



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 05:24 PM GMT

PDB ID : 3OG0
Title : Crystal structure of the E. coli ribosome bound to clindamycin. This file contains the 50S subunit of the second 70S ribosome.
Authors : Dunkle, J.A.; Xiong, L.; Mankin, A.S.; Cate, J.H.D.
Deposited on : 2010-08-16
Resolution : 3.29 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>

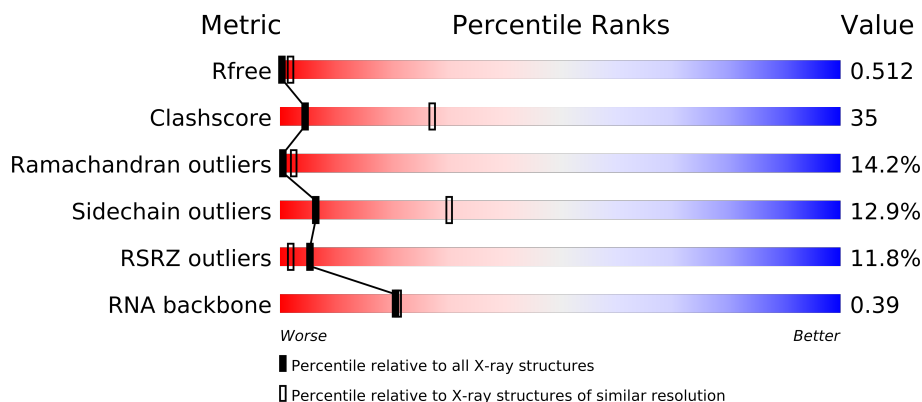
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.29 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	1151 (3.36-3.20)
Clashscore	79885	1464 (3.36-3.20)
Ramachandran outliers	78287	1435 (3.36-3.20)
Sidechain outliers	78261	1433 (3.36-3.20)
RSRZ outliers	66119	1152 (3.36-3.20)
RNA backbone	1838	1033 (3.86-2.70)

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	2903	
2	B	117	
3	C	271	
4	D	209	
5	E	201	
6	F	178	
7	G	176	
8	H	149	
9	I	141	
10	J	142	
11	K	122	
12	L	143	

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Mol	Chain	Length	Quality of chain
13	M	136	
14	N	120	
15	O	116	
16	P	114	
17	Q	117	
18	R	103	
19	S	110	
20	T	93	
21	U	102	
22	V	94	
23	W	79	
24	X	77	
25	Y	63	
26	Z	58	
27	0	56	
28	1	50	
29	2	46	
30	3	64	
31	4	38	

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	MG	A	2905	-	X
32	MG	A	2908	-	X
32	MG	A	2911	-	X
32	MG	A	2914	-	X
32	MG	A	2922	-	X
32	MG	A	2924	-	X
32	MG	A	2928	-	X
32	MG	A	2935	-	X
32	MG	A	2938	-	X
32	MG	A	2959	-	X
32	MG	A	2960	-	X
32	MG	A	2962	-	X
32	MG	A	2964	-	X
32	MG	A	2965	-	X
32	MG	A	2966	-	X
32	MG	A	2971	-	X
32	MG	A	2976	-	X
32	MG	A	2977	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	A	2980	-	X
32	MG	A	2983	-	X
32	MG	A	2987	-	X
32	MG	A	2988	-	X
32	MG	A	2993	-	X
32	MG	A	2994	-	X
32	MG	A	2997	-	X
32	MG	A	2999	-	X
32	MG	A	3001	-	X
32	MG	A	3010	-	X
32	MG	A	3011	-	X
32	MG	A	3017	-	X
32	MG	A	3029	-	X
32	MG	A	3032	-	X
32	MG	A	3035	-	X
32	MG	C	722	-	X
32	MG	J	747	-	X

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 90434 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 rRNA.

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

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

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

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

- Molecule 10 is a protein called 50S ribosomal protein L13.

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

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

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

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

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

- Molecule 18 is a protein called 50S ribosomal protein L21.

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

- Molecule 19 is a protein called 50S ribosomal protein L22.

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

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	102	Total	C	N	O			
			780	492	146	142	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

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

- Molecule 23 is a protein called 50S ribosomal protein L27.

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

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

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

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	0	56	Total	C	N	O	S			
			444	269	94	80	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	B	1	Total	Mg	0	0
			1	1		
32	A	132	Total	Mg	0	0
			132	132		
32	C	2	Total	Mg	0	0
			2	2		
32	J	1	Total	Mg	0	0
			1	1		
32	E	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	4	1	Total	Zn	0	0
			1	1		

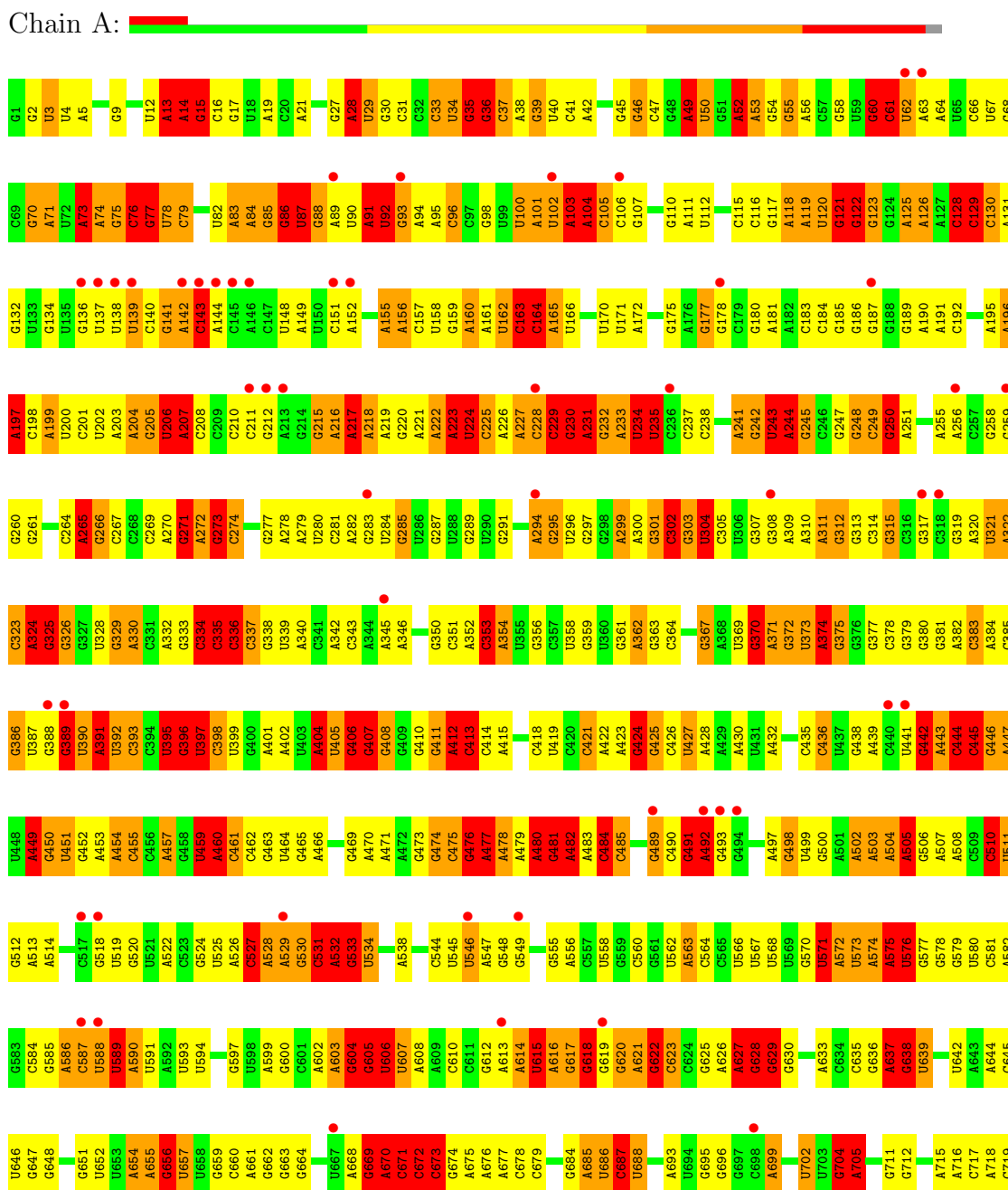
- Molecule 34 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	605	Total O 605 605	0	0
34	B	4	Total O 4 4	0	0
34	C	7	Total O 7 7	0	0
34	D	1	Total O 1 1	0	0
34	E	3	Total O 3 3	0	0
34	J	6	Total O 6 6	0	0
34	L	4	Total O 4 4	0	0
34	N	2	Total O 2 2	0	0
34	T	3	Total O 3 3	0	0
34	U	2	Total O 2 2	0	0
34	V	1	Total O 1 1	0	0
34	2	2	Total O 2 2	0	0
34	3	1	Total O 1 1	0	0
34	4	2	Total O 2 2	0	0

