



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:01 PM GMT

PDB ID : 3V25
Title : Crystal structure of RMF bound to the 70S ribosome. This PDB entry contains coordinates for the 50S subunit of the 2nd ribosome in the ASU
Authors : Polikanov, Y.S.; Blaha, G.M.; Steitz, T.A.
Deposited on : 2011-12-11
Resolution : 3.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

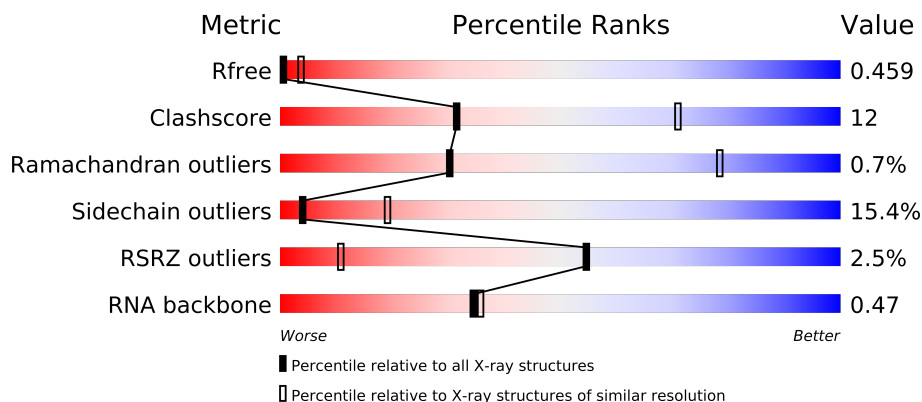
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2915	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	

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Mol	Chain	Length	Quality of chain
13	R	118	
14	S	112	
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 91067 atoms, of which 0 are hydrogen and 0 are deuterium.

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 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2814	Total	C	N	O	P	0	0	0
			60620	26978	11348	19481	2813			

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	203	Total	C	N	O	S	0	0	1
			1580	1007	298	273	2			

- Molecule 6 is a protein called 50S Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1038	668	180	189	1			

- Molecule 9 is a protein called 50S Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	149	Total	C	N	O	S	0	0	0
			1131	703	229	196	3			

- Molecule 12 is a protein called 50S Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	110	Total	C	N	O			
			865	544	172	149	0	0	0

- Molecule 15 is a protein called 50S Ribosomal Protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	T	131	Total	C	N	O	S		
			1063	666	213	183	1	0	0

- Molecule 16 is a protein called 50S Ribosomal Protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	U	116	Total	C	N	O	S		
			959	608	201	149	1	0	0

- Molecule 17 is a protein called 50S Ribosomal Protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S		
			771	495	140	135	1	0	0

- Molecule 18 is a protein called 50S Ribosomal Protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	W	112	Total	C	N	O	S		
			881	554	172	153	2	0	0

- Molecule 19 is a protein called 50S Ribosomal Protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	95	Total	C	N	O	S		
			742	483	134	124	1	0	0

- Molecule 20 is a protein called 50S Ribosomal Protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S		
			785	503	145	131	6	0	0

- Molecule 21 is a protein called 50S Ribosomal Protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S Ribosomal Protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			458	293	87	78			

- Molecule 26 is a protein called 50S Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a protein called 50S Ribosomal Protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	36	Total	C	N	O	S	0	0	0
			297	182	66	46	3			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	P	1	Total	Mg	0	0
			1	1		
32	D	1	Total	Mg	0	0
			1	1		
32	E	1	Total	Mg	0	0
			1	1		
32	B	5	Total	Mg	0	0
			5	5		
32	6	1	Total	Mg	0	0
			1	1		
32	7	1	Total	Mg	0	0
			1	1		
32	A	428	Total	Mg	0	0
			428	428		
32	8	1	Total	Mg	0	0
			1	1		
32	F	2	Total	Mg	0	0
			2	2		

- Molecule 33 is ZINC ION (three-letter code: ZN) (formula: Zn).

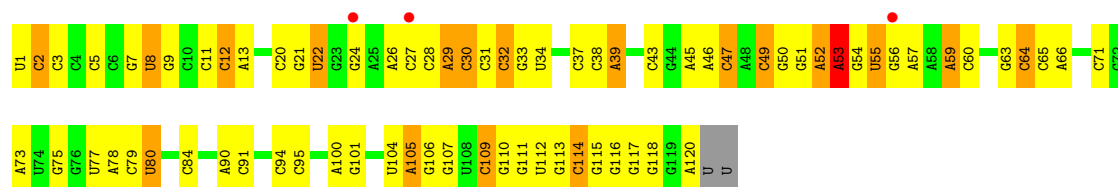
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	1	Total 1	Zn 1	0	0
33	Y	1	Total 1	Zn 1	0	0
33	4	1	Total 1	Zn 1	0	0
33	6	1	Total 1	Zn 1	0	0
33	5	1	Total 1	Zn 1	0	0

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	696	Total 696	O 696	0	0
34	B	9	Total 9	O 9	0	0
34	D	3	Total 3	O 3	0	0
34	E	1	Total 1	O 1	0	0
34	F	5	Total 5	O 5	0	0
34	P	5	Total 5	O 5	0	0
34	Q	2	Total 2	O 2	0	0
34	R	1	Total 1	O 1	0	0
34	V	1	Total 1	O 1	0	0
34	X	1	Total 1	O 1	0	0
34	Y	1	Total 1	O 1	0	0
34	0	1	Total 1	O 1	0	0
34	1	2	Total 2	O 2	0	0

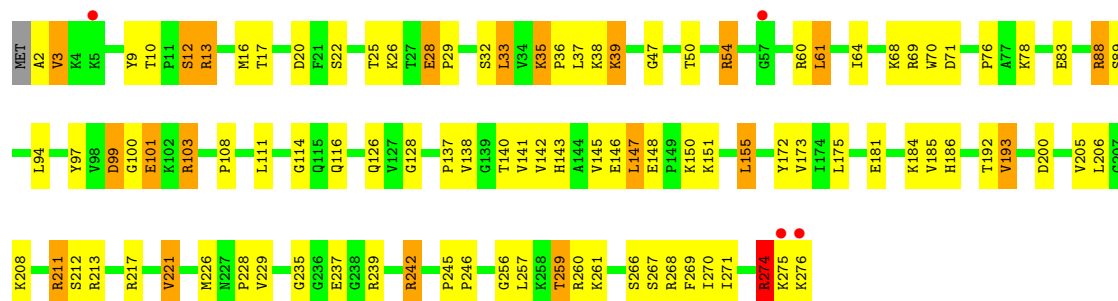


WORLDWIDE
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PROTEIN DATA BANK



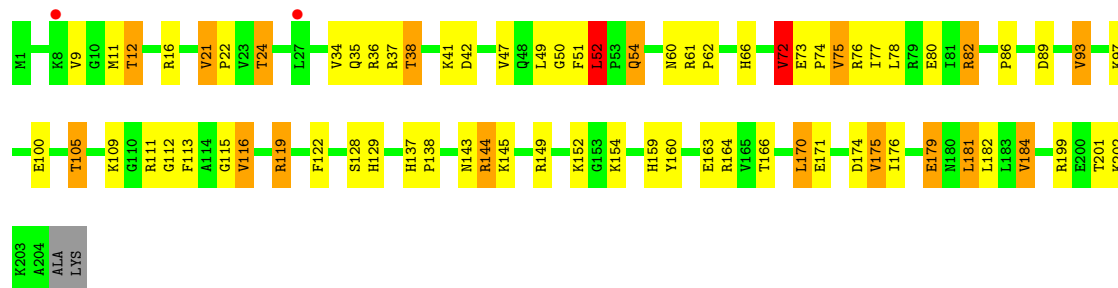
• Molecule 3: 50S Ribosomal Protein L2

Chain D:



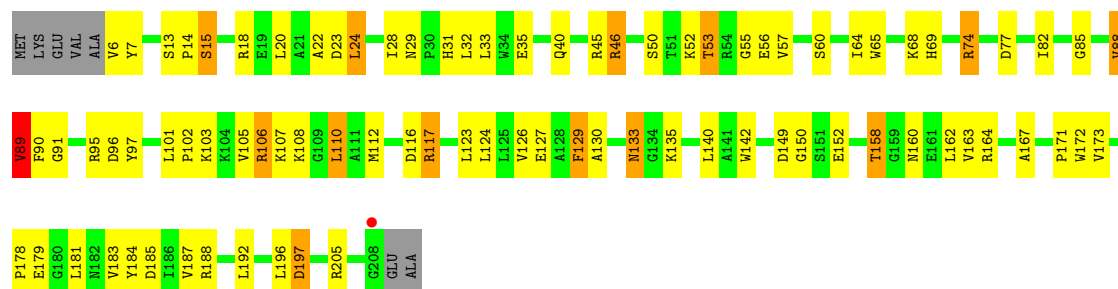
• Molecule 4: 50S Ribosomal Protein L3

Chain E:



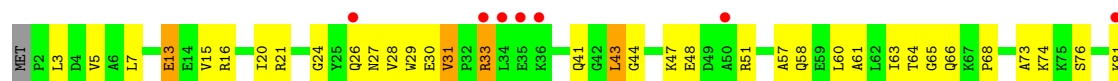
• Molecule 5: 50S Ribosomal Protein L4

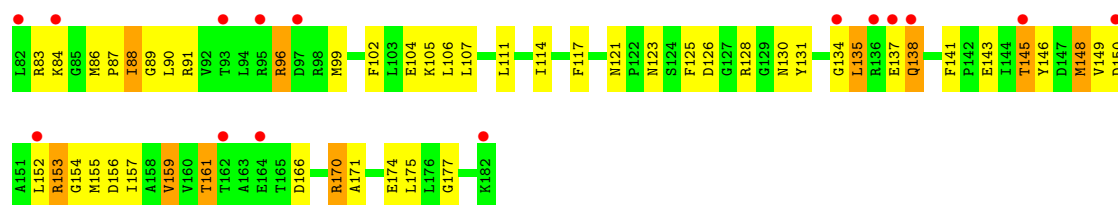
Chain F:



• Molecule 6: 50S Ribosomal Protein L5

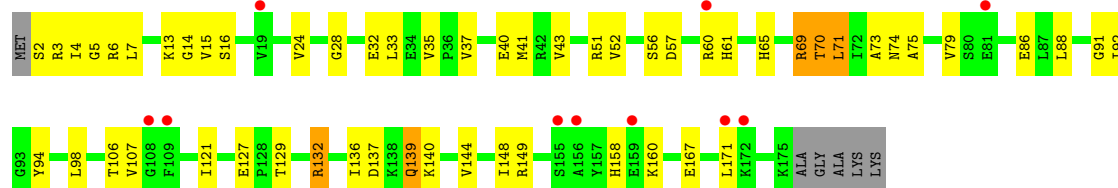
Chain G:





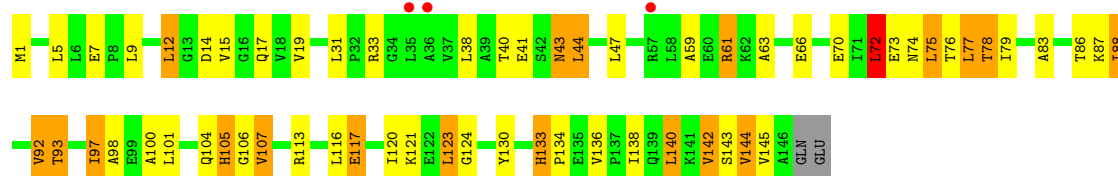
• Molecule 7: 50S Ribosomal Protein L6

Chain H:



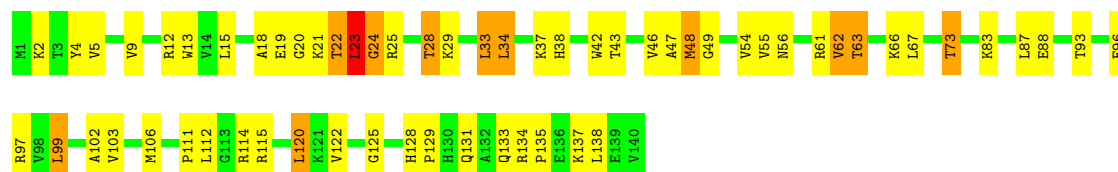
• Molecule 8: 50S Ribosomal Protein L9

Chain I:



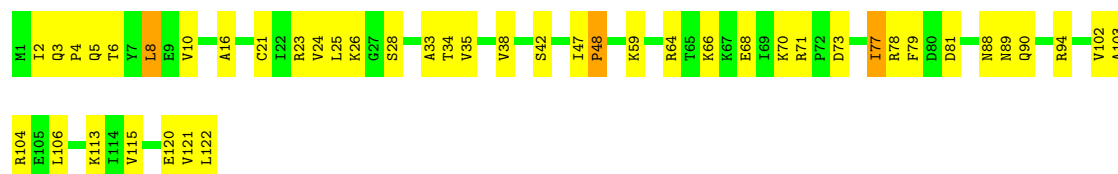
• Molecule 9: 50S Ribosomal Protein L13

Chain N:



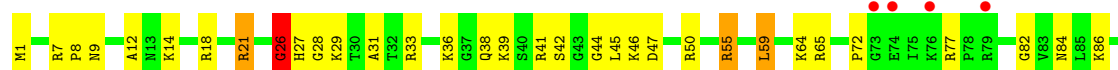
• Molecule 10: 50S Ribosomal Protein L14

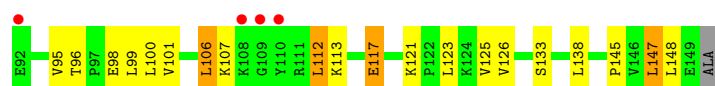
Chain O:



• Molecule 11: 50S Ribosomal Protein L15

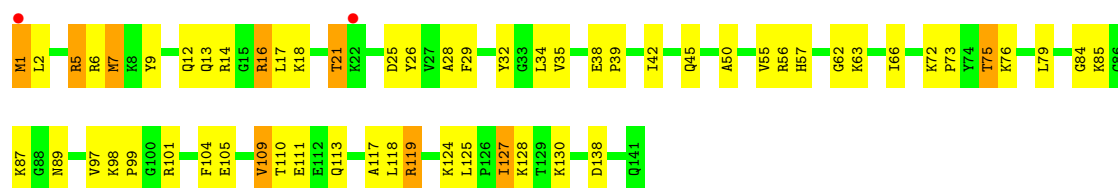
Chain P:





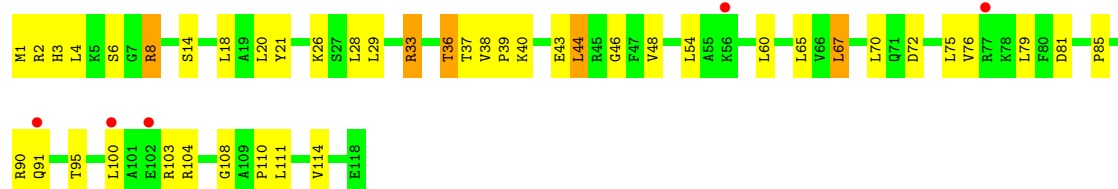
• Molecule 12: 50S Ribosomal Protein L16

Chain Q:



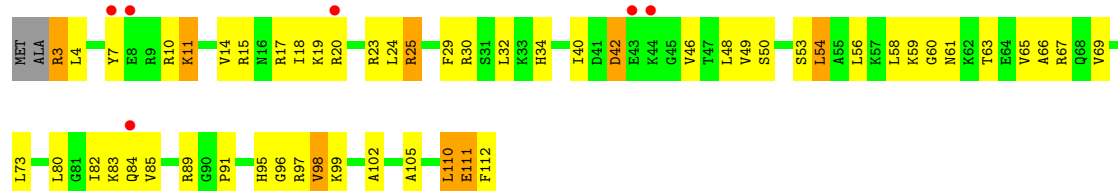
• Molecule 13: 50S Ribosomal Protein L17

Chain R:



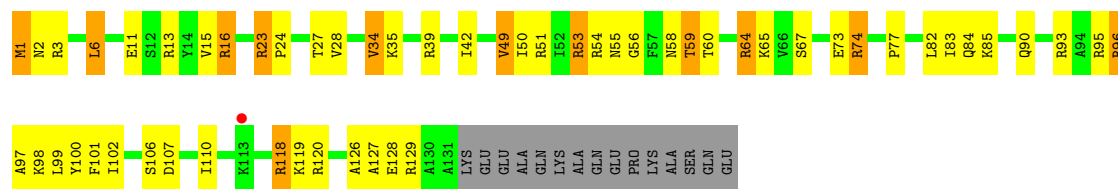
• Molecule 14: 50S Ribosomal Protein L18

Chain S:



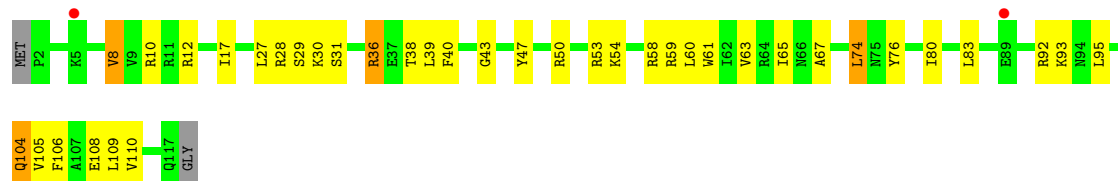
• Molecule 15: 50S Ribosomal Protein L19

