



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:39 AM GMT

PDB ID : 2QA4
Title : A more complete structure of the the L7/L12 stalk of the Haloarcula marismortui 50S large ribosomal subunit
Authors : Steitz, T.A.; Kavran, J.M.
Deposited on : 2007-06-14
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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

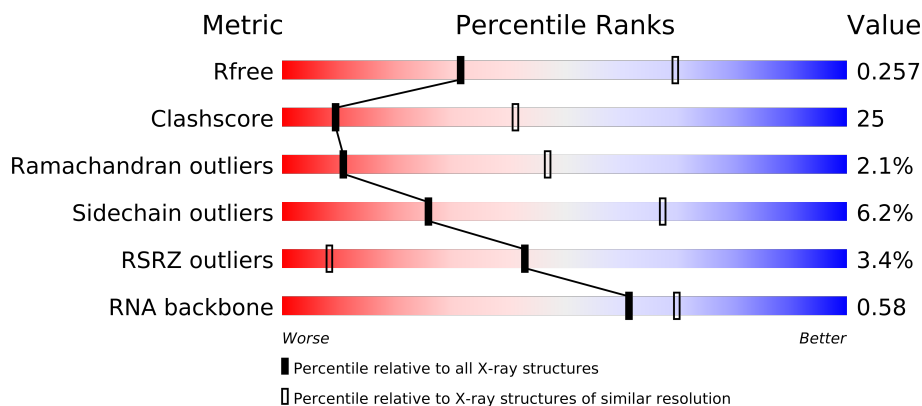
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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	A	240	
4	B	338	
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	I	162	

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Mol	Chain	Length	Quality of chain
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	67	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	92	
29	1	57	
30	2	50	
31	3	92	

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	1	-	X
32	MG	0	2924	-	X
32	MG	0	2927	-	X
32	MG	0	2933	-	X
32	MG	0	2934	-	X
32	MG	0	2935	-	X
32	MG	0	2937	-	X
32	MG	0	2938	-	X
32	MG	0	2940	-	X
32	MG	0	2942	-	X
32	MG	0	2943	-	X
32	MG	0	2945	-	X
32	MG	0	2946	-	X
32	MG	0	2947	-	X
32	MG	0	2948	-	X
32	MG	0	2949	-	X
32	MG	0	2951	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	2952	-	X
32	MG	0	2955	-	X
32	MG	0	2958	-	X
32	MG	0	2959	-	X
32	MG	0	2960	-	X
32	MG	0	2961	-	X
32	MG	0	2962	-	X
32	MG	0	2964	-	X
32	MG	0	2965	-	X
32	MG	0	2969	-	X
32	MG	0	2970	-	X
32	MG	0	2971	-	X
32	MG	0	2973	-	X
32	MG	0	2974	-	X
32	MG	0	2977	-	X
32	MG	0	2979	-	X
32	MG	0	2980	-	X
32	MG	0	2981	-	X
32	MG	0	2982	-	X
32	MG	0	2983	-	X
32	MG	0	2984	-	X
32	MG	0	2989	-	X
32	MG	0	2992	-	X
32	MG	0	2993	-	X
32	MG	0	2994	-	X
32	MG	0	2996	-	X
32	MG	0	2997	-	X
32	MG	0	2998	-	X
32	MG	0	2999	-	X
32	MG	0	3000	-	X
32	MG	0	3004	-	X
32	MG	0	3006	-	X
32	MG	0	3007	-	X
32	MG	0	3008	-	X
32	MG	0	3009	-	X
32	MG	0	3010	-	X
32	MG	0	3011	-	X
32	MG	0	3013	-	X
32	MG	0	3014	-	X
32	MG	0	3015	-	X
32	MG	0	3016	-	X
32	MG	0	3018	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	3019	-	X
32	MG	0	3021	-	X
32	MG	0	3022	-	X
32	MG	0	3023	-	X
32	MG	0	3024	-	X
32	MG	0	3025	-	X
32	MG	0	3026	-	X
32	MG	0	3027	-	X
32	MG	0	3029	-	X
32	MG	0	3030	-	X
32	MG	3	93	-	X
32	MG	A	240	-	X
32	MG	A	241	-	X
32	MG	B	338	-	X
32	MG	K	133	-	X
32	MG	Y	241	-	X
33	K	0	3031	-	X
34	NA	0	3032	-	X
34	NA	0	3033	-	X
34	NA	0	3034	-	X
34	NA	0	3036	-	X
34	NA	0	3038	-	X
34	NA	0	3039	-	X
34	NA	0	3041	-	X
34	NA	0	3043	-	X
34	NA	0	3044	-	X
34	NA	0	3046	-	X
34	NA	0	3048	-	X
34	NA	0	3049	-	X
34	NA	0	3050	-	X
34	NA	0	3051	-	X
34	NA	0	3052	-	X
34	NA	0	3054	-	X
34	NA	0	3056	-	X
34	NA	0	3057	-	X
34	NA	0	3060	-	X
34	NA	0	3063	-	X
34	NA	0	3064	-	X
34	NA	0	3067	-	X
34	NA	0	3068	-	X
34	NA	0	3069	-	X
34	NA	0	3072	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	3073	-	X
34	NA	0	3074	-	X
34	NA	0	3075	-	X
34	NA	0	3077	-	X
34	NA	0	3078	-	X
34	NA	0	3080	-	X
34	NA	0	3082	-	X
34	NA	0	3083	-	X
34	NA	0	3084	-	X
34	NA	0	3085	-	X
34	NA	0	3086	-	X
34	NA	0	3088	-	X
34	NA	0	3091	-	X
34	NA	0	3092	-	X
34	NA	0	3093	-	X
34	NA	0	3094	-	X
34	NA	0	3095	-	X
34	NA	0	3096	-	X
34	NA	0	3098	-	X
34	NA	0	3099	-	X
34	NA	0	3100	-	X
34	NA	0	3101	-	X
34	NA	0	3102	-	X
34	NA	0	3103	-	X
34	NA	0	3104	-	X
34	NA	9	125	-	X
34	NA	9	126	-	X
34	NA	S	85	-	X
35	CD	3	94	-	X
36	CL	0	3105	-	X
36	CL	0	3106	-	X
36	CL	0	3109	-	X
36	CL	0	3110	-	X
36	CL	0	3112	-	X
36	CL	A	243	-	X
36	CL	B	339	-	X
36	CL	J	147	-	X
36	CL	M	198	-	X
36	CL	O	117	-	X

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 92248 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	2753	Total	C	N	O	P	0	0	0
			58979	26332	10869	19036	2742			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	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 protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	125	Total	C	N	O	S	0	0	0
			959	592	162	203	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

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

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	LYS	CONFLICT	UNP P60617
H	166	SER	VAL	CONFLICT	UNP P60617
H	167	PRO	GLU	CONFLICT	UNP P60617
H	168	ALA	ARG	CONFLICT	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	170	ASN	ILE	CONFLICT	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	118	Total	C	N	O	S	0	0	0
			876	548	135	192	1			

- 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	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
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	GLY	CONFLICT	UNP P60618

- 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		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	UNP P60619

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	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	0	0
			1	1		
33	M	1	Total	K	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	73	Total	Na	0	0
			73	73		
34	J	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	A	1	Total	Na	0	0
			1	1		
34	R	2	Total	Na	0	0
			2	2		
34	9	3	Total	Na	0	0
			3	3		
34	L	1	Total	Na	0	0
			1	1		
34	S	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	O	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total 1	Cd 1	0	0
35	1	1	Total 1	Cd 1	0	0
35	3	1	Total 1	Cd 1	0	0
35	U	1	Total 1	Cd 1	0	0

