6-N1-C2	3.06	120.19	115.94
1	A	527	7MG	N3-C4-N9	4.16	133.00	126.75
1	A	1207	2MG	C6-N1-C2	4.63	122.05	115.31
1	A	516	PSU	C4-N3-C2	6.00	120.43	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1207	2MG	1	0
1	A	1402	4OC	1	0
1	A	1498	UR3	1	0
12	L	92	0TD	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 258 ligands modelled in this entry, 252 are monoatomic - leaving 6 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	NMY	A	1832	-	45,45,45	1.32	6 (13%)	58,67,67	1.34	7 (12%)
24	NMY	A	1833	-	45,45,45	1.32	3 (6%)	58,67,67	1.65	11 (18%)
24	NMY	A	1834	-	45,45,45	1.47	6 (13%)	58,67,67	1.83	16 (27%)
24	NMY	A	1835	-	45,45,45	1.32	4 (8%)	58,67,67	1.40	11 (18%)
24	NMY	A	1836	-	45,45,45	1.39	6 (13%)	58,67,67	1.81	12 (20%)
24	NMY	A	1837	-	45,45,45	1.45	8 (17%)	58,67,67	1.82	15 (25%)

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	NMY	A	1832	-	-	0/18/94/94	0/4/4/4
24	NMY	A	1833	-	-	0/18/94/94	0/4/4/4
24	NMY	A	1834	-	-	0/18/94/94	0/4/4/4
24	NMY	A	1835	-	-	0/18/94/94	0/4/4/4
24	NMY	A	1836	-	-	0/18/94/94	0/4/4/4
24	NMY	A	1837	-	-	0/18/94/94	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1832	NMY	C10-C9	2.00	1.57	1.53
24	A	1837	NMY	C20-C19	2.00	1.56	1.53
24	A	1837	NMY	C12-C7	2.03	1.58	1.53
24	A	1836	NMY	C20-C19	2.05	1.56	1.53
24	A	1837	NMY	C6-C5	2.06	1.57	1.52
24	A	1836	NMY	C21-C22	2.08	1.57	1.53
24	A	1837	NMY	C10-C11	2.11	1.56	1.52
24	A	1832	NMY	C10-C11	2.23	1.57	1.52
24	A	1834	NMY	C14-C15	2.25	1.58	1.53
24	A	1832	NMY	C18-C19	2.41	1.57	1.52
24	A	1835	NMY	C18-C19	2.42	1.57	1.52
24	A	1834	NMY	C21-C22	2.50	1.58	1.53
24	A	1834	NMY	C18-C19	2.51	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1832	NMY	C1-C2	2.66	1.57	1.52
24	A	1837	NMY	C18-C19	2.71	1.57	1.52
24	A	1835	NMY	C13-C14	2.75	1.56	1.52
24	A	1835	NMY	C1-C2	2.79	1.58	1.52
24	A	1834	NMY	C1-C2	2.82	1.58	1.52
24	A	1833	NMY	C13-C14	2.85	1.56	1.52
24	A	1833	NMY	C1-C2	2.85	1.58	1.52
24	A	1836	NMY	C13-C14	2.92	1.56	1.52
24	A	1832	NMY	C13-C14	2.93	1.56	1.52
24	A	1832	NMY	C3-C2	2.97	1.57	1.53
24	A	1836	NMY	C18-C19	3.00	1.58	1.52
24	A	1836	NMY	C3-C2	3.08	1.57	1.53
24	A	1835	NMY	C3-C2	3.09	1.57	1.53
24	A	1837	NMY	C13-C14	3.09	1.56	1.52
24	A	1836	NMY	C1-C2	3.25	1.58	1.52
24	A	1834	NMY	C3-C2	3.31	1.57	1.53
24	A	1837	NMY	C3-C2	3.34	1.57	1.53
24	A	1833	NMY	C3-C2	3.46	1.57	1.53
24	A	1837	NMY	C1-C2	3.82	1.60	1.52
24	A	1834	NMY	C13-C14	4.68	1.58	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1836	NMY	C14-C15-C16	-6.19	91.66	103.29
24	A	1833	NMY	O20-C20-C19	-4.47	102.76	110.31
24	A	1833	NMY	O21-C21-C20	-4.39	100.45	110.34
24	A	1837	NMY	C11-C10-C9	-4.14	101.35	111.21
24	A	1834	NMY	O20-C20-C19	-3.89	103.74	110.31
