



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:54 PM GMT

PDB ID : 2OTJ
Title : 13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
Resolution : 2.90 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>

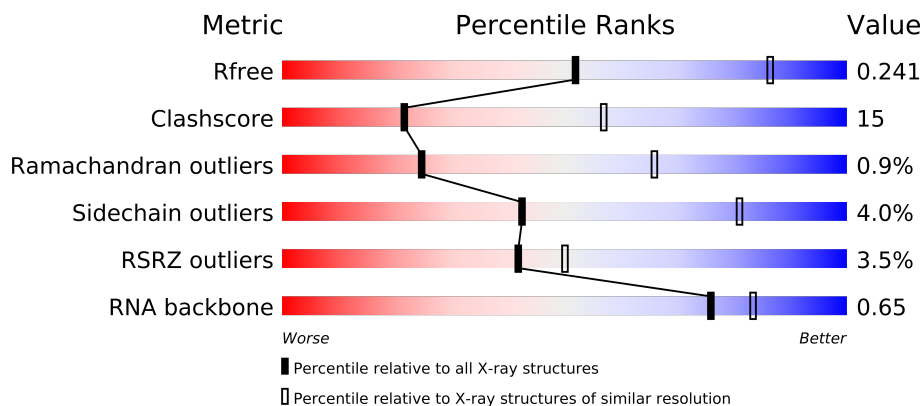
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	FAILED
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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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	A	240	
4	B	338	
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	

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Mol	Chain	Length	Quality of chain
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	
30	3	92	
31	I	161	

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	13T	0	9000	-	X
33	MG	0	8011	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8023	-	X
33	MG	0	8024	-	X
33	MG	0	8040	-	X
33	MG	0	8041	-	X
33	MG	0	8049	-	X
33	MG	0	8062	-	X
33	MG	0	8070	-	X
33	MG	0	8090	-	X
33	MG	0	8094	-	X
33	MG	0	8099	-	X
33	MG	0	8102	-	X
33	MG	0	8103	-	X
33	MG	0	8104	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8114	-	X
34	K	0	8401	-	X
35	NA	0	8502	-	X
35	NA	0	8503	-	X
35	NA	0	8506	-	X
35	NA	0	8507	-	X
35	NA	0	8508	-	X
35	NA	0	8515	-	X
35	NA	0	8516	-	X
35	NA	0	8518	-	X
35	NA	0	8520	-	X
35	NA	0	8521	-	X
35	NA	0	8523	-	X
35	NA	0	8525	-	X
35	NA	0	8526	-	X
35	NA	0	8527	-	X
35	NA	0	8528	-	X
35	NA	0	8531	-	X
35	NA	0	8532	-	X
35	NA	0	8535	-	X
35	NA	0	8539	-	X
35	NA	0	8540	-	X
35	NA	0	8542	-	X
35	NA	0	8543	-	X
35	NA	0	8549	-	X
35	NA	0	8550	-	X
35	NA	0	8555	-	X
35	NA	0	8556	-	X
35	NA	0	8557	-	X
35	NA	0	8558	-	X
35	NA	0	8559	-	X
35	NA	0	8560	-	X
35	NA	0	8561	-	X
35	NA	0	8562	-	X
35	NA	0	8563	-	X
35	NA	0	8564	-	X
35	NA	0	8565	-	X
35	NA	0	8566	-	X
35	NA	0	8567	-	X
35	NA	0	8568	-	X
35	NA	0	8569	-	X
35	NA	0	8570	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	8571	-	X
35	NA	0	8572	-	X
35	NA	0	8573	-	X
35	NA	0	8574	-	X
35	NA	0	8575	-	X
35	NA	0	8577	-	X
35	NA	0	8579	-	X
35	NA	0	8582	-	X
35	NA	0	8584	-	X
35	NA	0	8585	-	X
35	NA	9	8583	-	X
35	NA	H	8522	-	X
35	NA	L	8580	-	X
35	NA	R	8586	-	X
35	NA	S	8512	-	X
36	CL	0	8803	-	X
36	CL	0	8805	-	X
36	CL	0	8815	-	X
36	CL	0	8822	-	X
36	CL	A	8809	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99043 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 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
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 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 50S ribosomal protein L10E.

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

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 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	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 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			579	346	116	112	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

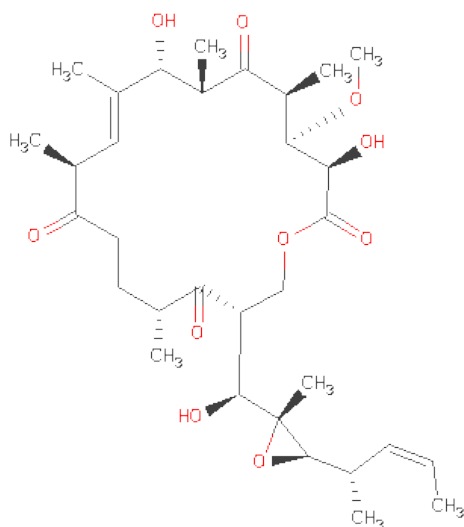
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is 13-DEOXYTEDANOLIDE (three-letter code: 13T) (formula: C₃₂H₅₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	0	1	Total	C	O	0	0
			42	32	10		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
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	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	3	2	Total	Mg	0	0
			2	2		

- 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	74	Total	Na	0	0
			74	74		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	J	3	Total 3	Cl 3	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	2	Total 2	Cl 2	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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

