



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:49 AM GMT

PDB ID : 1M1K  
Title : Co-crystal structure of azithromycin bound to the 50S ribosomal subunit of *Haloarcula marismortui*  
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2002-06-19  
Resolution : 3.20 Å(reported)

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

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

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

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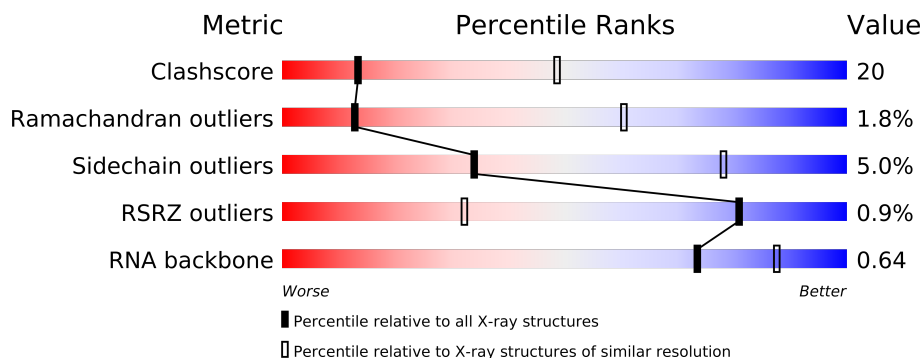
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	2922	
2	B	122	
3	C	239	
4	D	337	
5	E	246	
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	

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Mol	Chain	Length	Quality of chain
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	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
31	ZIT	A	8600	-	X
32	MG	1	8105	-	X
32	MG	A	8024	-	X
32	MG	A	8041	-	X
32	MG	A	8042	-	X
32	MG	A	8044	-	X
32	MG	A	8053	-	X
32	MG	A	8064	-	X
32	MG	A	8066	-	X
32	MG	A	8070	-	X
32	MG	A	8082	-	X
32	MG	A	8092	-	X
32	MG	A	8097	-	X
32	MG	A	8100	-	X
32	MG	A	8102	-	X
32	MG	A	8103	-	X
32	MG	A	8114	-	X
34	NA	A	8302	-	X
34	NA	A	8303	-	X
34	NA	A	8305	-	X
34	NA	A	8306	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	A	8307	-	X
34	NA	A	8310	-	X
34	NA	A	8313	-	X
34	NA	A	8315	-	X
34	NA	A	8316	-	X
34	NA	A	8318	-	X
34	NA	A	8321	-	X
34	NA	A	8323	-	X
34	NA	A	8325	-	X
34	NA	A	8326	-	X
34	NA	A	8328	-	X
34	NA	A	8329	-	X
34	NA	A	8331	-	X
34	NA	A	8335	-	X
34	NA	A	8340	-	X
34	NA	A	8341	-	X
34	NA	A	8342	-	X
34	NA	A	8349	-	X
34	NA	A	8350	-	X
34	NA	A	8352	-	X
34	NA	A	8354	-	X
34	NA	A	8355	-	X
34	NA	A	8356	-	X
34	NA	A	8358	-	X
34	NA	A	8359	-	X
34	NA	A	8360	-	X
34	NA	A	8361	-	X
34	NA	A	8362	-	X
34	NA	A	8363	-	X
34	NA	A	8364	-	X
34	NA	A	8365	-	X
34	NA	A	8366	-	X
34	NA	A	8367	-	X
34	NA	A	8368	-	X
34	NA	A	8369	-	X
34	NA	A	8370	-	X
34	NA	A	8371	-	X
34	NA	A	8372	-	X
34	NA	A	8373	-	X
34	NA	A	8374	-	X
34	NA	A	8375	-	X
34	NA	A	8376	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	A	8377	-	X
34	NA	A	8378	-	X
34	NA	A	8379	-	X
34	NA	A	8381	-	X
34	NA	A	8382	-	X
34	NA	A	8384	-	X
34	NA	A	8385	-	X
34	NA	B	8383	-	X
34	NA	J	8322	-	X
34	NA	M	8380	-	X
34	NA	S	8386	-	X
34	NA	T	8312	-	X
35	CL	4	8504	-	X
35	CL	A	8503	-	X
35	CL	A	8505	-	X
35	CL	A	8515	-	X
35	CL	A	8520	-	X
35	CL	A	8522	-	X
35	CL	C	8509	-	X
35	CL	D	8519	-	X
35	CL	K	8501	-	X
35	CL	O	8507	-	X
35	CL	R	8511	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	GB 3377779

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

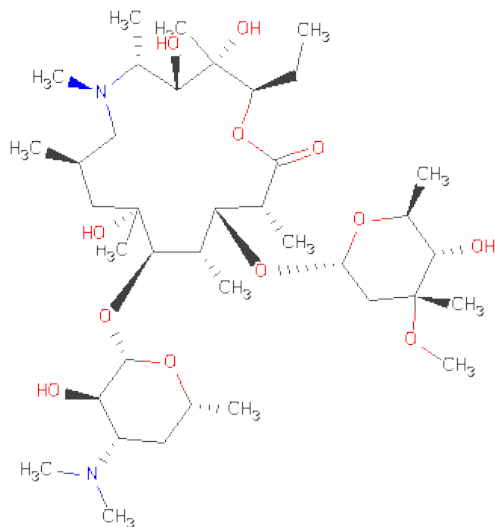
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is AZITHROMYCIN (three-letter code: ZIT) (formula: C<sub>38</sub>H<sub>72</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			52	38	2	12		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total	Mg	0	0
			1	1		
32	D	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	109	Total	Mg	0	0
			109	109		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	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	A	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	A	9	Total Cl 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5898	Total 5898	O 5898	0	0
37	B	140	Total 140	O 140	0	0
37	C	129	Total 129	O 129	0	0
37	D	152	Total 152	O 152	0	0
37	E	169	Total 169	O 169	0	0
37	F	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	21	Total 21	O 21	0	0
37	J	81	Total 81	O 81	0	0
37	K	56	Total 56	O 56	0	0
37	L	61	Total 61	O 61	0	0
37	M	81	Total 81	O 81	0	0
37	N	129	Total 129	O 129	0	0
37	O	68	Total 68	O 68	0	0
37	P	45	Total 45	O 45	0	0
37	Q	69	Total 69	O 69	0	0
37	R	56	Total 56	O 56	0	0
37	S	89	Total 89	O 89	0	0
37	T	36	Total 36	O 36	0	0
37	U	39	Total 39	O 39	0	0
37	V	27	Total 27	O 27	0	0
37	W	15	Total 15	O 15	0	0
37	X	73	Total 73	O 73	0	0
37	Y	30	Total 30	O 30	0	0
37	Z	93	Total 93	O 93	0	0
37	1	38	Total 38	O 38	0	0