24	A	1833	NMY	C11-C10-C9	-3.87	102.00	111.21
24	A	1836	NMY	O20-C20-C19	-3.55	104.31	110.31
24	A	1834	NMY	O21-C21-C20	-3.37	102.74	110.34
24	A	1836	NMY	O16-C13-C14	-3.33	100.10	104.78
24	A	1835	NMY	O21-C21-C20	-3.26	103.01	110.34
24	A	1835	NMY	O20-C20-C19	-3.22	104.86	110.31
24	A	1832	NMY	O20-C20-C19	-3.10	105.08	110.31
24	A	1834	NMY	C11-C10-C9	-3.06	103.92	111.21
24	A	1832	NMY	O21-C21-C20	-3.04	103.49	110.34
24	A	1837	NMY	O16-C13-C14	-3.02	100.55	104.78
24	A	1836	NMY	O21-C21-C20	-2.97	103.64	110.34
24	A	1833	NMY	O12-C12-C7	-2.93	104.44	109.87
24	A	1837	NMY	O20-C20-C19	-2.92	105.38	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1832	NMY	O18-C18-O22	-2.71	103.83	110.68
24	A	1834	NMY	O1-C1-O5	-2.66	103.96	110.68
24	A	1837	NMY	O21-C21-C20	-2.59	104.52	110.34
24	A	1835	NMY	C11-C10-C9	-2.56	105.11	111.21
24	A	1834	NMY	C18-O18-C15	-2.49	111.50	118.01
24	A	1837	NMY	O1-C1-O5	-2.47	104.44	110.68
24	A	1834	NMY	O22-C18-C19	-2.46	104.95	110.47
24	A	1835	NMY	O18-C18-O22	-2.46	104.47	110.68
24	A	1833	NMY	C18-O18-C15	-2.45	111.61	118.01
24	A	1836	NMY	O12-C12-C7	-2.42	105.38	109.87
24	A	1833	NMY	O20-C20-C21	-2.40	104.93	110.34
24	A	1835	NMY	O1-C1-O5	-2.39	104.64	110.68
24	A	1836	NMY	C18-O22-C22	-2.35	109.19	113.75
24	A	1832	NMY	C8-C7-C12	-2.29	106.60	110.11
24	A	1835	NMY	C13-O11-C11	-2.24	112.16	118.01
24	A	1834	NMY	C18-O22-C22	-2.19	109.50	113.75
24	A	1835	NMY	O16-C13-C14	-2.16	101.74	104.78
24	A	1837	NMY	C12-C11-C10	-2.11	106.80	111.44
24	A	1835	NMY	O12-C12-C11	-2.10	104.90	109.87
24	A	1833	NMY	C18-O22-C22	-2.07	109.72	113.75
24	A	1834	NMY	O20-C20-C21	-2.04	105.74	110.34
24	A	1836	NMY	C11-C10-C9	-2.02	106.39	111.21
24	A	1834	NMY	C14-C15-C16	-2.02	99.50	103.29
24	A	1837	NMY	O5-C5-C4	2.00	113.44	109.68
24	A	1837	NMY	C1-C2-N2	2.01	115.09	111.10
24	A	1835	NMY	O1-C10-C11	2.01	112.74	107.49
24	A	1832	NMY	O11-C13-C14	2.12	112.17	107.75
24	A	1833	NMY	O18-C18-C19	2.17	111.98	107.96
24	A	1834	NMY	C18-C19-N23	2.19	115.46	111.10
24	A	1835	NMY	O18-C18-C19	2.24	112.11	107.96
24	A	1832	NMY	O1-C1-C2	2.38	112.37	107.96
24	A	1834	NMY	O11-C11-C12	2.40	113.36	107.17
24	A	1837	NMY	O18-C18-C19	2.50	112.60	107.96
24	A	1836	NMY	O11-C11-C12	2.52	113.68	107.17
24	A	1837	NMY	O11-C11-C10	2.54	114.12	107.49
24	A	1834	NMY	C20-C21-C22	2.60	114.73	110.20
24	A	1833	NMY	O1-C1-C2	2.69	112.95	107.96
24	A	1837	NMY	O1-C1-C2	2.80	113.14	107.96
24	A	1837	NMY	O5-C5-C6	2.92	111.80	106.10
24	A	1836	NMY	O1-C1-C2	2.94	113.41	107.96
24	A	1834	NMY	O22-C22-C21	2.95	115.21	109.68
24	A	1833	NMY	O1-C10-C11	2.99	115.31	107.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	1835	NMY	O11-C13-C14	3.00	113.99	107.75
