



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:16 PM GMT

PDB ID : 3CCS
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.95 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>

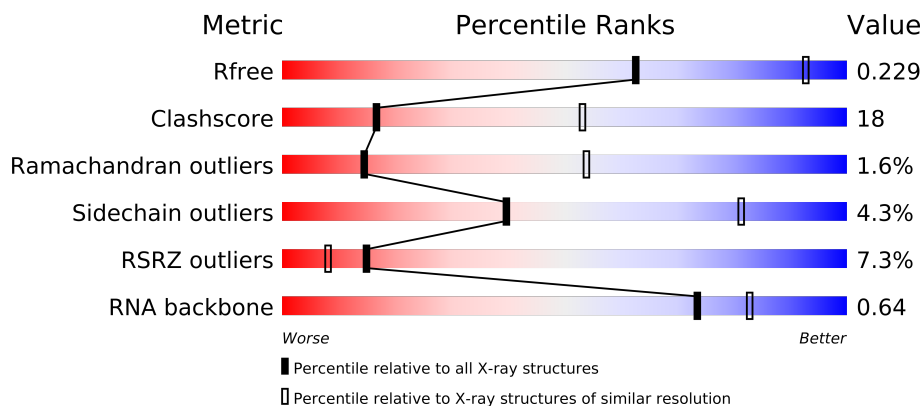
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.95 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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	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	8005	-	X
32	MG	0	8009	-	X
32	MG	0	8016	-	X
32	MG	0	8018	-	X
32	MG	0	8020	-	X
32	MG	0	8022	-	X
32	MG	0	8024	-	X
32	MG	0	8027	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8040	-	X
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8063	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8070	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8080	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	0	8089	-	X
32	MG	0	8092	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8502	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8527	-	X
34	NA	0	8528	-	X
34	NA	0	8530	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8537	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	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	8550	-	X
34	NA	0	8551	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8571	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
34	NA	9	8572	-	X
34	NA	B	8552	-	X
34	NA	H	8518	-	X
35	CL	0	8805	-	X
35	CL	0	8815	-	X
35	CL	0	8816	-	X
35	CL	0	8822	-	X
35	CL	A	8809	-	X
36	SR	0	8901	-	X
36	SR	0	8903	-	X
36	SR	0	8905	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8926	-	X
36	SR	0	8947	-	X
36	SR	0	8953	-	X
36	SR	0	8957	-	X
36	SR	0	8959	-	X
36	SR	0	8973	-	X
36	SR	0	8976	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8986	-	X
36	SR	0	8989	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	B	8987	-	X
36	SR	L	8969	-	X
36	SR	R	8912	-	X
37	CD	3	8704	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99121 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
			59019	26349	10873	19052	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	86	Total	Mg	0	0
			86	86		
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	2	Total	Mg	0	0
			2	2		
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	1	Total K 1 1	0	0
33	M	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	65	Total Na 65 65	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	B	1	Total Na 1 1	0	0
34	C	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
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	92	Total 92	Sr 92	0	0
36	1	2	Total 2	Sr 2	0	0
36	H	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	2	Total 2	Sr 2	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	L	1	Total 1	Sr 1	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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	5904	Total 5904	O 5904	0	0
38	9	149	Total 149	O 149	0	0
38	A	119	Total 119	O 119	0	0
38	B	152	Total 152	O 152	0	0
38	C	185	Total 185	O 185	0	0
38	D	42	Total 42	O 42	0	0
38	E	43	Total 43	O 43	0	0
38	F	26	Total 26	O 26	0	0
38	G	19	Total 19	O 19	0	0
38	H	65	Total 65	O 65	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	58	Total 58	O 58	0	0
38	L	85	Total 85	O 85	0	0
38	M	127	Total 127	O 127	0	0

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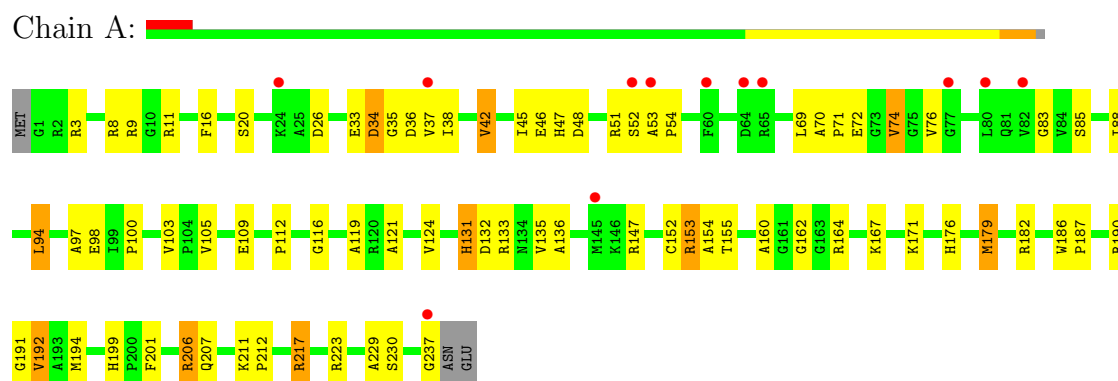
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	N	59	Total	O	0	0
			59	59		
38	O	39	Total	O	0	0
			39	39		
38	P	67	Total	O	0	0
			67	67		
38	Q	48	Total	O	0	0
			48	48		
38	R	77	Total	O	0	0
			77	77		
38	S	30	Total	O	0	0
			30	30		
38	T	36	Total	O	0	0
			36	36		
38	U	28	Total	O	0	0
			28	28		
38	V	13	Total	O	0	0
			13	13		
38	W	67	Total	O	0	0
			67	67		
38	X	21	Total	O	0	0
			21	21		
38	Y	100	Total	O	0	0
			100	100		
38	Z	31	Total	O	0	0
			31	31		
38	1	59	Total	O	0	0
			59	59		
38	2	43	Total	O	0	0
			43	43		
38	3	70	Total	O	0	0
			70	70		

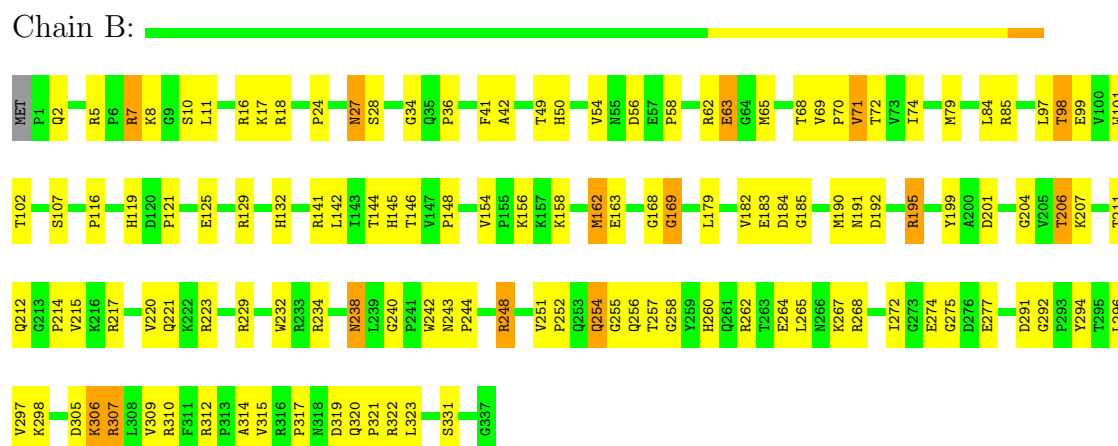
3 Residue-property plots

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.

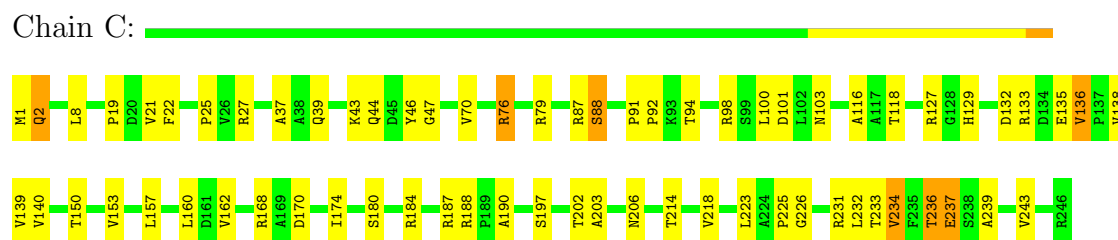
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

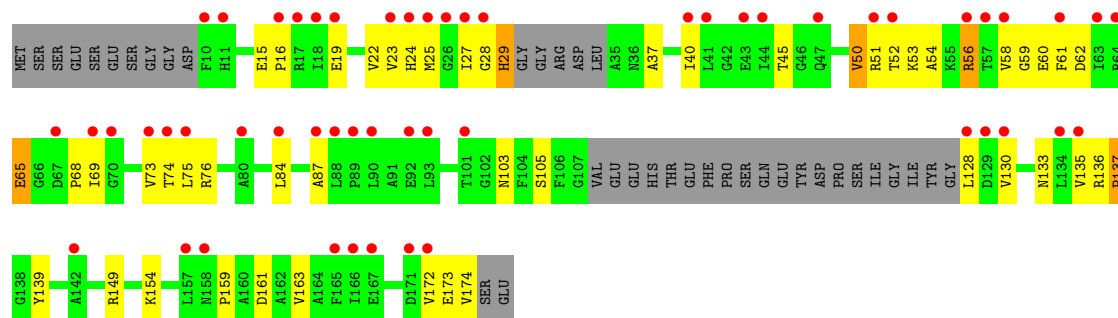


- Molecule 3: 50S ribosomal protein L4P



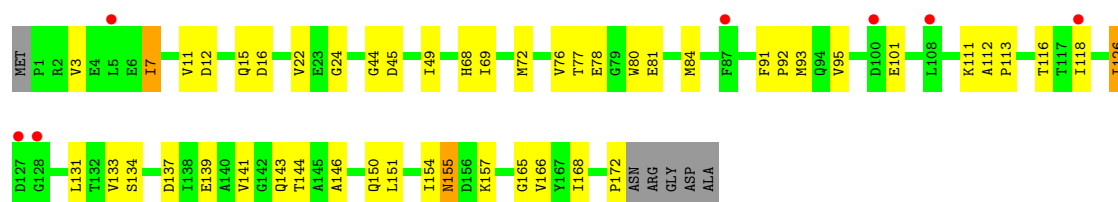
- Molecule 4: 50S ribosomal protein L5P

Chain D:



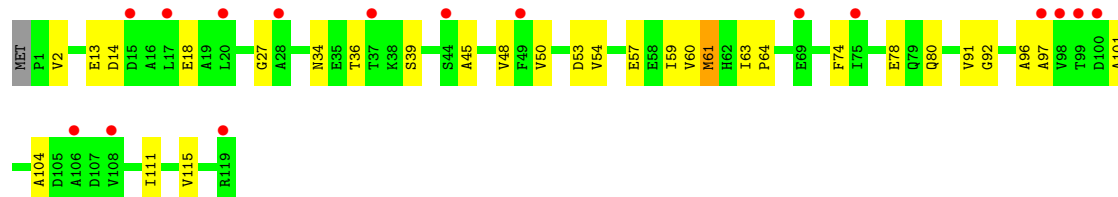
- Molecule 5: 50S ribosomal protein L6P

Chain E:



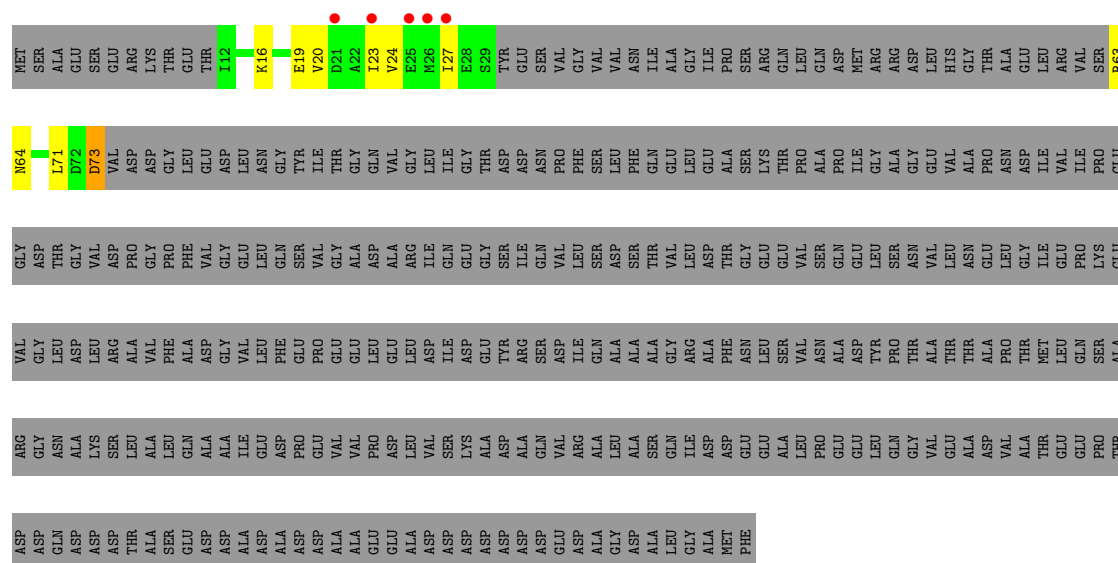
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



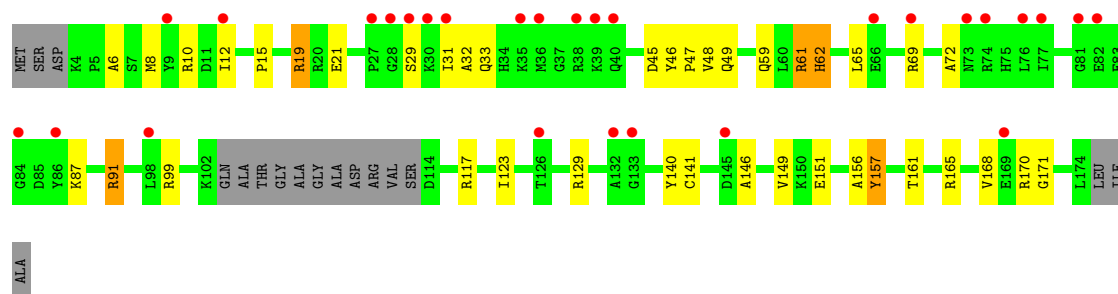
- Molecule 7: 50S ribosomal protein L10E

Chain G:



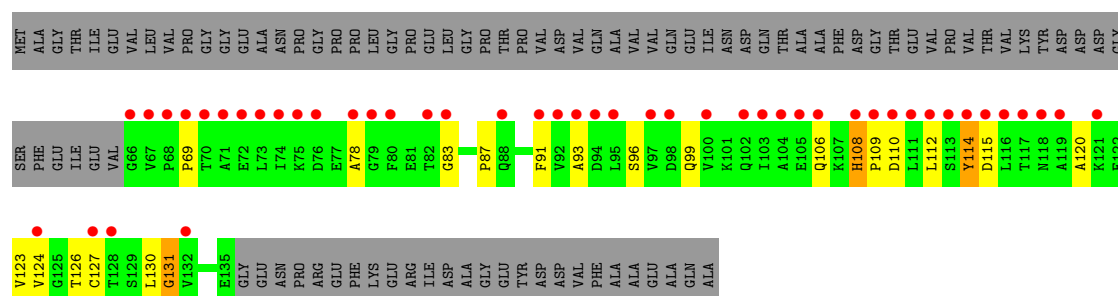
- Molecule 8: 50S ribosomal protein L10e

Chain H:



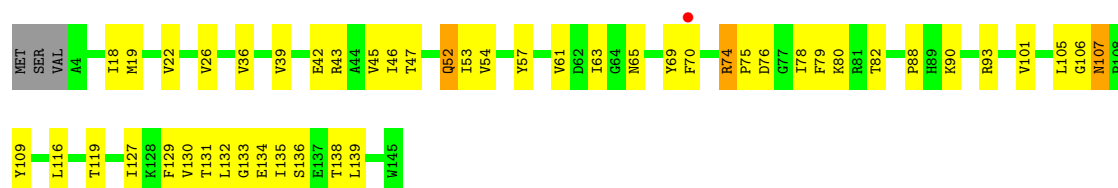
- Molecule 9: 50S ribosomal protein L11P

Chain I:



- Molecule 10: 50S ribosomal protein L13P

Chain J:



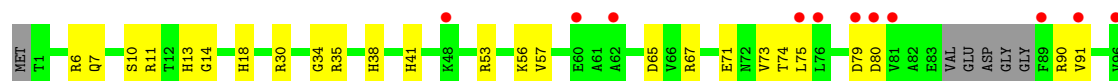
- Molecule 11: 50S ribosomal protein L14P

Chain K:



- Molecule 12: 50S ribosomal protein L15P

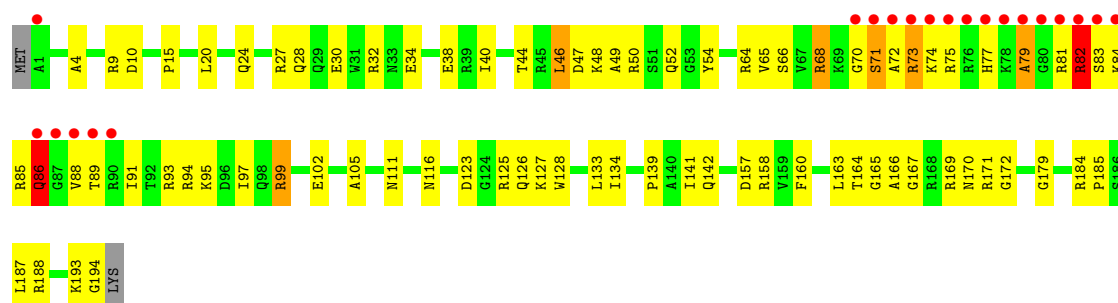
Chain L:





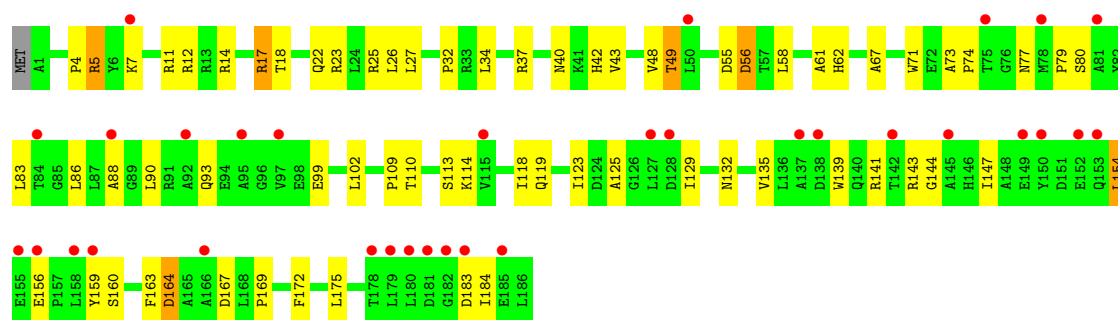
• Molecule 13: 50S ribosomal protein L15e

Chain M:



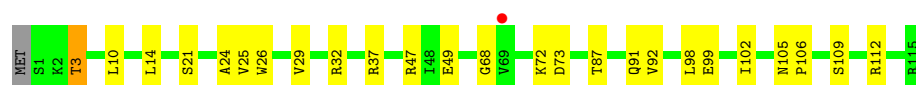
• Molecule 14: 50S ribosomal protein L18P

Chain N:



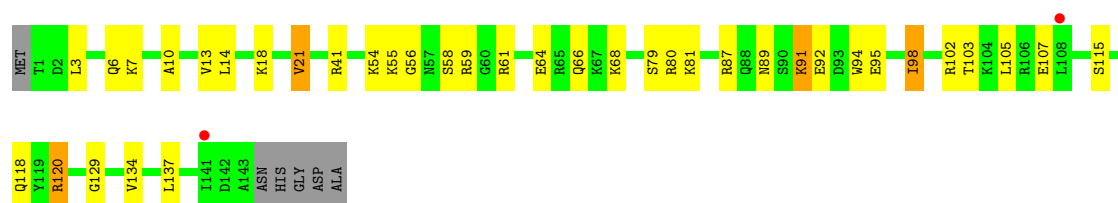
• Molecule 15: 50S ribosomal protein L18e

Chain O:



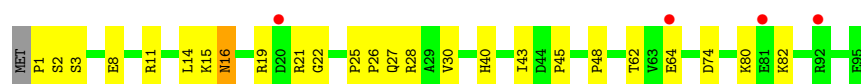
• Molecule 16: 50S ribosomal protein L19e

Chain P:



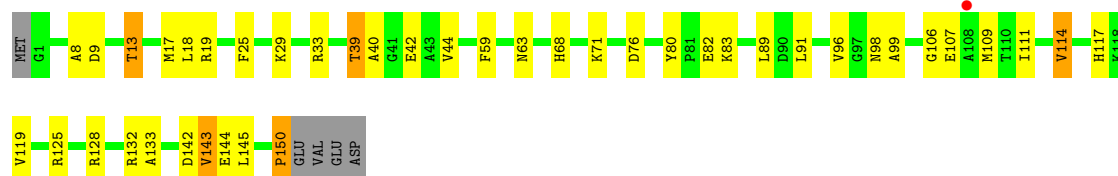
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



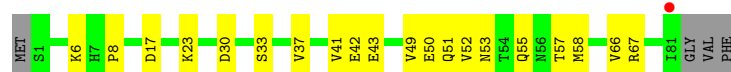
- Molecule 18: 50S ribosomal protein L22P

Chain R:



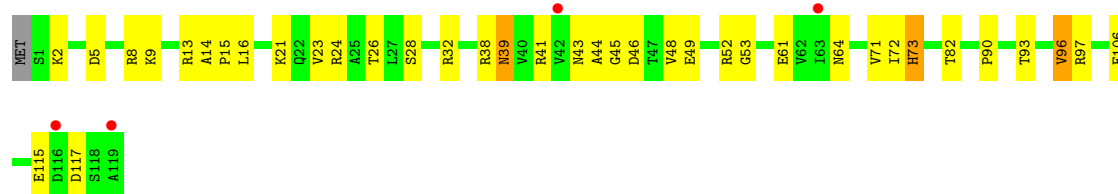
- Molecule 19: 50S ribosomal protein L23P

Chain S:



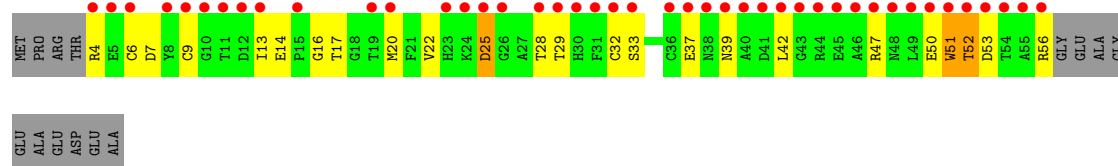
- Molecule 20: 50S ribosomal protein L24P

Chain T:



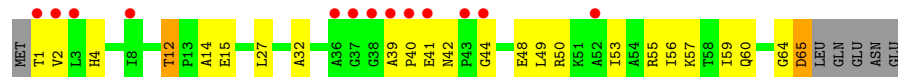
- Molecule 21: 50S ribosomal protein L24e

Chain U:



- Molecule 22: 50S ribosomal protein L29P

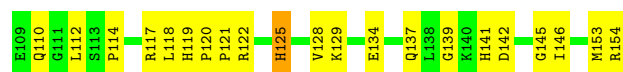
Chain V:



- Molecule 23: 50S ribosomal protein L30P

Chain W:





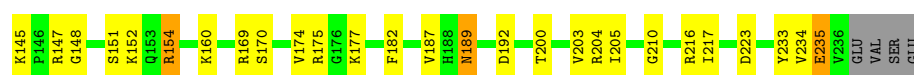
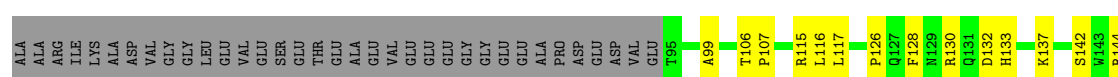
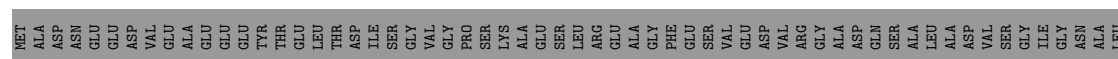
- Molecule 24: 50S ribosomal protein L31e

Chain X:



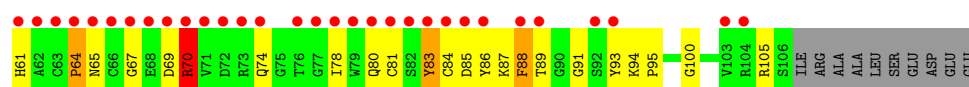
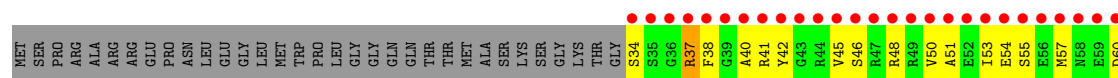
- Molecule 25: 50S ribosomal protein L32e

Chain Y:



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



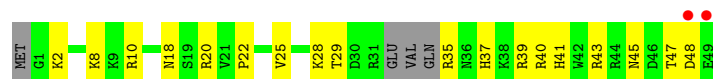
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



- Molecule 28: 50S ribosomal protein L39e

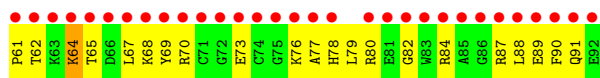
Chain 2:



- Molecule 29: 50S ribosomal protein L44E

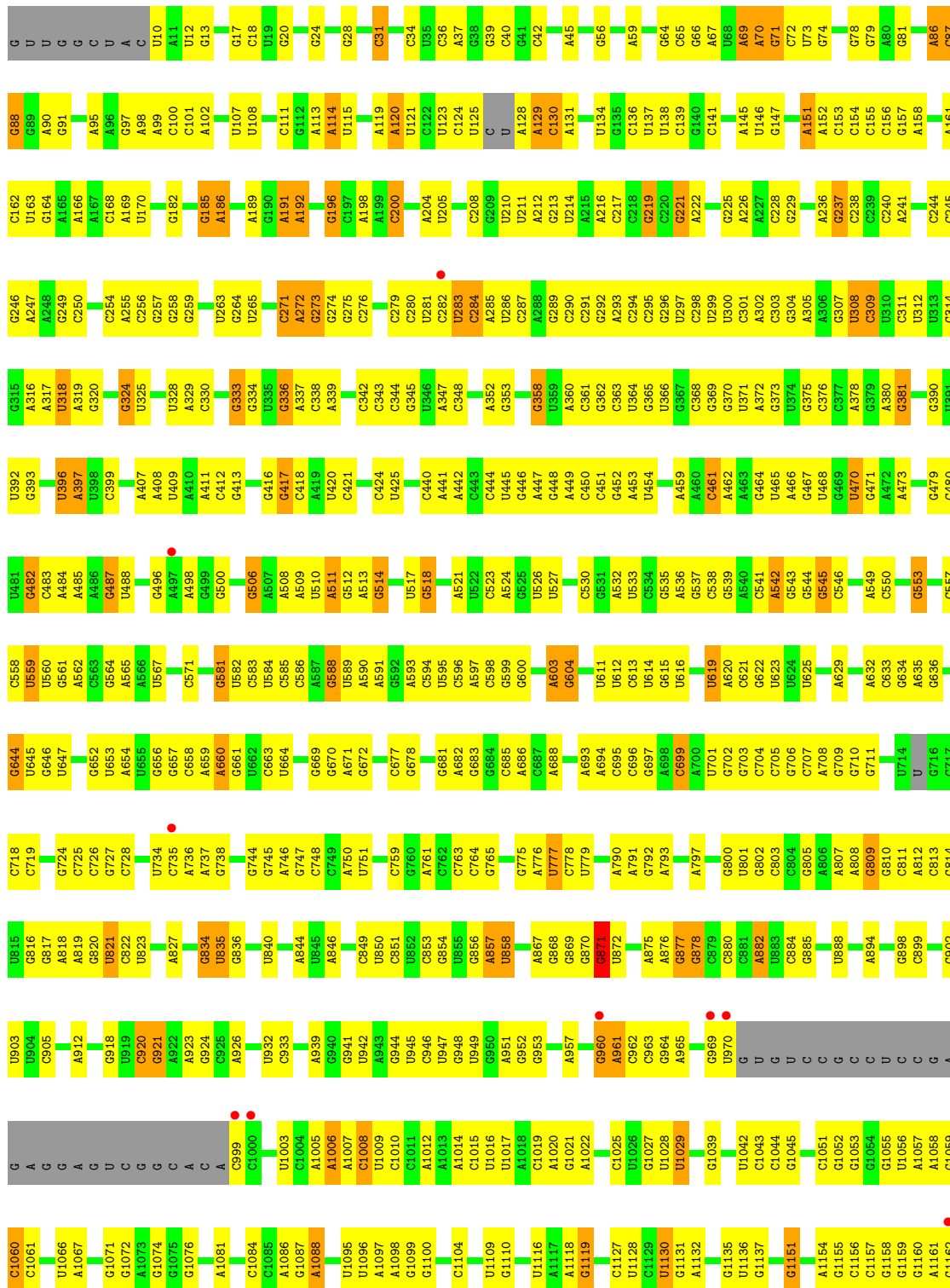
Chain 3:



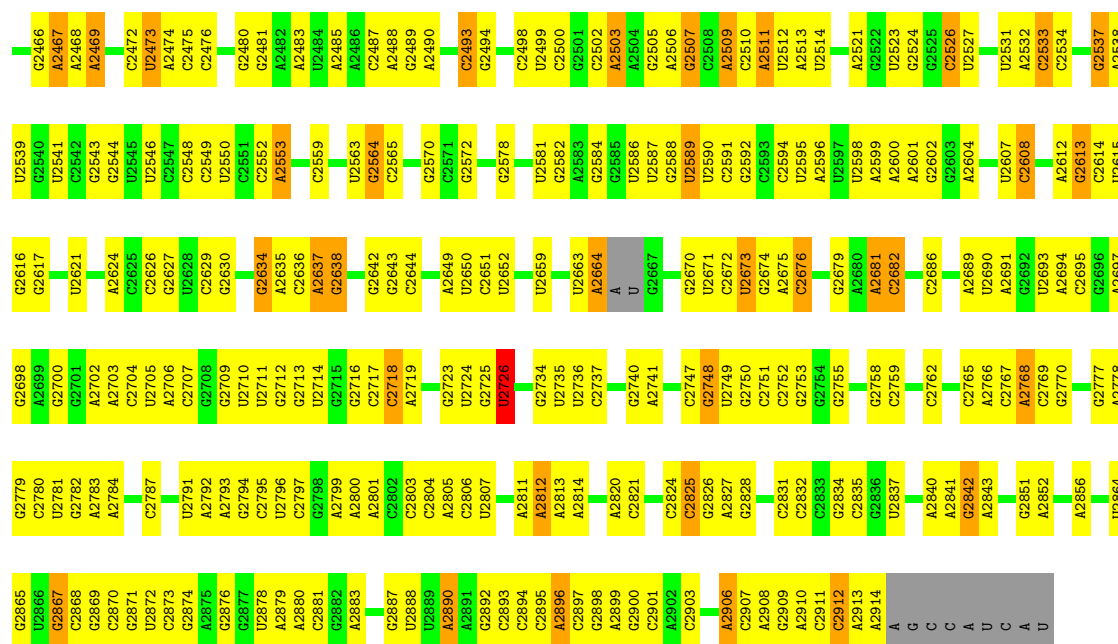


Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

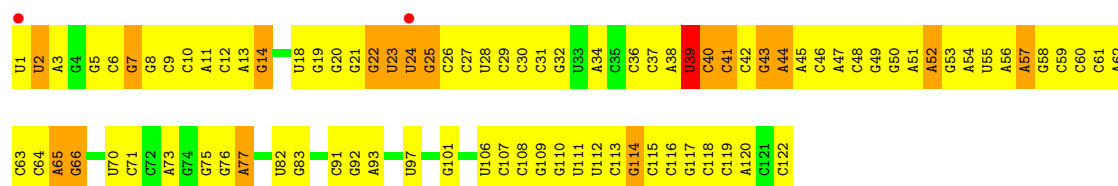


C2376	A	U	A2096	U1996	G1925	U1831	G1752	U1854	G1567	A1486	A1399	G1315	C1229	G1163
U2377	C	U	A2099	A1997	G1926	G1832	A1755	A1656	A1572	A1487	U1405	G1316	C1230	U1164
G2378	U	A	A2100	G1998	A1927	U1833	A1756	A1657	C1573	U1488	U1406	A1317	A1230	G1165
G2379	G	C	A2101	C2002	C1928	U1835	U1757	A1658	C1574	A1407	A1408	A1318		A1166
A2382	C	A	G2102	U2003	G1929	A1836	U1758		C1575	U1494	U1408	U1234		G1167
G2383	G2237	G	C2103	U2004	G1933	G1837	A1759	A1661	G1576	A1496	G1409	G1322		C1168
C2384	A2238	A	A2104	G2005	A1934	U1838	G1760	A1664	G1577	G1497	G1410	G1325		U1169
U2384	C2239	G	C2105	C2006	C1935	A1839	U1761	G1665	C1578	U1500	A1413	G1326		A1171
C2387	U2240	U	C2106	A2007	C1936	U1837	G1762	G1666		U1503	U1419	G1327		G1172
U2387	C2241	A	G	U2008	U1937	A1840	C1763	A1667		U1504	U1420	A1328		A1173
C2388	U2242	C	G	G2009	G1938	U1845	C1764	U1668		U1505	U1424	A1242		U1174
A2401	C2243	C	C	A2010	U1939	U1846	U1765			A1506		C1243		G1175
A2402	A2244	C	C	A2011	C1940	U1864	U1766			U1506		C1244		A1176
A2408	C2245	G	G	U2012	A1941	U1850	A1767					G1332		A1177
G2409	G2248	C	C	G2013	A1942	G1851	C1768					C1333		
A2409	C2249	G	C	U2017	G1943	C1852	U1770					C1334		U1180
G2410	G2250	C	G	A2018	G1947	C1853	U1771					C1335		A1181
G2411	G2251	U	U	C2019	U1948	C1854	U1772					C1336		A1182
G2412	A2252	A	A	U2022	G1949	C1855	G1773					U1337		C1183
A2413	G2253	C	C	A2022	C1950	C1856	G1774					U1338		C1184
C2414	G2254	G	G	U2032	G1951	C1864	G1777					C1339		U1185
A2415	A2255	G	G	U2033	U	A1865	C1778					G1340		C1186
G2416	G2256	C	C	G2034	A	G1868	A1778					C1341		U1187
C2417	G2257	G	G	C2035	C	A	A1779					C1342		A1188
U2418	A2258	C	C	U2036	U	U1871	C1780					G1343		A1189
A2419	G2259	C	C	A2037	U	C1872	G1787					C1344		G1190
G2420	C2260	A	A	C2038	U	U1873	U1788					U1266		A1191
C2421	U2261	C	C	U2039	U	G1874	U1789					C1267		A1192
U2422	A2262	C	C	G2040	U	C1875	G1790					U1346		C1268
A2423	G2263	G	G	U2041	G	G1876	G1791					U1347		A1193
G2424	C2264	C	C	G2042	A	U1877	C1792					U1350		A1194
A2425	A2265	C	C	U2043	C	C1878	C1793					C1351		
G2426	G2266	G	G	G2044	C	U1879	U1794					C1273		U1197
A2427	U2267	A	A	U2045	C	U1880	C1795					A1278		U1198
A2434	G2268	C	C	A2046	U1964	C1882	G1796					U1279		A1199
U2435	C2269	A	A	C2047	C1965	U1883	C1797					U1280		A1200
A2436	G2270	C	C	A2048	U1966	G1884	A1796					C1359		C1201
C2437	A2271	C	C	U2049	U1967	C1885	A1797					C1360		A1202
G2438	G2272	A	A	C2050	C1968	U1889	C1798					C1361		G1203
A2353	C2273	G	G	U2051	A1969	U1890	U1799					C1287		G1204
G2439	U2274	U	U	G2052	C1970	C1889	A1801					U1288		C1204
A2354	U2275	C	C	U2053	G1971	C1890	G1802					C1289		U1205
C2355	U2276	G	G	A2054	C2061	U1972	A1804					G1364		U1206
A2356	U2277	C	C	C2062	A2062	U1973	C1805					C1365		U1207
G2440	C2281	A	A	U2063	G1974	A1903	G1806					C1372		C1208
U2441	G2282	U	U	U2064	C1975	U1904	G1807					A1294		C1209
G2442	C2283	C	C	A2065	U1976	U1905						U1296		G1210
A2443	U2284	A	A	C2066	C1977	C1906	G1809					G1299		
G2444	G2285	C	C	U2067	U1978	C1907	C1810					G1300		
A2445	C2286	U	U	A2068	A1979	C1913	A1811					C1376		C1213
G2446	U2287	C	C	G2069	G1979	C1914	A1812					G1377		G1214
U2447	G2288	G	G	U2070	U1980	U1915	A1813					U1304		C1215
A2448	C2289	C	C	C2071	C1981	C1916	A1814					C1305		G1216
G2449	U2290	A	A	G2072	U1982	C1917	U1815					U1306		C1217
C2450	G2291	U	U	A2073	C1983	U1918	U1816					A1307		U1218
G2451	C2292	C	C	U2074	U1984	C1919	U1817					U1308		U1219
A2452	U2293	G	G	G2075	C1985	A1920	U1818					U1309		U1220
C2453	C2294	A	A	A2081	U1986	C1921	G1819					U1310		G1221
U2454	G2295	C	C	C2082	U1987	C1922	G1820					C1393		U1221
A2455	U2296	U	U	U2083	U1988	A1923	G1821					C1394		G1224
G2456	C2297	C	C	A2084	C1989	C1924	G1822					C1395		C1225
U2457	U2298	A	A	G2085	U1990	U1925	G1823					C1396		G1226
A2458	G2299	C	C	U2086	U1991	C1926	G1824					C1397		C1227
C2459	U2300	G	G	C2087	U1992	C1927	G1825					U1398		
U2460	A2301	U	U	A2088	U1993	A1928	G1826					U1399		
G2461	C2302	C	C	G2089	U1994	C1929	G1827					U1400		
A2462	U2303	A	A	U2090	U1995	C1930	G1828					U1401		
C2463	G2304	C	C	C2090	U1996	C1931	G1829					U1402		
U2464	U2305	G	G	A2091	U1997	A1932	G1830					U1403		
A2465	C2306	U	U	U2091	U1998	C1933	G1831					U1404		
G2466	G2307	C	C	G2092	U1999	C1934	G1832					U1405		
U2467	A2308	A	A	C2093	U2000	C1935	G1833					U1406		
A2468	U2309	C	C	U2094	U2001	A1936	G1834					U1407		
C2469	G2310	G	G	A2094	U2002	C1937	G1835					U1408		
U2469	C2311	C	C	U2095	U2003	U1938	G1836					U1409		
A2470	U2312	A	A	C2095	U2004	G1939	G1837					U1410		
G2471	G2313	U	U	G2096	U2005	U1940	G1838					U1411		
U2472	C2314	C	C	A2096	U2006	A1941	G1839					U1412		
A2473	G2315	C	C	U2097	U2007	C1942	G1840					U1413		
C2474	U2316	G	G	C2097	U2008	U1943	G1841					U1414		
G2475	C2317	U	U	A2098	U2009	G1944	G1842					U1415		
U2476	G2318	C	C	U2099	U2010	U1945	G1843					U1416		
A2477	U2319	A	A	G2099	U2011	C1946	G1844					U1417		
C2478	C2320	C	C	U2100	U2012	A1947	G1845					U1418		
U2479	U2321	G	G	C2101	U2013	G1948	G1846					U1419		
A2480	G2322	C	C	U2102	U2014	U1949	G1847					U1420		
C2481	C2323	A	A	G2103	U2015	C1949	G1848					U1421		
U2482	G2324	U	U	C2104	U2016	U1950	G1849					U1422		
A2483	U2325	C	C	U2105	U2017	G1951	G1850					U1423		
G2484	C2326	G	G	C2106	U2018	U1952	G1851					U1424		
U2485	U2327	A	A	A2107	U2019	C1953	G1852					U1425		
A2486	G2328	C	C	U2108	U2020	U1954	G1853					U1426		
C2487	C2329	U	U	G2109	U2021	U1955	G1854					U1427		
U2488	U2330	C	C	A2110	U2022	C1956	G1855					U1428		
G2489	G2331	G	G	U2109	U2023	U1957	G1856					U1429		
A2490	A2332	C	C	G2110	U2024	U1958	G1857					U1430		
U2491	C2333	A	A	U2110	U2025	C1959	G1858					U1431		
C2492	U2334	U	U	C2111	U2026	U1960	G1859					U1432		
G2493	G2335	C	C	U2111	U2027	U1961	G1860					U1433		
U2494	C2336	G	G	A2112	U2028	U1962	G1861					U1434		
A2495	U2337	A	A	C2113	U2029	U1963	G1862					U1435		
C2496	G2338	C	C	U2114	U2030	U1964	G1863					U1436		
U2497	A2339	C	C	G2115	U2031	U1965	G1864					U1437		
A2498	C2340	U	U	A2115	U2032	U1966	G1865					U1438		
G2499	U2341	C	C	C2116	U2033	U1967	G1866					U1439		
U2500	G2342	A	A	U2116	U2034	U1968	G1867					U1440		
A2501	C2343	C	C	G2117	U2035	U1969	G1868					U1441		
C2502	U2344	U	U	A2117	U2036	U1970	G1869					U1442		
G2503	G2345	C	C	U2118	U2037	U1971	G1870					U1443		
U2504	A2346	C	C	C2119	U2038	U1972	G1871					U1444		
A2505	C2347	A	A	U2119	U2039	U1973	G1872					U1445		
G2506	U2348	C	C	G2120	U2040	U1974	G1873					U1446		
U2507	A2349	U	U	A2120	U2041	U1975	G1874					U1447		
C2508	G2350	C	C	C2121	U2042	U1976	G1875					U1448		
U2509	U2351													



