



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 07:31 am BST

PDB ID : 4V9F  
Title : The re-refined crystal structure of the Haloarcula marismortui large ribosomal subunit at 2.4 Angstrom resolution: more complete structure of the L7/L12 and L1 stalk, L5 and LX proteins  
Authors : Gabdulkhakov, A.  
Deposited on : 2012-11-02  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

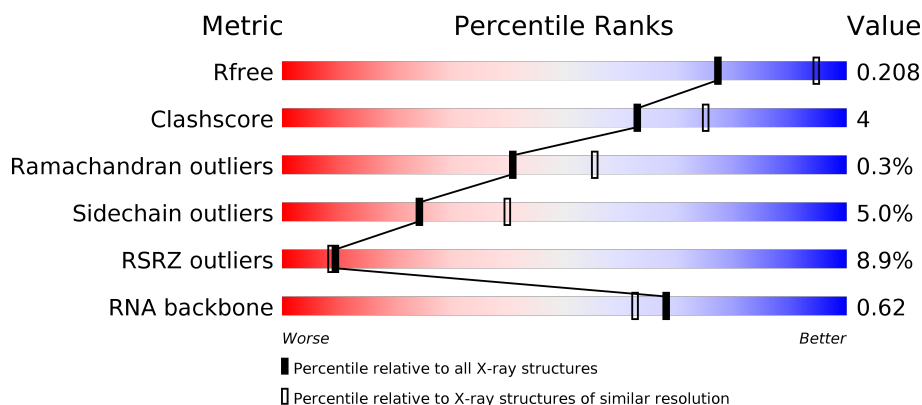
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2910	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• •</div> </div> </div>
2	9	122	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>6%</div> </div> </div>
3	A	240	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
4	B	338	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	255	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	67	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	92	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	
32	4	70	
32	5	70	
33	6	56	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	R	202	-	-	-	X
37	CL	9	203	-	-	X	-
38	ACY	0	8213	-	-	X	-

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 103831 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2808	Total	C	N	O	P	0	0	0
			60186	26859	11069	19451	2807			

- 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
			2599	1160	471	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	1130	345	383	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	166	Total	C	N	O	S	0	0	0
			1299	812	227	256	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	174	Total	C	N	O	S	0	0	0
			1376	850	230	292	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
			889	551	141	196	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	254	Total	C	N	O	S	0	0	0
			1805	1113	304	386	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	165	Total	C	N	O	S	0	0	0
			1320	822	246	246	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	145	Total	C	N	O	S	0	0	0
			1088	681	170	236	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	144	Total	C	N	O	S	0	0	0
			1132	704	201	224	3			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	149	Total	C	N	O	0	0	0
			1138	682	226	230			

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	195	Total	C	N	O	S	0	0	0
			1568	949	335	283	1			

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

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

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

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

- Molecule 18 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	144	Total	C	N	O	0	0	0
			1144	687	231	226			

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

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

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

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

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

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

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

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

- Molecule 23 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	56	Total	C	N	O	S	0	0	0
			435	259	81	90	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	90	Total	C	N	O	S	0	0	0
			714	438	137	138	1			

- Molecule 27 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	144	Total	C	N	O		0	0	0
			1146	696	230	220				

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	83	Total	C	N	O	S	0	0	0
			645	387	127	126	5			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	49	Total	C	N	O	S	0	0	0
			421	254	93	73	1			

- Molecule 31 is a protein called 50S ribosomal protein L44e.

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

- Molecule 32 is a protein called 50S ribosomal protein L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	4	58	Total	C	N	O	0	0	0
			290	174	58	58			
32	5	56	Total	C	N	O	0	0	0
			280	168	56	56			

- Molecule 33 is a protein called 50S ribosomal protein LX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	6	55	Total	C	N	O	0	0	0
			441	271	78	92			

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	125	Total	Mg	0	0
			125	125		
34	Y	4	Total	Mg	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	Mg 1	0	0
34	A	3	Total 3	Mg 3	0	0
34	T	1	Total 1	Mg 1	0	0
34	N	1	Total 1	Mg 1	0	0
34	9	1	Total 1	Mg 1	0	0
34	L	1	Total 1	Mg 1	0	0
34	3	1	Total 1	Mg 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total 2	K 2	0	0
35	O	1	Total 1	K 1	0	0

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	72	Total 72	Na 72	0	0
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	H	2	Total 2	Na 2	0	0
36	C	1	Total 1	Na 1	0	0
36	A	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0

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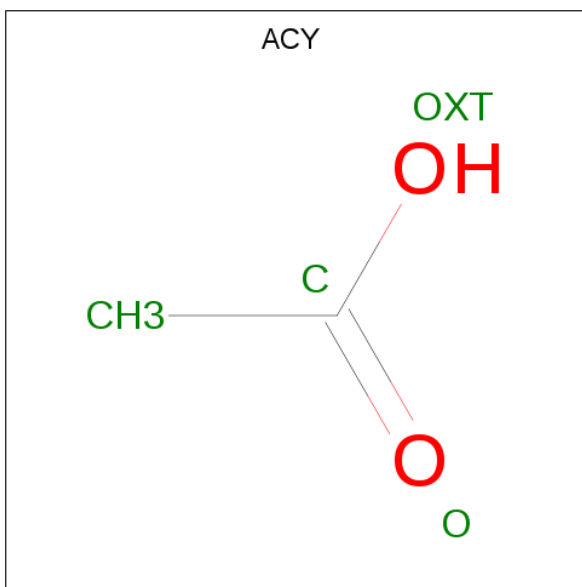
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	L	2	Total 2	Na 2	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	12	Total 12	Cl 12	0	0
37	G	1	Total 1	Cl 1	0	0
37	J	3	Total 3	Cl 3	0	0
37	Y	1	Total 1	Cl 1	0	0
37	B	2	Total 2	Cl 2	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	2	Total 2	Cl 2	0	0
37	R	2	Total 2	Cl 2	0	0
37	9	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	F	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	1	Total C O 4 2 2	0	0
38	0	1	Total C O 4 2 2	0	0
38	0	1	Total C O 4 2 2	0	0
38	W	1	Total C O 4 2 2	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	O	1	Total Cd 1 1	0	0
39	Z	1	Total Cd 1 1	0	0
39	1	1	Total Cd 1 1	0	0
39	3	1	Total Cd 1 1	0	0
39	U	1	Total Cd 1 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5924	Total 5924	O 5924	0	0
40	9	153	Total 153	O 153	0	0
40	A	126	Total 126	O 126	0	0
40	B	151	Total 151	O 151	0	0
40	C	171	Total 171	O 171	0	0
40	D	9	Total 9	O 9	0	0
40	E	44	Total 44	O 44	0	0
40	F	22	Total 22	O 22	0	0
40	G	3	Total 3	O 3	0	0
40	H	58	Total 58	O 58	0	0
40	I	1	Total 1	O 1	0	0
40	J	54	Total 54	O 54	0	0
40	K	59	Total 59	O 59	0	0
40	L	67	Total 67	O 67	0	0
40	M	133	Total 133	O 133	0	0
40	N	59	Total 59	O 59	0	0
40	O	45	Total 45	O 45	0	0
40	P	63	Total 63	O 63	0	0
40	Q	54	Total 54	O 54	0	0
40	R	72	Total 72	O 72	0	0
40	S	34	Total 34	O 34	0	0
40	T	39	Total 39	O 39	0	0