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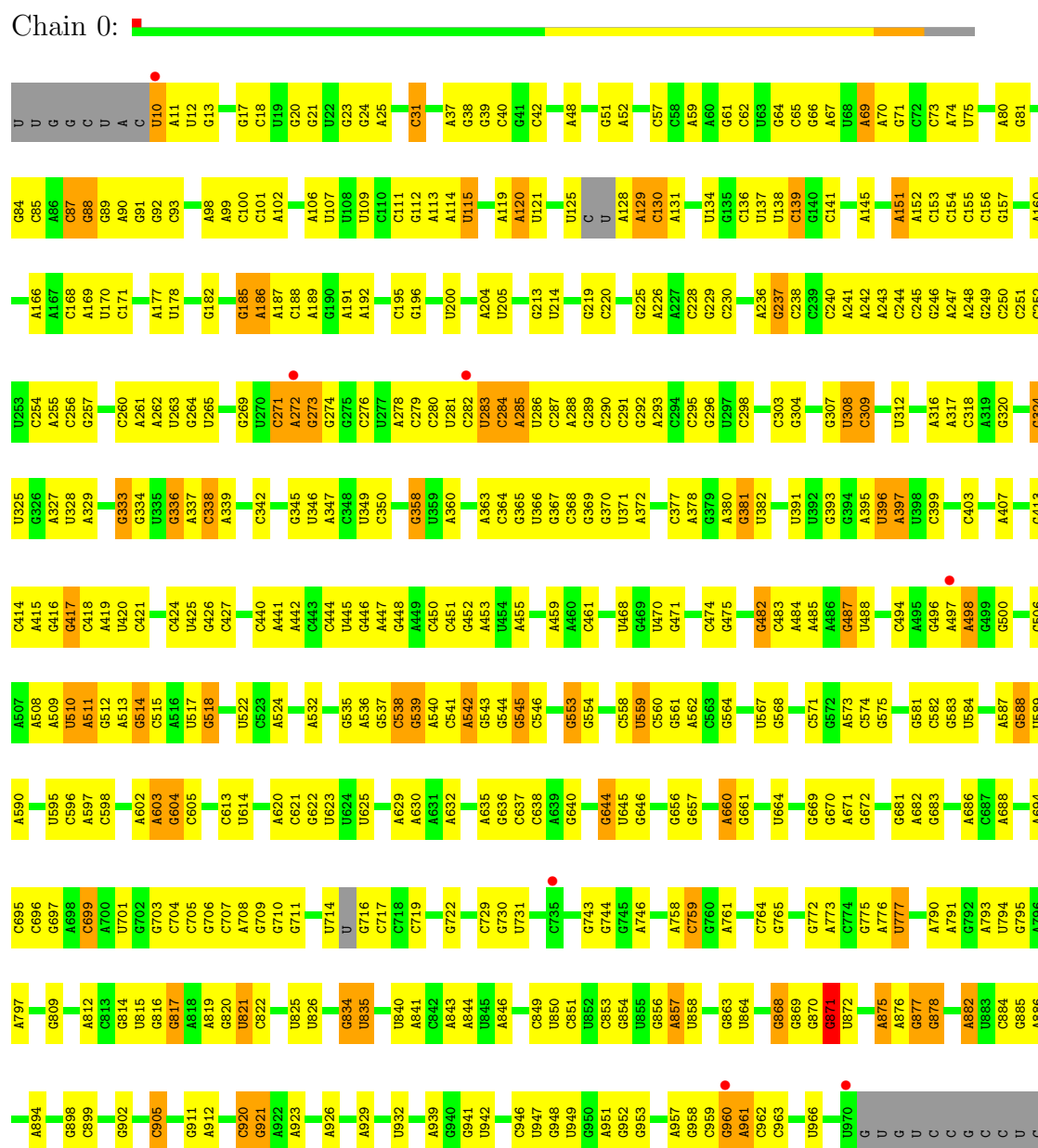
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	56	Total 56	O 56	0	0
38	Q	51	Total 51	O 51	0	0
38	R	80	Total 80	O 80	0	0
38	S	36	Total 36	O 36	0	0
38	T	33	Total 33	O 33	0	0
38	U	26	Total 26	O 26	0	0
38	V	11	Total 11	O 11	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	31	Total 31	O 31	0	0
38	1	56	Total 56	O 56	0	0
38	2	45	Total 45	O 45	0	0
38	3	66	Total 66	O 66	0	0
38	I	8	Total 8	O 8	0	0

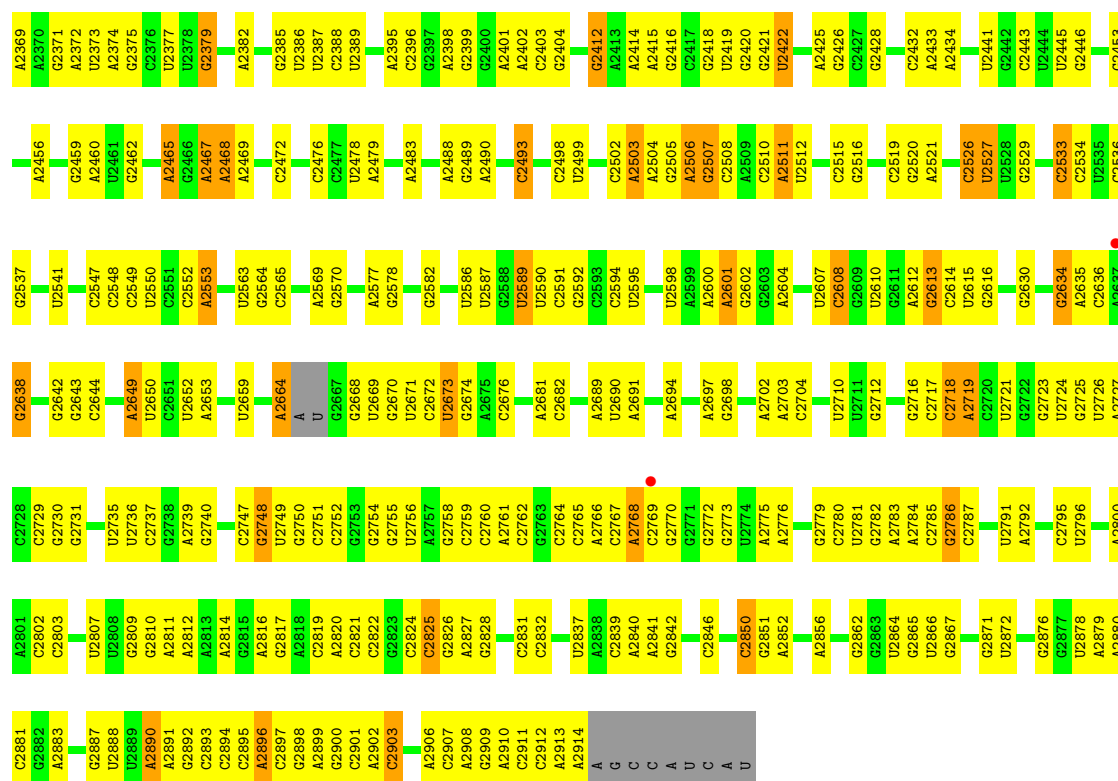
3 Residue-property plots

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

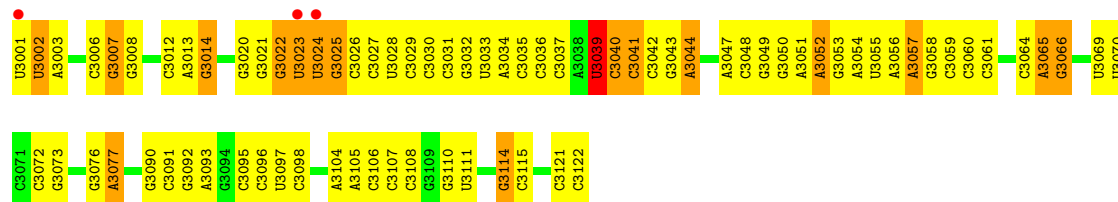


U2297	U2078	U1985	U1879	U1599	U1506	A1414	G1319	C1229	U1164	C1060	C
A	C	C	A	G	G	G	A	A	A	A	G
U	C	C	U	G	G	G	A	A	A	A	A
U	C	C	U	G	G	G	A	A	A	A	A
U	C	C	U	G	G	G	A	A	A	A	A
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
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C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C	C	C	C	C
C	C	C	C	C	C	C	C				