24	A	1836	NMY	O1-C10-C11	3.16	115.75	107.49
24	A	1837	NMY	O11-C11-C12	3.23	115.49	107.17
24	A	1834	NMY	O1-C10-C11	3.41	116.39	107.49
24	A	1836	NMY	O18-C18-C19	3.43	114.31	107.96
24	A	1834	NMY	O11-C13-C14	3.55	115.14	107.75
24	A	1832	NMY	O1-C10-C11	3.75	117.29	107.49
24	A	1837	NMY	O11-C13-C14	4.12	116.33	107.75
24	A	1833	NMY	O11-C11-C12	4.45	118.66	107.17
24	A	1834	NMY	O18-C18-C19	4.90	117.03	107.96
24	A	1836	NMY	O11-C13-C14	5.21	118.59	107.75
24	A	1837	NMY	O1-C10-C11	5.52	121.92	107.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	1832	NMY	1	0
24	A	1833	NMY	1	0
24	A	1834	NMY	3	0
24	A	1835	NMY	4	0
24	A	1836	NMY	2	0
24	A	1837	NMY	2	0

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

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	1500/1522 (98%)	-0.23	22 (1%) 76 71	51, 84, 177, 283	0
2	B	236/256 (92%)	-0.25	4 (1%) 73 67	60, 109, 189, 249	0
3	C	207/239 (86%)	-0.11	4 (1%) 70 63	50, 115, 159, 195	0
4	D	208/209 (99%)	-0.25	4 (1%) 70 63	63, 94, 134, 166	0
5	E	151/162 (93%)	-0.26	0 100 100	56, 75, 113, 167	0
6	F	101/101 (100%)	-0.46	1 (0%) 84 80	78, 118, 149, 179	0
7	G	155/156 (99%)	-0.29	3 (1%) 70 63	82, 115, 183, 212	0
8	H	138/138 (100%)	-0.46	1 (0%) 89 86	46, 72, 102, 140	0
9	I	127/128 (99%)	-0.01	2 (1%) 74 69	79, 121, 162, 198	0
10	J	99/105 (94%)	0.44	8 (8%) 15 11	73, 140, 218, 252	0
11	K	119/129 (92%)	-0.00	3 (2%) 61 54	68, 93, 129, 150	0
12	L	124/135 (91%)	-0.08	3 (2%) 62 55	58, 87, 126, 215	0
13	M	118/126 (93%)	-0.17	6 (5%) 32 25	84, 114, 146, 183	0
14	N	60/61 (98%)	0.21	2 (3%) 50 43	81, 108, 151, 202	0
15	O	88/89 (98%)	-0.14	1 (1%) 82 78	57, 89, 135, 169	0
16	P	84/88 (95%)	-0.28	0 100 100	62, 80, 107, 189	0
17	Q	104/105 (99%)	0.28	4 (3%) 44 37	59, 78, 125, 196	0
18	R	73/88 (82%)	0.00	2 (2%) 58 51	65, 97, 177, 232	0
19	S	81/93 (87%)	0.08	2 (2%) 61 54	47, 137, 180, 209	0
20	T	99/106 (93%)	-0.15	2 (2%) 68 62	64, 86, 136, 182	0
21	U	25/27 (92%)	1.30	5 (20%) 1 1	73, 106, 130, 206	0
All	All	3897/4063 (95%)	-0.16	79 (2%) 68 62	46, 94, 169, 283	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
17	Q	103	GLY	21.9
11	K	129	SER	18.4
17	Q	104	LYS	14.7
11	K	128	ALA	11.8
1	A	1129	C	9.5
17	Q	105	ALA	9.3
18	R	17	SER	6.1
17	Q	102	GLY	5.4
9	I	128	ARG	4.6
12	L	129	ALA	4.4
1	A	202	U	4.4
21	U	18	TYR	4.3
1	A	461	C	4.3
1	A	1006	C	4.3
2	B	125	PRO	4.3
1	A	1534	A	4.1
7	G	5	ARG	4.0
18	R	88	LYS	3.9
3	C	76	VAL	3.9
10	J	90	LEU	3.9
15	O	89	GLY	3.9
20	T	9	ASN	3.8
13	M	117	VAL	3.7
9	I	8	GLY	3.6
2	B	131	PRO	3.5
12	L	128	ALA	3.4
1	A	1034	G	3.4
1	A	82	U	3.4
21	U	17	THR	3.4
21	U	26	LYS	3.1
7	G	2	ALA	3.0
12	L	19	ARG	3.0
19	S	3	ARG	3.0
1	A	1542	U	3.0
14	N	12	ARG	2.9
10	J	33	GLN	2.9