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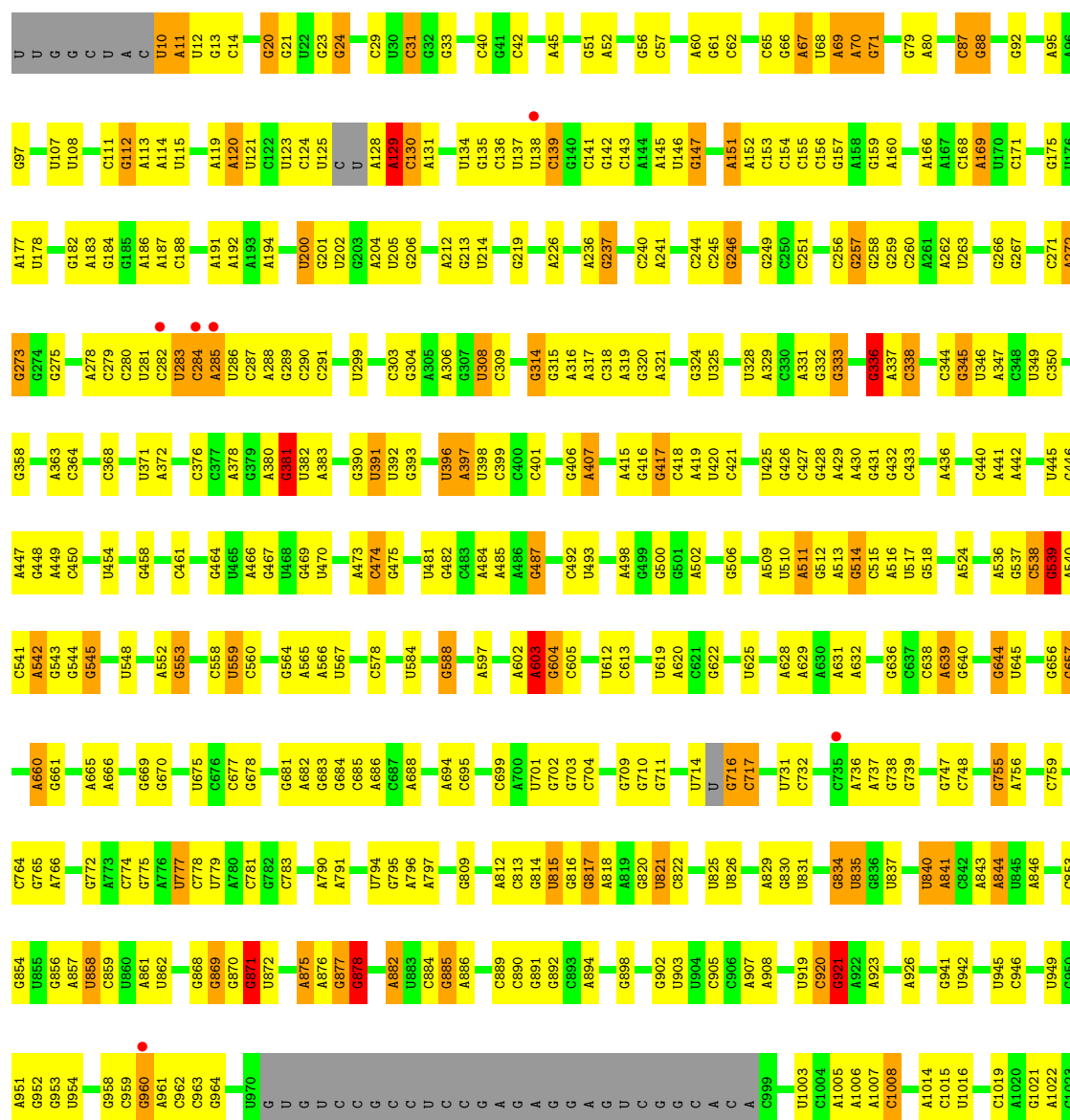
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	57	Total 57	O 57	0	0
37	3	39	Total 39	O 39	0	0
37	4	72	Total 72	O 72	0	0

### 3 Residue-property plots

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

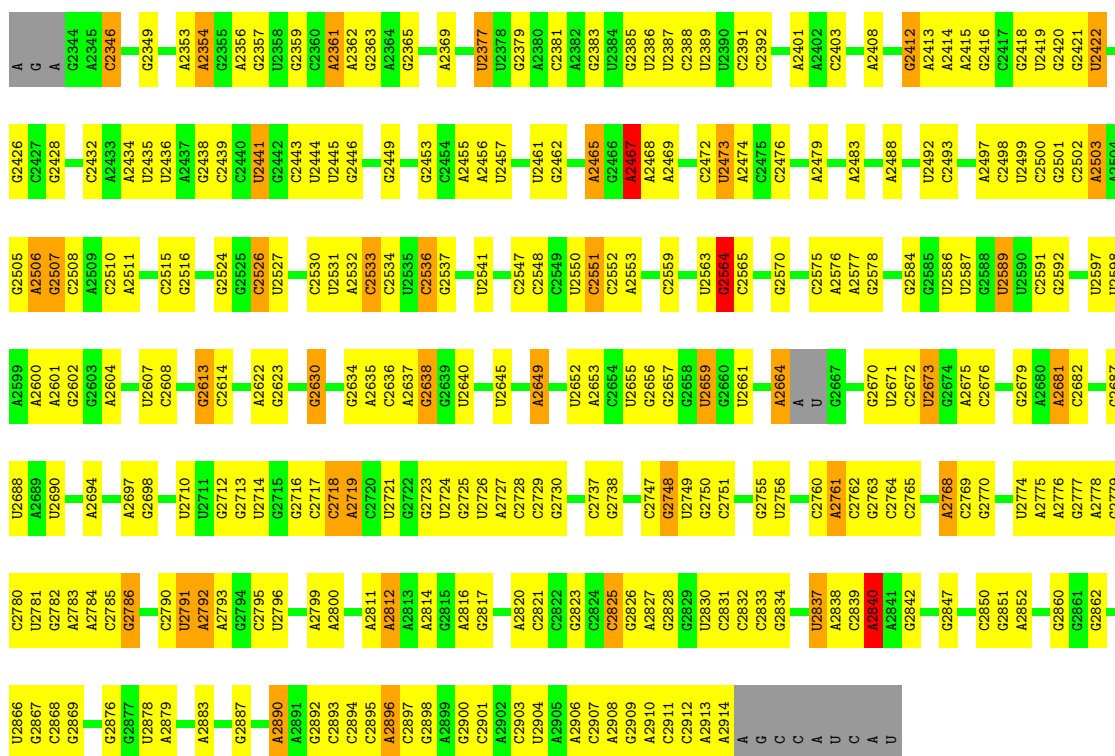
#### • Molecule 1: 23S rRNA

Chain A: 



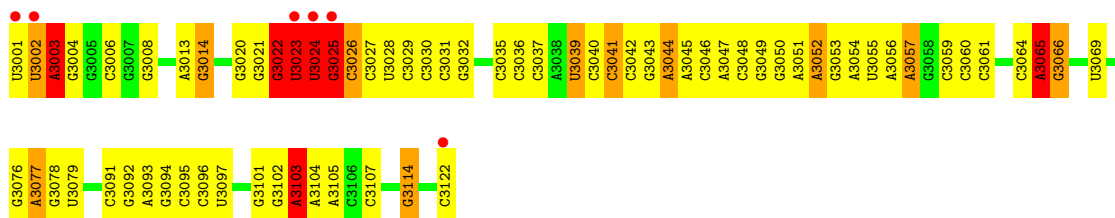






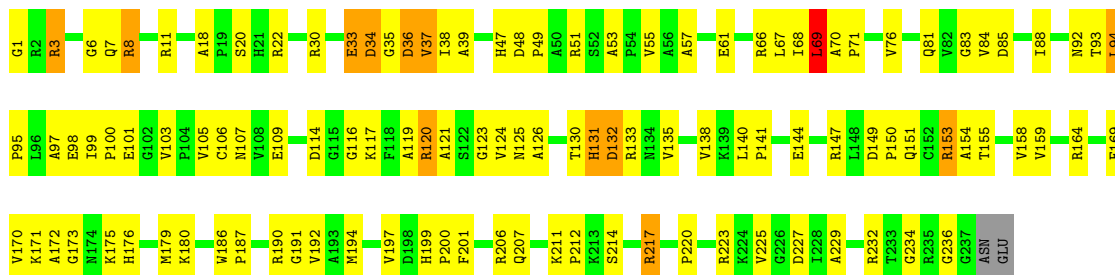
### • Molecule 2: 5S RRNA

Chain B:



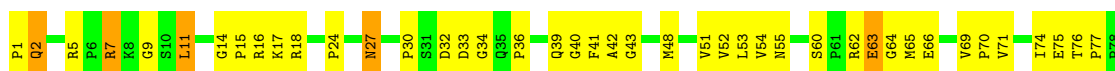
### • Molecule 3: RIBOSOMAL PROTEIN L2

Chain C:



### • Molecule 4: RIBOSOMAL PROTEIN L3

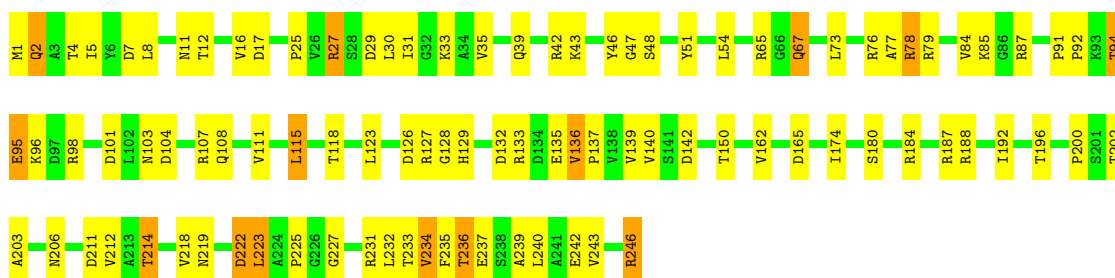
Chain D:





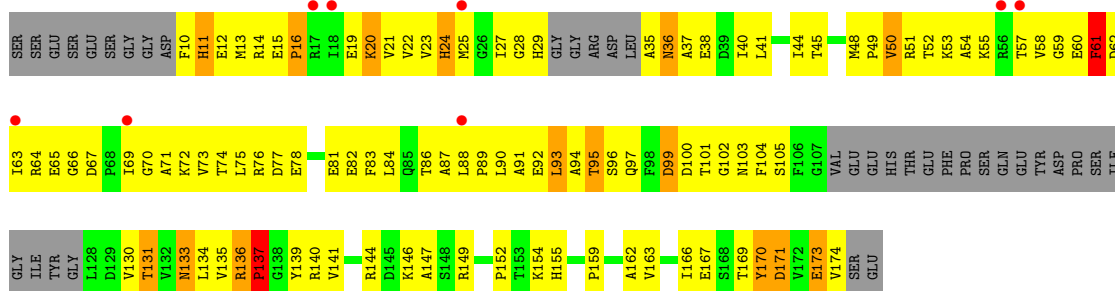
### • Molecule 5: RIBOSOMAL PROTEIN L4

Chain E:



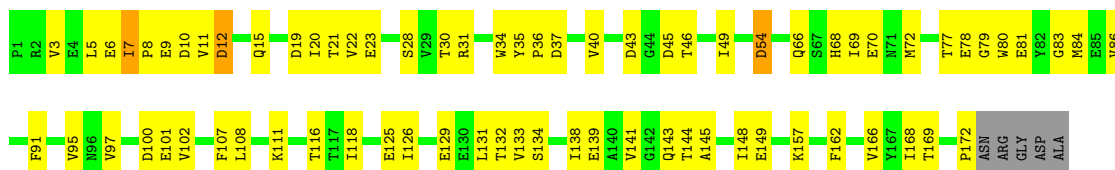
### • Molecule 6: RIBOSOMAL PROTEIN L5

Chain F:



### • Molecule 7: RIBOSOMAL PROTEIN L6

Chain G:



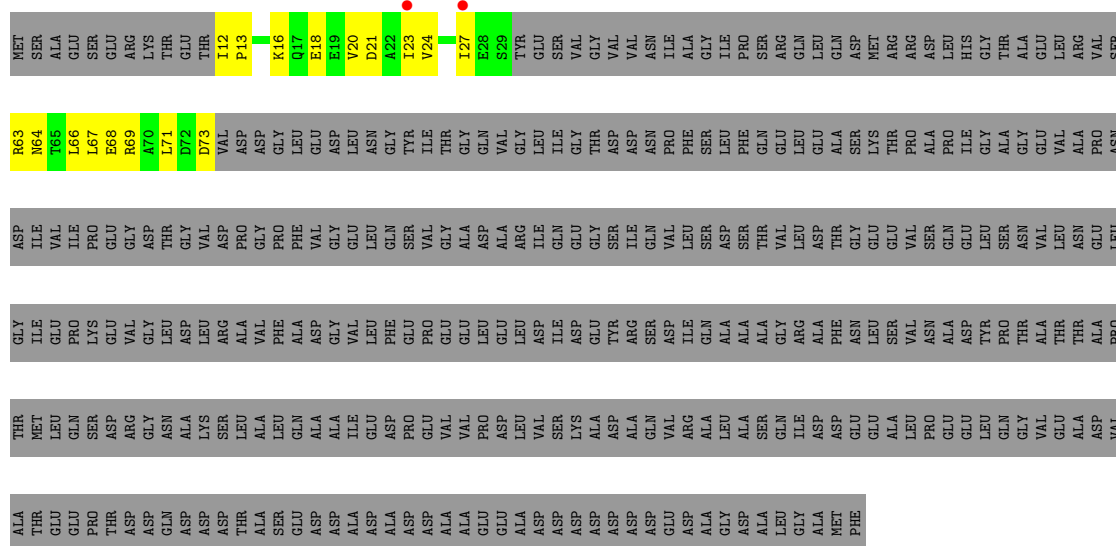
### • Molecule 8: RIBOSOMAL PROTEIN L7AE

Chain H:



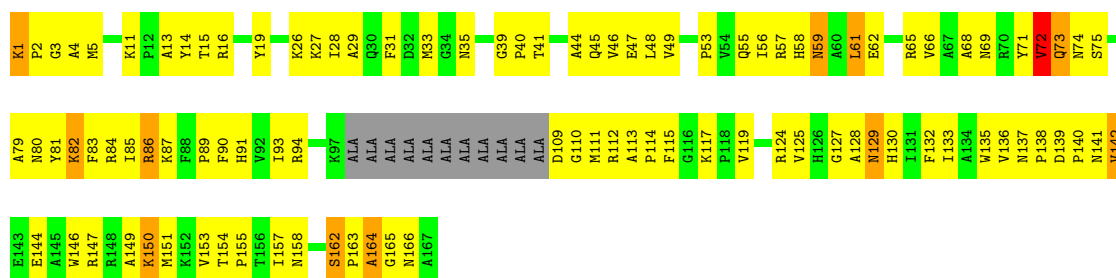
### • Molecule 9: RIBOSOMAL PROTEIN L10

Chain I:



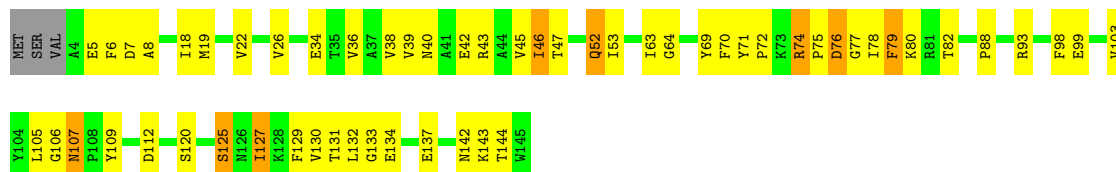
### • Molecule 10: RIBOSOMAL PROTEIN L10E

Chain J:



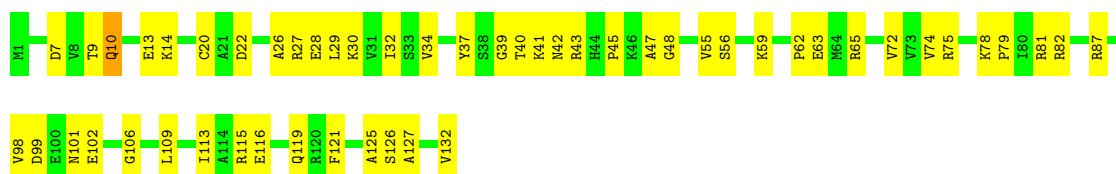
### • Molecule 11: RIBOSOMAL PROTEIN L13

Chain K:



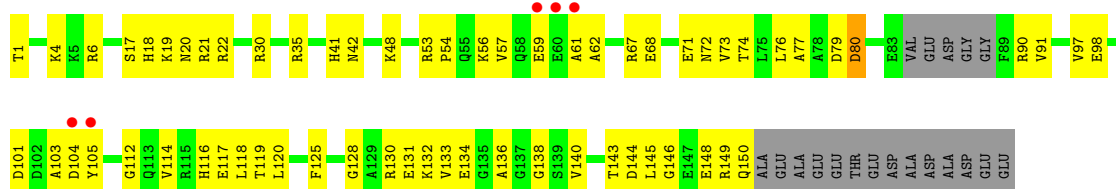
### • Molecule 12: RIBOSOMAL PROTEIN L14

Chain L:



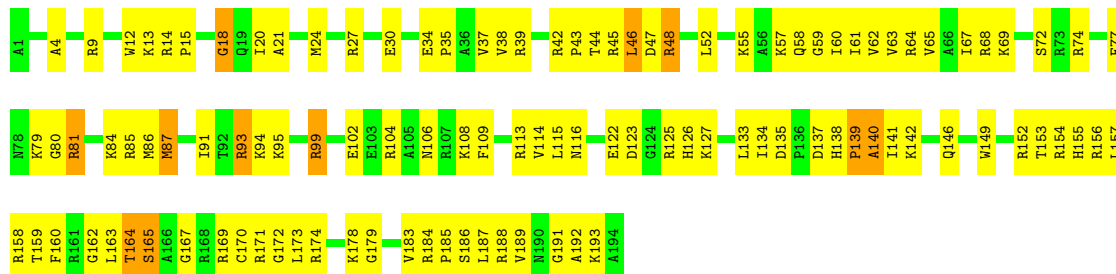
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M:



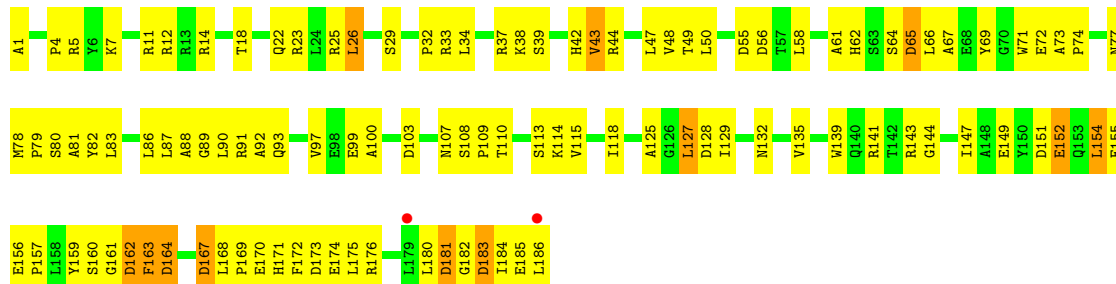
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N:



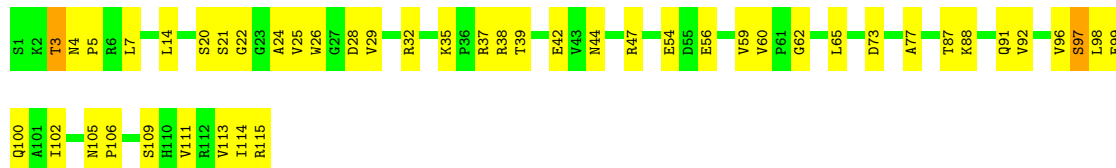
• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O:



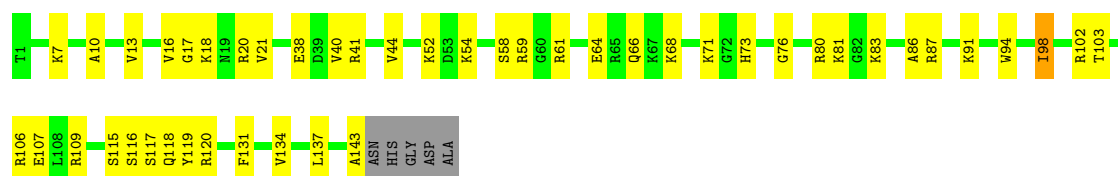
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P:



• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q:



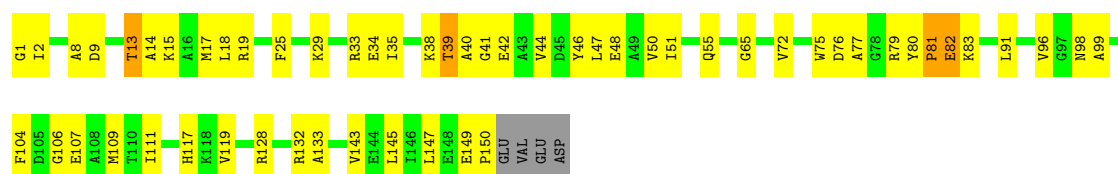
- Molecule 18: RIBOSOMAL PROTEIN L21E

Chain R:



- Molecule 19: RIBOSOMAL PROTEIN L22

Chain S:



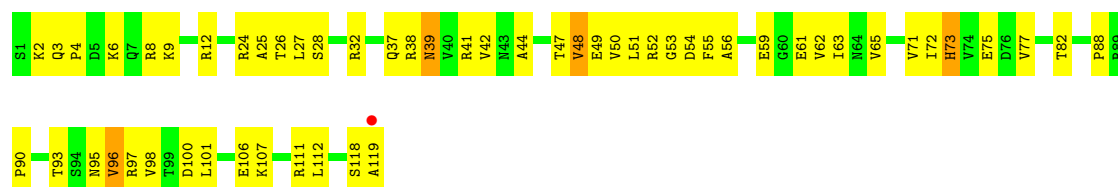
- Molecule 20: RIBOSOMAL PROTEIN L23

Chain T:



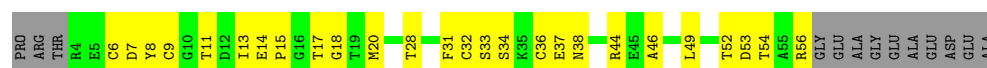
- Molecule 21: RIBOSOMAL PROTEIN L24

Chain U:



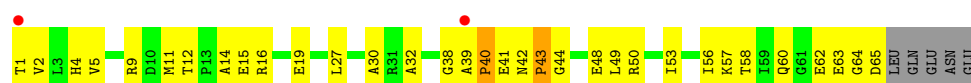
- Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V:



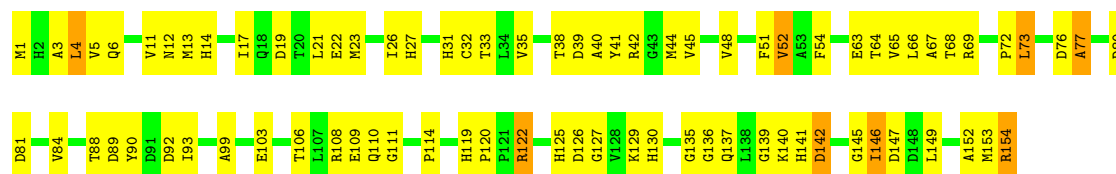
- Molecule 23: RIBOSOMAL PROTEIN L29

Chain W:



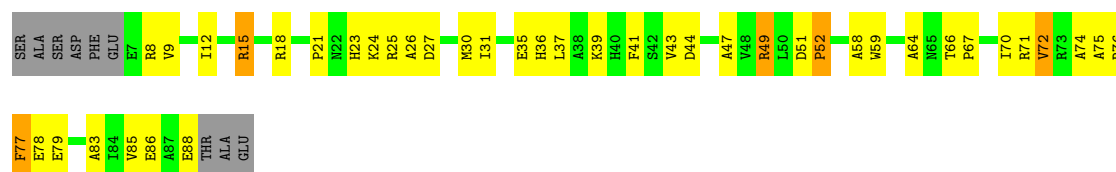
- Molecule 24: RIBOSOMAL PROTEIN L30

Chain X:



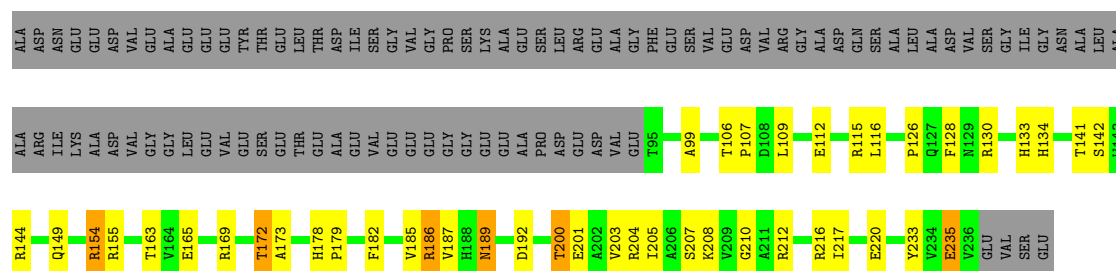
- Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y:



- Molecule 26: RIBOSOMAL PROTEIN L32E

Chain Z:



- Molecule 27: RIBOSOMAL PROTEIN L37Ae

Chain 1:



- Molecule 28: RIBOSOMAL PROTEIN L37E

Chain 2:

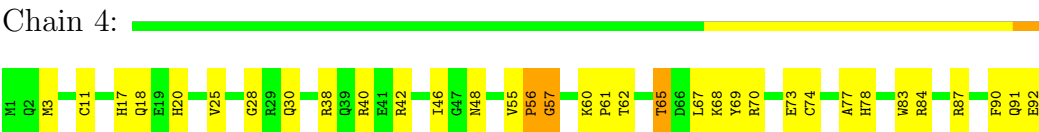


- Molecule 29: RIBOSOMAL PROTEIN L39E

Chain 3:



- Molecule 30: RIBOSOMAL PROTEIN L44E





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.75Å 301.57Å 574.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-3.20) 87.9 (49.69-3.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.250 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 366469 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, ZIT, CD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	1/66076 (0.0%)	0.76	33/103052 (0.0%)
2	B	0.92	16/2905 (0.6%)	0.98	20/4528 (0.4%)
3	C	0.47	0/1787	0.75	0/2409
4	D	0.52	0/2689	0.74	0/3652
5	E	0.49	0/1883	0.73	0/2551
6	F	0.43	0/1111	0.68	0/1498
7	G	0.48	0/1382	0.67	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.51	0/241	0.63	0/324
10	J	0.50	0/1246	0.82	2/1686 (0.1%)
11	K	0.53	0/1135	0.69	0/1530
12	L	0.57	1/1003 (0.1%)	0.78	0/1351
13	M	0.47	0/1126	0.76	0/1504
14	N	0.56	0/1633	0.81	1/2180 (0.0%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.49	0/873	0.69	0/1181
17	Q	0.49	0/1143	0.66	0/1521
18	R	0.52	0/748	0.78	0/1005
19	S	0.52	0/1172	0.77	0/1578
20	T	0.48	0/648	0.69	0/875
21	U	0.46	0/957	0.73	0/1289
22	V	0.47	0/417	0.67	0/562
23	W	0.43	0/502	0.63	0/675
24	X	0.52	0/1218	0.72	0/1655
25	Y	0.49	0/664	0.71	0/895
26	Z	0.50	0/1146	0.73	0/1536
27	1	0.52	0/575	0.75	0/763
28	2	0.57	0/437	0.78	0/578
29	3	0.45	0/398	0.63	0/527
30	4	0.57	0/771	0.73	0/1024
All	All	0.57	18/98255 (0.0%)	0.76	56/147027 (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	A	1	141
2	B	0	5
All	All	1	146

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3025	G	O3'-P	10.69	1.74	1.61
2	B	3025	G	C4'-O4'	9.77	1.58	1.45
2	B	3023	U	C2'-O2'	9.46	1.53	1.41
2	B	3026	C	P-O5'	-8.76	1.50	1.59
2	B	3003	A	C5'-C4'	8.50	1.61	1.51

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.12	63.13	105.20
1	A	1164	U	OP2-P-O3'	-17.65	66.37	105.20
1	A	1165	G	O5'-P-OP1	-12.66	94.31	105.70
2	B	3024	U	O5'-P-OP2	11.59	124.60	110.70
2	B	3026	C	O5'-P-OP2	-11.13	95.68	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	146	U	Sidechain
1	A	20	G	Sidechain
1	A	24	G	Sidechain
1	A	33	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	A	59017	0	29803	1165	0
2	B	2600	0	1326	84	0
3	C	1754	0	1763	129	0
4	D	2624	0	2533	180	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	84	0
8	H	885	0	854	66	0
9	I	240	0	231	25	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	56	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	159	0
15	O	1444	0	1401	142	0
16	P	864	0	873	46	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	28	0
19	S	1149	0	1122	64	0
20	T	641	0	605	22	0
21	U	949	0	923	55	0
22	V	410	0	364	36	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	59	0
27	1	563	0	597	51	0
28	2	430	0	426	28	0
29	3	393	0	406	30	0
30	4	755	0	728	41	0
31	A	52	0	72	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	1	0
32	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	C	1	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	4	0
35	L	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	2	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	38	0	0	8	0
37	2	57	0	0	4	0
37	3	39	0	0	4	0
37	4	72	0	0	12	0
37	A	5898	0	0	232	0
37	B	140	0	0	15	0
37	C	129	0	0	24	0
37	D	152	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	E	169	0	0	34	0
37	F	52	0	0	18	0
37	G	42	0	0	13	0
37	H	28	0	0	10	0
37	I	21	0	0	5	0
37	J	81	0	0	17	0
37	K	56	0	0	6	0
37	L	61	0	0	13	0
37	M	81	0	0	19	0
37	N	129	0	0	22	0
37	O	68	0	0	20	0
37	P	45	0	0	13	0
37	Q	69	0	0	6	0
37	R	56	0	0	3	0
37	S	89	0	0	8	0
37	T	36	0	0	4	0
37	U	39	0	0	5	0
37	V	27	0	0	5	0
37	W	15	0	0	3	0
37	X	73	0	0	7	0
37	Y	30	0	0	8	0
37	Z	93	0	0	14	0
All	All	98587	0	59571	3047	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 20.

The worst 5 of 3047 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.26	1.13
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.33	1.11
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.67	1.10
1:A:871:G:H8	1:A:871:G:H5'	1.14	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	C	235/239 (98%)	204 (87%)	26 (11%)	5 (2%)	11	55
4	D	335/337 (99%)	303 (90%)	23 (7%)	9 (3%)	8	46
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	43	88
6	F	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	1	5
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	14	62
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	6	38
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	11	55
12	L	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	15	64
13	M	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	16	66
14	N	192/194 (99%)	174 (91%)	15 (8%)	3 (2%)	14	63
15	O	184/186 (99%)	164 (89%)	13 (7%)	7 (4%)	5	34
16	P	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	25	76
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	30	80
18	R	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	21	72
19	S	148/154 (96%)	139 (94%)	8 (5%)	1 (1%)	30	80
20	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
21	U	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	25	76
22	V	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	11	56
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	6	39
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	30	80
25	Y	80/91 (88%)	71 (89%)	8 (10%)	1 (1%)	18	68
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	61 (86%)	8 (11%)	2 (3%)	8	44
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	10	53
All	All	3633/4235 (86%)	3285 (90%)	281 (8%)	67 (2%)	13	60