• Molecule 2: 5S ribosomal RNA

Chain 9:



• Molecule 3: 50S ribosomal protein L2P

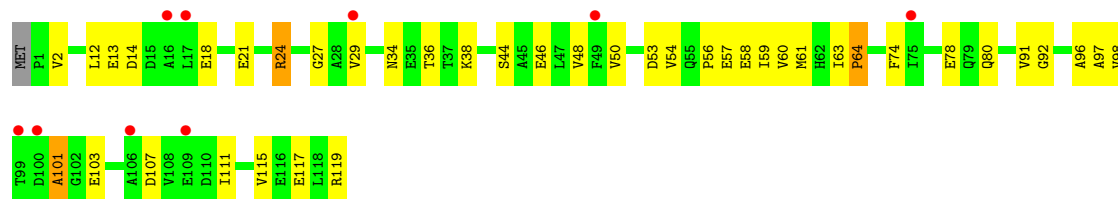
Chain A:



• Molecule 4: 50S ribosomal protein L3P

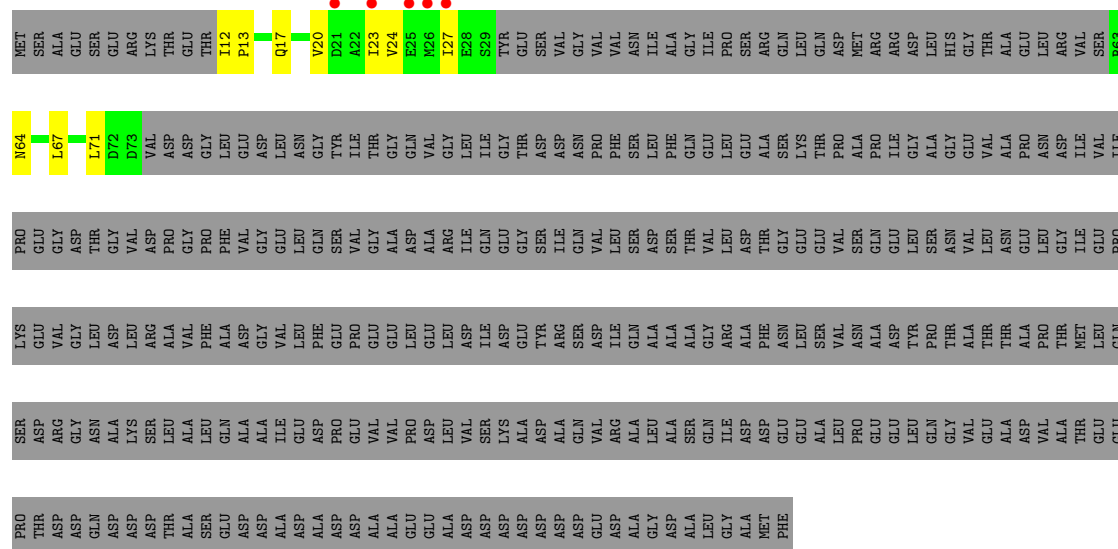
Chain B:





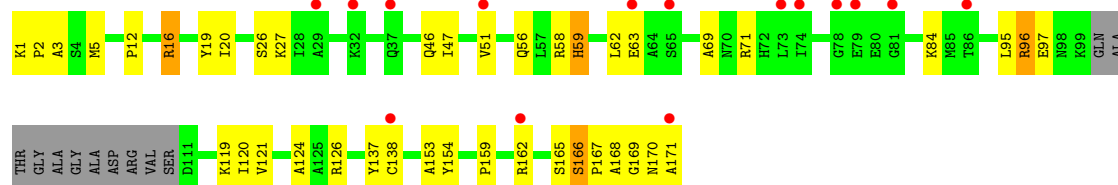
• Molecule 9: 50S ribosomal protein L10E

Chain G:



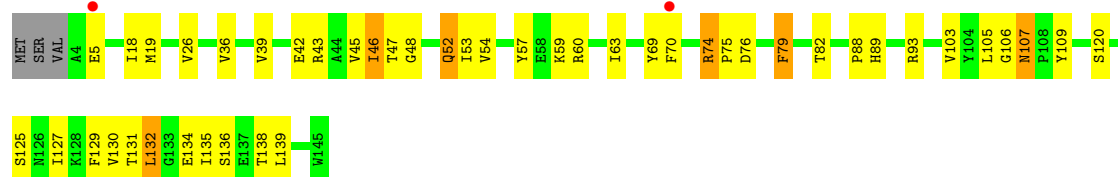
• Molecule 10: 50S ribosomal protein L10e

Chain H:



• Molecule 11: 50S ribosomal protein L13P

Chain J:



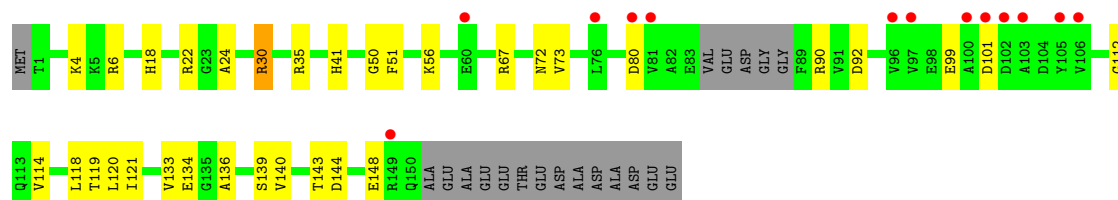
• Molecule 12: 50S ribosomal protein L14P

Chain K:



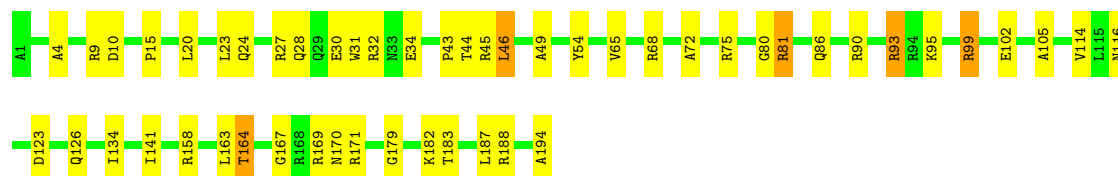
- Molecule 13: 50S ribosomal protein L15P

Chain L:



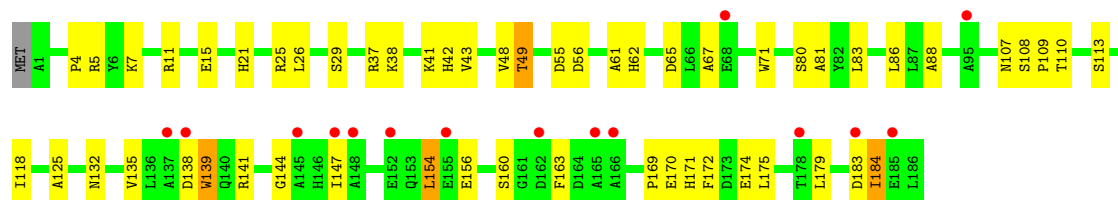
- Molecule 14: 50S ribosomal protein L15e

