wwPDB X-ray Structure Validation Summary Report (i)

Jul 3, 2024 – 02:38 PM EDT

PDB ID	:	1YJW
Title	:	Crystal Structure Of Quinupristin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors	:	Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on	:	2005-01-15
Resolution	:	2.90 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

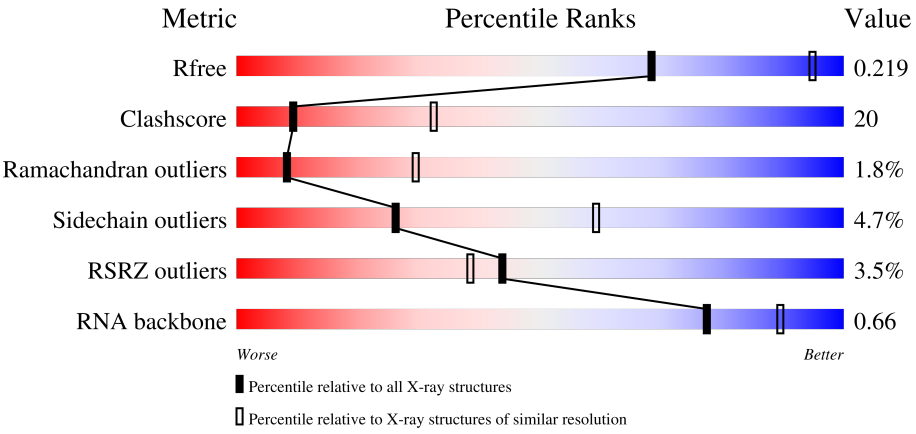
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

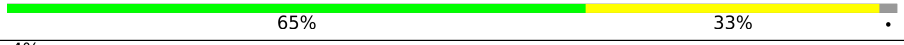
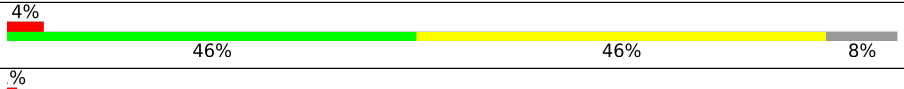
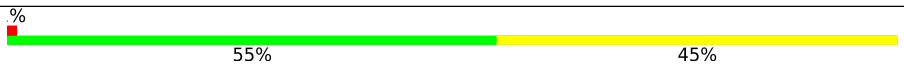
The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	2922	
2	1	57	
3	2	50	
4	3	92	