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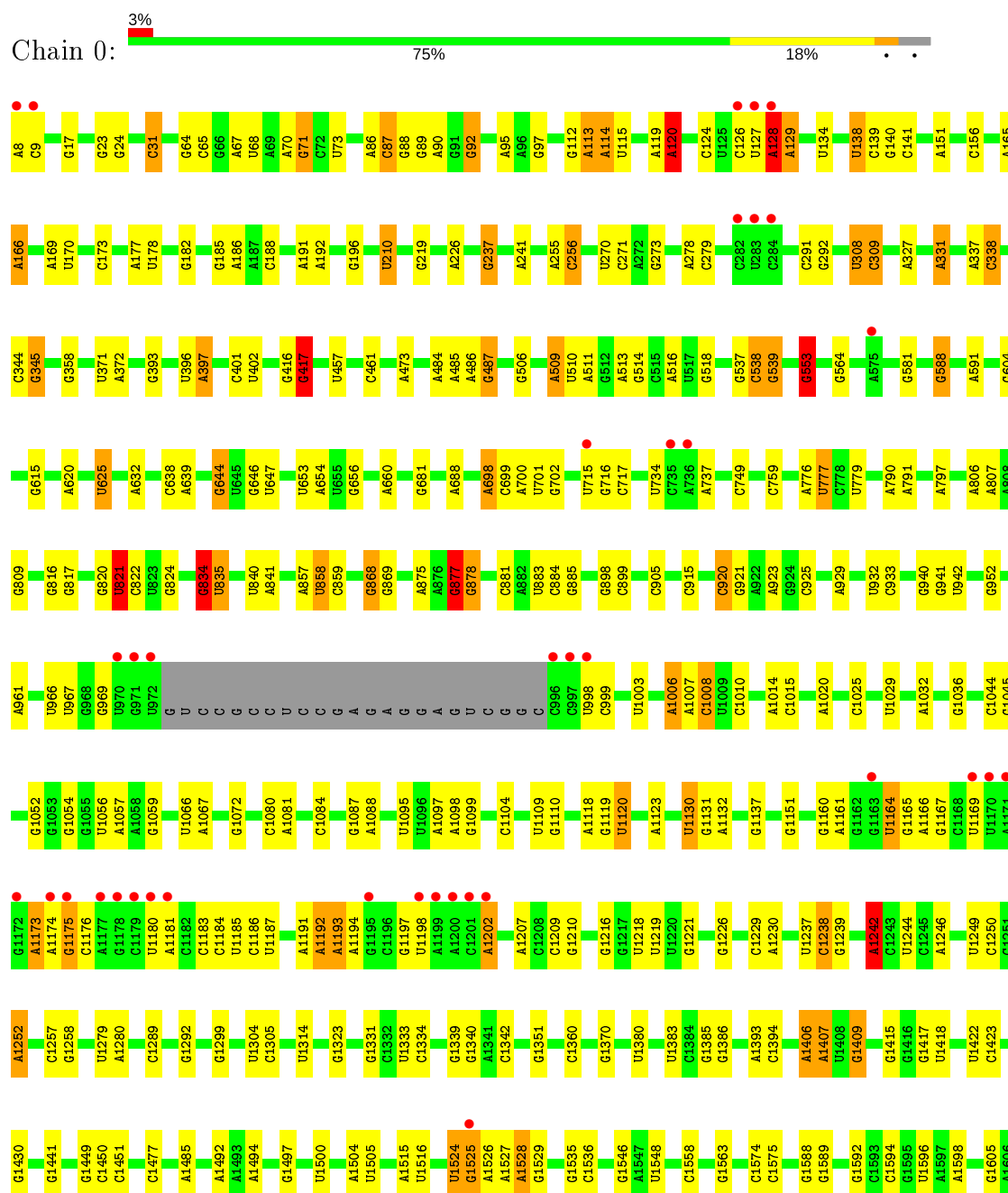
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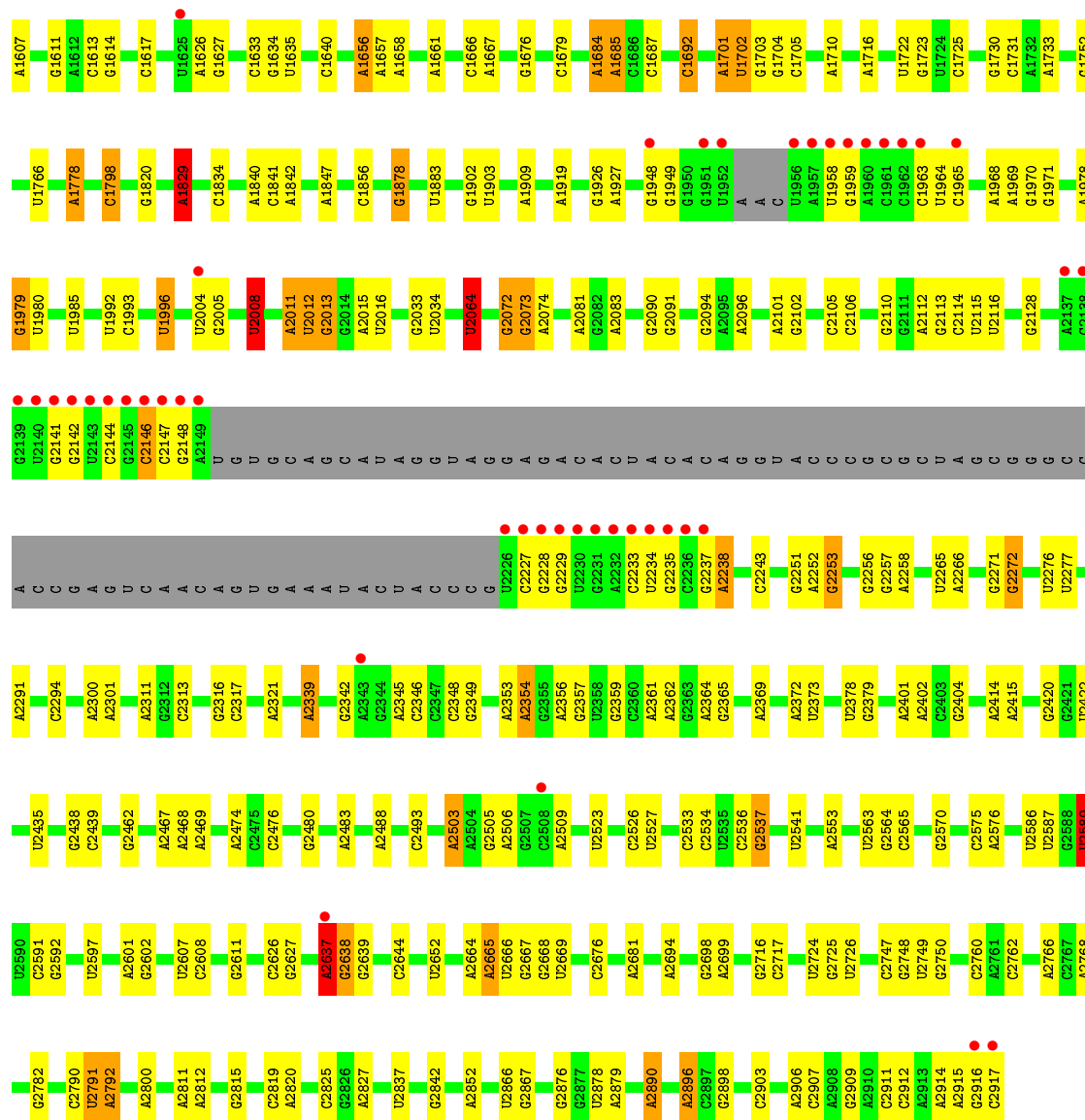
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40	U	23	Total 23	O 23	0	0
40	V	12	Total 12	O 12	0	0
40	W	64	Total 64	O 64	0	0
40	X	20	Total 20	O 20	0	0
40	Y	104	Total 104	O 104	0	0
40	Z	28	Total 28	O 28	0	0
40	1	50	Total 50	O 50	0	0
40	2	39	Total 39	O 39	0	0
40	3	63	Total 63	O 63	0	0
40	6	1	Total 1	O 1	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

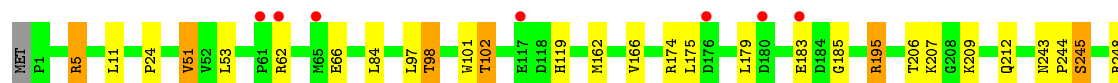
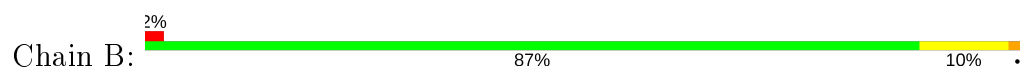




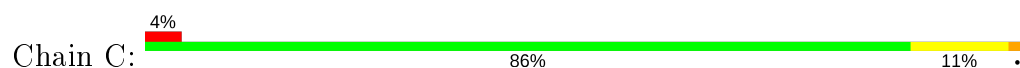




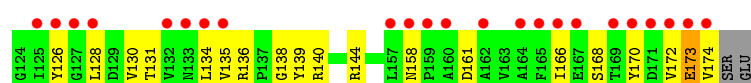
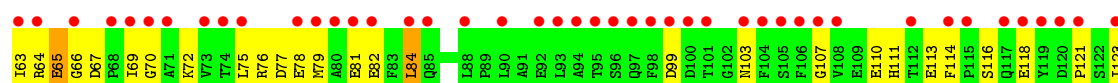
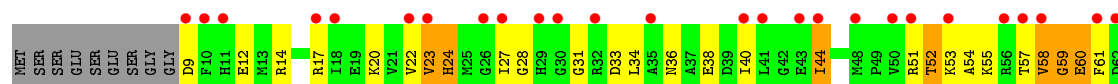
- Molecule 4: 50S ribosomal protein L3P