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

### 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	C	179/181 (99%)	166 (93%)	13 (7%)	20	62
4	D	282/282 (100%)	263 (93%)	19 (7%)	23	66
5	E	193/193 (100%)	175 (91%)	18 (9%)	13	46
6	F	117/147 (80%)	107 (92%)	10 (8%)	15	53
7	G	152/155 (98%)	148 (97%)	4 (3%)	59	90
8	H	92/92 (100%)	91 (99%)	1 (1%)	84	96
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	14	49
11	K	118/121 (98%)	108 (92%)	10 (8%)	15	53
12	L	106/106 (100%)	103 (97%)	3 (3%)	56	89
13	M	112/126 (89%)	108 (96%)	4 (4%)	47	85
14	N	166/166 (100%)	158 (95%)	8 (5%)	35	79
15	O	149/149 (100%)	143 (96%)	6 (4%)	42	83
16	P	93/93 (100%)	90 (97%)	3 (3%)	51	87
17	Q	113/116 (97%)	110 (97%)	3 (3%)	57	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	R	79/79 (100%)	75 (95%)	4 (5%)	33	77
19	S	117/121 (97%)	114 (97%)	3 (3%)	59	90
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	101 (96%)	4 (4%)	44	84
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	68	92
24	X	130/130 (100%)	122 (94%)	8 (6%)	26	70
25	Y	66/73 (90%)	61 (92%)	5 (8%)	19	60
26	Z	120/195 (62%)	112 (93%)	8 (7%)	23	66
27	1	56/56 (100%)	53 (95%)	3 (5%)	31	75
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	61	91
30	4	79/79 (100%)	78 (99%)	1 (1%)	80	95
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	34	78

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	72	VAL
11	K	125	SER
26	Z	163	THR
10	J	82	LYS
11	K	46	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	100	GLN
29	3	16	ASN
13	M	116	HIS
14	N	176	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	245 (8%)	36 (1%)
2	B	121/122 (99%)	14 (11%)	6 (4%)
All	All	2868/3044 (94%)	259 (9%)	42 (1%)

5 of 259 RNA backbone outliers are listed below:

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

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1450	C
1	A	1856	C
2	B	3025	G
1	A	1563	G
1	A	1692	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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
31	ZIT	A	8600	-	54,54,54	1.64	11 (20%)	83,83,83	1.28	8 (9%)

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
31	ZIT	A	8600	-	-	0/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	8600	ZIT	C2-C3	4.28	1.65	1.55
31	A	8600	ZIT	C7-C6	3.95	1.61	1.54
31	A	8600	ZIT	C3A-N3A	3.95	1.57	1.48
31	A	8600	ZIT	C11-N10	3.21	1.54	1.49
31	A	8600	ZIT	C2B-C3B	2.89	1.60	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	8600	ZIT	C6-C5-C4	-4.02	108.35	114.19
31	A	8600	ZIT	C21-N10-C9	3.13	113.83	110.02
31	A	8600	ZIT	O1A-C5-C6	2.90	110.17	106.28
31	A	8600	ZIT	C17-C2-C3	2.55	118.73	112.84
31	A	8600	ZIT	O1B-C3-C4	2.50	111.08	108.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.28	22 (0%) 83 35	27, 56, 101, 149	0
2	B	122/122 (100%)	-0.11	6 (4%) 28 6	43, 71, 98, 158	0
3	C	237/239 (99%)	-0.06	0 100 100	38, 62, 93, 114	0
4	D	337/337 (100%)	-0.13	0 100 100	29, 64, 90, 99	0
5	E	246/246 (100%)	-0.13	0 100 100	30, 58, 81, 92	0
6	F	140/176 (79%)	0.67	8 (5%) 23 5	61, 108, 124, 131	0
7	G	172/177 (97%)	0.10	0 100 100	50, 76, 97, 102	0
8	H	119/119 (100%)	0.14	0 100 100	62, 82, 106, 110	0
9	I	29/348 (8%)	0.93	2 (6%) 17 4	80, 100, 109, 109	0
10	J	156/167 (93%)	-0.06	0 100 100	43, 65, 94, 101	0
11	K	142/145 (97%)	-0.10	0 100 100	45, 57, 80, 97	0
12	L	132/132 (100%)	-0.17	0 100 100	38, 58, 80, 87	0
13	M	145/164 (88%)	0.22	5 (3%) 43 9	33, 77, 113, 123	0
14	N	194/194 (100%)	-0.14	0 100 100	42, 56, 73, 84	0
15	O	186/186 (100%)	0.13	2 (1%) 77 27	52, 74, 114, 124	0
16	P	115/115 (100%)	0.01	0 100 100	52, 66, 84, 88	0
17	Q	143/148 (96%)	0.14	0 100 100	45, 65, 80, 89	0
18	R	95/95 (100%)	-0.08	0 100 100	38, 54, 70, 82	0
19	S	150/154 (97%)	-0.13	0 100 100	40, 54, 74, 82	0
20	T	81/84 (96%)	-0.04	0 100 100	55, 71, 90, 97	0
21	U	119/119 (100%)	0.24	1 (0%) 83 35	52, 69, 92, 103	0
22	V	53/66 (80%)	-0.09	0 100 100	51, 64, 82, 89	0
23	W	65/70 (92%)	0.45	2 (3%) 47 10	62, 83, 118, 124	0
24	X	154/154 (100%)	-0.28	0 100 100	38, 56, 76, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	-0.00	0 100 100	53, 67, 91, 107	0
26	Z	142/240 (59%)	-0.11	0 100 100	33, 56, 77, 94	0
27	1	73/73 (100%)	0.01	1 (1%) 72 22	59, 71, 87, 94	0
28	2	56/56 (100%)	-0.28	0 100 100	35, 46, 51, 52	0
29	3	46/48 (95%)	0.04	0 100 100	44, 72, 96, 106	0
30	4	92/92 (100%)	0.13	0 100 100	44, 66, 79, 90	0
All	All	6577/7279 (90%)	-0.11	49 (0%) 81 38	27, 62, 101, 158	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3001	U	8.4
2	B	3024	U	4.7
2	B	3023	U	4.6
1	A	1173	A	4.4
1	A	735	C	3.5

