wwPDB X-ray Structure Validation Summary Report (i)

Feb 20, 2016 – 12:20 AM GMT

PDB ID	:	5DM6
Title	:	Crystal structure of the 50S ribosomal subunit from Deinococcus radiodurans
Authors	:	Kaminishi, T.; Schedlbauer, A.; Ochoa-Lizarralde, B.; Connell, S.R.; Fucini, P.
Deposited on	:	2015-09-08
Resolution	:	2.90 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
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:

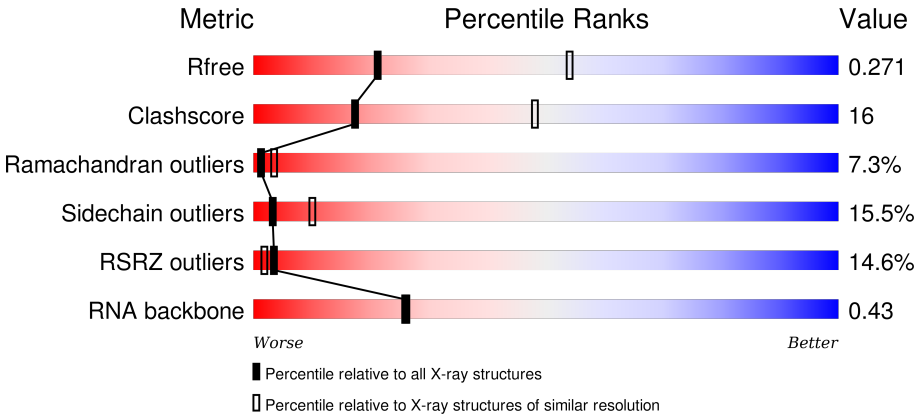
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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	0	224	89% 54% 38% 8%
2	A	274	11% 58% 37% 5%
3	B	205	3% 53% 40% 7%
4	C	197	8% 44% 46% 10%

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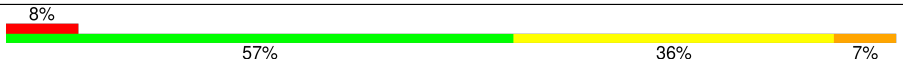
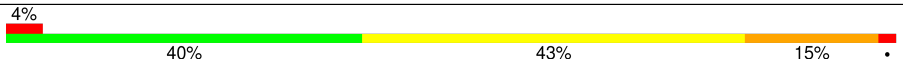
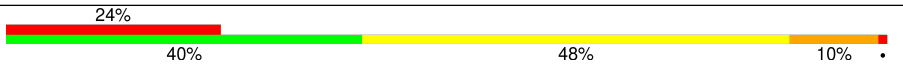
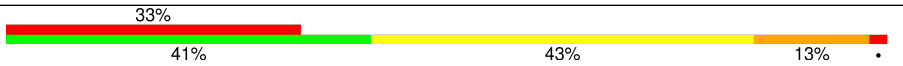
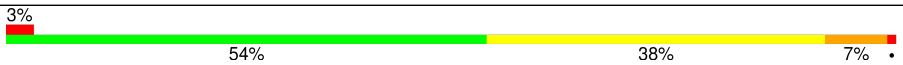
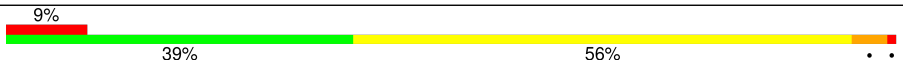
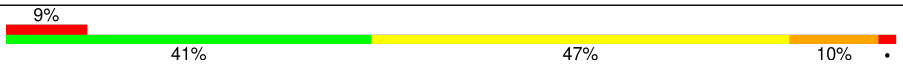
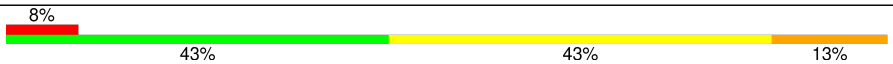
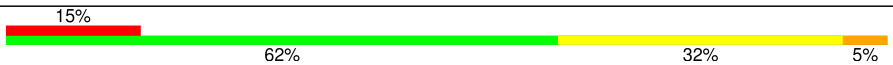
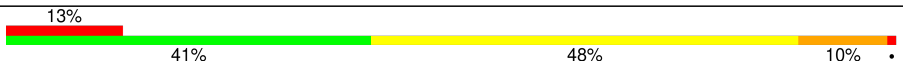
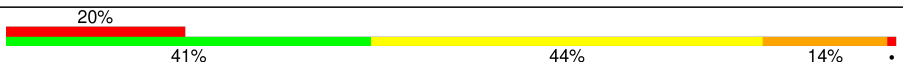
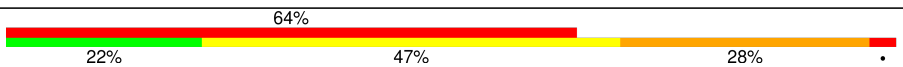
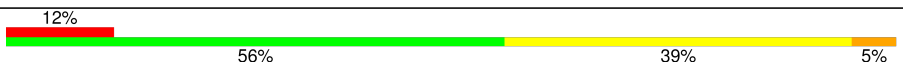
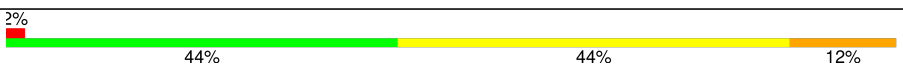
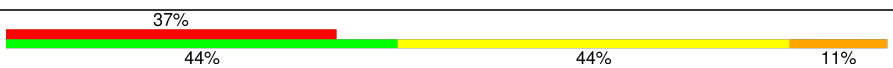
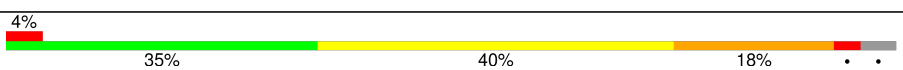
Mol	Chain	Length	Quality of chain
5	D	177	
6	E	171	
7	F	144	
8	G	142	
9	H	134	
10	I	141	
11	J	136	
12	K	113	
13	L	104	
14	M	109	
15	N	117	
16	O	94	
17	P	127	
18	Q	93	
19	R	110	
20	S	175	
21	T	84	
22	U	72	
23	V	66	
24	W	55	
25	Z	57	
26	1	54	
27	2	47	
28	3	65	
29	X	2881	

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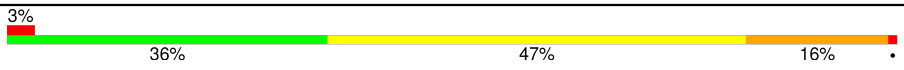
Mol	Chain	Length	Quality of chain
30	Y	122	

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
31	MG	X	6001	-	-	-	X
31	MG	X	6002	-	-	-	X
31	MG	X	6004	-	-	-	X
31	MG	X	6006	-	-	-	X
31	MG	X	6007	-	-	-	X
31	MG	X	6008	-	-	-	X
31	MG	X	6011	-	-	-	X
31	MG	X	6013	-	-	-	X
31	MG	X	6014	-	-	-	X
31	MG	X	6016	-	-	-	X
31	MG	X	6017	-	-	-	X
31	MG	X	6018	-	-	-	X
31	MG	X	6019	-	-	-	X
31	MG	X	6020	-	-	-	X
31	MG	X	6022	-	-	-	X
31	MG	X	6023	-	-	-	X
31	MG	X	6024	-	-	-	X
31	MG	X	6035	-	-	-	X
31	MG	X	6036	-	-	-	X
31	MG	X	6040	-	-	-	X
31	MG	X	6041	-	-	-	X
31	MG	X	6051	-	-	-	X
31	MG	X	6054	-	-	-	X
31	MG	X	6056	-	-	-	X
31	MG	X	6057	-	-	-	X
31	MG	X	6058	-	-	-	X
31	MG	X	6059	-	-	-	X
31	MG	X	6060	-	-	-	X
31	MG	X	6062	-	-	-	X
31	MG	X	6063	-	-	-	X
31	MG	X	6066	-	-	-	X
31	MG	X	6070	-	-	-	X
31	MG	X	6071	-	-	-	X
31	MG	X	6072	-	-	-	X
31	MG	X	6078	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	MG	X	6084	-	-	-	X
31	MG	X	6091	-	-	-	X
31	MG	X	6092	-	-	-	X
31	MG	X	6093	-	-	-	X
31	MG	X	6112	-	-	-	X
31	MG	X	6117	-	-	-	X
31	MG	X	6118	-	-	-	X
31	MG	X	6121	-	-	-	X
31	MG	X	6125	-	-	-	X
31	MG	X	6135	-	-	-	X
31	MG	X	6140	-	-	-	X
31	MG	X	6142	-	-	-	X
31	MG	X	6147	-	-	-	X
31	MG	X	6151	-	-	-	X
31	MG	X	6158	-	-	-	X
31	MG	X	6169	-	-	-	X
31	MG	X	6180	-	-	-	X
31	MG	X	6185	-	-	-	X

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 89337 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	224	Total	C	N	O	S	0	0	0
			1651	1031	302	313	5			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	274	Total	C	N	O	S	0	0	0
			2107	1313	423	368	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	LYS	ARG	conflict	UNP Q9RXJ9
A	25	ALA	THR	conflict	UNP Q9RXJ9
A	270	LEU	ILE	conflict	UNP Q9RXJ9

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	205	Total	C	N	O	S	0	0	0
			1540	965	295	272	8			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	197	Total	C	N	O	S	0	0	0
			1507	935	287	283	2			

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	177	Total	C	N	O	S	0	0	0
			1401	892	247	255	7			

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	171	Total	C	N	O	S	0	0	0
			1287	812	237	237	1			

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	144	Total	C	N	O	S	0	0	0
			1048	663	183	197	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	expression tag	UNP Q9RSS7
F	2	ARG	-	expression tag	UNP Q9RSS7
F	3	ARG	-	expression tag	UNP Q9RSS7

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	142	Total	C	N	O	S	0	0	0
			1115	704	209	199	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	134	Total	C	N	O	S	0	0	0
			997	614	198	180	5			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	141	Total	C	N	O	0	0	0
			1068	655	216	197			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	136	Total	C	N	O	S	0	0	0
			1091	696	202	186	7			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	113	Total	C	N	O	S	0	0	0
			879	541	178	158	2			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	104	Total	C	N	O	0	0	0
			778	476	159	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	26	LYS	ARG	conflict	UNP Q9RSL2

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	109	Total	C	N	O	0	0	0
			867	540	171	156			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	107	GLY	-	expression tag	UNP Q9RWB4
M	108	LYS	-	expression tag	UNP Q9RWB4
M	109	ALA	-	expression tag	UNP Q9RWB4
M	110	ALA	-	expression tag	UNP Q9RWB4

