



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:42 PM GMT

PDB ID : 1VQO
Title : The structure of CCPMN bound to the large ribosomal subunit haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.20 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>

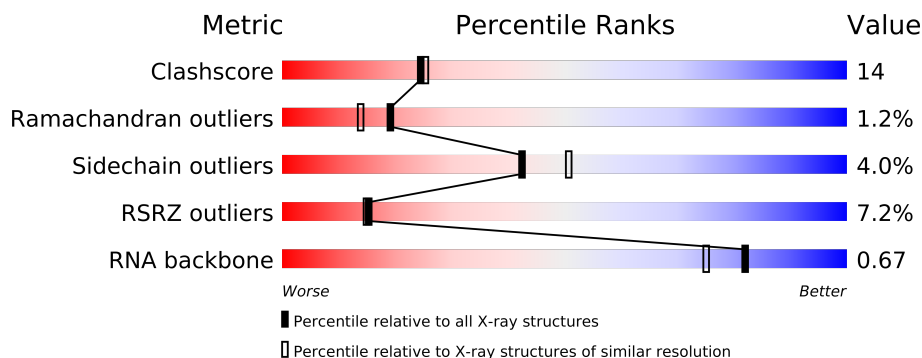
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.20 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))
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)
RNA backbone	1838	1120 (3.00-1.40)

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	0	2922	
2	9	122	
3	4	3	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8001	-	X
33	MG	0	8002	-	X
33	MG	0	8008	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8014	-	X
33	MG	0	8017	-	X
33	MG	0	8021	-	X
33	MG	0	8022	-	X
33	MG	0	8024	-	X
33	MG	0	8025	-	X
33	MG	0	8026	-	X
33	MG	0	8027	-	X
33	MG	0	8029	-	X
33	MG	0	8038	-	X
33	MG	0	8040	-	X
33	MG	0	8041	-	X
33	MG	0	8045	-	X
33	MG	0	8047	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8051	-	X
33	MG	0	8052	-	X
33	MG	0	8056	-	X
33	MG	0	8057	-	X
33	MG	0	8058	-	X
33	MG	0	8059	-	X
33	MG	0	8060	-	X
33	MG	0	8061	-	X
33	MG	0	8065	-	X
33	MG	0	8072	-	X
33	MG	0	8082	-	X
33	MG	0	8084	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8101	-	X
33	MG	0	8103	-	X
33	MG	0	8107	-	X
33	MG	0	8108	-	X
33	MG	0	8114	-	X
33	MG	0	8118	-	X
33	MG	9	8095	-	X
33	MG	A	8066	-	X
33	MG	B	8055	-	X
33	MG	K	8069	-	X
34	K	0	9001	-	X
35	NA	0	9101	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9111	-	X
35	NA	0	9116	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9122	-	X
35	NA	0	9125	-	X
35	NA	0	9129	-	X
35	NA	0	9132	-	X
35	NA	0	9141	-	X
35	NA	0	9149	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9152	-	X
35	NA	0	9154	-	X
35	NA	0	9155	-	X
35	NA	0	9156	-	X
35	NA	0	9157	-	X
35	NA	0	9158	-	X
35	NA	0	9163	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9169	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9173	-	X
35	NA	0	9175	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	9	9183	-	X
35	NA	B	9161	-	X
35	NA	R	9186	-	X
36	CL	0	9316	-	X
36	CL	0	9322	-	X
37	SR	0	9405	-	X
37	SR	0	9406	-	X
37	SR	0	9408	-	X
37	SR	0	9432	-	X
37	SR	0	9452	-	X
37	SR	0	9474	-	X
37	SR	0	9482	-	X
37	SR	0	9500	-	X
37	SR	0	9501	-	X
37	SR	0	9539	-	X
37	SR	0	9547	-	X
37	SR	0	9601	-	X
37	SR	0	9626	-	X
37	SR	B	9521	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99040 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	88	Total	Mg	0	0
			88	88		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	64	Total Na 64 64	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	D	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	9	Total Cl 9 9	0	0
36	J	3	Total Cl 3 3	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total 98	Sr 98	0	0
37	1	2	Total 2	Sr 2	0	0
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0
38	3	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5780	Total	O	0	0
			5780	5780		
39	9	136	Total	O	0	0
			136	136		
39	4	4	Total	O	0	0
			4	4		
39	A	124	Total	O	0	0
			124	124		
39	B	141	Total	O	0	0
			141	141		
39	C	177	Total	O	0	0
			177	177		
39	D	46	Total	O	0	0
			46	46		
39	E	43	Total	O	0	0
			43	43		
39	F	25	Total	O	0	0
			25	25		
39	G	16	Total	O	0	0
			16	16		
39	H	71	Total	O	0	0
			71	71		
39	J	58	Total	O	0	0
			58	58		
39	K	60	Total	O	0	0
			60	60		
39	L	82	Total	O	0	0
			82	82		
39	M	125	Total	O	0	0
			125	125		
39	N	62	Total	O	0	0
			62	62		
39	O	40	Total	O	0	0
			40	40		
39	P	60	Total	O	0	0
			60	60		

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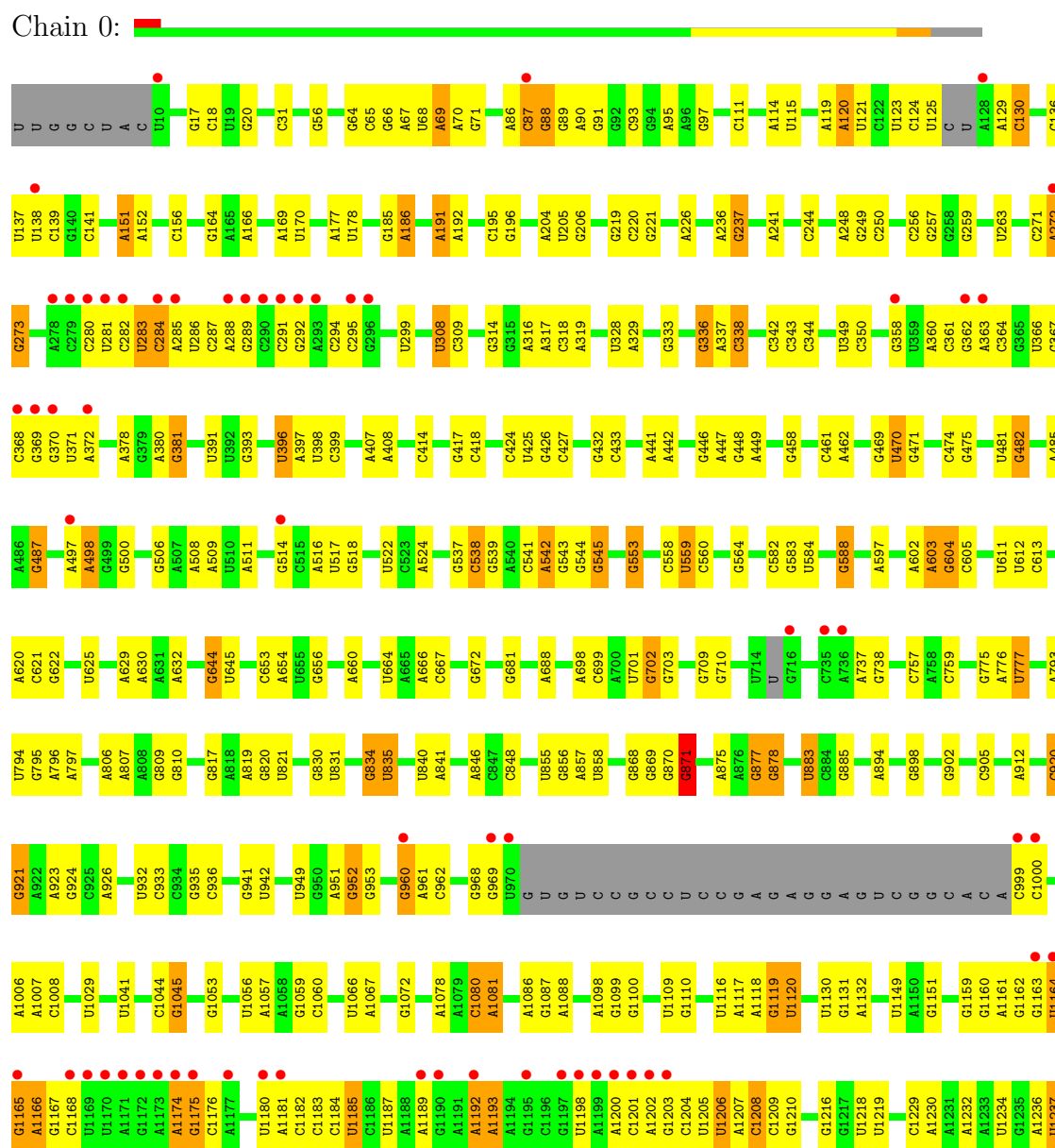
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	49	Total 49	O 49	0	0
39	R	83	Total 83	O 83	0	0
39	S	30	Total 30	O 30	0	0
39	T	36	Total 36	O 36	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	26	Total 26	O 26	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	29	Total 29	O 29	0	0
39	1	52	Total 52	O 52	0	0
39	2	40	Total 40	O 40	0	0
39	3	66	Total 66	O 66	0	0
39	I	8	Total 8	O 8	0	0