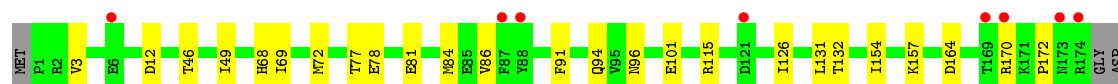
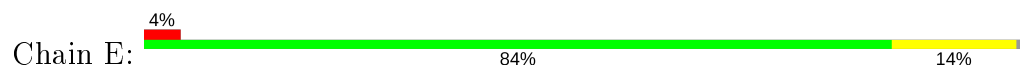
- Molecule 5: 50S ribosomal protein L4P



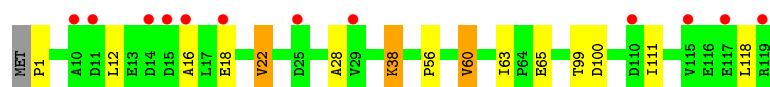
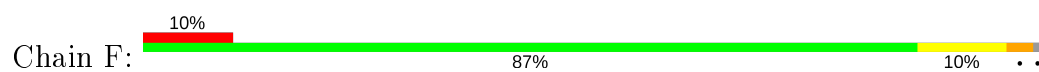
- Molecule 6: 50S ribosomal protein L5P



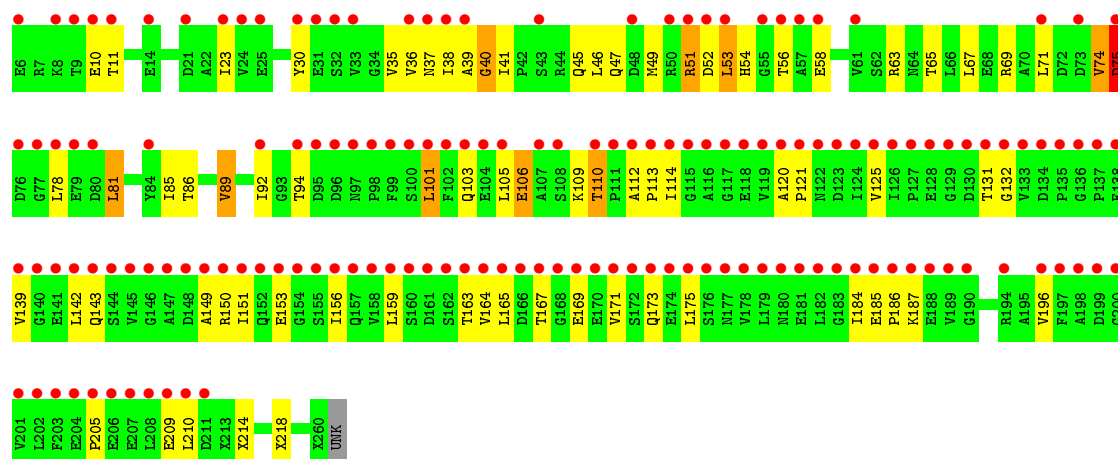
- Molecule 7: 50S ribosomal protein L6P



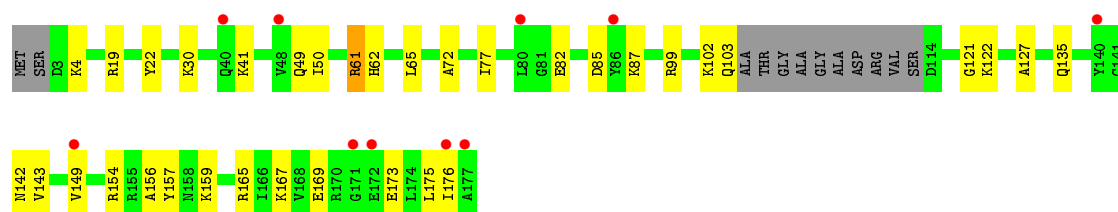
- Molecule 8: 50S ribosomal protein L7Ae



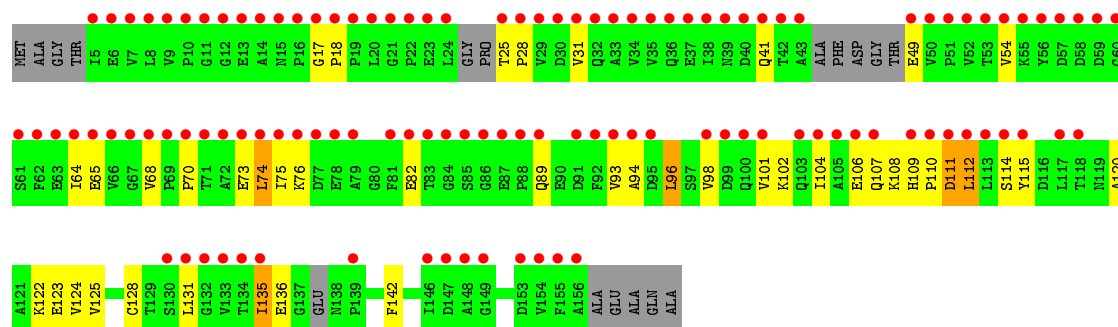
• Molecule 9: 50S ribosomal protein L10E



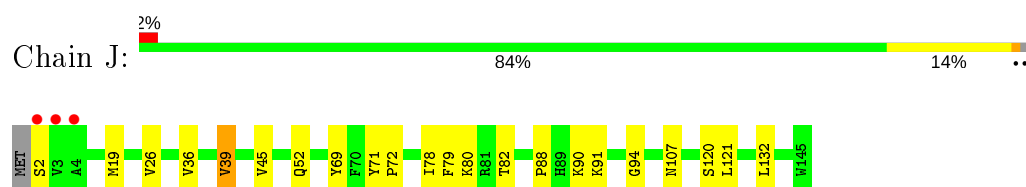
• Molecule 10: 50S ribosomal protein L10e



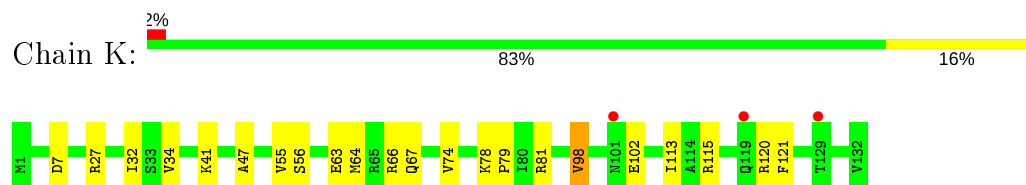
• Molecule 11: 50S ribosomal protein L11P



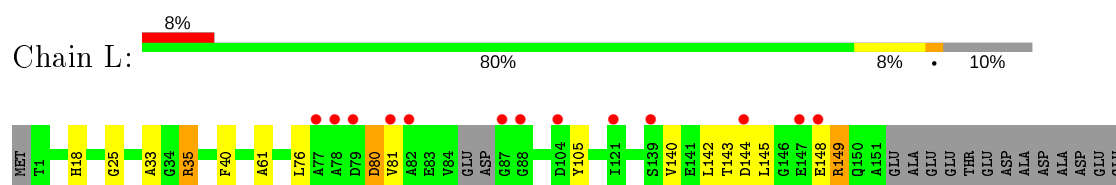
• Molecule 12: 50S ribosomal protein L13P



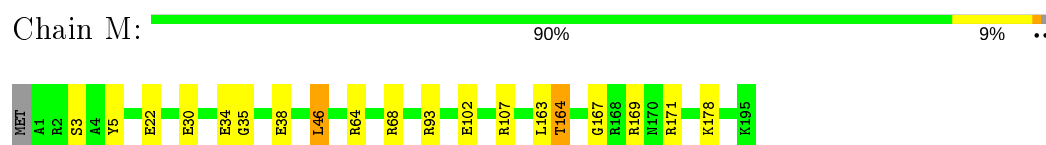
- Molecule 13: 50S ribosomal protein L14P



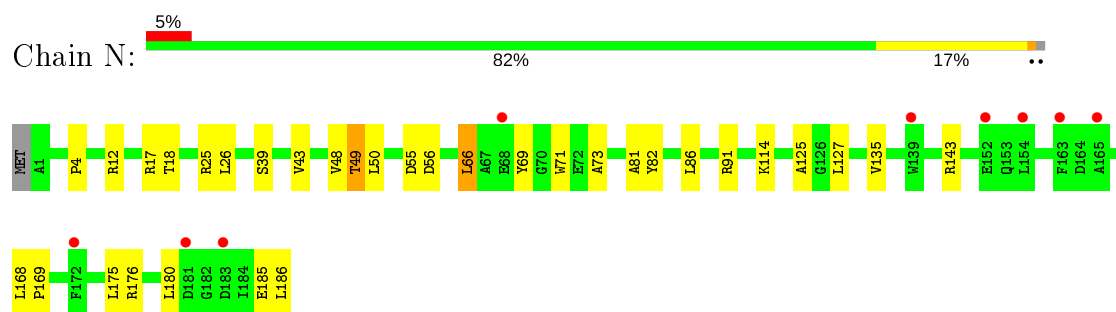
- Molecule 14: 50S ribosomal protein L15P



