



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 01:20 AM GMT

PDB ID : 2QAM
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with neomycin. This file contains the 50S subunit of the first 70S ribosome, with neomycin bound. The entire crystal structure contains two 70S ribosomes and is described in remark 400.
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-15
Resolution : 3.21 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>

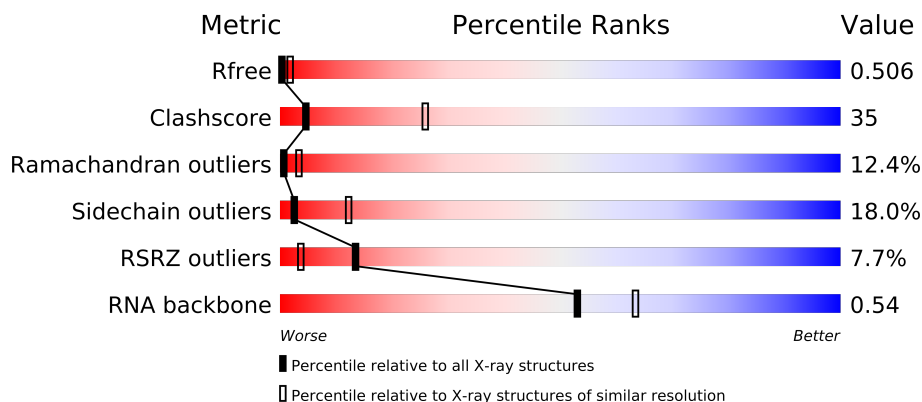
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.21 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	1205 (3.30-3.14)
Clashscore	79885	1072 (3.28-3.16)
Ramachandran outliers	78287	1052 (3.28-3.16)
Sidechain outliers	78261	1051 (3.28-3.16)
RSRZ outliers	66119	1206 (3.30-3.14)
RNA backbone	1838	1004 (3.74-2.70)

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	120	
2	B	2904	
3	I	141	
4	C	272	
5	D	209	
6	K	123	
7	P	114	
8	E	201	
9	Y	58	
10	0	56	
11	4	38	
12	1	54	

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Mol	Chain	Length	Quality of chain
13	3	64	
14	V	94	
15	2	46	
16	L	144	
17	M	136	
18	X	63	
19	H	149	
20	J	142	
21	N	127	
22	O	117	
23	Q	117	
24	S	110	
25	U	103	
26	F	178	
27	G	176	
28	R	103	
29	T	100	
30	Z	78	
31	W	84	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	NMY	B	2905	-	X
33	MG	B	3021	-	X
33	MG	B	3175	-	X
33	MG	B	3181	-	X
33	MG	B	3188	-	X
33	MG	B	3194	-	X
33	MG	B	3270	-	X
33	MG	B	3496	-	X
33	MG	B	3550	-	X
33	MG	B	3590	-	X

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 90298 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 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 2 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 6 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	K	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 7 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 9 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	Y	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 10 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 11 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 12 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 13 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 14 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	V	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 15 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	L	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	M	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 18 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	H	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	J	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	N	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	O	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 23 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	Q	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 24 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	S	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	U	102	Total	C	N	O		0	0	0
			779	492	146	141				

- Molecule 26 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	F	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 27 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	G	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 28 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	T	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

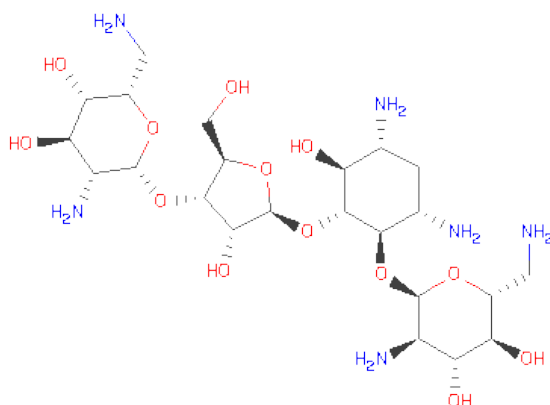
- Molecule 30 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	Z	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	W	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 32 is NEOMYCIN (three-letter code: NMY) (formula: $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$).



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

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	B	110	Total 110	Mg 110	0	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	4	1	Total 1	Zn 1	0	0

- Molecule 35 is water.

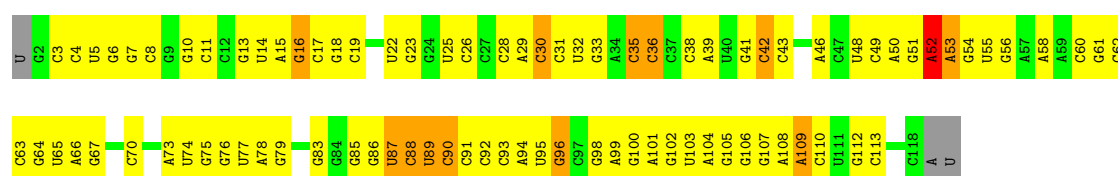
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	498	Total 498	O 498	0	0
35	C	5	Total 5	O 5	0	0
35	L	1	Total 1	O 1	0	0
35	N	1	Total 1	O 1	0	0
35	R	1	Total 1	O 1	0	0

3 Residue-property plots

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.