Chain T:



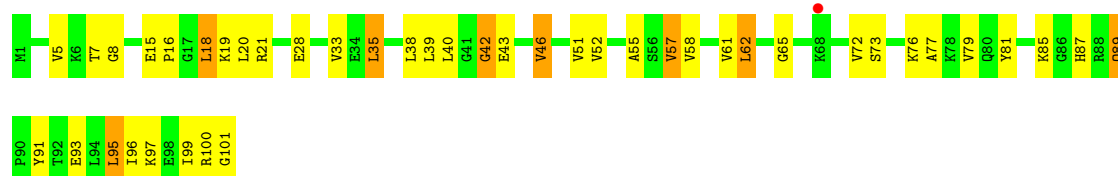
• Molecule 16: 50S Ribosomal Protein L20

Chain U:



- Molecule 17: 50S Ribosomal Protein L21

Chain V:



- Molecule 18: 50S Ribosomal Protein L22

Chain W:



- Molecule 19: 50S Ribosomal Protein L23

Chain X:



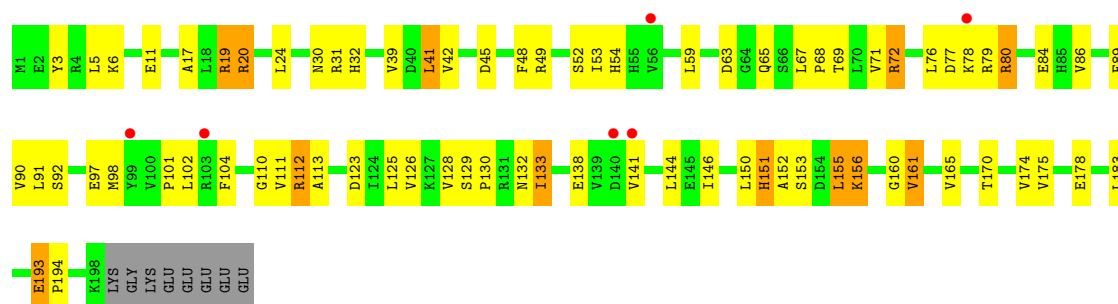
- Molecule 20: 50S Ribosomal Protein L24

Chain Y:



- Molecule 21: 50S Ribosomal Protein L25

Chain Z:



- Molecule 22: 50S Ribosomal Protein L27

Chain 0:





- Molecule 23: 50S Ribosomal Protein L28

Chain 1:



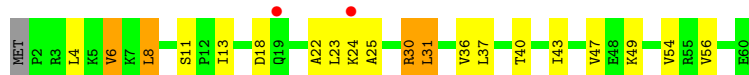
- Molecule 24: 50S Ribosomal Protein L29

Chain 2:



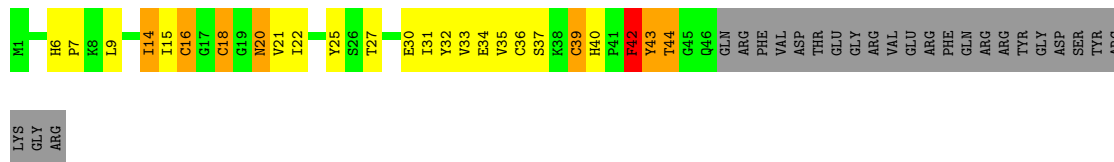
- Molecule 25: 50S Ribosomal Protein L30

Chain 3:



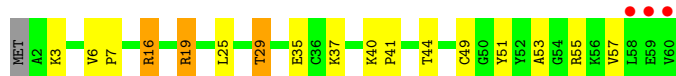
- Molecule 26: 50S Ribosomal Protein L31

Chain 4:



- Molecule 27: 50S Ribosomal Protein L32

Chain 5:



- Molecule 28: 50S Ribosomal Protein L33

Chain 6:

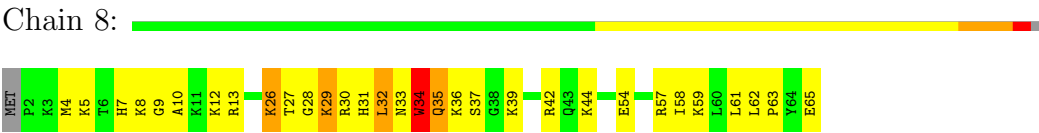


- Molecule 29: 50S Ribosomal Protein L34

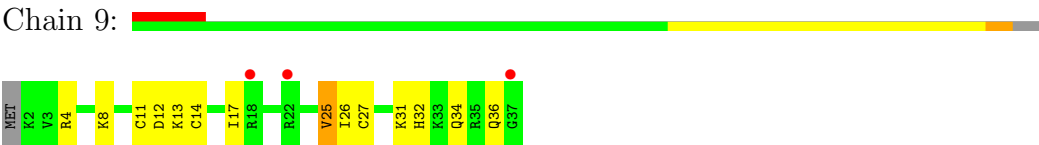
Chain 7:



• Molecule 30: 50S Ribosomal Protein L35



• Molecule 31: 50S Ribosomal Protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.24Å 451.44Å 621.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.00 49.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (49.75-3.00) 98.0 (49.75-3.00)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.218 , 0.254 0.457 , 0.459	Depositor DCC
R_{free} test set	57194 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 41.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 1142037 reflections	Xtriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	91067	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	A	1.16	149/67893 (0.2%)	1.60	1664/105982 (1.6%)
2	B	0.97	4/2878 (0.1%)	1.46	37/4490 (0.8%)
3	D	0.80	2/2186 (0.1%)	0.91	1/2944 (0.0%)
4	E	0.75	0/1588	0.92	0/2145
5	F	0.70	0/1615	0.90	2/2188 (0.1%)
6	G	0.59	0/1393	0.71	0/1892
7	H	0.60	0/1343	0.77	2/1820 (0.1%)
8	I	0.65	0/1053	0.84	1/1442 (0.1%)
9	N	0.65	0/1139	0.87	1/1538 (0.1%)
10	O	0.70	0/933	0.86	1/1257 (0.1%)
11	P	0.67	0/1148	0.93	2/1529 (0.1%)
12	Q	0.70	0/1143	0.86	0/1527
13	R	0.74	0/982	0.93	2/1312 (0.2%)
14	S	0.66	0/875	0.84	0/1168
15	T	0.66	0/1077	0.85	0/1444
16	U	0.79	0/977	0.88	0/1301
17	V	0.70	0/782	0.84	1/1049 (0.1%)
18	W	0.87	0/891	0.91	0/1197
19	X	0.78	0/756	0.84	1/1016 (0.1%)
20	Y	0.72	1/798 (0.1%)	0.87	1/1073 (0.1%)
21	Z	0.63	0/1555	0.80	1/2118 (0.0%)
22	0	0.73	0/602	0.81	0/804
23	1	0.77	0/752	0.99	2/1003 (0.2%)
24	2	0.71	0/590	0.83	0/781
25	3	0.64	0/463	0.82	0/623
26	4	0.70	0/358	0.82	1/487 (0.2%)
27	5	0.75	0/469	0.95	1/634 (0.2%)
28	6	0.92	2/456 (0.4%)	0.89	2/609 (0.3%)
29	7	0.92	0/426	1.00	0/561
30	8	0.73	1/516 (0.2%)	0.92	1/679 (0.1%)
31	9	0.68	0/300	0.83	0/395
All	All	1.05	159/97937 (0.2%)	1.45	1724/147008 (1.2%)

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
3	D	0	1
4	E	0	1
5	F	0	3
6	G	0	1
8	I	0	1
9	N	0	2
10	O	0	1
11	P	0	2
14	S	0	1
15	T	0	1
19	X	0	1
20	Y	0	1
23	1	0	1
26	4	0	2
30	8	0	2
All	All	0	21

The worst 5 of 159 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	A	N9-C4	-14.88	1.28	1.37
2	B	120	A	C6-N6	-11.72	1.24	1.33
28	6	13	CYS	CB-SG	-10.86	1.63	1.82
1	A	2296	U	C4-C5	10.51	1.53	1.43
1	A	2335	A	C6-N6	-9.99	1.25	1.33

The worst 5 of 1724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1779	U	C5-C6-N1	-22.12	111.64	122.70
1	A	2296	U	C5-C6-N1	-19.00	113.20	122.70
1	A	2104	G	N3-C2-N2	17.67	132.27	119.90
1	A	2296	U	N1-C2-N3	17.55	125.43	114.90
1	A	2296	U	C2-N3-C4	-17.29	116.62	127.00