13	M	118	ALA	2.9
14	N	13	THR	2.8
2	B	231	GLU	2.8
1	A	1005	A	2.7
19	S	10	PHE	2.7
6	F	101	ALA	2.7
21	U	25	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	103	VAL	2.7
1	A	1533	C	2.7
21	U	24	ARG	2.6
3	C	146	ALA	2.6
13	M	119	GLY	2.6
20	T	100	ILE	2.5
1	A	1003	G	2.5
4	D	32	ALA	2.5
4	D	35	ARG	2.5
1	A	1033	G	2.5
13	M	5	ALA	2.5
7	G	156	TRP	2.4
13	M	2	ALA	2.4
1	A	1038	C	2.4
11	K	127	LYS	2.4
1	A	1036	G	2.3
1	A	1025	U	2.3
10	J	71	LEU	2.2
4	D	9	CYS	2.2
1	A	216	G	2.2
4	D	33	MET	2.2
1	A	1544	U	2.2
1	A	83	U	2.2
1	A	1543	C	2.2
2	B	238	LEU	2.2
10	J	73	ASP	2.2
13	M	7	VAL	2.2
1	A	88	A	2.1
1	A	1032	G	2.1
10	J	6	ILE	2.1
8	H	1	MET	2.1
10	J	74	ILE	2.0
3	C	196	LEU	2.0
10	J	72	VAL	2.0
10	J	87	THR	2.0
1	A	81	U	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	5MC	A	967	21/22	0.97	0.14	-	59,76,83,84	0
1	5MC	A	1404	21/22	0.97	0.15	-	72,81,90,95	0
1	4OC	A	1402	22/23	0.98	0.16	-	70,75,83,91	0
1	PSU	A	516	20/21	0.94	0.16	-	87,90,100,100	0
1	2MG	A	1207	24/25	0.95	0.13	-	101,107,113,115	0
1	5MC	A	1400	21/22	0.95	0.20	-	67,83,106,112	0
1	5MC	A	1407	21/22	0.94	0.22	-	83,120,143,145	0
1	7MG	A	527	24/25	0.98	0.19	-	66,72,94,98	0
12	0TD	L	92	10/11	0.95	0.36	-	96,102,168,273	0
1	UR3	A	1498	21/22	0.96	0.22	-	71,77,98,103	0
1	M2G	A	966	25/26	0.98	0.13	-	70,81,95,98	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
22	MG	A	1687	1/1	0.96	1.11	51.68	60,60,60,60	0
22	MG	A	1690	1/1	0.93	1.55	43.89	70,70,70,70	0
22	MG	A	1618	1/1	0.91	0.86	39.83	58,58,58,58	0
22	MG	A	1646	1/1	0.95	0.56	23.06	58,58,58,58	0
22	MG	A	1625	1/1	0.96	0.58	21.67	57,57,57,57	0
22	MG	A	1635	1/1	0.96	0.49	21.00	41,41,41,41	0
22	MG	A	1624	1/1	0.97	0.53	19.75	39,39,39,39	0
22	MG	A	1696	1/1	0.93	0.53	18.77	45,45,45,45	0
22	MG	A	1705	1/1	0.99	0.81	18.28	61,61,61,61	0
22	MG	A	1615	1/1	0.82	0.59	16.42	95,95,95,95	0
22	MG	A	1629	1/1	0.97	0.49	16.13	43,43,43,43	0
22	MG	A	1660	1/1	0.86	0.44	15.78	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1688	1/1	0.90	0.54	14.67	41,41,41,41	0
22	MG	A	1670	1/1	0.92	0.28	13.74	57,57,57,57	0
22	MG	A	1708	1/1	0.97	0.40	12.33	63,63,63,63	0
22	MG	A	1651	1/1	0.90	0.46	11.56	77,77,77,77	0
23	K	A	1758	1/1	0.94	0.62	11.33	130,130,130,130	0
22	MG	A	1689	1/1	0.96	0.40	8.90	67,67,67,67	0
22	MG	A	1685	1/1	0.92	0.50	8.44	55,55,55,55	0
24	NMY	A	1837	42/42	0.86	0.28	7.78	57,138,186,186	0
22	MG	A	1643	1/1	0.94	0.26	7.11	54,54,54,54	0
22	MG	A	1637	1/1	0.97	0.37	6.82	67,67,67,67	0
22	MG	A	1702	1/1	0.98	0.29	6.03	40,40,40,40	0
22	MG	A	1727	1/1	0.88	0.25	5.88	54,54,54,54	0
22	MG	N	102	1/1	0.72	1.08	5.85	92,92,92,92	0
22	MG	A	1653	1/1	0.87	0.70	5.72	63,63,63,63	0
23	K	A	1745	1/1	0.98	0.22	4.62	142,142,142,142	0