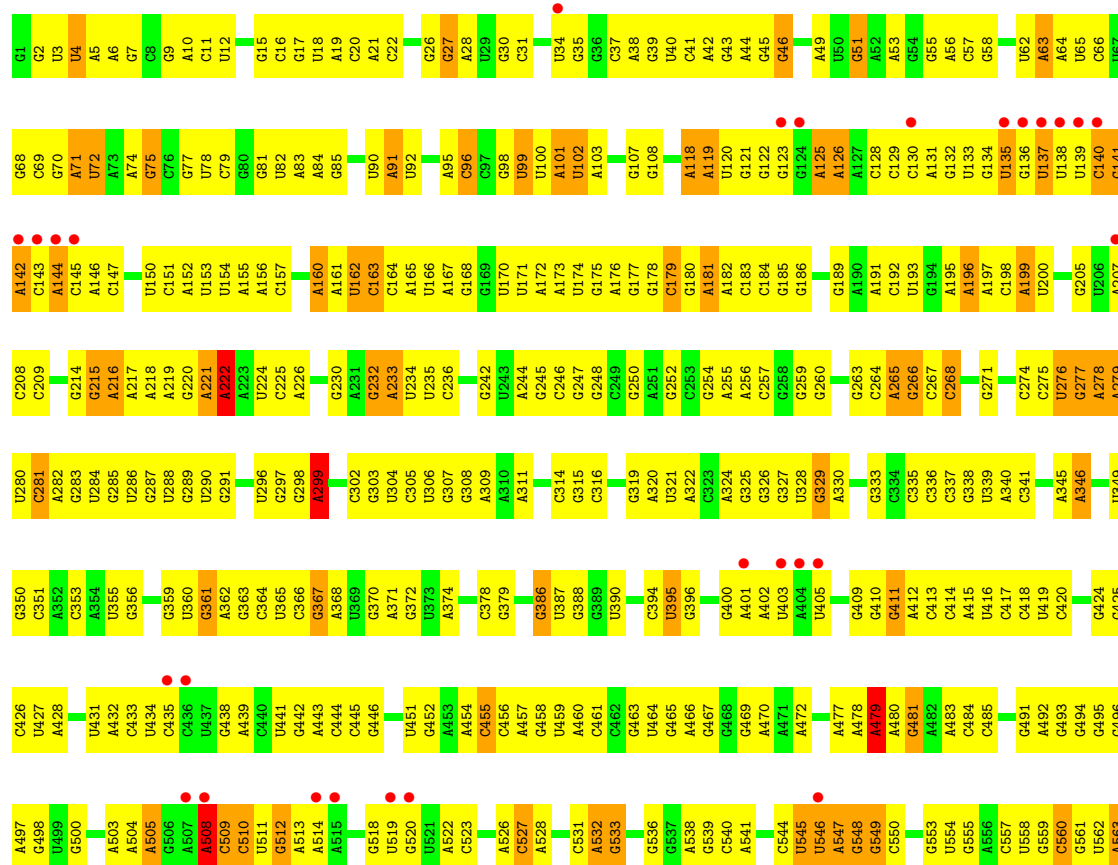
• Molecule 1: 5S rRNA

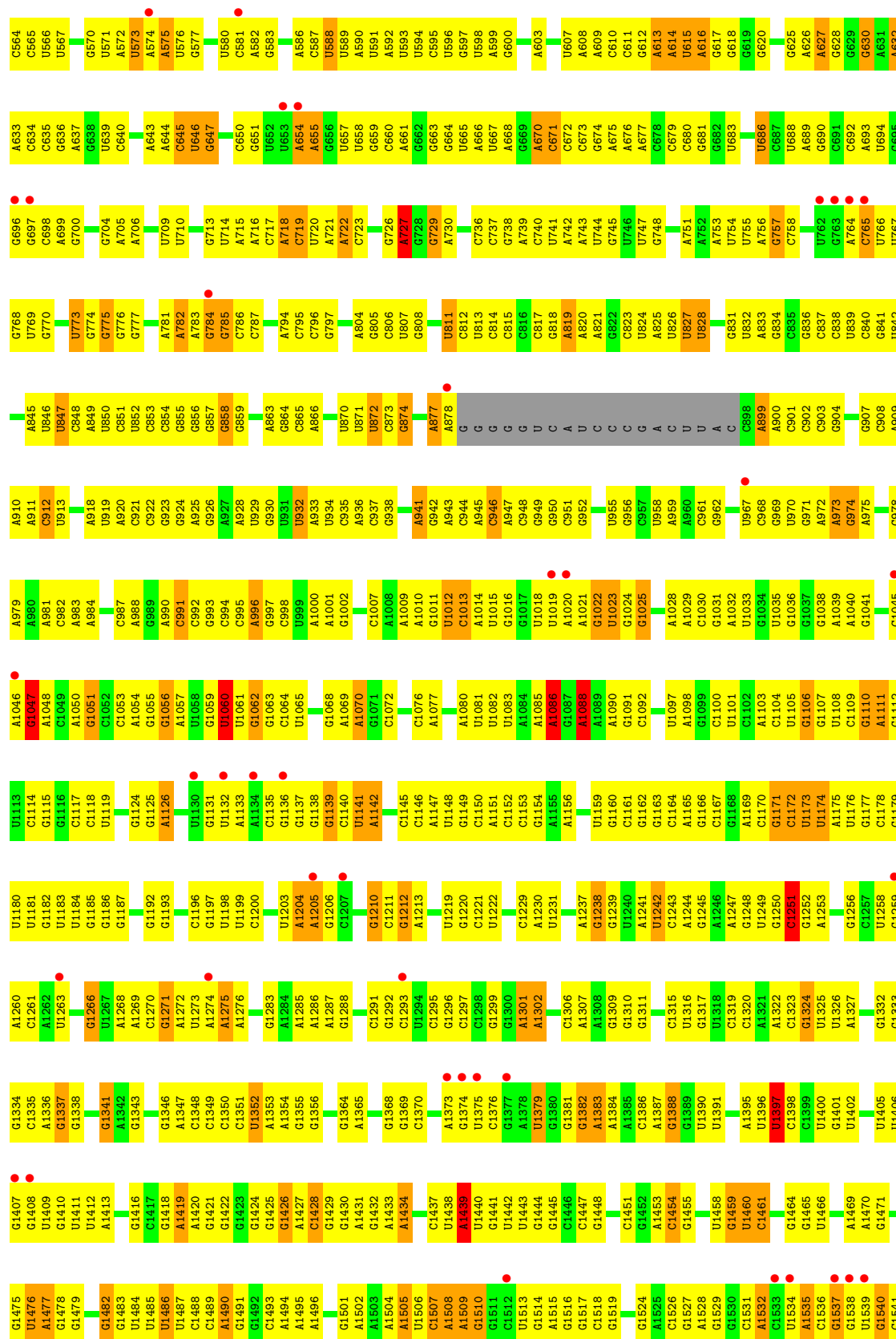
Chain A:



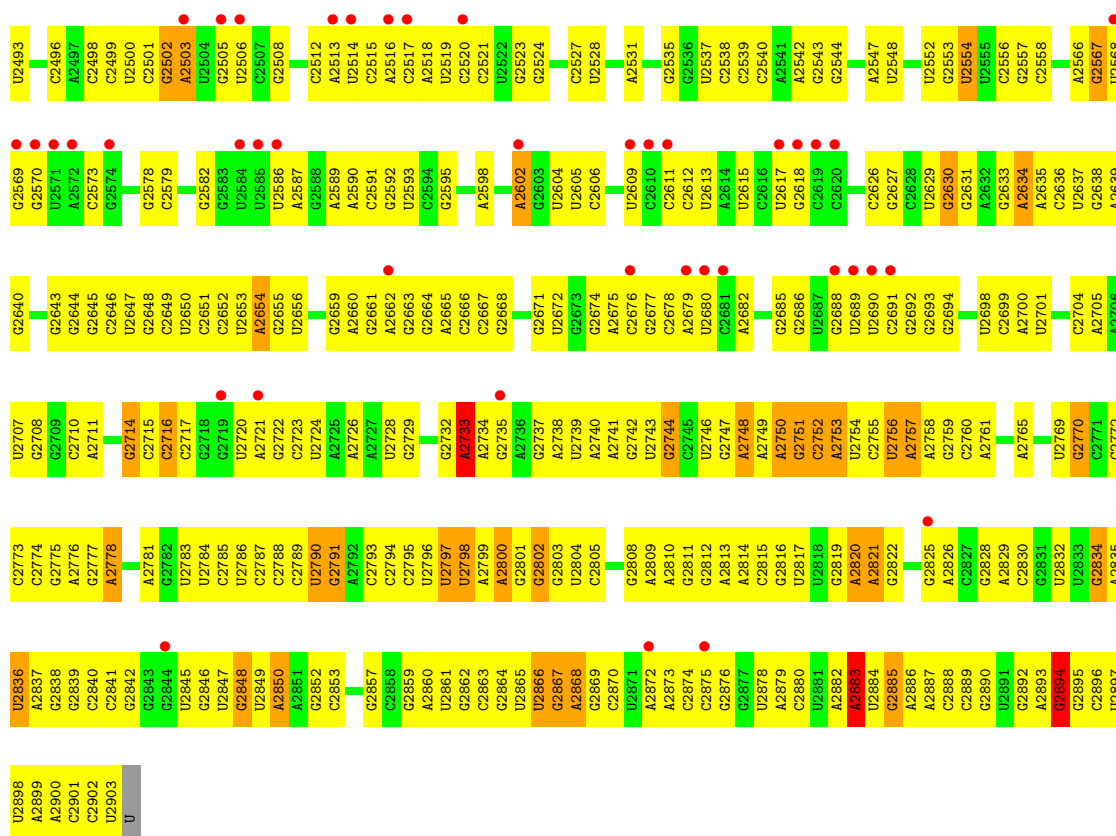
• Molecule 2: 23S rRNA

Chain B:



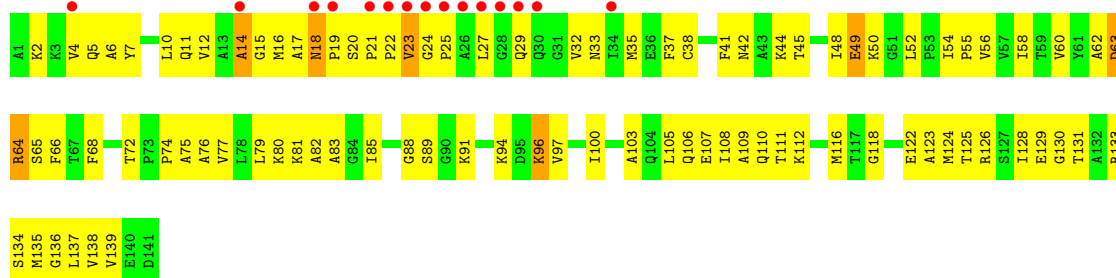






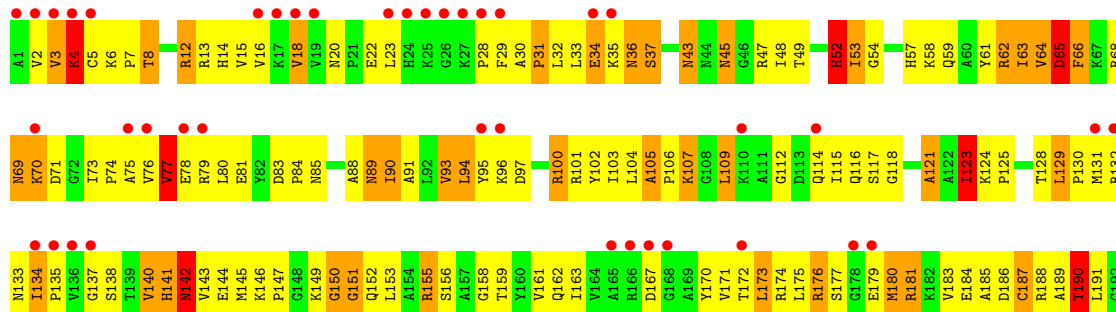
• Molecule 3: 50S ribosomal protein L11

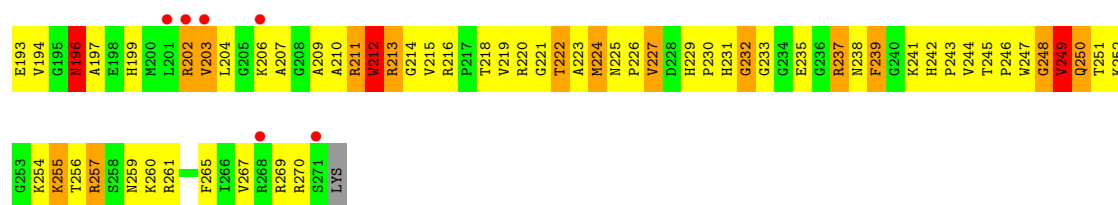
Chain I:



• Molecule 4: 50S ribosomal protein L2

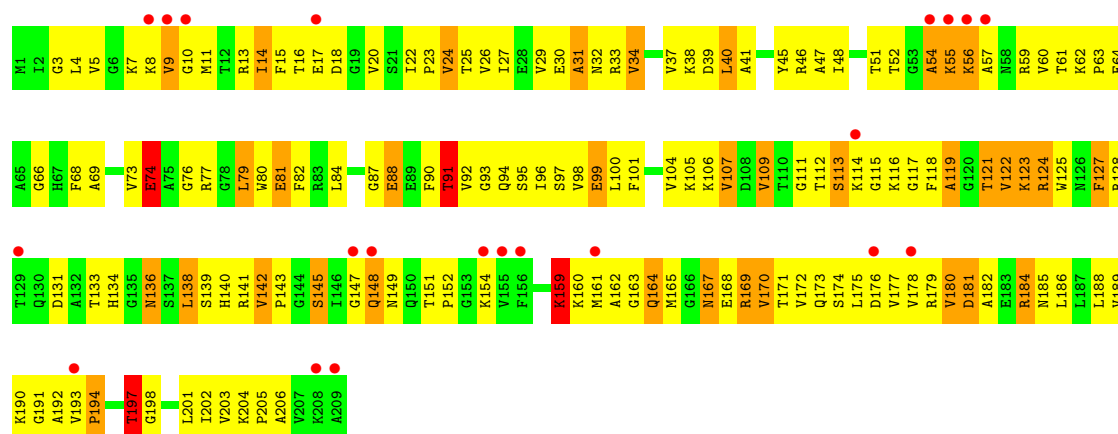
Chain C:





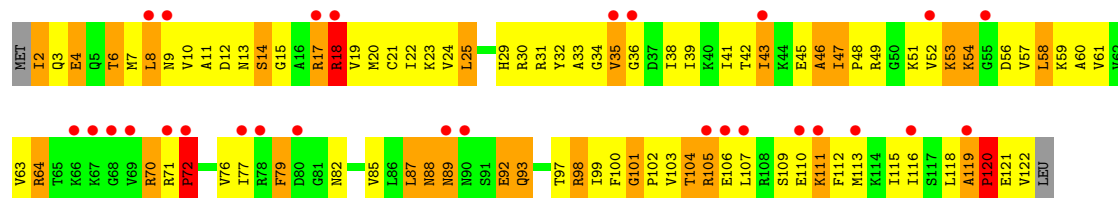
• Molecule 5: 50S ribosomal protein L3

Chain D:



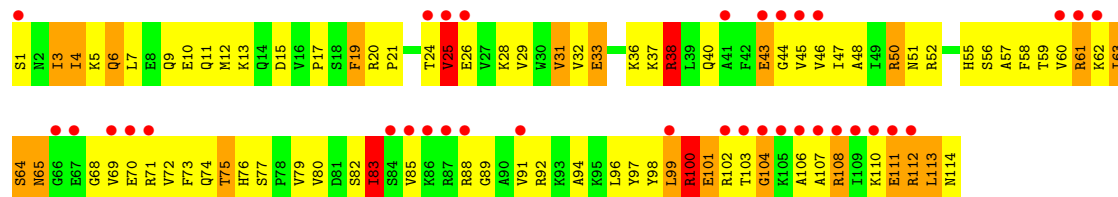
• Molecule 6: 50S ribosomal protein L14

Chain K:



• Molecule 7: 50S ribosomal protein L19

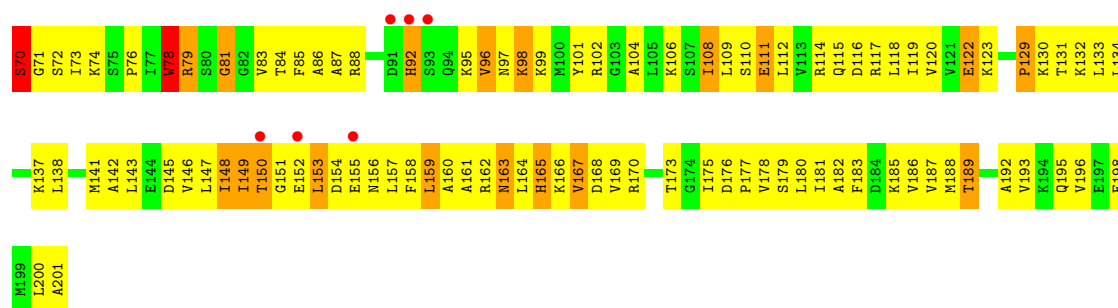
Chain P:



• Molecule 8: 50S ribosomal protein L4

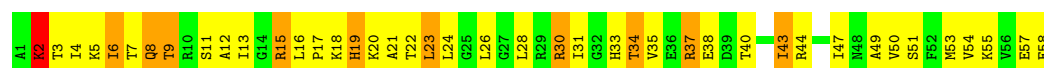
Chain E:





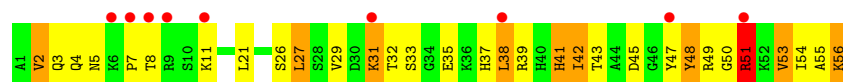
- Molecule 9: 50S ribosomal protein L30

Chain Y:



- Molecule 10: 50S ribosomal protein L32

Chain 0:



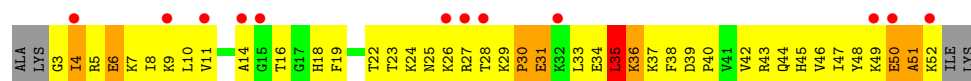
- Molecule 11: 50S ribosomal protein L36

Chain 4:



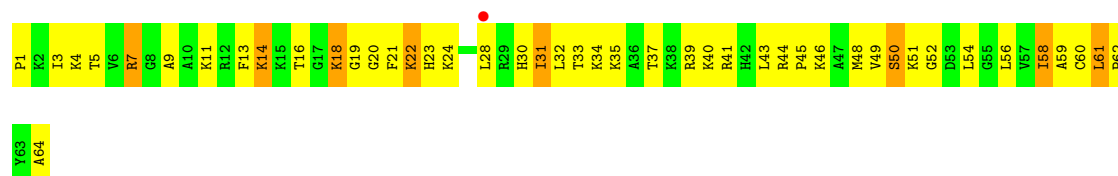
- Molecule 12: 50S ribosomal protein L33

Chain 1:



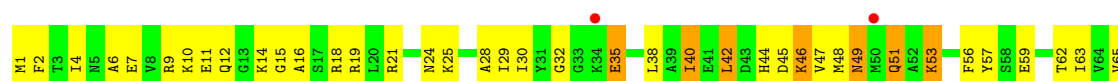
- Molecule 13: 50S ribosomal protein L35

Chain 3:



- Molecule 14: 50S ribosomal protein L25

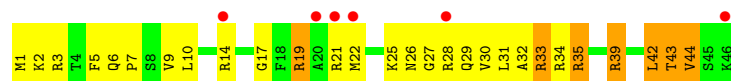
Chain V:





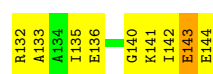
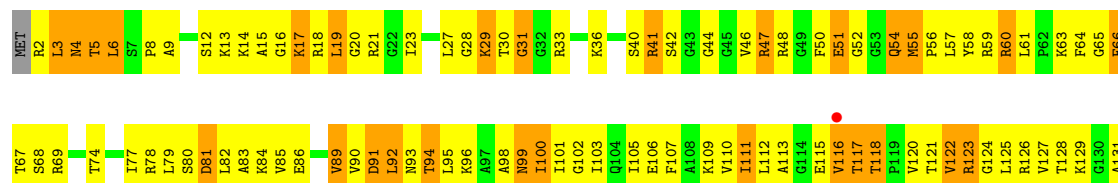
- Molecule 15: 50S ribosomal protein L34

Chain 2:



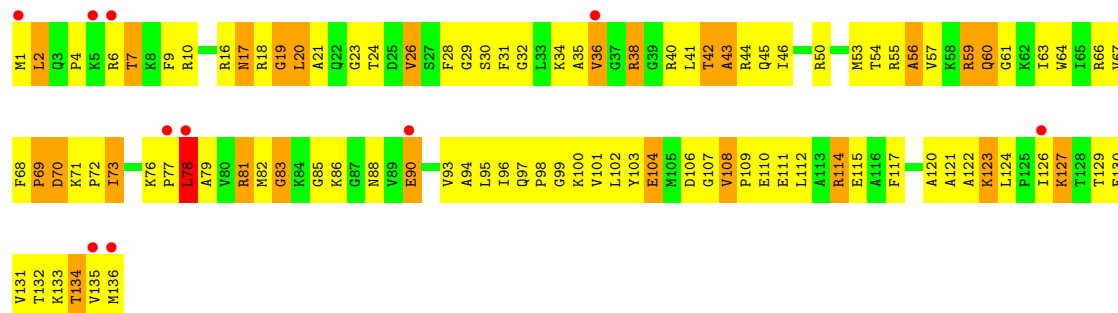
- Molecule 16: 50S ribosomal protein L15

Chain L:



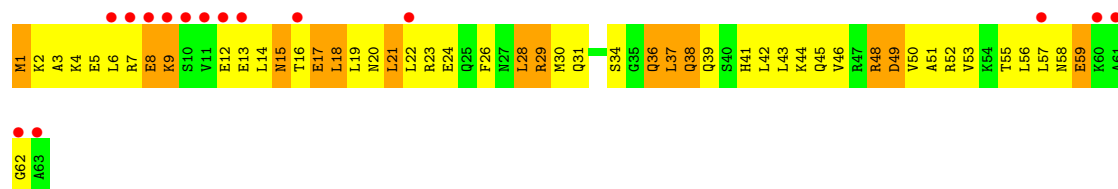
- Molecule 17: 50S ribosomal protein L16

Chain M:



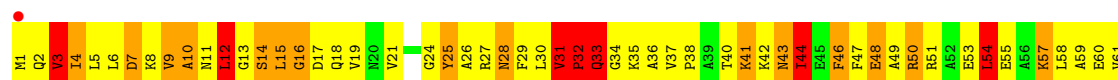
- Molecule 18: 50S ribosomal protein L29

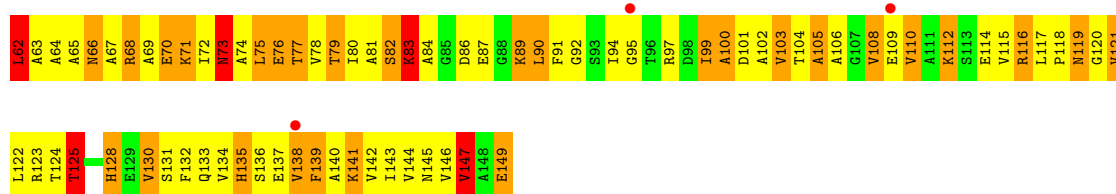
Chain X:



- Molecule 19: 50S ribosomal protein L9

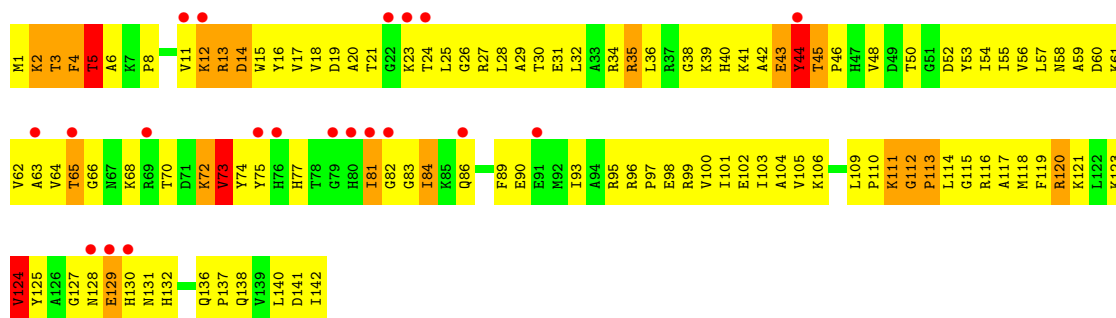
Chain H:





• Molecule 20: 50S ribosomal protein L13

Chain J:



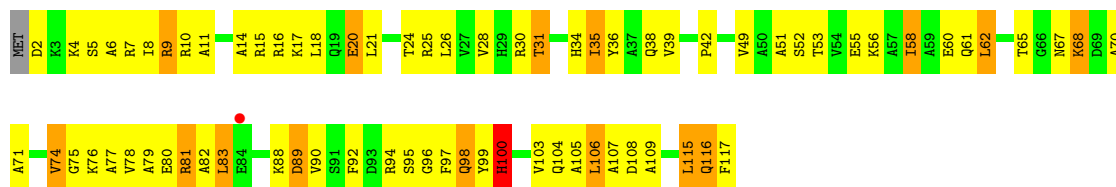
• Molecule 21: 50S ribosomal protein L17

Chain N:



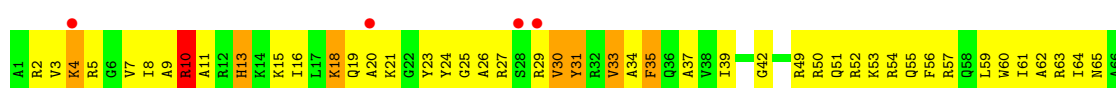
• Molecule 22: 50S ribosomal protein L18

Chain O:



• Molecule 23: 50S ribosomal protein L20

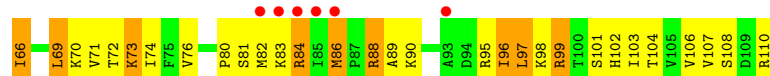
Chain Q:





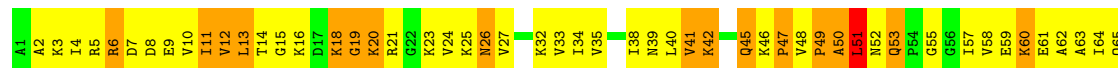
• Molecule 24: 50S ribosomal protein L22

Chain S:



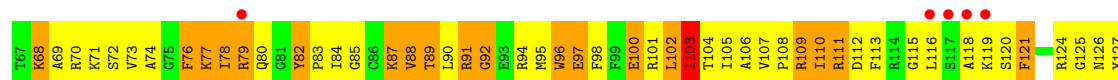
• Molecule 25: 50S ribosomal protein L24

Chain U:



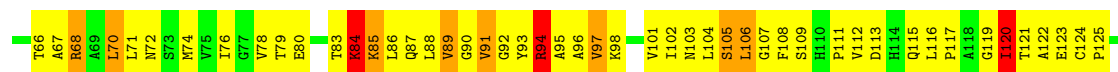
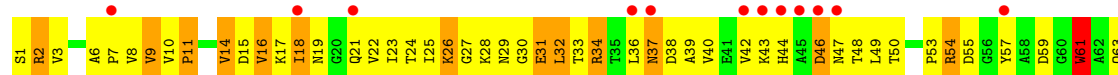
• Molecule 26: 50S ribosomal protein L5

Chain F:



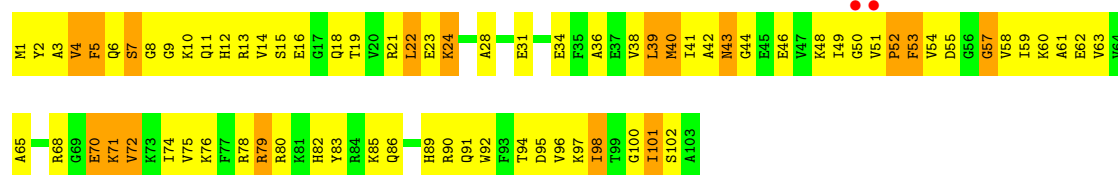
• Molecule 27: 50S ribosomal protein L6

Chain G:



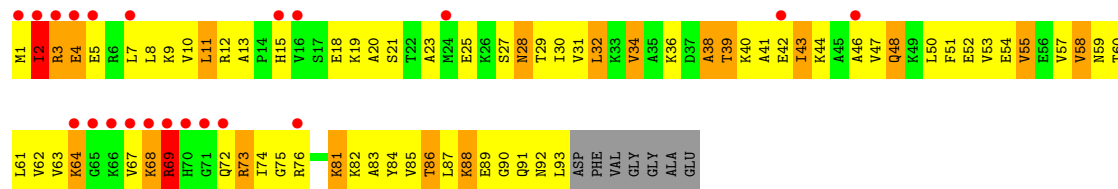
• Molecule 28: 50S ribosomal protein L21

Chain R:



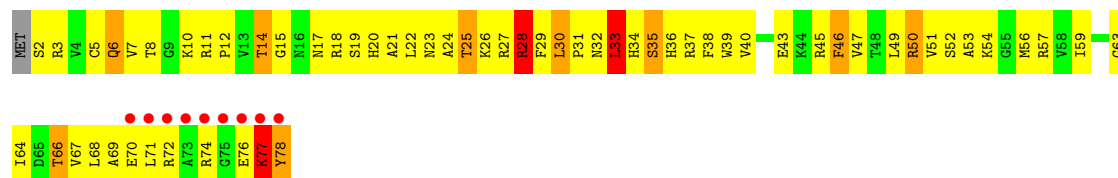
- Molecule 29: 50S ribosomal protein L23

Chain T:



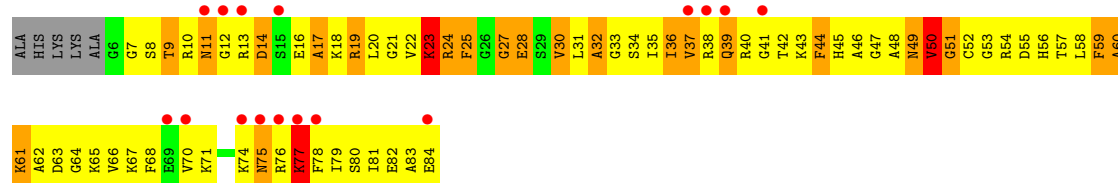
- Molecule 30: 50S ribosomal protein L28

Chain Z:



- Molecule 31: 50S ribosomal protein L27

Chain W:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.21 138.41 – 3.22	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-3.21) 66.6 (138.41-3.22)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 3.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.274 , 0.309 0.497 , 0.506	Depositor DCC
R_{free} test set	23931 reflections (3.82%)	DCC
Wilson B-factor (Å ²)	93.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 25.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 626512 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	90298	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, NMY

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/2803	0.75	1/4371 (0.0%)
2	B	0.28	8/68314 (0.0%)	0.77	42/106569 (0.0%)
3	I	0.24	0/1046	0.47	0/1410
4	C	0.22	0/2121	0.48	0/2852
5	D	0.24	0/1586	0.49	0/2134
6	K	0.24	0/939	0.56	0/1258
7	P	0.24	0/929	0.51	0/1242
8	E	0.24	0/1571	0.51	0/2113
9	Y	0.23	0/453	0.50	0/605
10	O	0.22	0/450	0.56	0/599
11	4	0.23	0/303	0.48	0/397
12	1	0.27	0/416	0.49	0/554
13	3	0.24	0/513	0.48	0/676
14	V	0.25	0/766	0.42	0/1025
15	2	0.26	0/380	0.47	0/498
16	L	0.23	0/1054	0.48	0/1403
17	M	0.25	0/1093	0.49	0/1460
18	X	0.24	0/510	0.53	0/677
19	H	0.25	0/1122	0.48	0/1515
20	J	0.23	0/1152	0.48	0/1551
21	N	0.24	0/973	0.52	0/1301
22	O	0.23	0/902	0.49	0/1209
23	Q	0.26	0/960	0.50	0/1278
24	S	0.22	0/864	0.52	0/1156
25	U	0.25	0/787	0.47	0/1051
26	F	0.26	0/1444	0.52	0/1937
27	G	0.23	0/1343	0.47	0/1816
28	R	0.25	0/829	0.49	0/1107
29	T	0.23	0/744	0.57	0/994
30	Z	0.25	0/635	0.52	0/848
31	W	0.28	0/603	0.53	0/797
All	All	0.27	8/97605 (0.0%)	0.71	43/146403 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	43