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

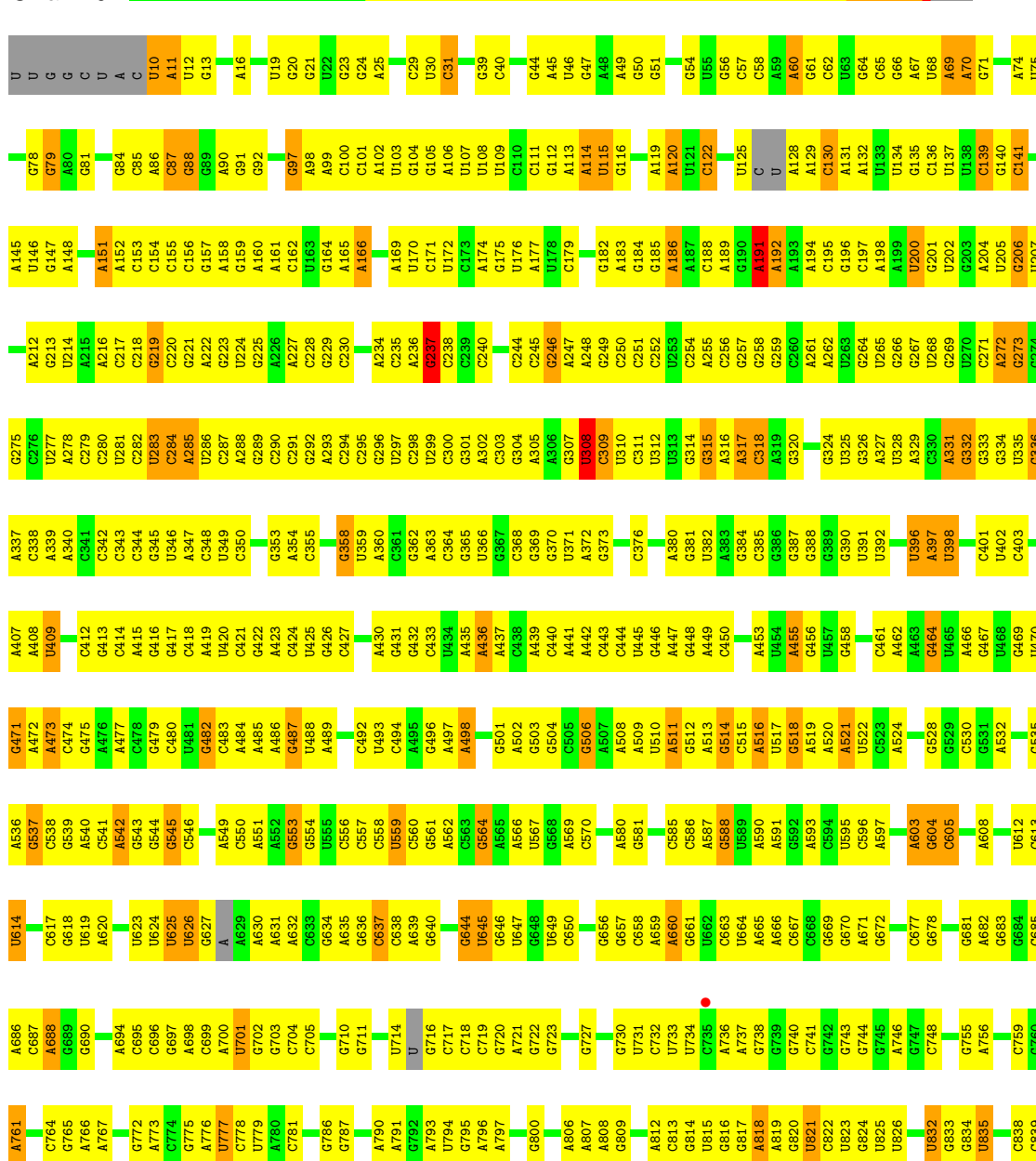
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	8	Total 8	Cl 8	0	0
36	J	3	Total 3	Cl 3	0	0
36	Q	1	Total 1	Cl 1	0	0
36	K	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

3 Residue-property plots

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

• Molecule 1: 23S RIBOSOMAL RNA

Chain 0:

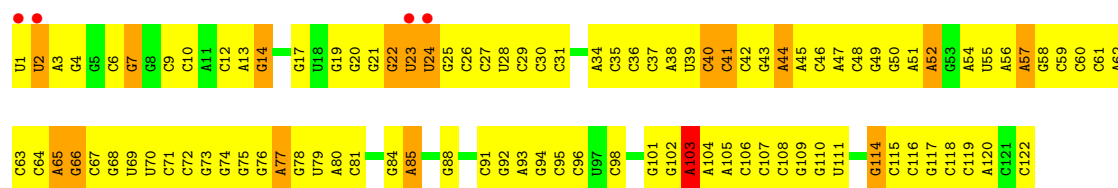


C1816	C1817	C1818	G1819	G1820	G1821	G1822	G1823	G1824	G1825	G1826	G1827	G1828	G1829	G1830	G1831	G1832	G1833	G1834	G1835	G1836	G1837	G1838	G1839	G1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878																																																																																																																																																																																																																																																																																														
U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878																																																																																																																																																																																																																																																																																															
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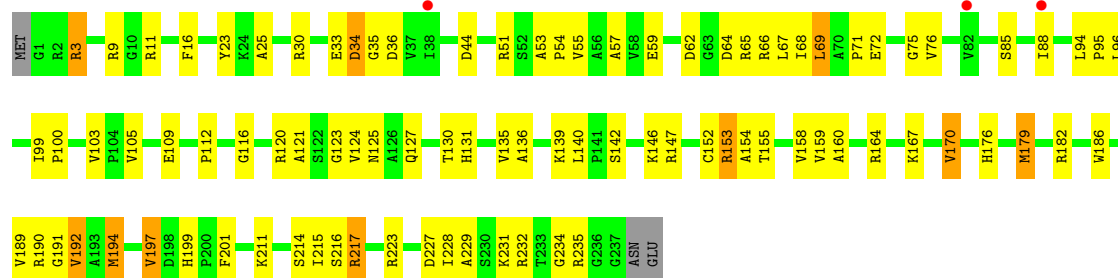
- Molecule 2: 5S RIBOSOMAL RNA

Chain 9:



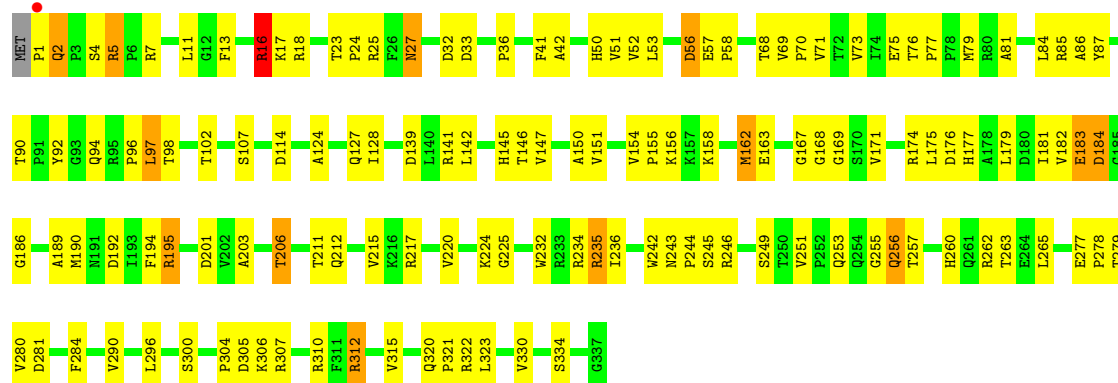
- Molecule 3: 50S ribosomal protein L2P

Chain A:



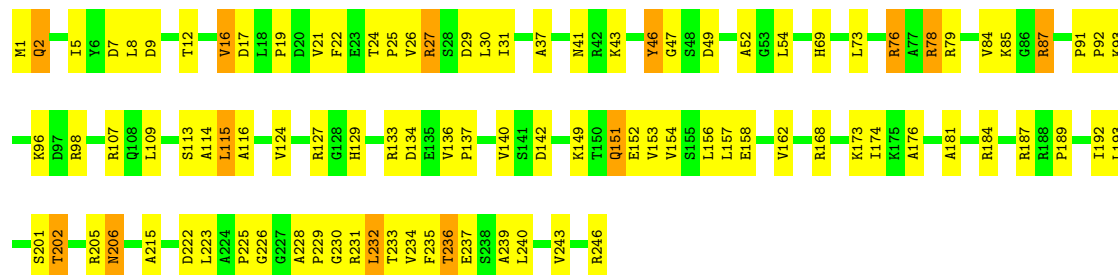
- Molecule 4: 50S ribosomal protein L3P

Chain B:



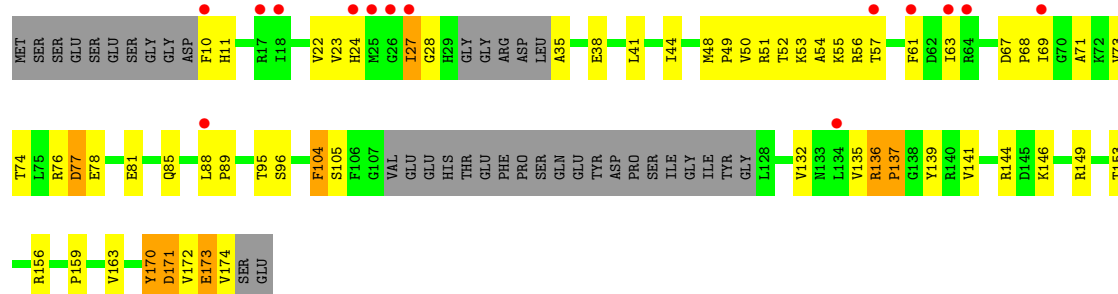
- Molecule 5: 50S ribosomal protein L4P

Chain C:



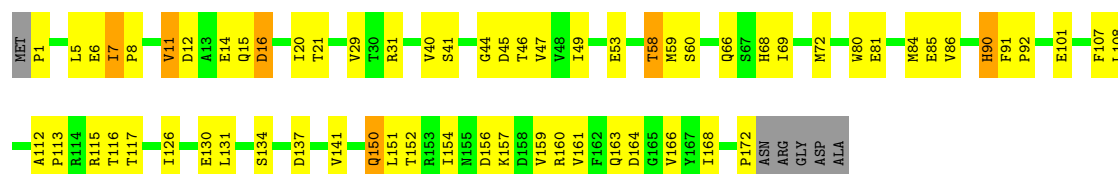
- Molecule 6: 50S ribosomal protein L5P

Chain D: 



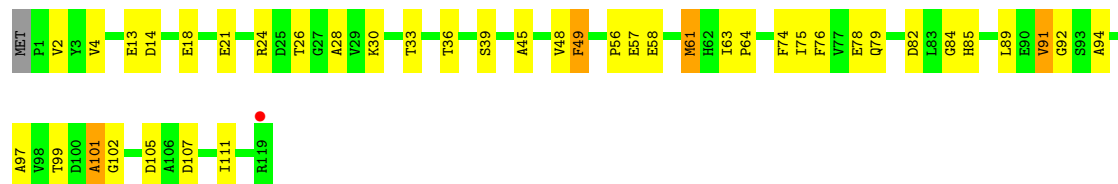
• Molecule 7: 50S ribosomal protein L6P

Chain E: 



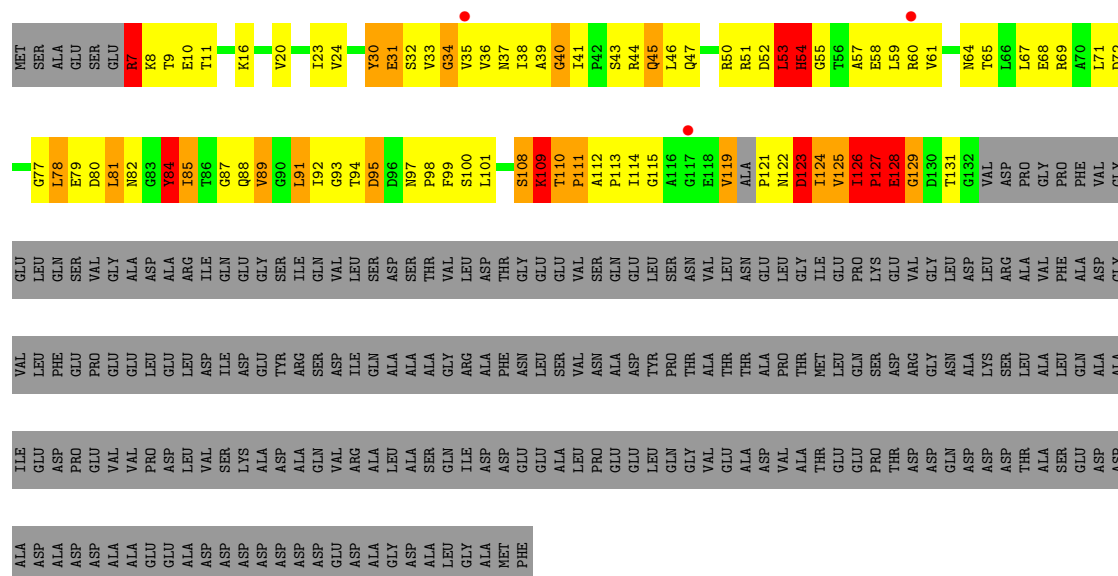
• Molecule 8: 50S ribosomal protein L7Ae

Chain F: 



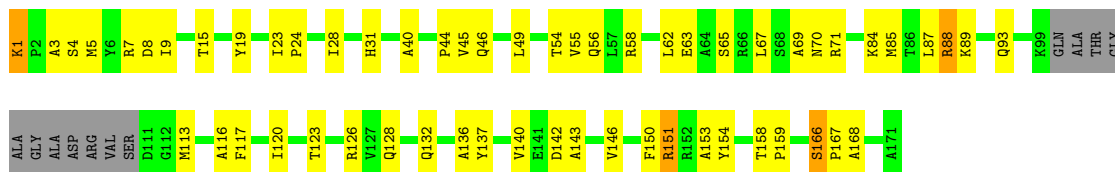
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMO

Chain G: 



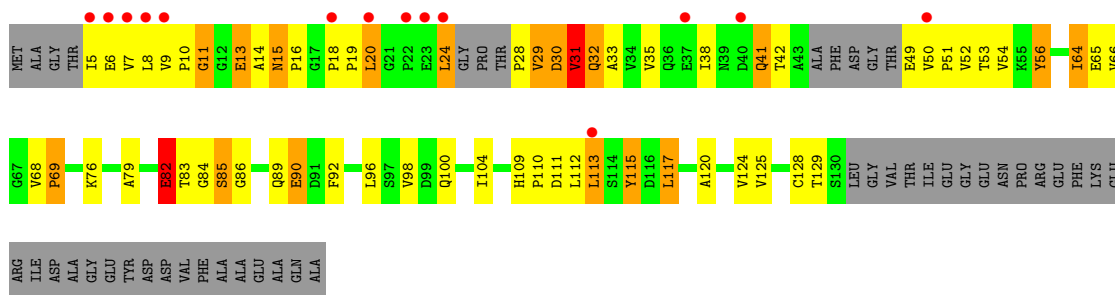
- Molecule 10: 50S ribosomal protein L10e

Chain H:



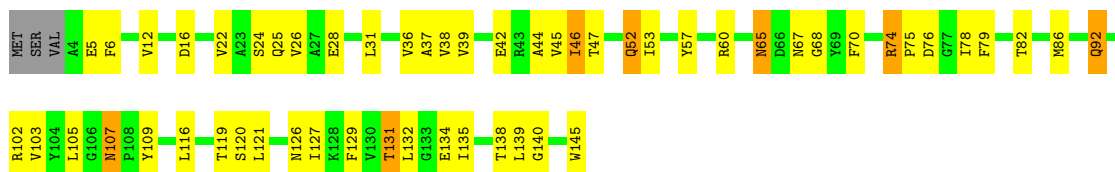
- Molecule 11: 50S ribosomal protein L11P

