wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2025 – 12:45 PM EST

PDB ID	:	4DV2
Title	:	Crystal structure of the Thermus thermophilus 30S ribosomal subunit with a 16S rRNA mutation, C912A
Authors	:	Demirci, H.; Murphy IV, F.; Murphy, E.; Gregory, S.T.; Dahlberg, A.E.; Jogl, G.
Deposited on	:	2012-02-22
Resolution	:	3.65 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

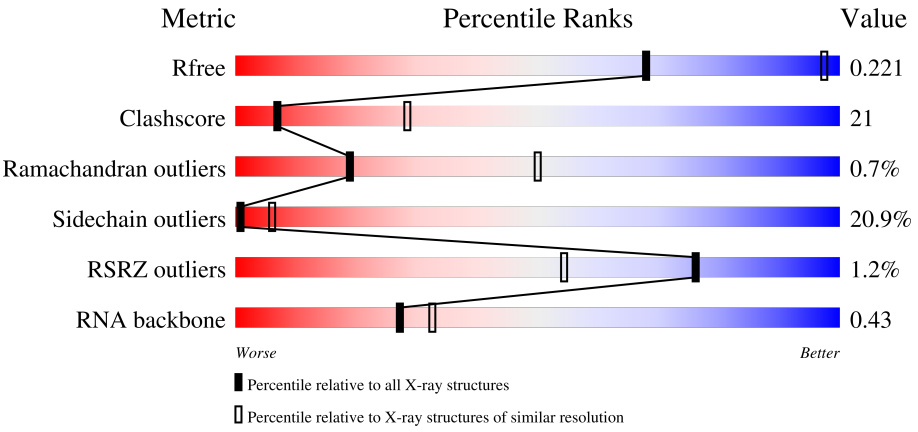
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.65 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}	164625	1000 (3.76-3.52)
Clashscore	180529	1046 (3.76-3.52)
Ramachandran outliers	177936	1031 (3.76-3.52)
Sidechain outliers	177891	1029 (3.76-3.52)
RSRZ outliers	164620	1682 (3.78-3.50)
RNA backbone	3690	1110 (4.26-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	1522	2% 20% 41% 30% 8%
2	B	256	% 41% 38% 12% 9%
3	C	239	% 30% 44% 12% 14%
4	D	209	3% 54% 36% 9%

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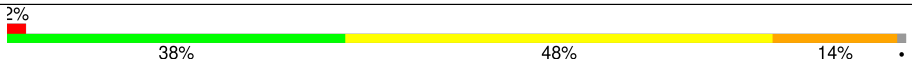
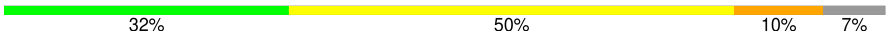
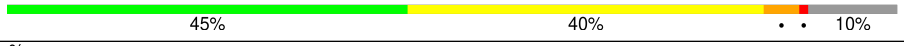
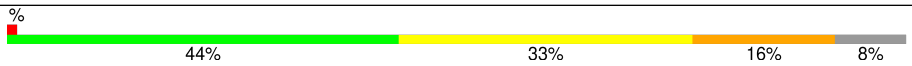
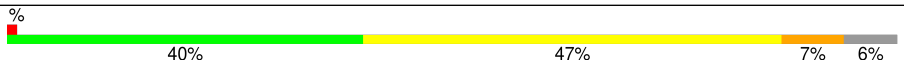
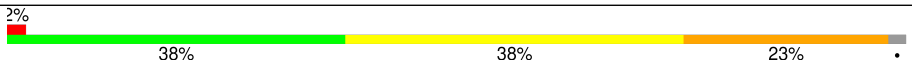
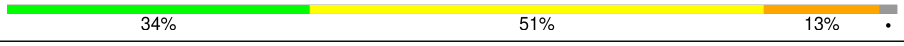
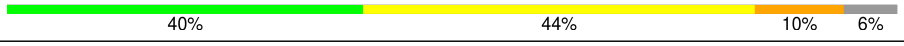
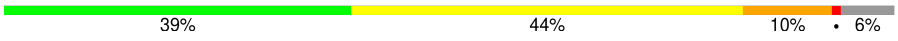
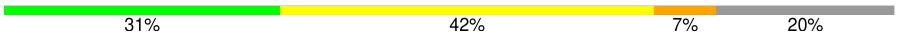
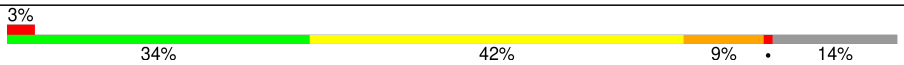
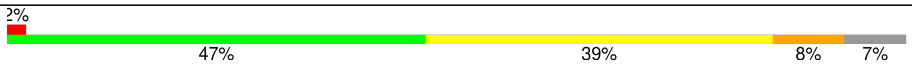
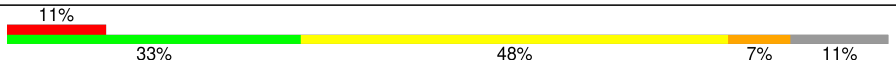
Mol	Chain	Length	Quality of chain
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	MG	A	1672	-	-	-	X
22	MG	A	1751	-	-	-	X

2 Entry composition (i)

There are 24 unique types of molecules in this entry. The entry contains 52441 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	1512	32646	14541	6041	10546	1518	0	6	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	912	A	C	engineered mutation	GB M26923.1
A	1534	C	A	conflict	GB M26923.1
A	1535	A	C	conflict	GB M26923.1

- Molecule 2 is a protein called ribosomal protein S2.

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

- Molecule 3 is a protein called ribosomal protein S3.

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

- Molecule 4 is a protein called ribosomal protein S4.

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

- Molecule 5 is a protein called ribosomal protein S5.

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

- 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	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 11 is a protein called ribosomal protein S11.

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

- Molecule 12 is a protein called ribosomal protein S12.

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

- Molecule 13 is a protein called 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	87	Total	C	N	O	S	0	0	0
			729	457	146	124	2			

- Molecule 16 is a protein called ribosomal protein S16.

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

- Molecule 17 is a protein called ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called ribosomal protein S18.

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

- Molecule 19 is a protein called ribosomal protein S19.

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

- Molecule 20 is a protein called ribosomal protein S20.

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

- Molecule 21 is a protein called ribosomal protein THX.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	268	Total 268	Mg 268	0	0
22	B	2	Total 2	Mg 2	0	0
22	C	2	Total 2	Mg 2	0	0
22	D	4	Total 4	Mg 4	0	0
22	E	1	Total 1	Mg 1	0	0
22	F	1	Total 1	Mg 1	0	0
22	I	1	Total 1	Mg 1	0	0
22	J	1	Total 1	Mg 1	0	0
22	L	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	M	2	Total Mg 2 2	0	0
22	P	2	Total Mg 2 2	0	0
22	Q	2	Total Mg 2 2	0	0
22	T	2	Total Mg 2 2	0	0

- Molecule 23 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 24 is water.

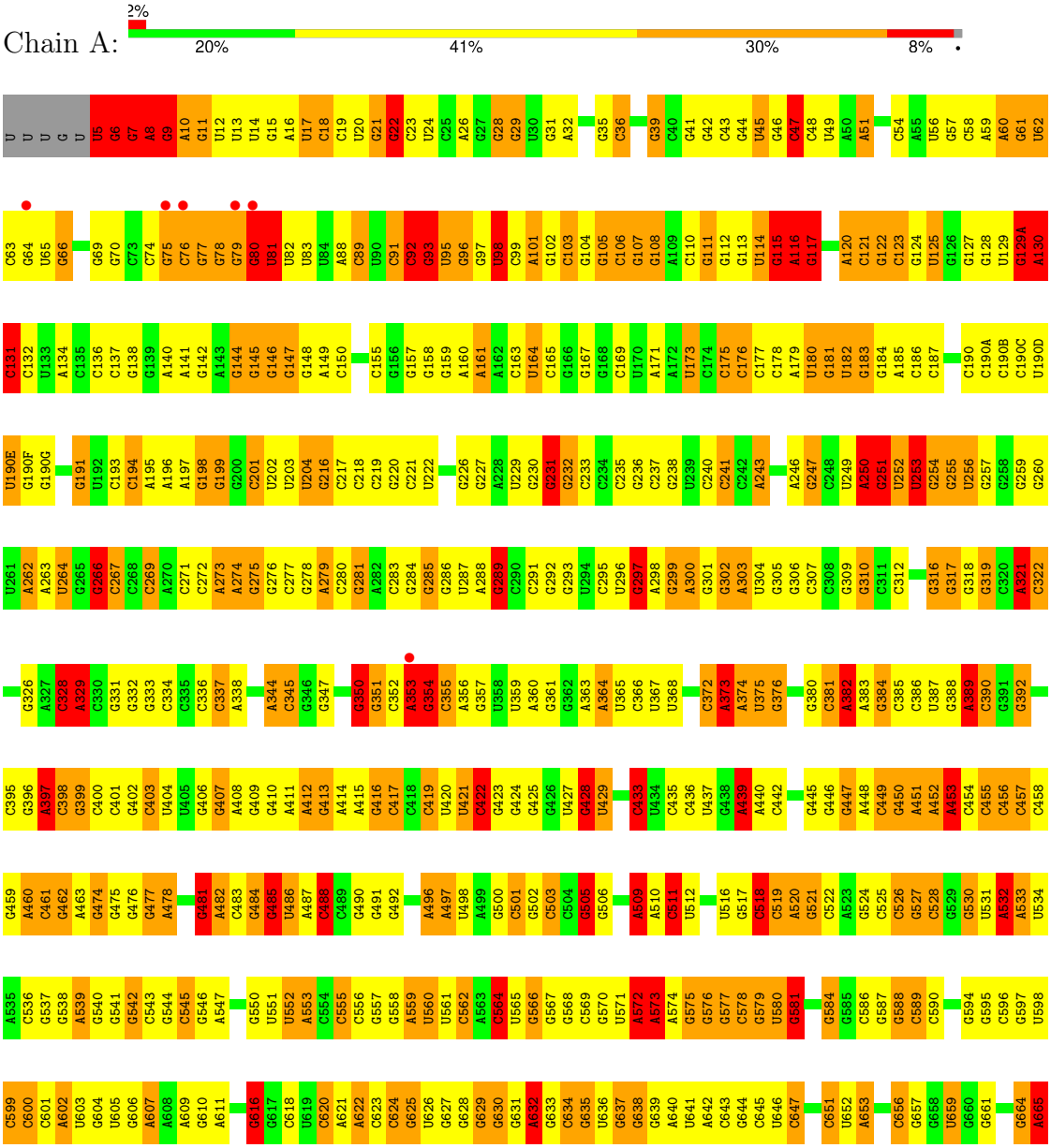
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	391	Total O 391 391	0	0
24	B	1	Total O 1 1	0	0
24	D	3	Total O 3 3	0	0
24	E	4	Total O 4 4	0	0
24	G	2	Total O 2 2	0	0
24	J	2	Total O 2 2	0	0
24	K	1	Total O 1 1	0	0
24	M	3	Total O 3 3	0	0
24	N	4	Total O 4 4	0	0
24	P	4	Total O 4 4	0	0
24	T	1	Total O 1 1	0	0