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1086	A	C5-C6	-16.18	1.26	1.41
2	B	1088	A	C6-N1	-10.58	1.28	1.35
2	B	1060	U	C2-N3	7.75	1.43	1.37
2	B	1086	A	N3-C4	-6.97	1.30	1.34
2	B	1086	A	N7-C5	-6.47	1.35	1.39

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2204	G	O5'-P-OP2	-28.20	76.86	110.70
2	B	2791	G	O5'-P-OP1	-27.64	77.53	110.70
2	B	2791	G	O5'-P-OP2	18.64	133.06	110.70
2	B	2204	G	O5'-P-OP1	17.75	132.00	110.70
2	B	2790	U	OP1-P-O3'	14.84	137.84	105.20

There are no chirality outliers.

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	221	A	Sidechain
2	B	222	A	Sidechain
2	B	232	G	Sidechain
2	B	299	A	Sidechain
2	B	51	G	Sidechain

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	2507	0	1270	96	0
2	B	60995	0	30678	2141	0
3	I	1032	0	1088	111	0
4	C	2082	0	2157	256	0
5	D	1565	0	1616	204	0
6	K	930	0	1000	117	0
7	P	917	0	965	116	0
8	E	1552	0	1619	185	0
9	Y	449	0	491	52	0
10	0	444	0	461	45	0
11	4	302	0	340	30	0
12	1	409	0	440	51	0
13	3	504	0	574	56	0
14	V	753	0	780	80	0
15	2	377	0	418	44	0
16	L	1045	0	1117	142	0
17	M	1074	0	1157	115	0
18	X	509	0	543	62	0
19	H	1111	0	1148	196	0
20	J	1129	0	1162	146	0
21	N	960	0	1000	116	0
22	O	892	0	923	79	0
23	Q	947	0	1022	142	0
24	S	857	0	922	103	0
25	U	779	0	834	125	0
26	F	1420	0	1460	229	0
27	G	1323	0	1374	187	0
28	R	816	0	839	97	0
29	T	738	0	807	129	0
30	Z	625	0	652	82	0
31	W	596	0	610	136	0
32	B	42	0	46	0	0
33	B	110	0	0	0	0
34	4	1	0	0	0	0
35	B	498	0	0	8	0
35	C	5	0	0	0	0
35	L	1	0	0	0	0
35	N	1	0	0	0	0
35	R	1	0	0	0	0
All	All	90298	0	59513	5215	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 35.

The worst 5 of 5215 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:H:31:VAL:HB	19:H:32:PRO:HD2	1.29	1.10
25:U:85:ARG:HD3	25:U:86:PHE:H	1.17	1.09
2:B:855:G:H21	31:W:23:LYS:HG2	0.99	1.07
2:B:126:A:H5'	15:2:19:ARG:HG3	1.40	1.03
5:D:10:GLY:HA3	5:D:26:VAL:H	1.20	1.03

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	I	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	36
4	C	269/272 (99%)	174 (65%)	49 (18%)	46 (17%)	0	1
5	D	207/209 (99%)	112 (54%)	63 (30%)	32 (16%)	0	1
6	K	119/123 (97%)	75 (63%)	28 (24%)	16 (13%)	0	2
7	P	112/114 (98%)	62 (55%)	35 (31%)	15 (13%)	0	2
8	E	199/201 (99%)	131 (66%)	51 (26%)	17 (8%)	1	9
9	Y	56/58 (97%)	36 (64%)	14 (25%)	6 (11%)	1	5
10	0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	8
11	4	36/38 (95%)	21 (58%)	7 (19%)	8 (22%)	0	0
12	1	48/54 (89%)	37 (77%)	5 (10%)	6 (12%)	1	3
13	3	62/64 (97%)	44 (71%)	13 (21%)	5 (8%)	1	10
14	V	92/94 (98%)	65 (71%)	23 (25%)	4 (4%)	4	31
15	2	44/46 (96%)	29 (66%)	14 (32%)	1 (2%)	10	52
16	L	141/144 (98%)	88 (62%)	30 (21%)	23 (16%)	0	1
17	M	134/136 (98%)	86 (64%)	31 (23%)	17 (13%)	0	3
18	X	61/63 (97%)	38 (62%)	18 (30%)	5 (8%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	H	147/149 (99%)	77 (52%)	41 (28%)	29 (20%)	0	0
20	J	140/142 (99%)	88 (63%)	36 (26%)	16 (11%)	1	4
21	N	118/127 (93%)	72 (61%)	34 (29%)	12 (10%)	1	6
22	O	114/117 (97%)	84 (74%)	25 (22%)	5 (4%)	4	29
23	Q	115/117 (98%)	73 (64%)	34 (30%)	8 (7%)	2	14
24	S	108/110 (98%)	69 (64%)	28 (26%)	11 (10%)	1	6
25	U	100/103 (97%)	53 (53%)	25 (25%)	22 (22%)	0	0
26	F	176/178 (99%)	107 (61%)	44 (25%)	25 (14%)	0	2
27	G	174/176 (99%)	100 (58%)	48 (28%)	26 (15%)	0	1
28	R	101/103 (98%)	65 (64%)	25 (25%)	11 (11%)	1	5
29	T	91/100 (91%)	50 (55%)	31 (34%)	10 (11%)	1	5
30	Z	75/78 (96%)	53 (71%)	18 (24%)	4 (5%)	3	24
31	W	77/84 (92%)	29 (38%)	27 (35%)	21 (27%)	0	0
All	All	3309/3397 (97%)	2076 (63%)	822 (25%)	411 (12%)	1	3

5 of 411 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	18	ASN
4	C	77	VAL
4	C	107	LYS
5	D	9	VAL
5	D	14	ILE

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	I	109/109 (100%)	107 (98%)	2 (2%)	71	93
4	C	216/217 (100%)	176 (82%)	40 (18%)	2	11
5	D	164/164 (100%)	142 (87%)	22 (13%)	6	26
6	K	102/104 (98%)	79 (78%)	23 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	P	99/99 (100%)	81 (82%)	18 (18%)	2	12
8	E	165/165 (100%)	136 (82%)	29 (18%)	3	13
9	Y	48/48 (100%)	38 (79%)	10 (21%)	2	8
10	O	47/47 (100%)	36 (77%)	11 (23%)	1	4
11	4	34/34 (100%)	28 (82%)	6 (18%)	3	13
12	1	45/48 (94%)	40 (89%)	5 (11%)	9	36
13	3	51/51 (100%)	47 (92%)	4 (8%)	18	58
14	V	78/78 (100%)	62 (80%)	16 (20%)	2	8
15	2	38/38 (100%)	32 (84%)	6 (16%)	4	16
16	L	102/103 (99%)	89 (87%)	13 (13%)	6	29
17	M	109/109 (100%)	91 (84%)	18 (16%)	3	14
18	X	55/55 (100%)	40 (73%)	15 (27%)	0	2
19	H	114/114 (100%)	64 (56%)	50 (44%)	0	0
20	J	116/116 (100%)	101 (87%)	15 (13%)	6	28
21	N	100/103 (97%)	87 (87%)	13 (13%)	6	28
22	O	86/87 (99%)	70 (81%)	16 (19%)	2	11
23	Q	89/89 (100%)	74 (83%)	15 (17%)	3	14
24	S	93/93 (100%)	79 (85%)	14 (15%)	4	19
25	U	83/84 (99%)	68 (82%)	15 (18%)	2	12
26	F	149/149 (100%)	114 (76%)	35 (24%)	1	4
27	G	137/137 (100%)	113 (82%)	24 (18%)	3	13
28	R	84/84 (100%)	73 (87%)	11 (13%)	6	28
29	T	80/84 (95%)	66 (82%)	14 (18%)	3	13
30	Z	67/68 (98%)	52 (78%)	15 (22%)	1	6
31	W	59/62 (95%)	45 (76%)	14 (24%)	1	4
All	All	2719/2739 (99%)	2230 (82%)	489 (18%)	2	12