Chain I:



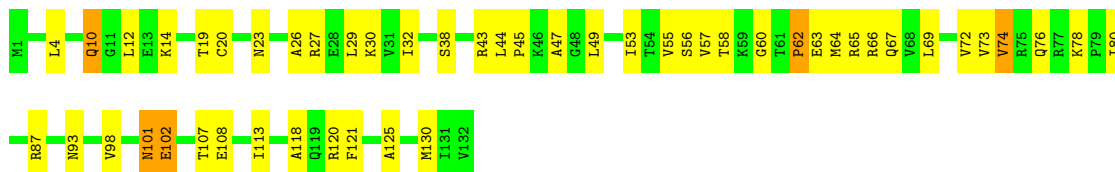
- Molecule 12: 50S ribosomal protein L13P

Chain J:



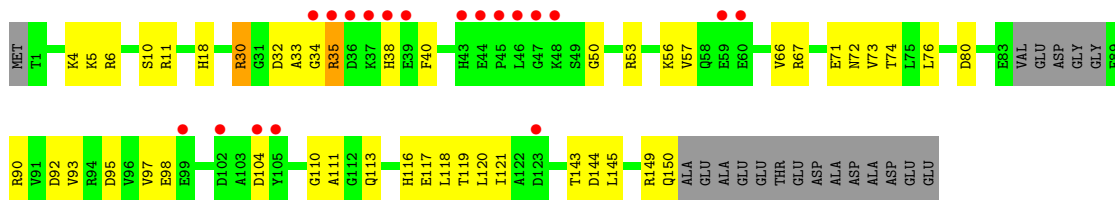
- Molecule 13: 50S ribosomal protein L14P

Chain K:



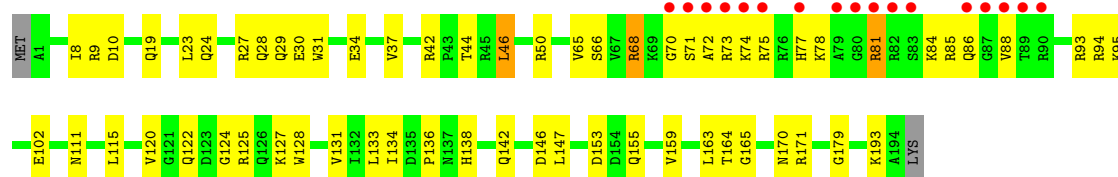
- Molecule 14: 50S ribosomal protein L15P

Chain L:



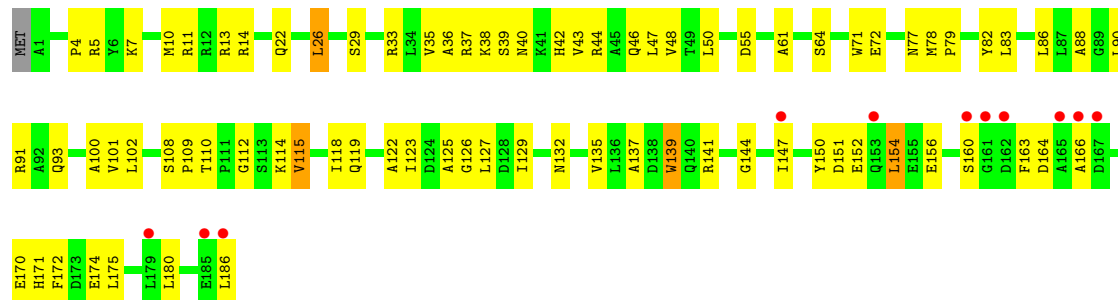
- Molecule 15: 50S ribosomal protein L15e

Chain M: 



- Molecule 16: 50S ribosomal protein L18P

Chain N: 



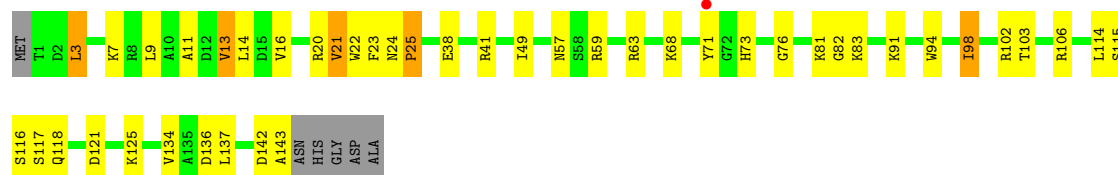
- Molecule 17: 50S ribosomal protein L18e

Chain O: 



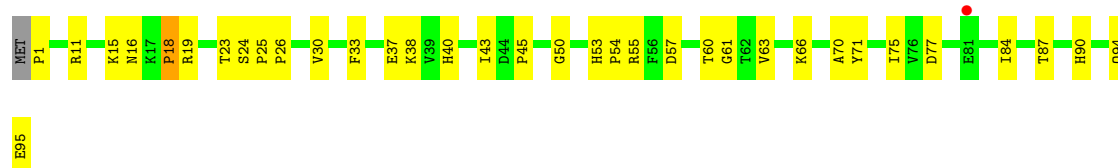
- Molecule 18: 50S ribosomal protein L19e

Chain P: 



- Molecule 19: 50S ribosomal protein L21e

Chain Q: 



- Molecule 20: 50S ribosomal protein L22P

Chain R: 



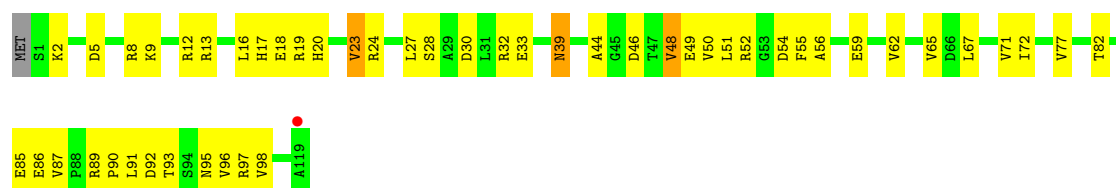
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



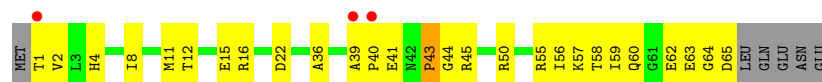
- Molecule 23: 50S ribosomal protein L24e

Chain U:



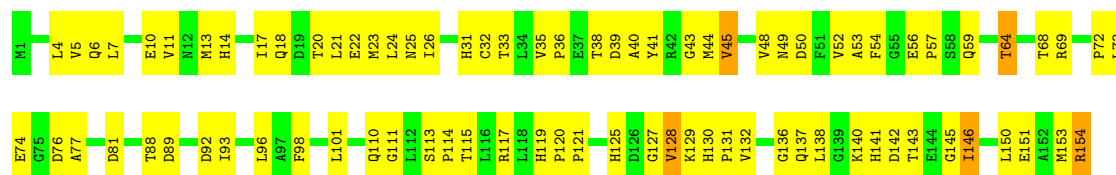
- Molecule 24: 50S ribosomal protein L29P

Chain V:



- Molecule 25: 50S ribosomal protein L30P

Chain W:



- Molecule 26: 50S RIBOSOMAL PROTEIN L31E

Chain X:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.49Å 302.43Å 578.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 49.83 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.00) 96.9 (49.83-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.241 , 0.288 0.257 , 0.257	Depositor DCC
R_{free} test set	18014 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	69.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 24.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 357596 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	92248	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% 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, NA, K, CD, OMU, UR3, 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	0.56	0/65932	0.75	36/102817 (0.0%)
2	9	0.42	0/2905	0.72	1/4528 (0.0%)
3	A	0.39	0/1786	0.69	0/2408
4	B	0.46	0/2690	0.76	0/3652
5	C	0.47	0/1884	0.76	1/2551 (0.0%)
6	D	0.36	0/1111	0.60	0/1498
7	E	0.45	0/1382	0.68	0/1880
8	F	0.34	0/901	0.58	0/1224
9	G	1.36	5/971 (0.5%)	1.67	22/1317 (1.7%)
10	H	0.41	0/1287	0.70	0/1725
11	I	4.03	6/890 (0.7%)	2.13	7/1216 (0.6%)
12	J	0.50	0/1136	0.70	0/1530
13	K	0.46	0/1001	0.77	0/1347
14	L	0.39	0/1130	0.68	0/1509
15	M	0.42	0/1583	0.68	0/2119
16	N	0.34	0/1474	0.66	0/1999
17	O	0.45	0/874	0.70	0/1181
18	P	0.42	0/1147	0.60	0/1528
19	Q	0.38	0/749	0.68	0/1005
20	R	0.50	0/1172	0.75	0/1578
21	S	0.42	0/648	0.64	0/875
22	T	0.42	0/958	0.71	0/1289
23	U	0.35	0/417	0.61	0/562
24	V	0.39	0/502	0.61	0/675
25	W	0.47	0/1219	0.77	0/1655
26	X	0.51	0/664	0.72	0/895
27	Y	0.48	0/1146	0.74	0/1536
28	Z	0.36	0/589	0.55	0/787
29	1	0.50	0/438	0.71	0/578
30	2	0.40	0/401	0.60	0/529
31	3	0.35	0/771	0.57	0/1024
All	All	0.66	11/99758 (0.0%)	0.77	67/149017 (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	6	93
2	9	0	1
9	G	0	8
11	I	2	4
All	All	8	106

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	24	LEU	CA-CB	82.97	3.44	1.53
11	I	24	LEU	CG-CD2	57.61	3.65	1.51
11	I	24	LEU	CG-CD1	50.48	3.38	1.51
11	I	24	LEU	CB-CG	34.68	2.53	1.52
9	G	54	HIS	CB-CG	28.65	2.01	1.50

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	24	LEU	CB-CA-C	-36.47	40.91	110.20
11	I	24	LEU	CD1-CG-CD2	-30.12	20.15	110.50
11	I	24	LEU	CB-CG-CD1	-29.18	61.40	111.00
11	I	24	LEU	CB-CG-CD2	-25.73	67.26	111.00
11	I	24	LEU	CA-CB-CG	-25.40	56.88	115.30

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1161	A	C1'
1	0	1167	G	C3',C1'
1	0	1193	A	C4',C3',C1'
11	I	24	LEU	CA
11	I	30	ASP	CA

5 of 106 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	116	G	Sidechain
1	0	191	A	Sidechain

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Mol	Chain	Res	Type	Group
1	0	206	G	Sidechain
1	0	49	A	Sidechain
1	0	79	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	58979	0	29793	2515	0
2	9	2600	0	1326	157	0
3	A	1753	0	1766	73	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	84	0
6	D	1094	0	1085	50	0
7	E	1357	0	1266	46	0
8	F	890	0	843	31	0
9	G	959	0	928	154	0
10	H	1266	0	1268	49	0
11	I	876	0	835	60	0
12	J	1120	0	1098	49	0
13	K	992	0	1031	44	0
14	L	1118	0	1076	34	0
15	M	1559	0	1567	63	0
16	N	1445	0	1401	73	0
17	O	865	0	873	28	0
18	P	1136	0	1123	39	0
19	Q	735	0	728	27	0
20	R	1149	0	1122	44	0
21	S	641	0	605	13	0
22	T	950	0	924	50	0
23	U	410	0	367	15	0
24	V	499	0	511	21	0
25	W	1196	0	1137	72	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	51	0
28	Z	578	0	543	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1	431	0	427	24	0
30	2	396	0	413	16	0
31	3	755	0	732	34	0
32	0	108	0	0	0	0
32	3	1	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
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	73	0	0	0	0
34	9	3	0	0	0	0
34	A	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	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	1	1	0	0	1	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	8	0	0	1	0
36	3	1	0	0	5	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	4	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	1	0
36	Q	1	0	0	1	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	92248	0	60923	3719	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 25.

The worst 5 of 3719 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:G:54:HIS:CB	9:G:54:HIS:CG	2.01	1.43
9:G:108:SER:O	9:G:109:LYS:HE3	1.32	1.30
1:O:1167:G:H5'	1:O:1168:C:OP2	1.34	1.28
9:G:33:VAL:C	9:G:123:ASP:OD2	1.72	1.27
9:G:35:VAL:HG21	9:G:122:ASN:OD1	1.37	1.25

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	11	47
4	B	335/338 (99%)	287 (86%)	38 (11%)	10 (3%)	7	34
5	C	244/246 (99%)	209 (86%)	28 (12%)	7 (3%)	7	35
6	D	134/177 (76%)	95 (71%)	34 (25%)	5 (4%)	5	28
7	E	170/178 (96%)	156 (92%)	12 (7%)	2 (1%)	19	64
8	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	8	39
9	G	121/348 (35%)	79 (65%)	29 (24%)	13 (11%)	1	3
10	H	156/171 (91%)	141 (90%)	11 (7%)	4 (3%)	8	39
11	I	112/162 (69%)	76 (68%)	28 (25%)	8 (7%)	2	9
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	16	60
13	K	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	15	58
14	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	30	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	M	192/196 (98%)	161 (84%)	31 (16%)	0	100	100
16	N	184/187 (98%)	162 (88%)	19 (10%)	3 (2%)	14	56
17	O	113/116 (97%)	103 (91%)	9 (8%)	1 (1%)	25	73
18	P	141/149 (95%)	129 (92%)	11 (8%)	1 (1%)	30	78
19	Q	93/96 (97%)	85 (91%)	5 (5%)	3 (3%)	6	33
20	R	148/155 (96%)	129 (87%)	18 (12%)	1 (1%)	30	78
21	S	79/85 (93%)	65 (82%)	14 (18%)	0	100	100
22	T	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	25	73
23	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	14	56
25	W	152/154 (99%)	134 (88%)	17 (11%)	1 (1%)	30	78
26	X	80/92 (87%)	66 (82%)	13 (16%)	1 (1%)	18	62
27	Y	140/241 (58%)	130 (93%)	7 (5%)	3 (2%)	11	47
28	Z	71/92 (77%)	64 (90%)	7 (10%)	0	100	100
29	1	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	12	51
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	21	67
All	All	3845/4442 (87%)	3329 (87%)	436 (11%)	80 (2%)	11	47

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	16	ARG
6	D	27	ILE
8	F	91	VAL
9	G	127	PRO
11	I	11	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	164 (92%)	15 (8%)	16	51
4	B	282/283 (100%)	264 (94%)	18 (6%)	25	66
5	C	193/193 (100%)	174 (90%)	19 (10%)	12	41
6	D	117/148 (79%)	109 (93%)	8 (7%)	22	63
7	E	152/156 (97%)	142 (93%)	10 (7%)	24	64
8	F	93/94 (99%)	92 (99%)	1 (1%)	84	97
9	G	106/283 (38%)	95 (90%)	11 (10%)	10	37
10	H	132/138 (96%)	124 (94%)	8 (6%)	26	68
11	I	99/130 (76%)	84 (85%)	15 (15%)	4	20
12	J	118/121 (98%)	107 (91%)	11 (9%)	13	45
13	K	106/106 (100%)	98 (92%)	8 (8%)	19	57
14	L	113/127 (89%)	108 (96%)	5 (4%)	39	82
15	M	158/160 (99%)	150 (95%)	8 (5%)	33	76
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	88
17	O	93/94 (99%)	89 (96%)	4 (4%)	40	82
18	P	113/117 (97%)	107 (95%)	6 (5%)	32	74
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	85
20	R	117/122 (96%)	113 (97%)	4 (3%)	49	88
21	S	71/74 (96%)	66 (93%)	5 (7%)	21	62
22	T	105/106 (99%)	99 (94%)	6 (6%)	29	71
23	U	44/53 (83%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	43	85
25	W	130/130 (100%)	121 (93%)	9 (7%)	22	62
26	X	66/74 (89%)	62 (94%)	4 (6%)	26	68
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	57
28	Z	60/74 (81%)	60 (100%)	0	100	100
29	1	46/47 (98%)	43 (94%)	3 (6%)	24	65
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	92
31	3	79/79 (100%)	78 (99%)	1 (1%)	80	96
All	All	3213/3620 (89%)	3014 (94%)	199 (6%)	26	67