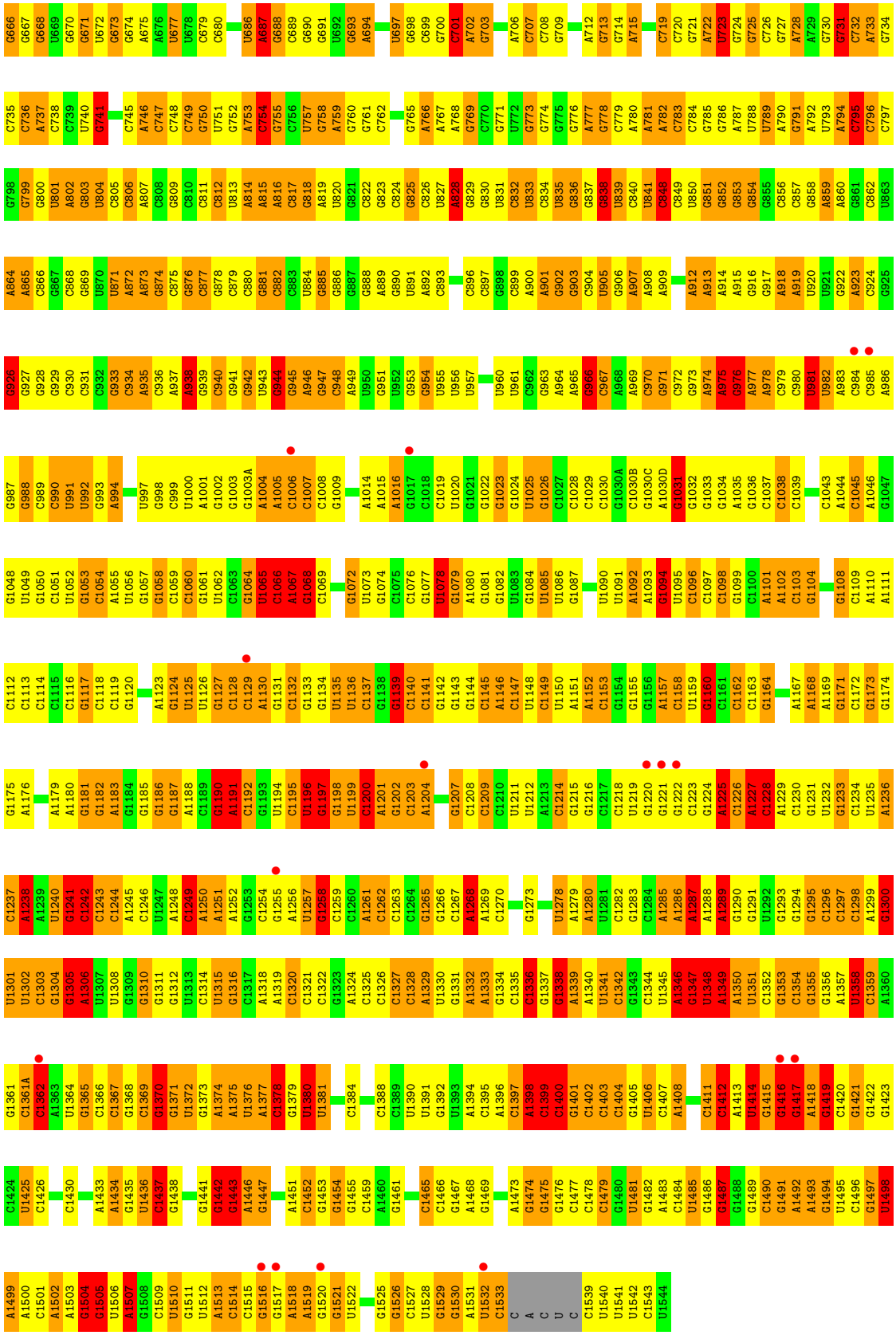
3 Residue-property plots (i)

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

- Molecule 1: 16S rRNA

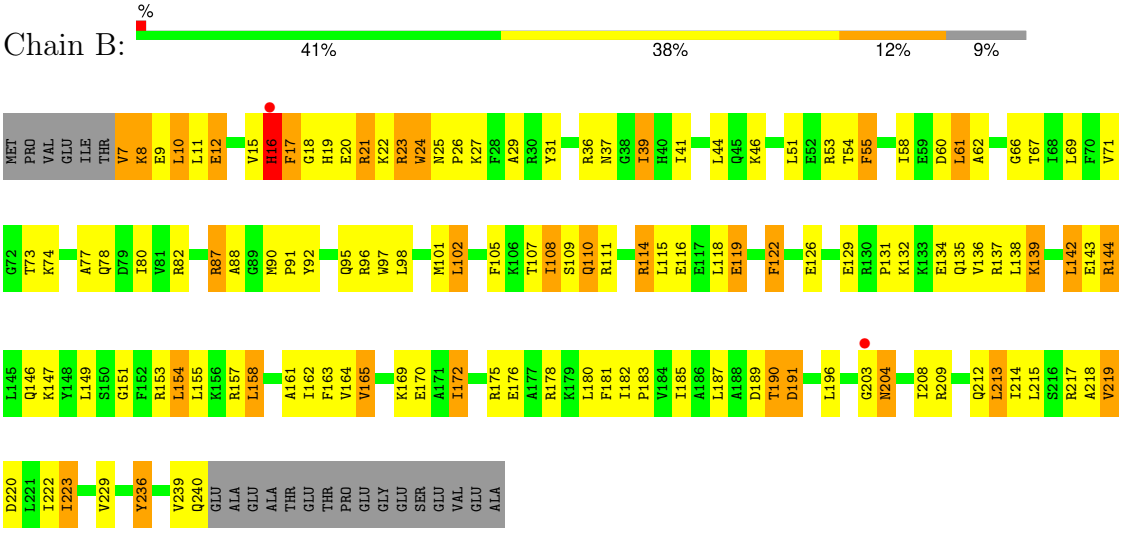
Chain A:





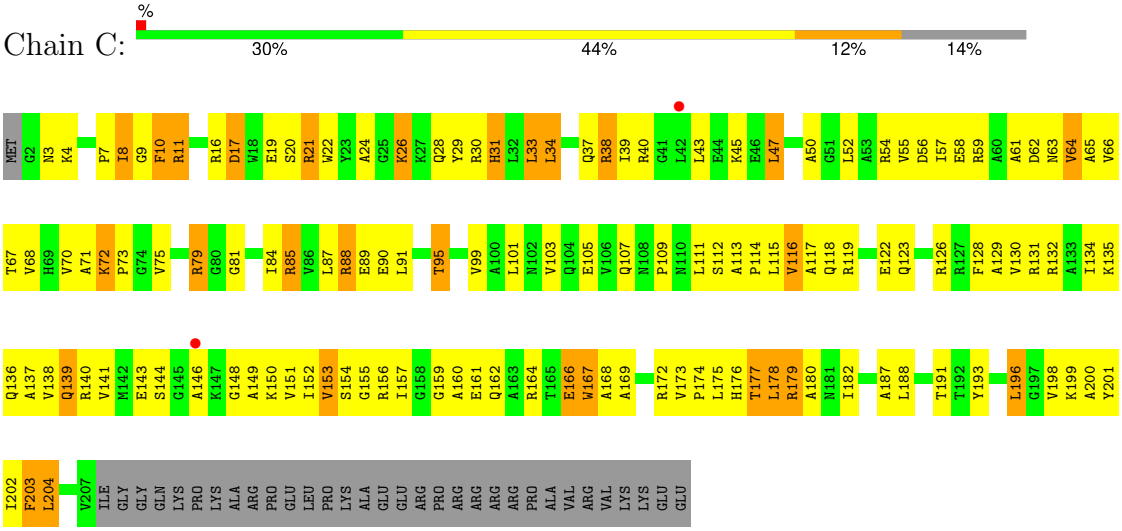
• Molecule 2: ribosomal protein S2

Chain B:



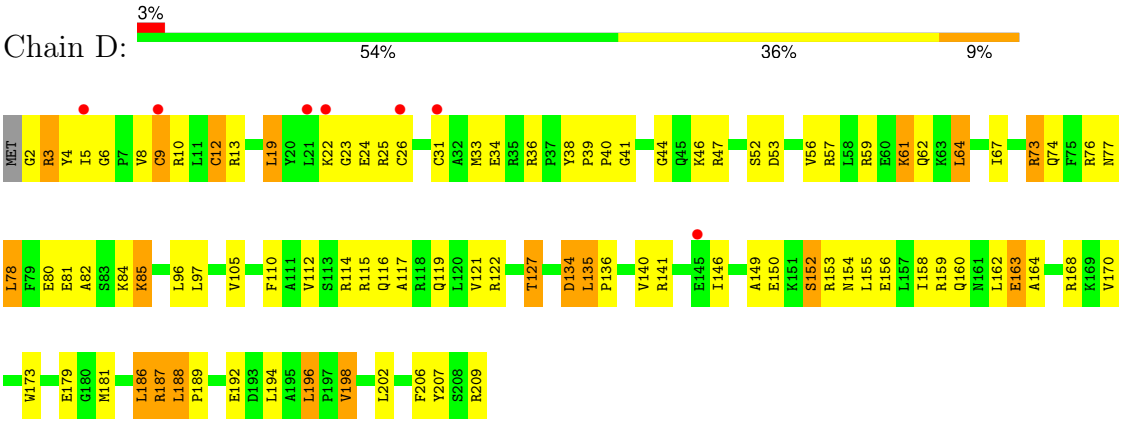
• Molecule 3: ribosomal protein S3

Chain C:



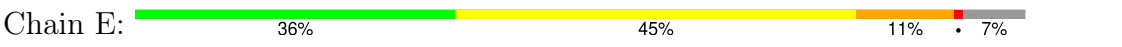
• Molecule 4: ribosomal protein S4

Chain D:



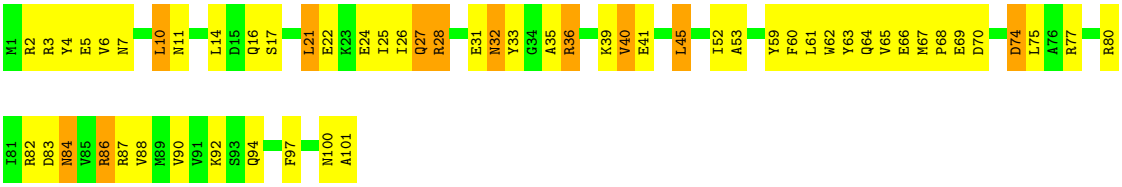
• Molecule 5: ribosomal protein S5

Chain E:



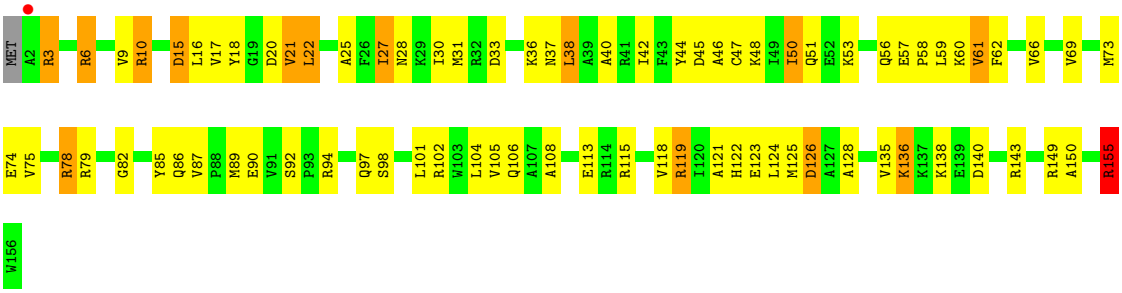
• Molecule 6: ribosomal protein S6

Chain F:



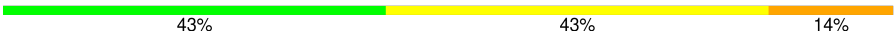
• Molecule 7: ribosomal protein S7

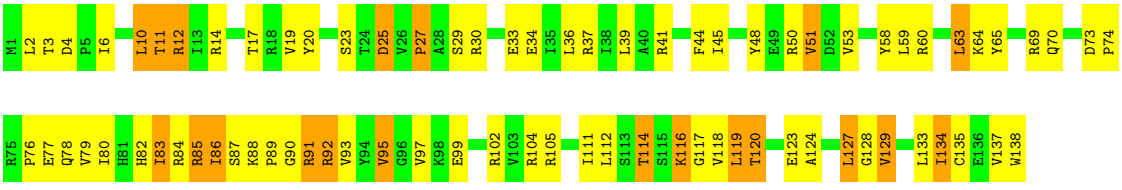
Chain G:



• Molecule 8: ribosomal protein S8

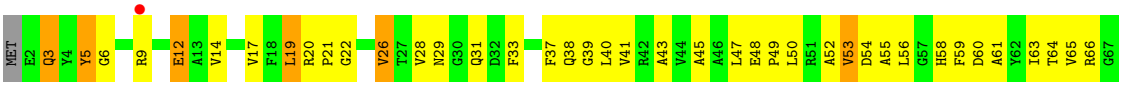
Chain H:

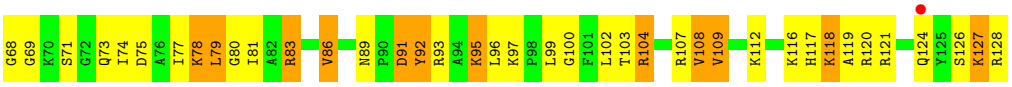




• Molecule 9: ribosomal protein S9

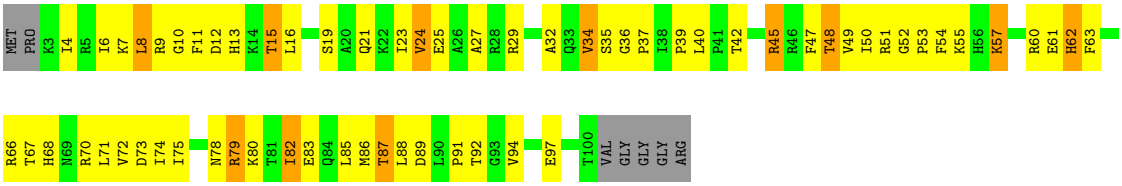
Chain I:





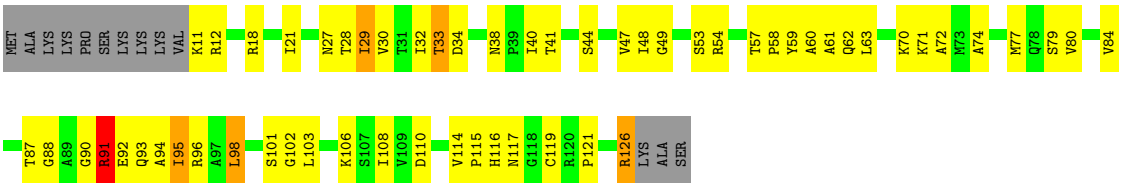
• Molecule 10: ribosomal protein S10

Chain J:



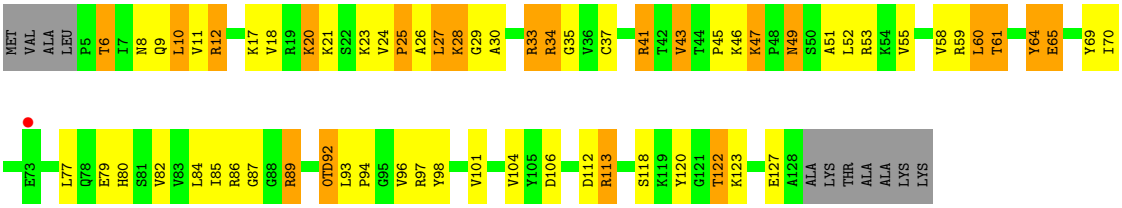
• Molecule 11: ribosomal protein S11

Chain K:



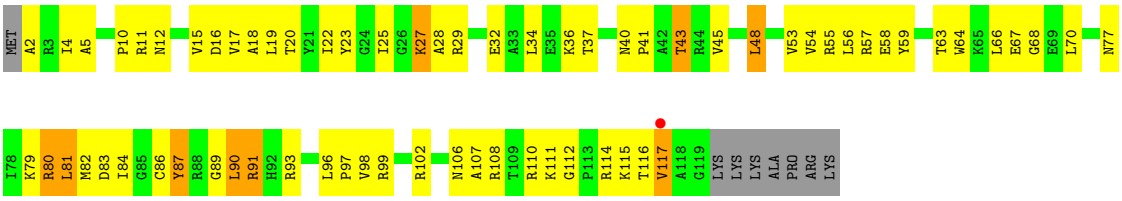
• Molecule 12: ribosomal protein S12

Chain L:



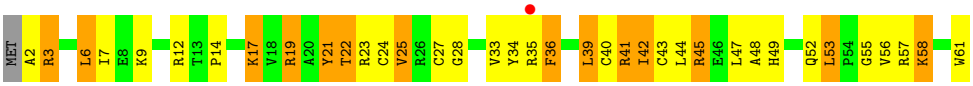
• Molecule 13: ribosomal protein S13

Chain M:



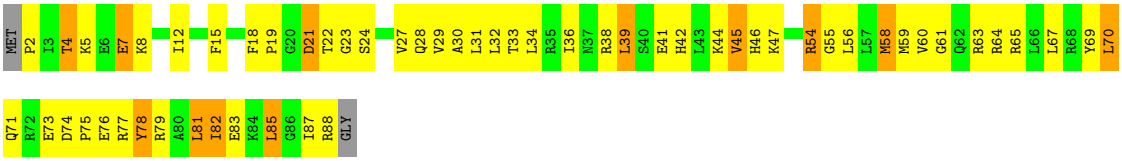
• Molecule 14: ribosomal protein S14

Chain N:



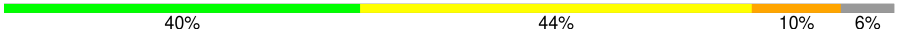
• Molecule 15: ribosomal protein S15

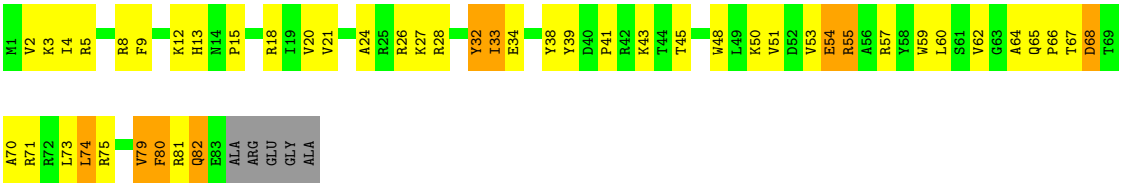
Chain O:



• Molecule 16: ribosomal protein S16

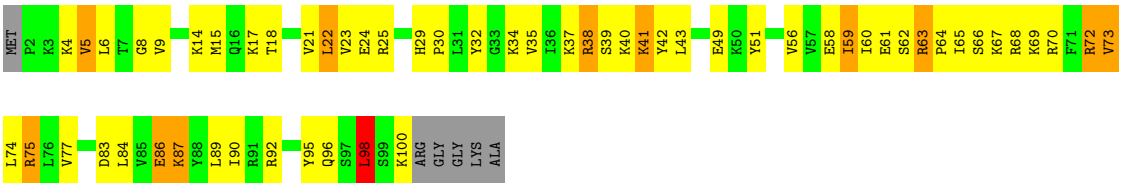
Chain P:





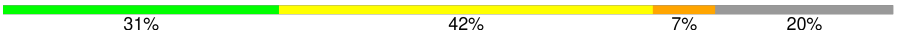
• Molecule 17: ribosomal protein S17

Chain Q:



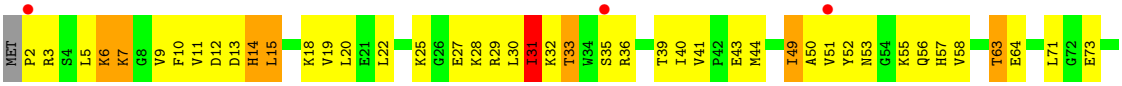
• Molecule 18: ribosomal protein S18

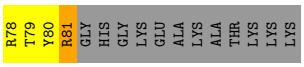
Chain R:



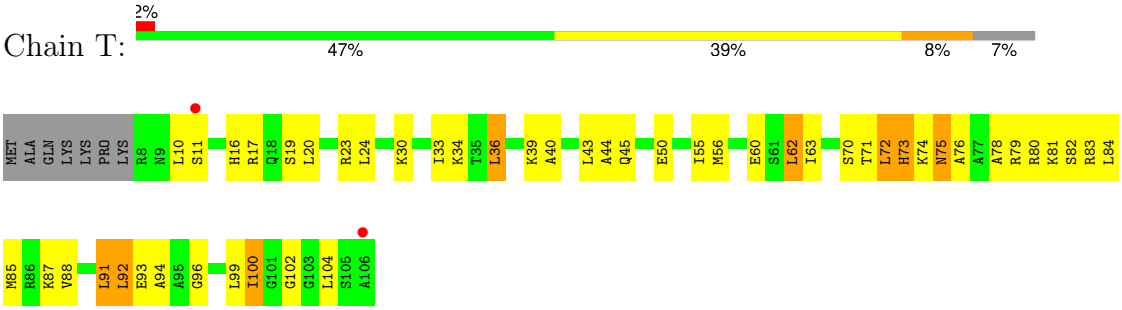
• Molecule 19: ribosomal protein S19

Chain S:

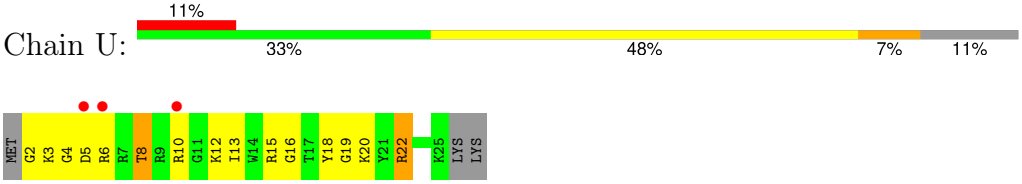




• Molecule 20: ribosomal protein S20



• 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	403.74Å 403.74Å 173.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 3.65 29.77 – 3.65	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.77-3.65) 96.6 (29.77-3.65)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.65Å)	Xtriage
Refinement program	PHENIX dev_978	Depositor
R, R_{free}	0.165 , 0.223 0.164 , 0.221	Depositor DCC
R_{free} test set	7644 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	137.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 129.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	52441	wwPDB-VP
Average B, all atoms (Å^2)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.20	163/36142 (0.5%)	1.88	1794/56401 (3.2%)
2	B	0.79	0/1935	0.96	1/2609 (0.0%)
3	C	0.58	0/1636	0.82	1/2205 (0.0%)
4	D	0.74	2/1733 (0.1%)	0.93	4/2318 (0.2%)
5	E	0.93	0/1162	1.12	4/1564 (0.3%)
6	F	0.65	0/856	0.84	0/1154
7	G	0.65	0/1276	0.83	0/1709
8	H	1.08	1/1136 (0.1%)	1.21	5/1527 (0.3%)
9	I	0.69	0/1029	0.86	1/1379 (0.1%)
10	J	0.57	0/805	0.83	0/1082
11	K	0.77	0/879	0.97	2/1187 (0.2%)
12	L	0.81	0/977	1.02	2/1306 (0.2%)
13	M	0.69	0/947	0.86	0/1270
14	N	0.59	0/501	0.85	0/664
15	O	0.80	0/740	1.05	3/987 (0.3%)
16	P	0.87	1/716 (0.1%)	1.00	1/963 (0.1%)
17	Q	1.01	0/836	1.21	6/1117 (0.5%)
18	R	0.74	0/579	0.98	1/768 (0.1%)
19	S	0.47	0/661	0.78	0/890
20	T	0.74	0/765	1.01	1/1007 (0.1%)
21	U	0.71	0/212	0.90	0/277
All	All	1.07	167/55523 (0.3%)	1.65	1826/82384 (2.2%)

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
2	B	0	1
3	C	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1
8	H	0	2
10	J	0	2
12	L	0	1
13	M	0	1
20	T	0	1
All	All	0	11

The worst 5 of 167 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	A	N3-C4	-11.90	1.27	1.34
1	A	279	A	N9-C4	-11.72	1.30	1.37
1	A	573	A	N7-C5	-10.54	1.32	1.39
1	A	1500	A	N3-C4	-9.71	1.29	1.34
1	A	1507	A	N9-C4	-9.58	1.32	1.37

The worst 5 of 1826 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1505	G	C8-N9-C4	-16.48	99.81	106.40
1	A	117	G	N1-C6-O6	15.84	129.41	119.90
1	A	279	A	C5-N7-C8	-15.12	96.34	103.90
1	A	722	A	N1-C6-N6	14.64	127.39	118.60
1	A	948	C	C6-N1-C2	14.42	126.07	120.30