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	O	94	Total	C	N	O	0	0	0
			742	465	139	138			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	127	Total	C	N	O	S	0	0	0
			1014	639	199	174	2			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	93	Total	C	N	O	S	0	0	0
			727	458	136	131	2			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	110	Total	C	N	O	S	0	0	0
			826	513	160	152	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	175	Total	C	N	O	S	0	0	0
			1346	849	236	255	6			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	84	Total	C	N	O	S	0	0	0
			626	393	122	110	1			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	72	Total	C	N	O	0	0	0
			553	341	116	96			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U	67	ILE	LEU	conflict	UNP Q9RRG8

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	66	Total	C	N	O	S	0	0	0
			534	327	107	97	3			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	55	Total	C	N	O	S	0	0	0
			424	264	82	76	2			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	57	Total	C	N	O	S	0	0	0
			453	278	93	77	5			

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	1	54	Total	C	N	O	S	0	0	0
			404	256	73	74	1			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	2	47	Total	C	N	O	S	0	0	0
			393	235	92	64	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	3	65	Total	C	N	O	S	0	0	0
			509	320	104	80	5			

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	X	2780	Total	C	N	O	P	0	0	0
			59673	26617	11011	19265	2780			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1510	U	UNK	conflict	GB 11612676

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Y	122	Total	C	N	O	P	0	0	0
			2601	1161	476	842	122			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

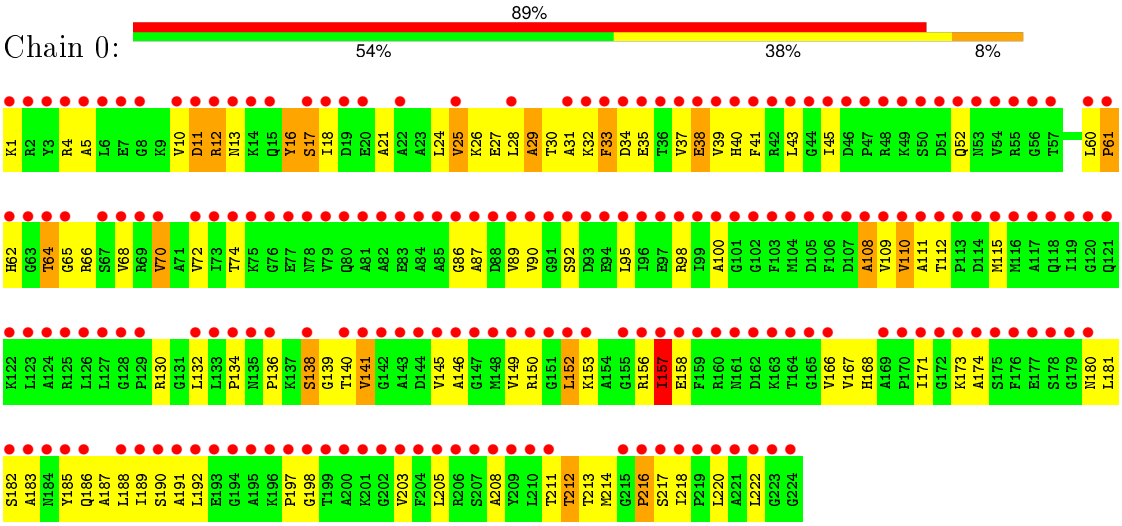
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	X	192	Total	Mg	0	0
			192	192		
31	Y	5	Total	Mg	0	0
			5	5		
31	M	1	Total	Mg	0	0
			1	1		

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.

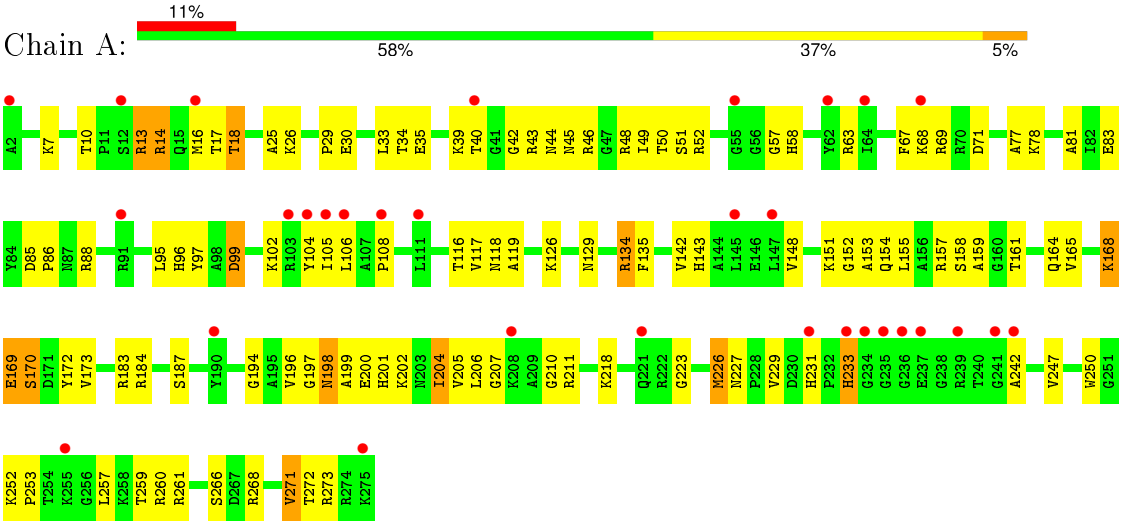
- Molecule 1: 50S ribosomal protein L1

Chain 0:



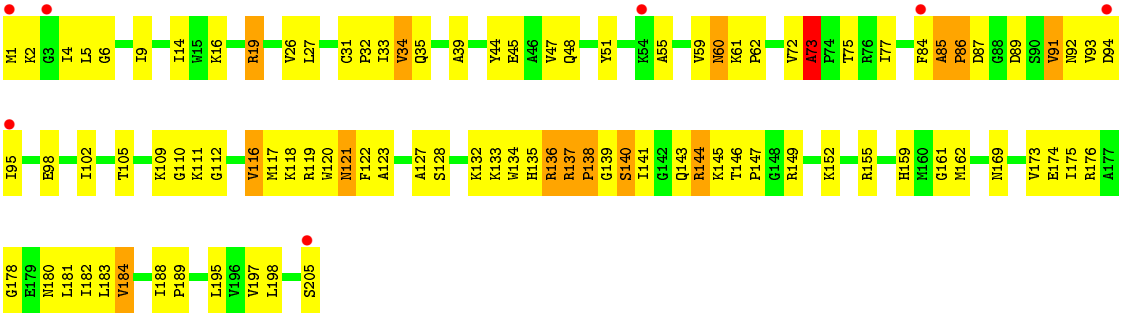
- Molecule 2: 50S ribosomal protein L2

Chain A:



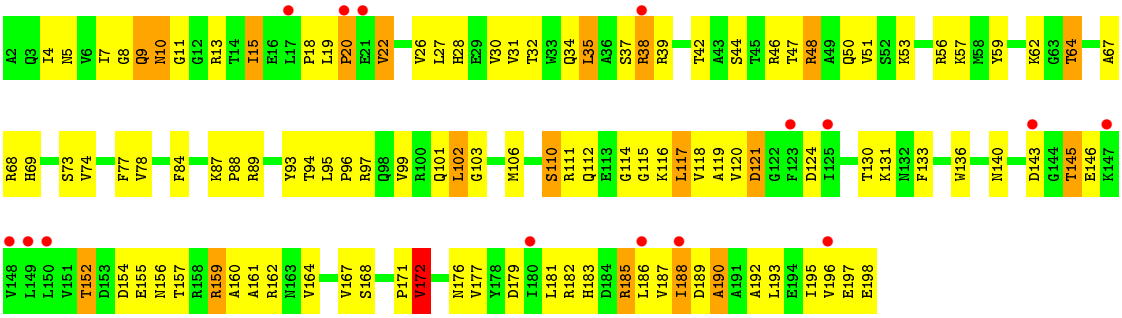
- Molecule 3: 50S ribosomal protein L3

Chain B:



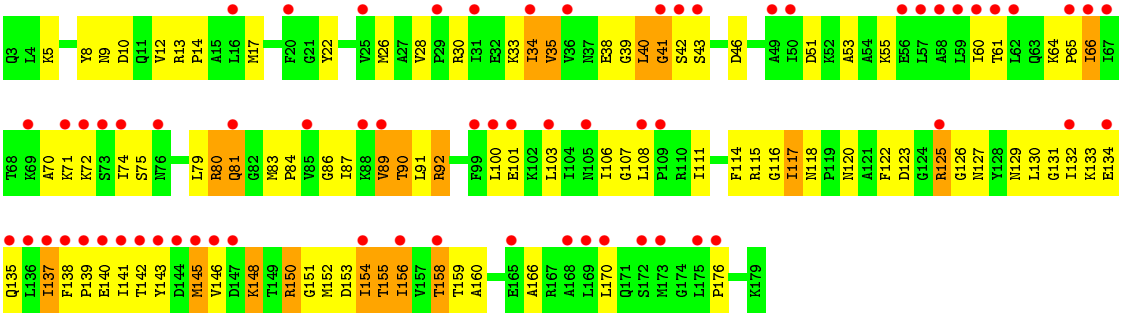
• Molecule 4: 50S ribosomal protein L4

Chain C:



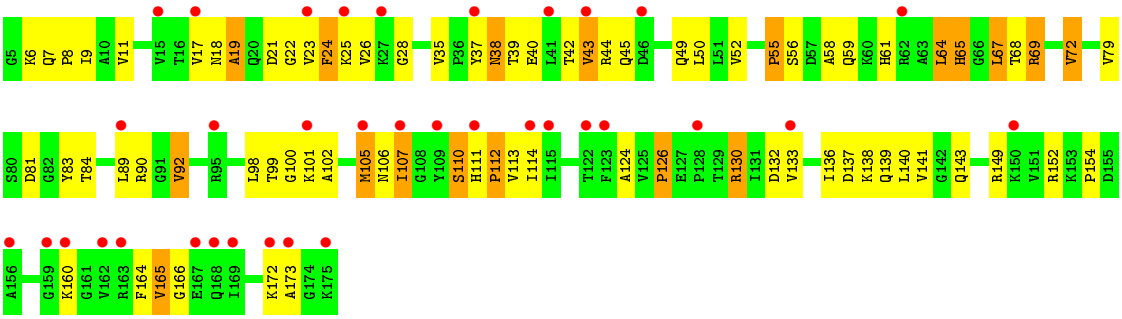
• Molecule 5: 50S ribosomal protein L5

Chain D:



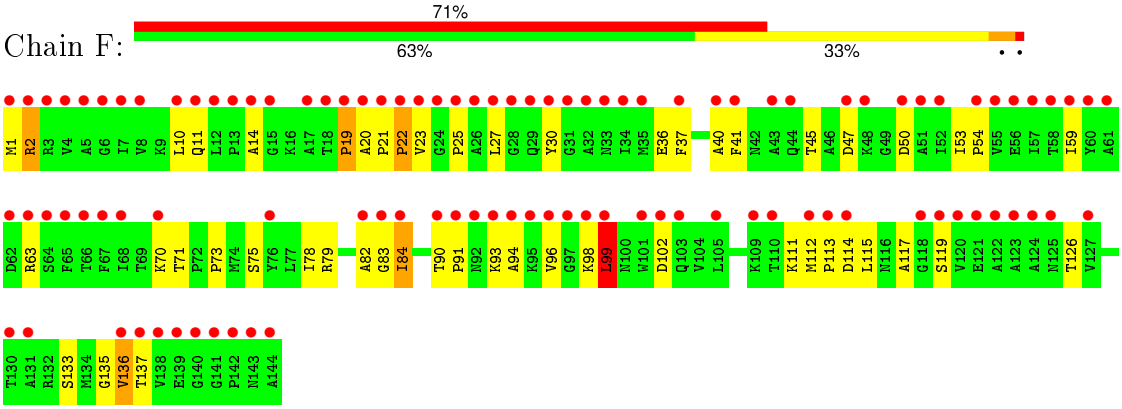
• Molecule 6: 50S ribosomal protein L6

Chain E:



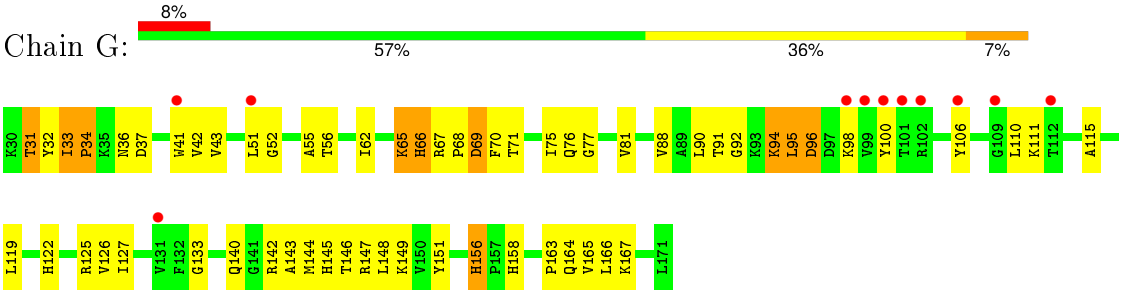
- Molecule 7: 50S ribosomal protein L11

Chain F:



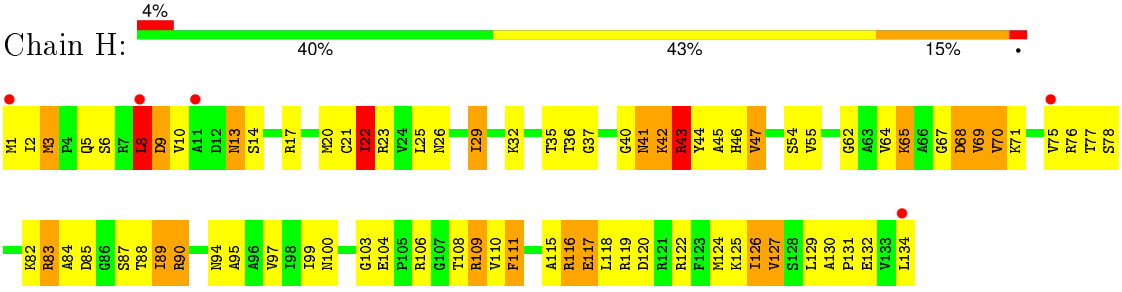
- Molecule 8: 50S ribosomal protein L13

Chain G:



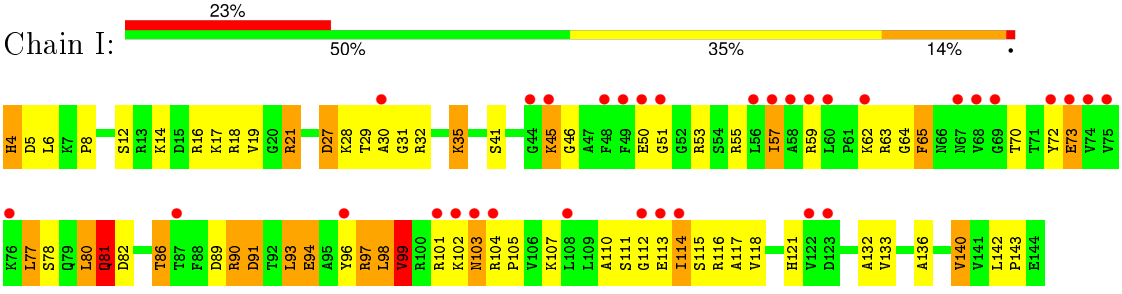
- Molecule 9: 50S ribosomal protein L14

Chain H:



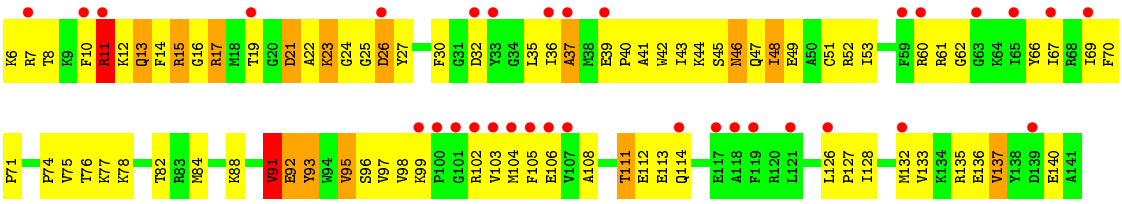
- Molecule 10: 50S ribosomal protein L15

Chain I:



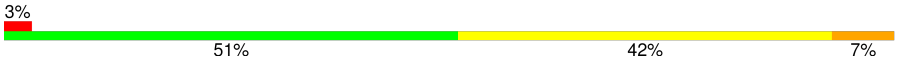
- Molecule 11: 50S ribosomal protein L16

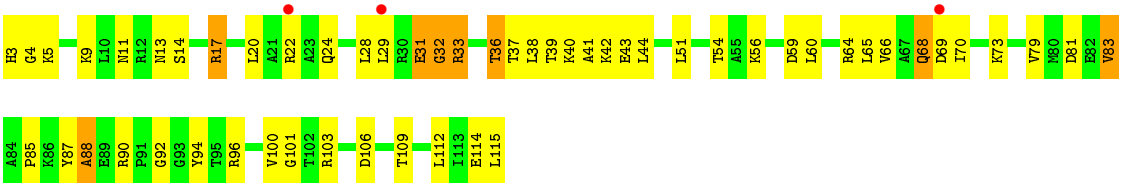
Chain J:



• Molecule 12: 50S ribosomal protein L17

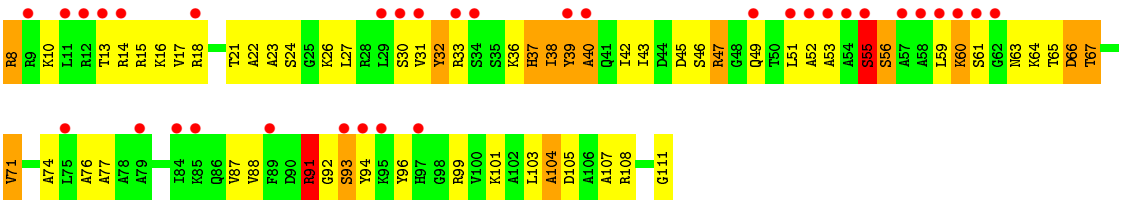
Chain K:





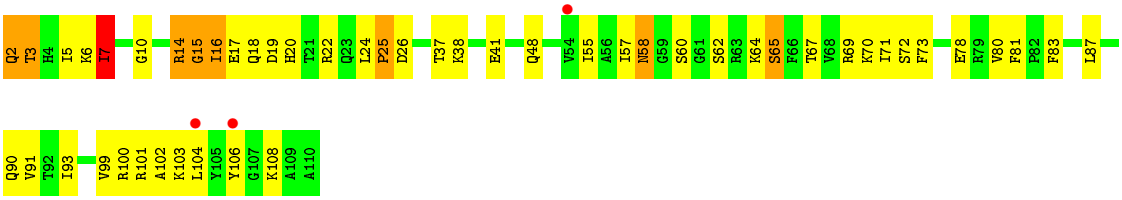
• Molecule 13: 50S ribosomal protein L18

Chain L:



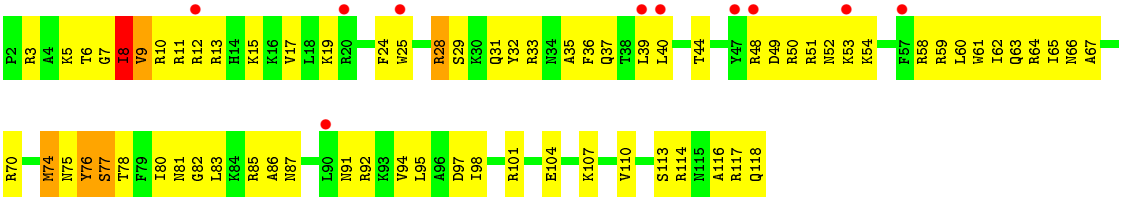
• Molecule 14: 50S ribosomal protein L19

Chain M:



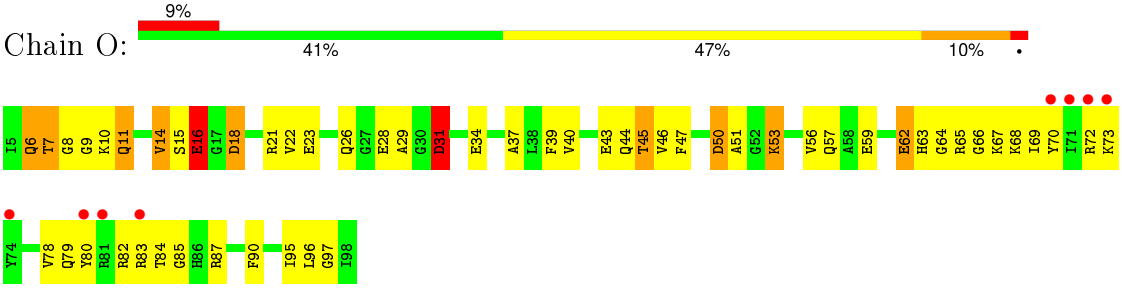
• Molecule 15: 50S ribosomal protein L20