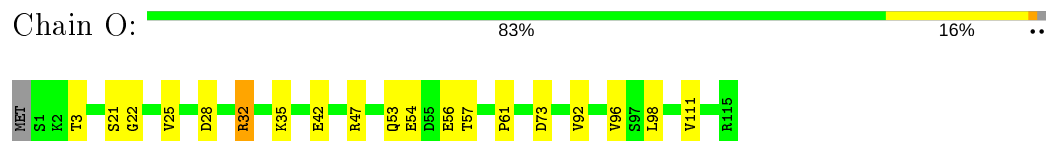
- Molecule 15: 50S ribosomal protein L15e



- Molecule 16: 50S ribosomal protein L18P



- Molecule 17: 50S ribosomal protein L18e

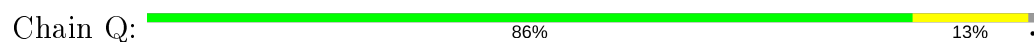


- Molecule 18: 50S ribosomal protein L19e

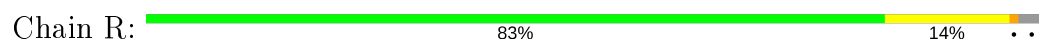




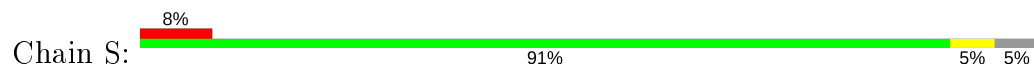
- Molecule 19: 50S ribosomal protein L21e



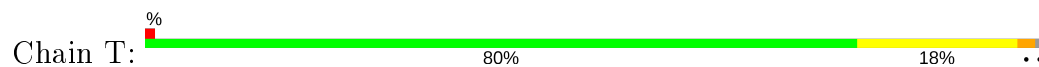
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



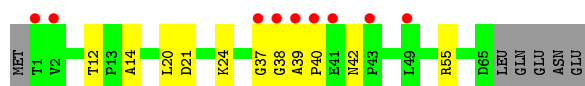
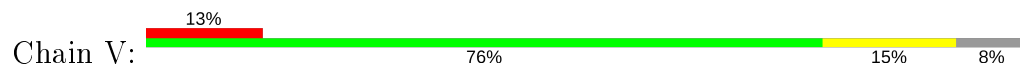
- Molecule 22: 50S ribosomal protein L24P



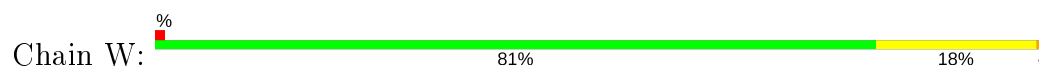
- Molecule 23: 50S ribosomal protein L24e



- Molecule 24: 50S ribosomal protein L29P

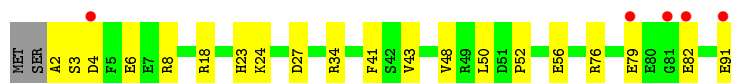
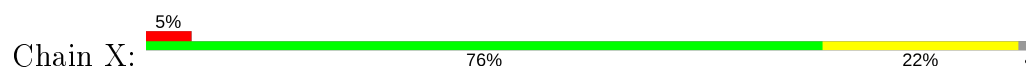


- Molecule 25: 50S ribosomal protein L30P

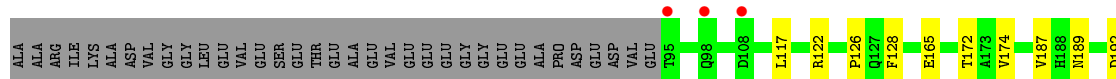




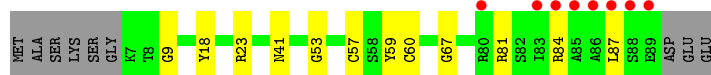
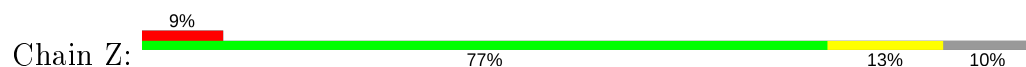
- Molecule 26: 50S ribosomal protein L31e



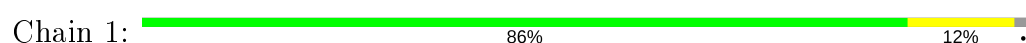
- Molecule 27: 50S ribosomal protein L32e



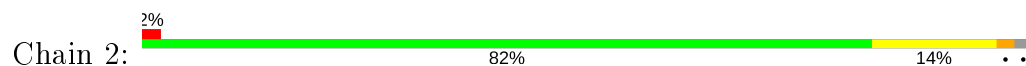
- Molecule 28: 50S ribosomal protein L37Ae



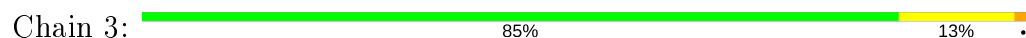
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e

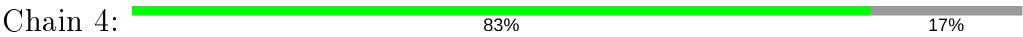


- Molecule 31: 50S ribosomal protein L44e

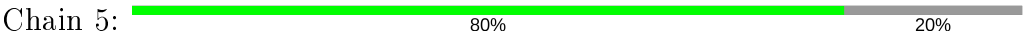




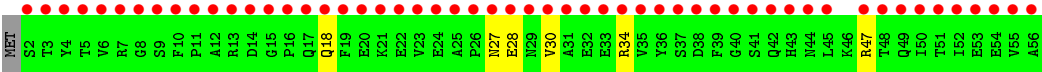
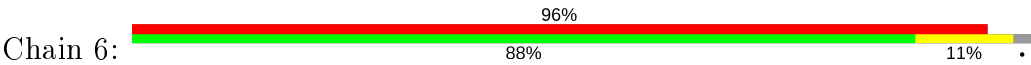
• Molecule 32: 50S ribosomal protein L12



• Molecule 32: 50S ribosomal protein L12



• Molecule 33: 50S ribosomal protein LX



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.48 – 2.40 89.24 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (85.48-2.40) 95.5 (89.24-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168), CNS	Depositor
R, $R_{free}$	0.166 , 0.206 0.168 , 0.208	Depositor DCC
$R_{free}$ test set	6982 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.3	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 45.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	103831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, CD, OMU, UR3, 1MA, ACY, 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	0.55	3/67259 (0.0%)	1.00	67/104899 (0.1%)
2	9	0.47	0/2904	0.91	0/4526
3	A	0.41	0/1786	0.62	1/2408 (0.0%)
4	B	0.39	0/2690	0.58	0/3652
5	C	0.46	0/1884	0.64	0/2552
6	D	0.32	0/1324	0.55	0/1791
7	E	0.38	0/1401	0.53	0/1905
8	F	0.39	0/900	0.52	0/1224
9	G	0.30	0/1585	0.58	1/2156 (0.0%)
10	H	0.41	0/1340	0.59	0/1795
11	I	0.29	0/1107	0.53	0/1512
12	J	0.40	0/1148	0.57	0/1548
13	K	0.42	0/1003	0.61	0/1351
14	L	0.45	0/1150	0.62	0/1536
15	M	0.46	0/1592	0.63	0/2127
16	N	0.37	0/1473	0.58	0/1999
17	O	0.40	0/874	0.55	0/1181
18	P	0.39	0/1155	0.52	0/1539
19	Q	0.44	0/748	0.61	0/1005
20	R	0.43	0/1172	0.58	0/1578
21	S	0.40	0/648	0.52	0/875
22	T	0.39	0/957	0.60	0/1289
23	U	0.40	0/443	0.52	0/597
24	V	0.39	0/502	0.46	0/675
25	W	0.40	0/1219	0.61	0/1655
26	X	0.38	0/725	0.55	0/978
27	Y	0.43	0/1162	0.56	0/1558
28	Z	0.40	0/656	0.57	0/877
29	1	0.55	0/438	0.74	0/578
30	2	0.45	0/427	0.55	0/566
31	3	0.46	0/771	0.55	0/1024
33	6	0.32	0/449	0.45	0/607



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.51	3/102892 (0.0%)	0.90	69/153563 (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
6	D	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	128	A	O3'-P	7.10	1.69	1.61
1	0	1656	A	O3'-P	-5.92	1.54	1.61
1	0	129	A	O3'-P	-5.40	1.54	1.61