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	77	ALA	Peptide
3	C	166	GLU	Peptide
3	C	179	ARG	Peptide
5	E	20	GLN	Peptide
8	H	27	PRO	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	32646	0	16503	873	1
2	B	1900	0	1951	105	0
3	C	1612	0	1677	109	0
4	D	1703	0	1763	68	0
5	E	1146	0	1207	71	0
6	F	843	0	857	46	0
7	G	1257	0	1296	60	0
8	H	1116	0	1177	71	0
9	I	1010	0	1037	78	0
10	J	792	0	835	59	0
11	K	864	0	881	41	0
12	L	972	0	1058	59	0
13	M	937	0	995	52	0
14	N	492	0	529	47	0
15	O	729	0	768	41	0
16	P	700	0	720	41	0
17	Q	823	0	893	58	0
18	R	574	0	644	37	0
19	S	647	0	673	35	0
20	T	763	0	861	37	0
21	U	208	0	221	14	0
22	A	268	0	0	0	0
22	B	2	0	0	0	0
22	C	2	0	0	0	0
22	D	4	0	0	0	0
22	E	1	0	0	0	0
22	F	1	0	0	0	0
22	I	1	0	0	0	0
22	J	1	0	0	0	0
22	L	1	0	0	0	0
22	M	2	0	0	0	0
22	P	2	0	0	0	0
22	Q	2	0	0	0	0
22	T	2	0	0	0	0
23	D	1	0	0	0	0
23	N	1	0	0	0	0
24	A	391	0	0	6	0
24	B	1	0	0	2	0
24	D	3	0	0	0	0
24	E	4	0	0	0	0
24	G	2	0	0	1	0
24	J	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	K	1	0	0	0	0
24	M	3	0	0	1	0
24	N	4	0	0	1	0
24	P	4	0	0	3	0
24	T	1	0	0	1	0
All	All	52441	0	36546	1809	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 1809 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:967:5MC:H4'	9:I:128:ARG:HG3	1.33	1.06
1:A:75:G:N2	1:A:76:C:N3	2.07	1.02
1:A:949:A:N6	24:A:2225:HOH:O	1.90	1.02
1:A:1152:A:H5"	10:J:13:HIS:HB2	1.44	1.00
20:T:50:GLU:HA	20:T:100:ILE:HG13	1.47	0.95

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:C:O2'	1:A:1338:G:O2'[3_545]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	232/256 (91%)	195 (84%)	33 (14%)	4 (2%)	7 32
3	C	204/239 (85%)	172 (84%)	32 (16%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	206/209 (99%)	197 (96%)	9 (4%)	0	100 100
5	E	148/162 (91%)	137 (93%)	10 (7%)	1 (1%)	19 50
6	F	99/101 (98%)	93 (94%)	6 (6%)	0	100 100
7	G	153/156 (98%)	139 (91%)	13 (8%)	1 (1%)	19 50
8	H	136/138 (99%)	125 (92%)	11 (8%)	0	100 100
9	I	125/128 (98%)	109 (87%)	15 (12%)	1 (1%)	16 47
10	J	96/105 (91%)	82 (85%)	12 (12%)	2 (2%)	5 29
11	K	114/129 (88%)	104 (91%)	10 (9%)	0	100 100
12	L	121/135 (90%)	111 (92%)	8 (7%)	2 (2%)	7 32
13	M	116/126 (92%)	99 (85%)	17 (15%)	0	100 100
14	N	58/61 (95%)	51 (88%)	7 (12%)	0	100 100
15	O	85/89 (96%)	80 (94%)	4 (5%)	1 (1%)	11 39
16	P	81/88 (92%)	77 (95%)	4 (5%)	0	100 100
17	Q	97/105 (92%)	88 (91%)	9 (9%)	0	100 100
18	R	68/88 (77%)	59 (87%)	9 (13%)	0	100 100
19	S	78/93 (84%)	69 (88%)	7 (9%)	2 (3%)	4 25
20	T	97/106 (92%)	81 (84%)	14 (14%)	2 (2%)	5 29
21	U	22/27 (82%)	19 (86%)	3 (14%)	0	100 100
All	All	2336/2541 (92%)	2087 (89%)	233 (10%)	16 (1%)	19 50

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
7	G	155	ARG
19	S	31	ILE
9	I	119	ALA
10	J	86	MET

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%)	153 (76%)	49 (24%)	0 4
3	C	160/188 (85%)	120 (75%)	40 (25%)	0 3
4	D	180/181 (99%)	151 (84%)	29 (16%)	2 11
5	E	115/123 (94%)	84 (73%)	31 (27%)	0 2
6	F	90/90 (100%)	73 (81%)	17 (19%)	1 7
7	G	126/127 (99%)	100 (79%)	26 (21%)	1 6
8	H	119/119 (100%)	95 (80%)	24 (20%)	1 6
9	I	98/99 (99%)	75 (76%)	23 (24%)	0 4
10	J	87/92 (95%)	65 (75%)	22 (25%)	0 3
11	K	88/99 (89%)	77 (88%)	11 (12%)	3 17
12	L	103/110 (94%)	78 (76%)	25 (24%)	0 4
13	M	94/101 (93%)	81 (86%)	13 (14%)	3 15
14	N	49/50 (98%)	33 (67%)	16 (33%)	0 1
15	O	79/80 (99%)	59 (75%)	20 (25%)	0 3
16	P	72/74 (97%)	59 (82%)	13 (18%)	1 8
17	Q	94/97 (97%)	80 (85%)	14 (15%)	2 13
18	R	61/77 (79%)	50 (82%)	11 (18%)	1 8
19	S	71/80 (89%)	56 (79%)	15 (21%)	1 6
20	T	76/82 (93%)	63 (83%)	13 (17%)	1 10
21	U	19/22 (86%)	17 (90%)	2 (10%)	5 23
All	All	1983/2111 (94%)	1569 (79%)	414 (21%)	1 6

5 of 414 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	92	TYR
12	L	52	LEU
20	T	19	SER
9	I	127	LYS
10	J	88	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	14	HIS
15	O	46	HIS
10	J	62	HIS
10	J	56	HIS
11	K	26	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1504/1522 (98%)	402 (26%)	50 (3%)

5 of 402 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	913	A
1	A	1067	A
1	A	1505	G
1	A	960	U
1	A	992	U

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

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	2MG	A	1207	1	18,26,27	1.54	4 (22%)	16,38,41	1.31	2 (12%)
1	PSU	A	1540	1	18,21,22	1.10	1 (5%)	21,30,33	1.72	4 (19%)
1	UR3	A	1498	1,22	19,22,23	1.41	3 (15%)	26,32,35	1.31	1 (3%)
1	MA6	A	1519[A]	1	19,26,27	1.04	1 (5%)	18,38,41	1.03	2 (11%)
1	PSU	A	516	1,22	18,21,22	1.24	2 (11%)	21,30,33	2.09	6 (28%)
1	7MG	A	527	1	23,26,27	3.47	4 (17%)	27,39,42	2.26	9 (33%)
1	M2G	A	966	1	20,27,28	1.51	4 (20%)	19,40,43	1.73	3 (15%)
1	5MC	A	1400	1	19,22,23	1.87	4 (21%)	26,32,35	1.27	4 (15%)
1	5MC	A	967	1	19,22,23	0.91	1 (5%)	26,32,35	1.07	2 (7%)
1	5MC	A	1404	1	19,22,23	1.33	2 (10%)	26,32,35	1.11	3 (11%)
1	5MC	A	1407	1	19,22,23	1.47	4 (21%)	26,32,35	0.98	1 (3%)
1	MA6	A	1518[A]	1	19,26,27	0.79	0	18,38,41	0.97	2 (11%)
12	0TD	L	92	12	8,9,10	1.36	0	6,11,13	2.64	3 (50%)
1	MA6	A	1519[B]	1	19,26,27	1.42	3 (15%)	18,38,41	0.67	0
1	MA6	A	1518[B]	1	19,26,27	1.43	3 (15%)	18,38,41	0.70	0
1	PSU	A	1541	1	18,21,22	1.17	1 (5%)	21,30,33	1.69	3 (14%)
1	4OC	A	1402	1	20,23,24	1.54	4 (20%)	25,32,35	0.87	0

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	-	2/5/27/28	0/3/3/3
1	PSU	A	1540	1	-	1/7/25/26	0/2/2/2
1	UR3	A	1498	1,22	-	2/7/25/26	0/2/2/2
1	MA6	A	1519[A]	1	-	2/7/29/30	0/3/3/3
1	PSU	A	516	1,22	-	0/7/25/26	0/2/2/2
1	7MG	A	527	1	-	2/7/37/38	0/3/3/3
1	M2G	A	966	1	-	4/7/29/30	0/3/3/3
1	5MC	A	1400	1	-	2/7/25/26	0/2/2/2
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1404	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518[A]	1	-	1/7/29/30	0/3/3/3
12	0TD	L	92	12	-	2/7/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519[B]	1	-	4/7/29/30	0/3/3/3
1	MA6	A	1518[B]	1	-	0/7/29/30	0/3/3/3
1	PSU	A	1541	1	-	0/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	3/9/29/30	0/2/2/2

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	7MG	C8-N9	-14.06	1.36	1.45
1	A	527	7MG	C5-N7	7.21	1.44	1.35
1	A	1400	5MC	C2-N1	5.01	1.50	1.40
1	A	966	M2G	C2-N3	4.48	1.37	1.30
1	A	1518[B]	MA6	C6-N1	4.45	1.38	1.32

