



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:20 PM GMT

PDB ID : 3CCM  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.55 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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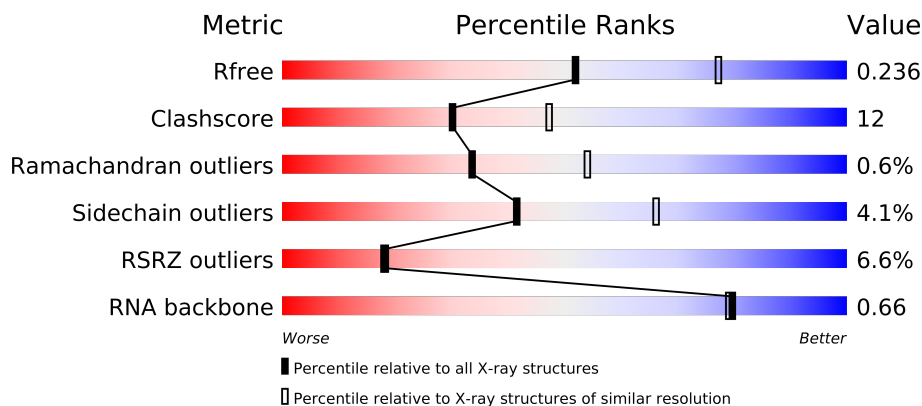
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.55 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	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)
RNA backbone	1838	1058 (3.10-1.98)

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  $\geq 3$ , 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	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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Mol	Chain	Length	Quality of chain
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

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	0	8004	-	X
32	MG	0	8006	-	X
32	MG	0	8007	-	X
32	MG	0	8008	-	X
32	MG	0	8009	-	X
32	MG	0	8012	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8019	-	X
32	MG	0	8028	-	X
32	MG	0	8030	-	X
32	MG	0	8032	-	X
32	MG	0	8037	-	X
32	MG	0	8038	-	X
32	MG	0	8039	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8044	-	X
32	MG	0	8045	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8050	-	X
32	MG	0	8055	-	X
32	MG	0	8056	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8063	-	X
32	MG	0	8065	-	X
32	MG	0	8066	-	X
32	MG	0	8068	-	X
32	MG	0	8071	-	X
32	MG	0	8073	-	X
32	MG	0	8076	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8081	-	X
32	MG	0	8085	-	X
32	MG	0	8092	-	X
32	MG	0	8093	-	X
32	MG	9	8074	-	X
32	MG	A	8051	-	X
32	MG	B	8042	-	X
34	NA	0	8502	-	X
34	NA	0	8504	-	X
34	NA	0	8505	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8516	-	X
34	NA	0	8517	-	X
34	NA	0	8518	-	X
34	NA	0	8520	-	X
34	NA	0	8521	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8542	-	X
34	NA	0	8545	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8552	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
35	CL	B	8819	-	X
36	SR	0	8902	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8907	-	X
36	SR	0	8910	-	X
36	SR	0	8918	-	X
36	SR	0	8922	-	X
36	SR	0	8926	-	X
36	SR	0	8927	-	X
36	SR	0	8938	-	X
36	SR	0	8949	-	X
36	SR	0	8955	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	8957	-	X
36	SR	0	8962	-	X
36	SR	0	8971	-	X
36	SR	0	8974	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8983	-	X
36	SR	0	8987	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	9000	-	X
36	SR	0	9002	-	X
36	SR	0	9007	-	X
36	SR	9	8968	-	X
36	SR	9	8980	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26348	10870	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	T	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	94	Total 94	Sr 94	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	1	Total 1	Sr 1	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5938	Total O 5938 5938	0	0
38	9	145	Total O 145 145	0	0
38	A	117	Total O 117 117	0	0
38	B	139	Total O 139 139	0	0
38	C	165	Total O 165 165	0	0
38	D	48	Total O 48 48	0	0
38	E	49	Total O 49 49	0	0
38	F	25	Total O 25 25	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	8	Total O 8 8	0	0
38	J	55	Total O 55 55	0	0
38	K	55	Total O 55 55	0	0
38	L	79	Total O 79 79	0	0
38	M	138	Total O 138 138	0	0
38	N	58	Total O 58 58	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	49	Total O 49 49	0	0
38	R	78	Total O 78 78	0	0
38	S	32	Total O 32 32	0	0

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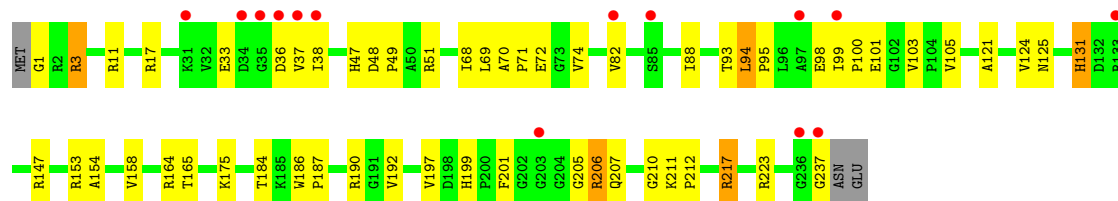
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	24	Total 24	O 24	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	29	Total 29	O 29	0	0
38	1	51	Total 51	O 51	0	0
38	2	37	Total 37	O 37	0	0
38	3	72	Total 72	O 72	0	0

### 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.

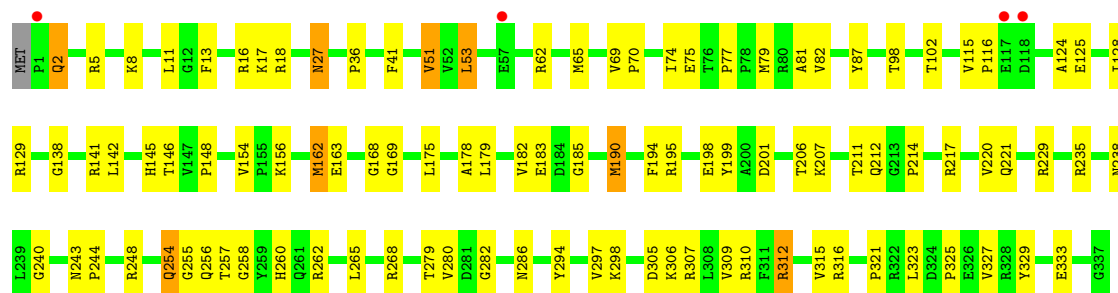
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



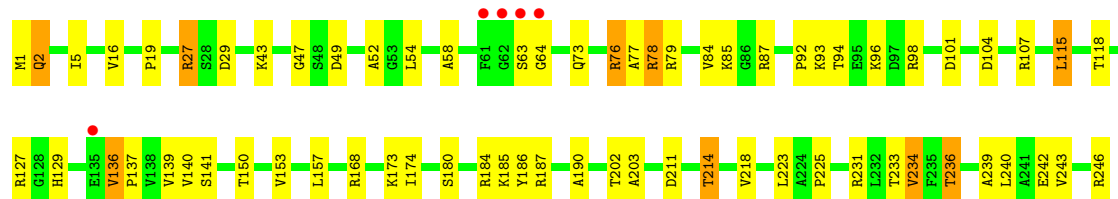
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