3 Residue-property plots

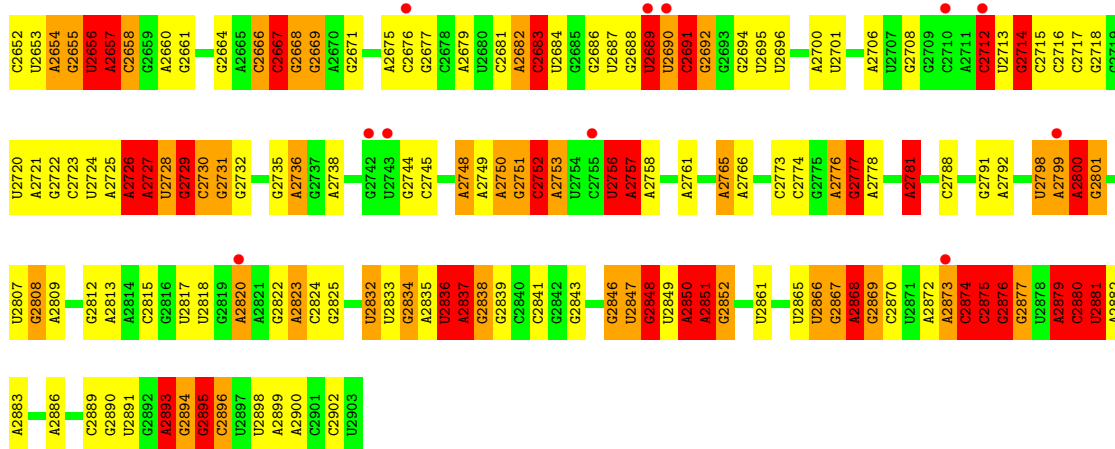
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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: 23S rRNA



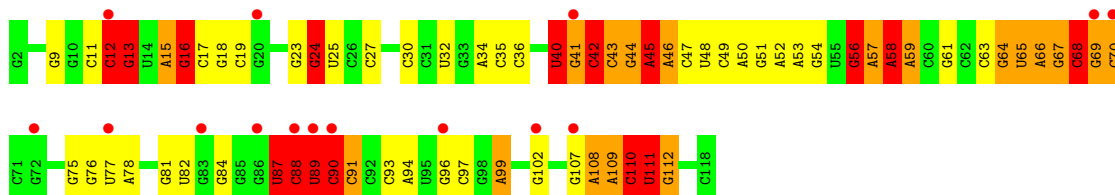






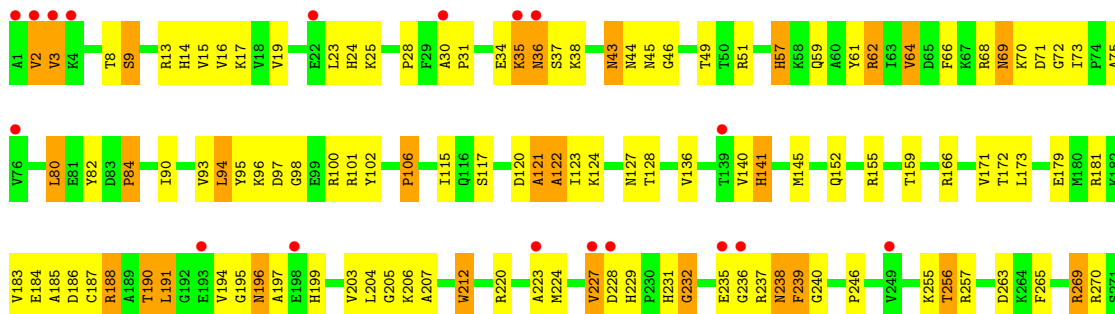
• Molecule 2: 5S rRNA

Chain B:



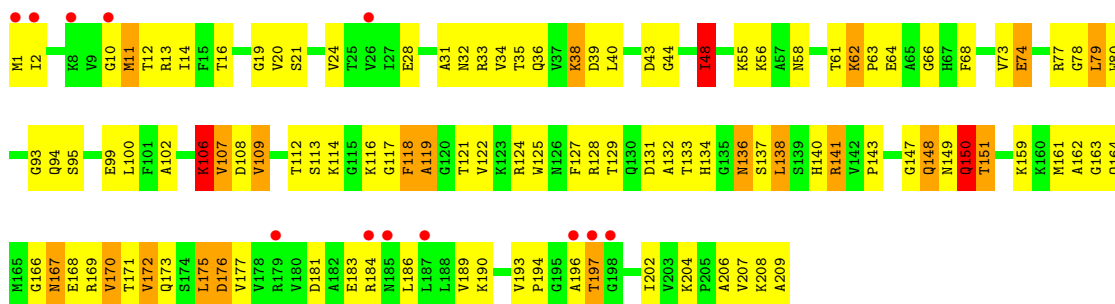
• Molecule 3: 50S ribosomal protein L2

Chain C:

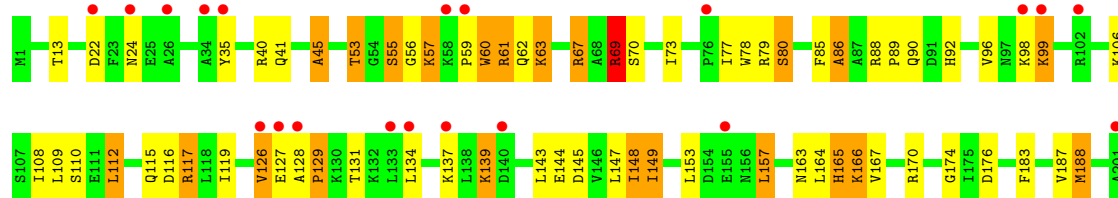


• Molecule 4: 50S ribosomal protein L3

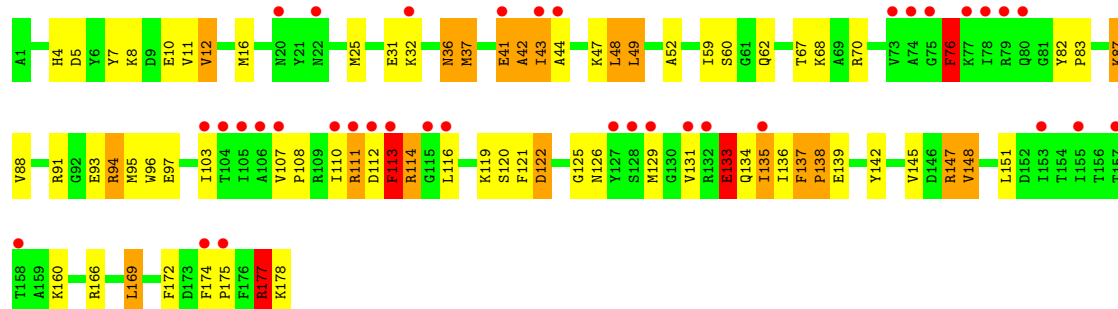
Chain D:



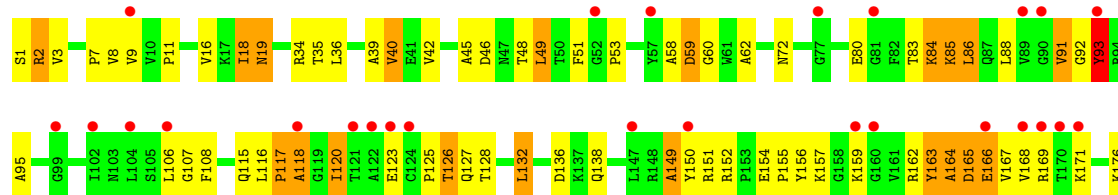
• Molecule 5: 50S ribosomal protein L4

Chain E: 

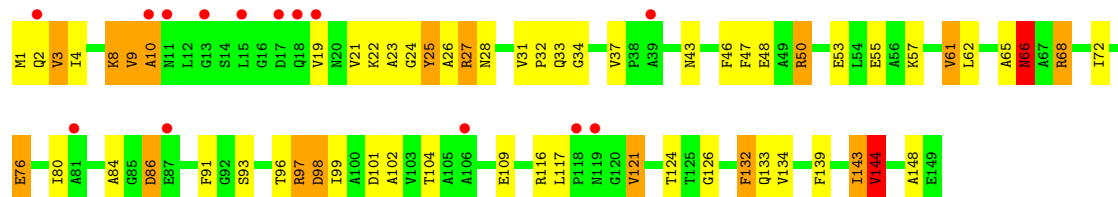
- Molecule 6: 50S ribosomal protein L5

Chain F: 

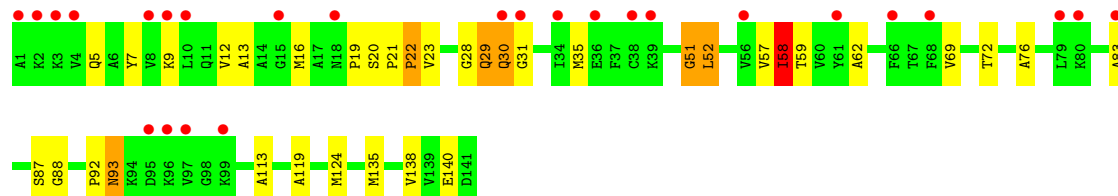
- Molecule 7: 50S ribosomal protein L6

Chain G: 

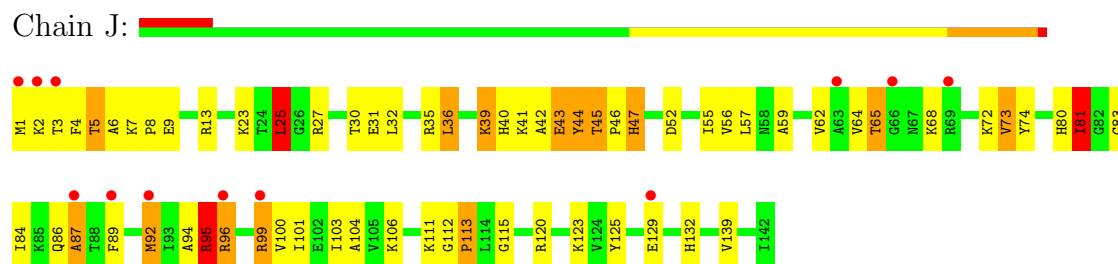
- Molecule 8: 50S ribosomal protein L9

Chain H: 

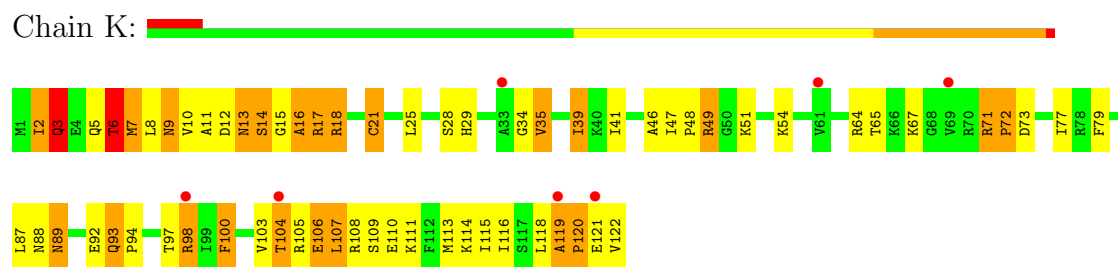
- Molecule 9: 50S ribosomal protein L11

Chain I: 

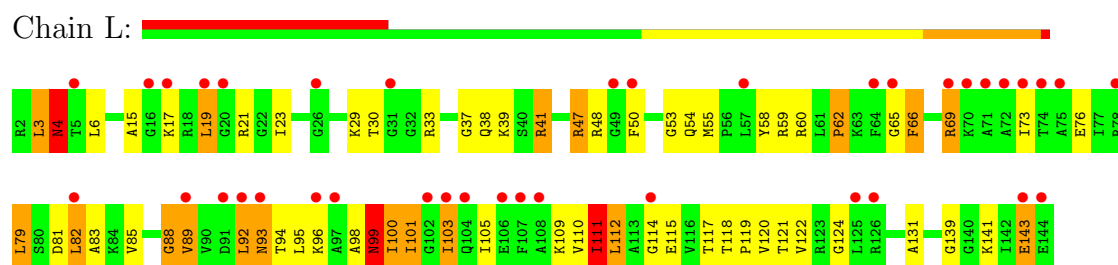
- Molecule 10: 50S ribosomal protein L13