3 Residue-property plots

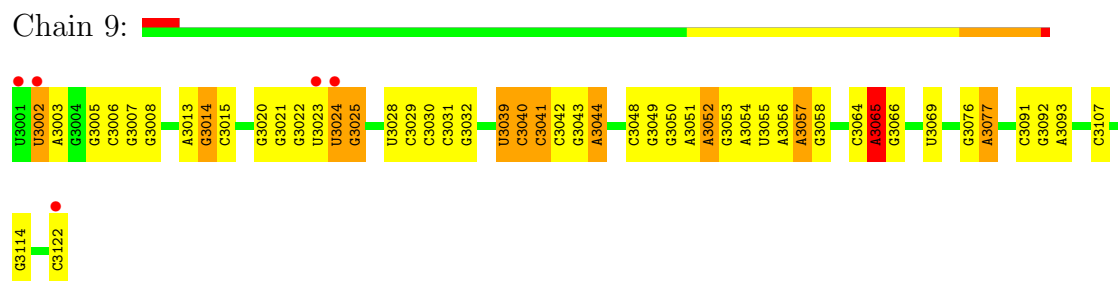
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal rna



C2857	C2858	A2761	C2762	C2644	C2645	U2551	C2426	C2427	U2320	U	C	A2038	A1941	A1778	G1681	A1528	A1369	C1238
U2856	G2867	C2765	U2661	A2649	U2645	C2532	C2428	U2435	A2321	A	U	A2039	A1942	A1779	A1682	G1529	A1372	G1239
G2876	G2877	C2768	U2662	U2643	U2644	C2534	U2436	U2437	G2324	C	G	U2043	C1946	C1787	A1684	G1552	U1372	A1242
A2879	A2880	G2779	G2663	U2644	U2645	U2536	C2443	U2438	C2329	C	U	G2044	G1948	G1789	A1685	G1555	G1376	U1243
C2881	G2882	C2780	U2664	U2645	U2646	U2537	U2443	U2439	U2330	C	U	A2054	G1949	U1798	C1687	U	C1377	C1245
A2883	G2884	U2781	A	U	U	C2541	U2456	U2457	G2337	C	G	U2064	G1950	C1798	C1687	C1589	U1378	A1246
A2885	A2886	G2782	G2667	U2646	U2647	C2549	G2462	U2458	G2338	C	U	A2067	G1951	U1817	C1692	C1561	U1380	C1250
A2887	A2888	A2783	C2668	U2647	U2648	C2552	A2465	U2459	C2340	C	A	A2068	U1951	G1818	C1700	C1562	C1384	C1251
A2890	A2891	G2785	U2670	U2648	U2649	C2553	A2466	U2460	A2344	C	U	G2072	U1952	G1819	C1701	G1563	A1384	A1252
C2895	A2896	C2786	U2671	U2649	U2650	U2554	A2467	U2461	A2345	C	U	A2074	U1953	G1820	U1702	C1564	C1400	C1253
C2903	A2904	C2791	C2676	U2650	U2651	C2555	C2472	U2462	C2347	C	U	C2080	U1954	U1835	A1717	C1594	C1400	C1268
A2906	C2907	C2795	G2679	A2680	C2682	C2556	C2476	U2463	C2348	C	U	G2091	U1955	U1836	C1715	C1595	A1406	U1278
A2908	C2909	U2796	A2681	C2683	C2684	C2557	C2477	U2464	A2353	C	U	G2092	U1956	U1837	C1716	C1596	A1407	U1279
C2911	C2912	A2811	A2697	U2681	U2682	C2558	C2478	U2465	A2354	C	U	A2095	U1957	U1838	C1717	C1597	A1408	U1280
A2913	A2914	C2812	C2698	U2682	U2683	C2559	C2479	U2466	A2355	C	U	A2096	U1958	U1839	C1718	C1598	A1409	U1281
A	G	C2813	C2699	U2683	U2684	C2560	C2480	U2467	A2356	C	U	U1967	U1959	U1840	C1719	C1599	A1410	U1282
G	C	A2814	C2700	U2684	U2685	C2561	C2481	U2468	A2357	C	U	C2100	U1960	U1841	C1720	C1600	A1411	U1283
C	C	G2815	C2701	U2685	U2686	C2562	C2482	U2469	A2358	C	U	A2101	U1961	U1842	C1721	C1601	A1412	U1284
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C	C	G2817	U2705	U2687	U2688	C2564	C2484	U2471	A2360	C	U	A2103	U1963	U1844	C1723	C1603	A1414	U1286
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G2826	A2827	G2828	C2718	C2719	C2720	C2501	C2500	C2491	A2363	C	U	G2111	U1966	U1847	C1726	C1606	A1436	C1305
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G2861	G2862	G2863	U2748	U2749	U2750	C2512	C2511	C2502	A2374	C	U	G2122	U1977	U1858	C1737	C1617	A1447	U1323
G2864	G2865	G2866	U2751	U2752	U2753	C2513	C2512	C2503	A2375	C	U	G2123	U1978	U1859	C1738	C1618	A1448	U1324
G2867	G2868	G2869	U2754	U2755	U2756	C2514	C2513	C2504	A2376	C	U	G2124	U1979	U1860	C1739	C1619	A1449	U1325
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G2873	G2874	G2875	U2760	U2761	U2762	C2516	C2515	C2506	A2378	C	U	G2126	U1981	U1862	C1741	C1621	A1451	U1327
G2876	G2877	G2878	U2763	U2764	U2765	C2517	C2516	C2507	A2379	C	U	G2127	U1982	U1863	C1742	C1622	A1452	U1328
G2879	G2880	G2881	U2766	U2767	U2768	C2518	C2517	C2508	A2380	C	U	G2128	U1983	U1864	C1743	C1623	A1453	U1329
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G2885	G2886	G2887	U2772	U2773	U2774	C2520	C2519	C2510	A2382	C	U	G2130	U1985	U1866	C1745	C1625	A1455	U1331
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G2891	G2892	G2893	U2778	U2779	U2780	C2522	C2521	C2512	A2384	C	U	G2132	U1987	U1868	C1747	C1627	A1457	U1333
G2894	G2895	G2896	U2781	U2782	U2783	C2523	C2522	C2513	A2385	C	U	G2133	U1988	U1869	C1748	C1628	A1458	U1334
G2897	G2898	G2899	U2784	U2785	U2786	C2524	C2523	C2514	A2386	C	U	G2134	U1989	U1870	C1749	C1629	A1459	U1335
G2900	G2901	G2902	U2787	U2788	U2789	C2525	C2524	C2515	A2387	C	U	G2135	U1990	U1871	C1750	C1630	A1460	U1336
G2903	G2904	G2905	U2790	U2791	U2792	C2526	C2525	C2516	A2388	C	U	G2136	U1991	U1872	C1751	C1631	A1461	U1337
G2906	G2907	G2908	U2793	U2794	U2795	C2527	C2526	C2517	A2389	C	U	G2137	U1992	U1873	C1752	C1632	A1462	U1338
G2909	G2910	G2911	U2796	U2797	U2798	C2528	C2527	C2518	A2390	C	U	G2138	U1993	U1874	C1753	C1633	A1463	U1339
G2912	G2913	G2914	U2799	U2800	U2801	C2529	C2528	C2519	A2391	C	U	G2139	U1994	U1875	C1754	C1634	A1464	U1340
G2915	G2916	G2917	U2802	U2803	U2804	C2530	C2529	C2520	A2392	C	U	G2140	U1995	U1876	C1755	C1635	A1465	U1341
G2918	G2919	G2920	U2805	U2806	U2807	C2531	C2530	C2521	A2393	C	U	G2141	U1996	U1877	C1756	C1636	A1466	U1342
G2921	G2922	G2923	U2808	U2809	U2810	C2532	C2531	C2522	A2394	C	U	G2142	U1997	U1878	C1757	C1637	A1467	U1343
G2924	G2925	G2926	U2811	U2812	U2813	C2533	C2532	C2523	A2395	C	U	G2143	U1998	U1879	C1758	C1638	A1468	U1344
G2927	G2928	G2929	U2814	U2815	U2816	C2534	C2533	C2524	A2396	C	U	G2144	U1999	U1880	C1759	C1639	A1469	U1345
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G2939	G2940	G2941	U2826	U2827	U2828	C2538	C2537	C2528	A2400	C	U	G2148	U2003	U1884	C1763	C1643	A1473	U1349
G2942	G2943	G2944	U2829	U2830	U2831	C2539	C2538	C2529	A2401	C	U	G2149	U2004	U1885	C1764	C1644	A1474	U1350
G2945	G2946	G2947	U2832	U2833	U2834	C2540	C2539	C2530	A2402	C	U	G2150	U2005	U1886	C1765	C1645	A1475	U1351
G2948	G2949	G2950	U2835	U2836	U2837	C2541	C2540	C2531	A2403	C	U	G2151	U2006	U1887	C1766	C1646	A1476	U1352
G2951	G2952	G2953	U2838	U2839	U2840	C2542	C2541	C2532	A2404	C	U	G2152	U2007	U1888	C1767	C1647	A1477	U1353
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G2960	G2961	G2962	U2847	U2848	U2849	C2545	C2544	C2535	A2407	C	U	G2155	U2010	U1891	C1770	C1650	A1480	U1356
G2963	G2964	G2965	U2850	U2851	U2852	C2546	C2545	C2536	A2408	C	U	G2156	U2011	U1892	C1771	C1651	A1481	U1357
G2966	G2967	G2968	U2853	U2854	U2855	C2547	C2546	C2537	A2409	C	U	G2157	U2012	U1893	C1772	C1652	A1482	U1358
G2969	G2970	G2971	U2856	U2857	U2858	C2548	C2547	C2538	A2410	C	U	G2158	U2013	U1894	C1773	C1653	A1483	U1359
G2972</																		