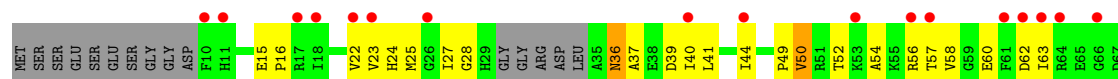
- Molecule 3: 50S ribosomal protein L4P

Chain C: 



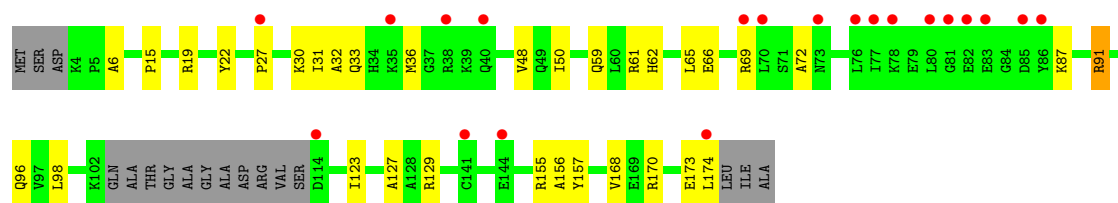
- Molecule 4: 50S ribosomal protein L5P

Chain D: 



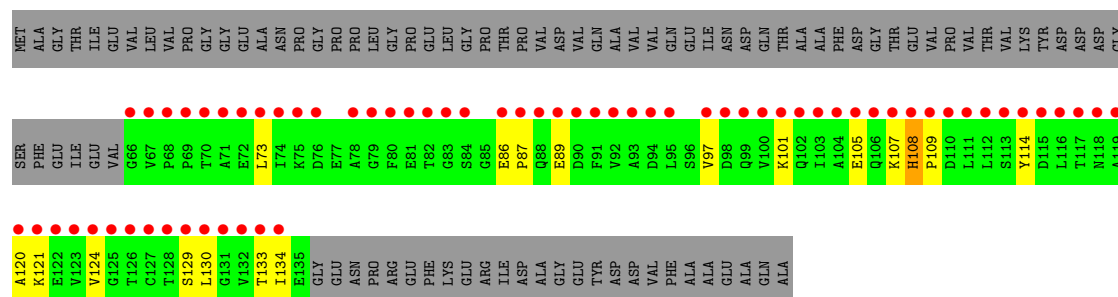






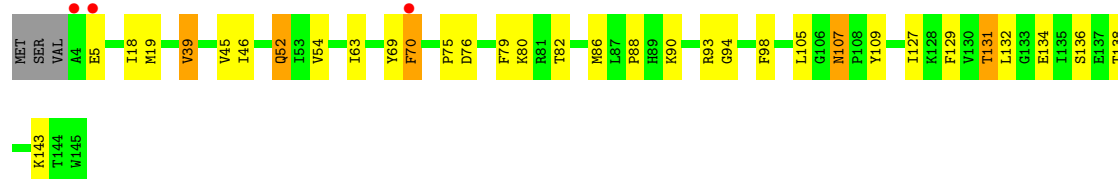
• Molecule 9: 50S ribosomal protein L11P

Chain I:



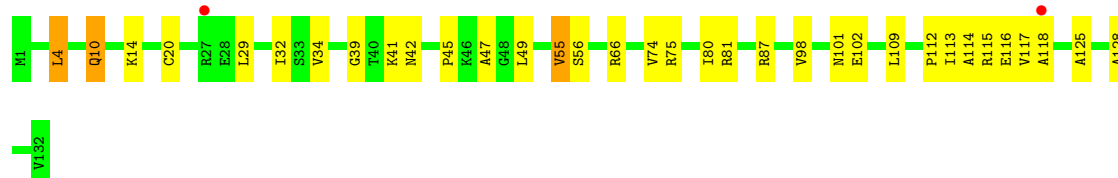
• Molecule 10: 50S ribosomal protein L13P

Chain J:



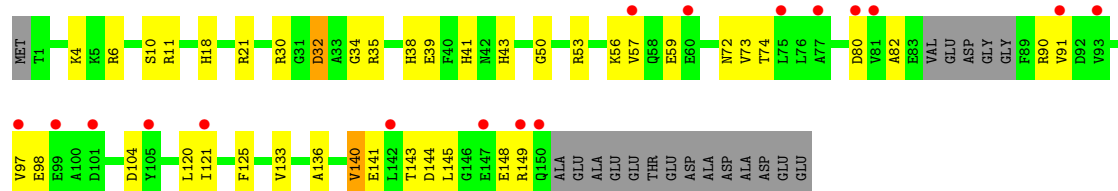
• Molecule 11: 50S ribosomal protein L14P

Chain K:



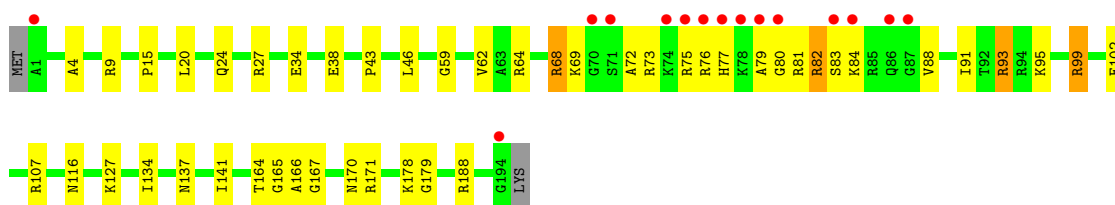
• Molecule 12: 50S ribosomal protein L15P

Chain L:



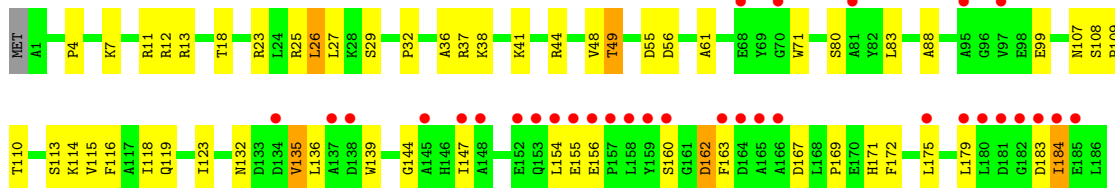
• Molecule 13: 50S ribosomal protein L15e

Chain M:



- Molecule 14: 50S ribosomal protein L18P

Chain N:



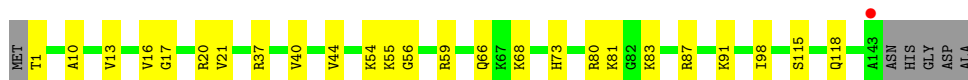
- Molecule 15: 50S ribosomal protein L18e

Chain O:



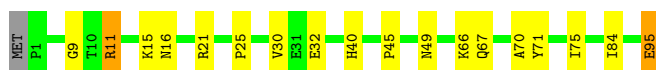
- Molecule 16: 50S ribosomal protein L19e

Chain P:



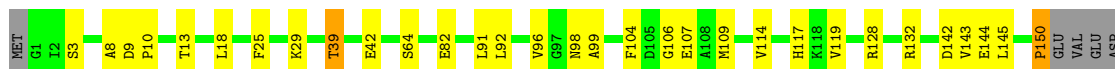
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



- Molecule 18: 50S ribosomal protein L22P

Chain R:



- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

- Molecule 21: 50S ribosomal protein L24e

- Molecule 22: 50S ribosomal protein L29P

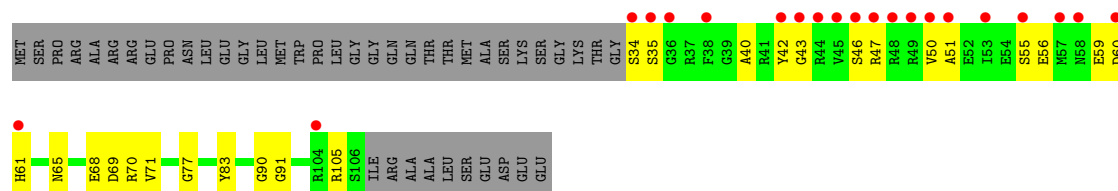
- Molecule 23: 50S ribosomal protein L30P

- Molecule 24: 50S ribosomal protein L31e

- Molecule 25: 50S ribosomal protein L32e

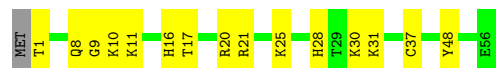
- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



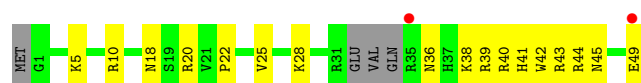
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



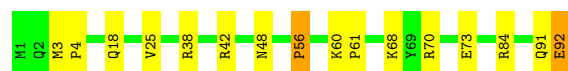
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



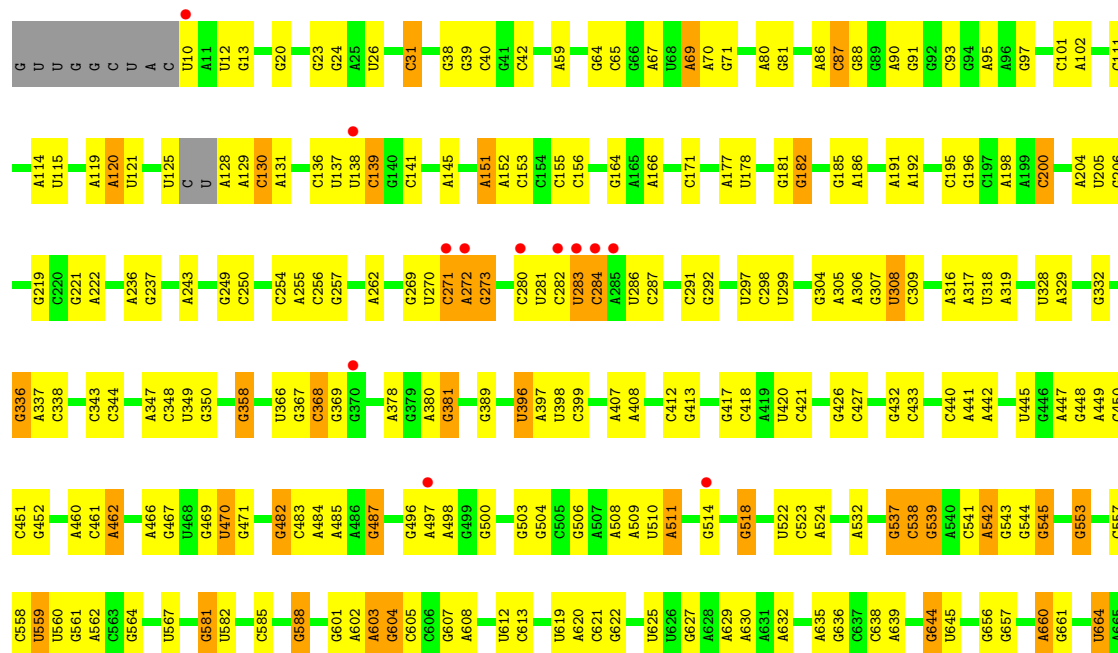
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