• 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, α , β , γ	212.24Å 299.19Å 575.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 85.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 91.7 (85.59-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.238 0.178 , 0.229	Depositor DCC
R_{free} test set	3430 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.7	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	0 of 667094 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: 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	0.34	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.39	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.57	0/1498
5	E	0.34	0/1382	0.56	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.32	0/241	0.47	0/324
8	H	0.33	0/1302	0.62	0/1743
9	I	0.32	0/526	0.54	0/716
10	J	0.39	0/1136	0.61	0/1530
11	K	0.37	0/1004	0.66	0/1351
12	L	0.34	0/1130	0.61	0/1509
13	M	0.40	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.61	0/1999
15	O	0.37	0/874	0.62	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.64	0/1005
18	R	1.27	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.36	0/648	0.59	0/875
20	T	0.34	0/958	0.66	0/1289
21	U	0.45	0/417	0.60	0/562
22	V	0.34	0/502	0.53	0/675
23	W	0.38	0/1219	0.65	0/1655
24	X	0.36	0/664	0.61	0/895
25	Y	0.38	0/1146	0.62	0/1536
26	Z	0.43	0/584	0.63	0/781
27	1	0.47	0/438	0.64	0/578
28	2	0.36	0/401	0.61	0/529
29	3	0.46	0/771	0.60	0/1024
30	0	0.42	0/65956	0.68	7/102865 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.42	7/98700 (0.0%)	0.67	14/147584 (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
23	W	0	1
30	0	0	34
All	All	1	35

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	27.15	2.85	1.50
18	R	150	PRO	CA-C	-18.51	1.15	1.52
18	R	150	PRO	CG-CD	13.84	1.96	1.50
18	R	150	PRO	C-O	11.87	1.47	1.23
18	R	150	PRO	N-CA	11.57	1.67	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.43	55.92	112.00
18	R	150	PRO	N-CA-C	-19.45	61.53	112.10
18	R	150	PRO	CA-N-CD	12.27	128.88	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.27	100.34	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	196	G	Sidechain
30	0	221	G	Sidechain
30	0	324	G	Sidechain
30	0	333	G	Sidechain
23	W	90	TYR	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	85	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	63	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	39	0
6	F	890	0	843	19	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	14	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	34	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	95	0
14	N	1445	0	1401	73	0
15	O	865	0	873	22	0
16	P	1136	0	1123	34	0
17	Q	735	0	729	28	0
18	R	1149	0	1122	41	0
19	S	641	0	605	15	0
20	T	950	0	924	36	0
21	U	410	0	368	26	0
22	V	499	0	511	21	0
23	W	1196	0	1137	58	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	39	0
26	Z	573	0	535	50	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	732	57	0
30	0	59019	0	29809	1661	0
31	9	2599	0	1325	128	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	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	1	0	0	0	0
33	M	1	0	0	0	0
34	0	65	0	0	0	0
34	9	2	0	0	0	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	H	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
35	0	10	0	0	3	0
35	3	1	0	0	1	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	2	0
36	0	92	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	2	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	L	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	0	5904	0	0	251	0
38	1	59	0	0	3	0
38	2	43	0	0	2	0
38	3	70	0	0	3	0
38	9	149	0	0	10	0
38	A	119	0	0	7	0
38	B	152	0	0	16	0
38	C	185	0	0	18	0
38	D	42	0	0	4	0
38	E	43	0	0	1	0
38	F	26	0	0	1	0
38	G	19	0	0	1	0
38	H	65	0	0	4	0
38	I	8	0	0	1	0
38	J	53	0	0	1	0
38	K	58	0	0	3	0
38	L	85	0	0	9	0
38	M	127	0	0	13	0
38	N	59	0	0	2	0
38	O	39	0	0	2	0
38	P	67	0	0	3	0
38	Q	48	0	0	1	0
38	R	77	0	0	2	0
38	S	30	0	0	2	0
38	T	36	0	0	3	0
38	U	28	0	0	4	0
38	V	13	0	0	2	0
38	W	67	0	0	3	0
38	X	21	0	0	2	0
38	Y	100	0	0	5	0
38	Z	31	0	0	7	0
All	All	99121	0	59922	2676	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 18.

The worst 5 of 2676 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	1.96	1.41
30:0:871:G:C8	30:0:871:G:H5'	1.77	1.19
10:J:82:THR:HG23	30:0:1242:A:H5'	1.23	1.16
30:0:1165:G:H1'	30:0:1174:A:H1'	1.17	1.14

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.19	1.13

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%)	202 (86%)	27 (12%)	6 (3%)	8	37
2	B	335/338 (99%)	309 (92%)	17 (5%)	9 (3%)	8	36
3	C	244/246 (99%)	222 (91%)	20 (8%)	2 (1%)	27	74
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	7	32
5	E	170/178 (96%)	157 (92%)	12 (7%)	1 (1%)	33	79
6	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	6	28
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	18	60
9	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	2	12
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	30	76
11	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	27	74
12	L	141/165 (86%)	120 (85%)	21 (15%)	0	100	100
13	M	192/196 (98%)	179 (93%)	9 (5%)	4 (2%)	11	45
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	10	43
15	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	21	66
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	30	76
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
20	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	U	51/67 (76%)	42 (82%)	8 (16%)	1 (2%)	11	47
22	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
23	W	152/154 (99%)	140 (92%)	10 (7%)	2 (1%)	18	60
24	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	9	38
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	58 (82%)	8 (11%)	5 (7%)	2	8
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	9	40
29	3	90/92 (98%)	74 (82%)	13 (14%)	3 (3%)	6	29
All	All	3705/4472 (83%)	3359 (91%)	286 (8%)	60 (2%)	14	54

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	37	VAL
1	A	74	VAL
4	D	65	GLU
4	D	137	PRO

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%)	171 (96%)	8 (4%)	38	80
2	B	282/283 (100%)	264 (94%)	18 (6%)	25	64
3	C	193/193 (100%)	182 (94%)	11 (6%)	29	70
4	D	117/148 (79%)	110 (94%)	7 (6%)	27	67
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	91
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	85
8	H	134/145 (92%)	126 (94%)	8 (6%)	27	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	58/130 (45%)	56 (97%)	2 (3%)	49	86
10	J	118/121 (98%)	113 (96%)	5 (4%)	40	82
11	K	106/106 (100%)	104 (98%)	2 (2%)	69	94
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	80
13	M	158/160 (99%)	148 (94%)	10 (6%)	25	65
14	N	149/150 (99%)	144 (97%)	5 (3%)	49	86
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	97
16	P	113/117 (97%)	107 (95%)	6 (5%)	32	73
17	Q	79/80 (99%)	78 (99%)	1 (1%)	80	96
18	R	117/122 (96%)	114 (97%)	3 (3%)	59	91
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
20	T	105/106 (99%)	99 (94%)	6 (6%)	29	70
21	U	44/53 (83%)	41 (93%)	3 (7%)	22	61
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	83
23	W	130/130 (100%)	124 (95%)	6 (5%)	37	79
24	X	66/74 (89%)	61 (92%)	5 (8%)	19	55
25	Y	120/196 (61%)	115 (96%)	5 (4%)	40	82
26	Z	60/94 (64%)	57 (95%)	3 (5%)	34	75
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	92
29	3	79/79 (100%)	76 (96%)	3 (4%)	44	84
All	All	3095/3646 (85%)	2963 (96%)	132 (4%)	40	81