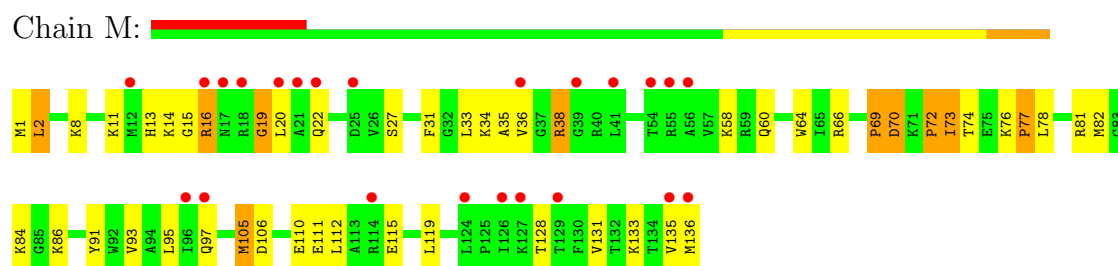
- Molecule 11: 50S ribosomal protein L14



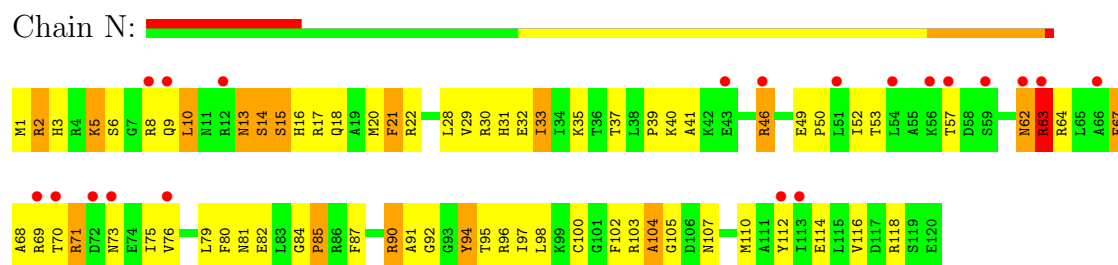
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16

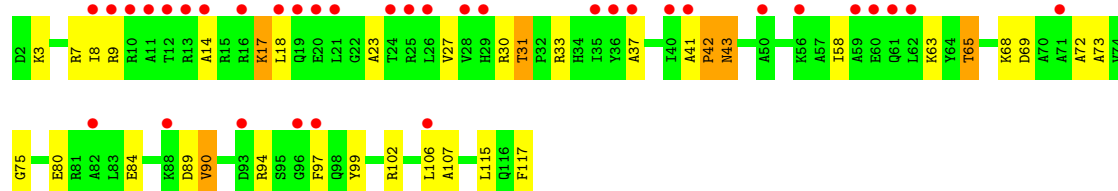


- Molecule 14: 50S ribosomal protein L17



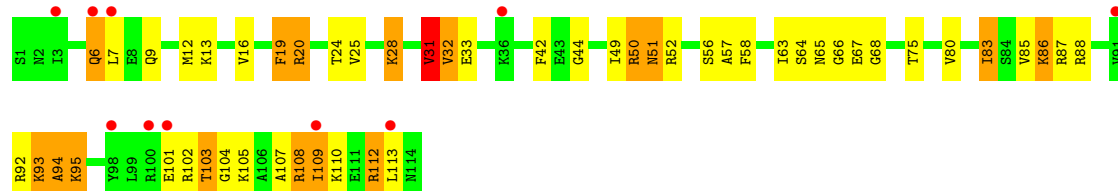
- Molecule 15: 50S ribosomal protein L18

Chain O: 



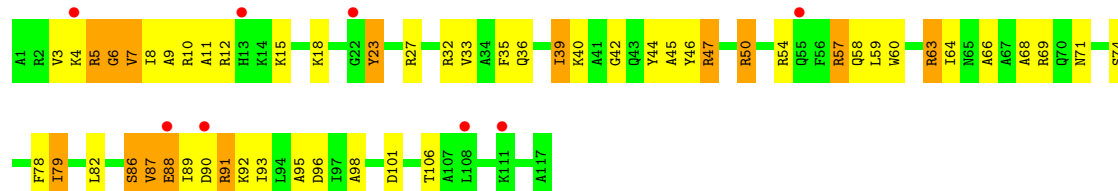
- Molecule 16: 50S ribosomal protein L19

Chain P: 



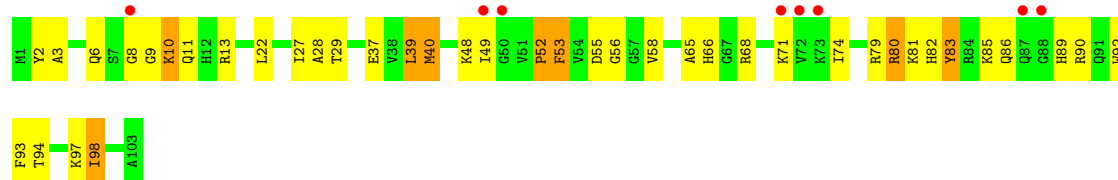
- Molecule 17: 50S ribosomal protein L20

Chain Q: 



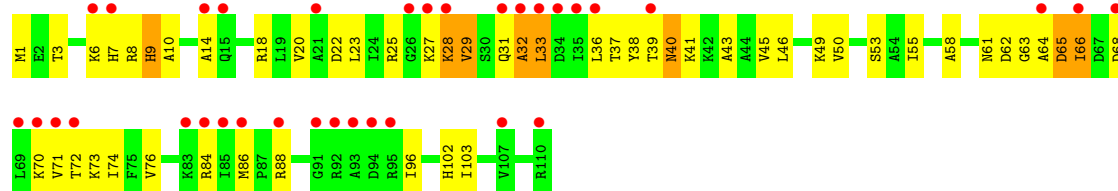
- Molecule 18: 50S ribosomal protein L21

Chain R: 



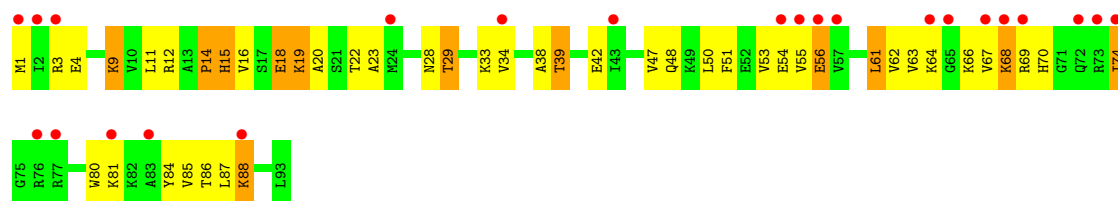
- Molecule 19: 50S ribosomal protein L22

Chain S: 



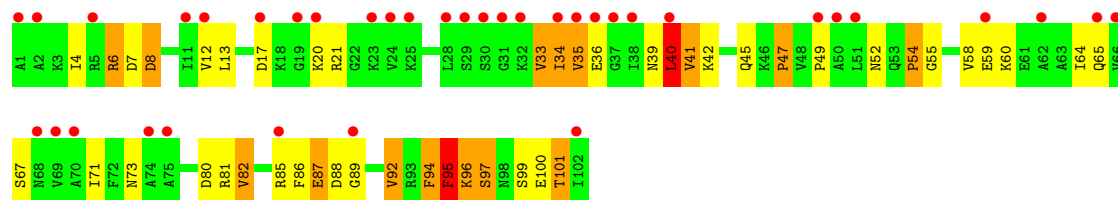
- Molecule 20: 50S ribosomal protein L23