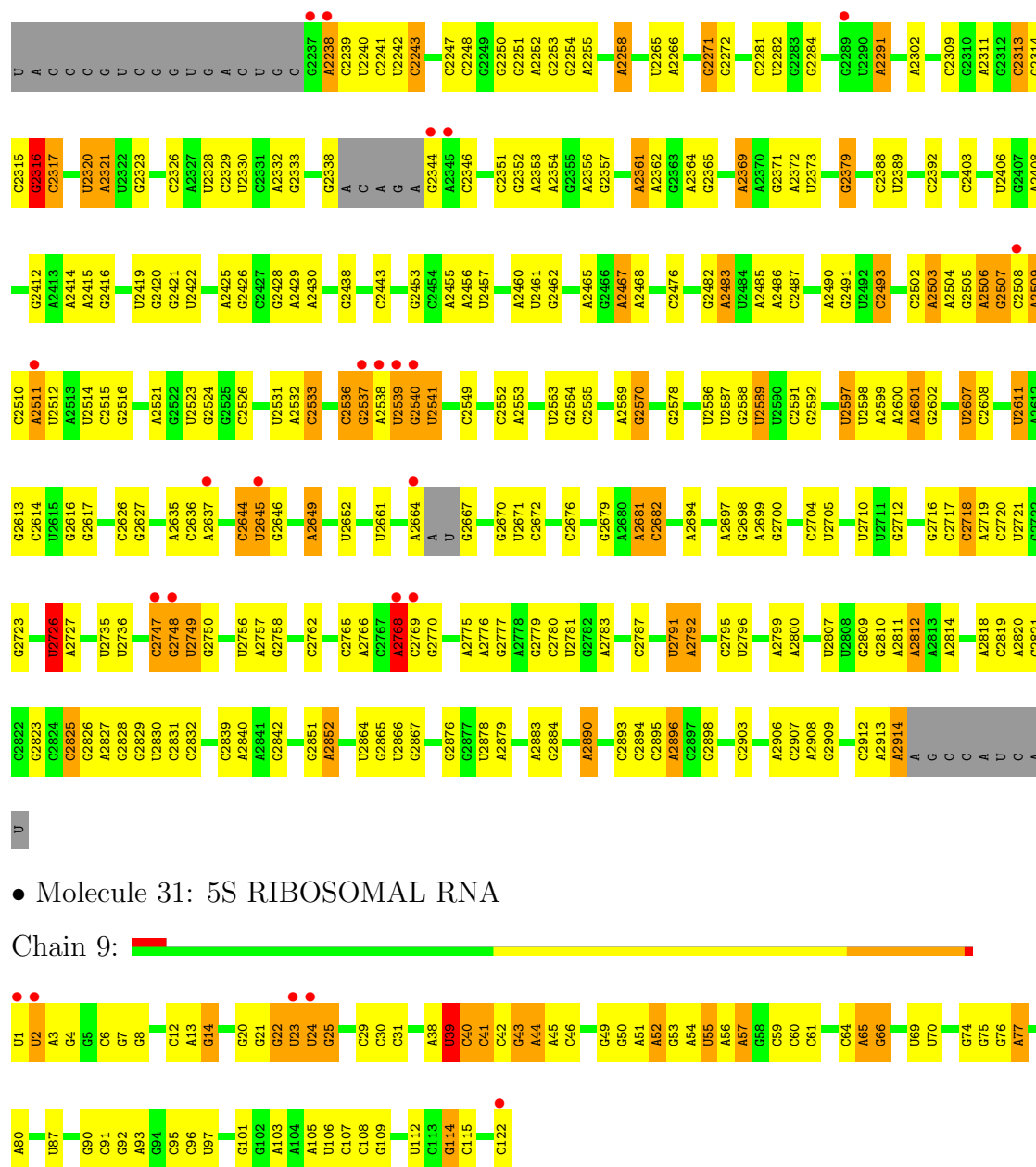


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:



WORLDWIDE  
 **PDB**  
PROTEIN DATA BANK



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 85.30 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 90.6 (85.30-2.39)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.201 , 0.240 0.203 , 0.236	Depositor DCC
$R_{free}$ test set	5933 reflections (0.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.9	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 691614 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, PSU

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	0.33	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.30	0/1111	0.56	1/1498 (0.1%)
5	E	0.31	0/1382	0.56	0/1880
6	F	0.33	0/901	0.56	0/1224
7	G	0.29	0/241	0.45	0/324
8	H	0.33	0/1302	0.64	0/1743
9	I	0.29	0/526	0.47	0/716
10	J	0.36	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.66	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.63	0/1999
15	O	0.32	0/874	0.60	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.35	0/749	0.69	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.33	0/648	0.56	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.34	0/417	0.55	0/562
22	V	0.30	0/502	0.51	0/675
23	W	0.33	0/1219	0.60	0/1655
24	X	0.32	0/664	0.57	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.36	0/584	0.60	0/781
27	1	0.39	0/438	0.65	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.38	0/771	0.57	0/1024
30	0	0.35	0/65953	0.69	25/102860 (0.0%)
31	9	0.30	0/2904	0.70	1/4526 (0.0%)
All	All	0.37	7/98697 (0.0%)	0.68	33/147579 (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
18	R	1	0
30	0	0	46
31	9	0	3
All	All	1	49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.57	2.82	1.50
18	R	150	PRO	CA-C	-19.00	1.14	1.52
18	R	150	PRO	CG-CD	14.11	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.60	1.67	1.47

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.33	56.17	112.00
18	R	150	PRO	N-CA-C	-19.61	61.12	112.10
18	R	150	PRO	CA-N-CD	12.19	128.76	111.70
18	R	150	PRO	N-CA-CB	10.92	116.40	103.30
30	0	1942	A	C5'-C4'-C3'	8.23	129.17	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 49 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	182	G	Sidechain
30	0	26	U	Sidechain
30	0	270	U	Sidechain
30	0	332	G	Sidechain
30	0	396	U	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	1753	0	1766	51	0
2	B	2625	0	2533	86	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	35	0
6	F	890	0	843	25	0
7	G	240	0	231	6	0
8	H	1282	0	1292	31	0
9	I	519	0	500	19	0
10	J	1120	0	1098	37	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	35	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	32	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	15	0
22	V	499	0	511	15	0
23	W	1196	0	1137	52	0
24	X	654	0	653	15	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	78	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	94	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	1	0	0	0	0
36	F	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	145	0	0	9	0
38	A	117	0	0	8	0
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0
38	H	71	0	0	5	0
38	I	8	0	0	0	0
38	J	55	0	0	1	0
38	K	55	0	0	2	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1801	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 1801 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
30:0:1160:G:H5'	30:0:1161:A:H5'	1.13	1.11

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	
1	A	235/240 (98%)	209 (89%)	24 (10%)	2 (1%)	25	41
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	33	54
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	10	15
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	25	41
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	15	25
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	16	27
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	11	16
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	8	10
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	25	41
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	9	11
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	16	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	21	34
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	33	54

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU
14	N	154	LEU
14	N	183	ASP
14	N	184	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	
1	A	179/182 (98%)	170 (95%)	9 (5%)	34	56
2	B	282/283 (100%)	268 (95%)	14 (5%)	34	56
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	31
4	D	117/148 (79%)	112 (96%)	5 (4%)	40	64
5	E	152/156 (97%)	147 (97%)	5 (3%)	50	75
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	96
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	71
8	H	134/145 (92%)	129 (96%)	5 (4%)	45	71
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	111 (94%)	7 (6%)	28	46
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	81
12	L	113/127 (89%)	109 (96%)	4 (4%)	48	73
13	M	158/160 (99%)	152 (96%)	6 (4%)	44	70
14	N	149/150 (99%)	145 (97%)	4 (3%)	57	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	93/94 (99%)	88 (95%)	5 (5%)	31	51
16	P	113/117 (97%)	110 (97%)	3 (3%)	57	82
17	Q	79/80 (99%)	76 (96%)	3 (4%)	44	70
18	R	117/122 (96%)	115 (98%)	2 (2%)	73	92
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	98 (93%)	7 (7%)	23	39
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	86
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	89
23	W	130/130 (100%)	124 (95%)	6 (5%)	37	60
24	X	66/74 (89%)	61 (92%)	5 (8%)	19	33
25	Y	120/196 (61%)	110 (92%)	10 (8%)	16	28
26	Z	60/94 (64%)	58 (97%)	2 (3%)	50	75
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	44	70
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	41	66

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	52	GLN
13	M	82	ARG
25	Y	174	VAL
10	J	79	PHE
11	K	55	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	137	ASN
17	Q	16	ASN
27	1	28	HIS
13	M	170	ASN
16	P	66	GLN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	259 (9%)	31 (1%)

5 of 259 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1684	A
30	0	1856	C
31	9	43	G
30	0	1685	A
30	0	1942	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OMU	0	2587	30	20,22,23	0.83	1 (5%)	24,31,34	0.75	0
30	OMG	0	2588	30	24,26,27	0.89	1 (4%)	32,38,41	4.86	3 (9%)
30	UR3	0	2619	30	20,22,23	0.73	0	23,32,35	0.88	0
30	PSU	0	2621	30	19,21,22	1.16	1 (5%)	23,30,33	1.09	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	1MA	0	628	30,34	23,25,26	0.81	0	32,37,40	0.92	1 (3%)