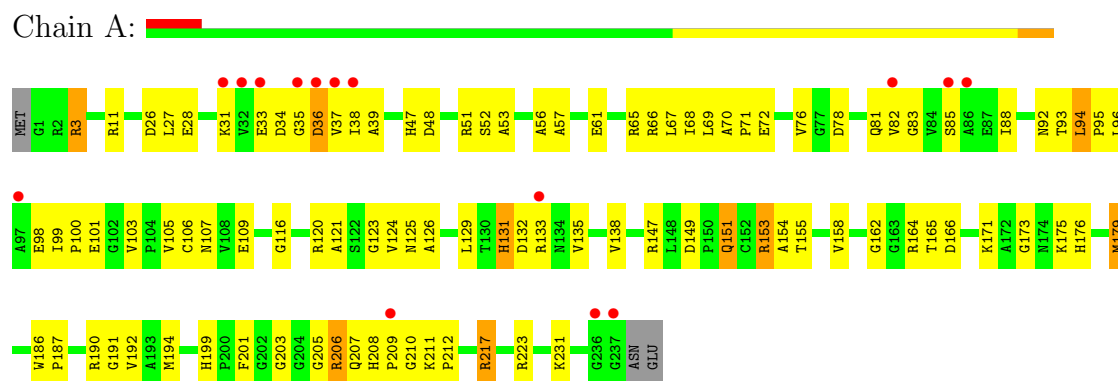
- Molecule 2: 5S ribosomal RNA



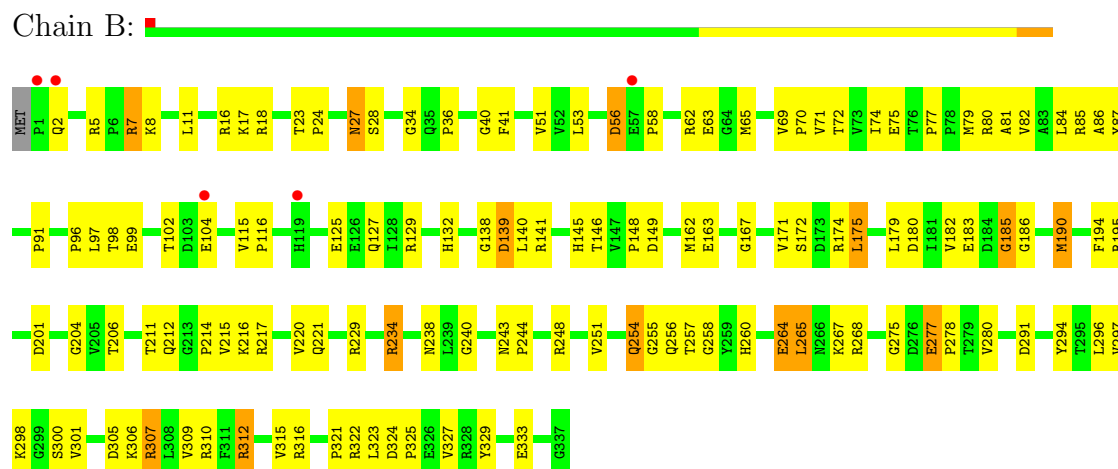
- Molecule 3: 5'-R(*CP*CP*(PPU))-3'



- Molecule 4: 50S ribosomal protein L2P

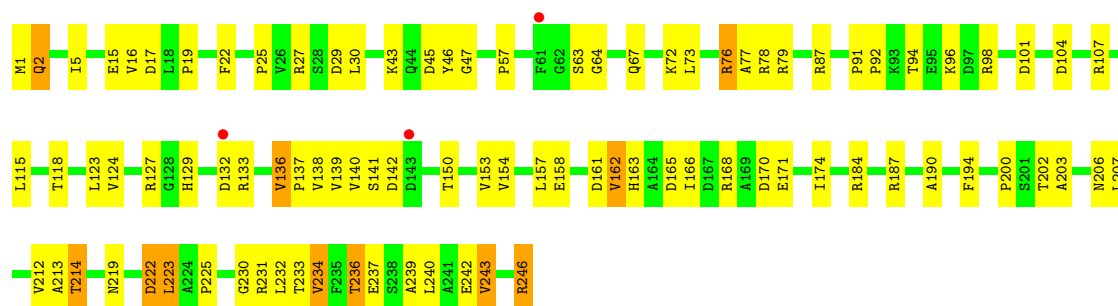


- Molecule 5: 50S ribosomal protein L3P



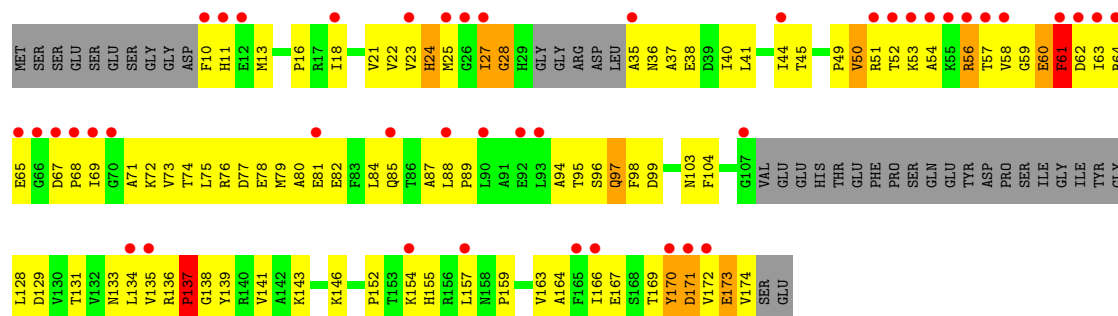
- Molecule 6: 50S ribosomal protein L4E





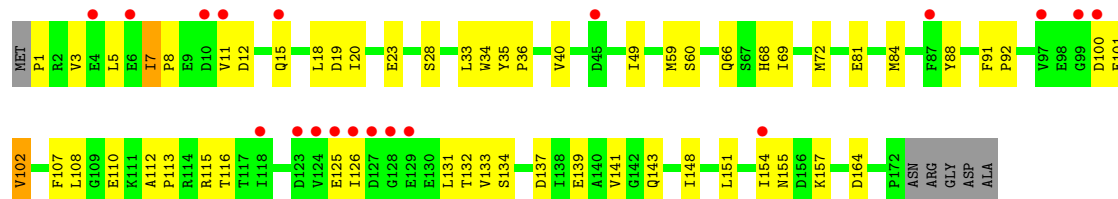
• Molecule 7: 50S ribosomal protein L5P

Chain D:



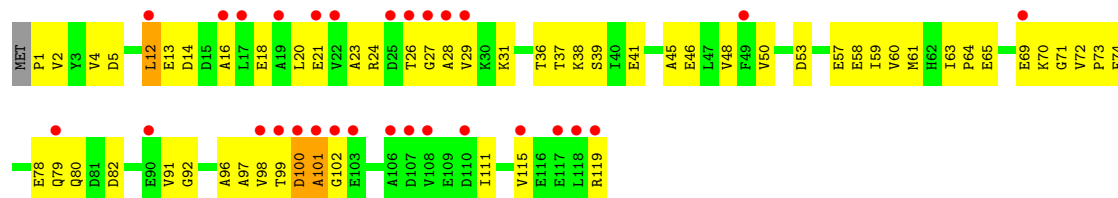
• Molecule 8: 50S ribosomal protein L6P

Chain E:



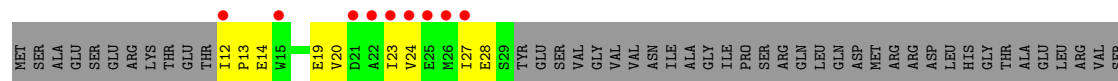
• Molecule 9: 50S ribosomal protein L7AE

Chain F:



• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

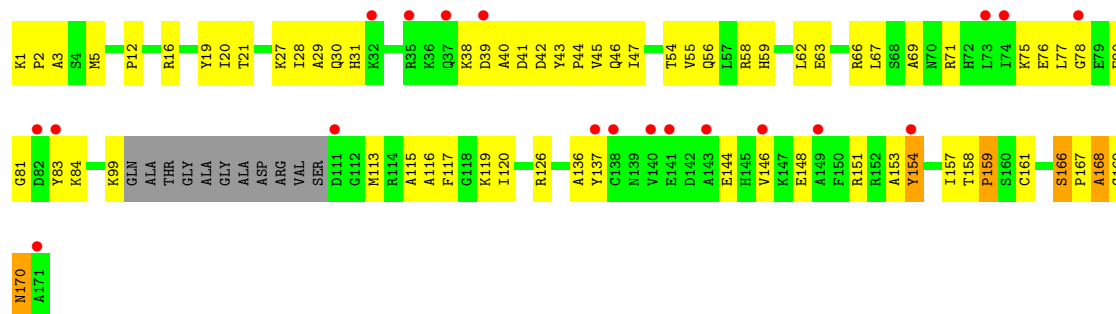
Chain G:





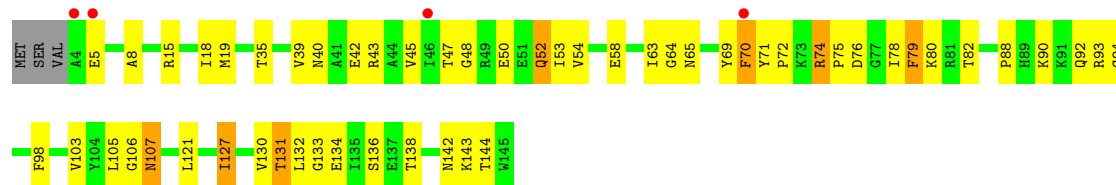
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



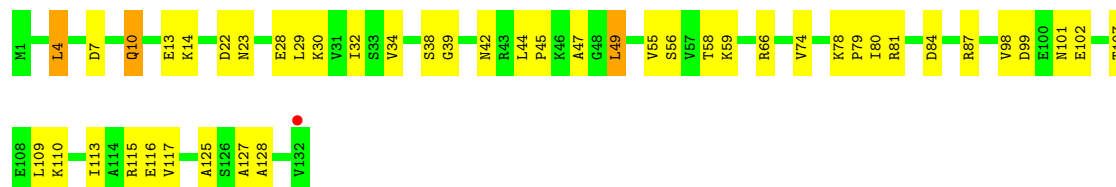
• Molecule 12: 50S ribosomal protein L13P