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2013	G	O5'-P-OP1	-12.13	94.78	105.70
1	0	518	G	O4'-C1'-N9	10.81	116.85	108.20
1	0	777	U	O5'-P-OP1	-9.99	96.71	105.70
1	0	128	A	OP2-P-O3'	9.70	126.53	105.20
1	0	920	C	O5'-P-OP1	-8.82	97.76	105.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	59	GLY	Peptide
6	D	65	GLU	Peptide

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	60186	0	30379	291	0
2	9	2599	0	1325	23	0
3	A	1753	0	1766	17	0
4	B	2625	0	2533	27	0
5	C	1859	0	1813	23	0
6	D	1299	0	1263	48	0
7	E	1376	0	1285	15	0
8	F	889	0	843	6	0
9	G	1805	0	1560	47	0
10	H	1320	0	1331	22	0
11	I	1088	0	1029	27	0
12	J	1132	0	1112	15	0
13	K	993	0	1027	12	0
14	L	1138	0	1096	10	0
15	M	1568	0	1586	19	0
16	N	1444	0	1401	16	0
17	O	865	0	873	10	0
18	P	1144	0	1129	9	0
19	Q	734	0	729	9	0
20	R	1149	0	1122	13	0
21	S	641	0	605	2	0
22	T	949	0	924	14	0
23	U	435	0	394	6	0
24	V	499	0	511	6	0
25	W	1196	0	1137	20	0
26	X	714	0	700	11	0
27	Y	1146	0	1148	10	0
28	Z	645	0	610	6	0
29	1	431	0	426	5	0
30	2	421	0	437	8	0
31	3	755	0	728	7	0
32	4	290	0	60	0	0
32	5	280	0	59	0	0
33	6	441	0	411	4	0
34	0	125	0	0	0	0
34	3	1	0	0	0	0
34	9	1	0	0	0	0
34	A	3	0	0	0	0
34	K	1	0	0	0	0
34	L	1	0	0	0	0
34	N	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	0	2	0	0	0	0
35	O	1	0	0	0	0
36	0	72	0	0	0	0
36	9	1	0	0	0	0
36	A	1	0	0	0	0
36	C	1	0	0	0	0
36	H	2	0	0	0	0
36	J	1	0	0	0	0
36	L	2	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	12	0	0	1	0
37	3	1	0	0	0	0
37	9	1	0	0	3	0
37	A	1	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	1	0
37	G	1	0	0	0	0
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	2	0	0	1	0
37	R	2	0	0	0	0
37	Y	1	0	0	0	0
38	0	12	0	9	4	0
38	W	4	0	3	1	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5924	0	0	16	0
40	1	50	0	0	0	0
40	2	39	0	0	1	0
40	3	63	0	0	0	0
40	6	1	0	0	1	0
40	9	153	0	0	3	0
40	A	126	0	0	2	0
40	B	151	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	C	171	0	0	6	0
40	D	9	0	0	3	0
40	E	44	0	0	2	0
40	F	22	0	0	0	0
40	G	3	0	0	0	0
40	H	58	0	0	2	0
40	I	1	0	0	0	0
40	J	54	0	0	0	0
40	K	59	0	0	1	0
40	L	67	0	0	1	0
40	M	133	0	0	8	0
40	N	59	0	0	1	0
40	O	45	0	0	1	0
40	P	63	0	0	1	0
40	Q	54	0	0	2	0
40	R	72	0	0	1	0
40	S	34	0	0	0	0
40	T	39	0	0	0	0
40	U	23	0	0	0	0
40	V	12	0	0	0	0
40	W	64	0	0	1	0
40	X	20	0	0	2	0
40	Y	104	0	0	2	0
40	Z	28	0	0	1	0
All	All	103831	0	63364	679	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 679 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:164:THR:HG22	15:M:167:GLY:H	1.28	0.97
5:C:236:THR:HG22	5:C:239:ALA:H	1.30	0.95
1:O:156:C:H5''	15:M:171:ARG:HD3	1.46	0.95
20:R:39:THR:HG22	20:R:42:GLU:H	1.33	0.94
1:O:1160:G:H5'	1:O:1161:A:H5'	1.58	0.85

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%)	223 (95%)	11 (5%)	1 (0%)	34	48
4	B	335/338 (99%)	327 (98%)	8 (2%)	0	100	100
5	C	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
6	D	164/177 (93%)	143 (87%)	18 (11%)	3 (2%)	8	10
7	E	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
8	F	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
9	G	204/255 (80%)	171 (84%)	28 (14%)	5 (2%)	5	6
10	H	161/177 (91%)	156 (97%)	4 (2%)	1 (1%)	25	36
11	I	141/162 (87%)	122 (86%)	17 (12%)	2 (1%)	11	15
12	J	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
13	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
14	L	145/165 (88%)	139 (96%)	5 (3%)	1 (1%)	22	32
15	M	193/196 (98%)	189 (98%)	4 (2%)	0	100	100
16	N	184/187 (98%)	179 (97%)	5 (3%)	0	100	100
17	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
18	P	142/149 (95%)	142 (100%)	0	0	100	100
19	Q	93/96 (97%)	93 (100%)	0	0	100	100
20	R	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
21	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
22	T	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
23	U	54/67 (81%)	53 (98%)	1 (2%)	0	100	100
24	V	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
25	W	152/154 (99%)	152 (100%)	0	0	100	100
26	X	88/92 (96%)	83 (94%)	5 (6%)	0	100	100
27	Y	142/241 (59%)	142 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	47/50 (94%)	46 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	2 (2%)	0	100	100
33	6	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
All	All	4083/4411 (93%)	3924 (96%)	146 (4%)	13 (0%)	41	55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	G	38	ILE
6	D	173	GLU
9	G	74	VAL
9	G	53	LEU
9	G	75	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%)	24	40
4	B	282/283 (100%)	268 (95%)	14 (5%)	24	40
5	C	193/193 (100%)	182 (94%)	11 (6%)	20	33
6	D	139/148 (94%)	124 (89%)	15 (11%)	6	9
7	E	154/156 (99%)	148 (96%)	6 (4%)	32	50
8	F	93/94 (99%)	85 (91%)	8 (9%)	10	16
9	G	174/174 (100%)	159 (91%)	15 (9%)	10	16
10	H	138/145 (95%)	133 (96%)	5 (4%)	35	54
11	I	120/130 (92%)	112 (93%)	8 (7%)	16	26
12	J	120/121 (99%)	115 (96%)	5 (4%)	30	47
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	L	114/127 (90%)	108 (95%)	6 (5%)	22	37
15	M	159/160 (99%)	154 (97%)	5 (3%)	40	60
16	N	149/150 (99%)	140 (94%)	9 (6%)	19	31
17	O	93/94 (99%)	85 (91%)	8 (9%)	10	16
18	P	114/117 (97%)	110 (96%)	4 (4%)	36	55
19	Q	79/80 (99%)	77 (98%)	2 (2%)	47	67
20	R	117/122 (96%)	112 (96%)	5 (4%)	29	46
21	S	71/74 (96%)	70 (99%)	1 (1%)	67	82
22	T	105/106 (99%)	98 (93%)	7 (7%)	16	26
23	U	47/53 (89%)	44 (94%)	3 (6%)	17	28
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	74
25	W	130/130 (100%)	126 (97%)	4 (3%)	40	60
26	X	72/74 (97%)	69 (96%)	3 (4%)	30	47
27	Y	122/196 (62%)	119 (98%)	3 (2%)	47	67
28	Z	67/74 (90%)	64 (96%)	3 (4%)	27	44
29	1	46/47 (98%)	45 (98%)	1 (2%)	52	71
30	2	45/46 (98%)	44 (98%)	1 (2%)	52	71
31	3	79/79 (100%)	76 (96%)	3 (4%)	33	51
33	6	48/49 (98%)	48 (100%)	0	100	100
All	All	3406/3567 (96%)	3237 (95%)	169 (5%)	24	40

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	G	173	GLN
12	J	80	LYS
26	X	43	VAL
10	H	4	LYS
11	I	74	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
19	Q	4	ASN

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Mol	Chain	Res	Type
20	R	123	GLN
25	W	2	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2804/2910 (96%)	263 (9%)	23 (0%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2925/3032 (96%)	279 (9%)	24 (0%)

5 of 279 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	9	C
1	0	17	G
1	0	31	C
1	0	67	A
1	0	70	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1080	C
1	0	1524	U
1	0	2791	U
1	0	1246	A
1	0	1504	A