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
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,34	-	1/8/25/26	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	3.00	1.43	1.37
30	0	2587	OMU	P-OP1	2.78	1.49	1.46
30	0	2588	OMG	P-OP1	2.42	1.49	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-26.91	130.52	134.14
30	0	2588	OMG	C6-N1-C2	3.22	125.15	119.51
30	0	628	1MA	C2-N3-C4	-3.18	110.79	116.23
30	0	2621	PSU	C5-C1'-C2'	-2.32	111.52	115.61
30	0	2588	OMG	C2-N3-C4	-2.18	112.03	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 305 ligands modelled in this entry, 305 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.28	14 (5%) 22 23	20, 40, 77, 100	0
2	B	337/338 (99%)	0.12	4 (1%) 75 78	21, 44, 73, 83	0
3	C	246/246 (100%)	0.10	5 (2%) 62 65	17, 36, 60, 73	0
4	D	140/177 (79%)	1.82	46 (32%) 1 1	48, 89, 116, 126	0
5	E	172/178 (96%)	0.57	9 (5%) 26 27	34, 59, 79, 85	0
6	F	119/120 (99%)	1.01	22 (18%) 2 2	34, 61, 91, 105	0
7	G	29/348 (8%)	2.08	14 (48%) 1 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.77	20 (12%) 5 4	32, 50, 85, 91	0
9	I	70/162 (43%)	5.34	66 (94%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.08	3 (2%) 60 64	27, 41, 63, 89	0
11	K	132/132 (100%)	-0.09	2 (1%) 70 73	23, 39, 63, 72	0
12	L	145/165 (87%)	0.73	17 (11%) 5 5	18, 55, 103, 118	0
13	M	194/196 (98%)	0.21	15 (7%) 13 13	23, 34, 54, 59	0
14	N	186/187 (99%)	0.87	32 (17%) 2 2	34, 52, 104, 112	0
15	O	115/116 (99%)	0.24	2 (1%) 67 70	31, 45, 61, 69	0
16	P	143/149 (95%)	0.00	1 (0%) 84 87	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.01	0 100 100	29, 37, 55, 66	0
18	R	150/155 (96%)	-0.05	0 100 100	23, 36, 57, 71	0
19	S	81/85 (95%)	0.53	9 (11%) 6 6	33, 48, 70, 81	0
20	T	119/120 (99%)	0.34	5 (4%) 35 37	29, 46, 74, 101	0
21	U	53/67 (79%)	0.48	1 (1%) 64 67	33, 46, 65, 74	0
22	V	65/71 (91%)	2.07	21 (32%) 1 1	41, 63, 106, 113	0
23	W	154/154 (100%)	0.14	2 (1%) 74 77	26, 42, 59, 71	0
24	X	82/92 (89%)	0.46	5 (6%) 21 21	34, 49, 77, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.09	3 (2%) 60 64	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.35	21 (28%) 1 1	36, 55, 72, 89	0
27	1	56/57 (98%)	-0.14	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.37	2 (4%) 34 36	25, 49, 74, 86	0
29	3	92/92 (100%)	0.23	0 100 100	27, 45, 60, 74	0
30	0	2754/2923 (94%)	-0.07	98 (3%) 41 43	14, 35, 77, 154	0
31	9	122/122 (100%)	-0.00	5 (4%) 35 38	29, 54, 76, 138	0
All	All	6651/7517 (88%)	0.26	444 (6%) 18 17	14, 41, 89, 156	0