Chain N:



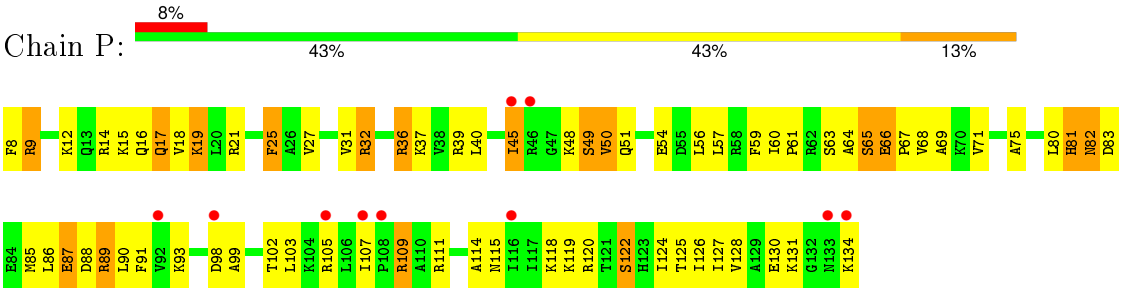
• Molecule 16: 50S ribosomal protein L21

Chain O:



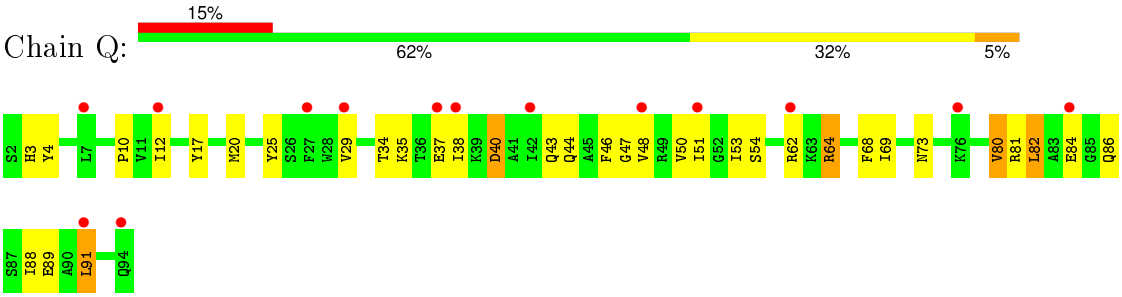
- Molecule 17: 50S ribosomal protein L22

Chain P:



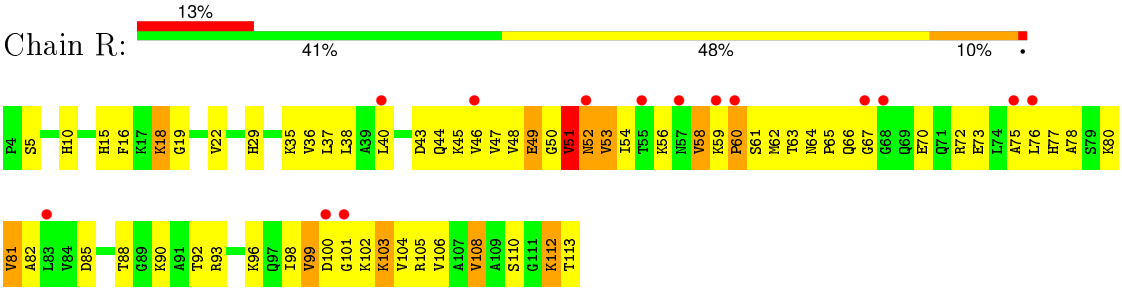
- Molecule 18: 50S ribosomal protein L23

Chain Q:



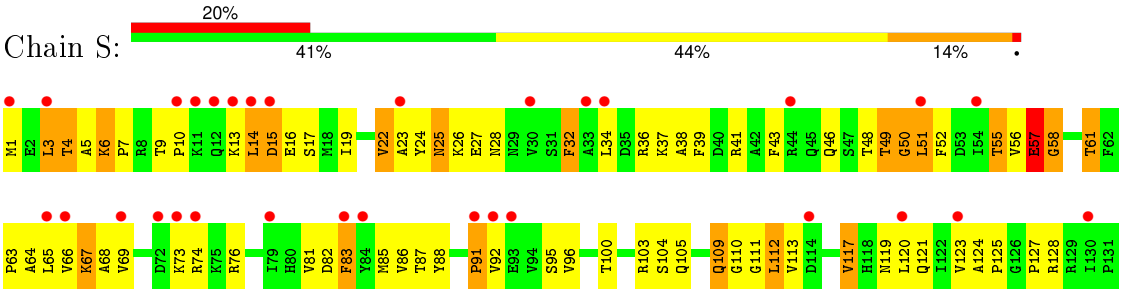
- Molecule 19: 50S ribosomal protein L24

Chain R:

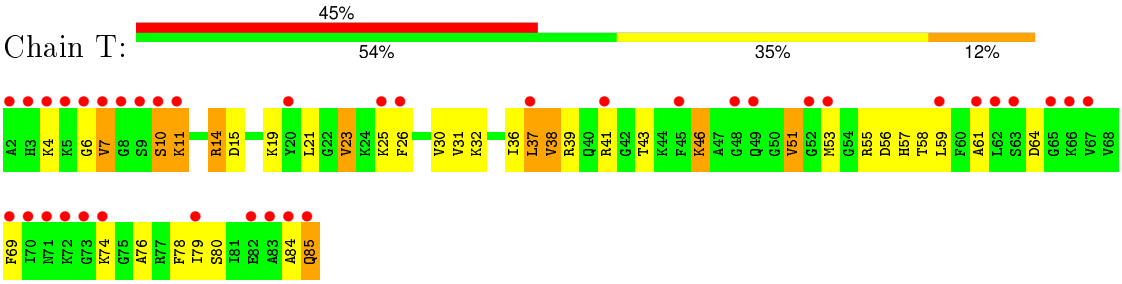


- Molecule 20: 50S ribosomal protein L25

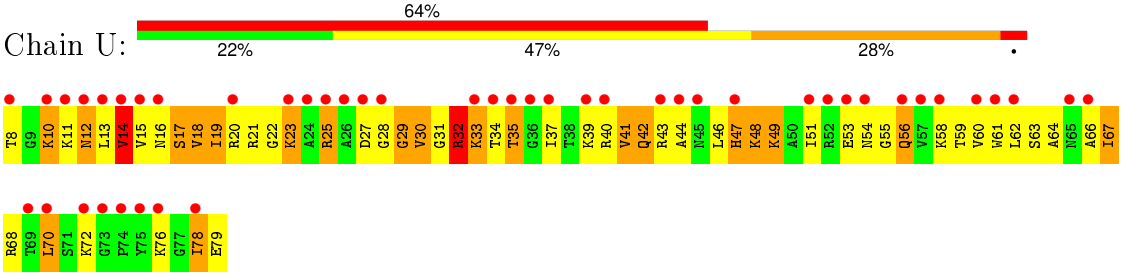
Chain S:



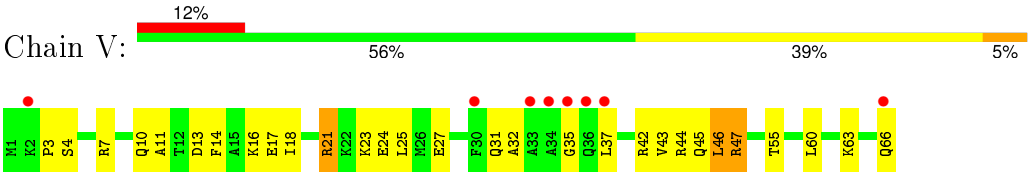
- Molecule 21: 50S ribosomal protein L27



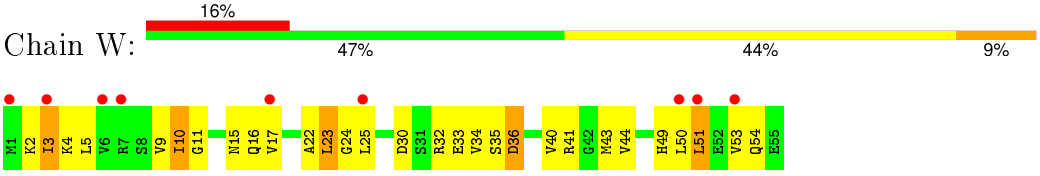
- Molecule 22: 50S ribosomal protein L28



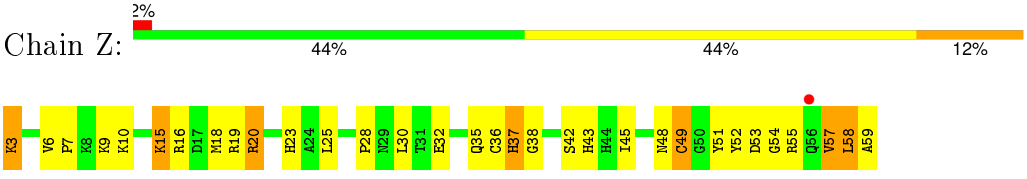
- Molecule 23: 50S ribosomal protein L29



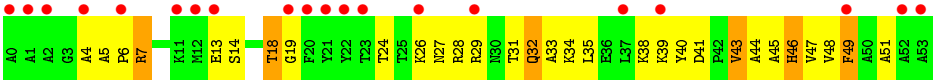
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



- Molecule 26: 50S ribosomal protein L33

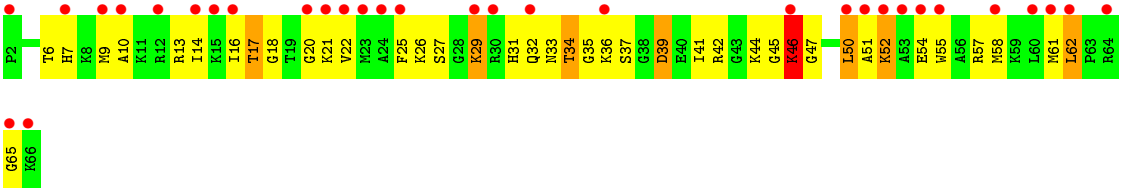


• Molecule 27: 50S ribosomal protein L34

Chain 2:

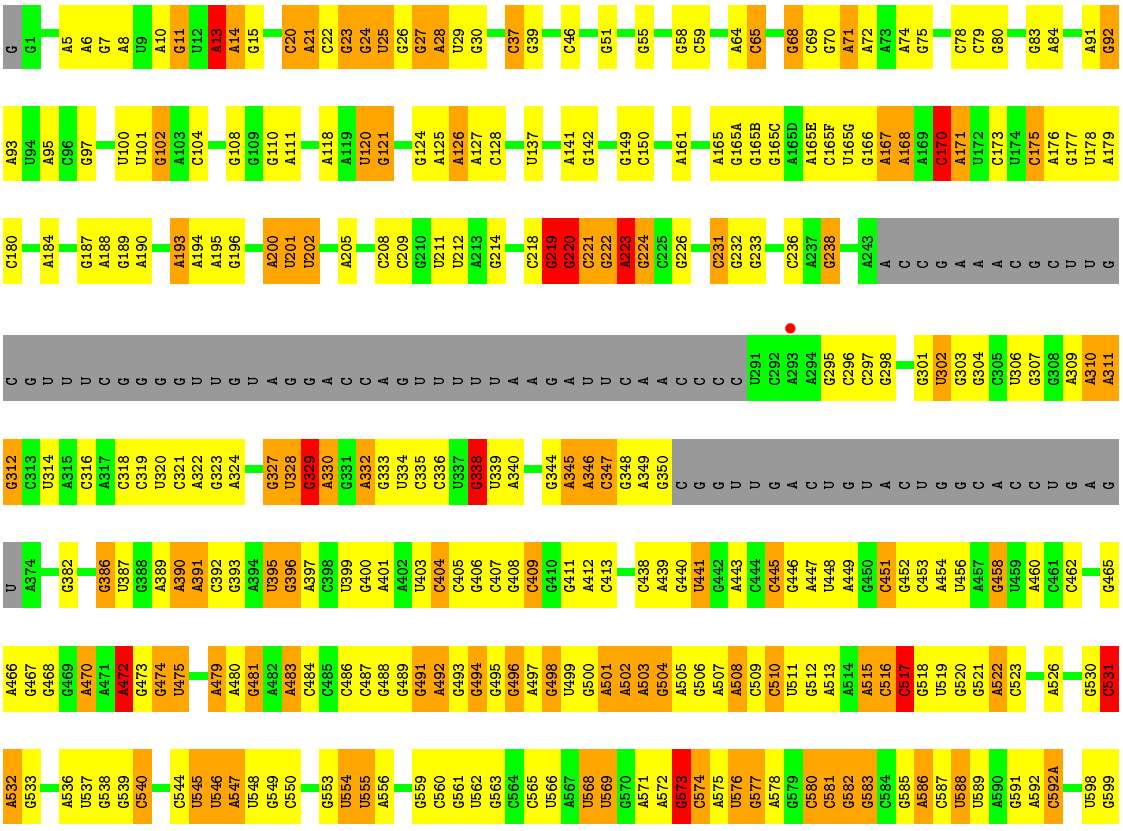
• Molecule 28: 50S ribosomal protein L35

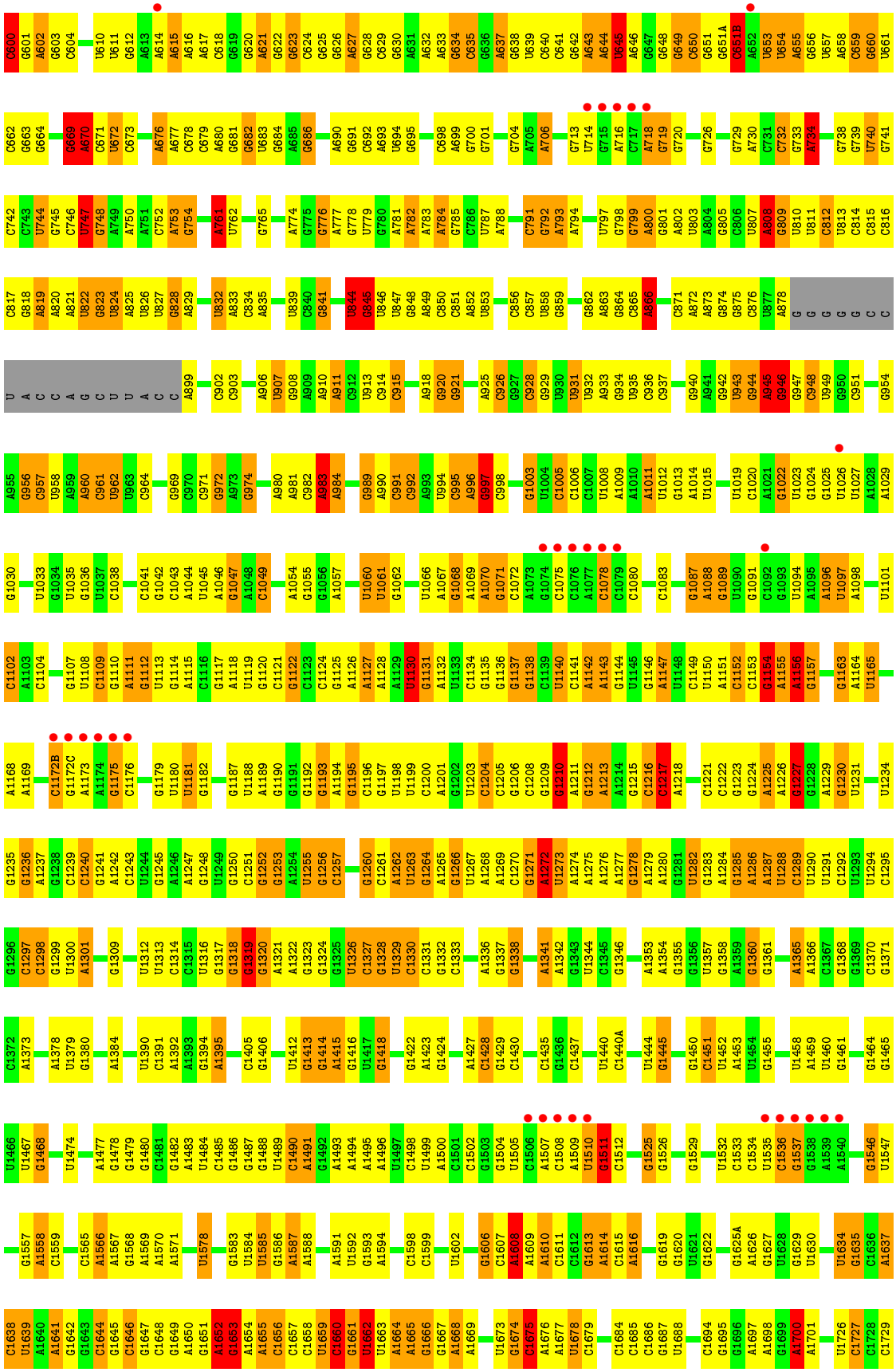
Chain 3:

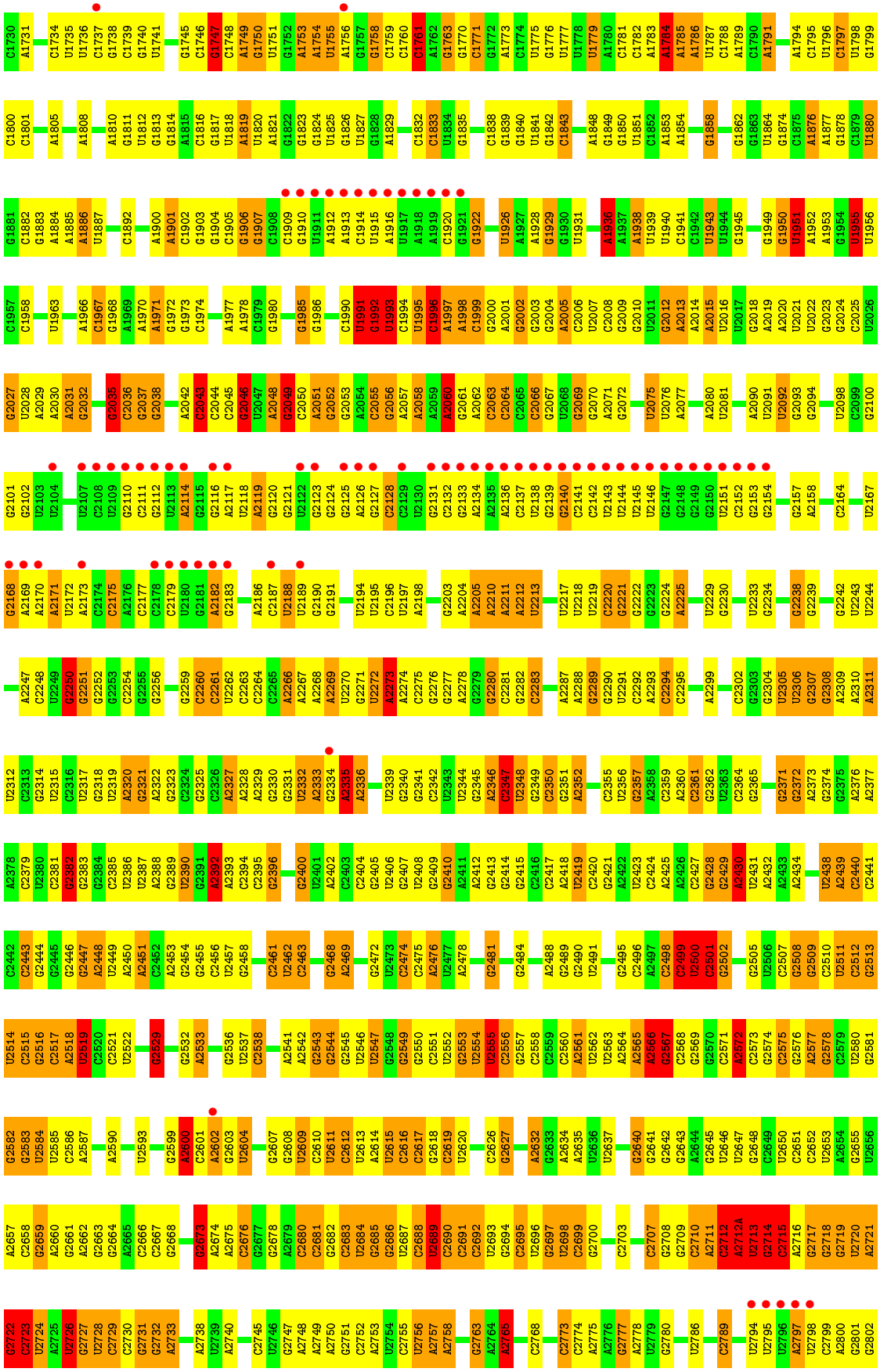


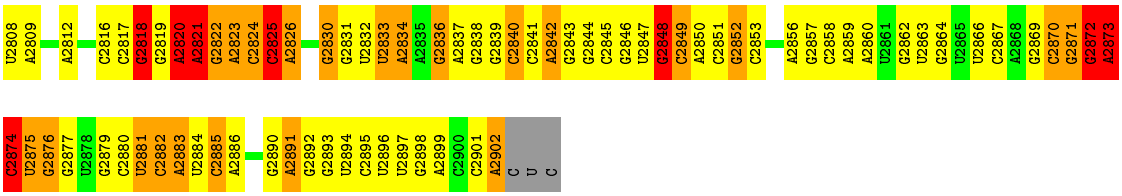
• Molecule 29: 23S ribosomal RNA

Chain X:

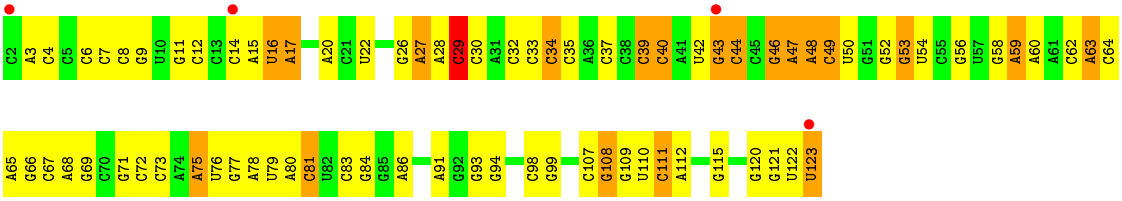








- Molecule 30: 5S ribosomal RNA



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	169.90Å 410.76Å 696.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.90 58.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (58.96-2.90) 81.6 (58.96-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.270 0.237 , 0.271	Depositor DCC
R_{free} test set	20602 reflections (4.74%)	DCC
Wilson B-factor (Å^2)	79.0	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 65.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	3 of 530819 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	89337	wwPDB-VP
Average B, all atoms (Å^2)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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

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	0	0.30	0/1674	0.49	0/2257
2	A	0.39	0/2149	0.59	0/2890
3	B	0.69	1/1568 (0.1%)	0.86	1/2105 (0.0%)
4	C	0.51	0/1530	0.73	1/2070 (0.0%)
5	D	0.36	0/1420	0.56	0/1903
6	E	0.39	0/1309	0.55	0/1771
7	F	0.33	0/1067	0.52	1/1446 (0.1%)
8	G	0.47	0/1139	0.67	0/1539
9	H	0.76	0/1007	0.91	2/1352 (0.1%)
10	I	0.52	0/1082	0.76	1/1448 (0.1%)
11	J	0.65	0/1114	0.78	0/1486
12	K	0.83	0/887	1.04	0/1188
13	L	0.52	0/784	0.73	0/1045
14	M	0.77	0/880	0.83	0/1179
15	N	0.64	0/994	0.80	1/1323 (0.1%)
16	O	0.53	0/751	0.73	0/1000
17	P	0.69	0/1027	0.83	0/1373
18	Q	0.45	0/738	0.59	0/988
19	R	0.54	0/836	0.72	0/1121
20	S	0.41	0/1371	0.67	0/1862
21	T	0.54	0/634	0.69	0/838
22	U	0.61	0/557	0.88	1/741 (0.1%)
23	V	0.41	0/538	0.57	0/714
24	W	0.51	0/426	0.68	0/568
25	Z	0.71	0/465	0.90	0/622
26	1	0.49	0/411	0.73	0/554
27	2	0.48	0/397	0.65	0/521
28	3	0.54	0/516	0.70	0/673
29	X	0.78	37/66826 (0.1%)	1.44	971/104247 (0.9%)
30	Y	0.64	0/2907	1.20	8/4529 (0.2%)
All	All	0.72	38/97004 (0.0%)	1.29	987/145353 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	B	0	3
4	C	0	1
8	G	0	1
25	Z	0	2
All	All	0	7

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	X	761	A	C6-N1	8.06	1.41	1.35
29	X	1999	C	N3-C4	-7.01	1.29	1.33
29	X	1638	C	N1-C6	-6.80	1.33	1.37
29	X	1661	G	C6-N1	-6.69	1.34	1.39
29	X	1661	G	C5-C4	-6.50	1.33	1.38

The worst 5 of 987 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	X	761	A	N1-C6-N6	22.08	131.85	118.60
29	X	761	A	C5-N7-C8	-17.56	95.12	103.90
29	X	2713	U	O5'-P-OP2	-17.29	89.95	110.70
29	X	761	A	C4-C5-N7	16.33	118.87	110.70
29	X	761	A	C5-C6-N6	-14.62	112.00	123.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	178	GLY	Peptide
3	B	73	ALA	Peptide
3	B	85	ALA	Peptide
4	C	187	VAL	Peptide
8	G	37	ASP	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	0	1651	0	1693	59	0
2	A	2107	0	2190	82	0
3	B	1540	0	1600	75	0
4	C	1507	0	1525	80	0
5	D	1401	0	1481	64	0
6	E	1287	0	1336	49	0
7	F	1048	0	1088	23	0
8	G	1115	0	1144	47	0
9	H	997	0	1046	67	0
10	I	1068	0	1103	60	0
11	J	1091	0	1125	64	0
12	K	879	0	930	43	0
13	L	778	0	820	38	0
14	M	867	0	890	43	0
15	N	978	0	1020	72	0
16	O	742	0	756	37	0
17	P	1014	0	1096	60	0
18	Q	727	0	753	25	0
19	R	826	0	881	54	0
20	S	1346	0	1372	65	0
21	T	626	0	655	33	0
22	U	553	0	604	59	0
23	V	534	0	558	16	0
24	W	424	0	470	20	0
25	Z	453	0	455	38	0
26	1	404	0	416	21	0
27	2	393	0	420	19	0
28	3	509	0	565	40	0
29	X	59673	0	30060	1282	0
30	Y	2601	0	1327	57	0
31	M	1	0	0	0	0
31	X	192	0	0	0	0
31	Y	5	0	0	0	0
All	All	89337	0	59379	2369	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 16.

The worst 5 of 2369 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)
12:K:103:ARG:HD2	29:X:1287:A:H5'	1.33	1.04
9:H:41:ASN:ND2	29:X:2674:A:O2'	1.91	1.04
15:N:48:ARG:HD2	29:X:1156:A:H61	1.20	1.03
8:G:31:THR:HG21	15:N:61:TRP:HE1	1.26	1.00
29:X:500:G:H22	29:X:503:A:H5"	1.26	0.97

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
1	0	222/224 (99%)	135 (61%)	65 (29%)	22 (10%)	1 2
2	A	272/274 (99%)	238 (88%)	25 (9%)	9 (3%)	5 20
3	B	203/205 (99%)	168 (83%)	24 (12%)	11 (5%)	2 7
4	C	195/197 (99%)	151 (77%)	30 (15%)	14 (7%)	1 3
5	D	175/177 (99%)	124 (71%)	39 (22%)	12 (7%)	1 4
6	E	169/171 (99%)	130 (77%)	22 (13%)	17 (10%)	1 2
7	F	142/144 (99%)	99 (70%)	34 (24%)	9 (6%)	2 5
8	G	140/142 (99%)	121 (86%)	13 (9%)	6 (4%)	3 13
9	H	132/134 (98%)	103 (78%)	19 (14%)	10 (8%)	1 3
10	I	139/141 (99%)	104 (75%)	23 (16%)	12 (9%)	1 2
11	J	134/136 (98%)	102 (76%)	20 (15%)	12 (9%)	1 2
12	K	111/113 (98%)	95 (86%)	11 (10%)	5 (4%)	3 12
13	L	102/104 (98%)	65 (64%)	21 (21%)	16 (16%)	0 0
14	M	107/109 (98%)	93 (87%)	7 (6%)	7 (6%)	1 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
15	N	115/117 (98%)	104 (90%)	8 (7%)	3 (3%)	7 26
16	O	92/94 (98%)	75 (82%)	11 (12%)	6 (6%)	1 4
17	P	125/127 (98%)	99 (79%)	16 (13%)	10 (8%)	1 3
18	Q	91/93 (98%)	87 (96%)	4 (4%)	0	100 100
19	R	108/110 (98%)	84 (78%)	14 (13%)	10 (9%)	1 2
20	S	173/175 (99%)	123 (71%)	32 (18%)	18 (10%)	1 1
21	T	82/84 (98%)	68 (83%)	11 (13%)	3 (4%)	4 17
22	U	70/72 (97%)	38 (54%)	16 (23%)	16 (23%)	0 0
23	V	64/66 (97%)	55 (86%)	5 (8%)	4 (6%)	2 5
24	W	53/55 (96%)	48 (91%)	3 (6%)	2 (4%)	4 16
25	Z	55/57 (96%)	41 (74%)	11 (20%)	3 (6%)	2 7
26	1	52/54 (96%)	33 (64%)	13 (25%)	6 (12%)	0 1
27	2	45/47 (96%)	40 (89%)	3 (7%)	2 (4%)	3 12
28	3	63/65 (97%)	47 (75%)	12 (19%)	4 (6%)	2 5
All	All	3431/3487 (98%)	2670 (78%)	512 (15%)	249 (7%)	1 3

5 of 249 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	28	LEU
1	0	30	THR
1	0	45	ILE
1	0	157	ILE
1	0	216	PRO

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
1	0	167/167 (100%)	150 (90%)	17 (10%)	9 27
2	A	214/214 (100%)	190 (89%)	24 (11%)	7 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	B	155/155 (100%)	139 (90%)	16 (10%)	9 26
4	C	157/157 (100%)	137 (87%)	20 (13%)	5 16
5	D	153/153 (100%)	131 (86%)	22 (14%)	4 12
6	E	136/136 (100%)	114 (84%)	22 (16%)	3 9
7	F	107/107 (100%)	97 (91%)	10 (9%)	11 32
8	G	118/118 (100%)	108 (92%)	10 (8%)	13 37
9	H	103/103 (100%)	76 (74%)	27 (26%)	0 2
10	I	108/108 (100%)	85 (79%)	23 (21%)	1 4
11	J	110/110 (100%)	89 (81%)	21 (19%)	2 5
12	K	90/90 (100%)	78 (87%)	12 (13%)	5 14
13	L	74/74 (100%)	52 (70%)	22 (30%)	0 1
14	M	92/92 (100%)	79 (86%)	13 (14%)	4 12
15	N	96/96 (100%)	86 (90%)	10 (10%)	9 26
16	O	75/75 (100%)	57 (76%)	18 (24%)	1 2
17	P	109/109 (100%)	92 (84%)	17 (16%)	3 10
18	Q	75/75 (100%)	69 (92%)	6 (8%)	15 40
19	R	91/91 (100%)	76 (84%)	15 (16%)	3 8
20	S	149/149 (100%)	117 (78%)	32 (22%)	1 4
21	T	62/62 (100%)	48 (77%)	14 (23%)	1 3
22	U	57/57 (100%)	42 (74%)	15 (26%)	0 2
23	V	54/54 (100%)	48 (89%)	6 (11%)	8 22
24	W	48/48 (100%)	43 (90%)	5 (10%)	9 26
25	Z	51/51 (100%)	43 (84%)	8 (16%)	3 9
26	1	38/38 (100%)	30 (79%)	8 (21%)	1 4
27	2	40/40 (100%)	33 (82%)	7 (18%)	2 7
28	3	51/51 (100%)	40 (78%)	11 (22%)	1 3
All	All	2780/2780 (100%)	2349 (84%)	431 (16%)	3 10