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	0	2587	1	14,22,23	0.70	0	14,31,34	0.67	0
1	OMG	0	2588	1	18,26,27	1.21	2 (11%)	20,38,41	2.29	7 (35%)
1	UR3	0	2619	1	14,22,23	0.78	0	15,32,35	0.76	1 (6%)
1	PSU	0	2621	1	17,21,22	1.37	2 (11%)	20,30,33	3.47	6 (30%)
1	1MA	0	628	1,36	15,25,26	1.51	3 (20%)	15,37,40	1.54	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	628	1MA	C6-C5	4.52	1.48	1.41
1	0	2588	OMG	C6-C5	3.89	1.48	1.41
1	0	2621	PSU	C4-C5	3.58	1.49	1.41
1	0	2621	PSU	C5-C1'	-2.90	1.49	1.52
1	0	2588	OMG	C5-C4	2.49	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-10.07	120.43	128.43
1	0	2621	PSU	C4-N3-C2	8.19	122.05	115.14
1	0	2621	PSU	C5-C4-N3	-5.53	118.24	125.36
1	0	2588	OMG	C6-N1-C2	4.36	122.86	115.93
1	0	2588	OMG	C6-C5-C4	-4.25	116.74	120.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 265 ligands modelled in this entry, 261 are monoatomic - leaving 4 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	$\# Z  > 2$
38	ACY	0	8212	-	1,3,3	1.36	0	0,3,3	0.00	-
38	ACY	0	8214	-	1,3,3	2.57	1 (100%)	0,3,3	0.00	-
38	ACY	W	201	-	1,3,3	1.96	0	0,3,3	0.00	-
38	ACY	0	8213	-	1,3,3	0.27	0	0,3,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	8214	ACY	CH3-C	2.57	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	8212	ACY	1	0
38	W	201	ACY	1	0
38	0	8213	ACY	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	211:ASP	C	213:UNK	N	3.25

## 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	0	2803/2910 (96%)	-0.18	81 (2%) 51 50	9, 28, 77, 221	0
2	9	122/122 (100%)	-0.50	3 (2%) 57 55	24, 44, 61, 127	0
3	A	237/240 (98%)	0.33	14 (5%) 22 21	12, 30, 63, 98	0
4	B	337/338 (99%)	0.23	7 (2%) 63 61	14, 35, 60, 72	0
5	C	246/246 (100%)	0.30	9 (3%) 41 41	10, 27, 48, 58	0
6	D	166/177 (93%)	2.43	93 (56%) 0 0	33, 81, 106, 113	0
7	E	174/178 (97%)	0.30	8 (4%) 32 31	30, 47, 64, 83	0
8	F	119/120 (99%)	0.68	12 (10%) 7 6	27, 46, 72, 78	0
9	G	206/255 (80%)	4.74	151 (73%) 0 0	57, 105, 173, 186	0
10	H	165/177 (93%)	0.41	10 (6%) 21 20	22, 37, 70, 94	0
11	I	145/162 (89%)	4.39	115 (79%) 0 0	81, 115, 155, 179	0
12	J	144/145 (99%)	0.06	3 (2%) 63 61	23, 33, 55, 82	0
13	K	132/132 (100%)	0.11	3 (2%) 60 58	19, 32, 49, 63	0
14	L	149/165 (90%)	0.76	13 (8%) 10 9	12, 41, 80, 88	0
15	M	195/196 (99%)	-0.05	0 100 100	14, 22, 34, 47	0
16	N	186/187 (99%)	0.32	9 (4%) 30 29	25, 41, 76, 101	0
17	O	115/116 (99%)	-0.20	0 100 100	23, 34, 50, 55	0
18	P	144/149 (96%)	-0.09	0 100 100	23, 34, 48, 60	0
19	Q	95/96 (98%)	0.02	0 100 100	19, 26, 41, 50	0
20	R	150/155 (96%)	0.05	0 100 100	16, 26, 45, 56	0
21	S	81/85 (95%)	0.36	7 (8%) 10 9	23, 36, 54, 63	0
22	T	119/120 (99%)	0.19	1 (0%) 86 84	21, 36, 55, 76	0
23	U	56/67 (83%)	0.28	2 (3%) 42 42	28, 36, 60, 103	0
24	V	65/71 (91%)	1.16	9 (13%) 2 2	30, 46, 78, 114	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.17	2 (1%) 77 75	22, 32, 47, 56	0
26	X	90/92 (97%)	0.26	5 (5%) 24 23	26, 39, 101, 111	0
27	Y	144/241 (59%)	0.09	7 (4%) 29 28	15, 28, 53, 104	0
28	Z	83/92 (90%)	0.44	8 (9%) 8 7	25, 39, 85, 108	0
29	1	56/57 (98%)	0.52	0 100 100	11, 16, 23, 24	0
30	2	49/50 (98%)	0.31	1 (2%) 65 63	20, 37, 64, 73	0
31	3	92/92 (100%)	0.03	0 100 100	16, 32, 46, 52	0
32	4	0/70	-	-	-	-
32	5	0/70	-	-	-	-
33	6	55/56 (98%)	5.17	54 (98%) 0 0	56, 98, 117, 122	0
All	All	7074/7583 (93%)	0.37	627 (8%) 9 9	9, 33, 102, 221	0

The worst 5 of 627 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	G	133	VAL	15.5
9	G	136	GLY	14.9
9	G	208	LEU	13.3
9	G	139	VAL	13.1
11	I	50	VAL	13.0