5 of 489 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	M	123	LYS
19	H	104	THR
29	T	32	LEU

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Mol	Chain	Res	Type
18	X	17	GLU
19	H	33	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
15	2	13	ASN
19	H	73	ASN
29	T	92	ASN
16	L	38	GLN
18	X	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	116/120 (96%)	17 (14%)	1 (0%)
2	B	2837/2904 (97%)	435 (15%)	18 (0%)
All	All	2953/3024 (97%)	452 (15%)	19 (0%)

5 of 452 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	G
1	A	25	U
1	A	26	C
1	A	30	C
1	A	35	C

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1419	A
2	B	2213	U
2	B	2756	U
2	B	1301	A
2	B	2832	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 112 ligands modelled in this entry, 111 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	NMY	B	2905	-	45,45,45	2.20	13 (28%)	67,67,67	1.25	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	NMY	B	2905	-	-	0/18/94/94	0/4/4/4

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	2905	NMY	C8-C7	6.21	1.57	1.52
32	B	2905	NMY	C8-C9	6.11	1.57	1.52
32	B	2905	NMY	O22-C18	4.54	1.53	1.41
32	B	2905	NMY	C3-C2	4.37	1.59	1.53
32	B	2905	NMY	O5-C1	3.43	1.50	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	2905	NMY	O22-C22-C23	4.02	111.91	106.97
32	B	2905	NMY	O11-C13-O16	3.58	114.93	111.51
32	B	2905	NMY	O18-C18-C19	3.22	114.46	108.09
32	B	2905	NMY	O5-C5-C6	3.03	110.70	106.97
32	B	2905	NMY	O11-C13-C14	2.80	112.50	107.50

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	117/120 (97%)	-0.28	0 100 100	49, 83, 138, 174	0
2	B	2841/2904 (97%)	0.06	161 (5%) 23 5	16, 60, 154, 180	0
3	I	141/141 (100%)	0.17	15 (10%) 7 2	93, 176, 180, 180	0
4	C	271/272 (99%)	0.83	46 (16%) 2 1	9, 50, 104, 180	0
5	D	209/209 (100%)	0.49	21 (10%) 8 2	20, 76, 135, 180	0
6	K	121/123 (98%)	1.19	28 (23%) 1 1	14, 72, 133, 180	0
7	P	114/114 (100%)	1.42	35 (30%) 1 1	35, 86, 151, 180	0
8	E	201/201 (100%)	-0.05	10 (4%) 28 6	10, 67, 144, 180	0
9	Y	58/58 (100%)	0.20	0 100 100	34, 74, 139, 180	0
10	0	56/56 (100%)	0.86	9 (16%) 2 1	15, 74, 151, 180	0
11	4	38/38 (100%)	0.15	4 (10%) 7 2	35, 91, 145, 151	0
12	1	50/54 (92%)	0.89	12 (24%) 1 1	52, 90, 134, 174	0
13	3	64/64 (100%)	0.07	1 (1%) 68 22	26, 59, 87, 158	0
14	V	94/94 (100%)	-0.12	3 (3%) 45 10	29, 97, 155, 178	0
15	2	46/46 (100%)	0.59	6 (13%) 4 1	14, 50, 83, 144	0
16	L	143/144 (99%)	0.07	1 (0%) 84 40	25, 70, 133, 180	0
17	M	136/136 (100%)	0.27	10 (7%) 14 4	21, 68, 136, 180	0
18	X	63/63 (100%)	1.26	15 (23%) 1 1	21, 81, 149, 175	0
19	H	149/149 (100%)	0.22	4 (2%) 52 12	31, 134, 180, 180	0
20	J	142/142 (100%)	0.74	20 (14%) 3 1	23, 82, 140, 169	0
21	N	120/127 (94%)	0.64	10 (8%) 11 3	24, 71, 139, 180	0
22	O	116/117 (99%)	-0.39	1 (0%) 81 35	35, 83, 145, 180	0
23	Q	117/117 (100%)	0.20	5 (4%) 34 7	10, 66, 129, 167	0
24	S	110/110 (100%)	0.38	8 (7%) 15 4	6, 62, 123, 152	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	U	102/103 (99%)	-0.36	1 (0%) 79 31	21, 77, 140, 180	0
26	F	178/178 (100%)	-0.14	8 (4%) 32 7	56, 128, 177, 180	0
27	G	176/176 (100%)	0.49	14 (7%) 12 3	49, 112, 163, 180	0
28	R	103/103 (100%)	-0.27	2 (1%) 64 19	25, 87, 151, 176	0
29	T	93/100 (93%)	1.24	21 (22%) 1 1	22, 77, 159, 180	0
30	Z	77/78 (98%)	0.63	9 (11%) 5 2	12, 51, 112, 143	0
31	W	79/84 (94%)	1.10	16 (20%) 1 1	18, 85, 141, 159	0
All	All	6325/6421 (98%)	0.24	496 (7%) 13 3	6, 70, 161, 180	0

The worst 5 of 496 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	T	3	ARG	10.0
18	X	63	ALA	9.1
2	B	137	U	8.9
29	T	1	MET	8.6
7	P	86	LYS	8.3