22	MG	A	1815	1/1	0.83	0.55	4.53	81,81,81,81	0
22	MG	A	1703	1/1	0.99	0.25	4.09	51,51,51,51	0
24	NMY	A	1835	42/42	0.88	0.23	3.55	105,127,145,147	0
22	MG	A	1654	1/1	0.96	0.26	3.48	50,50,50,50	0
22	MG	A	1707	1/1	0.99	0.25	2.94	85,85,85,85	0
22	MG	A	1825	1/1	0.88	0.22	2.71	63,63,63,63	0
24	NMY	A	1836	42/42	0.86	0.27	2.67	75,119,177,188	0
22	MG	A	1676	1/1	0.93	0.25	2.57	60,60,60,60	0
23	K	A	1731	1/1	0.84	0.23	2.53	121,121,121,121	0
22	MG	M	201	1/1	0.96	0.27	2.16	72,72,72,72	0
22	MG	A	1697	1/1	0.97	0.23	1.96	36,36,36,36	0
24	NMY	A	1834	42/42	0.86	0.28	1.91	62,120,200,201	0
23	K	A	1754	1/1	0.83	0.19	1.70	135,135,135,135	0
22	MG	N	103	1/1	0.77	0.30	1.62	57,57,57,57	0
22	MG	A	1693	1/1	0.94	0.29	1.53	72,72,72,72	0
22	MG	A	1728	1/1	0.90	0.32	1.44	55,55,55,55	0
22	MG	A	1608	1/1	0.89	0.14	1.29	73,73,73,73	0
24	NMY	A	1832	42/42	0.94	0.21	1.29	54,85,153,163	0
22	MG	A	1716	1/1	0.94	0.19	1.27	49,49,49,49	0
22	MG	A	1723	1/1	0.91	0.27	1.25	55,55,55,55	0
24	NMY	A	1833	42/42	0.95	0.18	0.97	55,78,103,105	0
22	MG	P	102	1/1	0.97	0.23	0.97	84,84,84,84	0
22	MG	A	1674	1/1	0.87	0.20	0.96	38,38,38,38	0
25	ZN	N	101	1/1	0.99	0.19	0.86	106,106,106,106	0
25	ZN	D	301	1/1	0.98	0.34	0.41	92,92,92,92	0
22	MG	A	1650	1/1	0.97	0.19	0.18	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1686	1/1	0.82	0.17	-0.44	54,54,54,54	0
22	MG	D	302	1/1	0.80	0.16	-0.62	63,63,63,63	0
22	MG	A	1695	1/1	0.95	0.15	-0.68	53,53,53,53	0
22	MG	Q	201	1/1	0.74	0.14	-0.98	71,71,71,71	0
22	MG	A	1717	1/1	0.95	0.10	-3.16	66,66,66,66	0
22	MG	A	1722	1/1	0.94	0.08	-3.70	35,35,35,35	0
22	MG	A	1638	1/1	0.93	0.09	-3.80	64,64,64,64	0
22	MG	A	1699	1/1	0.95	0.08	-	64,64,64,64	0
22	MG	P	101	1/1	0.82	0.45	-	68,68,68,68	0
22	MG	A	1785	1/1	0.89	0.21	-	67,67,67,67	0
22	MG	A	1682	1/1	0.77	1.21	-	84,84,84,84	0
22	MG	A	1806	1/1	0.79	0.76	-	76,76,76,76	0
22	MG	A	1656	1/1	0.92	0.20	-	57,57,57,57	0
23	K	A	1742	1/1	0.74	1.22	-	138,138,138,138	0
23	K	A	1743	1/1	0.91	0.31	-	137,137,137,137	0
22	MG	A	1610	1/1	0.85	0.23	-	89,89,89,89	0
22	MG	A	1718	1/1	0.84	0.59	-	84,84,84,84	0
22	MG	A	1711	1/1	0.85	0.57	-	90,90,90,90	0
23	K	A	1734	1/1	0.90	0.25	-	119,119,119,119	0
22	MG	A	1790	1/1	0.90	0.33	-	72,72,72,72	0
22	MG	A	1730	1/1	0.80	1.47	-	74,74,74,74	0
22	MG	A	1787	1/1	0.84	0.92	-	117,117,117,117	0
22	MG	A	1617	1/1	0.87	0.36	-	112,112,112,112	0
22	MG	B	303	1/1	0.82	0.09	-	83,83,83,83	0
22	MG	A	1644	1/1	0.88	0.46	-	62,62,62,62	0
22	MG	A	1807	1/1	0.93	0.53	-	78,78,78,78	0
22	MG	A	1603	1/1	0.91	0.78	-	69,69,69,69	0
23	K	A	1740	1/1	0.90	0.56	-	135,135,135,135	0
22	MG	A	1671	1/1	0.94	0.40	-	50,50,50,50	0
22	MG	A	1776	1/1	0.81	0.58	-	85,85,85,85	0