The worst 5 of 444 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	15.3
22	V	1	THR	15.0
4	D	63	ILE	14.3
22	V	40	PRO	12.9
30	0	2101	A	12.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
30	1MA	0	628	23/24	0.15	-0.03	20,23,25,25	0
30	UR3	0	2619	21/22	0.14	-0.53	43,48,52,56	0
30	OMU	0	2587	21/22	0.11	-0.57	23,27,29,29	0
30	PSU	0	2621	20/21	0.13	-0.97	29,31,42,42	0
30	OMG	0	2588	24/25	0.11	-2.12	23,29,30,31	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
36	SR	0	9007	1/1	1.30	163.44	178,178,178,178	0
36	SR	0	8962	1/1	1.13	128.50	165,165,165,165	0
32	MG	0	8065	1/1	0.85	63.20	68,68,68,68	0
34	NA	0	8555	1/1	0.67	60.02	59,59,59,59	0
36	SR	0	8955	1/1	0.20	56.57	140,140,140,140	0
34	NA	0	8521	1/1	0.57	53.37	70,70,70,70	0
36	SR	0	8949	1/1	0.49	48.62	184,184,184,184	0
32	MG	0	8073	1/1	0.29	47.26	72,72,72,72	0
32	MG	0	8049	1/1	0.48	46.20	78,78,78,78	0
34	NA	0	8567	1/1	0.38	37.36	59,59,59,59	0
34	NA	0	8548	1/1	0.27	34.70	41,41,41,41	0
32	MG	0	8040	1/1	0.36	33.47	81,81,81,81	0
36	SR	0	8902	1/1	0.55	32.32	112,112,112,112	0
34	NA	0	8562	1/1	0.39	30.34	61,61,61,61	0
34	NA	0	8554	1/1	0.30	29.56	55,55,55,55	0
36	SR	0	8987	1/1	0.70	29.48	199,199,199,199	0
34	NA	0	8561	1/1	0.28	27.28	67,67,67,67	0
36	SR	0	8983	1/1	0.24	27.02	151,151,151,151	0
32	MG	0	8018	1/1	0.23	26.45	13,13,13,13	0
32	MG	0	8030	1/1	0.26	25.72	51,51,51,51	0
34	NA	0	8505	1/1	0.36	25.25	37,37,37,37	0
32	MG	0	8092	1/1	0.18	25.02	53,53,53,53	0
32	MG	0	8038	1/1	0.38	22.30	80,80,80,80	0
32	MG	0	8017	1/1	0.53	21.98	67,67,67,67	0
34	NA	0	8509	1/1	0.15	21.92	60,60,60,60	0
36	SR	0	8994	1/1	0.45	21.92	173,173,173,173	0
34	NA	0	8569	1/1	0.32	21.12	61,61,61,61	0
34	NA	0	8549	1/1	0.37	20.95	73,73,73,73	0
36	SR	0	8991	1/1	0.27	19.94	171,171,171,171	0
32	MG	0	8085	1/1	0.26	18.72	90,90,90,90	0
32	MG	0	8037	1/1	0.29	18.23	77,77,77,77	0
34	NA	0	8552	1/1	0.32	18.16	51,51,51,51	0
34	NA	0	8502	1/1	0.20	18.15	52,52,52,52	0
32	MG	0	8006	1/1	0.27	17.16	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8044	1/1	0.23	16.25	62,62,62,62	0
34	NA	0	8518	1/1	0.47	15.40	81,81,81,81	0
32	MG	0	8039	1/1	0.28	14.53	42,42,42,42	0
34	NA	0	8575	1/1	0.45	13.65	78,78,78,78	0
34	NA	0	8553	1/1	0.24	13.26	61,61,61,61	0
34	NA	0	8547	1/1	0.24	12.89	49,49,49,49	0
34	NA	0	8530	1/1	0.26	12.14	41,41,41,41	0
36	SR	0	8997	1/1	0.19	12.13	115,115,115,115	0
32	MG	0	8050	1/1	0.51	12.01	63,63,63,63	0
34	NA	0	8558	1/1	0.22	11.73	39,39,39,39	0
32	MG	0	8063	1/1	0.29	11.57	74,74,74,74	0
34	NA	0	8535	1/1	0.23	11.13	55,55,55,55	0
34	NA	0	8563	1/1	0.36	11.11	64,64,64,64	0
36	SR	0	8976	1/1	0.27	10.99	122,122,122,122	0
36	SR	0	8922	1/1	0.51	10.69	164,164,164,164	0
32	MG	0	8032	1/1	0.16	10.68	42,42,42,42	0
32	MG	0	8047	1/1	0.34	10.07	66,66,66,66	0
32	MG	0	8009	1/1	0.27	10.02	1,1,1,1	0
32	MG	0	8028	1/1	0.24	9.85	1,1,1,1	0
36	SR	0	8910	1/1	0.21	9.62	60,60,60,60	0
36	SR	0	8996	1/1	0.26	9.36	173,173,173,173	0
36	SR	9	8980	1/1	0.18	9.34	144,144,144,144	0
36	SR	0	8905	1/1	0.22	9.26	43,43,43,43	0
32	MG	0	8041	1/1	0.22	9.23	52,52,52,52	0
34	NA	0	8542	1/1	0.26	8.83	44,44,44,44	0
34	NA	0	8536	1/1	0.12	8.44	62,62,62,62	0
32	MG	0	8076	1/1	0.18	8.43	52,52,52,52	0
32	MG	0	8008	1/1	0.21	8.37	27,27,27,27	0
32	MG	0	8019	1/1	0.20	8.31	18,18,18,18	0
34	NA	0	8559	1/1	0.18	8.24	67,67,67,67	0
34	NA	0	8511	1/1	0.18	7.81	61,61,61,61	0
36	SR	0	8971	1/1	0.15	7.80	153,153,153,153	0
32	MG	0	8071	1/1	0.24	7.75	73,73,73,73	0
36	SR	0	8918	1/1	0.19	7.70	45,45,45,45	0
32	MG	0	8012	1/1	0.19	7.42	4,4,4,4	0
32	MG	9	8074	1/1	0.26	7.36	42,42,42,42	0
36	SR	0	8989	1/1	0.24	7.14	149,149,149,149	0
34	NA	0	8524	1/1	0.19	6.92	27,27,27,27	0
32	MG	0	8079	1/1	0.23	6.86	52,52,52,52	0
32	MG	0	8045	1/1	0.23	6.72	40,40,40,40	0
34	NA	0	8516	1/1	0.24	6.71	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8048	1/1	0.22	6.68	55,55,55,55	0
32	MG	0	8081	1/1	0.18	6.62	65,65,65,65	0
36	SR	0	8957	1/1	0.28	6.60	149,149,149,149	0
32	MG	0	8062	1/1	0.26	6.55	46,46,46,46	0
34	NA	0	8571	1/1	0.21	6.51	83,83,83,83	0
32	MG	0	8055	1/1	0.21	6.46	12,12,12,12	0
36	SR	0	8974	1/1	0.26	6.11	119,119,119,119	0
36	SR	0	8903	1/1	0.15	5.89	36,36,36,36	0
32	MG	0	8014	1/1	0.19	5.56	23,23,23,23	0
32	MG	0	8066	1/1	0.23	5.51	67,67,67,67	0
32	MG	0	8068	1/1	0.15	5.33	50,50,50,50	0
34	NA	0	8564	1/1	0.17	5.27	49,49,49,49	0
32	MG	0	8004	1/1	0.17	5.24	13,13,13,13	0
34	NA	0	8574	1/1	0.23	5.22	47,47,47,47	0
32	MG	0	8007	1/1	0.20	5.19	53,53,53,53	0
32	MG	0	8078	1/1	0.20	5.18	52,52,52,52	0
36	SR	0	9002	1/1	0.21	4.71	141,141,141,141	0
34	NA	0	8508	1/1	0.17	4.62	36,36,36,36	0
32	MG	0	8093	1/1	0.15	4.55	29,29,29,29	0
32	MG	0	8061	1/1	0.21	4.38	17,17,17,17	0