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ILE
13	M	68	ARG
25	Y	189	ASN
10	J	74	ARG
12	L	99	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	93	GLN
17	Q	16	ASN
27	1	28	HIS
14	N	107	ASN
16	P	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	250 (9%)	21 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	269 (9%)	23 (0%)

5 of 269 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 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1474	C
31	9	43	G
30	0	1377	C
30	0	1506	U

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	0.70	0	24,31,34	0.76	0
30	OMG	0	2588	30	24,26,27	0.74	0	32,38,41	5.16	3 (9%)
30	UR3	0	2619	30	20,22,23	0.81	1 (5%)	23,32,35	0.80	0
30	PSU	0	2621	30	19,21,22	1.18	3 (15%)	23,30,33	1.09	2 (8%)
30	1MA	0	628	30	23,25,26	0.80	0	32,37,40	1.00	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	-	0/8/25/26	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.83	1.42	1.37
30	0	2621	PSU	P-OP1	2.29	1.49	1.46
30	0	2621	PSU	C6-N1	2.28	1.34	1.32
30	0	2619	UR3	P-OP1	2.02	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	-28.58	130.29	134.14
30	0	2588	OMG	C6-N1-C2	3.31	125.31	119.51
30	0	628	1MA	C2-N3-C4	-3.20	110.76	116.23
30	0	2588	OMG	C2-N3-C4	-2.37	111.76	115.09
30	0	2621	PSU	C5-C4-N3	-2.22	114.81	118.86

There are no chirality outliers.

There are no torsion outliers.

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, 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	237/240 (98%)	-0.11	12 (5%) 27 13	36, 71, 108, 128	0
2	B	337/338 (99%)	-0.40	0 100 100	38, 67, 98, 112	0
3	C	246/246 (100%)	-0.37	0 100 100	32, 56, 80, 91	0
4	D	140/177 (79%)	1.61	53 (37%) 1 0	89, 121, 144, 151	0
5	E	172/178 (96%)	-0.05	7 (4%) 35 17	57, 83, 104, 113	0
6	F	119/120 (99%)	0.58	16 (13%) 4 2	64, 88, 121, 131	0
7	G	29/348 (8%)	1.18	5 (17%) 2 2	92, 107, 116, 118	0
8	H	160/177 (90%)	0.72	28 (17%) 2 2	65, 89, 118, 127	0
9	I	70/162 (43%)	3.44	47 (67%) 0 0	145, 162, 177, 179	0
10	J	142/145 (97%)	-0.37	1 (0%) 84 44	47, 63, 86, 105	0
11	K	132/132 (100%)	-0.47	0 100 100	45, 63, 91, 100	0
12	L	145/165 (87%)	0.54	21 (14%) 3 2	41, 88, 131, 140	0
13	M	194/196 (98%)	0.28	21 (10%) 6 4	37, 53, 115, 122	0
14	N	186/187 (99%)	0.82	33 (17%) 2 2	70, 90, 134, 139	0
15	O	115/116 (99%)	-0.34	1 (0%) 81 39	46, 64, 81, 87	0
16	P	143/149 (95%)	-0.30	2 (1%) 72 34	48, 67, 85, 96	0
17	Q	95/96 (98%)	-0.00	4 (4%) 35 17	57, 69, 89, 97	0
18	R	150/155 (96%)	-0.52	1 (0%) 84 44	39, 56, 79, 95	0
19	S	81/85 (95%)	-0.23	1 (1%) 75 36	52, 70, 89, 104	0
20	T	119/120 (99%)	-0.07	4 (3%) 43 19	48, 67, 95, 125	0
21	U	53/67 (79%)	4.70	43 (81%) 0 0	112, 125, 131, 134	0
22	V	65/71 (91%)	0.95	13 (20%) 2 1	51, 83, 131, 135	0
23	W	154/154 (100%)	-0.36	1 (0%) 86 47	45, 62, 79, 92	0
24	X	82/92 (89%)	0.02	4 (4%) 28 14	54, 72, 95, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.55	0 100 100	30, 53, 78, 97	0
26	Z	73/116 (62%)	8.27	58 (79%) 0 0	111, 130, 139, 142	0
27	1	56/57 (98%)	-0.52	0 100 100	30, 39, 47, 65	0
28	2	46/50 (92%)	-0.14	2 (4%) 34 16	39, 72, 104, 110	0
29	3	92/92 (100%)	9.07	91 (98%) 0 0	123, 135, 142, 148	0
30	0	2754/2923 (94%)	-0.41	23 (0%) 83 42	25, 58, 106, 183	0
31	9	122/122 (100%)	-0.59	2 (1%) 68 32	51, 90, 111, 159	0
All	All	6651/7517 (88%)	0.12	494 (7%) 15 8	25, 66, 129, 183	0

The worst 5 of 494 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	58	ASN	29.0
29	3	41	GLU	22.2
29	3	35	TRP	21.5
26	Z	36	GLY	21.5
26	Z	35	SER	21.5