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	274	ARG	Peptide
4	E	72	VAL	Peptide
5	F	129	PHE	Peptide
5	F	85	GLY	Peptide
5	F	89	VAL	Mainchain

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60620	0	30560	940	0
2	B	2573	0	1304	52	0
3	D	2136	0	2218	67	0
4	E	1555	0	1607	52	0
5	F	1580	0	1621	65	0
6	G	1368	0	1324	56	0
7	H	1317	0	1376	31	0
8	I	1038	0	1040	38	0
9	N	1112	0	1180	37	0
10	O	923	0	981	28	0
11	P	1131	0	1201	39	0
12	Q	1122	0	1179	45	0
13	R	968	0	1033	29	0
14	S	865	0	905	52	0
15	T	1063	0	1103	40	0
16	U	959	0	1019	29	0
17	V	771	0	830	24	0
18	W	881	0	935	21	0
19	X	742	0	799	18	0
20	Y	785	0	828	27	0
21	Z	1522	0	1511	52	0
22	0	594	0	604	31	0
23	1	745	0	804	31	0
24	2	588	0	643	24	0
25	3	458	0	503	13	0
26	4	349	0	336	19	0
27	5	455	0	472	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	6	449	0	462	18	0
29	7	418	0	467	15	0
30	8	509	0	565	28	0
31	9	297	0	316	10	0
32	6	1	0	0	0	0
32	7	1	0	0	0	0
32	8	1	0	0	0	0
32	A	428	0	0	0	0
32	B	5	0	0	0	0
32	D	1	0	0	0	0
32	E	1	0	0	0	0
32	F	2	0	0	0	0
32	P	1	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	6	1	0	0	0	0
33	9	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	1	0	0	0	0
34	1	2	0	0	0	0
34	A	696	0	0	56	0
34	B	9	0	0	0	0
34	D	3	0	0	0	0
34	E	1	0	0	0	0
34	F	5	0	0	0	0
34	P	5	0	0	0	0
34	Q	2	0	0	0	0
34	R	1	0	0	0	0
34	V	1	0	0	0	0
34	X	1	0	0	0	0
34	Y	1	0	0	0	0
All	All	91067	0	59726	1702	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 1702 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2296:U:O4	1:A:2335:A:N6	1.79	1.15
23:1:21:ARG:HH11	23:1:21:ARG:HG2	1.27	0.99
1:A:2304:G:H1	1:A:2312:U:H3	1.12	0.97
1:A:1310:G:OP2	29:7:9:ARG:NH1	1.97	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:139(A):G:N2	19:X:44:GLU:OE1	1.99	0.96

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/276 (99%)	258 (94%)	14 (5%)	1 (0%)	43	87
4	E	202/206 (98%)	189 (94%)	11 (5%)	2 (1%)	22	70
5	F	201/210 (96%)	188 (94%)	12 (6%)	1 (0%)	38	84
6	G	179/182 (98%)	151 (84%)	27 (15%)	1 (1%)	33	81
7	H	172/180 (96%)	158 (92%)	12 (7%)	2 (1%)	19	64
8	I	144/148 (97%)	113 (78%)	29 (20%)	2 (1%)	16	60
9	N	138/140 (99%)	126 (91%)	7 (5%)	5 (4%)	5	29
10	O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	P	147/150 (98%)	134 (91%)	13 (9%)	0	100	100
12	Q	139/141 (99%)	125 (90%)	14 (10%)	0	100	100
13	R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	S	108/112 (96%)	97 (90%)	10 (9%)	1 (1%)	25	73
15	T	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
16	U	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
17	V	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
18	W	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
19	X	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	Y	105/110 (96%)	95 (90%)	8 (8%)	2 (2%)	12	51
21	Z	196/206 (95%)	177 (90%)	16 (8%)	3 (2%)	15	58
22	0	74/85 (87%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	1	95/98 (97%)	93 (98%)	1 (1%)	1 (1%)	21	67
24	2	68/72 (94%)	65 (96%)	3 (4%)	0	100	100
25	3	57/60 (95%)	53 (93%)	4 (7%)	0	100	100
26	4	44/71 (62%)	38 (86%)	6 (14%)	0	100	100
27	5	57/60 (95%)	52 (91%)	5 (9%)	0	100	100
28	6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
29	7	46/49 (94%)	45 (98%)	0	1 (2%)	10	45
30	8	62/65 (95%)	59 (95%)	1 (2%)	2 (3%)	6	33
31	9	34/37 (92%)	34 (100%)	0	0	100	100
All	All	3373/3526 (96%)	3121 (92%)	228 (7%)	24 (1%)	30	78

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	N	23	LEU
9	N	24	GLY
30	8	34	TRP
30	8	35	GLN
5	F	89	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/218 (99%)	180 (84%)	35 (16%)	3	17
4	E	163/166 (98%)	135 (83%)	28 (17%)	3	14
5	F	159/166 (96%)	133 (84%)	26 (16%)	3	16
6	G	128/156 (82%)	106 (83%)	22 (17%)	3	14
7	H	141/148 (95%)	127 (90%)	14 (10%)	11	40
8	I	98/124 (79%)	67 (68%)	31 (32%)	0	2
9	N	117/119 (98%)	93 (80%)	24 (20%)	2	9
10	O	98/100 (98%)	90 (92%)	8 (8%)	17	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	114/116 (98%)	100 (88%)	14 (12%)	7	28
12	Q	111/111 (100%)	96 (86%)	15 (14%)	6	24
13	R	101/101 (100%)	83 (82%)	18 (18%)	2	14
14	S	84/88 (96%)	72 (86%)	12 (14%)	5	22
15	T	110/127 (87%)	92 (84%)	18 (16%)	3	16
16	U	93/94 (99%)	84 (90%)	9 (10%)	12	42
17	V	80/82 (98%)	64 (80%)	16 (20%)	2	10
18	W	89/92 (97%)	76 (85%)	13 (15%)	5	21
19	X	75/78 (96%)	70 (93%)	5 (7%)	23	64
20	Y	80/91 (88%)	63 (79%)	17 (21%)	1	8
21	Z	159/179 (89%)	141 (89%)	18 (11%)	9	33
22	0	59/67 (88%)	54 (92%)	5 (8%)	15	51
23	1	78/83 (94%)	67 (86%)	11 (14%)	5	23
24	2	65/67 (97%)	58 (89%)	7 (11%)	9	35
25	3	49/52 (94%)	42 (86%)	7 (14%)	5	22
26	4	39/63 (62%)	29 (74%)	10 (26%)	1	4
27	5	50/52 (96%)	45 (90%)	5 (10%)	11	39
28	6	50/52 (96%)	37 (74%)	13 (26%)	1	4
29	7	41/42 (98%)	34 (83%)	7 (17%)	3	15
30	8	52/55 (94%)	43 (83%)	9 (17%)	3	14
31	9	32/34 (94%)	29 (91%)	3 (9%)	13	44
All	All	2730/2923 (93%)	2310 (85%)	420 (15%)	4	19

5 of 420 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	33	ARG
14	S	3	ARG
28	6	6	ARG
11	P	98	GLU
12	Q	109	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
10	O	88	ASN
15	T	58	ASN
30	8	7	HIS
10	O	89	ASN
12	Q	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2808/2915 (96%)	552 (19%)	63 (2%)
2	B	119/122 (97%)	21 (17%)	0
All	All	2927/3037 (96%)	573 (19%)	63 (2%)

5 of 573 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	15	G
1	A	34	C
1	A	36	G
1	A	45	C

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1047	G
1	A	1379	A
1	A	2712	U
1	A	1048	A
1	A	1106	G

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 446 ligands modelled in this entry, 446 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.