36	SR	0	8938	1/1	0.19	4.31	102,102,102,102	0
34	NA	0	8566	1/1	0.20	3.95	37,37,37,37	0
34	NA	0	8520	1/1	0.23	3.94	49,49,49,49	0
32	MG	A	8051	1/1	0.30	3.92	51,51,51,51	0
36	SR	0	8907	1/1	0.18	3.79	50,50,50,50	0
36	SR	9	8968	1/1	0.13	3.73	96,96,96,96	0
34	NA	0	8517	1/1	0.31	3.69	68,68,68,68	0
32	MG	0	8015	1/1	0.16	3.61	50,50,50,50	0
34	NA	0	8528	1/1	0.18	3.56	67,67,67,67	0
34	NA	0	8560	1/1	0.28	3.46	67,67,67,67	0
34	NA	0	8504	1/1	0.17	3.37	34,34,34,34	0
35	CL	B	8819	1/1	0.20	3.35	57,57,57,57	0
36	SR	0	8926	1/1	0.15	3.25	69,69,69,69	0
34	NA	0	8525	1/1	0.15	3.11	57,57,57,57	0
36	SR	0	8979	1/1	0.19	3.00	193,193,193,193	0
34	NA	0	8546	1/1	0.28	2.83	51,51,51,51	0
36	SR	0	9000	1/1	0.15	2.57	125,125,125,125	0
34	NA	0	8507	1/1	0.15	2.52	19,19,19,19	0
34	NA	0	8545	1/1	0.17	2.49	40,40,40,40	0
32	MG	0	8056	1/1	0.14	2.37	66,66,66,66	0
34	NA	0	8573	1/1	0.16	2.27	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8556	1/1	0.33	2.23	38,38,38,38	0
32	MG	B	8042	1/1	0.17	2.14	75,75,75,75	0
36	SR	0	8927	1/1	0.14	2.05	58,58,58,58	0
32	MG	0	8080	1/1	0.14	1.90	54,54,54,54	0
34	NA	0	8512	1/1	0.41	1.85	63,63,63,63	0
32	MG	0	8064	1/1	0.14	1.69	54,54,54,54	0
32	MG	0	8067	1/1	0.45	1.64	55,55,55,55	0
34	NA	0	8523	1/1	0.15	1.61	48,48,48,48	0
34	NA	0	8533	1/1	0.18	1.43	57,57,57,57	0
34	NA	0	8514	1/1	0.19	1.40	34,34,34,34	0
36	SR	0	8919	1/1	0.15	1.12	167,167,167,167	0
32	MG	0	8035	1/1	0.12	1.07	63,63,63,63	0
37	CD	Z	8703	1/1	0.20	1.05	67,67,67,67	0
36	SR	0	8914	1/1	0.17	0.91	67,67,67,67	0
33	K	0	8401	1/1	0.35	0.90	97,97,97,97	0
32	MG	0	8025	1/1	0.14	0.86	40,40,40,40	0
35	CL	0	8816	1/1	0.16	0.77	49,49,49,49	0
36	SR	0	8969	1/1	0.15	0.73	115,115,115,115	0
32	MG	0	8011	1/1	0.18	0.70	26,26,26,26	0
34	NA	0	8541	1/1	0.16	0.70	33,33,33,33	0
36	SR	0	8901	1/1	0.14	0.66	35,35,35,35	0
36	SR	0	8985	1/1	0.17	0.63	98,98,98,98	0
36	SR	0	8921	1/1	0.12	0.61	46,46,46,46	0
32	MG	0	8003	1/1	0.14	0.58	24,24,24,24	0
34	NA	9	8572	1/1	0.15	0.57	66,66,66,66	0
32	MG	0	8020	1/1	0.14	0.57	22,22,22,22	0
37	CD	U	8701	1/1	0.17	0.47	62,62,62,62	0
34	NA	0	8522	1/1	0.14	0.44	52,52,52,52	0
36	SR	0	9004	1/1	0.47	0.44	182,182,182,182	0
33	K	0	8402	1/1	0.19	0.34	77,77,77,77	0
36	SR	0	8906	1/1	0.17	0.31	50,50,50,50	0
36	SR	0	8982	1/1	0.12	0.30	116,116,116,116	0
36	SR	0	8947	1/1	0.16	0.29	73,73,73,73	0
34	NA	0	8570	1/1	0.13	0.29	35,35,35,35	0
37	CD	1	8702	1/1	0.13	0.22	54,54,54,54	0
32	MG	0	8082	1/1	0.28	0.18	63,63,63,63	0
32	MG	0	8084	1/1	0.14	0.03	59,59,59,59	0
34	NA	0	8534	1/1	0.23	0.02	56,56,56,56	0
36	SR	0	8908	1/1	0.12	0.00	46,46,46,46	0
36	SR	0	8986	1/1	0.17	-0.00	136,136,136,136	0
36	SR	0	8965	1/1	0.12	0.00	80,80,80,80	0
36	SR	0	8981	1/1	0.14	-0.02	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	C	8503	1/1	0.15	-0.08	19,19,19,19	0
32	MG	0	8036	1/1	0.12	-0.10	37,37,37,37	0
32	MG	0	8001	1/1	0.16	-0.10	9,9,9,9	0
36	SR	0	8972	1/1	0.16	-0.25	121,121,121,121	0
32	MG	0	8016	1/1	0.24	-0.25	75,75,75,75	0
36	SR	0	8944	1/1	0.14	-0.26	117,117,117,117	0
36	SR	0	8925	1/1	0.11	-0.27	55,55,55,55	0
34	NA	0	8550	1/1	0.16	-0.28	37,37,37,37	0
36	SR	0	8995	1/1	0.15	-0.35	94,94,94,94	0
36	SR	0	8992	1/1	0.12	-0.40	108,108,108,108	0
35	CL	J	8821	1/1	0.15	-0.41	52,52,52,52	0
32	MG	0	8058	1/1	0.14	-0.43	3,3,3,3	0
35	CL	0	8803	1/1	0.12	-0.48	38,38,38,38	0
32	MG	0	8022	1/1	0.12	-0.53	7,7,7,7	0
34	NA	0	8515	1/1	0.14	-0.56	28,28,28,28	0
37	CD	3	8704	1/1	0.14	-0.56	63,63,63,63	0
34	NA	J	8538	1/1	0.13	-0.57	47,47,47,47	0
32	MG	0	8005	1/1	0.15	-0.57	29,29,29,29	0
36	SR	A	8977	1/1	0.14	-0.59	88,88,88,88	0
36	SR	0	8956	1/1	0.12	-0.59	111,111,111,111	0
34	NA	0	8568	1/1	0.15	-0.61	33,33,33,33	0
35	CL	0	8822	1/1	0.13	-0.68	46,46,46,46	0
34	NA	0	8551	1/1	0.12	-0.73	40,40,40,40	0
36	SR	0	8909	1/1	0.11	-0.82	44,44,44,44	0
32	MG	0	8053	1/1	0.13	-0.83	45,45,45,45	0
34	NA	0	8513	1/1	0.14	-0.84	32,32,32,32	0
34	NA	R	8532	1/1	0.13	-0.89	32,32,32,32	0
36	SR	0	8954	1/1	0.10	-0.91	60,60,60,60	0
32	MG	T	8057	1/1	0.17	-0.92	32,32,32,32	0
34	NA	M	8539	1/1	0.11	-0.96	34,34,34,34	0
36	SR	0	8993	1/1	0.07	-1.01	154,154,154,154	0
32	MG	0	8026	1/1	0.11	-1.05	44,44,44,44	0
36	SR	A	8930	1/1	0.10	-1.08	57,57,57,57	0
32	MG	0	8002	1/1	0.15	-1.09	33,33,33,33	0
32	MG	0	8010	1/1	0.27	-1.10	69,69,69,69	0
36	SR	0	8960	1/1	0.09	-1.11	100,100,100,100	0
36	SR	R	8912	1/1	0.12	-1.13	55,55,55,55	0
36	SR	0	8998	1/1	0.13	-1.14	99,99,99,99	0
32	MG	0	8069	1/1	0.18	-1.24	75,75,75,75	0
32	MG	0	8070	1/1	0.11	-1.28	50,50,50,50	0
36	SR	0	8963	1/1	0.13	-1.33	135,135,135,135	0
36	SR	F	9005	1/1	0.11	-1.34	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8942	1/1	0.09	-1.46	55,55,55,55	0