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, 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
30	PSU	0	2621	20/21	0.17	0.81	39,41,53,53	0
30	UR3	0	2619	21/22	0.13	-0.13	47,49,51,54	0
30	OMU	0	2587	21/22	0.11	-0.56	43,47,50,51	0
30	1MA	0	628	23/24	0.14	-1.01	38,44,47,47	0
30	OMG	0	2588	24/25	0.12	-1.35	41,43,46,50	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, 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
36	SR	0	9007	1/1	1.81	199.06	200,200,200,200	0
34	NA	0	8549	1/1	0.67	169.41	56,56,56,56	0
36	SR	0	8982	1/1	2.34	119.04	200,200,200,200	0
36	SR	0	9006	1/1	0.69	105.36	200,200,200,200	0
34	NA	0	8545	1/1	0.82	62.44	58,58,58,58	0
34	NA	0	8562	1/1	0.93	51.50	82,82,82,82	0
34	NA	0	8547	1/1	0.88	48.75	67,67,67,67	0
35	CL	0	8822	1/1	0.45	48.55	88,88,88,88	0
34	NA	0	8551	1/1	0.67	45.33	63,63,63,63	0
32	MG	0	8089	1/1	0.27	44.00	65,65,65,65	0
34	NA	0	8505	1/1	0.78	39.77	53,53,53,53	0
34	NA	0	8565	1/1	0.39	32.94	78,78,78,78	0
34	NA	0	8554	1/1	1.02	31.89	69,69,69,69	0
34	NA	0	8574	1/1	0.53	28.22	60,60,60,60	0
36	SR	0	8996	1/1	0.50	27.21	200,200,200,200	0
34	NA	0	8564	1/1	0.34	25.99	69,69,69,69	0
34	NA	0	8524	1/1	0.54	24.82	73,73,73,73	0
36	SR	0	9004	1/1	0.89	24.30	200,200,200,200	0
36	SR	0	8994	1/1	0.60	24.22	200,200,200,200	0
34	NA	0	8509	1/1	0.17	20.58	69,69,69,69	0
36	SR	0	8983	1/1	0.40	19.51	197,197,197,197	0
34	NA	0	8536	1/1	0.21	17.67	64,64,64,64	0
34	NA	0	8566	1/1	0.35	17.46	63,63,63,63	0
34	NA	0	8528	1/1	0.56	16.75	76,76,76,76	0
36	SR	0	8986	1/1	0.80	16.64	200,200,200,200	0
36	SR	0	8909	1/1	0.15	16.00	93,93,93,93	0
32	MG	0	8040	1/1	0.36	15.79	86,86,86,86	0
32	MG	0	8030	1/1	0.48	15.78	90,90,90,90	0
34	NA	0	8530	1/1	0.50	15.53	74,74,74,74	0
36	SR	B	8987	1/1	0.62	14.32	200,200,200,200	0
32	MG	0	8031	1/1	0.31	13.91	83,83,83,83	0
36	SR	0	8997	1/1	0.25	13.65	189,189,189,189	0
34	NA	0	8508	1/1	0.31	13.60	52,52,52,52	0
34	NA	0	8542	1/1	0.51	13.43	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8556	1/1	0.96	12.79	71,71,71,71	0
34	NA	0	8546	1/1	0.64	12.71	94,94,94,94	0
33	K	0	8401	1/1	0.59	12.58	139,139,139,139	0
34	NA	H	8518	1/1	0.54	12.54	91,91,91,91	0
34	NA	0	8525	1/1	0.18	11.92	75,75,75,75	0
36	SR	0	8957	1/1	0.34	11.89	200,200,200,200	0
34	NA	0	8571	1/1	0.17	11.12	79,79,79,79	0
34	NA	0	8561	1/1	0.32	11.05	65,65,65,65	0
34	NA	0	8567	1/1	0.28	10.91	78,78,78,78	0
34	NA	9	8572	1/1	0.32	10.77	88,88,88,88	0
35	CL	0	8815	1/1	0.19	10.61	89,89,89,89	0
36	SR	L	8969	1/1	0.24	9.01	200,200,200,200	0
36	SR	0	8905	1/1	0.25	8.98	72,72,72,72	0
35	CL	A	8809	1/1	0.31	8.86	104,104,104,104	0
34	NA	0	8555	1/1	0.42	8.84	52,52,52,52	0
32	MG	0	8078	1/1	0.30	8.71	65,65,65,65	0
36	SR	0	8924	1/1	0.19	8.52	124,124,124,124	0
32	MG	0	8022	1/1	0.19	7.88	33,33,33,33	0
34	NA	0	8559	1/1	0.18	7.62	77,77,77,77	0
32	MG	0	8092	1/1	0.17	7.56	76,76,76,76	0
32	MG	0	8047	1/1	0.35	7.41	66,66,66,66	0
36	SR	0	8959	1/1	0.24	7.27	200,200,200,200	0
34	NA	0	8521	1/1	0.28	7.26	64,64,64,64	0
36	SR	0	8976	1/1	0.25	7.16	193,193,193,193	0
32	MG	0	8063	1/1	0.29	7.00	116,116,116,116	0
34	NA	0	8507	1/1	0.21	7.00	43,43,43,43	0
34	NA	0	8527	1/1	0.29	6.94	72,72,72,72	0
34	NA	B	8552	1/1	0.29	6.93	89,89,89,89	0
34	NA	0	8514	1/1	0.32	6.79	55,55,55,55	0
34	NA	0	8575	1/1	0.27	6.73	103,103,103,103	0
34	NA	0	8558	1/1	0.31	6.32	58,58,58,58	0
36	SR	0	8914	1/1	0.28	5.92	133,133,133,133	0
36	SR	0	8903	1/1	0.18	5.92	57,57,57,57	0
34	NA	0	8513	1/1	0.36	5.91	68,68,68,68	0
34	NA	0	8544	1/1	0.18	5.83	79,79,79,79	0
35	CL	0	8805	1/1	0.17	5.74	98,98,98,98	0
34	NA	0	8535	1/1	0.23	5.70	67,67,67,67	0
34	NA	0	8548	1/1	0.16	5.70	56,56,56,56	0
32	MG	0	8048	1/1	0.23	5.46	29,29,29,29	0
36	SR	0	8973	1/1	0.16	5.09	146,146,146,146	0
36	SR	0	8926	1/1	0.14	5.07	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8049	1/1	0.25	4.88	64,64,64,64	0
35	CL	0	8816	1/1	0.41	4.85	85,85,85,85	0
34	NA	0	8550	1/1	0.25	4.73	71,71,71,71	0
32	MG	0	8082	1/1	0.21	4.65	76,76,76,76	0
36	SR	0	8925	1/1	0.13	4.64	98,98,98,98	0
32	MG	0	8018	1/1	0.19	4.48	33,33,33,33	0
32	MG	0	8037	1/1	0.14	4.37	77,77,77,77	0
36	SR	0	8989	1/1	0.20	4.37	178,178,178,178	0
32	MG	0	8085	1/1	0.15	4.17	76,76,76,76	0
34	NA	0	8553	1/1	0.25	4.12	89,89,89,89	0
32	MG	0	8009	1/1	0.24	3.92	34,34,34,34	0
36	SR	0	8901	1/1	0.17	3.55	66,66,66,66	0
36	SR	0	8947	1/1	0.23	3.22	200,200,200,200	0
34	NA	0	8506	1/1	0.18	3.13	83,83,83,83	0
36	SR	R	8912	1/1	0.18	3.08	95,95,95,95	0
32	MG	0	8079	1/1	0.17	3.07	66,66,66,66	0
32	MG	0	8027	1/1	0.12	2.67	47,47,47,47	0
32	MG	0	8005	1/1	0.22	2.63	42,42,42,42	0
32	MG	0	8016	1/1	0.18	2.61	40,40,40,40	0
32	MG	0	8070	1/1	0.17	2.56	66,66,66,66	0
34	NA	0	8502	1/1	0.17	2.50	69,69,69,69	0
34	NA	0	8541	1/1	0.22	2.39	64,64,64,64	0
32	MG	0	8024	1/1	0.17	2.35	62,62,62,62	0
36	SR	0	8992	1/1	0.18	2.35	159,159,159,159	0
32	MG	0	8029	1/1	0.15	2.25	59,59,59,59	0
34	NA	0	8519	1/1	0.21	2.23	52,52,52,52	0
34	NA	0	8537	1/1	0.17	2.23	50,50,50,50	0
32	MG	0	8020	1/1	0.14	2.20	41,41,41,41	0
32	MG	A	8051	1/1	0.32	2.00	94,94,94,94	0
36	SR	0	8904	1/1	0.19	1.94	57,57,57,57	0
36	SR	0	8975	1/1	0.13	1.94	149,149,149,149	0
32	MG	0	8003	1/1	0.19	1.87	38,38,38,38	0
32	MG	0	8091	1/1	0.13	1.75	56,56,56,56	0
32	MG	0	8014	1/1	0.18	1.67	37,37,37,37	0
32	MG	0	8011	1/1	0.20	1.67	25,25,25,25	0
34	NA	0	8501	1/1	0.14	1.61	39,39,39,39	0
36	SR	0	8922	1/1	0.20	1.56	168,168,168,168	0
32	MG	0	8028	1/1	0.17	1.55	34,34,34,34	0
32	MG	0	8064	1/1	0.17	1.54	45,45,45,45	0
36	SR	0	8998	1/1	0.17	1.39	178,178,178,178	0
36	SR	0	8943	1/1	0.12	1.34	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	CL	J	8801	1/1	0.20	1.26	95,95,95,95	0
32	MG	0	8036	1/1	0.12	1.25	48,48,48,48	0
36	SR	0	8946	1/1	0.18	1.23	137,137,137,137	0
32	MG	K	8054	1/1	0.17	1.23	57,57,57,57	0
35	CL	R	8806	1/1	0.17	1.21	58,58,58,58	0
35	CL	0	8814	1/1	0.16	1.18	79,79,79,79	0
34	NA	0	8568	1/1	0.22	1.14	54,54,54,54	0
32	MG	0	8023	1/1	0.16	1.04	28,28,28,28	0
34	NA	0	8523	1/1	0.17	1.03	54,54,54,54	0
32	MG	0	8008	1/1	0.13	0.98	31,31,31,31	0
32	MG	0	8061	1/1	0.19	0.95	36,36,36,36	0
32	MG	0	8066	1/1	0.16	0.95	69,69,69,69	0
36	SR	0	8906	1/1	0.21	0.91	67,67,67,67	0
32	MG	0	8084	1/1	0.16	0.89	35,35,35,35	0
34	NA	0	8526	1/1	0.09	0.83	46,46,46,46	0
32	MG	0	8080	1/1	0.64	0.79	83,83,83,83	0
35	CL	0	8817	1/1	0.14	0.70	72,72,72,72	0
32	MG	0	8015	1/1	0.13	0.56	45,45,45,45	0
32	MG	0	8007	1/1	0.17	0.53	36,36,36,36	0
35	CL	N	8807	1/1	0.27	0.46	87,87,87,87	0
32	MG	0	8043	1/1	0.13	0.46	52,52,52,52	0
36	SR	0	8964	1/1	0.11	0.45	134,134,134,134	0
32	MG	0	8039	1/1	0.19	0.43	84,84,84,84	0
32	MG	0	8019	1/1	0.18	0.43	29,29,29,29	0
36	SR	1	8952	1/1	0.15	0.42	90,90,90,90	0
34	NA	R	8532	1/1	0.13	0.38	50,50,50,50	0
34	NA	0	8516	1/1	0.16	0.37	39,39,39,39	0
32	MG	0	8081	1/1	0.13	0.37	88,88,88,88	0
35	CL	0	8811	1/1	0.21	0.35	81,81,81,81	0
32	MG	0	8062	1/1	0.18	0.34	56,56,56,56	0
36	SR	0	8917	1/1	0.14	0.33	114,114,114,114	0
32	MG	0	8041	1/1	0.16	0.31	36,36,36,36	0
36	SR	0	9002	1/1	0.12	0.22	193,193,193,193	0
34	NA	0	8560	1/1	0.54	0.22	118,118,118,118	0
36	SR	0	8931	1/1	0.10	0.20	111,111,111,111	0