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, 95th 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	2814/2915 (96%)	-0.05	57 (2%) 62 12	34, 56, 138, 189	0
2	B	120/122 (98%)	0.22	3 (2%) 54 11	63, 90, 111, 129	0
3	D	275/276 (99%)	0.04	4 (1%) 70 16	36, 55, 72, 119	0
4	E	204/206 (99%)	0.02	2 (0%) 79 22	35, 61, 84, 101	0
5	F	203/210 (96%)	0.00	1 (0%) 88 36	34, 67, 96, 136	0
6	G	181/182 (99%)	0.66	22 (12%) 5 1	92, 126, 146, 156	0
7	H	174/180 (96%)	0.32	10 (5%) 23 5	70, 92, 107, 122	0
8	I	146/148 (98%)	0.17	3 (2%) 60 12	60, 108, 127, 131	0
9	N	140/140 (100%)	-0.05	0 100 100	45, 63, 89, 101	0
10	O	122/122 (100%)	-0.05	0 100 100	46, 62, 82, 86	0
11	P	149/150 (99%)	0.28	8 (5%) 25 5	38, 70, 102, 111	0
12	Q	141/141 (100%)	0.10	2 (1%) 72 18	47, 67, 85, 94	0
13	R	118/118 (100%)	0.12	5 (4%) 35 7	42, 55, 73, 82	0
14	S	110/112 (98%)	0.32	6 (5%) 24 5	64, 82, 99, 110	0
15	T	131/146 (89%)	0.05	1 (0%) 83 26	55, 67, 101, 118	0
16	U	116/118 (98%)	0.06	2 (1%) 67 15	40, 56, 76, 86	0
17	V	101/101 (100%)	0.05	1 (0%) 79 22	40, 72, 90, 98	0
18	W	112/113 (99%)	-0.22	0 100 100	40, 48, 69, 95	0
19	X	95/96 (98%)	-0.07	0 100 100	47, 56, 80, 102	0
20	Y	107/110 (97%)	0.55	13 (12%) 5 1	59, 72, 96, 116	0
21	Z	198/206 (96%)	0.28	6 (3%) 48 9	73, 92, 115, 132	0
22	0	76/85 (89%)	0.14	0 100 100	53, 61, 76, 90	0
23	1	97/98 (98%)	0.15	2 (2%) 60 12	41, 61, 91, 108	0
24	2	70/72 (97%)	0.21	5 (7%) 16 4	55, 71, 88, 112	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	3	59/60 (98%)	0.14	2 (3%) 43 8	49, 64, 92, 112	0
26	4	46/71 (64%)	-0.12	0 100 100	113, 141, 152, 163	0
27	5	59/60 (98%)	-0.03	3 (5%) 27 6	37, 55, 73, 95	0
28	6	53/54 (98%)	0.05	1 (1%) 64 13	56, 65, 79, 82	0
29	7	48/49 (97%)	0.41	4 (8%) 11 3	36, 40, 64, 83	0
30	8	64/65 (98%)	0.03	0 100 100	46, 53, 62, 72	0
31	9	36/37 (97%)	0.83	3 (8%) 11 3	58, 68, 81, 91	0
All	All	6365/6563 (96%)	0.06	166 (2%) 54 10	34, 62, 126, 189	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2117	A	7.5
7	H	171	LEU	7.3
5	F	208	GLY	7.0
1	A	2116	G	6.2
1	A	652(B)	A	5.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3123	1/1	0.27	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3348	1/1	0.24	-	50,50,50,50	0
32	MG	A	3010	1/1	0.55	-	60,60,60,60	0
32	MG	A	3150	1/1	0.53	-	58,58,58,58	0
32	MG	A	3017	1/1	0.23	-	41,41,41,41	0
32	MG	A	3070	1/1	0.44	-	50,50,50,50	0
32	MG	A	3042	1/1	0.30	-	51,51,51,51	0
32	MG	A	3119	1/1	0.26	-	53,53,53,53	0
32	MG	A	3294	1/1	0.23	-	50,50,50,50	0
32	MG	A	3363	1/1	0.23	-	50,50,50,50	0
32	MG	A	3030	1/1	0.22	-	43,43,43,43	0
32	MG	A	3263	1/1	0.16	-	39,39,39,39	0
32	MG	A	3272	1/1	0.13	-	35,35,35,35	0
32	MG	A	3388	1/1	0.44	-	69,69,69,69	0
32	MG	A	3002	1/1	0.16	-	59,59,59,59	0
32	MG	A	3032	1/1	0.11	-	74,74,74,74	0
32	MG	A	3340	1/1	0.17	-	41,41,41,41	0
32	MG	A	3410	1/1	0.15	-	45,45,45,45	0
32	MG	A	3039	1/1	0.63	-	49,49,49,49	0
32	MG	A	3399	1/1	0.10	-	85,85,85,85	0
32	MG	A	3051	1/1	0.25	-	54,54,54,54	0
32	MG	A	3101	1/1	0.51	-	71,71,71,71	0
32	MG	A	3049	1/1	0.86	-	43,43,43,43	0
33	ZN	5	101	1/1	0.06	-	65,65,65,65	0
32	MG	A	3360	1/1	0.05	-	63,63,63,63	0
32	MG	A	3132	1/1	0.52	-	64,64,64,64	0
32	MG	A	3122	1/1	0.27	-	35,35,35,35	0
32	MG	B	205	1/1	0.11	-	70,70,70,70	0
32	MG	A	3131	1/1	0.49	-	78,78,78,78	0
32	MG	A	3343	1/1	0.50	-	100,100,100,100	0
32	MG	A	3216	1/1	0.31	-	53,53,53,53	0
32	MG	A	3256	1/1	0.43	-	56,56,56,56	0
32	MG	A	3108	1/1	0.34	-	46,46,46,46	0
32	MG	A	3267	1/1	0.09	-	54,54,54,54	0
32	MG	A	3330	1/1	0.12	-	62,62,62,62	0
32	MG	A	3087	1/1	0.96	-	82,82,82,82	0
32	MG	A	3261	1/1	0.15	-	70,70,70,70	0
32	MG	A	3068	1/1	0.37	-	53,53,53,53	0
32	MG	A	3283	1/1	0.12	-	52,52,52,52	0
32	MG	A	3231	1/1	0.24	-	43,43,43,43	0
32	MG	A	3240	1/1	0.46	-	38,38,38,38	0
32	MG	A	3331	1/1	0.11	-	53,53,53,53	0
32	MG	A	3194	1/1	0.16	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3242	1/1	0.28	-	35,35,35,35	0
32	MG	A	3018	1/1	0.45	-	39,39,39,39	0
32	MG	A	3223	1/1	0.28	-	64,64,64,64	0
32	MG	A	3179	1/1	0.24	-	51,51,51,51	0
32	MG	A	3065	1/1	0.31	-	32,32,32,32	0
32	MG	D	301	1/1	0.07	-	40,40,40,40	0
32	MG	A	3006	1/1	0.32	-	48,48,48,48	0
32	MG	A	3180	1/1	0.49	-	59,59,59,59	0
32	MG	A	3098	1/1	0.35	-	61,61,61,61	0
32	MG	A	3361	1/1	0.21	-	72,72,72,72	0
32	MG	A	3063	1/1	0.32	-	58,58,58,58	0
32	MG	A	3359	1/1	0.12	-	67,67,67,67	0
32	MG	A	3207	1/1	1.70	-	79,79,79,79	0
32	MG	A	3023	1/1	0.32	-	57,57,57,57	0
32	MG	A	3059	1/1	0.69	-	52,52,52,52	0
32	MG	A	3342	1/1	0.17	-	51,51,51,51	0
32	MG	A	3050	1/1	0.73	-	71,71,71,71	0
32	MG	B	203	1/1	0.33	-	61,61,61,61	0
32	MG	A	3184	1/1	0.44	-	42,42,42,42	0
32	MG	A	3384	1/1	0.12	-	63,63,63,63	0
32	MG	A	3102	1/1	0.39	-	57,57,57,57	0
32	MG	A	3210	1/1	0.35	-	38,38,38,38	0
32	MG	A	3115	1/1	0.24	-	34,34,34,34	0
32	MG	A	3407	1/1	0.20	-	79,79,79,79	0
32	MG	A	3095	1/1	0.61	-	64,64,64,64	0
32	MG	A	3220	1/1	0.22	-	47,47,47,47	0
32	MG	A	3135	1/1	0.75	-	64,64,64,64	0
32	MG	A	3165	1/1	1.22	-	59,59,59,59	0
32	MG	A	3217	1/1	0.21	-	38,38,38,38	0