Chain M:



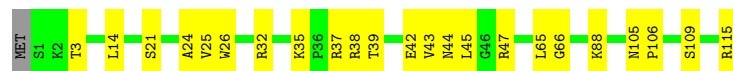
- Molecule 15: 50S ribosomal protein L18P

Chain N:



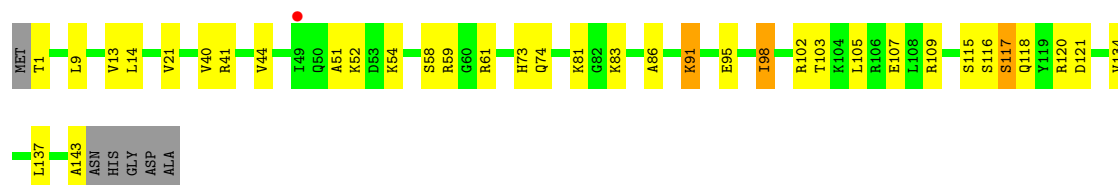
- Molecule 16: 50S ribosomal protein L18e

Chain O:



- Molecule 17: 50S ribosomal protein L19e

Chain P:



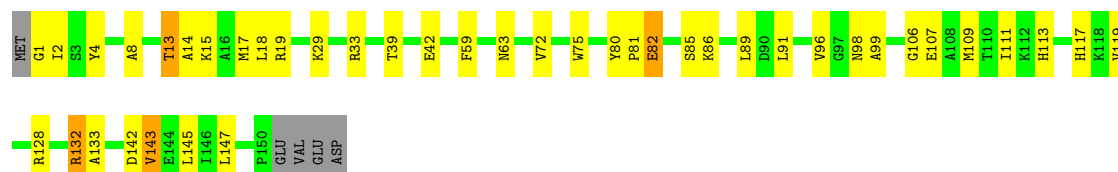
- Molecule 18: 50S ribosomal protein L21e

Chain Q: 



- Molecule 19: 50S ribosomal protein L22P

Chain R: 



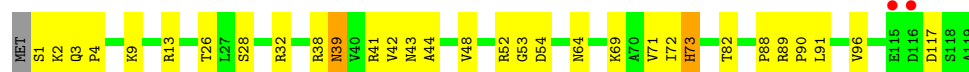
- Molecule 20: 50S ribosomal protein L23P

Chain S: 



- Molecule 21: 50S ribosomal protein L24P

Chain T: 



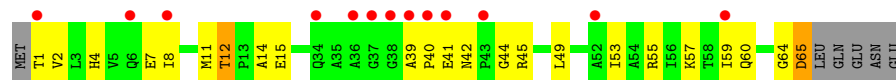
- Molecule 22: 50S ribosomal protein L24e

Chain U: 



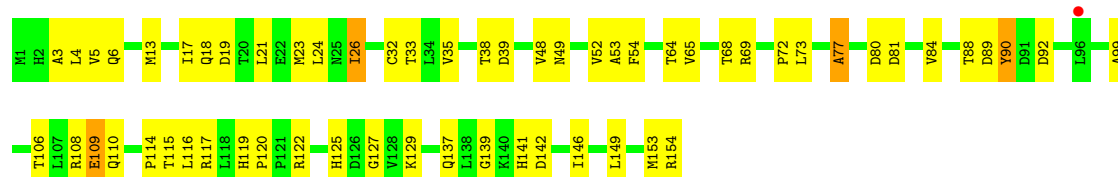
- Molecule 23: 50S ribosomal protein L29P

Chain V: 



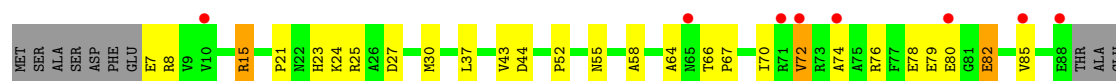
- Molecule 24: 50S ribosomal protein L30P

Chain W: 



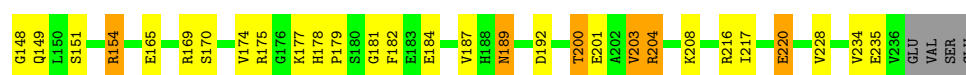
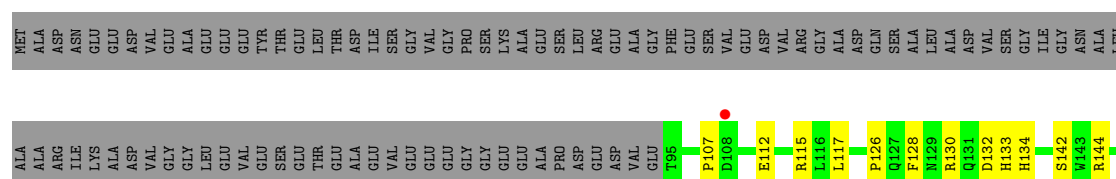
- Molecule 25: 50S ribosomal protein L31e

Chain X:



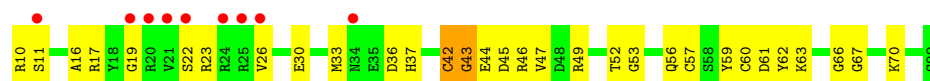
- Molecule 26: 50S ribosomal protein L32e

Chain Y:



- Molecule 27: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 28: 50S ribosomal protein L37e

Chain 1:



- Molecule 29: 50S ribosomal protein L39e

Chain 2:



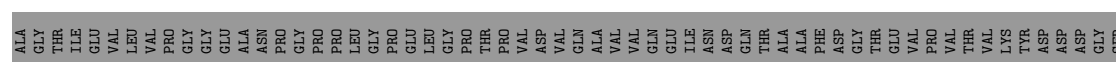
- Molecule 30: 50S ribosomal protein L44E

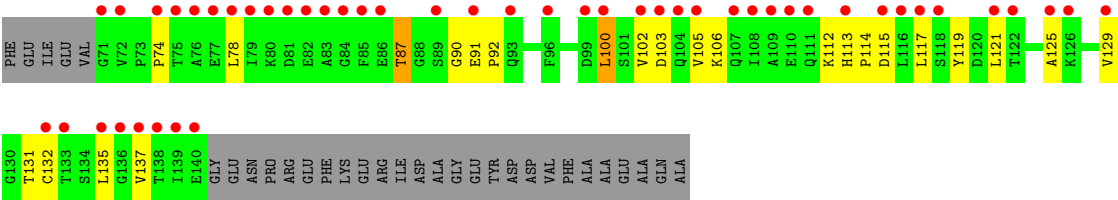
Chain 3:



- Molecule 31: 50S ribosomal protein L11P

Chain I:





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 91.7 (85.48-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.86Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.193 , 0.238 0.212 , 0.241	Depositor DCC
R_{free} test set	3809 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 422682 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99043	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, UR3, CD, OMU, 13T, 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	0.39	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.69	1/4528 (0.0%)
3	A	0.35	0/1786	0.66	0/2408
4	B	0.34	0/2690	0.66	0/3652
5	C	0.39	0/1884	0.66	0/2551
6	D	0.33	0/1111	0.58	0/1498
7	E	0.34	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.33	0/241	0.49	0/324
10	H	0.38	0/1287	0.65	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.35	0/1130	0.64	0/1509
14	M	0.37	0/1584	0.63	0/2119
15	N	0.31	0/1474	0.65	1/1999 (0.1%)
16	O	0.36	0/874	0.61	1/1181 (0.1%)
17	P	0.35	0/1147	0.55	0/1528
18	Q	0.37	0/749	0.68	0/1005
19	R	0.36	0/1172	0.64	0/1578
20	S	0.35	0/648	0.59	0/875
21	T	0.34	0/958	0.63	0/1289
22	U	0.36	0/417	0.56	0/562
23	V	0.35	0/502	0.56	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.59	0/895
26	Y	0.36	0/1146	0.63	0/1536
27	Z	0.39	0/590	0.64	0/787
28	1	0.40	0/438	0.63	0/578
29	2	0.37	0/401	0.56	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.35	0/526	0.57	0/716
All	All	0.38	0/98693	0.67	17/147577 (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	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.37	130.11	109.50
2	9	3039	U	N1-C1'-C2'	6.50	122.45	114.00
1	0	2316	G	C5'-C4'-C3'	-6.49	105.61	116.00
1	0	1504	A	C1'-O4'-C4'	-6.21	104.93	109.90
1	0	1942	A	C5'-C4'-C3'	6.20	125.92	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	131	A	Sidechain
1	0	220	C	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	48	A	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	1337	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	78	0
4	B	2625	0	2533	112	0
5	C	1859	0	1816	74	0
6	D	1094	0	1085	56	0
7	E	1357	0	1266	38	0
8	F	890	0	843	32	0
9	G	240	0	231	9	0
10	H	1266	0	1268	39	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	40	0
13	L	1118	0	1076	28	0
14	M	1560	0	1568	45	0
15	N	1445	0	1401	45	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	41	0
20	S	641	0	605	14	0
21	T	950	0	923	25	0
22	U	410	0	364	21	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	25	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	21	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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
35	0	74	0	0	2	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	1	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	2	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	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	0	0
36	R	1	0	0	0	0
36	Y	2	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0
38	A	112	0	0	8	0
38	B	142	0	0	21	0
38	C	170	0	0	16	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2276	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 15.

The worst 5 of 2276 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H8	1:0:871:G:H5'	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5''	1.37	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
3	A	235/240 (98%)	212 (90%)	21 (9%)	2 (1%)	25 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	19	57
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	27	68
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	10	37
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	33	76
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	8	32
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	12	42
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	16	52
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100	100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	10	37
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	30	72
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	21	60
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	66
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	18	54
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	18	54
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	8	29
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	25	66

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP

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%)	170 (95%)	9 (5%)	34	73
4	B	282/283 (100%)	268 (95%)	14 (5%)	34	73
5	C	193/193 (100%)	178 (92%)	15 (8%)	18	46
6	D	117/148 (79%)	115 (98%)	2 (2%)	73	94
7	E	152/156 (97%)	149 (98%)	3 (2%)	68	92
8	F	93/94 (99%)	89 (96%)	4 (4%)	40	78
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	126 (96%)	6 (4%)	38	77
11	J	118/121 (98%)	110 (93%)	8 (7%)	22	55
12	K	106/106 (100%)	104 (98%)	2 (2%)	69	93
13	L	113/127 (89%)	107 (95%)	6 (5%)	32	70
14	M	158/158 (100%)	149 (94%)	9 (6%)	29	66
15	N	149/150 (99%)	146 (98%)	3 (2%)	68	92
16	O	93/94 (99%)	92 (99%)	1 (1%)	84	97
17	P	113/117 (97%)	109 (96%)	4 (4%)	48	85
18	Q	79/80 (99%)	78 (99%)	1 (1%)	80	96
19	R	117/122 (96%)	113 (97%)	4 (3%)	49	86
20	S	71/74 (96%)	70 (99%)	1 (1%)	78	96
21	T	105/106 (99%)	99 (94%)	6 (6%)	29	66
22	U	44/52 (85%)	43 (98%)	1 (2%)	63	92
23	V	51/57 (90%)	49 (96%)	2 (4%)	43	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	130/130 (100%)	124 (95%)	6 (5%)	37	76
25	X	66/74 (89%)	61 (92%)	5 (8%)	19	48
26	Y	120/196 (61%)	114 (95%)	6 (5%)	34	73
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	45 (98%)	1 (2%)	64	92
29	2	42/46 (91%)	40 (95%)	2 (5%)	35	74
30	3	79/79 (100%)	78 (99%)	1 (1%)	80	96
31	I	58/129 (45%)	56 (97%)	2 (3%)	49	86
All	All	3093/3602 (86%)	2969 (96%)	124 (4%)	42	81

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	79	PHE
14	M	10	ASP
26	Y	200	THR
11	J	93	ARG
12	K	132	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	137	ASN
18	Q	40	HIS
29	2	45	ASN
14	M	170	ASN
17	P	50	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	241 (8%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	259 (9%)	34 (1%)

5 of 259 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1246	A
1	0	1474	C
1	0	2718	C
1	0	1377	C
1	0	699	C

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

Mogul failed to run properly - this section will therefore be empty.