5 of 199 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	9	VAL
12	J	79	PHE
26	X	76	ARG
11	I	15	ASN
11	I	90	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	24	GLN
16	N	107	ASN
27	Y	189	ASN
15	M	58	GLN
16	N	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2741/2922 (93%)	291 (10%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	4 (3%)
All	All	2862/3044 (94%)	307 (10%)	39 (1%)

5 of 307 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1506	U
2	9	43	G
1	0	1377	C
1	0	1450	C

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

4 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	0.85	1 (5%)	24,31,34	0.71	0
1	OMG	0	2588	1	24,26,27	0.81	0	32,38,41	5.37	4 (12%)
1	UR3	0	2619	1	20,22,23	0.77	1 (5%)	23,32,35	0.91	0
1	PSU	0	2621	1	19,21,22	1.12	2 (10%)	23,30,33	1.11	2 (8%)

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	-	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.31	1.43	1.37
1	0	2587	OMU	P-OP1	2.93	1.50	1.46
1	0	2621	PSU	C6-N1	2.22	1.34	1.32
1	0	2619	UR3	C6-C5	-2.09	1.32	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-29.79	130.13	134.14
1	0	2588	OMG	C6-N1-C2	3.07	124.87	119.51
1	0	2621	PSU	O2'-C2'-C1'	-2.88	105.35	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	N2-C2-N1	-2.32	115.30	117.86
1	0	2588	OMG	C2-N3-C4	-2.32	111.83	115.09

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 231 ligands modelled in this entry, 231 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	2753/2922 (94%)	-0.34	6 (0%) 93 54	17, 56, 120, 184	0
2	9	122/122 (100%)	-0.07	4 (3%) 44 8	41, 89, 136, 181	0
3	A	237/240 (98%)	0.16	3 (1%) 74 19	34, 90, 133, 148	0
4	B	337/338 (99%)	-0.07	1 (0%) 91 48	25, 60, 100, 112	0
5	C	246/246 (100%)	-0.09	0 100 100	29, 58, 91, 106	0
6	D	140/177 (79%)	0.72	14 (10%) 8 2	89, 146, 170, 178	0
7	E	172/178 (96%)	0.04	0 100 100	46, 73, 100, 109	0
8	F	119/120 (99%)	0.07	1 (0%) 83 26	74, 110, 150, 166	0
9	G	125/348 (35%)	0.54	3 (2%) 56 11	100, 133, 165, 168	0
10	H	160/171 (93%)	0.06	0 100 100	51, 76, 109, 120	0
11	I	118/162 (72%)	1.12	14 (11%) 5 1	20, 181, 199, 200	0
12	J	142/145 (97%)	-0.11	0 100 100	31, 54, 83, 99	0
13	K	132/132 (100%)	-0.05	0 100 100	33, 61, 98, 103	0
14	L	145/165 (87%)	0.87	19 (13%) 4 1	49, 111, 158, 162	0
15	M	194/196 (98%)	0.40	17 (8%) 10 3	2, 62, 161, 180	0
16	N	186/187 (99%)	0.47	11 (5%) 22 5	62, 106, 176, 189	0
17	O	115/116 (99%)	0.01	0 100 100	48, 70, 88, 91	0
18	P	143/149 (95%)	0.23	1 (0%) 84 28	44, 68, 103, 109	0
19	Q	95/96 (98%)	0.13	1 (1%) 77 21	52, 74, 87, 100	0
20	R	150/155 (96%)	-0.12	0 100 100	30, 48, 74, 81	0
21	S	81/85 (95%)	0.09	0 100 100	56, 87, 108, 123	0
22	T	119/120 (99%)	0.30	1 (0%) 83 26	51, 74, 106, 139	0
23	U	53/67 (79%)	0.62	2 (3%) 38 7	96, 108, 126, 133	0
24	V	65/71 (91%)	0.43	3 (4%) 31 7	66, 105, 145, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.19	0	100	100	38, 55, 81, 95	0
26	X	82/92 (89%)	-0.00	0	100	100	43, 63, 84, 95	0
27	Y	142/241 (58%)	-0.05	0	100	100	23, 51, 87, 106	0
28	Z	73/92 (79%)	3.32	41 (56%)	0	0	164, 174, 200, 200	0
29	1	56/57 (98%)	-0.07	0	100	100	28, 43, 56, 65	0
30	2	46/50 (92%)	0.66	5 (10%)	6	2	48, 87, 150, 152	0
31	3	92/92 (100%)	4.82	83 (90%)	0	0	184, 198, 200, 200	0
All	All	6794/7486 (90%)	0.07	230 (3%)	43	8	2, 67, 162, 200	0

The worst 5 of 230 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	3	33	MET	13.1
31	3	31	THR	11.7
31	3	34	LYS	9.7
31	3	82	GLY	9.5
31	3	32	GLY	9.3