32	MG	A	3125	1/1	0.97	-	63,63,63,63	0
32	MG	F	302	1/1	1.13	-	64,64,64,64	0
32	MG	A	3080	1/1	0.43	-	51,51,51,51	0
32	MG	A	3420	1/1	0.17	-	75,75,75,75	0
32	MG	A	3147	1/1	0.24	-	36,36,36,36	0
32	MG	A	3034	1/1	0.24	-	65,65,65,65	0
32	MG	A	3249	1/1	0.45	-	39,39,39,39	0
32	MG	A	3145	1/1	0.43	-	78,78,78,78	0
32	MG	A	3209	1/1	0.13	-	53,53,53,53	0
32	MG	A	3332	1/1	0.11	-	56,56,56,56	0
32	MG	A	3282	1/1	0.17	-	61,61,61,61	0
32	MG	A	3003	1/1	0.62	-	64,64,64,64	0
32	MG	A	3202	1/1	0.29	-	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3398	1/1	0.56	-	95,95,95,95	0
32	MG	A	3110	1/1	0.42	-	60,60,60,60	0
32	MG	A	3107	1/1	0.75	-	70,70,70,70	0
32	MG	A	3254	1/1	0.35	-	59,59,59,59	0
32	MG	A	3061	1/1	0.20	-	54,54,54,54	0
32	MG	A	3028	1/1	0.26	-	52,52,52,52	0
32	MG	A	3375	1/1	0.12	-	61,61,61,61	0
32	MG	A	3044	1/1	0.65	-	43,43,43,43	0
32	MG	A	3215	1/1	0.67	-	69,69,69,69	0
32	MG	A	3345	1/1	0.24	-	76,76,76,76	0
32	MG	A	3386	1/1	0.29	-	72,72,72,72	0
32	MG	A	3016	1/1	0.22	-	42,42,42,42	0
32	MG	A	3327	1/1	0.13	-	47,47,47,47	0
32	MG	A	3072	1/1	0.31	-	38,38,38,38	0
32	MG	A	3159	1/1	0.41	-	55,55,55,55	0
32	MG	A	3086	1/1	0.29	-	65,65,65,65	0
32	MG	A	3413	1/1	0.09	-	89,89,89,89	0
32	MG	A	3252	1/1	0.25	-	43,43,43,43	0
32	MG	A	3146	1/1	0.21	-	70,70,70,70	0
32	MG	A	3255	1/1	0.26	-	59,59,59,59	0
32	MG	A	3276	1/1	0.16	-	46,46,46,46	0
32	MG	A	3204	1/1	0.60	-	75,75,75,75	0
32	MG	A	3367	1/1	0.20	-	57,57,57,57	0
32	MG	A	3310	1/1	0.19	-	67,67,67,67	0
32	MG	A	3100	1/1	0.53	-	79,79,79,79	0
32	MG	A	3266	1/1	0.16	-	43,43,43,43	0
32	MG	A	3027	1/1	0.69	-	72,72,72,72	0
32	MG	A	3157	1/1	0.33	-	59,59,59,59	0
32	MG	A	3198	1/1	0.31	-	67,67,67,67	0
32	MG	A	3230	1/1	0.20	-	46,46,46,46	0
32	MG	A	3289	1/1	0.41	-	43,43,43,43	0
32	MG	A	3109	1/1	0.48	-	60,60,60,60	0
32	MG	A	3387	1/1	0.15	-	58,58,58,58	0
33	ZN	6	101	1/1	0.09	-	86,86,86,86	0
32	MG	A	3419	1/1	0.10	-	69,69,69,69	0
32	MG	E	301	1/1	0.27	-	37,37,37,37	0
32	MG	A	3192	1/1	0.56	-	77,77,77,77	0
32	MG	A	3011	1/1	0.24	-	41,41,41,41	0
32	MG	A	3040	1/1	0.36	-	46,46,46,46	0
32	MG	A	3339	1/1	0.09	-	39,39,39,39	0
32	MG	A	3013	1/1	0.50	-	71,71,71,71	0
32	MG	A	3071	1/1	0.25	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3238	1/1	0.32	-	67,67,67,67	0
32	MG	A	3138	1/1	0.88	-	70,70,70,70	0
32	MG	A	3060	1/1	0.34	-	65,65,65,65	0
32	MG	A	3347	1/1	0.29	-	54,54,54,54	0
32	MG	A	3302	1/1	0.12	-	38,38,38,38	0
32	MG	A	3311	1/1	0.16	-	64,64,64,64	0
32	MG	A	3093	1/1	0.30	-	71,71,71,71	0
32	MG	A	3408	1/1	0.29	-	72,72,72,72	0
32	MG	A	3218	1/1	0.22	-	48,48,48,48	0
32	MG	A	3334	1/1	0.39	-	87,87,87,87	0
32	MG	A	3274	1/1	0.15	-	51,51,51,51	0
32	MG	A	3389	1/1	0.27	-	67,67,67,67	0
32	MG	A	3337	1/1	0.12	-	48,48,48,48	0
32	MG	A	3164	1/1	0.36	-	55,55,55,55	0
32	MG	A	3036	1/1	0.23	-	39,39,39,39	0
32	MG	A	3008	1/1	0.39	-	43,43,43,43	0
32	MG	B	201	1/1	0.40	-	75,75,75,75	0
32	MG	A	3193	1/1	0.30	-	75,75,75,75	0
32	MG	A	3246	1/1	0.37	-	44,44,44,44	0
32	MG	A	3379	1/1	0.15	-	79,79,79,79	0
32	MG	A	3148	1/1	0.20	-	41,41,41,41	0
32	MG	A	3189	1/1	0.56	-	50,50,50,50	0
32	MG	A	3094	1/1	0.20	-	46,46,46,46	0
32	MG	A	3167	1/1	0.21	-	39,39,39,39	0
32	MG	A	3221	1/1	0.77	-	104,104,104,104	0
32	MG	A	3047	1/1	0.40	-	58,58,58,58	0
32	MG	B	202	1/1	0.31	-	86,86,86,86	0
32	MG	A	3412	1/1	0.30	-	68,68,68,68	0
32	MG	A	3082	1/1	0.40	-	62,62,62,62	0
32	MG	A	3299	1/1	0.16	-	55,55,55,55	0
32	MG	A	3425	1/1	0.16	-	40,40,40,40	0
32	MG	A	3318	1/1	0.16	-	57,57,57,57	0
32	MG	A	3203	1/1	0.19	-	82,82,82,82	0
32	MG	A	3090	1/1	0.42	-	63,63,63,63	0
32	MG	A	3280	1/1	0.13	-	42,42,42,42	0
32	MG	A	3219	1/1	0.32	-	69,69,69,69	0
32	MG	A	3045	1/1	0.49	-	65,65,65,65	0
32	MG	A	3033	1/1	0.64	-	68,68,68,68	0
32	MG	A	3121	1/1	0.32	-	56,56,56,56	0
32	MG	P	201	1/1	0.48	-	58,58,58,58	0
32	MG	A	3414	1/1	0.07	-	32,32,32,32	0
32	MG	A	3041	1/1	0.26	-	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3365	1/1	0.19	-	68,68,68,68	0
32	MG	A	3213	1/1	0.24	-	58,58,58,58	0
32	MG	A	3264	1/1	0.06	-	58,58,58,58	0
32	MG	A	3344	1/1	0.13	-	89,89,89,89	0
32	MG	A	3141	1/1	0.46	-	62,62,62,62	0
32	MG	A	3303	1/1	0.14	-	55,55,55,55	0
32	MG	A	3133	1/1	0.20	-	44,44,44,44	0
32	MG	A	3356	1/1	0.61	-	68,68,68,68	0
32	MG	A	3161	1/1	0.35	-	56,56,56,56	0
32	MG	A	3426	1/1	0.14	-	81,81,81,81	0
32	MG	A	3333	1/1	0.41	-	72,72,72,72	0
32	MG	A	3397	1/1	0.48	-	60,60,60,60	0
32	MG	B	204	1/1	0.23	-	74,74,74,74	0
32	MG	A	3114	1/1	0.39	-	46,46,46,46	0
32	MG	A	3373	1/1	0.10	-	50,50,50,50	0
32	MG	A	3309	1/1	0.21	-	65,65,65,65	0
32	MG	A	3067	1/1	0.20	-	61,61,61,61	0
32	MG	A	3285	1/1	0.15	-	46,46,46,46	0
32	MG	A	3224	1/1	0.28	-	53,53,53,53	0
32	MG	A	3118	1/1	0.45	-	52,52,52,52	0
32	MG	A	3143	1/1	0.22	-	47,47,47,47	0
32	MG	A	3316	1/1	0.13	-	66,66,66,66	0
32	MG	A	3022	1/1	0.51	-	49,49,49,49	0
32	MG	A	3055	1/1	0.33	-	67,67,67,67	0
32	MG	A	3196	1/1	0.21	-	55,55,55,55	0
32	MG	A	3341	1/1	0.13	-	35,35,35,35	0
32	MG	A	3286	1/1	0.07	-	37,37,37,37	0
32	MG	A	3077	1/1	0.29	-	60,60,60,60	0