5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

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%)	-0.29	26 (0%) 81 88	23, 50, 93, 150	0
2	9	122/122 (100%)	-0.52	3 (2%) 54 64	43, 69, 91, 151	0
3	A	237/240 (98%)	-0.18	6 (2%) 54 64	32, 55, 86, 105	0
4	B	337/338 (99%)	-0.25	1 (0%) 91 95	33, 60, 82, 90	0
5	C	246/246 (100%)	-0.42	0 100 100	30, 50, 73, 82	0
6	D	140/177 (79%)	1.47	50 (35%) 1 1	63, 103, 124, 130	0
7	E	172/178 (96%)	-0.05	3 (1%) 67 76	55, 73, 90, 96	0
8	F	119/120 (99%)	0.47	9 (7%) 14 17	57, 74, 96, 106	0
9	G	29/348 (8%)	0.99	5 (17%) 2 3	81, 94, 103, 103	0
10	H	160/171 (93%)	0.51	15 (9%) 9 11	52, 67, 93, 100	0
11	J	142/145 (97%)	-0.34	2 (1%) 72 80	45, 56, 74, 94	0
12	K	132/132 (100%)	-0.44	1 (0%) 83 89	41, 54, 75, 81	0
13	L	145/165 (87%)	0.34	13 (8%) 10 12	32, 71, 107, 118	0
14	M	194/194 (100%)	-0.50	0 100 100	36, 47, 60, 64	0
15	N	186/187 (99%)	0.18	15 (8%) 12 15	50, 67, 110, 119	0
16	O	115/116 (99%)	-0.24	0 100 100	44, 59, 71, 76	0
17	P	143/149 (95%)	-0.22	1 (0%) 84 90	46, 60, 70, 75	0
18	Q	95/96 (98%)	-0.40	0 100 100	43, 52, 64, 72	0
19	R	150/155 (96%)	-0.35	0 100 100	38, 50, 68, 73	0
20	S	81/85 (95%)	-0.05	3 (3%) 39 47	52, 65, 81, 85	0
21	T	119/120 (99%)	-0.09	2 (1%) 67 76	47, 62, 83, 96	0
22	U	53/66 (80%)	-0.17	1 (1%) 64 72	51, 61, 75, 81	0
23	V	65/71 (91%)	1.31	13 (20%) 2 2	59, 79, 109, 114	0
24	W	154/154 (100%)	-0.35	1 (0%) 86 91	42, 56, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.23	8 (9%) 8 10	52, 64, 87, 97	0
26	Y	142/241 (58%)	-0.55	1 (0%) 84 90	30, 51, 70, 86	0
27	Z	73/73 (100%)	0.38	9 (12%) 5 6	58, 69, 80, 94	0
28	1	56/57 (98%)	-0.47	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	0.23	3 (6%) 18 22	41, 69, 90, 99	0
30	3	92/92 (100%)	-0.34	0 100 100	42, 60, 71, 82	0
31	I	70/161 (43%)	3.38	48 (68%) 0 0	109, 119, 135, 135	0
All	All	6651/7463 (89%)	-0.12	239 (3%) 42 48	23, 57, 100, 151	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	I	118	SER	9.7
31	I	109	ALA	9.1
6	D	63	ILE	9.0
31	I	75	THR	8.6
13	L	100	ALA	8.5