## 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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMG	0	2588	24/25	0.98	0.15	15,17,20,22	0
1	UR3	0	2619	21/22	0.98	0.15	16,18,21,26	0
1	PSU	0	2621	20/21	0.99	0.18	14,17,20,21	0
1	1MA	0	628	23/24	0.99	0.18	13,15,17,18	0
1	OMU	0	2587	21/22	0.99	0.13	15,18,20,22	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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	MG	0	8203	1/1	0.55	0.27	43,43,43,43	0
34	MG	0	8084	1/1	0.73	0.31	37,37,37,37	0
36	NA	R	202	1/1	0.75	0.40	48,48,48,48	0
34	MG	0	8068	1/1	0.81	0.09	34,34,34,34	0
34	MG	0	8050	1/1	0.82	0.52	73,73,73,73	0
34	MG	0	8208	1/1	0.83	0.08	45,45,45,45	0
34	MG	0	8065	1/1	0.84	0.06	40,40,40,40	0
38	ACY	0	8213	4/4	0.85	0.38	34,39,40,49	0
34	MG	0	8061	1/1	0.85	0.07	30,30,30,30	0
38	ACY	0	8214	4/4	0.85	0.27	28,35,37,39	0
34	MG	0	8100	1/1	0.85	0.13	42,42,42,42	0
37	CL	O	203	1/1	0.85	0.16	56,56,56,56	0
36	NA	0	8118	1/1	0.86	0.17	41,41,41,41	0
36	NA	0	8178	1/1	0.86	0.19	60,60,60,60	0
36	NA	0	8144	1/1	0.87	0.23	37,37,37,37	0
34	MG	0	8087	1/1	0.87	0.11	22,22,22,22	0
34	MG	0	8047	1/1	0.88	0.14	49,49,49,49	0
36	NA	0	8172	1/1	0.88	0.29	33,33,33,33	0
37	CL	0	8209	1/1	0.88	0.10	54,54,54,54	0
34	MG	0	8086	1/1	0.88	0.10	38,38,38,38	0
34	MG	0	8201	1/1	0.88	0.24	42,42,42,42	0
37	CL	9	203	1/1	0.89	0.07	59,59,59,59	0
34	MG	0	8094	1/1	0.89	0.18	32,32,32,32	0
34	MG	0	8096	1/1	0.89	0.19	43,43,43,43	0
36	NA	0	8168	1/1	0.89	0.31	43,43,43,43	0
36	NA	0	8179	1/1	0.89	0.09	43,43,43,43	0
34	MG	A	301	1/1	0.89	0.11	42,42,42,42	0
36	NA	9	202	1/1	0.90	0.21	42,42,42,42	0
36	NA	0	8134	1/1	0.90	0.17	46,46,46,46	0
34	MG	0	8079	1/1	0.90	0.09	27,27,27,27	0
34	MG	0	8034	1/1	0.90	0.10	25,25,25,25	0
34	MG	0	8072	1/1	0.90	0.15	15,15,15,15	0
34	MG	3	101	1/1	0.90	0.10	27,27,27,27	0
34	MG	0	8052	1/1	0.90	0.04	36,36,36,36	0
34	MG	0	8195	1/1	0.90	0.19	45,45,45,45	0
36	NA	0	8141	1/1	0.91	0.08	30,30,30,30	0
34	MG	0	8076	1/1	0.91	0.12	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CL	G	301	1/1	0.91	0.11	58,58,58,58	0
34	MG	0	8207	1/1	0.91	0.09	33,33,33,33	0
34	MG	0	8205	1/1	0.91	0.24	43,43,43,43	0
35	K	0	8109	1/1	0.91	0.10	44,44,44,44	0
34	MG	0	8098	1/1	0.91	0.06	33,33,33,33	0
37	CL	B	402	1/1	0.91	0.48	62,62,62,62	0
38	ACY	0	8212	4/4	0.91	0.33	35,39,41,43	0
34	MG	0	8196	1/1	0.91	0.14	39,39,39,39	0
34	MG	0	8006	1/1	0.91	0.10	22,22,22,22	0
36	NA	0	8167	1/1	0.91	0.19	29,29,29,29	0
34	MG	0	8204	1/1	0.91	0.13	33,33,33,33	0
36	NA	0	8132	1/1	0.91	0.14	23,23,23,23	0
34	MG	0	8202	1/1	0.92	0.15	33,33,33,33	0
34	MG	0	8022	1/1	0.92	0.16	23,23,23,23	0
36	NA	0	8148	1/1	0.92	0.15	21,21,21,21	0
34	MG	0	8091	1/1	0.92	0.12	20,20,20,20	0
34	MG	0	8043	1/1	0.92	0.07	29,29,29,29	0
34	MG	0	8071	1/1	0.92	0.06	37,37,37,37	0
36	NA	0	8156	1/1	0.92	0.43	33,33,33,33	0
36	NA	0	8130	1/1	0.92	0.21	31,31,31,31	0
34	MG	0	8104	1/1	0.92	0.13	26,26,26,26	0
34	MG	0	8197	1/1	0.92	0.18	31,31,31,31	0
35	K	O	204	1/1	0.92	0.18	77,77,77,77	0
36	NA	C	301	1/1	0.93	0.17	20,20,20,20	0
34	MG	0	8037	1/1	0.93	0.08	29,29,29,29	0
34	MG	0	8092	1/1	0.93	0.23	25,25,25,25	0
34	MG	0	8069	1/1	0.93	0.09	29,29,29,29	0
36	NA	H	202	1/1	0.93	0.26	39,39,39,39	0
36	NA	0	8161	1/1	0.93	0.27	29,29,29,29	0
36	NA	0	8119	1/1	0.93	0.22	32,32,32,32	0
34	MG	0	8014	1/1	0.93	0.15	19,19,19,19	0
34	MG	0	8013	1/1	0.93	0.18	16,16,16,16	0
34	MG	Y	304	1/1	0.93	0.10	33,33,33,33	0
34	MG	0	8040	1/1	0.93	0.11	26,26,26,26	0
35	K	0	8211	1/1	0.93	0.14	51,51,51,51	0
34	MG	0	8026	1/1	0.94	0.17	19,19,19,19	0
36	NA	0	8174	1/1	0.94	0.32	28,28,28,28	0
36	NA	0	8166	1/1	0.94	0.10	38,38,38,38	0
34	MG	0	8085	1/1	0.94	0.07	28,28,28,28	0
34	MG	0	8078	1/1	0.94	0.09	27,27,27,27	0
36	NA	0	8149	1/1	0.94	0.39	28,28,28,28	0
34	MG	0	8023	1/1	0.94	0.17	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	8180	1/1	0.94	0.27	37,37,37,37	0
36	NA	0	8170	1/1	0.94	0.26	38,38,38,38	0
36	NA	0	8121	1/1	0.94	0.21	20,20,20,20	0
34	MG	0	8074	1/1	0.94	0.10	30,30,30,30	0
36	NA	0	8110	1/1	0.94	0.17	26,26,26,26	0
34	MG	0	8075	1/1	0.94	0.14	28,28,28,28	0
34	MG	0	8191	1/1	0.94	0.11	31,31,31,31	0
34	MG	0	8046	1/1	0.94	0.11	37,37,37,37	0
34	MG	0	8097	1/1	0.94	0.12	34,34,34,34	0
34	MG	0	8198	1/1	0.94	0.15	39,39,39,39	0
34	MG	0	8064	1/1	0.94	0.12	20,20,20,20	0
36	NA	0	8117	1/1	0.94	0.15	24,24,24,24	0
34	MG	0	8206	1/1	0.94	0.21	33,33,33,33	0
36	NA	0	8171	1/1	0.94	0.12	39,39,39,39	0
36	NA	0	8165	1/1	0.95	0.21	29,29,29,29	0
34	MG	0	8108	1/1	0.95	0.06	20,20,20,20	0
36	NA	0	8175	1/1	0.95	0.19	30,30,30,30	0
34	MG	0	8045	1/1	0.95	0.05	35,35,35,35	0
36	NA	0	8169	1/1	0.95	0.17	30,30,30,30	0
34	MG	0	8106	1/1	0.95	0.12	29,29,29,29	0
34	MG	0	8007	1/1	0.95	0.16	18,18,18,18	0
34	MG	0	8058	1/1	0.95	0.10	18,18,18,18	0
36	NA	0	8111	1/1	0.95	0.17	25,25,25,25	0
36	NA	0	8124	1/1	0.95	0.27	32,32,32,32	0
37	CL	J	203	1/1	0.95	0.11	42,42,42,42	0
36	NA	0	8131	1/1	0.95	0.13	28,28,28,28	0
34	MG	0	8027	1/1	0.95	0.10	30,30,30,30	0
34	MG	L	204	1/1	0.95	0.10	26,26,26,26	0
34	MG	0	8090	1/1	0.95	0.10	19,19,19,19	0
36	NA	L	201	1/1	0.95	0.19	24,24,24,24	0
34	MG	0	8080	1/1	0.95	0.04	31,31,31,31	0
34	MG	0	8036	1/1	0.95	0.12	21,21,21,21	0
34	MG	N	202	1/1	0.95	0.13	58,58,58,58	0
34	MG	0	8062	1/1	0.95	0.09	35,35,35,35	0
34	MG	0	8105	1/1	0.96	0.09	23,23,23,23	0
34	MG	0	8056	1/1	0.96	0.13	25,25,25,25	0
36	NA	R	201	1/1	0.96	0.10	29,29,29,29	0
34	MG	0	8031	1/1	0.96	0.15	15,15,15,15	0
34	MG	0	8041	1/1	0.96	0.13	25,25,25,25	0
34	MG	0	8081	1/1	0.96	0.15	42,42,42,42	0
34	MG	0	8033	1/1	0.96	0.10	16,16,16,16	0
34	MG	0	8088	1/1	0.96	0.06	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8066	1/1	0.96	0.10	27,27,27,27	0
36	NA	0	8164	1/1	0.96	0.23	39,39,39,39	0
34	MG	0	8089	1/1	0.96	0.09	23,23,23,23	0
36	NA	0	8162	1/1	0.96	0.37	25,25,25,25	0
34	MG	0	8032	1/1	0.96	0.14	17,17,17,17	0
36	NA	0	8139	1/1	0.96	0.12	29,29,29,29	0
34	MG	0	8083	1/1	0.96	0.08	34,34,34,34	0