32	MG	A	3177	1/1	0.56	-	62,62,62,62	0
32	MG	A	3074	1/1	0.09	-	70,70,70,70	0
32	MG	A	3188	1/1	0.16	-	57,57,57,57	0
32	MG	A	3128	1/1	0.52	-	59,59,59,59	0
32	MG	A	3404	1/1	0.11	-	35,35,35,35	0
32	MG	A	3417	1/1	0.25	-	50,50,50,50	0
32	MG	8	101	1/1	0.31	-	49,49,49,49	0
32	MG	A	3305	1/1	0.14	-	39,39,39,39	0
32	MG	A	3385	1/1	0.20	-	71,71,71,71	0
32	MG	A	3225	1/1	0.26	-	65,65,65,65	0
32	MG	A	3091	1/1	0.62	-	66,66,66,66	0
32	MG	A	3160	1/1	0.60	-	55,55,55,55	0
32	MG	A	3298	1/1	0.16	-	62,62,62,62	0
32	MG	A	3313	1/1	0.24	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3092	1/1	0.26	-	39,39,39,39	0
32	MG	A	3378	1/1	0.15	-	91,91,91,91	0
32	MG	A	3314	1/1	0.28	-	75,75,75,75	0
32	MG	A	3308	1/1	0.18	-	56,56,56,56	0
32	MG	A	3195	1/1	0.88	-	66,66,66,66	0
32	MG	A	3323	1/1	0.32	-	36,36,36,36	0
32	MG	A	3172	1/1	0.33	-	60,60,60,60	0
32	MG	A	3162	1/1	0.16	-	46,46,46,46	0
32	MG	A	3287	1/1	0.18	-	52,52,52,52	0
32	MG	A	3268	1/1	0.07	-	34,34,34,34	0
32	MG	A	3346	1/1	0.18	-	85,85,85,85	0
32	MG	A	3007	1/1	0.38	-	54,54,54,54	0
32	MG	A	3099	1/1	0.29	-	62,62,62,62	0
32	MG	A	3251	1/1	0.20	-	42,42,42,42	0
32	MG	A	3081	1/1	0.37	-	55,55,55,55	0
32	MG	A	3021	1/1	0.47	-	61,61,61,61	0
32	MG	A	3262	1/1	0.28	-	46,46,46,46	0
32	MG	A	3052	1/1	0.51	-	75,75,75,75	0
32	MG	A	3166	1/1	0.16	-	42,42,42,42	0
32	MG	A	3129	1/1	0.22	-	39,39,39,39	0
32	MG	A	3247	1/1	0.27	-	67,67,67,67	0
32	MG	A	3064	1/1	0.21	-	56,56,56,56	0
32	MG	A	3151	1/1	0.58	-	38,38,38,38	0
32	MG	A	3377	1/1	0.31	-	94,94,94,94	0
32	MG	A	3300	1/1	0.16	-	36,36,36,36	0
32	MG	A	3144	1/1	0.31	-	35,35,35,35	0
32	MG	A	3066	1/1	0.19	-	48,48,48,48	0
33	ZN	9	101	1/1	0.04	-	87,87,87,87	0
32	MG	A	3245	1/1	0.17	-	52,52,52,52	0
32	MG	A	3326	1/1	0.06	-	34,34,34,34	0
32	MG	A	3183	1/1	0.55	-	47,47,47,47	0
32	MG	A	3416	1/1	0.13	-	39,39,39,39	0
32	MG	A	3158	1/1	0.36	-	48,48,48,48	0
32	MG	A	3269	1/1	0.13	-	57,57,57,57	0
32	MG	A	3015	1/1	0.24	-	61,61,61,61	0
32	MG	A	3024	1/1	0.93	-	49,49,49,49	0
32	MG	A	3250	1/1	0.21	-	41,41,41,41	0
32	MG	A	3075	1/1	0.34	-	66,66,66,66	0
33	ZN	Y	201	1/1	0.03	-	128,128,128,128	0
32	MG	A	3124	1/1	0.22	-	80,80,80,80	0
32	MG	A	3004	1/1	0.78	-	44,44,44,44	0
32	MG	A	3236	1/1	0.61	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	3155	1/1	0.33	-	69,69,69,69	0
32	MG	A	3369	1/1	0.28	-	50,50,50,50	0
32	MG	A	3402	1/1	0.25	-	53,53,53,53	0
32	MG	A	3259	1/1	0.43	-	56,56,56,56	0
32	MG	A	3153	1/1	0.26	-	57,57,57,57	0
32	MG	A	3201	1/1	0.15	-	48,48,48,48	0
32	MG	A	3175	1/1	0.68	-	59,59,59,59	0
32	MG	A	3306	1/1	0.24	-	49,49,49,49	0
32	MG	A	3393	1/1	0.21	-	37,37,37,37	0
32	MG	A	3037	1/1	0.17	-	41,41,41,41	0
32	MG	A	3427	1/1	0.13	-	44,44,44,44	0
32	MG	A	3403	1/1	0.19	-	70,70,70,70	0
32	MG	A	3170	1/1	0.28	-	50,50,50,50	0
32	MG	A	3054	1/1	0.77	-	61,61,61,61	0
32	MG	A	3197	1/1	0.14	-	74,74,74,74	0
32	MG	A	3035	1/1	1.05	-	49,49,49,49	0
32	MG	A	3111	1/1	0.26	-	42,42,42,42	0
32	MG	A	3260	1/1	0.22	-	46,46,46,46	0
32	MG	A	3152	1/1	0.31	-	62,62,62,62	0
32	MG	A	3366	1/1	0.27	-	78,78,78,78	0
32	MG	A	3053	1/1	0.35	-	43,43,43,43	0
32	MG	A	3228	1/1	0.52	-	67,67,67,67	0
32	MG	A	3358	1/1	0.33	-	63,63,63,63	0
32	MG	A	3248	1/1	0.21	-	41,41,41,41	0
32	MG	A	3182	1/1	0.30	-	39,39,39,39	0
32	MG	A	3351	1/1	0.11	-	40,40,40,40	0
32	MG	A	3304	1/1	0.10	-	88,88,88,88	0
32	MG	A	3227	1/1	0.46	-	55,55,55,55	0
32	MG	A	3335	1/1	0.20	-	42,42,42,42	0
32	MG	A	3383	1/1	0.30	-	49,49,49,49	0
32	MG	A	3112	1/1	0.15	-	51,51,51,51	0
32	MG	A	3297	1/1	0.14	-	54,54,54,54	0
32	MG	A	3097	1/1	0.27	-	40,40,40,40	0
32	MG	A	3257	1/1	0.30	-	64,64,64,64	0
32	MG	A	3149	1/1	0.42	-	58,58,58,58	0
32	MG	A	3271	1/1	0.23	-	37,37,37,37	0
32	MG	A	3243	1/1	0.39	-	47,47,47,47	0
32	MG	A	3422	1/1	0.08	-	130,130,130,130	0
32	MG	A	3273	1/1	0.21	-	48,48,48,48	0
32	MG	A	3400	1/1	0.28	-	59,59,59,59	0
32	MG	A	3395	1/1	0.22	-	65,65,65,65	0
32	MG	A	3048	1/1	0.26	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3025	1/1	0.23	-	51,51,51,51	0
32	MG	A	3174	1/1	0.52	-	61,61,61,61	0
32	MG	A	3005	1/1	0.17	-	36,36,36,36	0
32	MG	A	3181	1/1	0.16	-	50,50,50,50	0
32	MG	A	3428	1/1	0.07	-	72,72,72,72	0
32	MG	A	3222	1/1	0.38	-	80,80,80,80	0
32	MG	A	3239	1/1	0.24	-	63,63,63,63	0
32	MG	A	3126	1/1	0.48	-	72,72,72,72	0
32	MG	A	3353	1/1	0.24	-	37,37,37,37	0
32	MG	A	3043	1/1	0.58	-	72,72,72,72	0
32	MG	A	3026	1/1	0.20	-	53,53,53,53	0
32	MG	A	3130	1/1	0.33	-	49,49,49,49	0
32	MG	A	3073	1/1	0.69	-	71,71,71,71	0
32	MG	A	3096	1/1	0.36	-	62,62,62,62	0
32	MG	A	3301	1/1	0.10	-	37,37,37,37	0
32	MG	A	3372	1/1	0.21	-	44,44,44,44	0
32	MG	A	3139	1/1	0.87	-	74,74,74,74	0
32	MG	A	3185	1/1	0.47	-	47,47,47,47	0
32	MG	A	3329	1/1	0.17	-	69,69,69,69	0
32	MG	A	3411	1/1	0.13	-	37,37,37,37	0
32	MG	A	3423	1/1	0.07	-	60,60,60,60	0
32	MG	A	3200	1/1	0.30	-	37,37,37,37	0
32	MG	A	3325	1/1	0.60	-	94,94,94,94	0
32	MG	A	3085	1/1	0.39	-	58,58,58,58	0
32	MG	A	3352	1/1	0.18	-	41,41,41,41	0
32	MG	A	3038	1/1	0.58	-	50,50,50,50	0
32	MG	A	3178	1/1	0.51	-	78,78,78,78	0