Chain T: 



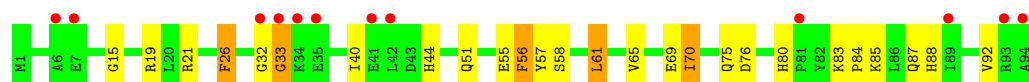
• Molecule 21: 50S ribosomal protein L24

Chain U:



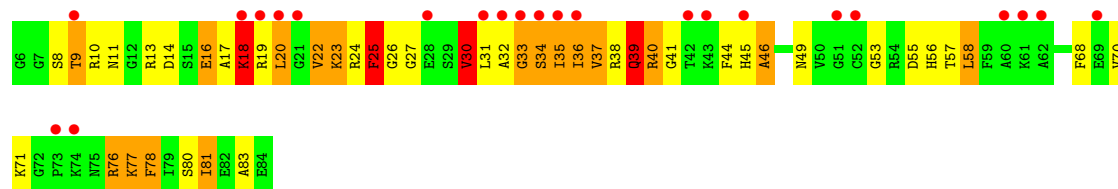
• Molecule 22: 50S ribosomal protein L25

Chain V:



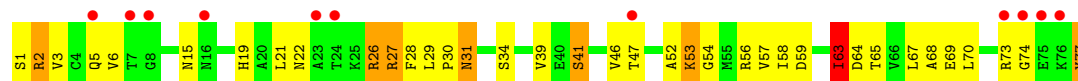
• Molecule 23: 50S ribosomal protein L27

Chain W:



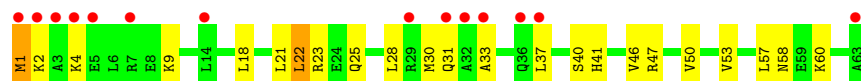
• Molecule 24: 50S ribosomal protein L28

Chain X:



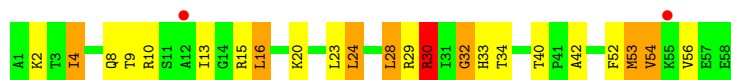
• Molecule 25: 50S ribosomal protein L29

Chain Y:



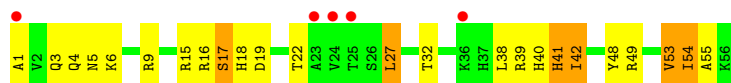
• Molecule 26: 50S ribosomal protein L30

Chain Z:



- Molecule 27: 50S ribosomal protein L32

Chain 0:



- Molecule 28: 50S ribosomal protein L33

Chain 1:



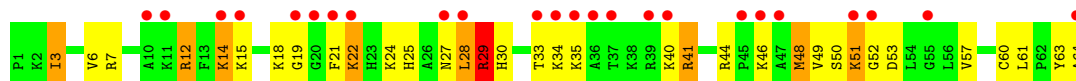
- Molecule 29: 50S ribosomal protein L34

Chain 2:



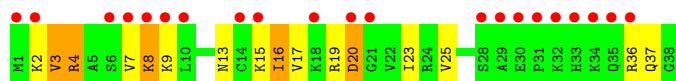
- Molecule 30: 50S ribosomal protein L35

Chain 3:



- Molecule 31: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.08Å 434.46Å 618.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.35 – 3.29 76.35 – 3.29	Depositor EDS
% Data completeness (in resolution range)	77.5 (76.35-3.29) 77.5 (76.35-3.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.189 , 0.241 0.508 , 0.512	Depositor DCC
R_{free} test set	10670 reflections (1.61%)	DCC
Wilson B-factor (Å ²)	66.6	Xtriage
Anisotropy	0.324	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 700316 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	90434	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	0.45	2/68314 (0.0%)	1.23	934/106569 (0.9%)
2	B	0.43	1/2803 (0.0%)	1.07	30/4371 (0.7%)
3	C	0.29	0/2122	0.51	0/2852
4	D	0.28	0/1586	0.54	0/2134
5	E	0.24	0/1571	0.46	0/2113
6	F	0.22	0/1444	0.45	0/1937
7	G	0.22	0/1343	0.44	0/1816
8	H	0.25	0/1122	0.51	2/1515 (0.1%)
9	I	0.20	0/1046	0.42	0/1410
10	J	0.26	0/1152	0.55	1/1551 (0.1%)
11	K	0.29	0/948	0.52	0/1268
12	L	0.25	0/1054	0.50	0/1403
13	M	0.27	0/1093	0.46	0/1460
14	N	0.26	0/974	0.48	0/1301
15	O	0.21	0/902	0.40	0/1209
16	P	0.27	0/929	0.47	0/1242
17	Q	0.27	0/960	0.44	0/1278
18	R	0.26	0/829	0.49	0/1107
19	S	0.26	0/864	0.50	0/1156
20	T	0.22	0/745	0.45	0/994
21	U	0.22	0/788	0.45	0/1051
22	V	0.23	0/766	0.42	0/1025
23	W	0.25	0/603	0.46	0/797
24	X	0.26	0/635	0.52	0/848
25	Y	0.21	0/510	0.42	0/677
26	Z	0.25	0/453	0.50	0/605
27	0	0.26	0/450	0.48	0/599
28	1	0.24	0/417	0.44	0/554
29	2	0.25	0/380	0.47	0/498
30	3	0.25	0/513	0.49	0/676
31	4	0.32	0/303	0.45	0/397
All	All	0.40	3/97619 (0.0%)	1.09	967/146413 (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
6	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	107	G	O3'-P	-8.40	1.51	1.61
1	A	1929	G	O3'-P	6.36	1.68	1.61
1	A	901	C	O3'-P	5.98	1.68	1.61

The worst 5 of 967 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2586	U	N1-C1'-C2'	-16.52	92.53	114.00
1	A	2283	C	N1-C1'-C2'	-14.98	94.52	114.00
1	A	2197	U	P-O3'-C3'	14.29	136.85	119.70
1	A	2137	U	N1-C1'-C2'	-14.24	95.49	114.00
1	A	2504	U	N1-C1'-C2'	-14.02	95.77	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	177	ARG	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	60995	0	0	2300	0
2	B	2507	0	0	90	0
3	C	2083	0	0	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1565	0	0	68	0
5	E	1552	0	0	42	0
6	F	1420	0	12	41	0
7	G	1323	0	0	34	0
8	H	1111	0	0	30	0
9	I	1032	0	0	13	0
10	J	1129	0	0	47	0
11	K	939	0	0	35	0
12	L	1045	0	0	49	0
13	M	1074	0	0	26	0
14	N	961	0	0	49	0
15	O	892	0	0	20	0
16	P	917	0	0	34	0
17	Q	947	0	0	42	0
18	R	816	0	0	27	0
19	S	857	0	0	26	0
20	T	739	0	0	27	0
21	U	780	0	0	24	0
22	V	753	0	0	12	0
23	W	596	0	0	39	0
24	X	625	0	0	26	0
25	Y	509	0	0	15	0
26	Z	449	0	0	10	0
27	0	444	0	0	18	0
28	1	410	0	0	12	0
29	2	377	0	0	11	0
30	3	504	0	0	22	0
31	4	302	0	0	8	0
32	A	132	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	E	1	0	0	0	0
32	J	1	0	0	0	0
33	4	1	0	0	0	0
34	2	2	0	0	0	0
34	3	1	0	0	0	0
34	4	2	0	0	0	0
34	A	605	0	0	12	0
34	B	4	0	0	0	0
34	C	7	0	0	0	0
34	D	1	0	0	0	0
34	E	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	J	6	0	0	0	0
34	L	4	0	0	0	0
34	N	2	0	0	0	0
34	T	3	0	0	0	0
34	U	2	0	0	0	0
34	V	1	0	0	0	0
All	All	90434	0	12	3069	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 3069 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:2093:G:O6	1:A:2225:A:C8	2.08	1.07
1:A:1116:G:C2	1:A:1117:C:C5	2.51	0.98
1:A:1116:G:C2	1:A:1117:C:C6	2.52	0.98
1:A:1116:G:N3	1:A:1117:C:C6	2.33	0.95
2:B:69:G:C8	2:B:70:C:C5	2.55	0.94