Chain J:



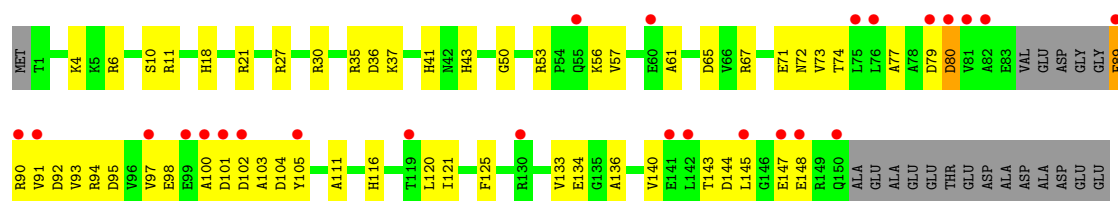
• Molecule 13: 50S ribosomal protein L14P

Chain K:



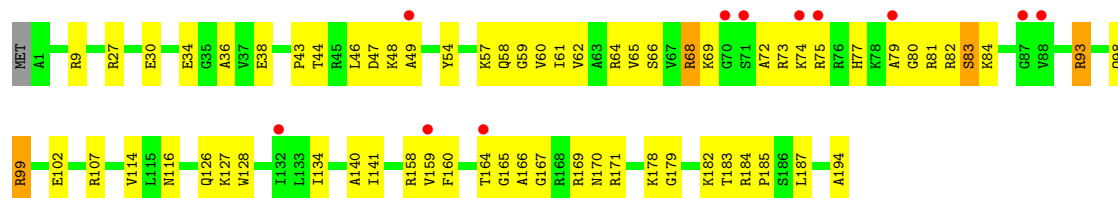
• Molecule 14: 50S ribosomal protein L15P

Chain L:



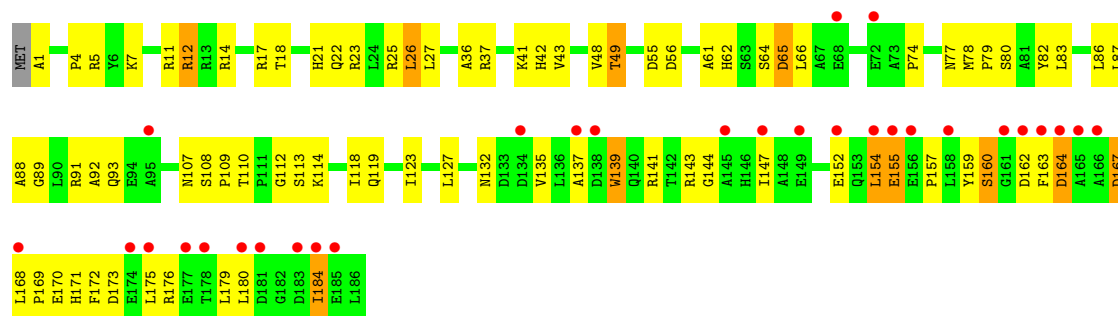
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



• Molecule 16: 50S ribosomal protein L18P

Chain N:



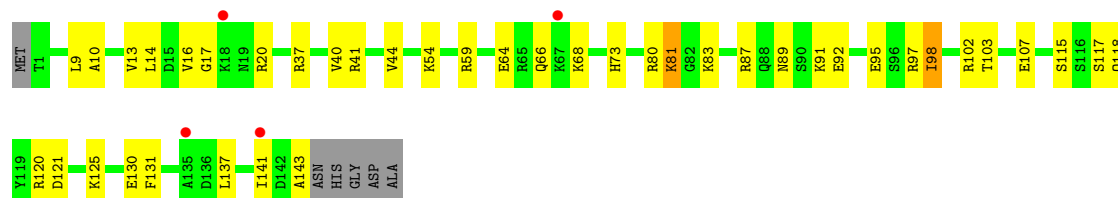
• Molecule 17: 50S ribosomal protein L18e

Chain O:



• Molecule 18: 50S ribosomal protein L19E

Chain P:



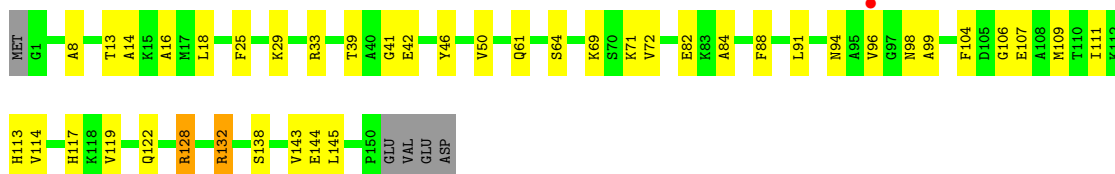
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



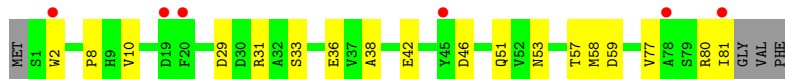
- Molecule 20: 50S ribosomal protein L22P

Chain R:



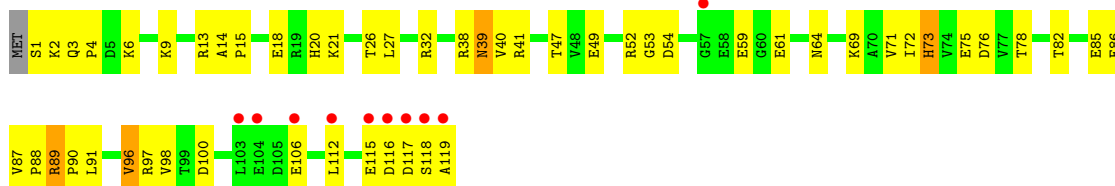
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



- Molecule 23: 50S ribosomal protein L24E

Chain U:



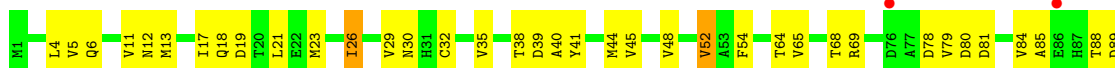
- Molecule 24: 50S ribosomal protein L29P

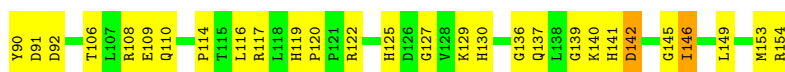
Chain V:



- Molecule 25: 50S ribosomal protein L30P

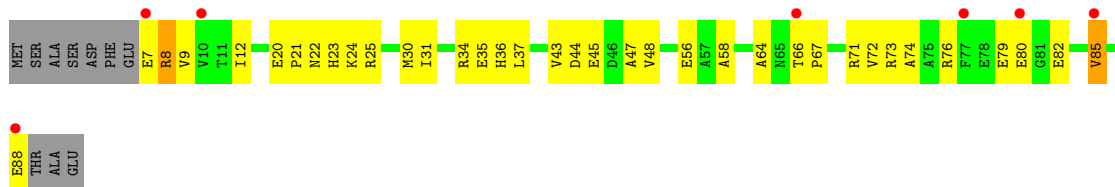
Chain W:





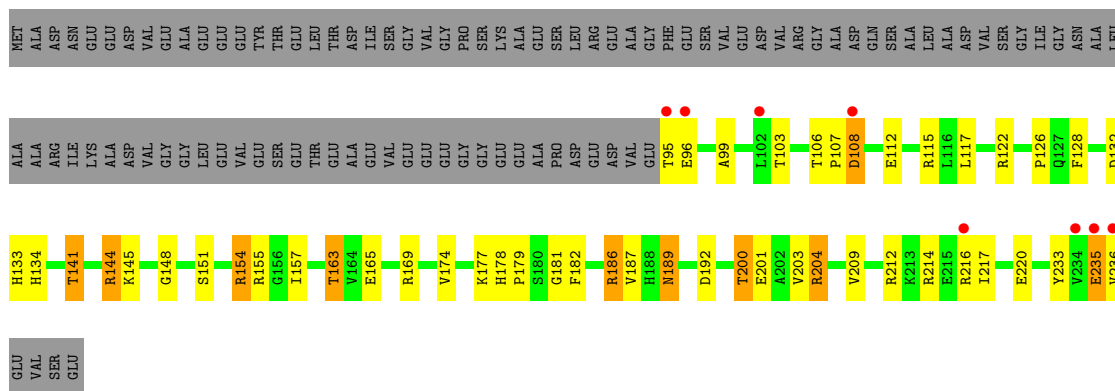
- Molecule 26: 50S ribosomal protein L31e

Chain X:



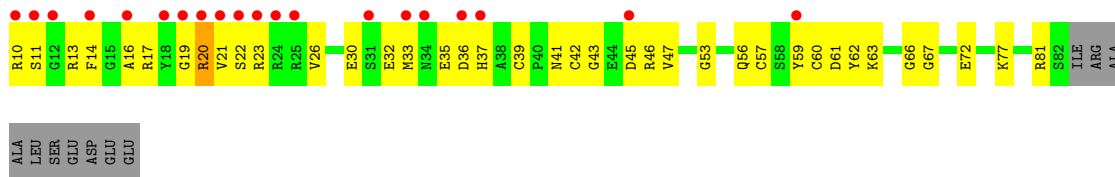
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