34	MG	0	8001	1/1	0.96	0.17	16,16,16,16	0
36	NA	0	8115	1/1	0.96	0.13	32,32,32,32	0
34	MG	0	8051	1/1	0.96	0.08	32,32,32,32	0
34	MG	0	8063	1/1	0.96	0.21	19,19,19,19	0
36	NA	0	8146	1/1	0.96	0.20	22,22,22,22	0
34	MG	0	8019	1/1	0.96	0.08	23,23,23,23	0
34	MG	0	8073	1/1	0.96	0.20	10,10,10,10	0
38	ACY	W	201	4/4	0.96	0.29	46,47,48,49	0
36	NA	A	304	1/1	0.96	0.09	28,28,28,28	0
34	MG	0	8095	1/1	0.96	0.16	34,34,34,34	0
34	MG	0	8049	1/1	0.96	0.10	36,36,36,36	0
36	NA	0	8154	1/1	0.96	0.15	24,24,24,24	0
34	MG	0	8028	1/1	0.96	0.09	21,21,21,21	0
34	MG	0	8194	1/1	0.97	0.14	35,35,35,35	0
36	NA	0	8163	1/1	0.97	0.13	18,18,18,18	0
34	MG	0	8093	1/1	0.97	0.21	42,42,42,42	0
34	MG	0	8200	1/1	0.97	0.20	37,37,37,37	0
36	NA	0	8125	1/1	0.97	0.19	19,19,19,19	0
36	NA	0	8173	1/1	0.97	0.22	25,25,25,25	0
36	NA	0	8150	1/1	0.97	0.12	36,36,36,36	0
34	MG	0	8107	1/1	0.97	0.06	32,32,32,32	0
36	NA	S	101	1/1	0.97	0.14	25,25,25,25	0
34	MG	Y	303	1/1	0.97	0.28	38,38,38,38	0
36	NA	0	8127	1/1	0.97	0.20	22,22,22,22	0
34	MG	0	8082	1/1	0.97	0.18	17,17,17,17	0
36	NA	0	8138	1/1	0.97	0.11	20,20,20,20	0
36	NA	0	8177	1/1	0.97	0.15	33,33,33,33	0
36	NA	0	8128	1/1	0.97	0.15	19,19,19,19	0
37	CL	L	203	1/1	0.97	0.11	29,29,29,29	0
34	MG	0	8054	1/1	0.97	0.21	10,10,10,10	0
36	NA	0	8160	1/1	0.97	0.18	26,26,26,26	0
36	NA	M	201	1/1	0.97	0.22	15,15,15,15	0
36	NA	0	8147	1/1	0.97	0.23	23,23,23,23	0
34	MG	0	8002	1/1	0.97	0.15	19,19,19,19	0
34	MG	0	8016	1/1	0.97	0.12	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	8176	1/1	0.97	0.32	37,37,37,37	0
34	MG	0	8060	1/1	0.97	0.14	22,22,22,22	0
37	CL	0	8181	1/1	0.97	0.17	29,29,29,29	0
34	MG	0	8199	1/1	0.97	0.10	55,55,55,55	0
34	MG	A	303	1/1	0.97	0.16	23,23,23,23	0
34	MG	0	8057	1/1	0.97	0.06	23,23,23,23	0
34	MG	0	8099	1/1	0.97	0.07	26,26,26,26	0
37	CL	0	8210	1/1	0.97	0.17	49,49,49,49	0
34	MG	0	8077	1/1	0.97	0.11	24,24,24,24	0
36	NA	0	8123	1/1	0.97	0.19	23,23,23,23	0
34	MG	0	8018	1/1	0.97	0.12	22,22,22,22	0
36	NA	0	8145	1/1	0.97	0.10	31,31,31,31	0
36	NA	0	8135	1/1	0.97	0.09	29,29,29,29	0
37	CL	J	202	1/1	0.97	0.11	34,34,34,34	0
36	NA	0	8158	1/1	0.97	0.14	28,28,28,28	0
34	MG	9	201	1/1	0.97	0.07	54,54,54,54	0
36	NA	0	8143	1/1	0.97	0.24	13,13,13,13	0
34	MG	Y	305	1/1	0.98	0.14	33,33,33,33	0
36	NA	0	8116	1/1	0.98	0.17	29,29,29,29	0
36	NA	Q	101	1/1	0.98	0.08	25,25,25,25	0
36	NA	0	8120	1/1	0.98	0.19	21,21,21,21	0
36	NA	L	202	1/1	0.98	0.15	24,24,24,24	0
34	MG	0	8067	1/1	0.98	0.12	33,33,33,33	0
37	CL	3	103	1/1	0.98	0.07	33,33,33,33	0
34	MG	0	8101	1/1	0.98	0.12	19,19,19,19	0
36	NA	0	8136	1/1	0.98	0.21	20,20,20,20	0
34	MG	0	8055	1/1	0.98	0.07	31,31,31,31	0
34	MG	0	8029	1/1	0.98	0.10	22,22,22,22	0
34	MG	0	8020	1/1	0.98	0.11	17,17,17,17	0
34	MG	0	8030	1/1	0.98	0.10	17,17,17,17	0
37	CL	M	202	1/1	0.98	0.15	21,21,21,21	0
36	NA	0	8155	1/1	0.98	0.08	34,34,34,34	0
36	NA	0	8112	1/1	0.98	0.17	19,19,19,19	0
37	CL	R	204	1/1	0.98	0.12	34,34,34,34	0
34	MG	0	8035	1/1	0.98	0.10	27,27,27,27	0
37	CL	O	202	1/1	0.98	0.07	36,36,36,36	0
39	CD	3	102	1/1	0.98	0.13	39,39,39,39	0
37	CL	0	8182	1/1	0.98	0.09	26,26,26,26	0
34	MG	T	201	1/1	0.98	0.07	47,47,47,47	0
36	NA	0	8157	1/1	0.98	0.19	24,24,24,24	0
37	CL	R	203	1/1	0.98	0.14	30,30,30,30	0
36	NA	0	8159	1/1	0.98	0.23	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	8153	1/1	0.98	0.29	29,29,29,29	0
34	MG	Y	301	1/1	0.98	0.12	19,19,19,19	0
36	NA	0	8122	1/1	0.98	0.26	16,16,16,16	0
34	MG	0	8025	1/1	0.98	0.08	25,25,25,25	0
34	MG	0	8053	1/1	0.98	0.09	22,22,22,22	0
37	CL	0	8186	1/1	0.98	0.17	25,25,25,25	0
34	MG	K	201	1/1	0.98	0.10	25,25,25,25	0
36	NA	0	8140	1/1	0.98	0.19	21,21,21,21	0
34	MG	0	8044	1/1	0.98	0.11	21,21,21,21	0
36	NA	0	8126	1/1	0.98	0.30	23,23,23,23	0
36	NA	J	201	1/1	0.98	0.13	27,27,27,27	0
34	MG	0	8042	1/1	0.98	0.07	28,28,28,28	0
34	MG	0	8017	1/1	0.98	0.25	11,11,11,11	0
36	NA	0	8192	1/1	0.98	0.09	22,22,22,22	0
36	NA	0	8129	1/1	0.98	0.12	37,37,37,37	0
37	CL	N	201	1/1	0.98	0.11	36,36,36,36	0
34	MG	0	8015	1/1	0.98	0.21	15,15,15,15	0
37	CL	J	204	1/1	0.98	0.13	36,36,36,36	0
37	CL	Y	302	1/1	0.98	0.12	26,26,26,26	0
36	NA	H	201	1/1	0.98	0.16	19,19,19,19	0
34	MG	A	302	1/1	0.98	0.12	20,20,20,20	0
34	MG	0	8039	1/1	0.98	0.07	27,27,27,27	0
37	CL	F	201	1/1	0.98	0.10	33,33,33,33	0
36	NA	0	8152	1/1	0.98	0.22	17,17,17,17	0
37	CL	A	305	1/1	0.98	0.11	35,35,35,35	0
34	MG	0	8008	1/1	0.98	0.13	13,13,13,13	0
37	CL	0	8189	1/1	0.98	0.08	35,35,35,35	0
34	MG	0	8003	1/1	0.98	0.12	12,12,12,12	0
36	NA	0	8114	1/1	0.98	0.16	19,19,19,19	0
34	MG	0	8012	1/1	0.99	0.13	23,23,23,23	0
34	MG	0	8193	1/1	0.99	0.14	14,14,14,14	0
39	CD	O	201	1/1	0.99	0.07	58,58,58,58	0
34	MG	0	8038	1/1	0.99	0.17	13,13,13,13	0
34	MG	0	8004	1/1	0.99	0.20	13,13,13,13	0
34	MG	0	8048	1/1	0.99	0.07	33,33,33,33	0
37	CL	0	8185	1/1	0.99	0.12	32,32,32,32	0
37	CL	0	8190	1/1	0.99	0.19	31,31,31,31	0
34	MG	0	8024	1/1	0.99	0.24	17,17,17,17	0
39	CD	U	8401	1/1	0.99	0.12	39,39,39,39	0
37	CL	0	8187	1/1	0.99	0.13	38,38,38,38	0
37	CL	0	8188	1/1	0.99	0.14	30,30,30,30	0
36	NA	0	8137	1/1	0.99	0.17	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CL	0	8183	1/1	0.99	0.10	25,25,25,25	0
37	CL	0	8184	1/1	0.99	0.10	26,26,26,26	0
34	MG	0	8005	1/1	0.99	0.19	13,13,13,13	0
36	NA	0	8142	1/1	0.99	0.06	28,28,28,28	0
34	MG	0	8011	1/1	0.99	0.14	16,16,16,16	0
34	MG	0	8009	1/1	0.99	0.19	15,15,15,15	0
34	MG	0	8059	1/1	0.99	0.25	21,21,21,21	0
36	NA	0	8133	1/1	0.99	0.19	28,28,28,28	0
34	MG	0	8103	1/1	0.99	0.08	15,15,15,15	0
34	MG	0	8102	1/1	0.99	0.16	24,24,24,24	0
34	MG	0	8070	1/1	0.99	0.08	22,22,22,22	0
39	CD	Z	101	1/1	0.99	0.16	38,38,38,38	0
34	MG	0	8021	1/1	0.99	0.12	17,17,17,17	0
36	NA	0	8113	1/1	0.99	0.15	19,19,19,19	0
36	NA	0	8151	1/1	0.99	0.19	11,11,11,11	0
34	MG	0	8010	1/1	0.99	0.19	14,14,14,14	0
37	CL	B	401	1/1	0.99	0.14	24,24,24,24	0
39	CD	1	101	1/1	1.00	0.11	37,37,37,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.