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	M2G	O6-C6-N1	-5.75	113.80	120.62
1	A	516	PSU	N1-C2-N3	5.36	120.82	115.17
12	L	92	0TD	CSB-SB-CB	-5.06	93.27	102.36
1	A	516	PSU	C4-N3-C2	-4.89	119.64	126.37
1	A	527	7MG	C5-C6-N1	4.74	119.29	110.94

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	7MG	O4'-C4'-C5'-O5'
1	A	966	M2G	N1-C2-N2-CM1
1	A	966	M2G	N1-C2-N2-CM2
1	A	966	M2G	N3-C2-N2-CM1
1	A	966	M2G	N3-C2-N2-CM2

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1498	UR3	5	0
1	A	1519[A]	MA6	3	0
1	A	966	M2G	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1400	5MC	1	0
1	A	967	5MC	6	0
1	A	1404	5MC	1	0
1	A	1518[A]	MA6	2	0
12	L	92	0TD	2	0
1	A	1519[B]	MA6	2	0
1	A	1518[B]	MA6	3	0
1	A	1402	4OC	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 291 ligands modelled in this entry, 291 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1498/1522 (98%)	-0.52	23 (1%) 71 50	56, 156, 308, 384	4 (0%)
2	B	234/256 (91%)	-0.66	2 (0%) 81 61	105, 165, 249, 269	0
3	C	206/239 (86%)	-0.34	2 (0%) 79 59	164, 235, 290, 329	0
4	D	208/209 (99%)	-0.49	7 (3%) 48 31	99, 159, 211, 239	0
5	E	150/162 (92%)	-0.86	0 100 100	79, 122, 163, 194	0
6	F	101/101 (100%)	-0.69	0 100 100	130, 175, 208, 240	0
7	G	155/156 (99%)	-0.53	1 (0%) 85 69	150, 203, 268, 323	0
8	H	138/138 (100%)	-0.82	0 100 100	74, 108, 152, 181	0
9	I	127/128 (99%)	-0.27	2 (1%) 70 49	173, 226, 272, 298	0
10	J	98/105 (93%)	-0.26	0 100 100	194, 237, 302, 326	0
11	K	116/129 (89%)	-0.72	0 100 100	111, 146, 197, 222	0
12	L	123/135 (91%)	-0.54	1 (0%) 82 64	79, 155, 195, 227	0
13	M	118/126 (93%)	-0.44	1 (0%) 82 64	139, 190, 229, 290	0
14	N	60/61 (98%)	-0.11	1 (1%) 69 47	185, 222, 274, 306	0
15	O	87/89 (97%)	-0.79	0 100 100	92, 132, 179, 209	0
16	P	83/88 (94%)	-0.55	0 100 100	110, 146, 187, 230	0
17	Q	99/105 (94%)	-0.72	0 100 100	95, 125, 176, 185	0
18	R	70/88 (79%)	-0.70	0 100 100	107, 145, 200, 231	0
19	S	80/93 (86%)	-0.13	3 (3%) 44 29	197, 254, 313, 320	0
20	T	99/106 (93%)	-0.44	2 (2%) 64 44	112, 149, 204, 232	0
21	U	24/27 (88%)	0.36	3 (12%) 9 8	169, 204, 229, 238	0
All	All	3874/4063 (95%)	-0.53	48 (1%) 76 54	56, 166, 278, 384	4 (0%)

The worst 5 of 48 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	985	C	6.2
20	T	106	ALA	5.5
1	A	1204	A	3.8
4	D	31	CYS	3.8
9	I	9	ARG	3.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
1	PSU	A	1541	20/21	0.89	0.10	223,263,279,284	0
1	PSU	A	1540	20/21	0.91	0.09	271,280,285,287	0
1	5MC	A	967	21/22	0.95	0.06	162,170,190,199	0
1	PSU	A	516	20/21	0.95	0.06	162,181,197,197	0
1	M2G	A	966	25/26	0.95	0.07	165,177,184,186	0
1	5MC	A	1400	21/22	0.96	0.07	114,142,154,174	0
1	4OC	A	1402	22/23	0.96	0.13	124,137,170,187	0
1	7MG	A	527	24/25	0.96	0.08	116,135,155,161	0
1	2MG	A	1207	24/25	0.96	0.12	263,291,297,309	0
1	MA6	A	1518[A]	24/25	0.97	0.14	118,131,141,143	24
1	MA6	A	1518[B]	24/25	0.97	0.14	126,135,138,138	24
1	5MC	A	1407	21/22	0.97	0.07	149,172,180,188	0
1	UR3	A	1498	21/22	0.97	0.10	117,143,151,155	0
12	0TD	L	92	10/11	0.97	0.08	157,170,178,331	0
1	5MC	A	1404	21/22	0.98	0.09	112,135,164,183	0
1	MA6	A	1519[B]	24/25	0.99	0.10	106,118,129,130	24
1	MA6	A	1519[A]	24/25	0.99	0.10	109,115,125,137	24