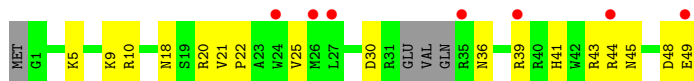
- Molecule 29: 50S ribosomal protein L37e

Chain 1:

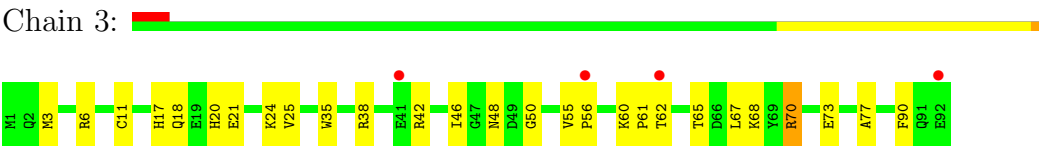


- Molecule 30: 50S ribosomal protein L39e

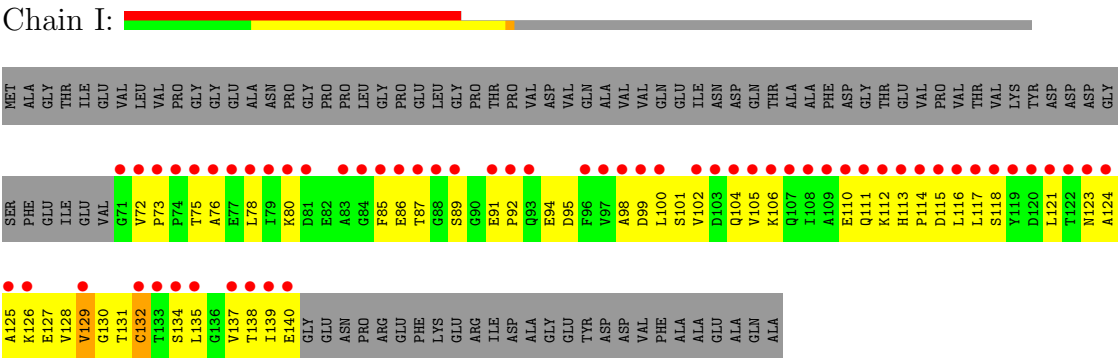
Chain 2:



- Molecule 31: 50S ribosomal protein L44E



● Molecule 32: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.04Å 299.41Å 575.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 49.39 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.20) 88.8 (49.39-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.246 0.214 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 892831 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99040	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, PPU, 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	0	0.37	0/65959	0.70	24/102870 (0.0%)
2	9	0.33	0/2905	0.71	1/4528 (0.0%)
3	4	0.43	0/40	0.63	0/60
4	A	0.32	0/1786	0.64	0/2408
5	B	0.35	0/2690	0.67	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.32	0/1382	0.57	0/1880
9	F	0.32	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.35	0/1136	0.61	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.66	0/1509
15	M	0.34	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.59	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	1/1005 (0.1%)
20	R	0.35	0/1172	0.67	1/1578 (0.1%)
21	S	0.31	0/648	0.56	0/875
22	T	0.29	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.25	0/502	0.51	0/675
25	W	0.34	0/1219	0.61	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.66	0/1536
28	Z	0.32	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.49	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98732	0.68	28/147637 (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
1	0	1	40
2	9	0	1
All	All	1	41

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.80	131.06	109.50
1	0	871	G	C5'-C4'-O4'	-8.85	98.48	109.10
1	0	1942	A	C5'-C4'-C3'	8.20	129.12	116.00
1	0	777	U	O4'-C1'-N1	6.82	113.66	108.20
1	0	1819	G	C5'-C4'-C3'	6.76	126.81	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 41 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	191	A	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	718	0
2	9	2600	0	1326	56	0
3	4	74	0	51	2	0
4	A	1753	0	1766	117	0
5	B	2625	0	2532	131	0
6	C	1859	0	1816	111	0
7	D	1094	0	1085	101	0
8	E	1357	0	1266	53	0
9	F	890	0	843	52	0
10	G	240	0	231	15	0
11	H	1266	0	1268	68	0
12	J	1120	0	1098	68	0
13	K	992	0	1031	49	0
14	L	1118	0	1076	59	0
15	M	1560	0	1568	67	0
16	N	1445	0	1401	89	0
17	O	865	0	873	38	0
18	P	1136	0	1123	40	0
19	Q	735	0	728	18	0
20	R	1149	0	1122	46	0
21	S	641	0	605	17	0
22	T	950	0	924	53	0
23	U	410	0	364	26	0
24	V	499	0	511	37	0
25	W	1196	0	1137	76	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	55	0
28	Z	578	0	539	33	0
29	1	431	0	426	24	0
30	2	396	0	413	23	0
31	3	755	0	728	23	0
32	I	519	0	500	54	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5780	0	0	111	0
39	1	52	0	0	3	0
39	2	40	0	0	2	0
39	3	66	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	4	4	0	0	0	0
39	9	136	0	0	10	0
39	A	124	0	0	12	0
39	B	141	0	0	19	0
39	C	177	0	0	16	0
39	D	46	0	0	10	0
39	E	43	0	0	1	0
39	F	25	0	0	4	0
39	G	16	0	0	3	0
39	H	71	0	0	8	0
39	I	8	0	0	0	0
39	J	58	0	0	3	0
39	K	60	0	0	8	0
39	L	82	0	0	12	0
39	M	125	0	0	6	0
39	N	62	0	0	7	0
39	O	40	0	0	4	0
39	P	60	0	0	4	0
39	Q	49	0	0	3	0
39	R	83	0	0	5	0
39	S	30	0	0	0	0
39	T	36	0	0	4	0
39	U	28	0	0	4	0
39	V	12	0	0	1	0
39	W	68	0	0	4	0
39	X	26	0	0	6	0
39	Y	93	0	0	11	0
39	Z	29	0	0	2	0
All	All	99040	0	59949	2117	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 14.

The worst 5 of 2117 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.32	1.10
6:C:236:THR:HG22	6:C:239:ALA:H	1.10	1.10
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.34	1.10
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.32	1.08
2:9:3006:C:H5''	16:N:37:ARG:NH1	1.68	1.07

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	
4	A	235/240 (98%)	208 (88%)	25 (11%)	2 (1%)	25	21
5	B	335/338 (99%)	315 (94%)	16 (5%)	4 (1%)	19	14
6	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
7	D	134/177 (76%)	107 (80%)	16 (12%)	11 (8%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	105 (90%)	8 (7%)	4 (3%)	6	2
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	137 (88%)	15 (10%)	4 (3%)	8	4
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	11	5
13	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
14	L	141/165 (86%)	119 (84%)	20 (14%)	2 (1%)	16	12
15	M	192/195 (98%)	183 (95%)	8 (4%)	1 (0%)	38	38
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	5	2
17	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
20	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	21
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	14	9
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	62 (87%)	6 (8%)	3 (4%)	4	1
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	7	3
All	All	3705/4431 (84%)	3432 (93%)	228 (6%)	45 (1%)	19	14

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	27	LEU
5	B	139	ASP
11	H	166	SER
11	H	168	ALA
12	J	143	LYS

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	
4	A	179/182 (98%)	168 (94%)	11 (6%)	26	28
5	B	282/283 (100%)	265 (94%)	17 (6%)	27	29
6	C	193/193 (100%)	176 (91%)	17 (9%)	14	13
7	D	117/148 (79%)	111 (95%)	6 (5%)	33	38
8	E	152/156 (97%)	147 (97%)	5 (3%)	50	60
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	92
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	128 (97%)	4 (3%)	53	64
12	J	118/121 (98%)	111 (94%)	7 (6%)	28	30
13	K	106/106 (100%)	102 (96%)	4 (4%)	44	53
14	L	113/127 (89%)	110 (97%)	3 (3%)	57	68
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	62
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	59
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	113/117 (97%)	111 (98%)	2 (2%)	71	82
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	53
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	84
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	53
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	79
25	W	130/130 (100%)	125 (96%)	5 (4%)	44	53
26	X	66/74 (89%)	62 (94%)	4 (6%)	26	28
27	Y	120/196 (61%)	107 (89%)	13 (11%)	9	8
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	73
31	3	79/79 (100%)	78 (99%)	1 (1%)	80	89
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2970 (96%)	123 (4%)	42	51

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	164	ASP
13	K	4	LEU
27	Y	163	THR
11	H	84	LYS
12	J	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	170	ASN
19	Q	16	ASN
30	2	18	ASN
16	N	107	ASN
18	P	50	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	2 (1%)
3	4	1/3 (33%)	0	0
All	All	2867/3047 (94%)	248 (8%)	37 (1%)

5 of 248 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1692	C
1	0	2852	A
1	0	1563	G
1	0	1684	A