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	OMU	0	2587	21/22	0.18	1.18	33,36,42,43	0
1	OMG	0	2588	24/25	0.15	-0.11	38,42,48,49	0
1	PSU	0	2621	20/21	0.15	-0.45	35,37,44,44	0
1	UR3	0	2619	21/22	0.18	-0.46	34,42,44,47	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
32	MG	0	3029	1/1	0.91	218.67	69,69,69,69	0
34	NA	0	3100	1/1	1.82	140.80	56,56,56,56	0
32	MG	0	3026	1/1	0.92	85.78	79,79,79,79	0
32	MG	0	2980	1/1	0.49	71.64	48,48,48,48	0
32	MG	0	3011	1/1	0.85	52.65	71,71,71,71	0
36	CL	0	3109	1/1	0.74	51.63	135,135,135,135	0
32	MG	0	3015	1/1	0.44	46.64	53,53,53,53	0
36	CL	0	3106	1/1	1.13	45.59	120,120,120,120	0
34	NA	0	3044	1/1	0.60	40.46	46,46,46,46	0
32	MG	0	2989	1/1	0.69	39.09	56,56,56,56	0
34	NA	0	3075	1/1	0.55	38.27	41,41,41,41	0
34	NA	0	3033	1/1	0.34	36.90	60,60,60,60	0
34	NA	0	3104	1/1	0.55	36.74	34,34,34,34	0
32	MG	0	2984	1/1	0.68	35.28	59,59,59,59	0
34	NA	0	3057	1/1	0.57	31.48	124,124,124,124	0
34	NA	0	3085	1/1	0.42	30.74	15,15,15,15	0
34	NA	0	3103	1/1	0.74	29.94	198,198,198,198	0
32	MG	0	2962	1/1	0.56	28.94	60,60,60,60	0
34	NA	0	3050	1/1	1.20	28.61	137,137,137,137	0
34	NA	0	3032	1/1	0.45	26.66	30,30,30,30	0
34	NA	0	3091	1/1	0.38	26.16	31,31,31,31	0
34	NA	9	125	1/1	0.42	25.60	78,78,78,78	0
34	NA	9	126	1/1	0.98	22.96	91,91,91,91	0
32	MG	0	3004	1/1	0.59	22.95	27,27,27,27	0
34	NA	0	3039	1/1	0.54	22.28	29,29,29,29	0
34	NA	0	3080	1/1	0.89	22.06	57,57,57,57	0
34	NA	0	3077	1/1	0.59	20.52	119,119,119,119	0
32	MG	0	2945	1/1	0.35	18.76	27,27,27,27	0
32	MG	0	3018	1/1	0.33	18.54	78,78,78,78	0
32	MG	0	2981	1/1	0.49	18.12	44,44,44,44	0
32	MG	0	2998	1/1	0.48	17.87	73,73,73,73	0
32	MG	0	2938	1/1	0.40	17.37	42,42,42,42	0
34	NA	0	3078	1/1	0.27	16.66	78,78,78,78	0
34	NA	0	3067	1/1	0.30	16.52	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	2942	1/1	0.48	15.71	16,16,16,16	0
32	MG	0	3024	1/1	0.32	15.65	1,1,1,1	0
32	MG	K	133	1/1	0.41	15.05	35,35,35,35	0
34	NA	0	3098	1/1	0.53	14.48	62,62,62,62	0
32	MG	0	2947	1/1	0.24	14.39	15,15,15,15	0
34	NA	0	3051	1/1	0.36	14.22	49,49,49,49	0
36	CL	0	3112	1/1	0.54	13.73	96,96,96,96	0
32	MG	0	2958	1/1	0.41	13.72	33,33,33,33	0
32	MG	0	3021	1/1	0.27	13.65	20,20,20,20	0
34	NA	0	3094	1/1	0.46	13.51	116,116,116,116	0
33	K	0	3031	1/1	0.53	13.36	153,153,153,153	0
32	MG	0	2964	1/1	0.32	13.01	50,50,50,50	0
32	MG	0	3006	1/1	0.47	12.94	49,49,49,49	0
32	MG	0	2973	1/1	0.33	12.22	51,51,51,51	0
32	MG	0	2992	1/1	0.36	12.20	52,52,52,52	0
32	MG	0	2960	1/1	0.34	11.82	11,11,11,11	0
34	NA	0	3102	1/1	0.36	11.69	47,47,47,47	0
36	CL	O	117	1/1	1.61	11.62	127,127,127,127	0
32	MG	0	2993	1/1	0.59	11.61	78,78,78,78	0
34	NA	0	3068	1/1	0.27	11.44	68,68,68,68	0
34	NA	0	3095	1/1	0.60	11.08	126,126,126,126	0
34	NA	0	3083	1/1	0.42	11.04	27,27,27,27	0
32	MG	0	3014	1/1	0.31	10.93	87,87,87,87	0
32	MG	0	2969	1/1	0.37	10.84	38,38,38,38	0
32	MG	0	2971	1/1	0.48	10.58	200,200,200,200	0
32	MG	0	2943	1/1	0.39	10.37	23,23,23,23	0
34	NA	0	3038	1/1	0.29	10.31	67,67,67,67	0
34	NA	0	3084	1/1	0.35	10.19	62,62,62,62	0
36	CL	A	243	1/1	0.67	9.98	90,90,90,90	0
34	NA	0	3046	1/1	0.23	9.70	26,26,26,26	0
32	MG	0	2951	1/1	0.33	9.67	11,11,11,11	0
32	MG	0	3025	1/1	0.45	9.42	57,57,57,57	0
34	NA	0	3082	1/1	0.51	9.23	43,43,43,43	0
32	MG	0	2955	1/1	0.28	9.04	11,11,11,11	0
34	NA	0	3073	1/1	0.26	8.91	25,25,25,25	0
32	MG	0	2933	1/1	0.34	8.66	1,1,1,1	0
32	MG	0	2996	1/1	0.25	8.42	21,21,21,21	0
34	NA	0	3069	1/1	0.30	8.35	58,58,58,58	0
32	MG	0	3022	1/1	0.44	8.28	44,44,44,44	0
32	MG	0	2940	1/1	0.34	8.17	24,24,24,24	0
32	MG	Y	241	1/1	0.43	8.02	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	2965	1/1	0.20	8.00	47,47,47,47	0
32	MG	0	3007	1/1	0.28	7.86	54,54,54,54	0
32	MG	0	2946	1/1	0.33	7.73	200,200,200,200	0
34	NA	0	3092	1/1	0.28	7.60	45,45,45,45	0
34	NA	0	3093	1/1	0.44	7.54	116,116,116,116	0
34	NA	0	3054	1/1	0.37	7.45	63,63,63,63	0
34	NA	S	85	1/1	0.67	7.29	64,64,64,64	0
34	NA	0	3043	1/1	0.33	7.26	115,115,115,115	0
32	MG	0	2934	1/1	0.35	7.25	22,22,22,22	0
32	MG	0	3009	1/1	0.28	7.19	40,40,40,40	0
34	NA	0	3099	1/1	1.03	7.02	56,56,56,56	0
32	MG	0	2937	1/1	0.27	6.98	14,14,14,14	0
32	MG	0	3019	1/1	0.30	6.91	41,41,41,41	0
32	MG	0	2935	1/1	0.33	6.62	28,28,28,28	0
32	MG	A	240	1/1	0.49	6.40	56,56,56,56	0
32	MG	0	2994	1/1	0.23	6.37	14,14,14,14	0
32	MG	0	3023	1/1	0.28	6.27	29,29,29,29	0
32	MG	0	2959	1/1	0.26	6.15	39,39,39,39	0
34	NA	0	3056	1/1	0.33	6.08	42,42,42,42	0
32	MG	0	2961	1/1	0.22	5.89	41,41,41,41	0
34	NA	0	3064	1/1	0.28	5.60	60,60,60,60	0
34	NA	0	3034	1/1	0.51	5.58	91,91,91,91	0
34	NA	0	3086	1/1	0.57	5.00	26,26,26,26	0
32	MG	0	2948	1/1	0.23	4.98	18,18,18,18	0
32	MG	0	2983	1/1	0.26	4.89	43,43,43,43	0
32	MG	0	2970	1/1	0.20	4.66	32,32,32,32	0
32	MG	0	1	1/1	0.28	4.58	26,26,26,26	0
36	CL	M	198	1/1	0.35	4.52	77,77,77,77	0
34	NA	0	3096	1/1	0.22	4.18	47,47,47,47	0
32	MG	0	2979	1/1	0.26	3.86	20,20,20,20	0
34	NA	0	3041	1/1	0.26	3.83	70,70,70,70	0
34	NA	0	3052	1/1	0.35	3.77	72,72,72,72	0
32	MG	0	3008	1/1	0.23	3.77	52,52,52,52	0
36	CL	0	3110	1/1	0.31	3.77	56,56,56,56	0
32	MG	A	241	1/1	0.38	3.75	142,142,142,142	0
32	MG	0	3010	1/1	0.18	3.37	56,56,56,56	0
32	MG	0	2949	1/1	0.24	3.33	45,45,45,45	0