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	A	8306	1/1	0.36	142.07	41,41,41,41	0
34	NA	A	8384	1/1	1.25	121.61	90,90,90,90	0
34	NA	A	8342	1/1	0.33	83.79	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	A	8515	1/1	0.69	80.71	110,110,110,110	0
34	NA	A	8374	1/1	1.43	74.57	89,89,89,89	0
34	NA	A	8385	1/1	0.62	69.55	73,73,73,73	0
34	NA	A	8356	1/1	0.65	68.48	78,78,78,78	0
34	NA	A	8360	1/1	0.89	46.29	59,59,59,59	0
34	NA	A	8363	1/1	0.95	43.09	79,79,79,79	0
34	NA	A	8318	1/1	0.43	42.82	45,45,45,45	0
34	NA	A	8362	1/1	0.64	35.87	62,62,62,62	0
34	NA	A	8378	1/1	1.04	34.74	48,48,48,48	0
32	MG	A	8042	1/1	0.24	33.33	52,52,52,52	0
34	NA	A	8307	1/1	0.46	31.60	48,48,48,48	0
34	NA	A	8321	1/1	0.47	30.94	42,42,42,42	0
34	NA	B	8383	1/1	0.41	28.92	40,40,40,40	0
34	NA	A	8303	1/1	0.42	28.25	54,54,54,54	0
32	MG	A	8064	1/1	0.53	27.42	36,36,36,36	0
34	NA	A	8323	1/1	0.46	27.14	57,57,57,57	0
34	NA	A	8377	1/1	0.32	22.44	68,68,68,68	0
34	NA	A	8371	1/1	0.35	22.39	48,48,48,48	0
34	NA	A	8354	1/1	0.47	21.97	54,54,54,54	0
34	NA	A	8326	1/1	0.91	21.81	92,92,92,92	0
34	NA	A	8316	1/1	0.41	21.35	61,61,61,61	0
34	NA	A	8329	1/1	0.51	20.79	70,70,70,70	0
34	NA	A	8358	1/1	0.57	20.05	107,107,107,107	0
35	CL	A	8522	1/1	0.71	19.98	83,83,83,83	0
32	MG	A	8066	1/1	0.69	17.72	48,48,48,48	0
34	NA	A	8340	1/1	0.43	17.14	56,56,56,56	0
34	NA	J	8322	1/1	0.47	15.45	62,62,62,62	0
34	NA	M	8380	1/1	0.72	15.19	75,75,75,75	0
32	MG	A	8024	1/1	0.77	14.87	79,79,79,79	0
34	NA	A	8350	1/1	0.28	14.46	43,43,43,43	0
35	CL	A	8505	1/1	0.46	14.41	92,92,92,92	0
34	NA	A	8352	1/1	0.31	14.39	56,56,56,56	0
34	NA	A	8361	1/1	0.47	13.46	46,46,46,46	0
32	MG	A	8082	1/1	0.23	13.17	83,83,83,83	0
34	NA	A	8370	1/1	0.18	11.57	42,42,42,42	0
35	CL	A	8503	1/1	0.53	10.88	74,74,74,74	0
34	NA	A	8359	1/1	0.42	10.83	75,75,75,75	0
34	NA	A	8335	1/1	0.30	10.57	61,61,61,61	0
34	NA	A	8372	1/1	0.45	10.26	87,87,87,87	0
34	NA	A	8376	1/1	0.27	9.46	49,49,49,49	0
34	NA	A	8315	1/1	0.28	9.12	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8369	1/1	0.32	9.08	55,55,55,55	0
34	NA	A	8373	1/1	0.45	8.44	67,67,67,67	0
34	NA	S	8386	1/1	0.48	7.66	97,97,97,97	0
34	NA	A	8382	1/1	0.27	7.21	74,74,74,74	0
34	NA	A	8349	1/1	0.31	7.16	57,57,57,57	0
34	NA	A	8302	1/1	0.23	7.03	52,52,52,52	0
35	CL	O	8507	1/1	0.47	6.98	84,84,84,84	0
32	MG	A	8041	1/1	0.27	6.84	69,69,69,69	0
34	NA	A	8313	1/1	0.22	6.77	66,66,66,66	0
35	CL	D	8519	1/1	0.45	6.01	65,65,65,65	0
32	MG	A	8092	1/1	0.30	5.90	95,95,95,95	0
31	ZIT	A	8600	52/52	0.34	5.74	81,91,95,96	0
34	NA	A	8341	1/1	0.23	5.69	63,63,63,63	0
34	NA	A	8368	1/1	0.21	5.54	65,65,65,65	0
34	NA	A	8366	1/1	0.29	5.53	79,79,79,79	0
34	NA	A	8305	1/1	0.23	5.40	46,46,46,46	0
34	NA	A	8355	1/1	0.48	5.21	60,60,60,60	0
32	MG	1	8105	1/1	0.50	4.98	38,38,38,38	0
32	MG	A	8102	1/1	0.26	4.62	75,75,75,75	0
35	CL	C	8509	1/1	0.28	4.43	69,69,69,69	0
34	NA	A	8375	1/1	0.29	4.12	86,86,86,86	0
34	NA	A	8364	1/1	0.22	4.10	52,52,52,52	0
32	MG	A	8097	1/1	0.20	4.08	45,45,45,45	0
34	NA	A	8325	1/1	0.20	3.93	62,62,62,62	0
35	CL	R	8511	1/1	0.58	3.88	102,102,102,102	0
34	NA	A	8365	1/1	0.54	3.76	76,76,76,76	0
32	MG	A	8053	1/1	0.17	3.27	40,40,40,40	0
35	CL	4	8504	1/1	0.61	3.24	93,93,93,93	0
32	MG	A	8114	1/1	0.24	3.18	47,47,47,47	0
32	MG	A	8103	1/1	0.18	2.99	76,76,76,76	0
34	NA	A	8310	1/1	0.21	2.93	29,29,29,29	0
35	CL	A	8520	1/1	0.17	2.75	65,65,65,65	0
34	NA	A	8328	1/1	0.24	2.71	61,61,61,61	0
32	MG	A	8100	1/1	0.17	2.71	88,88,88,88	0
34	NA	A	8367	1/1	0.21	2.66	38,38,38,38	0
34	NA	A	8379	1/1	0.20	2.62	52,52,52,52	0
32	MG	A	8044	1/1	0.19	2.60	58,58,58,58	0
34	NA	A	8331	1/1	0.19	2.30	55,55,55,55	0
32	MG	A	8070	1/1	0.17	2.26	46,46,46,46	0
34	NA	A	8381	1/1	0.18	2.26	61,61,61,61	0
34	NA	T	8312	1/1	0.29	2.20	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	K	8501	1/1	0.32	2.08	81,81,81,81	0
32	MG	A	8060	1/1	0.19	1.99	51,51,51,51	0
32	MG	A	8098	1/1	0.24	1.89	52,52,52,52	0
32	MG	A	8050	1/1	0.28	1.81	67,67,67,67	0
35	CL	P	8508	1/1	0.39	1.77	97,97,97,97	0
34	NA	S	8337	1/1	0.20	1.68	58,58,58,58	0
35	CL	K	8516	1/1	0.27	1.63	53,53,53,53	0
34	NA	A	8330	1/1	0.21	1.53	57,57,57,57	0
32	MG	A	8067	1/1	0.22	1.24	51,51,51,51	0
34	NA	U	8343	1/1	0.23	0.99	38,38,38,38	0
35	CL	A	8514	1/1	0.21	0.87	57,57,57,57	0
32	MG	A	8099	1/1	0.16	0.84	55,55,55,55	0
35	CL	S	8506	1/1	0.22	0.77	69,69,69,69	0
32	MG	A	8049	1/1	0.19	0.48	74,74,74,74	0
34	NA	A	8308	1/1	0.16	0.48	53,53,53,53	0
35	CL	A	8510	1/1	0.33	0.47	97,97,97,97	0
32	MG	A	8013	1/1	0.17	0.29	56,56,56,56	0
34	NA	C	8345	1/1	0.21	0.09	57,57,57,57	0
32	MG	A	8112	1/1	0.18	0.02	50,50,50,50	0
34	NA	A	8336	1/1	0.17	0.02	85,85,85,85	0
34	NA	E	8304	1/1	0.19	-0.03	32,32,32,32	0
34	NA	A	8332	1/1	0.15	-0.15	50,50,50,50	0
34	NA	A	8314	1/1	0.16	-0.41	48,48,48,48	0
32	MG	L	8069	1/1	0.16	-0.49	79,79,79,79	0
35	CL	A	8513	1/1	0.14	-0.69	67,67,67,67	0
36	CD	I	8403	1/1	0.12	-0.81	77,77,77,77	0
32	MG	A	8058	1/1	0.17	-0.83	62,62,62,62	0
35	CL	K	8521	1/1	0.17	-0.91	64,64,64,64	0
32	MG	Z	8109	1/1	0.15	-0.92	61,61,61,61	0
34	NA	K	8346	1/1	0.20	-0.92	33,33,33,33	0
34	NA	A	8311	1/1	0.13	-0.94	63,63,63,63	0
32	MG	A	8113	1/1	0.15	-0.95	53,53,53,53	0