34	NA	0	8569	1/1	0.16	0.14	50,50,50,50	0
36	SR	9	8980	1/1	0.11	0.12	183,183,183,183	0
36	SR	A	8929	1/1	0.15	0.02	139,139,139,139	0
36	SR	0	8949	1/1	0.13	0.00	117,117,117,117	0
32	MG	0	8045	1/1	0.11	-0.03	31,31,31,31	0
36	SR	0	8951	1/1	0.09	-0.07	155,155,155,155	0
36	SR	0	8921	1/1	0.12	-0.11	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	3	8999	1/1	0.26	-0.12	187,187,187,187	0
32	MG	0	8012	1/1	0.16	-0.15	25,25,25,25	0
34	NA	0	8512	1/1	0.16	-0.22	56,56,56,56	0
32	MG	0	8006	1/1	0.12	-0.22	44,44,44,44	0
34	NA	0	8529	1/1	0.08	-0.23	48,48,48,48	0
34	NA	0	8573	1/1	0.15	-0.25	73,73,73,73	0
35	CL	O	8808	1/1	0.19	-0.30	86,86,86,86	0
36	SR	0	8953	1/1	0.56	-0.32	200,200,200,200	0
32	MG	0	8083	1/1	0.09	-0.33	55,55,55,55	0
36	SR	0	8995	1/1	0.15	-0.35	150,150,150,150	0
34	NA	0	8511	1/1	0.11	-0.38	81,81,81,81	0
36	SR	0	8907	1/1	0.11	-0.44	63,63,63,63	0
37	CD	U	8701	1/1	0.43	-0.48	200,200,200,200	0
34	NA	Q	8540	1/1	0.14	-0.49	79,79,79,79	0
34	NA	C	8503	1/1	0.15	-0.50	46,46,46,46	0
36	SR	0	8981	1/1	0.12	-0.53	161,161,161,161	0
36	SR	0	8911	1/1	0.11	-0.54	88,88,88,88	0
34	NA	J	8538	1/1	0.14	-0.54	78,78,78,78	0
33	K	M	8402	1/1	0.13	-0.55	87,87,87,87	0
32	MG	0	8090	1/1	0.16	-0.55	97,97,97,97	0
34	NA	0	8522	1/1	0.10	-0.56	82,82,82,82	0
32	MG	0	8010	1/1	0.15	-0.60	72,72,72,72	0
36	SR	H	8972	1/1	0.13	-0.60	164,164,164,164	0
36	SR	A	8930	1/1	0.13	-0.64	142,142,142,142	0
37	CD	3	8704	1/1	0.72	-0.67	200,200,200,200	0
36	SR	0	8935	1/1	0.10	-0.69	103,103,103,103	0
36	SR	0	8993	1/1	0.11	-0.71	167,167,167,167	0
37	CD	Z	8703	1/1	0.45	-0.71	200,200,200,200	0
36	SR	0	8936	1/1	0.11	-0.72	95,95,95,95	0
36	SR	0	8956	1/1	0.11	-0.74	169,169,169,169	0
36	SR	0	8918	1/1	0.11	-0.76	85,85,85,85	0
32	MG	0	8071	1/1	0.12	-0.77	60,60,60,60	0
36	SR	0	8984	1/1	0.09	-0.79	119,119,119,119	0
36	SR	0	8954	1/1	0.11	-0.80	108,108,108,108	0
36	SR	0	8937	1/1	0.15	-0.82	113,113,113,113	0
36	SR	0	8979	1/1	0.11	-0.88	196,196,196,196	0
34	NA	0	8520	1/1	0.09	-0.88	56,56,56,56	0
36	SR	0	8948	1/1	0.10	-0.91	115,115,115,115	0
36	SR	0	8934	1/1	0.12	-0.95	133,133,133,133	0
34	NA	9	8543	1/1	0.18	-0.96	61,61,61,61	0
34	NA	0	8504	1/1	0.12	-1.06	40,40,40,40	0
36	SR	0	8977	1/1	0.06	-1.07	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8515	1/1	0.13	-1.09	32,32,32,32	0
34	NA	0	8563	1/1	0.13	-1.11	117,117,117,117	0
35	CL	J	8821	1/1	0.10	-1.13	77,77,77,77	0
36	SR	0	8915	1/1	0.10	-1.13	126,126,126,126	0
36	SR	0	9001	1/1	0.11	-1.14	177,177,177,177	0
36	SR	3	8932	1/1	0.33	-1.14	178,178,178,178	0
32	MG	0	8058	1/1	0.05	-1.15	18,18,18,18	0
36	SR	0	8990	1/1	0.14	-1.18	137,137,137,137	0
32	MG	0	8026	1/1	0.08	-1.19	50,50,50,50	0
32	MG	B	8042	1/1	0.07	-1.29	69,69,69,69	0
36	SR	0	8902	1/1	0.13	-1.35	68,68,68,68	0
36	SR	0	8958	1/1	0.08	-1.36	116,116,116,116	0
35	CL	0	8813	1/1	0.08	-1.36	60,60,60,60	0
32	MG	0	8060	1/1	0.06	-1.38	53,53,53,53	0
37	CD	O	8705	1/1	0.08	-1.44	100,100,100,100	0
36	SR	F	9005	1/1	0.07	-1.45	147,147,147,147	0
32	MG	0	8068	1/1	0.10	-1.45	56,56,56,56	0
34	NA	0	8534	1/1	0.12	-1.50	50,50,50,50	0
36	SR	0	8908	1/1	0.10	-1.51	85,85,85,85	0
36	SR	0	8923	1/1	0.10	-1.54	109,109,109,109	0
34	NA	0	8557	1/1	0.07	-1.57	65,65,65,65	0
36	SR	0	8985	1/1	0.06	-1.60	164,164,164,164	0
36	SR	0	8933	1/1	0.04	-1.61	135,135,135,135	0
36	SR	9	9003	1/1	0.09	-1.61	187,187,187,187	0
34	NA	0	8533	1/1	0.09	-1.65	70,70,70,70	0
35	CL	0	8803	1/1	0.09	-1.67	60,60,60,60	0
36	SR	0	8938	1/1	0.08	-1.70	183,183,183,183	0
36	SR	0	9008	1/1	0.14	-1.75	92,92,92,92	0
36	SR	0	8968	1/1	0.07	-1.84	177,177,177,177	0
37	CD	1	8702	1/1	0.09	-1.86	61,61,61,61	0
32	MG	0	8053	1/1	0.06	-1.87	63,63,63,63	0
35	CL	J	8802	1/1	0.05	-1.88	67,67,67,67	0
36	SR	0	8940	1/1	0.10	-1.89	93,93,93,93	0
35	CL	B	8819	1/1	0.14	-1.90	69,69,69,69	0
34	NA	0	8570	1/1	0.08	-1.92	61,61,61,61	0
32	MG	0	8088	1/1	0.12	-2.06	35,35,35,35	0
32	MG	0	8017	1/1	0.11	-2.15	40,40,40,40	0
32	MG	0	8044	1/1	0.07	-2.21	58,58,58,58	0
36	SR	0	8991	1/1	0.07	-2.21	180,180,180,180	0
36	SR	0	8910	1/1	0.08	-2.26	108,108,108,108	0
32	MG	T	8057	1/1	0.08	-2.28	65,65,65,65	0
36	SR	0	8919	1/1	0.10	-2.29	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8073	1/1	0.07	-2.34	72,72,72,72	0
32	MG	0	8025	1/1	0.09	-2.35	37,37,37,37	0
36	SR	0	8960	1/1	0.03	-2.37	151,151,151,151	0
32	MG	0	8004	1/1	0.12	-2.49	29,29,29,29	0
35	CL	0	8812	1/1	0.06	-2.74	61,61,61,61	0
32	MG	0	8033	1/1	0.07	-2.74	63,63,63,63	0
32	MG	0	8059	1/1	0.09	-2.80	51,51,51,51	0
32	MG	0	8093	1/1	0.09	-2.85	36,36,36,36	0
36	SR	0	8988	1/1	0.06	-2.88	173,173,173,173	0
32	MG	0	8002	1/1	0.11	-2.96	40,40,40,40	0
32	MG	0	8052	1/1	0.06	-2.97	44,44,44,44	0
32	MG	Y	8086	1/1	0.07	-2.99	50,50,50,50	0
32	MG	0	8076	1/1	0.07	-3.06	40,40,40,40	0
32	MG	0	8067	1/1	0.09	-3.20	35,35,35,35	0
35	CL	L	8810	1/1	0.05	-3.31	64,64,64,64	0
32	MG	0	8046	1/1	0.11	-3.32	45,45,45,45	0
36	SR	0	8941	1/1	0.09	-3.42	114,114,114,114	0
32	MG	0	8021	1/1	0.08	-3.42	33,33,33,33	0
36	SR	9	8978	1/1	0.05	-3.51	157,157,157,157	0
36	SR	0	8962	1/1	0.12	-3.55	172,172,172,172	0
32	MG	0	8038	1/1	0.08	-3.55	74,74,74,74	0
32	MG	0	8001	1/1	0.12	-3.64	36,36,36,36	0
36	SR	1	8913	1/1	0.09	-3.64	95,95,95,95	0
36	SR	0	8939	1/1	0.05	-3.67	144,144,144,144	0
32	MG	0	8032	1/1	0.04	-3.73	52,52,52,52	0
35	CL	M	8818	1/1	0.05	-3.83	49,49,49,49	0
32	MG	0	8077	1/1	0.07	-3.89	48,48,48,48	0
36	SR	S	8961	1/1	0.08	-3.93	128,128,128,128	0
36	SR	0	8928	1/1	0.03	-3.98	137,137,137,137	0
36	SR	0	8916	1/1	0.04	-3.98	105,105,105,105	0
32	MG	0	8087	1/1	0.10	-4.08	38,38,38,38	0
32	MG	0	8069	1/1	0.10	-4.09	102,102,102,102	0
32	MG	0	8034	1/1	0.06	-4.14	50,50,50,50	0
36	SR	0	8945	1/1	0.08	-4.24	105,105,105,105	0
34	NA	S	8510	1/1	0.03	-4.41	44,44,44,44	0
32	MG	0	8075	1/1	0.05	-4.42	55,55,55,55	0
34	NA	M	8539	1/1	0.08	-4.48	42,42,42,42	0
36	SR	0	8965	1/1	0.05	-4.58	134,134,134,134	0
32	MG	0	8072	1/1	0.10	-4.71	59,59,59,59	0
32	MG	0	8055	1/1	0.06	-4.88	62,62,62,62	0
36	SR	0	8944	1/1	0.07	-5.01	172,172,172,172	0
32	MG	0	8035	1/1	0.07	-5.16	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8531	1/1	0.06	-5.25	39,39,39,39	0
36	SR	0	8970	1/1	0.05	-5.31	125,125,125,125	0
36	SR	0	8920	1/1	0.04	-5.36	127,127,127,127	0
32	MG	0	8065	1/1	0.05	-5.49	42,42,42,42	0
32	MG	9	8074	1/1	0.06	-5.77	87,87,87,87	0
32	MG	0	8013	1/1	0.05	-5.98	28,28,28,28	0
32	MG	A	8050	1/1	0.03	-6.11	64,64,64,64	0
36	SR	B	8950	1/1	0.15	-6.14	130,130,130,130	0
32	MG	0	8056	1/1	0.05	-6.29	57,57,57,57	0
34	NA	0	8517	1/1	0.07	-6.30	38,38,38,38	0
36	SR	0	9000	1/1	0.06	-6.48	183,183,183,183	0
35	CL	Y	8820	1/1	0.07	-6.81	52,52,52,52	0
36	SR	0	8967	1/1	0.05	-7.04	131,131,131,131	0
35	CL	3	8804	1/1	0.19	-8.70	128,128,128,128	0
36	SR	0	8966	1/1	0.08	-9.90	105,105,105,105	0
36	SR	0	8927	1/1	0.08	-10.10	181,181,181,181	0
36	SR	0	8974	1/1	0.08	-11.82	166,166,166,166	0
36	SR	0	8942	1/1	0.07	-19.05	124,124,124,124	0
36	SR	0	8971	1/1	0.05	-63.00	192,192,192,192	0
36	SR	0	8955	1/1	0.07	-64.35	200,200,200,200	0
36	SR	0	8963	1/1	0.08	-	133,133,133,133	0

6.5 Other polymers ⓘ

There are no such residues in this entry.