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	C	269/271 (99%)	177 (66%)	55 (20%)	37 (14%)	0	3
4	D	207/209 (99%)	134 (65%)	39 (19%)	34 (16%)	0	1
5	E	199/201 (99%)	122 (61%)	51 (26%)	26 (13%)	0	3
6	F	176/178 (99%)	98 (56%)	46 (26%)	32 (18%)	0	1
7	G	174/176 (99%)	100 (58%)	43 (25%)	31 (18%)	0	1
8	H	147/149 (99%)	71 (48%)	58 (40%)	18 (12%)	1	4
9	I	139/141 (99%)	78 (56%)	43 (31%)	18 (13%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	140/142 (99%)	90 (64%)	30 (21%)	20 (14%)	0	2
11	K	120/122 (98%)	83 (69%)	13 (11%)	24 (20%)	0	1
12	L	141/143 (99%)	81 (57%)	42 (30%)	18 (13%)	0	3
13	M	134/136 (98%)	93 (69%)	24 (18%)	17 (13%)	0	3
14	N	118/120 (98%)	72 (61%)	30 (25%)	16 (14%)	0	3
15	O	114/116 (98%)	76 (67%)	26 (23%)	12 (10%)	1	7
16	P	112/114 (98%)	65 (58%)	27 (24%)	20 (18%)	0	1
17	Q	115/117 (98%)	78 (68%)	24 (21%)	13 (11%)	1	5
18	R	101/103 (98%)	67 (66%)	25 (25%)	9 (9%)	1	10
19	S	108/110 (98%)	75 (69%)	21 (19%)	12 (11%)	1	6
20	T	91/93 (98%)	47 (52%)	28 (31%)	16 (18%)	0	1
21	U	100/102 (98%)	50 (50%)	23 (23%)	27 (27%)	0	0
22	V	92/94 (98%)	61 (66%)	24 (26%)	7 (8%)	2	15
23	W	77/79 (98%)	34 (44%)	22 (29%)	21 (27%)	0	0
24	X	75/77 (97%)	46 (61%)	24 (32%)	5 (7%)	2	18
25	Y	61/63 (97%)	40 (66%)	16 (26%)	5 (8%)	1	12
26	Z	56/58 (97%)	35 (62%)	15 (27%)	6 (11%)	1	6
27	0	54/56 (96%)	37 (68%)	12 (22%)	5 (9%)	1	9
28	1	48/50 (96%)	33 (69%)	10 (21%)	5 (10%)	1	7
29	2	44/46 (96%)	32 (73%)	6 (14%)	6 (14%)	0	3
30	3	62/64 (97%)	40 (64%)	17 (27%)	5 (8%)	1	13
31	4	36/38 (95%)	24 (67%)	6 (17%)	6 (17%)	0	1
All	All	3310/3368 (98%)	2039 (62%)	800 (24%)	471 (14%)	0	2

5 of 471 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	9	SER
3	C	28	PRO
3	C	186	ASP
3	C	232	GLY
3	C	239	PHE

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	C	216/216 (100%)	189 (88%)	27 (12%)	7	32
4	D	164/164 (100%)	139 (85%)	25 (15%)	4	21
5	E	165/165 (100%)	148 (90%)	17 (10%)	10	42
6	F	149/149 (100%)	127 (85%)	22 (15%)	4	22
7	G	137/137 (100%)	121 (88%)	16 (12%)	8	36
8	H	114/114 (100%)	98 (86%)	16 (14%)	5	25
9	I	109/109 (100%)	103 (94%)	6 (6%)	30	75
10	J	116/116 (100%)	103 (89%)	13 (11%)	9	38
11	K	103/103 (100%)	82 (80%)	21 (20%)	2	8
12	L	102/102 (100%)	89 (87%)	13 (13%)	6	31
13	M	109/109 (100%)	103 (94%)	6 (6%)	30	75
14	N	100/100 (100%)	80 (80%)	20 (20%)	2	9
15	O	86/86 (100%)	78 (91%)	8 (9%)	13	48
16	P	99/99 (100%)	89 (90%)	10 (10%)	11	42
17	Q	89/89 (100%)	75 (84%)	14 (16%)	4	19
18	R	84/84 (100%)	71 (84%)	13 (16%)	4	20
19	S	93/93 (100%)	79 (85%)	14 (15%)	4	21
20	T	80/80 (100%)	74 (92%)	6 (8%)	19	62
21	U	83/83 (100%)	73 (88%)	10 (12%)	7	34
22	V	78/78 (100%)	70 (90%)	8 (10%)	10	42
23	W	59/59 (100%)	44 (75%)	15 (25%)	1	3
24	X	67/67 (100%)	57 (85%)	10 (15%)	4	22
25	Y	55/55 (100%)	52 (94%)	3 (6%)	30	75
26	Z	48/48 (100%)	40 (83%)	8 (17%)	3	16
27	0	47/47 (100%)	40 (85%)	7 (15%)	4	22
28	1	45/45 (100%)	41 (91%)	4 (9%)	14	51
29	2	38/38 (100%)	35 (92%)	3 (8%)	18	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	3	51/51 (100%)	40 (78%)	11 (22%)	1	7
31	4	34/34 (100%)	29 (85%)	5 (15%)	4	23
All	All	2720/2720 (100%)	2369 (87%)	351 (13%)	6	30

5 of 351 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	105	ARG
14	N	94	TYR
27	O	27	LEU
12	L	3	LEU
13	M	78	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2839/2903 (97%)	1062 (37%)	506 (17%)
2	B	116/117 (99%)	38 (32%)	15 (12%)
All	All	2955/3020 (97%)	1100 (37%)	521 (17%)

5 of 1100 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	A
1	A	14	A
1	A	15	G
1	A	16	C
1	A	28	A

5 of 521 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1329	U
1	A	1654	A
1	A	2752	C
1	A	1388	G
1	A	1508	A