5 of 431 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	26	ASP
13	L	71	VAL

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Mol	Chain	Res	Type
25	Z	9	LYS
11	J	92	GLU
12	K	60	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	127	ASN
8	G	161	GLN
18	Q	86	GLN
5	D	120	ASN
15	N	91	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	X	2776/2881 (96%)	655 (23%)	41 (1%)
30	Y	121/122 (99%)	35 (28%)	1 (0%)
All	All	2897/3003 (96%)	690 (23%)	42 (1%)

5 of 690 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
29	X	13	A
29	X	14	A
29	X	22	C
29	X	28	A
29	X	46	C

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
29	X	1413	G
29	X	1586	G
29	X	2756	U
29	X	1414	G
29	X	1510	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 198 ligands modelled in this entry, 198 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	224/224 (100%)	5.93	199 (88%) 0 0	238, 259, 280, 290	0
2	A	274/274 (100%)	0.53	31 (11%) 7 4	93, 135, 154, 161	0
3	B	205/205 (100%)	0.24	7 (3%) 49 41	60, 89, 107, 124	0
4	C	197/197 (100%)	0.37	15 (7%) 17 11	77, 125, 145, 159	0
5	D	177/177 (100%)	1.65	66 (37%) 0 0	155, 174, 190, 197	0
6	E	171/171 (100%)	0.84	35 (20%) 1 1	110, 148, 175, 177	0
7	F	144/144 (100%)	3.55	102 (70%) 0 0	213, 230, 235, 237	0
8	G	142/142 (100%)	0.27	11 (7%) 16 11	79, 112, 127, 144	0
9	H	134/134 (100%)	0.03	5 (3%) 45 38	62, 79, 94, 111	0
10	I	141/141 (100%)	0.98	33 (23%) 1 0	86, 138, 155, 161	0
11	J	136/136 (100%)	1.04	33 (24%) 1 0	94, 113, 135, 141	0
12	K	113/113 (100%)	0.14	3 (2%) 58 52	61, 72, 83, 88	0
13	L	104/104 (100%)	1.48	34 (32%) 1 0	121, 136, 153, 162	0
14	M	109/109 (100%)	-0.19	3 (2%) 56 50	65, 80, 98, 127	0
15	N	117/117 (100%)	0.40	10 (8%) 13 8	80, 107, 127, 133	0
16	O	94/94 (100%)	0.08	8 (8%) 13 8	89, 122, 141, 152	0
17	P	127/127 (100%)	0.40	10 (7%) 15 10	71, 85, 109, 156	0
18	Q	93/93 (100%)	0.94	14 (15%) 3 1	98, 124, 140, 144	0
19	R	110/110 (100%)	0.57	14 (12%) 5 3	110, 121, 146, 157	0
20	S	175/175 (100%)	0.72	35 (20%) 1 1	124, 151, 164, 168	0
21	T	84/84 (100%)	2.25	38 (45%) 0 0	102, 117, 133, 146	0
22	U	72/72 (100%)	2.89	46 (63%) 0 0	117, 148, 161, 164	0
23	V	66/66 (100%)	0.35	8 (12%) 6 3	129, 141, 159, 163	0
24	W	55/55 (100%)	0.70	9 (16%) 2 1	95, 110, 126, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	57/57 (100%)	-0.12	1 (1%) 71 68	74, 82, 104, 112	0
26	1	54/54 (100%)	1.46	20 (37%) 0 0	125, 136, 152, 168	0
27	2	47/47 (100%)	0.21	1 (2%) 67 62	91, 108, 116, 117	0
28	3	65/65 (100%)	2.08	32 (49%) 0 0	107, 118, 127, 129	0
29	X	2780/2881 (96%)	-0.13	108 (3%) 43 36	51, 111, 221, 347	0
30	Y	122/122 (100%)	-0.53	4 (3%) 50 42	96, 136, 161, 172	0
All	All	6389/6490 (98%)	0.57	935 (14%) 3 2	51, 119, 242, 347	0

The worst 5 of 935 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	X	2137	C	31.1
29	X	1916	A	26.7
1	0	54	VAL	23.5
29	X	2112	G	20.1
1	0	86	GLY	19.9