23	K	A	1747	1/1	0.90	0.45	-	112,112,112,112	0
22	MG	A	1642	1/1	0.27	0.70	-	68,68,68,68	0
22	MG	A	1665	1/1	0.85	0.42	-	84,84,84,84	0
22	MG	A	1762	1/1	0.81	0.39	-	89,89,89,89	0
22	MG	A	1623	1/1	0.91	1.33	-	86,86,86,86	0
23	K	A	1738	1/1	0.83	0.29	-	133,133,133,133	0
22	MG	A	1704	1/1	0.99	0.52	-	60,60,60,60	0
22	MG	A	1799	1/1	0.80	0.34	-	98,98,98,98	0
23	K	A	1760	1/1	0.75	0.53	-	145,145,145,145	0
22	MG	A	1777	1/1	0.87	0.57	-	96,96,96,96	0
22	MG	A	1640	1/1	0.98	0.30	-	47,47,47,47	0
22	MG	A	1681	1/1	0.93	0.44	-	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1725	1/1	0.85	0.63	-	76,76,76,76	0
22	MG	A	1823	1/1	0.86	0.11	-	107,107,107,107	0
22	MG	A	1706	1/1	0.93	0.78	-	73,73,73,73	0
22	MG	A	1621	1/1	0.96	0.47	-	82,82,82,82	0
22	MG	A	1601	1/1	0.95	0.19	-	76,76,76,76	0
22	MG	A	1798	1/1	0.92	0.91	-	85,85,85,85	0
22	MG	A	1645	1/1	0.89	0.84	-	79,79,79,79	0
22	MG	A	1819	1/1	0.85	0.24	-	85,85,85,85	0
22	MG	C	301	1/1	0.88	0.22	-	66,66,66,66	0
22	MG	A	1661	1/1	0.81	0.56	-	69,69,69,69	0
22	MG	A	1803	1/1	0.84	0.22	-	66,66,66,66	0
22	MG	A	1658	1/1	0.85	1.09	-	76,76,76,76	0
22	MG	E	201	1/1	0.96	0.45	-	64,64,64,64	0
22	MG	A	1669	1/1	0.95	0.21	-	51,51,51,51	0
22	MG	A	1812	1/1	0.90	0.21	-	103,103,103,103	0
22	MG	A	1719	1/1	0.88	0.15	-	62,62,62,62	0
23	K	A	1757	1/1	0.93	0.29	-	143,143,143,143	0
22	MG	L	201	1/1	0.86	0.29	-	99,99,99,99	0
23	K	A	1746	1/1	0.94	0.45	-	149,149,149,149	0
23	K	A	1753	1/1	0.79	0.36	-	127,127,127,127	0
22	MG	A	1721	1/1	0.82	0.29	-	77,77,77,77	0
22	MG	H	202	1/1	0.84	0.46	-	49,49,49,49	0
22	MG	A	1796	1/1	0.85	0.40	-	89,89,89,89	0
22	MG	A	1680	1/1	0.93	0.75	-	46,46,46,46	0
22	MG	A	1605	1/1	0.94	0.64	-	44,44,44,44	0
22	MG	A	1714	1/1	0.95	1.07	-	94,94,94,94	0
22	MG	A	1775	1/1	0.67	0.66	-	84,84,84,84	0
22	MG	A	1634	1/1	0.99	0.29	-	40,40,40,40	0
22	MG	A	1673	1/1	0.92	0.41	-	57,57,57,57	0
22	MG	D	303	1/1	0.91	0.78	-	89,89,89,89	0
22	MG	A	1791	1/1	0.92	0.45	-	78,78,78,78	0
22	MG	A	1811	1/1	0.90	0.28	-	79,79,79,79	0
22	MG	F	201	1/1	0.66	0.43	-	95,95,95,95	0
23	K	A	1736	1/1	0.94	0.56	-	108,108,108,108	0
22	MG	A	1824	1/1	0.91	0.20	-	103,103,103,103	0
22	MG	A	1632	1/1	0.91	0.56	-	64,64,64,64	0
23	K	A	1749	1/1	0.86	0.67	-	115,115,115,115	0
22	MG	A	1616	1/1	0.71	0.83	-	84,84,84,84	0
22	MG	A	1774	1/1	0.87	0.56	-	98,98,98,98	0
22	MG	A	1664	1/1	0.68	0.52	-	94,94,94,94	0
22	MG	A	1817	1/1	0.87	0.36	-	103,103,103,103	0
22	MG	A	1607	1/1	0.94	0.76	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1813	1/1	0.90	0.64	-	88,88,88,88	0
22	MG	A	1622	1/1	0.95	0.36	-	65,65,65,65	0
22	MG	A	1827	1/1	0.90	0.15	-	102,102,102,102	0
22	MG	A	1830	1/1	0.87	0.06	-	293,293,293,293	0