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 138 ligands modelled in this entry, 138 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	2841/2903 (97%)	0.70	215 (7%) 14 4	49, 122, 252, 460	0
2	B	117/117 (100%)	0.88	15 (12%) 4 2	95, 169, 224, 274	0
3	C	271/271 (100%)	0.60	18 (6%) 18 4	51, 96, 147, 192	0
4	D	209/209 (100%)	0.68	12 (5%) 23 5	50, 111, 176, 290	0
5	E	201/201 (100%)	0.59	20 (9%) 8 2	62, 197, 395, 486	0
6	F	178/178 (100%)	1.06	36 (20%) 2 1	183, 225, 286, 338	0
7	G	176/176 (100%)	0.80	26 (14%) 3 1	95, 195, 279, 335	0
8	H	149/149 (100%)	0.29	14 (9%) 9 3	82, 181, 277, 319	0
9	I	141/141 (100%)	1.13	26 (18%) 2 1	210, 324, 369, 408	0
10	J	142/142 (100%)	0.65	12 (8%) 11 3	63, 102, 163, 184	0
11	K	122/122 (100%)	0.58	7 (5%) 23 5	52, 95, 164, 236	0
12	L	143/143 (100%)	1.36	38 (26%) 1 1	58, 159, 278, 348	0
13	M	136/136 (100%)	0.85	23 (16%) 2 1	44, 105, 164, 196	0
14	N	120/120 (100%)	1.11	20 (16%) 2 1	79, 127, 200, 268	0
15	O	116/116 (100%)	1.61	35 (30%) 1 1	124, 169, 240, 292	0
16	P	114/114 (100%)	0.65	10 (8%) 10 3	62, 114, 174, 238	0
17	Q	117/117 (100%)	0.77	8 (6%) 17 4	66, 103, 194, 288	0
18	R	103/103 (100%)	0.50	8 (7%) 13 4	67, 130, 227, 316	0
19	S	110/110 (100%)	1.59	34 (30%) 1 1	59, 130, 231, 279	0
20	T	93/93 (100%)	1.40	23 (24%) 1 1	123, 205, 306, 347	0
21	U	102/102 (100%)	1.95	37 (36%) 1 0	123, 285, 434, 557	0
22	V	94/94 (100%)	0.83	12 (12%) 4 2	97, 143, 194, 233	0
23	W	79/79 (100%)	1.45	23 (29%) 1 1	82, 140, 238, 284	0
24	X	77/77 (100%)	1.01	11 (14%) 3 1	78, 117, 171, 236	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	63/63 (100%)	1.26	14 (22%) 1 1	143, 309, 433, 440	0
26	Z	58/58 (100%)	0.40	2 (3%) 43 10	78, 119, 208, 217	0
27	0	56/56 (100%)	0.74	5 (8%) 10 3	63, 139, 242, 298	0
28	1	50/50 (100%)	0.57	3 (6%) 21 5	99, 170, 210, 236	0
29	2	46/46 (100%)	1.15	7 (15%) 3 1	81, 118, 175, 233	0
30	3	64/64 (100%)	1.65	24 (37%) 1 0	65, 128, 183, 257	0
31	4	38/38 (100%)	2.52	21 (55%) 0 0	79, 137, 187, 227	0
All	All	6326/6388 (99%)	0.83	759 (11%) 5 2	44, 132, 301, 557	0

The worst 5 of 759 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1537	G	14.0
5	E	127	GLU	13.5
25	Y	3	ALA	11.9
9	I	9	LYS	11.1
6	F	129	MET	11.0