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

6 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	$\# Z > 2$
1	OMU	0	2587	1	20,22,23	0.79	1 (5%)	24,31,34	0.85	0
1	OMG	0	2588	1,3	24,26,27	0.83	0	32,38,41	5.07	4 (12%)
1	UR3	0	2619	1	20,22,23	0.79	0	23,32,35	0.81	0
1	PSU	0	2621	1	19,21,22	1.30	3 (15%)	23,30,33	1.08	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	0	628	1	23,25,26	0.81	0	32,37,40	1.00	1 (3%)
3	PPU	4	76	1,3	38,40,41	1.07	2 (5%)	54,57,60	0.92	2 (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
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3
3	PPU	4	76	1,3	-	0/26/43/44	0/2/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.02	1.26	1.42
1	0	2621	PSU	C2-N1	3.39	1.43	1.37
1	0	2621	PSU	C6-N1	2.75	1.34	1.32
1	0	2621	PSU	P-OP1	2.61	1.49	1.46
1	0	2587	OMU	P-OP1	2.44	1.49	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.02	130.37	134.14
3	4	76	PPU	C2-N1-C6	3.45	119.00	111.53
1	0	2588	OMG	C6-N1-C2	3.30	125.29	119.51
1	0	628	1MA	C2-N3-C4	-3.12	110.90	116.23
3	4	76	PPU	C4'-C3'-N3'	-2.49	108.25	113.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	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 312 ligands modelled in this entry, 312 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	0	2754/2922 (94%)	-0.17	96 (3%) 42 42	26, 46, 90, 148	0
2	9	122/122 (100%)	0.08	5 (4%) 35 36	39, 62, 87, 147	0
3	4	3/3 (100%)	-0.02	0 100 100	52, 52, 57, 62	0
4	A	237/240 (98%)	0.40	15 (6%) 19 19	30, 52, 82, 104	0
5	B	337/338 (99%)	0.12	5 (1%) 70 71	31, 50, 72, 85	0
6	C	246/246 (100%)	-0.02	3 (1%) 75 76	28, 47, 68, 81	0
7	D	140/177 (79%)	1.63	44 (31%) 1 1	56, 90, 119, 127	0
8	E	172/178 (96%)	0.66	19 (11%) 6 6	42, 60, 78, 83	0
9	F	119/120 (99%)	1.09	29 (24%) 1 1	47, 71, 99, 108	0
10	G	29/348 (8%)	2.38	15 (51%) 0 0	68, 89, 97, 98	0
11	H	160/171 (93%)	0.63	19 (11%) 5 5	44, 60, 92, 99	0
12	J	142/145 (97%)	-0.03	4 (2%) 50 51	36, 47, 66, 86	0
13	K	132/132 (100%)	-0.23	1 (0%) 83 85	34, 45, 66, 69	0
14	L	145/165 (87%)	0.73	25 (17%) 2 2	30, 64, 110, 119	0
15	M	194/195 (99%)	0.43	11 (5%) 23 23	35, 46, 67, 79	0
16	N	186/187 (99%)	0.79	30 (16%) 2 2	44, 62, 104, 112	0
17	O	115/116 (99%)	0.07	2 (1%) 67 68	41, 53, 66, 74	0
18	P	143/149 (95%)	0.17	4 (2%) 50 51	40, 51, 65, 78	0
19	Q	95/96 (98%)	0.04	3 (3%) 45 46	41, 47, 63, 74	0
20	R	150/155 (96%)	-0.09	1 (0%) 84 86	31, 44, 62, 70	0
21	S	81/85 (95%)	0.37	6 (7%) 14 14	43, 62, 82, 95	0
22	T	119/120 (99%)	0.58	10 (8%) 11 10	43, 56, 79, 107	0
23	U	53/66 (80%)	0.35	3 (5%) 23 23	42, 51, 67, 75	0
24	V	65/71 (91%)	2.02	23 (35%) 1 0	54, 78, 111, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.00	2 (1%) 74 74	36, 48, 69, 78	0
26	X	82/92 (89%)	0.52	7 (8%) 11 10	41, 53, 79, 97	0
27	Y	142/241 (58%)	0.12	8 (5%) 24 23	31, 43, 62, 82	0
28	Z	73/83 (87%)	1.07	20 (27%) 1 1	49, 73, 86, 92	0
29	1	56/57 (98%)	-0.46	0 100 100	30, 35, 42, 50	0
30	2	46/50 (92%)	0.69	7 (15%) 3 3	38, 58, 73, 83	0
31	3	92/92 (100%)	0.19	4 (4%) 34 34	37, 55, 68, 79	0
32	I	70/162 (43%)	4.93	60 (85%) 0 0	107, 120, 137, 139	0
All	All	6654/7478 (88%)	0.21	481 (7%) 15 15	26, 51, 95, 148	0

The worst 5 of 481 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	16.1
24	V	1	THR	15.2
7	D	63	ILE	12.9
32	I	133	THR	12.6
24	V	39	ALA	11.6