22	MG	A	1678	1/1	0.97	0.29	-	35,35,35,35	0
22	MG	A	1795	1/1	0.81	0.43	-	96,96,96,96	0
22	MG	A	1666	1/1	0.88	0.71	-	72,72,72,72	0
22	MG	A	1611	1/1	0.88	0.44	-	49,49,49,49	0
22	MG	A	1657	1/1	0.81	0.27	-	70,70,70,70	0
22	MG	A	1710	1/1	0.94	0.37	-	90,90,90,90	0
22	MG	A	1647	1/1	0.63	0.46	-	83,83,83,83	0
22	MG	A	1612	1/1	0.82	1.30	-	93,93,93,93	0
23	K	A	1732	1/1	0.96	0.18	-	104,104,104,104	0
23	K	A	1741	1/1	0.89	0.97	-	154,154,154,154	0
22	MG	A	1609	1/1	0.93	0.94	-	86,86,86,86	0
22	MG	A	1792	1/1	0.85	0.85	-	68,68,68,68	0
22	MG	A	1641	1/1	0.95	0.80	-	37,37,37,37	0
22	MG	A	1765	1/1	0.83	0.64	-	55,55,55,55	0
23	K	A	1751	1/1	0.80	0.33	-	160,160,160,160	0
22	MG	H	201	1/1	0.86	0.21	-	74,74,74,74	0
22	MG	A	1766	1/1	0.78	0.41	-	61,61,61,61	0
22	MG	A	1782	1/1	0.83	0.57	-	82,82,82,82	0
22	MG	A	1626	1/1	0.86	0.39	-	79,79,79,79	0
22	MG	A	1628	1/1	0.97	0.60	-	57,57,57,57	0
22	MG	A	1720	1/1	0.79	0.38	-	75,75,75,75	0
22	MG	A	1805	1/1	0.84	1.01	-	79,79,79,79	0
22	MG	A	1636	1/1	0.96	0.46	-	64,64,64,64	0
22	MG	A	1773	1/1	0.74	0.56	-	69,69,69,69	0
23	K	A	1756	1/1	0.82	0.61	-	151,151,151,151	0
22	MG	A	1679	1/1	0.88	0.57	-	62,62,62,62	0
22	MG	A	1788	1/1	0.31	0.41	-	88,88,88,88	0
22	MG	A	1677	1/1	0.95	0.93	-	63,63,63,63	0
22	MG	B	301	1/1	0.91	0.29	-	96,96,96,96	0
22	MG	A	1672	1/1	0.93	0.40	-	83,83,83,83	0
22	MG	A	1604	1/1	0.95	0.17	-	79,79,79,79	0
22	MG	C	302	1/1	0.62	0.72	-	106,106,106,106	0
22	MG	A	1797	1/1	0.84	0.17	-	68,68,68,68	0
22	MG	A	1783	1/1	0.83	0.40	-	73,73,73,73	0
22	MG	A	1786	1/1	0.78	0.79	-	71,71,71,71	0
23	K	A	1733	1/1	0.86	0.66	-	112,112,112,112	0
23	K	A	1739	1/1	0.85	0.30	-	140,140,140,140	0
22	MG	A	1620	1/1	0.93	1.23	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1821	1/1	0.83	0.45	-	73,73,73,73	0
22	MG	A	1764	1/1	0.94	0.21	-	65,65,65,65	0
22	MG	A	1713	1/1	0.95	0.50	-	61,61,61,61	0
22	MG	A	1639	1/1	0.97	0.27	-	28,28,28,28	0
22	MG	A	1781	1/1	0.80	0.55	-	87,87,87,87	0
22	MG	A	1810	1/1	0.82	0.55	-	65,65,65,65	0
22	MG	A	1655	1/1	0.78	0.34	-	93,93,93,93	0
23	K	A	1737	1/1	0.81	0.13	-	134,134,134,134	0
23	K	A	1735	1/1	0.73	0.83	-	152,152,152,152	0
22	MG	A	1770	1/1	0.65	0.55	-	102,102,102,102	0
22	MG	A	1761	1/1	0.64	0.53	-	51,51,51,51	0
22	MG	A	1816	1/1	0.87	0.55	-	67,67,67,67	0
22	MG	A	1801	1/1	0.43	1.33	-	80,80,80,80	0
22	MG	A	1648	1/1	0.96	0.82	-	56,56,56,56	0
22	MG	A	1784	1/1	0.93	0.64	-	90,90,90,90	0
22	MG	A	1684	1/1	0.87	0.52	-	68,68,68,68	0
22	MG	A	1698	1/1	0.98	0.64	-	47,47,47,47	0
22	MG	A	1652	1/1	0.88	0.48	-	64,64,64,64	0
22	MG	A	1683	1/1	0.76	0.19	-	77,77,77,77	0
22	MG	A	1613	1/1	0.92	0.55	-	86,86,86,86	0
22	MG	A	1667	1/1	0.51	0.66	-	98,98,98,98	0
22	MG	A	1828	1/1	0.89	0.22	-	95,95,95,95	0