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.14	1.88	36,38,39,40	0
1	1MA	0	628	23/24	0.16	0.60	33,35,36,37	0
1	OMU	0	2587	21/22	0.12	-0.73	38,39,40,41	0
1	OMG	0	2588	24/25	0.13	-0.79	37,38,39,40	0
1	PSU	0	2621	20/21	0.11	-2.06	30,32,39,40	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
35	NA	0	8577	1/1	1.06	95.15	81,81,81,81	0
35	NA	0	8584	1/1	0.78	59.12	90,90,90,90	0
35	NA	0	8558	1/1	0.60	55.99	75,75,75,75	0
34	K	0	8401	1/1	0.68	46.16	84,84,84,84	0
35	NA	0	8575	1/1	0.40	36.84	72,72,72,72	0
35	NA	0	8506	1/1	0.73	35.77	49,49,49,49	0
35	NA	0	8585	1/1	0.36	32.93	65,65,65,65	0
33	MG	0	8024	1/1	1.15	30.81	65,65,65,65	0
35	NA	0	8528	1/1	0.49	27.23	54,54,54,54	0
35	NA	0	8574	1/1	0.42	26.22	67,67,67,67	0
35	NA	0	8531	1/1	0.42	26.09	57,57,57,57	0
35	NA	0	8559	1/1	0.45	25.35	53,53,53,53	0
35	NA	0	8550	1/1	0.50	23.34	65,65,65,65	0
36	CL	0	8822	1/1	0.40	23.21	90,90,90,90	0
35	NA	0	8567	1/1	0.43	21.62	61,61,61,61	0
35	NA	0	8516	1/1	0.41	20.57	49,49,49,49	0
35	NA	0	8502	1/1	0.20	19.88	57,57,57,57	0
35	NA	0	8565	1/1	0.73	18.73	47,47,47,47	0
35	NA	0	8525	1/1	0.34	17.53	59,59,59,59	0
35	NA	0	8562	1/1	0.43	16.70	70,70,70,70	0
35	NA	0	8556	1/1	0.42	16.21	61,61,61,61	0
35	NA	0	8518	1/1	0.34	16.16	58,58,58,58	0
35	NA	0	8563	1/1	0.34	14.96	68,68,68,68	0
35	NA	0	8571	1/1	0.24	14.91	59,59,59,59	0
35	NA	0	8564	1/1	0.33	13.51	49,49,49,49	0
35	NA	0	8570	1/1	0.39	13.40	65,65,65,65	0
35	NA	0	8521	1/1	0.40	13.26	77,77,77,77	0
33	MG	0	8114	1/1	0.33	13.23	54,54,54,54	0
35	NA	0	8579	1/1	0.33	12.31	65,65,65,65	0
35	NA	0	8503	1/1	0.29	11.92	1,1,1,1	0
35	NA	0	8526	1/1	0.25	11.49	70,70,70,70	0
35	NA	0	8555	1/1	1.00	11.36	85,85,85,85	0
35	NA	0	8572	1/1	0.35	11.26	73,73,73,73	0
35	NA	0	8532	1/1	0.23	10.84	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8102	1/1	0.24	10.70	50,50,50,50	0
35	NA	0	8523	1/1	0.29	10.11	38,38,38,38	0
35	NA	0	8573	1/1	0.22	10.10	56,56,56,56	0
33	MG	0	8040	1/1	0.29	9.92	53,53,53,53	0
35	NA	0	8582	1/1	0.29	9.39	85,85,85,85	0
35	NA	0	8507	1/1	0.23	9.27	69,69,69,69	0
35	NA	0	8540	1/1	0.24	8.52	50,50,50,50	0
33	MG	0	8099	1/1	0.32	8.46	70,70,70,70	0
33	MG	0	8049	1/1	0.16	8.46	36,36,36,36	0
35	NA	0	8535	1/1	0.33	8.36	54,54,54,54	0
35	NA	0	8568	1/1	0.19	8.16	87,87,87,87	0
33	MG	0	8011	1/1	0.18	7.81	39,39,39,39	0
33	MG	0	8103	1/1	0.19	7.56	78,78,78,78	0
33	MG	0	8062	1/1	0.22	6.99	13,13,13,13	0
33	MG	0	8104	1/1	0.35	6.90	78,78,78,78	0
35	NA	0	8561	1/1	0.24	6.48	50,50,50,50	0
35	NA	0	8560	1/1	0.25	6.14	60,60,60,60	0
35	NA	0	8539	1/1	0.25	6.13	40,40,40,40	0
35	NA	0	8508	1/1	0.27	6.02	58,58,58,58	0
33	MG	0	8090	1/1	0.33	5.65	73,73,73,73	0
33	MG	0	8041	1/1	0.22	5.61	68,68,68,68	0
35	NA	0	8520	1/1	0.22	5.48	36,36,36,36	0
35	NA	0	8549	1/1	0.23	5.03	53,53,53,53	0
35	NA	0	8566	1/1	0.15	5.03	48,48,48,48	0
35	NA	0	8527	1/1	0.23	4.82	61,61,61,61	0
35	NA	0	8515	1/1	0.21	4.60	49,49,49,49	0
35	NA	L	8580	1/1	0.23	4.17	1,1,1,1	0
35	NA	S	8512	1/1	0.45	4.17	57,57,57,57	0
35	NA	0	8542	1/1	0.29	4.15	15,15,15,15	0
36	CL	0	8815	1/1	0.15	3.76	89,89,89,89	0
32	13T	0	9000	42/42	0.24	3.69	58,67,73,74	0
35	NA	R	8586	1/1	0.34	3.67	23,23,23,23	0
36	CL	A	8809	1/1	0.18	3.41	82,82,82,82	0
33	MG	0	8013	1/1	0.18	3.30	38,38,38,38	0
33	MG	0	8094	1/1	0.14	3.05	59,59,59,59	0
33	MG	0	8070	1/1	0.16	3.00	43,43,43,43	0
35	NA	H	8522	1/1	0.34	2.99	77,77,77,77	0
35	NA	0	8543	1/1	0.18	2.99	35,35,35,35	0
33	MG	0	8023	1/1	0.23	2.92	61,61,61,61	0
35	NA	0	8569	1/1	0.24	2.84	64,64,64,64	0
36	CL	0	8803	1/1	0.17	2.79	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8557	1/1	0.14	2.63	45,45,45,45	0
36	CL	0	8805	1/1	0.15	2.57	71,71,71,71	0
33	MG	0	8012	1/1	0.15	2.56	39,39,39,39	0
35	NA	9	8583	1/1	0.15	2.17	73,73,73,73	0
33	MG	B	8055	1/1	0.15	1.69	64,64,64,64	0
33	MG	0	8081	1/1	0.16	1.69	43,43,43,43	0
33	MG	0	8050	1/1	0.17	1.58	74,74,74,74	0
33	MG	0	8018	1/1	0.15	1.43	39,39,39,39	0
33	MG	0	8060	1/1	0.17	1.28	45,45,45,45	0
33	MG	0	8084	1/1	0.14	1.14	58,58,58,58	0
33	MG	9	8095	1/1	0.14	1.11	77,77,77,77	0
35	NA	0	8510	1/1	0.14	0.97	45,45,45,45	0
33	MG	0	8058	1/1	0.13	0.93	42,42,42,42	0
33	MG	3	8118	1/1	0.19	0.84	50,50,50,50	0
36	CL	Y	8817	1/1	0.16	0.73	70,70,70,70	0
35	NA	J	8546	1/1	0.23	0.63	39,39,39,39	0
35	NA	0	8541	1/1	0.12	0.62	46,46,46,46	0
33	MG	0	8043	1/1	0.12	0.62	47,47,47,47	0
33	MG	Y	8109	1/1	0.18	0.62	44,44,44,44	0
33	MG	0	8054	1/1	0.15	0.60	30,30,30,30	0
33	MG	0	8089	1/1	0.14	0.36	62,62,62,62	0
35	NA	0	8552	1/1	0.12	0.35	68,68,68,68	0
35	NA	0	8533	1/1	0.11	0.22	39,39,39,39	0
35	NA	9	8551	1/1	0.33	0.10	92,92,92,92	0
33	MG	0	8004	1/1	0.16	0.08	37,37,37,37	0
36	CL	J	8821	1/1	0.18	-0.05	77,77,77,77	0
33	MG	0	8007	1/1	0.17	-0.06	26,26,26,26	0
33	MG	0	8079	1/1	0.14	-0.12	27,27,27,27	0
33	MG	0	8098	1/1	0.12	-0.14	42,42,42,42	0
35	NA	0	8530	1/1	0.10	-0.26	45,45,45,45	0
35	NA	0	8519	1/1	0.15	-0.34	17,17,17,17	0
35	NA	0	8524	1/1	0.12	-0.55	48,48,48,48	0
33	MG	0	8107	1/1	0.11	-0.57	38,38,38,38	0
35	NA	Q	8548	1/1	0.13	-0.60	46,46,46,46	0
36	CL	0	8816	1/1	0.12	-0.62	69,69,69,69	0
36	CL	J	8802	1/1	0.14	-0.64	76,76,76,76	0
33	MG	0	8009	1/1	0.15	-0.65	36,36,36,36	0
33	MG	0	8038	1/1	0.12	-0.70	31,31,31,31	0
33	MG	0	8113	1/1	0.15	-0.70	44,44,44,44	0
33	MG	0	8045	1/1	0.12	-0.72	67,67,67,67	0