32	MG	0	2927	1/1	0.22	3.33	18,18,18,18	0
32	MG	B	338	1/1	0.50	3.33	43,43,43,43	0
34	NA	0	3036	1/1	0.25	3.31	49,49,49,49	0
32	MG	0	2974	1/1	0.25	3.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	3088	1/1	0.27	3.15	33,33,33,33	0
36	CL	B	339	1/1	0.39	3.06	61,61,61,61	0
32	MG	0	3000	1/1	0.21	3.05	7,7,7,7	0
32	MG	0	2924	1/1	0.26	3.03	35,35,35,35	0
34	NA	0	3048	1/1	0.22	2.96	46,46,46,46	0
32	MG	0	3013	1/1	0.29	2.94	41,41,41,41	0
36	CL	0	3105	1/1	0.22	2.94	59,59,59,59	0
34	NA	0	3072	1/1	0.21	2.75	65,65,65,65	0
32	MG	0	2977	1/1	0.44	2.70	43,43,43,43	0
34	NA	0	3074	1/1	0.57	2.42	66,66,66,66	0
32	MG	0	2999	1/1	0.18	2.41	25,25,25,25	0
32	MG	0	2982	1/1	0.23	2.41	14,14,14,14	0
36	CL	J	147	1/1	0.30	2.41	69,69,69,69	0
32	MG	0	2952	1/1	0.20	2.40	4,4,4,4	0
34	NA	0	3063	1/1	0.26	2.36	162,162,162,162	0
34	NA	0	3101	1/1	0.19	2.30	43,43,43,43	0
34	NA	0	3060	1/1	0.18	2.25	101,101,101,101	0
32	MG	0	3030	1/1	0.20	2.20	46,46,46,46	0
32	MG	0	2997	1/1	0.21	2.17	59,59,59,59	0
34	NA	0	3049	1/1	0.28	2.14	28,28,28,28	0
32	MG	0	3016	1/1	0.22	2.08	43,43,43,43	0
32	MG	0	2988	1/1	0.29	1.83	52,52,52,52	0
34	NA	0	3037	1/1	0.19	1.82	61,61,61,61	0
32	MG	0	2954	1/1	0.23	1.81	29,29,29,29	0
34	NA	C	247	1/1	0.32	1.81	41,41,41,41	0
34	NA	0	3097	1/1	0.20	1.77	50,50,50,50	0
32	MG	0	2985	1/1	0.18	1.66	34,34,34,34	0
34	NA	R	155	1/1	0.25	1.61	31,31,31,31	0
32	MG	0	2928	1/1	0.17	1.55	32,32,32,32	0
32	MG	0	2929	1/1	0.20	1.51	14,14,14,14	0
32	MG	0	2986	1/1	0.21	1.48	53,53,53,53	0
36	CL	Q	97	1/1	0.40	1.43	93,93,93,93	0
36	CL	K	134	1/1	0.25	1.43	55,55,55,55	0
32	MG	0	2939	1/1	0.23	1.36	20,20,20,20	0
36	CL	0	3111	1/1	0.26	1.28	54,54,54,54	0
32	MG	0	3027	1/1	0.87	1.23	110,110,110,110	0
34	NA	0	3058	1/1	0.18	1.14	61,61,61,61	0
34	NA	R	156	1/1	0.25	1.05	53,53,53,53	0
32	MG	0	3012	1/1	0.17	0.95	39,39,39,39	0
36	CL	R	157	1/1	0.21	0.91	55,55,55,55	0
32	MG	0	2967	1/1	0.26	0.85	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	3042	1/1	0.20	0.82	32,32,32,32	0
34	NA	A	242	1/1	0.27	0.82	55,55,55,55	0
32	MG	0	3017	1/1	0.33	0.80	166,166,166,166	0
32	MG	0	2987	1/1	0.16	0.80	35,35,35,35	0
32	MG	0	2975	1/1	0.16	0.80	45,45,45,45	0
32	MG	0	3020	1/1	0.21	0.79	84,84,84,84	0
34	NA	J	146	1/1	0.29	0.65	41,41,41,41	0
35	CD	O	116	1/1	0.24	0.54	200,200,200,200	0
34	NA	0	3089	1/1	0.14	0.44	51,51,51,51	0
34	NA	0	3081	1/1	0.17	0.43	49,49,49,49	0
32	MG	0	2963	1/1	0.20	0.25	72,72,72,72	0
36	CL	0	3108	1/1	0.38	0.12	72,72,72,72	0
33	K	M	196	1/1	0.30	0.12	127,127,127,127	0
32	MG	0	2991	1/1	0.18	0.07	20,20,20,20	0
34	NA	0	3076	1/1	0.17	-0.02	51,51,51,51	0
32	MG	0	2968	1/1	0.14	-0.03	60,60,60,60	0
32	MG	0	2950	1/1	0.20	-0.04	17,17,17,17	0
34	NA	0	3065	1/1	0.18	-0.14	27,27,27,27	0
32	MG	0	2932	1/1	0.17	-0.22	10,10,10,10	0
34	NA	Q	96	1/1	0.24	-0.22	64,64,64,64	0
32	MG	3	93	1/1	0.94	-0.24	69,69,69,69	0
34	NA	0	3040	1/1	0.16	-0.28	29,29,29,29	0
35	CD	3	94	1/1	0.65	-0.31	200,200,200,200	0
34	NA	0	3090	1/1	0.23	-0.32	81,81,81,81	0
34	NA	0	3059	1/1	0.20	-0.39	53,53,53,53	0
32	MG	0	2941	1/1	0.15	-0.40	15,15,15,15	0
34	NA	0	3047	1/1	0.35	-0.40	53,53,53,53	0
34	NA	H	172	1/1	0.17	-0.42	43,43,43,43	0
32	MG	0	2972	1/1	0.15	-0.47	109,109,109,109	0
32	MG	9	123	1/1	0.20	-0.48	37,37,37,37	0
36	CL	Y	242	1/1	0.17	-0.52	27,27,27,27	0
32	MG	0	2956	1/1	0.16	-0.52	24,24,24,24	0
34	NA	0	3070	1/1	0.17	-0.59	27,27,27,27	0
36	CL	L	166	1/1	0.27	-0.64	68,68,68,68	0
32	MG	0	2978	1/1	0.18	-0.77	46,46,46,46	0
32	MG	0	2944	1/1	0.17	-0.85	25,25,25,25	0
32	MG	0	3001	1/1	0.15	-0.98	38,38,38,38	0
34	NA	0	3045	1/1	0.14	-1.04	33,33,33,33	0
32	MG	0	2936	1/1	0.16	-1.04	17,17,17,17	0
32	MG	0	2925	1/1	0.16	-1.11	5,5,5,5	0
34	NA	0	3071	1/1	0.11	-1.14	27,27,27,27	0
36	CL	J	149	1/1	0.16	-1.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	3003	1/1	0.16	-1.18	26,26,26,26	0
36	CL	N	187	1/1	0.23	-1.18	64,64,64,64	0
32	MG	0	2957	1/1	0.12	-1.19	37,37,37,37	0
35	CD	Z	93	1/1	0.35	-1.26	200,200,200,200	0
32	MG	0	2926	1/1	0.10	-1.31	17,17,17,17	0
34	NA	0	3061	1/1	0.11	-1.37	39,39,39,39	0
34	NA	9	124	1/1	0.18	-1.45	34,34,34,34	0
32	MG	0	3005	1/1	0.14	-1.47	47,47,47,47	0
32	MG	0	2966	1/1	0.12	-1.56	46,46,46,46	0
34	NA	0	3066	1/1	0.13	-1.62	9,9,9,9	0
34	NA	M	197	1/1	0.15	-1.68	28,28,28,28	0
32	MG	T	120	1/1	0.17	-1.69	38,38,38,38	0
35	CD	1	57	1/1	0.06	-1.71	76,76,76,76	0
36	CL	0	3107	1/1	0.12	-1.88	55,55,55,55	0
34	NA	0	3062	1/1	0.06	-1.90	38,38,38,38	0
32	MG	0	2990	1/1	0.13	-1.96	31,31,31,31	0
34	NA	0	3055	1/1	0.12	-2.01	36,36,36,36	0
34	NA	0	3035	1/1	0.12	-2.12	17,17,17,17	0
36	CL	J	148	1/1	0.11	-2.13	49,49,49,49	0
34	NA	L	165	1/1	0.08	-2.15	42,42,42,42	0
36	CL	3	95	1/1	0.26	-2.15	124,124,124,124	0
32	MG	0	2930	1/1	0.10	-2.20	55,55,55,55	0
32	MG	0	2995	1/1	0.11	-2.26	13,13,13,13	0
32	MG	0	2976	1/1	0.12	-2.28	19,19,19,19	0
32	MG	0	2931	1/1	0.10	-3.30	27,27,27,27	0
34	NA	0	3079	1/1	0.10	-3.42	53,53,53,53	0
34	NA	0	3053	1/1	0.09	-3.43	19,19,19,19	0
35	CD	U	67	1/1	0.06	-3.62	134,134,134,134	0
32	MG	0	2953	1/1	0.11	-5.66	8,8,8,8	0
32	MG	0	3002	1/1	0.13	-6.08	20,20,20,20	0
34	NA	0	3087	1/1	0.06	-9.38	22,22,22,22	0
32	MG	0	3028	1/1	0.57	-	66,66,66,66	0

6.5 Other polymers ⓘ

There are no such residues in this entry.