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
33	MG	B	3270	1/1	0.33	16.90	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	NMY	B	2905	42/42	0.77	12.40	100,100,100,100	42
33	MG	B	3194	1/1	0.33	8.08	136,136,136,136	0
33	MG	B	3181	1/1	0.33	6.16	45,45,45,45	0
33	MG	B	3590	1/1	0.26	5.73	54,54,54,54	0
33	MG	B	3021	1/1	0.34	4.85	39,39,39,39	0
33	MG	B	3550	1/1	0.36	4.09	41,41,41,41	0
33	MG	B	3496	1/1	0.54	3.98	57,57,57,57	0
33	MG	B	3175	1/1	0.35	3.34	47,47,47,47	0
33	MG	B	3509	1/1	0.41	1.40	75,75,75,75	0
33	MG	B	3289	1/1	0.36	1.38	41,41,41,41	0
33	MG	B	3206	1/1	0.44	1.25	36,36,36,36	0
33	MG	B	3400	1/1	0.33	1.16	15,15,15,15	0
33	MG	B	3188	1/1	0.55	0.96	55,55,55,55	0
33	MG	B	3600	1/1	0.23	0.88	32,32,32,32	0
33	MG	B	3349	1/1	0.15	0.87	41,41,41,41	0
33	MG	B	3418	1/1	0.40	0.62	67,67,67,67	0
33	MG	B	3382	1/1	0.14	0.16	34,34,34,34	0
33	MG	B	3412	1/1	0.26	0.16	52,52,52,52	0
33	MG	B	3369	1/1	0.36	0.10	24,24,24,24	0
33	MG	B	3050	1/1	0.13	-0.03	82,82,82,82	0
33	MG	B	3561	1/1	0.17	-0.31	138,138,138,138	0
33	MG	B	3555	1/1	0.17	-0.36	68,68,68,68	0
33	MG	B	3044	1/1	0.18	-0.37	64,64,64,64	0
33	MG	B	3471	1/1	0.24	-0.42	59,59,59,59	0
33	MG	B	3157	1/1	0.15	-0.44	32,32,32,32	0
33	MG	B	3253	1/1	0.21	-0.45	67,67,67,67	0
33	MG	B	3344	1/1	0.20	-0.47	30,30,30,30	0
33	MG	B	3145	1/1	0.14	-0.55	54,54,54,54	0
33	MG	B	3505	1/1	0.30	-0.64	49,49,49,49	0
33	MG	B	3516	1/1	0.14	-0.74	36,36,36,36	0
33	MG	B	3221	1/1	0.11	-0.76	131,131,131,131	0
33	MG	B	3061	1/1	0.17	-0.81	25,25,25,25	0
33	MG	B	3428	1/1	0.14	-0.84	13,13,13,13	0
33	MG	B	3359	1/1	0.16	-0.84	31,31,31,31	0
33	MG	B	3028	1/1	0.17	-0.87	5,5,5,5	0
33	MG	B	3376	1/1	0.12	-0.91	44,44,44,44	0
33	MG	B	3240	1/1	0.11	-0.98	170,170,170,170	0
33	MG	B	3103	1/1	0.13	-1.01	45,45,45,45	0
33	MG	B	3537	1/1	0.13	-1.06	32,32,32,32	0
33	MG	B	3444	1/1	0.14	-1.12	32,32,32,32	0
33	MG	B	3450	1/1	0.12	-1.12	75,75,75,75	0
33	MG	B	3433	1/1	0.18	-1.15	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	3066	1/1	0.19	-1.27	41,41,41,41	0
33	MG	B	3531	1/1	0.11	-1.28	42,42,42,42	0
33	MG	B	3169	1/1	0.13	-1.32	36,36,36,36	0
33	MG	B	3488	1/1	0.09	-1.35	66,66,66,66	0
33	MG	B	3164	1/1	0.10	-1.40	32,32,32,32	0
33	MG	B	3259	1/1	0.14	-1.44	46,46,46,46	0
33	MG	B	3596	1/1	0.09	-1.48	25,25,25,25	0
33	MG	B	3201	1/1	0.07	-1.61	32,32,32,32	0
33	MG	B	3439	1/1	0.05	-1.61	37,37,37,37	0
33	MG	B	3353	1/1	0.18	-1.62	29,29,29,29	0
34	ZN	4	617	1/1	0.07	-1.66	72,72,72,72	0
33	MG	B	3512	1/1	0.29	-1.79	32,32,32,32	0
33	MG	B	3232	1/1	0.12	-1.80	28,28,28,28	0
33	MG	B	3338	1/1	0.14	-1.86	30,30,30,30	0
33	MG	B	3577	1/1	0.14	-1.88	8,8,8,8	0
33	MG	B	3423	1/1	0.21	-1.89	31,31,31,31	0
33	MG	B	3464	1/1	0.13	-1.89	52,52,52,52	0
33	MG	B	3586	1/1	0.10	-1.93	33,33,33,33	0
33	MG	B	3568	1/1	0.09	-2.03	28,28,28,28	0
33	MG	B	3085	1/1	0.15	-2.09	18,18,18,18	0
33	MG	B	3096	1/1	0.07	-2.13	43,43,43,43	0
33	MG	B	3543	1/1	0.11	-2.20	80,80,80,80	0
33	MG	B	3217	1/1	0.04	-2.26	50,50,50,50	0
33	MG	B	3302	1/1	0.07	-2.28	25,25,25,25	0
33	MG	B	3406	1/1	0.15	-2.28	29,29,29,29	0
33	MG	B	3227	1/1	0.08	-2.31	28,28,28,28	0
33	MG	B	3612	1/1	0.09	-2.40	81,81,81,81	0
33	MG	B	3235	1/1	0.10	-2.44	8,8,8,8	0
33	MG	B	3078	1/1	0.07	-2.57	27,27,27,27	0
33	MG	B	3499	1/1	0.10	-2.61	45,45,45,45	0
33	MG	B	3110	1/1	0.07	-2.67	45,45,45,45	0
33	MG	B	3364	1/1	0.11	-2.67	26,26,26,26	0
33	MG	B	3032	1/1	0.05	-2.72	5,5,5,5	0
33	MG	B	3265	1/1	0.07	-2.77	46,46,46,46	0
33	MG	B	3090	1/1	0.06	-2.87	28,28,28,28	0
33	MG	B	3521	1/1	0.11	-2.89	93,93,93,93	0
33	MG	B	3331	1/1	0.10	-3.00	76,76,76,76	0
33	MG	B	3038	1/1	0.08	-3.00	64,64,64,64	0
33	MG	B	3492	1/1	0.07	-3.01	41,41,41,41	0
33	MG	B	3124	1/1	0.08	-3.04	22,22,22,22	0
33	MG	B	3582	1/1	0.06	-3.15	21,21,21,21	0
33	MG	B	3135	1/1	0.11	-3.15	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	3484	1/1	0.07	-3.15	44,44,44,44	0
33	MG	B	3282	1/1	0.06	-3.19	18,18,18,18	0
33	MG	B	3573	1/1	0.05	-3.34	37,37,37,37	0
33	MG	B	3476	1/1	0.06	-3.37	5,5,5,5	0
33	MG	B	3007	1/1	0.07	-3.55	24,24,24,24	0
33	MG	B	3457	1/1	0.08	-3.58	37,37,37,37	0
33	MG	B	3151	1/1	0.05	-3.63	34,34,34,34	0
33	MG	B	3001	1/1	0.07	-3.71	24,24,24,24	0
33	MG	B	3295	1/1	0.12	-3.72	59,59,59,59	0
33	MG	B	3212	1/1	0.09	-3.83	42,42,42,42	0
33	MG	B	3321	1/1	0.05	-3.90	34,34,34,34	0
33	MG	B	3607	1/1	0.10	-4.02	30,30,30,30	0
33	MG	B	3141	1/1	0.04	-4.08	14,14,14,14	0
33	MG	B	3326	1/1	0.09	-4.27	20,20,20,20	0
33	MG	B	3389	1/1	0.05	-4.62	55,55,55,55	0
33	MG	B	3130	1/1	0.04	-4.80	41,41,41,41	0
33	MG	B	3316	1/1	0.09	-4.85	58,58,58,58	0
33	MG	B	3309	1/1	0.07	-5.09	46,46,46,46	0
33	MG	B	3246	1/1	0.07	-5.14	108,108,108,108	0
33	MG	B	3072	1/1	0.06	-5.33	42,42,42,42	0
33	MG	B	3528	1/1	0.03	-6.26	46,46,46,46	0
33	MG	B	3056	1/1	0.14	-6.57	66,66,66,66	0
33	MG	B	3480	1/1	0.08	-7.32	21,21,21,21	0
33	MG	B	3014	1/1	0.05	-7.79	38,38,38,38	0
33	MG	B	3394	1/1	0.07	-9.15	32,32,32,32	0
33	MG	B	3276	1/1	0.05	-15.76	14,14,14,14	0
33	MG	B	3117	1/1	0.13	-18.44	22,22,22,22	0

6.5 Other polymers ⓘ

There are no such residues in this entry.