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
1	UR3	0	2619	21/22	0.15	-0.07	45,45,49,50	0
3	PPU	4	76	37/38	0.14	-0.12	48,54,66,71	0
1	1MA	0	628	23/24	0.12	-0.45	29,33,36,37	0
1	OMG	0	2588	24/25	0.11	-0.47	30,35,40,41	0
1	OMU	0	2587	21/22	0.10	-0.97	33,36,38,39	0
1	PSU	0	2621	20/21	0.10	-1.14	37,40,50,51	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
37	SR	0	9601	1/1	0.68	1125.00	200,200,200,200	0
37	SR	0	9501	1/1	0.34	461.00	200,200,200,200	0
35	NA	0	9152	1/1	0.66	191.08	78,78,78,78	0
35	NA	0	9179	1/1	1.28	129.10	100,100,100,100	0
37	SR	0	9547	1/1	1.19	105.44	200,200,200,200	0
35	NA	B	9161	1/1	0.76	89.60	62,62,62,62	0
35	NA	0	9118	1/1	0.20	57.27	60,60,60,60	0
33	MG	0	8092	1/1	0.65	55.50	81,81,81,81	0
33	MG	0	8047	1/1	0.47	55.20	91,91,91,91	0
37	SR	0	9500	1/1	1.46	54.79	200,200,200,200	0
35	NA	0	9125	1/1	0.68	52.04	115,115,115,115	0
33	MG	0	8022	1/1	0.77	41.43	74,74,74,74	0
35	NA	0	9158	1/1	0.31	40.91	63,63,63,63	0
35	NA	0	9184	1/1	0.70	38.54	102,102,102,102	0
33	MG	0	8084	1/1	0.76	30.59	74,74,74,74	0
35	NA	0	9149	1/1	0.21	28.30	42,42,42,42	0
33	MG	0	8082	1/1	0.24	26.98	107,107,107,107	0
33	MG	0	8108	1/1	0.26	26.50	74,74,74,74	0
33	MG	0	8094	1/1	0.21	24.98	67,67,67,67	0
35	NA	0	9120	1/1	0.25	21.59	64,64,64,64	0
36	CL	0	9322	1/1	0.23	21.34	53,53,53,53	0
35	NA	0	9173	1/1	0.34	20.97	70,70,70,70	0
33	MG	0	8085	1/1	0.29	20.96	91,91,91,91	0
33	MG	0	8013	1/1	0.35	20.27	22,22,22,22	0
37	SR	0	9626	1/1	0.28	19.77	128,128,128,128	0
33	MG	0	8025	1/1	0.34	18.98	25,25,25,25	0
35	NA	0	9170	1/1	0.38	18.62	94,94,94,94	0
33	MG	0	8024	1/1	1.64	18.49	77,77,77,77	0
35	NA	0	9164	1/1	0.28	18.40	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8040	1/1	0.37	17.79	100,100,100,100	0
37	SR	B	9521	1/1	0.50	17.54	199,199,199,199	0
35	NA	R	9186	1/1	0.43	17.29	69,69,69,69	0
33	MG	0	8072	1/1	0.27	17.04	96,96,96,96	0
35	NA	0	9129	1/1	0.20	16.70	85,85,85,85	0
33	MG	0	8107	1/1	0.20	15.30	67,67,67,67	0
33	MG	0	8059	1/1	0.28	15.10	78,78,78,78	0
33	MG	0	8052	1/1	0.34	14.50	68,68,68,68	0
35	NA	0	9182	1/1	0.26	13.60	78,78,78,78	0
35	NA	0	9111	1/1	0.12	13.56	57,57,57,57	0
35	NA	0	9172	1/1	0.40	13.49	70,70,70,70	0
33	MG	0	8012	1/1	0.26	13.32	41,41,41,41	0
37	SR	0	9539	1/1	0.21	12.85	162,162,162,162	0
35	NA	0	9175	1/1	0.26	11.41	52,52,52,52	0
35	NA	0	9171	1/1	0.22	11.33	61,61,61,61	0
35	NA	0	9106	1/1	0.21	10.78	37,37,37,37	0
33	MG	0	8118	1/1	0.18	10.28	76,76,76,76	0
37	SR	0	9482	1/1	0.20	9.99	102,102,102,102	0
33	MG	0	8038	1/1	0.22	9.87	20,20,20,20	0
35	NA	0	9185	1/1	0.28	9.63	46,46,46,46	0
35	NA	0	9107	1/1	0.25	9.60	61,61,61,61	0
33	MG	0	8001	1/1	0.25	9.17	20,20,20,20	0
33	MG	0	8008	1/1	0.19	9.16	17,17,17,17	0
35	NA	0	9102	1/1	0.21	8.93	57,57,57,57	0
33	MG	0	8089	1/1	0.12	8.50	54,54,54,54	0
37	SR	0	9406	1/1	0.16	8.27	38,38,38,38	0
33	MG	0	8060	1/1	0.30	8.25	71,71,71,71	0
35	NA	0	9169	1/1	0.45	8.14	104,104,104,104	0
33	MG	0	8114	1/1	0.19	7.98	63,63,63,63	0
33	MG	0	8103	1/1	0.16	7.17	62,62,62,62	0
34	K	0	9001	1/1	0.36	7.16	116,116,116,116	0
33	MG	0	8041	1/1	0.17	6.67	50,50,50,50	0
33	MG	K	8069	1/1	0.20	6.35	29,29,29,29	0
35	NA	0	9122	1/1	0.34	6.31	96,96,96,96	0
33	MG	0	8090	1/1	0.51	6.19	80,80,80,80	0
33	MG	0	8065	1/1	0.41	6.13	93,93,93,93	0
35	NA	0	9157	1/1	0.13	6.08	47,47,47,47	0
33	MG	0	8029	1/1	0.21	5.97	33,33,33,33	0
33	MG	0	8061	1/1	0.13	5.74	95,95,95,95	0
35	NA	9	9183	1/1	0.19	5.72	66,66,66,66	0
33	MG	0	8051	1/1	0.17	5.44	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8021	1/1	0.17	5.24	55,55,55,55	0
37	SR	0	9474	1/1	0.11	5.18	112,112,112,112	0
35	NA	0	9177	1/1	0.20	5.06	63,63,63,63	0
37	SR	0	9432	1/1	0.11	5.03	62,62,62,62	0
33	MG	0	8026	1/1	0.15	4.95	27,27,27,27	0
33	MG	0	8045	1/1	0.30	4.81	84,84,84,84	0
35	NA	0	9165	1/1	0.30	4.57	47,47,47,47	0
35	NA	0	9178	1/1	0.19	4.39	51,51,51,51	0
33	MG	0	8014	1/1	0.34	4.26	73,73,73,73	0
35	NA	0	9101	1/1	0.14	4.22	47,47,47,47	0
35	NA	0	9132	1/1	0.19	4.12	51,51,51,51	0
33	MG	9	8095	1/1	0.19	4.09	46,46,46,46	0
33	MG	0	8017	1/1	0.13	3.82	28,28,28,28	0
37	SR	0	9405	1/1	0.14	3.75	60,60,60,60	0
33	MG	0	8027	1/1	0.18	3.75	39,39,39,39	0
35	NA	0	9116	1/1	0.18	3.72	58,58,58,58	0
33	MG	0	8058	1/1	0.25	3.48	45,45,45,45	0
35	NA	0	9141	1/1	0.14	3.35	62,62,62,62	0
36	CL	0	9316	1/1	0.21	3.33	69,69,69,69	0
37	SR	0	9452	1/1	0.17	3.13	114,114,114,114	0
33	MG	A	8066	1/1	0.17	3.02	53,53,53,53	0
35	NA	0	9163	1/1	0.16	2.60	66,66,66,66	0
35	NA	0	9156	1/1	0.12	2.57	53,53,53,53	0
35	NA	0	9154	1/1	0.16	2.40	59,59,59,59	0
33	MG	0	8101	1/1	0.14	2.34	59,59,59,59	0
33	MG	0	8056	1/1	0.20	2.26	46,46,46,46	0
37	SR	0	9408	1/1	0.13	2.15	39,39,39,39	0
35	NA	0	9155	1/1	0.27	2.05	55,55,55,55	0
33	MG	B	8055	1/1	0.20	2.03	108,108,108,108	0
33	MG	0	8002	1/1	0.15	2.02	28,28,28,28	0
33	MG	0	8057	1/1	0.20	2.01	85,85,85,85	0
33	MG	0	8080	1/1	0.16	1.94	47,47,47,47	0
37	SR	0	9529	1/1	0.15	1.82	138,138,138,138	0
37	SR	0	9515	1/1	0.15	1.57	87,87,87,87	0
33	MG	0	8104	1/1	0.23	1.38	76,76,76,76	0
37	SR	S	9470	1/1	0.12	1.38	100,100,100,100	0
35	NA	0	9128	1/1	0.12	1.20	45,45,45,45	0
35	NA	0	9174	1/1	0.10	1.18	65,65,65,65	0
36	CL	A	9309	1/1	0.20	1.08	68,68,68,68	0
35	NA	0	9117	1/1	0.16	1.02	39,39,39,39	0
33	MG	0	8097	1/1	0.13	0.97	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8074	1/1	0.19	0.93	23,23,23,23	0
37	SR	0	9407	1/1	0.11	0.90	43,43,43,43	0
33	MG	0	8020	1/1	0.15	0.87	37,37,37,37	0
33	MG	0	8070	1/1	0.14	0.86	26,26,26,26	0
33	MG	0	8015	1/1	0.12	0.83	34,34,34,34	0
35	NA	0	9140	1/1	0.18	0.77	60,60,60,60	0
33	MG	0	8050	1/1	0.14	0.75	93,93,93,93	0
33	MG	0	8028	1/1	0.12	0.73	37,37,37,37	0
35	NA	C	9104	1/1	0.17	0.69	34,34,34,34	0
37	SR	H	9486	1/1	0.16	0.62	109,109,109,109	0
37	SR	A	9437	1/1	0.13	0.58	67,67,67,67	0
33	MG	0	8076	1/1	0.11	0.54	61,61,61,61	0
33	MG	0	8003	1/1	0.15	0.49	32,32,32,32	0
33	MG	0	8091	1/1	0.11	0.46	45,45,45,45	0
35	NA	M	9147	1/1	0.16	0.33	43,43,43,43	0
35	NA	0	9166	1/1	0.10	0.30	67,67,67,67	0
35	NA	0	9113	1/1	0.11	0.25	65,65,65,65	0
36	CL	B	9319	1/1	0.11	0.21	52,52,52,52	0
35	NA	0	9139	1/1	0.15	0.17	52,52,52,52	0
35	NA	0	9136	1/1	0.10	-0.13	34,34,34,34	0
33	MG	0	8079	1/1	0.10	-0.16	34,34,34,34	0
35	NA	0	9162	1/1	0.11	-0.17	58,58,58,58	0
37	SR	F	9595	1/1	0.14	-0.22	105,105,105,105	0
33	MG	0	8004	1/1	0.09	-0.23	30,30,30,30	0
33	MG	0	8102	1/1	0.10	-0.27	56,56,56,56	0
37	SR	0	9537	1/1	0.12	-0.28	154,154,154,154	0
33	MG	0	8054	1/1	0.11	-0.37	58,58,58,58	0
34	K	0	9002	1/1	0.12	-0.37	89,89,89,89	0
35	NA	0	9126	1/1	0.10	-0.38	59,59,59,59	0
35	NA	0	9110	1/1	0.11	-0.43	46,46,46,46	0
36	CL	J	9301	1/1	0.10	-0.45	53,53,53,53	0
35	NA	S	9112	1/1	0.11	-0.45	59,59,59,59	0
33	MG	0	8093	1/1	0.11	-0.52	42,42,42,42	0
33	MG	0	8096	1/1	0.12	-0.58	46,46,46,46	0
37	SR	0	9477	1/1	0.10	-0.61	84,84,84,84	0
33	MG	0	8046	1/1	0.09	-0.62	40,40,40,40	0
33	MG	0	8099	1/1	0.11	-0.70	59,59,59,59	0
37	SR	0	9509	1/1	0.11	-0.70	81,81,81,81	0
35	NA	0	9181	1/1	0.09	-0.70	50,50,50,50	0
37	SR	R	9418	1/1	0.11	-0.74	54,54,54,54	0
37	SR	0	9414	1/1	0.10	-0.76	52,52,52,52	0