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	2922	1/1	0.82	217.67	247,247,247,247	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	J	747	1/1	1.35	89.15	230,230,230,230	0
32	MG	A	2924	1/1	1.08	80.88	199,199,199,199	0
32	MG	A	2965	1/1	1.22	66.07	211,211,211,211	0
32	MG	A	2999	1/1	0.71	62.62	102,102,102,102	0
32	MG	A	2964	1/1	1.38	32.62	229,229,229,229	0
32	MG	A	2935	1/1	0.81	14.78	121,121,121,121	0
32	MG	A	2976	1/1	0.61	14.24	274,274,274,274	0
32	MG	A	2960	1/1	0.45	12.40	227,227,227,227	0
32	MG	A	2962	1/1	0.37	12.09	200,200,200,200	0
32	MG	A	3011	1/1	0.55	10.81	185,185,185,185	0
32	MG	C	722	1/1	0.69	10.51	129,129,129,129	0
32	MG	A	3029	1/1	0.52	9.36	200,200,200,200	0
32	MG	A	2966	1/1	0.49	9.23	278,278,278,278	0
32	MG	A	2908	1/1	0.79	8.94	309,309,309,309	0
32	MG	A	2994	1/1	0.36	8.15	116,116,116,116	0
32	MG	A	2938	1/1	0.32	7.88	194,194,194,194	0
32	MG	A	3010	1/1	0.64	6.52	161,161,161,161	0
32	MG	A	2987	1/1	0.51	5.51	144,144,144,144	0
32	MG	A	2911	1/1	0.36	5.23	148,148,148,148	0
32	MG	A	3001	1/1	0.26	5.20	172,172,172,172	0
32	MG	A	2983	1/1	0.60	5.02	108,108,108,108	0
32	MG	A	3035	1/1	0.81	4.94	174,174,174,174	0
32	MG	A	2928	1/1	1.17	4.13	278,278,278,278	0
32	MG	A	2997	1/1	0.65	4.05	107,107,107,107	0
32	MG	A	3032	1/1	1.24	3.52	233,233,233,233	0
32	MG	A	2993	1/1	0.56	3.44	165,165,165,165	0
32	MG	A	2977	1/1	0.33	3.31	190,190,190,190	0
32	MG	A	2959	1/1	0.65	3.10	197,197,197,197	0
32	MG	A	2914	1/1	0.40	3.00	127,127,127,127	0
32	MG	A	3017	1/1	0.32	2.91	167,167,167,167	0
32	MG	A	2980	1/1	0.30	2.84	222,222,222,222	0
32	MG	A	2988	1/1	0.36	2.24	87,87,87,87	0
32	MG	A	2905	1/1	0.28	2.20	180,180,180,180	0
32	MG	A	2936	1/1	0.45	1.98	95,95,95,95	0
32	MG	A	2950	1/1	0.33	1.78	95,95,95,95	0
32	MG	A	2910	1/1	0.20	1.78	254,254,254,254	0
32	MG	A	2961	1/1	0.25	1.77	204,204,204,204	0
32	MG	A	3014	1/1	0.28	1.71	109,109,109,109	0
32	MG	A	2971	1/1	0.63	1.63	209,209,209,209	0
32	MG	A	2940	1/1	0.42	1.48	197,197,197,197	0
32	MG	C	272	1/1	0.41	1.35	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	2917	1/1	0.32	1.23	172,172,172,172	0
32	MG	A	2981	1/1	0.41	1.17	180,180,180,180	0
32	MG	A	3008	1/1	0.28	1.15	262,262,262,262	0
32	MG	A	2986	1/1	0.24	1.01	204,204,204,204	0
32	MG	A	3034	1/1	0.42	0.90	212,212,212,212	0
32	MG	B	590	1/1	0.25	0.57	104,104,104,104	0
32	MG	A	3018	1/1	0.27	0.34	65,65,65,65	0
32	MG	A	2958	1/1	0.27	0.26	120,120,120,120	0
32	MG	A	2912	1/1	0.22	0.14	69,69,69,69	0
32	MG	A	2949	1/1	0.25	0.02	151,151,151,151	0
32	MG	A	3027	1/1	0.33	-0.05	176,176,176,176	0
32	MG	A	2909	1/1	0.30	-0.06	211,211,211,211	0
32	MG	A	2984	1/1	0.21	-0.07	142,142,142,142	0
32	MG	A	2995	1/1	0.26	-0.21	229,229,229,229	0
32	MG	A	3024	1/1	0.24	-0.28	84,84,84,84	0
32	MG	A	3006	1/1	0.23	-0.34	44,44,44,44	0
32	MG	A	2906	1/1	0.26	-0.48	236,236,236,236	0
32	MG	A	2927	1/1	0.24	-0.57	89,89,89,89	0
32	MG	A	2931	1/1	0.25	-0.62	143,143,143,143	0
32	MG	A	3007	1/1	0.22	-0.73	47,47,47,47	0
32	MG	A	2945	1/1	0.23	-0.79	161,161,161,161	0
32	MG	A	3031	1/1	0.18	-0.84	214,214,214,214	0
32	MG	A	2907	1/1	0.21	-0.86	114,114,114,114	0
32	MG	A	2951	1/1	0.15	-0.86	218,218,218,218	0
32	MG	A	2975	1/1	0.13	-0.87	187,187,187,187	0
32	MG	A	2920	1/1	0.22	-0.88	204,204,204,204	0
32	MG	A	3030	1/1	0.20	-0.90	142,142,142,142	0
32	MG	A	2969	1/1	0.19	-0.96	61,61,61,61	0
32	MG	A	2996	1/1	0.25	-1.06	114,114,114,114	0
32	MG	A	2974	1/1	0.21	-1.07	133,133,133,133	0
32	MG	A	3023	1/1	0.19	-1.10	109,109,109,109	0
32	MG	A	2998	1/1	0.13	-1.12	95,95,95,95	0
32	MG	A	3013	1/1	0.17	-1.16	153,153,153,153	0
32	MG	A	3016	1/1	0.20	-1.19	148,148,148,148	0
32	MG	A	3000	1/1	0.24	-1.27	144,144,144,144	0
32	MG	A	2930	1/1	0.23	-1.28	253,253,253,253	0
32	MG	A	3012	1/1	0.22	-1.29	174,174,174,174	0
32	MG	A	2982	1/1	0.20	-1.32	142,142,142,142	0
32	MG	A	2992	1/1	0.19	-1.33	99,99,99,99	0
32	MG	A	2989	1/1	0.18	-1.33	139,139,139,139	0
32	MG	A	2933	1/1	0.19	-1.38	68,68,68,68	0
32	MG	A	2916	1/1	0.20	-1.40	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	2918	1/1	0.24	-1.42	183,183,183,183	0
33	ZN	4	781	1/1	0.19	-1.47	161,161,161,161	0
32	MG	A	2947	1/1	0.21	-1.52	156,156,156,156	0
32	MG	A	2946	1/1	0.15	-1.57	100,100,100,100	0
32	MG	A	3033	1/1	0.18	-1.66	85,85,85,85	0
32	MG	A	3025	1/1	0.17	-1.70	153,153,153,153	0
32	MG	A	2915	1/1	0.19	-1.73	64,64,64,64	0
32	MG	A	2925	1/1	0.25	-1.80	69,69,69,69	0
32	MG	A	2926	1/1	0.16	-1.91	87,87,87,87	0
32	MG	A	3009	1/1	0.16	-1.93	92,92,92,92	0
32	MG	A	2948	1/1	0.17	-1.98	78,78,78,78	0
32	MG	A	3004	1/1	0.14	-1.99	67,67,67,67	0
32	MG	A	3021	1/1	0.15	-2.05	76,76,76,76	0
32	MG	A	3003	1/1	0.18	-2.13	78,78,78,78	0
32	MG	A	2954	1/1	0.13	-2.20	57,57,57,57	0
32	MG	A	3015	1/1	0.15	-2.24	131,131,131,131	0
32	MG	A	2942	1/1	0.16	-2.49	65,65,65,65	0
32	MG	A	3002	1/1	0.19	-2.52	68,68,68,68	0
32	MG	A	2991	1/1	0.12	-2.54	87,87,87,87	0
32	MG	E	202	1/1	0.12	-2.61	131,131,131,131	0
32	MG	A	2957	1/1	0.15	-2.64	96,96,96,96	0
32	MG	A	2979	1/1	0.18	-2.74	93,93,93,93	0
32	MG	A	2985	1/1	0.10	-2.93	197,197,197,197	0
32	MG	A	2973	1/1	0.21	-3.07	56,56,56,56	0
32	MG	A	2955	1/1	0.19	-3.07	89,89,89,89	0
32	MG	A	2970	1/1	0.15	-3.09	83,83,83,83	0
32	MG	A	2921	1/1	0.17	-3.20	226,226,226,226	0
32	MG	A	2919	1/1	0.12	-3.24	87,87,87,87	0
32	MG	A	2904	1/1	0.12	-3.41	151,151,151,151	0
32	MG	A	3022	1/1	0.13	-3.44	93,93,93,93	0
32	MG	A	3026	1/1	0.12	-3.45	61,61,61,61	0
32	MG	A	3028	1/1	0.12	-3.47	82,82,82,82	0
32	MG	A	2972	1/1	0.11	-3.52	69,69,69,69	0
32	MG	A	2968	1/1	0.13	-3.59	49,49,49,49	0
32	MG	A	2929	1/1	0.09	-3.62	109,109,109,109	0
32	MG	A	2937	1/1	0.14	-3.71	125,125,125,125	0
32	MG	A	2939	1/1	0.07	-4.02	82,82,82,82	0
32	MG	A	2943	1/1	0.16	-4.32	70,70,70,70	0
32	MG	A	2934	1/1	0.15	-4.72	105,105,105,105	0
32	MG	A	2978	1/1	0.19	-4.75	174,174,174,174	0
32	MG	A	2952	1/1	0.28	-5.00	172,172,172,172	0
32	MG	A	2941	1/1	0.13	-5.01	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	2963	1/1	0.11	-5.16	105,105,105,105	0
32	MG	A	3005	1/1	0.17	-5.20	86,86,86,86	0
32	MG	A	3019	1/1	0.15	-5.21	77,77,77,77	0
32	MG	A	2953	1/1	0.13	-5.26	106,106,106,106	0
32	MG	A	2944	1/1	0.13	-6.31	82,82,82,82	0
32	MG	A	3020	1/1	0.09	-6.76	71,71,71,71	0
32	MG	A	2967	1/1	0.09	-8.97	70,70,70,70	0
32	MG	A	2932	1/1	0.18	-12.74	112,112,112,112	0
32	MG	A	2990	1/1	0.12	-17.38	179,179,179,179	0
32	MG	A	2956	1/1	0.04	-20.20	67,67,67,67	0
32	MG	A	2923	1/1	0.12	-21.02	49,49,49,49	0
32	MG	A	2913	1/1	0.73	-	218,218,218,218	0

6.5 Other polymers ⓘ

There are no such residues in this entry.