37	CD	U	8701	1/1	0.09	-0.78	67,67,67,67	0
33	MG	0	8087	1/1	0.08	-0.78	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8056	1/1	0.12	-0.81	56,56,56,56	0
35	NA	A	8545	1/1	0.12	-0.86	61,61,61,61	0
35	NA	0	8509	1/1	0.12	-0.87	48,48,48,48	0
34	K	0	8402	1/1	0.14	-0.90	61,61,61,61	0
35	NA	0	8505	1/1	0.13	-0.94	37,37,37,37	0
36	CL	3	8804	1/1	0.10	-1.02	56,56,56,56	0
35	NA	0	8534	1/1	0.08	-1.03	40,40,40,40	0
33	MG	0	8001	1/1	0.12	-1.04	44,44,44,44	0
35	NA	0	8576	1/1	0.14	-1.04	33,33,33,33	0
33	MG	0	8017	1/1	0.15	-1.05	31,31,31,31	0
33	MG	0	8077	1/1	0.15	-1.12	36,36,36,36	0
33	MG	0	8052	1/1	0.12	-1.13	68,68,68,68	0
35	NA	R	8537	1/1	0.13	-1.16	45,45,45,45	0
33	MG	0	8047	1/1	0.12	-1.18	57,57,57,57	0
37	CD	O	8705	1/1	0.11	-1.22	186,186,186,186	0
33	MG	0	8086	1/1	0.05	-1.27	42,42,42,42	0
35	NA	0	8517	1/1	0.12	-1.28	37,37,37,37	0
33	MG	0	8080	1/1	0.14	-1.30	39,39,39,39	0
37	CD	Z	8703	1/1	0.09	-1.35	71,71,71,71	0
33	MG	A	8065	1/1	0.13	-1.35	45,45,45,45	0
36	CL	0	8812	1/1	0.09	-1.36	49,49,49,49	0
36	CL	O	8808	1/1	0.11	-1.43	67,67,67,67	0
36	CL	N	8807	1/1	0.12	-1.52	71,71,71,71	0
33	MG	0	8064	1/1	0.10	-1.56	41,41,41,41	0
37	CD	3	8704	1/1	0.08	-1.58	65,65,65,65	0
33	MG	0	8085	1/1	0.12	-1.59	48,48,48,48	0
36	CL	0	8814	1/1	0.10	-1.60	57,57,57,57	0
33	MG	3	8078	1/1	0.10	-1.60	16,16,16,16	0
36	CL	J	8801	1/1	0.08	-1.61	58,58,58,58	0
33	MG	0	8096	1/1	0.10	-1.67	48,48,48,48	0
33	MG	0	8076	1/1	0.07	-1.67	49,49,49,49	0
33	MG	0	8015	1/1	0.14	-1.69	35,35,35,35	0
35	NA	0	8511	1/1	0.09	-1.79	56,56,56,56	0
33	MG	0	8074	1/1	0.04	-1.81	30,30,30,30	0
33	MG	0	8010	1/1	0.15	-1.84	11,11,11,11	0
33	MG	T	8073	1/1	0.10	-1.85	57,57,57,57	0
37	CD	1	8702	1/1	0.07	-1.88	65,65,65,65	0
36	CL	L	8810	1/1	0.08	-1.95	59,59,59,59	0
33	MG	0	8053	1/1	0.13	-1.96	43,43,43,43	0
35	NA	C	8504	1/1	0.07	-1.97	35,35,35,35	0
35	NA	0	8529	1/1	0.08	-1.98	68,68,68,68	0
33	MG	0	8106	1/1	0.06	-1.98	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8020	1/1	0.11	-2.04	39,39,39,39	0
33	MG	0	8061	1/1	0.14	-2.04	44,44,44,44	0
33	MG	A	8066	1/1	0.05	-2.09	73,73,73,73	0
35	NA	0	8554	1/1	0.13	-2.10	42,42,42,42	0
33	MG	0	8035	1/1	0.11	-2.13	46,46,46,46	0
36	CL	M	8818	1/1	0.09	-2.14	44,44,44,44	0
33	MG	0	8100	1/1	0.09	-2.43	42,42,42,42	0
33	MG	0	8039	1/1	0.08	-2.52	64,64,64,64	0
33	MG	0	8029	1/1	0.13	-2.54	42,42,42,42	0
33	MG	0	8117	1/1	0.10	-2.54	34,34,34,34	0
36	CL	Y	8820	1/1	0.05	-2.55	44,44,44,44	0
35	NA	0	8514	1/1	0.11	-2.61	38,38,38,38	0
33	MG	0	8028	1/1	0.06	-2.63	33,33,33,33	0
35	NA	0	8538	1/1	0.09	-2.65	55,55,55,55	0
33	MG	0	8051	1/1	0.11	-2.90	56,56,56,56	0
35	NA	M	8547	1/1	0.08	-2.92	41,41,41,41	0
33	MG	0	8083	1/1	0.08	-2.98	41,41,41,41	0
33	MG	0	8032	1/1	0.06	-3.01	35,35,35,35	0
36	CL	0	8811	1/1	0.07	-3.03	58,58,58,58	0
33	MG	0	8042	1/1	0.06	-3.04	33,33,33,33	0
36	CL	B	8819	1/1	0.08	-3.08	53,53,53,53	0
33	MG	0	8006	1/1	0.08	-3.19	36,36,36,36	0
33	MG	0	8101	1/1	0.08	-3.21	45,45,45,45	0
36	CL	0	8813	1/1	0.07	-3.39	54,54,54,54	0
33	MG	0	8003	1/1	0.10	-3.40	36,36,36,36	0
33	MG	0	8037	1/1	0.06	-3.60	42,42,42,42	0
33	MG	0	8092	1/1	0.09	-3.74	72,72,72,72	0
35	NA	0	8578	1/1	0.10	-3.74	57,57,57,57	0
33	MG	0	8034	1/1	0.09	-3.80	25,25,25,25	0
35	NA	0	8581	1/1	0.06	-3.93	42,42,42,42	0
33	MG	K	8069	1/1	0.06	-3.98	51,51,51,51	0
33	MG	0	8116	1/1	0.08	-4.08	56,56,56,56	0
33	MG	0	8008	1/1	0.06	-4.17	29,29,29,29	0
33	MG	0	8068	1/1	0.08	-4.22	56,56,56,56	0
33	MG	0	8072	1/1	0.09	-4.24	57,57,57,57	0
33	MG	0	8097	1/1	0.08	-4.28	45,45,45,45	0
35	NA	0	8513	1/1	0.07	-4.38	72,72,72,72	0
33	MG	0	8059	1/1	0.06	-4.41	39,39,39,39	0
33	MG	0	8048	1/1	0.07	-4.63	49,49,49,49	0
33	MG	0	8026	1/1	0.08	-4.82	33,33,33,33	0
33	MG	0	8005	1/1	0.10	-4.89	32,32,32,32	0
33	MG	0	8014	1/1	0.06	-4.93	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8091	1/1	0.08	-5.05	65,65,65,65	0
33	MG	0	8088	1/1	0.10	-5.14	33,33,33,33	0
33	MG	0	8112	1/1	0.07	-5.15	39,39,39,39	0
33	MG	0	8046	1/1	0.07	-5.18	56,56,56,56	0
33	MG	0	8067	1/1	0.06	-5.22	37,37,37,37	0
35	NA	0	8536	1/1	0.07	-5.33	54,54,54,54	0
33	MG	0	8057	1/1	0.05	-5.34	41,41,41,41	0
33	MG	0	8021	1/1	0.08	-5.53	37,37,37,37	0
33	MG	0	8093	1/1	0.10	-5.56	61,61,61,61	0
33	MG	0	8022	1/1	0.08	-5.62	37,37,37,37	0
36	CL	R	8806	1/1	0.02	-5.73	49,49,49,49	0
33	MG	0	8027	1/1	0.02	-5.79	40,40,40,40	0
33	MG	0	8075	1/1	0.04	-5.89	56,56,56,56	0
35	NA	0	8553	1/1	0.08	-5.99	44,44,44,44	0
33	MG	0	8016	1/1	0.07	-6.20	18,18,18,18	0
33	MG	0	8044	1/1	0.08	-6.38	55,55,55,55	0
33	MG	0	8111	1/1	0.07	-6.57	46,46,46,46	0
33	MG	0	8036	1/1	0.05	-6.71	41,41,41,41	0
33	MG	0	8110	1/1	0.10	-6.72	53,53,53,53	0
33	MG	0	8108	1/1	0.05	-6.79	77,77,77,77	0
33	MG	0	8033	1/1	0.04	-7.10	38,38,38,38	0
33	MG	0	8002	1/1	0.03	-7.11	40,40,40,40	0
33	MG	0	8030	1/1	0.05	-7.27	35,35,35,35	0
33	MG	0	8063	1/1	0.09	-8.53	63,63,63,63	0
33	MG	0	8071	1/1	0.06	-8.79	50,50,50,50	0
33	MG	0	8025	1/1	0.08	-12.68	43,43,43,43	0
35	NA	0	8544	1/1	0.06	-13.08	29,29,29,29	0
33	MG	0	8019	1/1	0.05	-15.18	34,34,34,34	0
35	NA	0	8501	1/1	0.04	-15.46	50,50,50,50	0
33	MG	0	8031	1/1	0.10	-22.32	30,30,30,30	0
33	MG	0	8115	1/1	0.07	-29.00	45,45,45,45	0
33	MG	0	8082	1/1	0.36	-	84,84,84,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.