33	MG	0	8063	1/1	0.11	-0.76	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	9417	1/1	0.09	-0.77	59,59,59,59	0
35	NA	R	9137	1/1	0.10	-0.78	36,36,36,36	0
37	SR	0	9433	1/1	0.09	-0.81	76,76,76,76	0
37	SR	0	9590	1/1	0.12	-0.85	178,178,178,178	0
37	SR	1	9419	1/1	0.10	-0.85	40,40,40,40	0
38	CD	U	9201	1/1	0.10	-0.86	48,48,48,48	0
36	CL	M	9318	1/1	0.15	-0.87	41,41,41,41	0
35	NA	J	9146	1/1	0.10	-0.90	55,55,55,55	0
33	MG	0	8088	1/1	0.08	-0.90	45,45,45,45	0
37	SR	0	9430	1/1	0.10	-0.93	44,44,44,44	0
37	SR	A	9497	1/1	0.07	-1.00	91,91,91,91	0
35	NA	0	9114	1/1	0.09	-1.07	46,46,46,46	0
37	SR	0	9440	1/1	0.03	-1.08	61,61,61,61	0
35	NA	0	9168	1/1	0.09	-1.08	57,57,57,57	0
36	CL	R	9306	1/1	0.10	-1.10	44,44,44,44	0
33	MG	0	8042	1/1	0.09	-1.11	60,60,60,60	0
35	NA	0	9124	1/1	0.06	-1.12	47,47,47,47	0
38	CD	Z	9203	1/1	0.07	-1.12	78,78,78,78	0
37	SR	0	9413	1/1	0.09	-1.13	44,44,44,44	0
35	NA	0	9134	1/1	0.07	-1.18	51,51,51,51	0
33	MG	T	8073	1/1	0.12	-1.20	46,46,46,46	0
37	SR	0	9420	1/1	0.10	-1.22	56,56,56,56	0
37	SR	L	9409	1/1	0.09	-1.26	40,40,40,40	0
33	MG	0	8030	1/1	0.09	-1.27	39,39,39,39	0
37	SR	0	9450	1/1	0.07	-1.31	62,62,62,62	0
37	SR	0	9475	1/1	0.08	-1.32	77,77,77,77	0
37	SR	0	9421	1/1	0.07	-1.33	64,64,64,64	0
36	CL	J	9321	1/1	0.04	-1.38	53,53,53,53	0
35	NA	0	9127	1/1	0.10	-1.42	57,57,57,57	0
35	NA	0	9105	1/1	0.09	-1.49	43,43,43,43	0
35	NA	D	9151	1/1	0.15	-1.50	63,63,63,63	0
36	CL	J	9302	1/1	0.05	-1.50	48,48,48,48	0
37	SR	0	9545	1/1	0.03	-1.51	79,79,79,79	0
37	SR	0	9415	1/1	0.09	-1.51	50,50,50,50	0
37	SR	0	9568	1/1	0.08	-1.52	75,75,75,75	0
37	SR	0	9504	1/1	0.08	-1.57	105,105,105,105	0
35	NA	0	9108	1/1	0.08	-1.60	35,35,35,35	0
37	SR	0	9451	1/1	0.08	-1.61	62,62,62,62	0
37	SR	0	9447	1/1	0.07	-1.61	67,67,67,67	0
38	CD	O	9205	1/1	0.07	-1.62	75,75,75,75	0
37	SR	0	9534	1/1	0.09	-1.65	100,100,100,100	0
37	SR	0	9410	1/1	0.11	-1.68	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	R	9138	1/1	0.07	-1.69	56,56,56,56	0
37	SR	0	9490	1/1	0.08	-1.69	109,109,109,109	0
35	NA	0	9159	1/1	0.09	-1.73	46,46,46,46	0
37	SR	0	9462	1/1	0.09	-1.75	64,64,64,64	0
37	SR	0	9488	1/1	0.07	-1.75	76,76,76,76	0
37	SR	0	9424	1/1	0.11	-1.76	45,45,45,45	0
38	CD	3	9204	1/1	0.04	-1.79	60,60,60,60	0
36	CL	0	9315	1/1	0.08	-1.79	58,58,58,58	0
37	SR	0	9416	1/1	0.09	-1.82	43,43,43,43	0
37	SR	0	9517	1/1	0.06	-1.86	91,91,91,91	0
36	CL	0	9311	1/1	0.06	-1.91	57,57,57,57	0
36	CL	O	9308	1/1	0.06	-1.94	60,60,60,60	0
33	MG	0	8068	1/1	0.10	-1.96	46,46,46,46	0
35	NA	0	9160	1/1	0.08	-1.97	39,39,39,39	0
37	SR	0	9530	1/1	0.10	-1.99	84,84,84,84	0
35	NA	Q	9148	1/1	0.07	-1.99	44,44,44,44	0
37	SR	0	9422	1/1	0.08	-2.11	54,54,54,54	0
37	SR	0	9467	1/1	0.07	-2.17	67,67,67,67	0
37	SR	0	9431	1/1	0.10	-2.25	55,55,55,55	0
37	SR	0	9446	1/1	0.06	-2.27	83,83,83,83	0
36	CL	L	9310	1/1	0.08	-2.33	54,54,54,54	0
33	MG	0	8067	1/1	0.09	-2.41	42,42,42,42	0
35	NA	0	9115	1/1	0.07	-2.42	39,39,39,39	0
36	CL	0	9314	1/1	0.08	-2.46	45,45,45,45	0
37	SR	0	9505	1/1	0.10	-2.49	85,85,85,85	0
33	MG	0	8019	1/1	0.07	-2.50	58,58,58,58	0
33	MG	0	8036	1/1	0.08	-2.50	60,60,60,60	0
33	MG	Y	8109	1/1	0.08	-2.51	41,41,41,41	0
37	SR	A	9436	1/1	0.04	-2.58	61,61,61,61	0
37	SR	0	9423	1/1	0.07	-2.60	54,54,54,54	0
33	MG	0	8116	1/1	0.06	-2.62	62,62,62,62	0
37	SR	0	9468	1/1	0.04	-2.64	113,113,113,113	0
33	MG	0	8032	1/1	0.07	-2.65	43,43,43,43	0
35	NA	0	9130	1/1	0.07	-2.66	49,49,49,49	0
37	SR	0	9443	1/1	0.08	-2.68	57,57,57,57	0
37	SR	0	9461	1/1	0.04	-2.74	76,76,76,76	0
37	SR	0	9427	1/1	0.09	-2.76	52,52,52,52	0
37	SR	0	9483	1/1	0.07	-2.77	68,68,68,68	0
37	SR	0	9449	1/1	0.07	-2.78	59,59,59,59	0
37	SR	0	9428	1/1	0.03	-2.79	49,49,49,49	0
37	SR	3	9439	1/1	0.04	-2.81	63,63,63,63	0
37	SR	0	9425	1/1	0.09	-2.81	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	9303	1/1	0.09	-2.88	46,46,46,46	0
36	CL	K	9312	1/1	0.05	-2.90	46,46,46,46	0
37	SR	1	9460	1/1	0.07	-2.94	52,52,52,52	0
37	SR	0	9448	1/1	0.04	-2.94	60,60,60,60	0
35	NA	0	9143	1/1	0.07	-3.00	43,43,43,43	0
37	SR	0	9455	1/1	0.06	-3.07	67,67,67,67	0
38	CD	1	9202	1/1	0.04	-3.07	51,51,51,51	0
33	MG	0	8115	1/1	0.08	-3.19	56,56,56,56	0
37	SR	0	9444	1/1	0.03	-3.20	50,50,50,50	0
37	SR	0	9581	1/1	0.06	-3.27	121,121,121,121	0
36	CL	0	9313	1/1	0.08	-3.47	51,51,51,51	0
35	NA	0	9123	1/1	0.08	-3.51	41,41,41,41	0
37	SR	0	9532	1/1	0.07	-3.56	103,103,103,103	0
37	SR	0	9442	1/1	0.07	-3.58	59,59,59,59	0
37	SR	0	9473	1/1	0.03	-3.65	69,69,69,69	0
36	CL	3	9304	1/1	0.06	-3.71	55,55,55,55	0
36	CL	0	9305	1/1	0.06	-3.72	54,54,54,54	0
33	MG	0	8039	1/1	0.06	-3.75	65,65,65,65	0
35	NA	0	9131	1/1	0.06	-3.78	48,48,48,48	0
37	SR	0	9566	1/1	0.04	-3.82	77,77,77,77	0
33	MG	0	8037	1/1	0.08	-3.84	39,39,39,39	0
37	SR	0	9434	1/1	0.08	-3.92	55,55,55,55	0
36	CL	N	9307	1/1	0.11	-4.05	52,52,52,52	0
37	SR	0	9560	1/1	0.06	-4.12	97,97,97,97	0
37	SR	0	9508	1/1	0.05	-4.17	80,80,80,80	0
33	MG	0	8112	1/1	0.05	-4.19	43,43,43,43	0
33	MG	0	8075	1/1	0.07	-4.21	36,36,36,36	0
33	MG	0	8044	1/1	0.06	-4.27	39,39,39,39	0
37	SR	0	9411	1/1	0.11	-4.30	40,40,40,40	0
33	MG	0	8098	1/1	0.06	-4.36	39,39,39,39	0
33	MG	0	8005	1/1	0.06	-4.36	35,35,35,35	0
37	SR	0	9426	1/1	0.06	-4.40	67,67,67,67	0
37	SR	0	9456	1/1	0.06	-4.66	69,69,69,69	0
37	SR	0	9465	1/1	0.06	-4.72	100,100,100,100	0
37	SR	0	9435	1/1	0.07	-4.77	65,65,65,65	0
37	SR	0	9457	1/1	0.06	-4.98	47,47,47,47	0
37	SR	0	9469	1/1	0.04	-5.04	79,79,79,79	0
37	SR	0	9506	1/1	0.03	-5.18	66,66,66,66	0
33	MG	0	8117	1/1	0.07	-5.22	43,43,43,43	0
37	SR	0	9498	1/1	0.04	-5.28	59,59,59,59	0
36	CL	0	9317	1/1	0.06	-5.41	50,50,50,50	0
33	MG	0	8009	1/1	0.09	-5.43	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8110	1/1	0.05	-5.48	36,36,36,36	0
37	SR	0	9466	1/1	0.03	-5.49	84,84,84,84	0
33	MG	0	8043	1/1	0.07	-5.51	49,49,49,49	0
33	MG	0	8031	1/1	0.06	-5.51	50,50,50,50	0
37	SR	0	9489	1/1	0.04	-5.66	85,85,85,85	0
35	NA	0	9135	1/1	0.07	-5.68	50,50,50,50	0
35	NA	0	9167	1/1	0.07	-5.69	56,56,56,56	0
37	SR	0	9429	1/1	0.07	-5.72	60,60,60,60	0
37	SR	0	9480	1/1	0.04	-5.78	87,87,87,87	0
36	CL	Y	9320	1/1	0.04	-6.00	43,43,43,43	0
37	SR	0	9478	1/1	0.06	-6.03	70,70,70,70	0
37	SR	9	9588	1/1	0.08	-6.24	114,114,114,114	0
37	SR	0	9441	1/1	0.05	-6.36	60,60,60,60	0
35	NA	0	9150	1/1	0.09	-6.64	38,38,38,38	0
37	SR	0	9438	1/1	0.04	-6.67	63,63,63,63	0
33	MG	0	8113	1/1	0.08	-6.85	50,50,50,50	0
37	SR	0	9459	1/1	0.07	-8.09	101,101,101,101	0
37	SR	0	9629	1/1	0.05	-8.17	65,65,65,65	0
33	MG	0	8106	1/1	0.03	-8.19	43,43,43,43	0
37	SR	B	9458	1/1	0.04	-8.23	68,68,68,68	0
37	SR	0	9445	1/1	0.05	-9.00	56,56,56,56	0
37	SR	0	9412	1/1	0.10	-9.84	42,42,42,42	0
37	SR	0	9454	1/1	0.03	-10.03	74,74,74,74	0
37	SR	9	9503	1/1	0.03	-11.45	114,114,114,114	0
37	SR	9	9481	1/1	0.04	-11.62	80,80,80,80	0
37	SR	0	9453	1/1	0.04	-11.65	69,69,69,69	0
37	SR	0	9585	1/1	0.05	-12.01	83,83,83,83	0
37	SR	0	9570	1/1	0.03	-13.68	98,98,98,98	0
37	SR	0	9464	1/1	0.03	-13.82	74,74,74,74	0
37	SR	0	9495	1/1	0.07	-14.37	88,88,88,88	0
33	MG	0	8083	1/1	0.07	-14.71	54,54,54,54	0
37	SR	0	9522	1/1	0.04	-18.57	104,104,104,104	0
37	SR	0	9484	1/1	0.11	-	147,147,147,147	0

6.5 Other polymers ⓘ

There are no such residues in this entry.