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6158	1/1	0.86	2.46	137.84	114,114,114,114	0
31	MG	X	6036	1/1	0.94	0.84	68.71	82,82,82,82	0
31	MG	X	6169	1/1	0.94	0.57	64.22	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6011	1/1	0.86	0.45	61.47	89,89,89,89	0
31	MG	X	6147	1/1	0.87	1.00	59.12	82,82,82,82	0
31	MG	X	6112	1/1	0.94	0.68	55.61	84,84,84,84	0
31	MG	X	6142	1/1	0.86	0.77	55.05	89,89,89,89	0
31	MG	X	6014	1/1	0.78	0.42	51.05	91,91,91,91	0
31	MG	X	6118	1/1	0.93	0.72	49.43	90,90,90,90	0
31	MG	X	6063	1/1	0.96	1.29	45.95	87,87,87,87	0
31	MG	X	6180	1/1	0.77	1.58	39.84	101,101,101,101	0
31	MG	X	6056	1/1	0.92	0.88	37.40	85,85,85,85	0
31	MG	X	6057	1/1	0.87	0.99	35.04	93,93,93,93	0
31	MG	X	6091	1/1	0.94	1.11	30.96	88,88,88,88	0
31	MG	X	6013	1/1	0.83	0.57	29.03	76,76,76,76	0
31	MG	X	6121	1/1	0.79	0.80	28.44	99,99,99,99	0
31	MG	X	6001	1/1	0.92	0.56	28.42	69,69,69,69	0
31	MG	X	6072	1/1	0.85	0.55	27.26	102,102,102,102	0
31	MG	X	6040	1/1	0.94	0.78	24.98	80,80,80,80	0
31	MG	X	6019	1/1	0.91	0.80	21.60	77,77,77,77	0
31	MG	X	6066	1/1	0.86	1.07	21.45	84,84,84,84	0
31	MG	X	6125	1/1	0.97	0.46	21.03	123,123,123,123	0
31	MG	X	6023	1/1	0.87	0.52	20.86	97,97,97,97	0
31	MG	X	6093	1/1	0.51	0.69	20.29	106,106,106,106	0
31	MG	X	6185	1/1	0.95	0.59	19.04	109,109,109,109	0
31	MG	X	6060	1/1	0.97	0.68	18.05	80,80,80,80	0
31	MG	X	6004	1/1	0.92	0.35	15.58	76,76,76,76	0
31	MG	X	6135	1/1	0.86	0.75	15.29	91,91,91,91	0
31	MG	X	6058	1/1	0.76	0.52	14.49	97,97,97,97	0
31	MG	X	6024	1/1	0.93	0.61	14.32	87,87,87,87	0
31	MG	X	6070	1/1	0.96	0.58	13.52	107,107,107,107	0
31	MG	X	6017	1/1	0.91	0.48	13.23	83,83,83,83	0
31	MG	X	6008	1/1	0.88	0.42	11.77	81,81,81,81	0
31	MG	X	6151	1/1	0.86	0.34	11.47	98,98,98,98	0
31	MG	X	6062	1/1	0.94	0.41	11.36	85,85,85,85	0
31	MG	X	6006	1/1	0.81	0.48	11.02	69,69,69,69	0
31	MG	X	6016	1/1	0.84	0.35	10.88	77,77,77,77	0
31	MG	X	6041	1/1	0.70	0.35	10.81	83,83,83,83	0
31	MG	X	6059	1/1	0.90	0.45	10.29	87,87,87,87	0
31	MG	X	6018	1/1	0.82	0.46	10.26	74,74,74,74	0
31	MG	X	6020	1/1	0.77	0.34	10.10	79,79,79,79	0
31	MG	X	6007	1/1	0.93	0.46	9.93	70,70,70,70	0
31	MG	X	6140	1/1	0.91	1.02	8.58	97,97,97,97	0
31	MG	X	6022	1/1	0.80	0.40	7.87	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6035	1/1	0.89	0.43	7.82	86,86,86,86	0
31	MG	X	6054	1/1	0.95	0.54	7.23	92,92,92,92	0
31	MG	X	6002	1/1	0.93	0.33	6.46	78,78,78,78	0
31	MG	X	6071	1/1	0.91	0.39	6.20	81,81,81,81	0
31	MG	X	6117	1/1	0.78	0.36	5.70	90,90,90,90	0
31	MG	X	6084	1/1	0.92	0.30	3.98	93,93,93,93	0
31	MG	X	6051	1/1	0.91	0.39	3.84	69,69,69,69	0
31	MG	X	6092	1/1	0.93	0.26	3.57	93,93,93,93	0
31	MG	X	6078	1/1	0.94	0.57	1.90	93,93,93,93	0
31	MG	X	6030	1/1	0.85	1.19	-	83,83,83,83	0
31	MG	X	6190	1/1	0.84	1.32	-	129,129,129,129	0
31	MG	X	6155	1/1	0.83	0.33	-	115,115,115,115	0
31	MG	X	6065	1/1	0.96	0.61	-	81,81,81,81	0
31	MG	X	6109	1/1	0.85	0.31	-	101,101,101,101	0
31	MG	X	6165	1/1	0.88	0.98	-	99,99,99,99	0
31	MG	X	6021	1/1	0.90	0.70	-	75,75,75,75	0
31	MG	X	6153	1/1	0.96	0.62	-	113,113,113,113	0
31	MG	X	6150	1/1	0.94	0.69	-	111,111,111,111	0
31	MG	X	6085	1/1	0.77	0.36	-	101,101,101,101	0
31	MG	X	6128	1/1	0.93	0.81	-	97,97,97,97	0
31	MG	X	6113	1/1	0.77	0.53	-	115,115,115,115	0
31	MG	X	6144	1/1	0.65	0.36	-	87,87,87,87	0
31	MG	X	6163	1/1	0.93	0.37	-	156,156,156,156	0
31	MG	Y	201	1/1	0.87	0.85	-	112,112,112,112	0
31	MG	X	6034	1/1	0.88	0.81	-	90,90,90,90	0
31	MG	X	6010	1/1	0.92	0.83	-	69,69,69,69	0
31	MG	X	6111	1/1	0.77	0.70	-	98,98,98,98	0
31	MG	X	6152	1/1	0.95	0.93	-	112,112,112,112	0
31	MG	X	6106	1/1	0.94	0.54	-	80,80,80,80	0
31	MG	X	6098	1/1	0.65	1.03	-	97,97,97,97	0
31	MG	X	6183	1/1	0.58	0.71	-	105,105,105,105	0
31	MG	X	6069	1/1	0.96	0.51	-	91,91,91,91	0
31	MG	X	6045	1/1	0.92	1.02	-	89,89,89,89	0
31	MG	X	6101	1/1	0.93	0.88	-	89,89,89,89	0
31	MG	X	6176	1/1	0.88	0.50	-	107,107,107,107	0
31	MG	X	6191	1/1	0.74	1.56	-	101,101,101,101	0
31	MG	X	6175	1/1	0.64	0.41	-	121,121,121,121	0
31	MG	X	6075	1/1	0.91	0.85	-	103,103,103,103	0
31	MG	X	6131	1/1	0.94	0.86	-	101,101,101,101	0
31	MG	X	6139	1/1	0.95	0.54	-	126,126,126,126	0
31	MG	X	6047	1/1	0.89	0.54	-	74,74,74,74	0
31	MG	Y	202	1/1	0.91	0.43	-	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6009	1/1	0.97	0.67	-	69,69,69,69	0
31	MG	X	6077	1/1	0.94	0.64	-	98,98,98,98	0
31	MG	Y	205	1/1	0.83	0.90	-	129,129,129,129	0
31	MG	X	6087	1/1	0.97	0.54	-	98,98,98,98	0
31	MG	X	6083	1/1	0.88	0.80	-	91,91,91,91	0
31	MG	X	6055	1/1	0.90	0.64	-	90,90,90,90	0
31	MG	X	6105	1/1	0.87	1.40	-	118,118,118,118	0
31	MG	X	6089	1/1	0.95	0.51	-	90,90,90,90	0
31	MG	X	6156	1/1	0.79	0.63	-	105,105,105,105	0
31	MG	X	6127	1/1	0.86	0.59	-	122,122,122,122	0
31	MG	X	6108	1/1	0.36	0.63	-	120,120,120,120	0
31	MG	X	6115	1/1	0.88	0.73	-	103,103,103,103	0
31	MG	X	6080	1/1	0.83	0.71	-	108,108,108,108	0
31	MG	X	6177	1/1	0.49	0.59	-	113,113,113,113	0
31	MG	X	6043	1/1	0.97	0.85	-	69,69,69,69	0
31	MG	X	6050	1/1	0.97	0.50	-	84,84,84,84	0
31	MG	X	6074	1/1	0.86	0.74	-	80,80,80,80	0
31	MG	X	6052	1/1	0.85	0.52	-	97,97,97,97	0
31	MG	X	6096	1/1	0.97	1.19	-	89,89,89,89	0
31	MG	X	6189	1/1	0.87	0.75	-	120,120,120,120	0
31	MG	X	6148	1/1	0.99	0.57	-	130,130,130,130	0
31	MG	X	6015	1/1	0.91	0.55	-	77,77,77,77	0
31	MG	X	6026	1/1	0.94	0.41	-	91,91,91,91	0
31	MG	X	6114	1/1	0.88	0.55	-	91,91,91,91	0
31	MG	X	6027	1/1	0.89	1.03	-	86,86,86,86	0
31	MG	X	6170	1/1	0.73	1.96	-	127,127,127,127	0
31	MG	X	6167	1/1	0.56	0.56	-	103,103,103,103	0
31	MG	X	6146	1/1	0.79	1.51	-	129,129,129,129	0
31	MG	X	6164	1/1	0.81	0.99	-	124,124,124,124	0
31	MG	X	6038	1/1	0.71	0.67	-	85,85,85,85	0
31	MG	X	6187	1/1	0.77	0.57	-	92,92,92,92	0
31	MG	X	6116	1/1	0.97	0.59	-	106,106,106,106	0
31	MG	X	6048	1/1	0.78	0.80	-	102,102,102,102	0
31	MG	X	6088	1/1	0.94	0.87	-	99,99,99,99	0
31	MG	X	6049	1/1	0.96	0.67	-	88,88,88,88	0
31	MG	X	6137	1/1	0.85	0.57	-	135,135,135,135	0
31	MG	X	6046	1/1	0.56	0.40	-	91,91,91,91	0
31	MG	X	6119	1/1	0.46	0.53	-	128,128,128,128	0
31	MG	X	6076	1/1	0.92	0.73	-	102,102,102,102	0
31	MG	X	6188	1/1	0.91	0.44	-	98,98,98,98	0
31	MG	X	6138	1/1	0.75	0.77	-	94,94,94,94	0
31	MG	Y	204	1/1	0.87	0.96	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6095	1/1	0.92	0.85	-	79,79,79,79	0
31	MG	X	6032	1/1	0.94	0.34	-	78,78,78,78	0
31	MG	X	6166	1/1	0.96	0.73	-	106,106,106,106	0
31	MG	X	6044	1/1	0.94	0.29	-	73,73,73,73	0
31	MG	Y	203	1/1	0.97	0.96	-	102,102,102,102	0
31	MG	M	201	1/1	0.95	0.93	-	69,69,69,69	0
31	MG	X	6110	1/1	0.81	0.38	-	130,130,130,130	0
31	MG	X	6012	1/1	0.86	0.50	-	82,82,82,82	0
31	MG	X	6182	1/1	0.88	0.97	-	120,120,120,120	0
31	MG	X	6122	1/1	0.82	0.46	-	100,100,100,100	0
31	MG	X	6168	1/1	0.91	0.84	-	107,107,107,107	0
31	MG	X	6104	1/1	0.91	0.59	-	86,86,86,86	0
31	MG	X	6064	1/1	0.91	0.63	-	96,96,96,96	0
31	MG	X	6184	1/1	0.96	0.76	-	102,102,102,102	0
31	MG	X	6033	1/1	0.93	0.53	-	98,98,98,98	0
31	MG	X	6192	1/1	0.77	0.69	-	138,138,138,138	0
31	MG	X	6178	1/1	0.93	0.58	-	103,103,103,103	0
31	MG	X	6102	1/1	0.94	0.25	-	89,89,89,89	0
31	MG	X	6141	1/1	0.74	0.60	-	122,122,122,122	0
31	MG	X	6160	1/1	0.87	0.68	-	104,104,104,104	0
31	MG	X	6133	1/1	0.72	1.20	-	111,111,111,111	0
31	MG	X	6186	1/1	0.72	1.02	-	134,134,134,134	0
31	MG	X	6031	1/1	0.96	0.53	-	69,69,69,69	0
31	MG	X	6073	1/1	0.95	0.79	-	85,85,85,85	0
31	MG	X	6029	1/1	0.94	0.43	-	69,69,69,69	0
31	MG	X	6003	1/1	0.85	0.49	-	70,70,70,70	0
31	MG	X	6082	1/1	0.91	0.75	-	83,83,83,83	0
31	MG	X	6134	1/1	0.99	0.67	-	112,112,112,112	0
31	MG	X	6086	1/1	0.98	0.92	-	87,87,87,87	0
31	MG	X	6171	1/1	0.82	0.80	-	111,111,111,111	0
31	MG	X	6081	1/1	0.93	0.42	-	78,78,78,78	0
31	MG	X	6162	1/1	0.67	0.81	-	111,111,111,111	0
31	MG	X	6103	1/1	0.94	0.32	-	117,117,117,117	0
31	MG	X	6099	1/1	0.73	0.68	-	89,89,89,89	0
31	MG	X	6005	1/1	0.96	0.89	-	69,69,69,69	0
31	MG	X	6132	1/1	0.89	0.54	-	94,94,94,94	0
31	MG	X	6053	1/1	0.98	0.84	-	91,91,91,91	0
31	MG	X	6149	1/1	0.88	0.59	-	94,94,94,94	0
31	MG	X	6123	1/1	0.88	0.48	-	130,130,130,130	0
31	MG	X	6061	1/1	0.95	0.71	-	83,83,83,83	0
31	MG	X	6129	1/1	0.93	0.89	-	104,104,104,104	0
31	MG	X	6068	1/1	0.94	0.66	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
31	MG	X	6090	1/1	0.83	0.45	-	117,117,117,117	0
31	MG	X	6174	1/1	0.85	0.71	-	87,87,87,87	0
31	MG	X	6130	1/1	0.94	0.67	-	108,108,108,108	0
31	MG	X	6100	1/1	0.83	0.58	-	97,97,97,97	0
31	MG	X	6145	1/1	0.94	0.20	-	104,104,104,104	0
31	MG	X	6124	1/1	0.87	1.13	-	107,107,107,107	0
31	MG	X	6097	1/1	0.93	1.25	-	93,93,93,93	0
31	MG	X	6161	1/1	0.93	0.68	-	95,95,95,95	0
31	MG	X	6120	1/1	0.93	1.03	-	102,102,102,102	0
31	MG	X	6028	1/1	0.84	0.33	-	88,88,88,88	0
31	MG	X	6173	1/1	0.85	1.90	-	102,102,102,102	0
31	MG	X	6143	1/1	0.86	1.04	-	100,100,100,100	0
31	MG	X	6025	1/1	0.97	0.45	-	83,83,83,83	0
31	MG	X	6179	1/1	0.61	0.54	-	117,117,117,117	0
31	MG	X	6172	1/1	0.84	0.66	-	124,124,124,124	0
31	MG	X	6037	1/1	0.89	0.41	-	86,86,86,86	0
31	MG	X	6126	1/1	0.94	1.19	-	94,94,94,94	0
31	MG	X	6181	1/1	0.97	0.32	-	121,121,121,121	0
31	MG	X	6039	1/1	0.89	1.17	-	104,104,104,104	0
31	MG	X	6136	1/1	0.83	0.81	-	122,122,122,122	0
31	MG	X	6079	1/1	0.95	0.35	-	102,102,102,102	0
31	MG	X	6107	1/1	0.79	0.75	-	113,113,113,113	0
31	MG	X	6159	1/1	0.49	0.44	-	111,111,111,111	0
31	MG	X	6154	1/1	0.83	1.09	-	113,113,113,113	0
31	MG	X	6042	1/1	0.98	0.59	-	83,83,83,83	0
31	MG	X	6094	1/1	0.94	0.45	-	92,92,92,92	0
31	MG	X	6157	1/1	0.82	0.31	-	111,111,111,111	0
31	MG	X	6067	1/1	0.91	0.49	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.