35	CL	O	8808	1/1	0.09	-1.49	52,52,52,52	0
36	SR	0	8924	1/1	0.09	-1.50	50,50,50,50	0
36	SR	0	8911	1/1	0.10	-1.51	48,48,48,48	0
36	SR	0	9001	1/1	0.09	-1.57	142,142,142,142	0
34	NA	9	8543	1/1	0.15	-1.60	60,60,60,60	0
34	NA	Q	8540	1/1	0.08	-1.65	39,39,39,39	0
34	NA	0	8506	1/1	0.10	-1.68	44,44,44,44	0
32	MG	0	8043	1/1	0.10	-1.71	51,51,51,51	0
35	CL	J	8801	1/1	0.08	-1.72	42,42,42,42	0
35	CL	0	8812	1/1	0.09	-1.72	43,43,43,43	0
32	MG	0	8023	1/1	0.10	-1.73	30,30,30,30	0
36	SR	A	8929	1/1	0.08	-1.75	78,78,78,78	0
34	NA	0	8544	1/1	0.10	-1.80	53,53,53,53	0
35	CL	L	8810	1/1	0.13	-1.81	43,43,43,43	0
32	MG	0	8013	1/1	0.10	-1.83	41,41,41,41	0
32	MG	0	8060	1/1	0.08	-1.88	41,41,41,41	0
32	MG	0	8075	1/1	0.10	-1.92	37,37,37,37	0
35	CL	0	8811	1/1	0.11	-1.93	54,54,54,54	0
34	NA	0	8557	1/1	0.10	-2.01	63,63,63,63	0
36	SR	1	8913	1/1	0.10	-2.02	32,32,32,32	0
36	SR	0	8946	1/1	0.13	-2.04	75,75,75,75	0
36	SR	0	8940	1/1	0.09	-2.08	62,62,62,62	0
35	CL	N	8807	1/1	0.10	-2.14	43,43,43,43	0
34	NA	0	8529	1/1	0.06	-2.15	29,29,29,29	0
32	MG	Y	8086	1/1	0.10	-2.16	30,30,30,30	0
34	NA	0	8565	1/1	0.09	-2.17	39,39,39,39	0
36	SR	0	8959	1/1	0.08	-2.28	129,129,129,129	0
32	MG	0	8090	1/1	0.10	-2.29	51,51,51,51	0
36	SR	S	8961	1/1	0.09	-2.39	98,98,98,98	0
35	CL	A	8809	1/1	0.12	-2.41	51,51,51,51	0
36	SR	3	8999	1/1	0.10	-2.45	63,63,63,63	0
36	SR	B	8950	1/1	0.10	-2.62	83,83,83,83	0
35	CL	J	8802	1/1	0.07	-2.63	49,49,49,49	0
36	SR	0	8915	1/1	0.09	-2.67	58,58,58,58	0
32	MG	0	8052	1/1	0.09	-2.72	29,29,29,29	0
36	SR	0	8917	1/1	0.12	-2.76	46,46,46,46	0
36	SR	0	8975	1/1	0.06	-2.79	114,114,114,114	0
36	SR	1	8952	1/1	0.11	-2.80	47,47,47,47	0
34	NA	T	8537	1/1	0.08	-2.83	26,26,26,26	0
36	SR	0	8966	1/1	0.09	-2.92	68,68,68,68	0
34	NA	0	8526	1/1	0.08	-2.99	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8943	1/1	0.06	-3.01	49,49,49,49	0
32	MG	0	8077	1/1	0.07	-3.04	34,34,34,34	0
32	MG	0	8031	1/1	0.08	-3.05	39,39,39,39	0
32	MG	0	8087	1/1	0.09	-3.06	33,33,33,33	0
32	MG	0	8072	1/1	0.10	-3.16	36,36,36,36	0
34	NA	S	8510	1/1	0.06	-3.20	32,32,32,32	0
32	MG	K	8054	1/1	0.09	-3.24	20,20,20,20	0
32	MG	0	8021	1/1	0.09	-3.42	24,24,24,24	0
36	SR	0	8964	1/1	0.07	-3.48	76,76,76,76	0
36	SR	0	8967	1/1	0.09	-3.56	86,86,86,86	0
35	CL	Y	8820	1/1	0.04	-3.61	27,27,27,27	0
32	MG	0	8083	1/1	0.05	-3.63	35,35,35,35	0
36	SR	0	8945	1/1	0.08	-3.67	71,71,71,71	0
35	CL	0	8817	1/1	0.09	-3.75	33,33,33,33	0
36	SR	0	9008	1/1	0.09	-3.85	59,59,59,59	0
35	CL	M	8818	1/1	0.08	-4.01	22,22,22,22	0
36	SR	0	8951	1/1	0.07	-4.06	99,99,99,99	0
36	SR	0	8973	1/1	0.09	-4.12	79,79,79,79	0
36	SR	0	8935	1/1	0.07	-4.17	54,54,54,54	0
36	SR	0	8953	1/1	0.06	-4.21	76,76,76,76	0
36	SR	0	8916	1/1	0.08	-4.24	45,45,45,45	0
36	SR	9	9003	1/1	0.06	-4.42	122,122,122,122	0
36	SR	3	8932	1/1	0.07	-4.52	65,65,65,65	0
34	NA	0	8527	1/1	0.11	-4.67	35,35,35,35	0
36	SR	0	8939	1/1	0.09	-4.68	62,62,62,62	0
35	CL	3	8804	1/1	0.05	-4.75	48,48,48,48	0
32	MG	0	8034	1/1	0.07	-4.92	25,25,25,25	0
36	SR	0	8941	1/1	0.10	-5.01	60,60,60,60	0
35	CL	0	8805	1/1	0.06	-5.16	39,39,39,39	0
36	SR	0	8970	1/1	0.09	-5.31	73,73,73,73	0
36	SR	0	8948	1/1	0.09	-5.33	57,57,57,57	0
32	MG	0	8027	1/1	0.06	-5.47	36,36,36,36	0
32	MG	0	8091	1/1	0.11	-5.50	50,50,50,50	0
32	MG	0	8046	1/1	0.10	-5.54	1,1,1,1	0
36	SR	0	8936	1/1	0.09	-5.72	44,44,44,44	0
36	SR	0	8937	1/1	0.11	-6.02	53,53,53,53	0
36	SR	0	8931	1/1	0.08	-6.24	61,61,61,61	0
35	CL	0	8815	1/1	0.07	-6.35	38,38,38,38	0
32	MG	0	8029	1/1	0.09	-6.46	35,35,35,35	0
36	SR	0	8934	1/1	0.07	-6.68	52,52,52,52	0
36	SR	0	8958	1/1	0.08	-6.88	57,57,57,57	0
35	CL	0	8814	1/1	0.06	-7.01	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8984	1/1	0.07	-7.51	75,75,75,75	0
35	CL	R	8806	1/1	0.08	-7.71	28,28,28,28	0
32	MG	0	8088	1/1	0.06	-7.75	25,25,25,25	0
36	SR	0	8978	1/1	0.08	-7.77	47,47,47,47	0
34	NA	0	8501	1/1	0.07	-7.91	30,30,30,30	0
32	MG	0	8059	1/1	0.09	-7.94	31,31,31,31	0
36	SR	0	8988	1/1	0.11	-8.25	110,110,110,110	0
37	CD	O	8705	1/1	0.04	-8.42	88,88,88,88	0
32	MG	0	8033	1/1	0.07	-8.55	45,45,45,45	0
34	NA	0	8519	1/1	0.07	-8.73	29,29,29,29	0
36	SR	0	8904	1/1	0.05	-8.78	20,20,20,20	0
36	SR	0	8928	1/1	0.07	-9.18	67,67,67,67	0
35	CL	0	8813	1/1	0.06	-9.26	34,34,34,34	0
32	MG	0	8024	1/1	0.13	-9.72	45,45,45,45	0
36	SR	0	8920	1/1	0.06	-9.89	63,63,63,63	0
36	SR	0	8923	1/1	0.08	-10.89	54,54,54,54	0
36	SR	0	8933	1/1	0.05	-12.30	54,54,54,54	0
34	NA	0	8531	1/1	0.06	-12.79	17,17,17,17	0
36	SR	0	8990	1/1	0.12	-12.83	132,132,132,132	0
32	MG	0	8089	1/1	0.12	-59.00	48,48,48,48	0
36	SR	0	9006	1/1	0.43	-	199,199,199,199	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.