34	NA	A	8353	1/1	0.13	-1.00	46,46,46,46	0
33	K	A	8202	1/1	0.15	-1.01	61,61,61,61	0
32	MG	A	8080	1/1	0.14	-1.03	65,65,65,65	0
34	NA	A	8333	1/1	0.12	-1.04	51,51,51,51	0
32	MG	A	8101	1/1	0.14	-1.04	60,60,60,60	0
33	K	A	8201	1/1	0.14	-1.04	70,70,70,70	0
32	MG	A	8086	1/1	0.11	-1.04	56,56,56,56	0
32	MG	A	8116	1/1	0.11	-1.11	54,54,54,54	0
35	CL	N	8518	1/1	0.20	-1.13	65,65,65,65	0
32	MG	A	8085	1/1	0.15	-1.14	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CD	4	8404	1/1	0.11	-1.15	75,75,75,75	0
34	NA	A	8357	1/1	0.10	-1.16	64,64,64,64	0
34	NA	A	8324	1/1	0.09	-1.17	48,48,48,48	0
32	MG	A	8090	1/1	0.14	-1.25	47,47,47,47	0
35	CL	K	8502	1/1	0.14	-1.28	87,87,87,87	0
32	MG	A	8059	1/1	0.14	-1.31	56,56,56,56	0
32	MG	A	8004	1/1	0.11	-1.33	60,60,60,60	0
36	CD	V	8401	1/1	0.10	-1.34	75,75,75,75	0
32	MG	A	8063	1/1	0.15	-1.36	92,92,92,92	0
32	MG	A	8081	1/1	0.14	-1.37	67,67,67,67	0
34	NA	J	8309	1/1	0.15	-1.38	43,43,43,43	0
32	MG	A	8057	1/1	0.17	-1.43	54,54,54,54	0
32	MG	A	8071	1/1	0.13	-1.51	85,85,85,85	0
35	CL	A	8517	1/1	0.14	-1.54	52,52,52,52	0
34	NA	A	8319	1/1	0.13	-1.57	57,57,57,57	0
32	MG	A	8047	1/1	0.16	-1.59	81,81,81,81	0
34	NA	B	8351	1/1	0.12	-1.60	54,54,54,54	0
32	MG	A	8106	1/1	0.10	-1.78	71,71,71,71	0
34	NA	A	8334	1/1	0.12	-1.78	45,45,45,45	0
36	CD	2	8402	1/1	0.08	-1.79	70,70,70,70	0
32	MG	4	8078	1/1	0.08	-1.92	54,54,54,54	0
35	CL	L	8512	1/1	0.11	-1.95	55,55,55,55	0
32	MG	A	8096	1/1	0.10	-1.96	64,64,64,64	0
32	MG	A	8107	1/1	0.04	-2.22	60,60,60,60	0
32	MG	U	8073	1/1	0.07	-2.32	62,62,62,62	0
32	MG	A	8008	1/1	0.12	-2.35	61,61,61,61	0
32	MG	A	8087	1/1	0.10	-2.45	75,75,75,75	0
32	MG	A	8005	1/1	0.14	-2.52	60,60,60,60	0
32	MG	A	8017	1/1	0.06	-2.54	42,42,42,42	0
32	MG	A	8032	1/1	0.12	-2.56	63,63,63,63	0
32	MG	D	8055	1/1	0.07	-2.71	51,51,51,51	0
32	MG	A	8062	1/1	0.09	-2.73	61,61,61,61	0
32	MG	A	8076	1/1	0.08	-2.89	75,75,75,75	0
32	MG	A	8033	1/1	0.12	-3.10	36,36,36,36	0
34	NA	R	8348	1/1	0.07	-3.17	39,39,39,39	0
32	MG	A	8074	1/1	0.03	-3.28	52,52,52,52	0
32	MG	A	8012	1/1	0.10	-3.41	35,35,35,35	0
32	MG	A	8011	1/1	0.10	-3.44	44,44,44,44	0
34	NA	S	8338	1/1	0.08	-3.46	49,49,49,49	0
34	NA	N	8347	1/1	0.10	-3.47	23,23,23,23	0
32	MG	A	8068	1/1	0.04	-3.49	56,56,56,56	0
34	NA	A	8317	1/1	0.04	-3.49	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8056	1/1	0.08	-3.51	61,61,61,61	0
32	MG	A	8104	1/1	0.07	-3.53	50,50,50,50	0
32	MG	A	8027	1/1	0.06	-3.57	51,51,51,51	0
34	NA	A	8344	1/1	0.07	-3.60	39,39,39,39	0
34	NA	A	8301	1/1	0.13	-3.82	42,42,42,42	0
32	MG	A	8003	1/1	0.08	-3.99	26,26,26,26	0
32	MG	A	8094	1/1	0.10	-4.17	66,66,66,66	0
32	MG	A	8015	1/1	0.09	-4.22	57,57,57,57	0
32	MG	A	8079	1/1	0.09	-4.29	42,42,42,42	0
32	MG	A	8016	1/1	0.12	-4.34	50,50,50,50	0
32	MG	A	8021	1/1	0.08	-4.35	32,32,32,32	0
32	MG	A	8018	1/1	0.10	-4.35	54,54,54,54	0
32	MG	A	8043	1/1	0.09	-4.56	56,56,56,56	0
32	MG	A	8037	1/1	0.12	-4.67	61,61,61,61	0
32	MG	A	8108	1/1	0.10	-4.77	85,85,85,85	0
32	MG	A	8052	1/1	0.11	-4.79	58,58,58,58	0
32	MG	A	8083	1/1	0.12	-4.81	51,51,51,51	0
32	MG	A	8045	1/1	0.11	-4.83	58,58,58,58	0
32	MG	A	8035	1/1	0.07	-4.85	60,60,60,60	0
32	MG	A	8093	1/1	0.09	-4.90	59,59,59,59	0
32	MG	A	8030	1/1	0.10	-5.03	40,40,40,40	0
32	MG	C	8065	1/1	0.03	-5.07	40,40,40,40	0
32	MG	A	8007	1/1	0.10	-5.14	42,42,42,42	0
32	MG	A	8115	1/1	0.07	-5.26	43,43,43,43	0
32	MG	A	8089	1/1	0.11	-5.59	70,70,70,70	0
32	MG	A	8019	1/1	0.07	-5.61	24,24,24,24	0
32	MG	A	8022	1/1	0.04	-5.67	55,55,55,55	0
32	MG	A	8026	1/1	0.10	-5.83	49,49,49,49	0
32	MG	A	8036	1/1	0.05	-6.13	46,46,46,46	0
32	MG	A	8034	1/1	0.04	-6.23	32,32,32,32	0
32	MG	A	8117	1/1	0.07	-6.38	33,33,33,33	0
32	MG	A	8039	1/1	0.06	-6.46	67,67,67,67	0
32	MG	A	8001	1/1	0.09	-6.54	41,41,41,41	0
32	MG	A	8077	1/1	0.08	-6.56	37,37,37,37	0
32	MG	A	8029	1/1	0.09	-6.77	50,50,50,50	0
32	MG	A	8038	1/1	0.06	-6.80	29,29,29,29	0
32	MG	A	8111	1/1	0.08	-6.83	62,62,62,62	0
32	MG	A	8054	1/1	0.06	-6.97	52,52,52,52	0
32	MG	A	8010	1/1	0.08	-7.15	43,43,43,43	0
32	MG	A	8110	1/1	0.10	-7.41	35,35,35,35	0
32	MG	A	8040	1/1	0.11	-7.42	63,63,63,63	0
32	MG	A	8075	1/1	0.10	-8.21	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8028	1/1	0.05	-8.35	57,57,57,57	0
32	MG	A	8048	1/1	0.07	-8.37	41,41,41,41	0
32	MG	B	8095	1/1	0.07	-8.40	98,98,98,98	0
32	MG	A	8046	1/1	0.08	-8.41	72,72,72,72	0
32	MG	A	8051	1/1	0.11	-8.45	66,66,66,66	0
32	MG	A	8020	1/1	0.07	-8.98	36,36,36,36	0
32	MG	A	8084	1/1	0.06	-9.06	41,41,41,41	0
32	MG	A	8014	1/1	0.07	-9.42	24,24,24,24	0
34	NA	A	8327	1/1	0.10	-10.17	44,44,44,44	0
32	MG	A	8002	1/1	0.07	-10.33	43,43,43,43	0
32	MG	A	8025	1/1	0.04	-11.09	54,54,54,54	0
34	NA	A	8320	1/1	0.10	-12.13	32,32,32,32	0
32	MG	A	8006	1/1	0.03	-12.46	54,54,54,54	0
32	MG	A	8072	1/1	0.11	-12.57	65,65,65,65	0
32	MG	A	8061	1/1	0.04	-13.48	37,37,37,37	0
32	MG	A	8091	1/1	0.06	-13.72	58,58,58,58	0
32	MG	A	8031	1/1	0.03	-16.43	44,44,44,44	0
32	MG	A	8009	1/1	0.06	-16.65	46,46,46,46	0
36	CD	P	8405	1/1	0.08	-17.36	152,152,152,152	0
32	MG	A	8088	1/1	0.12	-21.64	64,64,64,64	0
34	NA	A	8339	1/1	0.04	-24.85	33,33,33,33	0
32	MG	A	8023	1/1	0.03	-56.13	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.