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
22	MG	B	301	1/1	0.42	0.24	154,154,154,154	0
22	MG	A	1672	1/1	0.52	0.52	130,130,130,130	0
22	MG	A	1779	1/1	0.58	0.09	159,159,159,159	0
22	MG	M	202	1/1	0.60	0.11	122,122,122,122	0
22	MG	A	1626	1/1	0.64	0.31	150,150,150,150	0
22	MG	A	1776	1/1	0.73	0.14	129,129,129,129	0
22	MG	A	1679	1/1	0.73	0.23	177,177,177,177	0
22	MG	A	1751	1/1	0.74	0.50	136,136,136,136	0
22	MG	A	1840	1/1	0.75	0.16	149,149,149,149	0
22	MG	A	1769	1/1	0.76	0.24	142,142,142,142	0
22	MG	A	1742	1/1	0.76	0.23	132,132,132,132	0
22	MG	A	1864	1/1	0.79	0.25	123,123,123,123	0
22	MG	A	1783	1/1	0.79	0.39	133,133,133,133	0
22	MG	A	1780	1/1	0.79	0.34	162,162,162,162	0
22	MG	A	1768	1/1	0.80	0.37	118,118,118,118	0
22	MG	A	1713	1/1	0.80	0.66	106,106,106,106	0
22	MG	A	1656	1/1	0.81	0.21	133,133,133,133	0
22	MG	A	1773	1/1	0.81	0.14	164,164,164,164	0
22	MG	A	1685	1/1	0.81	0.36	116,116,116,116	0
22	MG	A	1799	1/1	0.81	0.37	287,287,287,287	0
22	MG	A	1744	1/1	0.82	0.17	151,151,151,151	0
22	MG	A	1668	1/1	0.82	0.24	111,111,111,111	0
22	MG	A	1863	1/1	0.83	0.15	103,103,103,103	0
22	MG	A	1689	1/1	0.83	0.07	238,238,238,238	0
22	MG	A	1825	1/1	0.83	0.13	404,404,404,404	0
22	MG	A	1601	1/1	0.83	0.26	137,137,137,137	0
22	MG	A	1680	1/1	0.84	0.15	139,139,139,139	0
22	MG	A	1782	1/1	0.84	0.36	144,144,144,144	0
22	MG	A	1823	1/1	0.84	0.18	168,168,168,168	0
22	MG	A	1765	1/1	0.85	0.51	390,390,390,390	0
22	MG	A	1859	1/1	0.85	0.24	132,132,132,132	0
22	MG	C	301	1/1	0.85	0.20	150,150,150,150	0
22	MG	A	1618	1/1	0.85	0.35	125,125,125,125	0
22	MG	T	201	1/1	0.85	0.09	155,155,155,155	0
22	MG	A	1724	1/1	0.86	0.44	146,146,146,146	0
22	MG	A	1729	1/1	0.86	0.25	120,120,120,120	0
22	MG	A	1671	1/1	0.86	0.20	162,162,162,162	0
22	MG	A	1720	1/1	0.86	0.21	109,109,109,109	0
22	MG	A	1847	1/1	0.86	0.17	145,145,145,145	0
22	MG	A	1748	1/1	0.86	0.27	144,144,144,144	0
22	MG	A	1763	1/1	0.87	0.10	240,240,240,240	0
22	MG	A	1716	1/1	0.87	0.12	95,95,95,95	0
22	MG	A	1631	1/1	0.87	0.44	118,118,118,118	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1704	1/1	0.87	0.09	118,118,118,118	0
22	MG	A	1816	1/1	0.87	0.15	170,170,170,170	0
22	MG	A	1749	1/1	0.87	0.19	121,121,121,121	0
22	MG	A	1664	1/1	0.87	0.12	126,126,126,126	0
22	MG	A	1758	1/1	0.87	0.19	107,107,107,107	0
22	MG	A	1674	1/1	0.88	0.09	168,168,168,168	0
22	MG	A	1745	1/1	0.88	0.11	127,127,127,127	0
22	MG	A	1867	1/1	0.88	0.18	139,139,139,139	0
22	MG	A	1756	1/1	0.88	0.24	140,140,140,140	0
22	MG	A	1608	1/1	0.88	0.33	127,127,127,127	0
22	MG	D	304	1/1	0.88	0.15	106,106,106,106	0
22	MG	A	1771	1/1	0.88	0.24	158,158,158,158	0
22	MG	A	1760	1/1	0.88	0.15	137,137,137,137	0
22	MG	A	1846	1/1	0.89	0.08	131,131,131,131	0
22	MG	A	1607	1/1	0.89	0.08	165,165,165,165	0
22	MG	A	1853	1/1	0.89	0.05	91,91,91,91	0
22	MG	A	1726	1/1	0.89	0.53	106,106,106,106	0
22	MG	A	1677	1/1	0.89	0.35	125,125,125,125	0
22	MG	A	1788	1/1	0.89	0.10	330,330,330,330	0
22	MG	A	1735	1/1	0.89	0.48	114,114,114,114	0
22	MG	A	1813	1/1	0.89	0.12	210,210,210,210	0
22	MG	A	1692	1/1	0.89	0.10	167,167,167,167	0
22	MG	A	1717	1/1	0.89	1.16	146,146,146,146	0
22	MG	L	201	1/1	0.89	0.07	122,122,122,122	0
22	MG	A	1778	1/1	0.89	0.10	137,137,137,137	0
22	MG	Q	201	1/1	0.89	0.17	140,140,140,140	0
22	MG	A	1693	1/1	0.89	0.44	146,146,146,146	0
22	MG	A	1820	1/1	0.90	0.06	495,495,495,495	0
22	MG	A	1623	1/1	0.90	0.07	125,125,125,125	0
22	MG	A	1865	1/1	0.90	0.17	120,120,120,120	0
22	MG	A	1695	1/1	0.90	0.12	125,125,125,125	0
22	MG	A	1795	1/1	0.90	0.15	253,253,253,253	0
22	MG	A	1845	1/1	0.90	0.33	106,106,106,106	0
22	MG	A	1798	1/1	0.90	0.17	208,208,208,208	0
22	MG	A	1640	1/1	0.90	0.23	111,111,111,111	0
22	MG	A	1709	1/1	0.90	0.08	165,165,165,165	0
22	MG	A	1856	1/1	0.90	0.26	108,108,108,108	0
22	MG	A	1736	1/1	0.90	0.08	99,99,99,99	0
22	MG	A	1609	1/1	0.91	0.13	113,113,113,113	0
22	MG	A	1790	1/1	0.91	0.20	159,159,159,159	0
22	MG	A	1838	1/1	0.91	0.29	386,386,386,386	0
22	MG	A	1762	1/1	0.91	0.21	219,219,219,219	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1843	1/1	0.91	0.44	163,163,163,163	0
22	MG	A	1620	1/1	0.91	0.22	136,136,136,136	0
22	MG	A	1737	1/1	0.91	0.22	142,142,142,142	0
22	MG	D	305	1/1	0.91	0.23	122,122,122,122	0
22	MG	A	1801	1/1	0.91	0.22	152,152,152,152	0
22	MG	A	1739	1/1	0.91	0.08	126,126,126,126	0
22	MG	A	1667	1/1	0.91	0.16	274,274,274,274	0
22	MG	A	1655	1/1	0.91	0.16	141,141,141,141	0
22	MG	A	1603	1/1	0.92	0.14	111,111,111,111	0
22	MG	A	1691	1/1	0.92	0.18	136,136,136,136	0
22	MG	A	1644	1/1	0.92	0.09	253,253,253,253	0
22	MG	A	1678	1/1	0.92	0.18	143,143,143,143	0
22	MG	A	1722	1/1	0.92	0.29	129,129,129,129	0
22	MG	A	1792	1/1	0.92	0.12	398,398,398,398	0
22	MG	A	1635	1/1	0.92	0.25	151,151,151,151	0
22	MG	A	1703	1/1	0.92	0.10	138,138,138,138	0
22	MG	A	1639	1/1	0.92	0.15	173,173,173,173	0
22	MG	A	1753	1/1	0.92	0.21	169,169,169,169	0
22	MG	A	1659	1/1	0.92	0.29	95,95,95,95	0
22	MG	A	1710	1/1	0.92	0.15	162,162,162,162	0
22	MG	A	1777	1/1	0.93	0.06	93,93,93,93	0
22	MG	A	1803	1/1	0.93	0.17	147,147,147,147	0
22	MG	A	1805	1/1	0.93	0.45	153,153,153,153	0
22	MG	A	1636	1/1	0.93	0.43	112,112,112,112	0
22	MG	A	1621	1/1	0.93	0.08	118,118,118,118	0
22	MG	D	302	1/1	0.93	0.13	142,142,142,142	0
22	MG	D	303	1/1	0.93	0.13	141,141,141,141	0
22	MG	A	1687	1/1	0.93	0.07	151,151,151,151	0
22	MG	A	1849	1/1	0.93	0.45	123,123,123,123	0
22	MG	A	1774	1/1	0.93	0.53	134,134,134,134	0
22	MG	A	1752	1/1	0.93	0.14	90,90,90,90	0
22	MG	A	1827	1/1	0.93	0.08	148,148,148,148	0
22	MG	Q	202	1/1	0.93	0.09	105,105,105,105	0
22	MG	A	1829	1/1	0.93	0.35	286,286,286,286	0
22	MG	A	1730	1/1	0.94	0.12	107,107,107,107	0
22	MG	A	1854	1/1	0.94	0.06	94,94,94,94	0
22	MG	A	1855	1/1	0.94	0.18	139,139,139,139	0
22	MG	A	1731	1/1	0.94	0.17	103,103,103,103	0
22	MG	A	1857	1/1	0.94	0.09	115,115,115,115	0
22	MG	A	1858	1/1	0.94	0.20	90,90,90,90	0
22	MG	A	1732	1/1	0.94	0.23	134,134,134,134	0
22	MG	A	1860	1/1	0.94	0.13	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1755	1/1	0.94	0.17	131,131,131,131	0
22	MG	A	1697	1/1	0.94	0.11	139,139,139,139	0
22	MG	A	1682	1/1	0.94	0.13	137,137,137,137	0
22	MG	A	1661	1/1	0.94	0.14	148,148,148,148	0
22	MG	A	1721	1/1	0.94	0.11	128,128,128,128	0
22	MG	B	302	1/1	0.94	0.08	166,166,166,166	0
22	MG	A	1828	1/1	0.94	0.23	156,156,156,156	0
22	MG	A	1787	1/1	0.94	0.19	140,140,140,140	0
22	MG	A	1653	1/1	0.94	0.05	118,118,118,118	0
22	MG	A	1743	1/1	0.94	0.40	135,135,135,135	0
22	MG	A	1766	1/1	0.94	0.17	282,282,282,282	0
22	MG	E	201	1/1	0.94	0.10	152,152,152,152	0
22	MG	I	201	1/1	0.94	0.34	143,143,143,143	0
22	MG	J	201	1/1	0.94	0.08	497,497,497,497	0
22	MG	A	1665	1/1	0.94	0.13	117,117,117,117	0
22	MG	A	1696	1/1	0.94	0.07	193,193,193,193	0
22	MG	A	1727	1/1	0.94	0.19	178,178,178,178	0
22	MG	A	1714	1/1	0.94	0.21	116,116,116,116	0