22	MG	A	1831	1/1	0.70	0.08	-	285,285,285,285	0
22	MG	A	1631	1/1	0.95	0.35	-	63,63,63,63	0
22	MG	A	1724	1/1	0.84	0.30	-	51,51,51,51	0
22	MG	A	1768	1/1	0.80	0.67	-	50,50,50,50	0
22	MG	A	1826	1/1	0.77	0.19	-	81,81,81,81	0
23	K	A	1748	1/1	0.78	0.52	-	136,136,136,136	0
22	MG	A	1793	1/1	0.92	1.09	-	69,69,69,69	0
22	MG	A	1633	1/1	0.60	0.36	-	93,93,93,93	0
22	MG	A	1809	1/1	0.72	0.18	-	74,74,74,74	0
22	MG	A	1779	1/1	0.95	0.15	-	82,82,82,82	0
22	MG	A	1800	1/1	0.76	0.33	-	98,98,98,98	0
22	MG	A	1729	1/1	0.95	0.22	-	64,64,64,64	0
23	K	A	1744	1/1	0.93	0.46	-	121,121,121,121	0
22	MG	A	1700	1/1	0.97	0.20	-	38,38,38,38	0
22	MG	A	1769	1/1	0.93	0.47	-	73,73,73,73	0
22	MG	A	1627	1/1	0.95	0.13	-	90,90,90,90	0
22	MG	A	1675	1/1	0.72	1.03	-	75,75,75,75	0
22	MG	A	1659	1/1	0.80	0.32	-	94,94,94,94	0
22	MG	A	1789	1/1	0.89	0.37	-	97,97,97,97	0
22	MG	A	1663	1/1	0.93	0.70	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
22	MG	A	1691	1/1	0.88	0.46	-	82,82,82,82	0
22	MG	A	1802	1/1	0.82	0.21	-	108,108,108,108	0
22	MG	A	1602	1/1	0.72	0.32	-	114,114,114,114	0
22	MG	A	1692	1/1	0.92	0.88	-	72,72,72,72	0
22	MG	A	1794	1/1	0.79	0.30	-	73,73,73,73	0
22	MG	B	302	1/1	0.83	0.36	-	84,84,84,84	0
22	MG	A	1726	1/1	0.84	0.43	-	70,70,70,70	0
22	MG	M	202	1/1	0.81	0.29	-	85,85,85,85	0
22	MG	A	1715	1/1	0.90	0.36	-	68,68,68,68	0
22	MG	A	1822	1/1	0.79	0.28	-	101,101,101,101	0
22	MG	A	1662	1/1	0.97	0.17	-	51,51,51,51	0
22	MG	A	1778	1/1	0.70	0.23	-	88,88,88,88	0
22	MG	A	1709	1/1	0.94	0.54	-	66,66,66,66	0
22	MG	A	1808	1/1	0.72	0.89	-	79,79,79,79	0
22	MG	A	1818	1/1	0.67	0.31	-	90,90,90,90	0
22	MG	A	1694	1/1	0.57	0.75	-	83,83,83,83	0
22	MG	A	1820	1/1	0.87	0.14	-	65,65,65,65	0
22	MG	A	1772	1/1	0.82	0.70	-	66,66,66,66	0
22	MG	A	1701	1/1	0.98	0.39	-	44,44,44,44	0
22	MG	A	1829	1/1	0.70	0.22	-	104,104,104,104	0
22	MG	A	1712	1/1	0.85	0.23	-	75,75,75,75	0
23	K	A	1750	1/1	0.76	1.10	-	143,143,143,143	0
22	MG	A	1614	1/1	0.69	0.54	-	72,72,72,72	0
23	K	A	1759	1/1	0.83	0.13	-	145,145,145,145	0
22	MG	A	1606	1/1	0.97	1.42	-	72,72,72,72	0
22	MG	A	1814	1/1	0.60	1.16	-	87,87,87,87	0
22	MG	A	1767	1/1	0.83	0.67	-	62,62,62,62	0
22	MG	A	1780	1/1	0.86	0.33	-	75,75,75,75	0
22	MG	A	1804	1/1	0.92	0.23	-	56,56,56,56	0
22	MG	A	1649	1/1	0.97	0.48	-	40,40,40,40	0
22	MG	A	1619	1/1	0.86	0.36	-	77,77,77,77	0
22	MG	A	1668	1/1	0.89	0.30	-	66,66,66,66	0
23	K	A	1752	1/1	0.98	0.62	-	115,115,115,115	0
22	MG	A	1630	1/1	0.80	0.51	-	60,60,60,60	0
22	MG	A	1763	1/1	0.71	0.21	-	68,68,68,68	0
22	MG	A	1771	1/1	0.92	0.69	-	58,58,58,58	0
23	K	A	1755	1/1	0.79	0.53	-	147,147,147,147	0

6.5 Other polymers (i)

There are no such residues in this entry.