32	MG	A	3120	1/1	0.28	-	47,47,47,47	0
32	MG	A	3270	1/1	0.18	-	47,47,47,47	0
32	MG	A	3083	1/1	0.22	-	51,51,51,51	0
32	MG	A	3390	1/1	0.12	-	56,56,56,56	0
32	MG	A	3127	1/1	1.72	-	78,78,78,78	0
32	MG	A	3140	1/1	0.34	-	46,46,46,46	0
32	MG	A	3088	1/1	0.27	-	53,53,53,53	0
32	MG	A	3370	1/1	0.23	-	40,40,40,40	0
32	MG	A	3154	1/1	0.75	-	52,52,52,52	0
32	MG	A	3187	1/1	0.71	-	66,66,66,66	0
32	MG	A	3265	1/1	0.21	-	59,59,59,59	0
32	MG	A	3069	1/1	0.28	-	60,60,60,60	0
32	MG	A	3350	1/1	0.23	-	61,61,61,61	0
32	MG	A	3062	1/1	0.34	-	53,53,53,53	0
32	MG	A	3076	1/1	0.51	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3190	1/1	0.21	-	66,66,66,66	0
32	MG	A	3237	1/1	0.18	-	39,39,39,39	0
32	MG	A	3046	1/1	0.54	-	53,53,53,53	0
32	MG	A	3258	1/1	0.20	-	44,44,44,44	0
32	MG	A	3278	1/1	0.23	-	40,40,40,40	0
32	MG	A	3396	1/1	0.19	-	52,52,52,52	0
32	MG	A	3205	1/1	0.38	-	53,53,53,53	0
32	MG	A	3229	1/1	0.32	-	54,54,54,54	0
32	MG	A	3106	1/1	0.35	-	80,80,80,80	0
32	MG	A	3380	1/1	0.22	-	53,53,53,53	0
32	MG	A	3312	1/1	0.31	-	54,54,54,54	0
32	MG	A	3029	1/1	0.33	-	43,43,43,43	0
32	MG	A	3019	1/1	0.43	-	53,53,53,53	0
32	MG	A	3406	1/1	0.21	-	65,65,65,65	0
32	MG	A	3142	1/1	0.19	-	42,42,42,42	0
32	MG	F	301	1/1	0.49	-	58,58,58,58	0
32	MG	A	3405	1/1	0.19	-	59,59,59,59	0
32	MG	A	3296	1/1	0.16	-	71,71,71,71	0
32	MG	A	3392	1/1	0.28	-	56,56,56,56	0
32	MG	A	3105	1/1	0.36	-	47,47,47,47	0
32	MG	A	3235	1/1	0.30	-	39,39,39,39	0
32	MG	A	3241	1/1	0.13	-	53,53,53,53	0
32	MG	A	3291	1/1	0.24	-	50,50,50,50	0
32	MG	A	3211	1/1	0.13	-	64,64,64,64	0
32	MG	A	3136	1/1	0.69	-	60,60,60,60	0
32	MG	A	3031	1/1	0.28	-	68,68,68,68	0
32	MG	A	3319	1/1	0.19	-	53,53,53,53	0
32	MG	A	3349	1/1	0.17	-	78,78,78,78	0
32	MG	A	3020	1/1	0.20	-	52,52,52,52	0
32	MG	A	3232	1/1	0.46	-	56,56,56,56	0
32	MG	A	3295	1/1	0.16	-	66,66,66,66	0
32	MG	A	3113	1/1	0.52	-	39,39,39,39	0
32	MG	A	3169	1/1	0.17	-	53,53,53,53	0
32	MG	A	3137	1/1	0.30	-	65,65,65,65	0
32	MG	A	3012	1/1	0.12	-	52,52,52,52	0
32	MG	A	3418	1/1	0.07	-	97,97,97,97	0
32	MG	A	3324	1/1	0.20	-	95,95,95,95	0
32	MG	A	3084	1/1	0.54	-	54,54,54,54	0
32	MG	A	3176	1/1	0.45	-	58,58,58,58	0
32	MG	A	3338	1/1	0.13	-	44,44,44,44	0
32	MG	A	3381	1/1	0.34	-	63,63,63,63	0
32	MG	A	3409	1/1	0.12	-	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3244	1/1	0.30	-	41,41,41,41	0
32	MG	A	3253	1/1	0.34	-	63,63,63,63	0
32	MG	A	3057	1/1	0.31	-	55,55,55,55	0
32	MG	A	3322	1/1	0.14	-	64,64,64,64	0
32	MG	A	3104	1/1	0.86	-	56,56,56,56	0
32	MG	A	3320	1/1	0.18	-	35,35,35,35	0
32	MG	A	3156	1/1	0.30	-	72,72,72,72	0
32	MG	A	3277	1/1	0.14	-	40,40,40,40	0
32	MG	A	3368	1/1	0.30	-	51,51,51,51	0
32	MG	A	3421	1/1	0.18	-	79,79,79,79	0
32	MG	A	3186	1/1	0.23	-	54,54,54,54	0
32	MG	A	3199	1/1	0.21	-	69,69,69,69	0
32	MG	A	3233	1/1	0.16	-	36,36,36,36	0
32	MG	A	3293	1/1	0.17	-	42,42,42,42	0
32	MG	A	3401	1/1	0.16	-	49,49,49,49	0
32	MG	A	3315	1/1	0.12	-	94,94,94,94	0
32	MG	A	3328	1/1	0.10	-	44,44,44,44	0
32	MG	A	3214	1/1	0.19	-	53,53,53,53	0
32	MG	A	3226	1/1	0.20	-	51,51,51,51	0
32	MG	A	3307	1/1	0.25	-	48,48,48,48	0
32	MG	A	3357	1/1	0.20	-	49,49,49,49	0
32	MG	A	3173	1/1	0.35	-	69,69,69,69	0
32	MG	A	3116	1/1	0.26	-	44,44,44,44	0
32	MG	6	102	1/1	0.41	-	64,64,64,64	0
32	MG	A	3371	1/1	0.12	-	38,38,38,38	0
32	MG	A	3134	1/1	0.23	-	42,42,42,42	0
33	ZN	4	101	1/1	0.05	-	176,176,176,176	0
32	MG	A	3275	1/1	0.18	-	42,42,42,42	0
32	MG	A	3206	1/1	0.25	-	52,52,52,52	0
32	MG	A	3089	1/1	0.17	-	70,70,70,70	0
32	MG	A	3234	1/1	0.29	-	44,44,44,44	0
32	MG	A	3009	1/1	0.30	-	46,46,46,46	0
32	MG	A	3163	1/1	0.27	-	58,58,58,58	0
32	MG	A	3056	1/1	0.26	-	51,51,51,51	0
32	MG	A	3424	1/1	0.28	-	94,94,94,94	0
32	MG	A	3391	1/1	0.20	-	81,81,81,81	0
32	MG	A	3079	1/1	0.32	-	52,52,52,52	0
32	MG	A	3288	1/1	0.12	-	42,42,42,42	0
32	MG	A	3364	1/1	0.11	-	35,35,35,35	0
32	MG	A	3281	1/1	0.11	-	48,48,48,48	0
32	MG	A	3078	1/1	0.59	-	73,73,73,73	0
32	MG	A	3336	1/1	0.31	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	3362	1/1	0.23	-	67,67,67,67	0
32	MG	A	3321	1/1	0.11	-	36,36,36,36	0
32	MG	A	3382	1/1	0.25	-	57,57,57,57	0
32	MG	7	101	1/1	0.33	-	52,52,52,52	0
32	MG	A	3058	1/1	0.86	-	60,60,60,60	0
32	MG	A	3279	1/1	0.07	-	36,36,36,36	0
32	MG	A	3355	1/1	0.19	-	53,53,53,53	0
32	MG	A	3103	1/1	0.56	-	33,33,33,33	0
32	MG	A	3374	1/1	0.09	-	43,43,43,43	0
32	MG	A	3191	1/1	0.78	-	63,63,63,63	0
32	MG	A	3117	1/1	0.45	-	57,57,57,57	0
32	MG	A	3292	1/1	0.42	-	52,52,52,52	0
32	MG	A	3001	1/1	0.34	-	35,35,35,35	0
32	MG	A	3376	1/1	0.19	-	98,98,98,98	0
32	MG	A	3014	1/1	0.58	-	41,41,41,41	0
32	MG	A	3354	1/1	0.09	-	42,42,42,42	0
32	MG	A	3394	1/1	0.13	-	37,37,37,37	0
32	MG	A	3415	1/1	0.18	-	81,81,81,81	0
32	MG	A	3284	1/1	0.20	-	50,50,50,50	0
32	MG	A	3212	1/1	0.89	-	74,74,74,74	0
32	MG	A	3290	1/1	0.16	-	39,39,39,39	0
32	MG	A	3171	1/1	0.30	-	49,49,49,49	0
32	MG	A	3208	1/1	0.32	-	60,60,60,60	0
32	MG	A	3168	1/1	0.42	-	52,52,52,52	0
32	MG	A	3317	1/1	0.06	-	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.