22	MG	A	1851	1/1	0.94	0.14	126,126,126,126	0
22	MG	A	1746	1/1	0.95	0.46	126,126,126,126	0
22	MG	A	1811	1/1	0.95	0.24	242,242,242,242	0
22	MG	A	1733	1/1	0.95	0.12	91,91,91,91	0
22	MG	A	1764	1/1	0.95	0.12	290,290,290,290	0
22	MG	A	1819	1/1	0.95	0.42	141,141,141,141	0
22	MG	A	1701	1/1	0.95	0.19	216,216,216,216	0
22	MG	A	1861	1/1	0.95	0.11	135,135,135,135	0
22	MG	A	1784	1/1	0.95	0.20	318,318,318,318	0
22	MG	A	1711	1/1	0.95	0.16	85,85,85,85	0
22	MG	A	1688	1/1	0.95	0.29	113,113,113,113	0
22	MG	A	1646	1/1	0.95	0.38	143,143,143,143	0
22	MG	A	1791	1/1	0.95	0.10	160,160,160,160	0
22	MG	A	1830	1/1	0.95	0.10	199,199,199,199	0
22	MG	A	1836	1/1	0.95	0.20	231,231,231,231	0
22	MG	A	1754	1/1	0.95	0.09	107,107,107,107	0
22	MG	A	1794	1/1	0.95	0.25	422,422,422,422	0
22	MG	A	1705	1/1	0.95	0.11	118,118,118,118	0
22	MG	A	1797	1/1	0.95	0.47	367,367,367,367	0
22	MG	A	1707	1/1	0.95	0.39	120,120,120,120	0
22	MG	F	201	1/1	0.95	0.09	149,149,149,149	0
22	MG	A	1708	1/1	0.95	0.12	113,113,113,113	0
22	MG	A	1800	1/1	0.95	0.10	389,389,389,389	0
22	MG	A	1850	1/1	0.95	0.06	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1698	1/1	0.95	0.18	192,192,192,192	0
22	MG	P	101	1/1	0.95	0.16	90,90,90,90	0
22	MG	P	102	1/1	0.95	0.08	128,128,128,128	0
22	MG	A	1852	1/1	0.95	0.44	121,121,121,121	0
22	MG	A	1761	1/1	0.95	0.30	156,156,156,156	0
22	MG	A	1804	1/1	0.95	0.29	305,305,305,305	0
22	MG	T	202	1/1	0.95	0.46	96,96,96,96	0
22	MG	A	1652	1/1	0.96	0.13	126,126,126,126	0
22	MG	A	1817	1/1	0.96	0.19	297,297,297,297	0
22	MG	A	1818	1/1	0.96	0.34	247,247,247,247	0
22	MG	A	1605	1/1	0.96	0.12	102,102,102,102	0
22	MG	A	1666	1/1	0.96	0.17	147,147,147,147	0
22	MG	A	1862	1/1	0.96	0.11	99,99,99,99	0
22	MG	A	1785	1/1	0.96	0.20	394,394,394,394	0
22	MG	A	1786	1/1	0.96	0.13	234,234,234,234	0
22	MG	A	1654	1/1	0.96	0.05	117,117,117,117	0
22	MG	A	1747	1/1	0.96	0.11	137,137,137,137	0
22	MG	A	1612	1/1	0.96	0.04	136,136,136,136	0
22	MG	A	1686	1/1	0.96	0.14	124,124,124,124	0
22	MG	A	1833	1/1	0.96	0.06	450,450,450,450	0
22	MG	A	1767	1/1	0.96	0.09	184,184,184,184	0
22	MG	A	1750	1/1	0.96	0.08	128,128,128,128	0
22	MG	A	1616	1/1	0.96	0.11	79,79,79,79	0
22	MG	A	1841	1/1	0.96	0.14	175,175,175,175	0
22	MG	A	1796	1/1	0.96	0.20	383,383,383,383	0
22	MG	A	1770	1/1	0.96	0.58	166,166,166,166	0
22	MG	A	1602	1/1	0.96	0.18	168,168,168,168	0
22	MG	A	1673	1/1	0.96	0.23	130,130,130,130	0
22	MG	A	1604	1/1	0.96	0.17	141,141,141,141	0
22	MG	M	201	1/1	0.96	0.19	388,388,388,388	0
22	MG	A	1775	1/1	0.96	0.10	101,101,101,101	0
22	MG	A	1663	1/1	0.96	0.18	148,148,148,148	0
22	MG	A	1741	1/1	0.96	0.20	111,111,111,111	0
22	MG	A	1757	1/1	0.96	0.12	123,123,123,123	0
22	MG	A	1807	1/1	0.96	0.11	141,141,141,141	0
22	MG	A	1725	1/1	0.96	0.06	142,142,142,142	0
22	MG	A	1759	1/1	0.96	0.28	98,98,98,98	0
23	ZN	N	101	1/1	0.96	0.06	395,395,395,395	0
22	MG	A	1719	1/1	0.97	0.17	143,143,143,143	0
22	MG	A	1835	1/1	0.97	0.21	317,317,317,317	0
22	MG	A	1738	1/1	0.97	0.35	102,102,102,102	0
22	MG	A	1619	1/1	0.97	0.08	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1868	1/1	0.97	0.18	139,139,139,139	0
22	MG	A	1702	1/1	0.97	0.15	322,322,322,322	0
22	MG	A	1648	1/1	0.97	0.13	82,82,82,82	0
22	MG	A	1650	1/1	0.97	0.13	118,118,118,118	0
22	MG	A	1781	1/1	0.97	0.38	116,116,116,116	0
22	MG	A	1627	1/1	0.97	0.07	96,96,96,96	0
22	MG	A	1628	1/1	0.97	0.10	69,69,69,69	0
22	MG	A	1848	1/1	0.97	0.10	166,166,166,166	0
22	MG	A	1629	1/1	0.97	0.19	106,106,106,106	0
22	MG	A	1728	1/1	0.97	0.09	129,129,129,129	0
22	MG	A	1814	1/1	0.97	0.21	224,224,224,224	0
22	MG	A	1641	1/1	0.97	0.07	78,78,78,78	0
22	MG	A	1694	1/1	0.97	0.10	376,376,376,376	0
22	MG	A	1613	1/1	0.97	0.13	117,117,117,117	0
22	MG	A	1789	1/1	0.97	0.25	174,174,174,174	0
22	MG	A	1681	1/1	0.97	0.06	162,162,162,162	0
22	MG	A	1669	1/1	0.97	0.14	145,145,145,145	0
22	MG	A	1734	1/1	0.97	0.35	99,99,99,99	0
22	MG	A	1793	1/1	0.97	0.06	182,182,182,182	0
22	MG	A	1772	1/1	0.97	0.19	126,126,126,126	0
22	MG	A	1670	1/1	0.97	0.06	129,129,129,129	0
22	MG	A	1700	1/1	0.97	0.28	438,438,438,438	0
22	MG	A	1610	1/1	0.98	0.11	110,110,110,110	0
22	MG	A	1683	1/1	0.98	0.12	237,237,237,237	0
22	MG	A	1649	1/1	0.98	0.11	145,145,145,145	0
22	MG	A	1611	1/1	0.98	0.04	182,182,182,182	0
22	MG	A	1637	1/1	0.98	0.06	329,329,329,329	0
22	MG	A	1821	1/1	0.98	0.21	399,399,399,399	0
22	MG	A	1706	1/1	0.98	0.10	151,151,151,151	0
22	MG	A	1638	1/1	0.98	0.08	124,124,124,124	0
22	MG	A	1826	1/1	0.98	0.21	447,447,447,447	0
22	MG	A	1617	1/1	0.98	0.04	97,97,97,97	0
22	MG	A	1690	1/1	0.98	0.07	160,160,160,160	0
22	MG	A	1606	1/1	0.98	0.07	114,114,114,114	0
22	MG	A	1866	1/1	0.98	0.18	149,149,149,149	0
22	MG	A	1624	1/1	0.98	0.24	68,68,68,68	0
22	MG	A	1831	1/1	0.98	0.08	191,191,191,191	0
22	MG	A	1832	1/1	0.98	0.20	364,364,364,364	0
22	MG	A	1712	1/1	0.98	0.23	103,103,103,103	0
22	MG	A	1834	1/1	0.98	0.18	232,232,232,232	0
22	MG	C	302	1/1	0.98	0.07	163,163,163,163	0
22	MG	A	1643	1/1	0.98	0.13	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	MG	A	1675	1/1	0.98	0.14	275,275,275,275	0
22	MG	A	1837	1/1	0.98	0.17	226,226,226,226	0
22	MG	A	1802	1/1	0.98	0.11	137,137,137,137	0
22	MG	A	1839	1/1	0.98	0.34	318,318,318,318	0
22	MG	A	1715	1/1	0.98	0.07	148,148,148,148	0
22	MG	A	1633	1/1	0.98	0.03	105,105,105,105	0
22	MG	A	1662	1/1	0.98	0.08	144,144,144,144	0
22	MG	A	1844	1/1	0.98	0.15	276,276,276,276	0
22	MG	A	1806	1/1	0.98	0.20	408,408,408,408	0
22	MG	A	1645	1/1	0.98	0.13	132,132,132,132	0
22	MG	A	1808	1/1	0.98	0.08	278,278,278,278	0
22	MG	A	1809	1/1	0.98	0.08	330,330,330,330	0
22	MG	A	1810	1/1	0.98	0.02	122,122,122,122	0
22	MG	A	1634	1/1	0.98	0.10	73,73,73,73	0
22	MG	A	1699	1/1	0.98	0.06	117,117,117,117	0
22	MG	A	1647	1/1	0.98	0.10	110,110,110,110	0
22	MG	A	1815	1/1	0.98	0.06	197,197,197,197	0
22	MG	A	1615	1/1	0.99	0.05	86,86,86,86	0
22	MG	A	1625	1/1	0.99	0.30	214,214,214,214	0
22	MG	A	1658	1/1	0.99	0.08	123,123,123,123	0
22	MG	A	1642	1/1	0.99	0.12	176,176,176,176	0
22	MG	A	1822	1/1	0.99	0.32	333,333,333,333	0
22	MG	A	1660	1/1	0.99	0.04	129,129,129,129	0
22	MG	A	1824	1/1	0.99	0.29	435,435,435,435	0
22	MG	A	1718	1/1	0.99	0.10	96,96,96,96	0
22	MG	A	1630	1/1	0.99	0.09	129,129,129,129	0
22	MG	A	1651	1/1	0.99	0.08	173,173,173,173	0
22	MG	A	1684	1/1	0.99	0.18	128,128,128,128	0
22	MG	A	1622	1/1	0.99	0.05	75,75,75,75	0
22	MG	A	1812	1/1	0.99	0.13	365,365,365,365	0
22	MG	A	1723	1/1	0.99	0.03	122,122,122,122	0
22	MG	A	1632	1/1	0.99	0.08	231,231,231,231	0
22	MG	A	1614	1/1	0.99	0.06	152,152,152,152	0
22	MG	A	1740	1/1	0.99	0.11	107,107,107,107	0
23	ZN	D	301	1/1	0.99	0.20	127,127,127,127	0
22	MG	A	1676	1/1	0.99	0.13	136,136,136,136	0
22	MG	A	1842	1/1	1.00	0.24	244,244,244,244	0
22	MG	A	1657	1/1	1.00	0.06	124,124,124,124	0

6.5 Other polymers (i)

There are no such residues in this entry.