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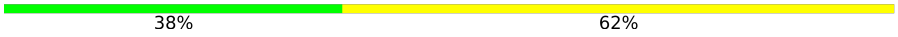
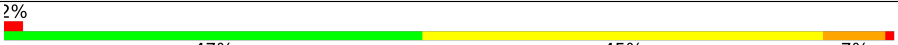
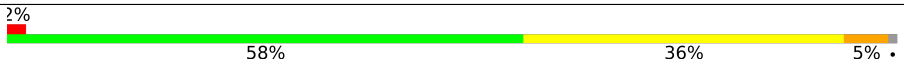
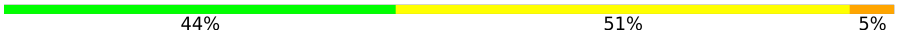
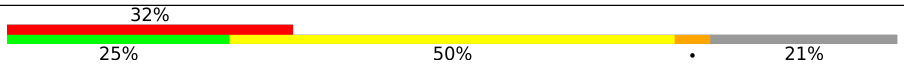
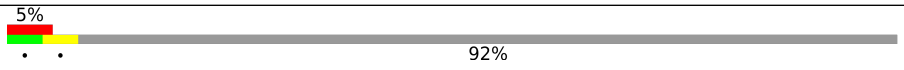
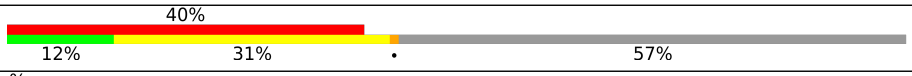
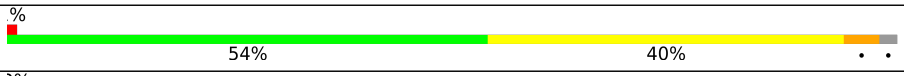
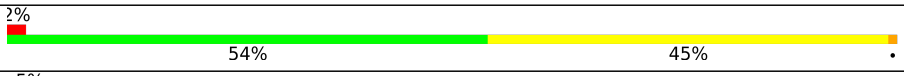
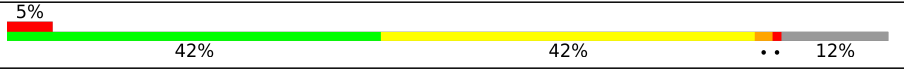
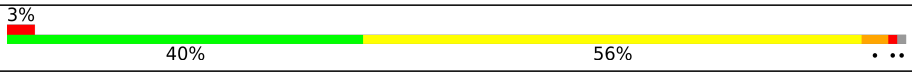
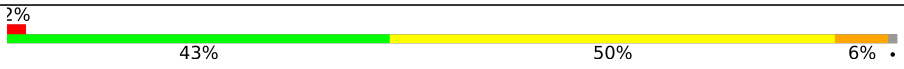
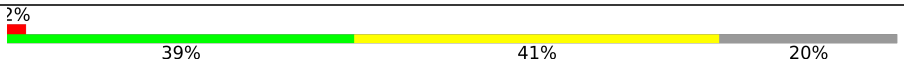
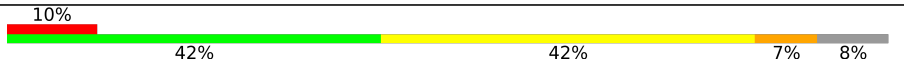
Mol	Chain	Length	Quality of chain
5	4	8	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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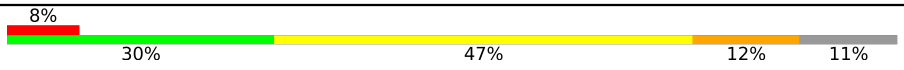
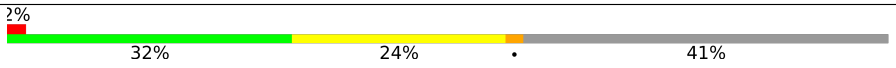
Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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
35	NA	0	3120	-	-	-	X
35	NA	0	3134	-	-	-	X
35	NA	0	3174	-	-	-	X
35	NA	0	3175	-	-	-	X
35	NA	0	3183	-	-	-	X
35	NA	9	203	-	-	-	X
35	NA	R	202	-	-	-	X
36	CL	0	3189	-	-	X	-
36	CL	N	201	-	-	X	-

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 99111 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	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	2099	A	G	conflict	GB 55229667

- Molecule 2 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	4	8	Total	C	N	O	S	0	0	0
			73	53	9	10	1			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S ribosomal protein L2.

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

- Molecule 8 is a protein called 50S ribosomal protein L3.

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

- Molecule 9 is a protein called 50S ribosomal protein L4.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called 50S ribosomal protein L5.

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

- Molecule 11 is a protein called 50S ribosomal protein L6.

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

- Molecule 12 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 13 is a protein called 50S ribosomal protein L10.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 14 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 15 is a protein called 50S ribosomal protein L11.

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

- Molecule 16 is a protein called 50S ribosomal protein L13.

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

- Molecule 17 is a protein called 50S ribosomal protein L14.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618

- Molecule 20 is a protein called 50S ribosomal protein L18.

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

- Molecule 21 is a protein called 50S ribosomal protein L18e.

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

- Molecule 22 is a protein called 50S ribosomal protein L19e.

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

- Molecule 23 is a protein called 50S ribosomal protein L21e.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L23.

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

- Molecule 26 is a protein called 50S ribosomal protein L24.

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

- Molecule 27 is a protein called 50S ribosomal protein L24e.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L31e.

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

- Molecule 31 is a protein called 50S ribosomal protein L32e.

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

- Molecule 32 is a protein called 50S ribosomal protein L37Ae.

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total 109	Mg 109	0	0
33	3	1	Total 1	Mg 1	0	0
33	4	1	Total 1	Mg 1	0	0
33	9	1	Total 1	Mg 1	0	0
33	A	1	Total 1	Mg 1	0	0
33	B	1	Total 1	Mg 1	0	0
33	K	1	Total 1	Mg 1	0	0
33	T	1	Total 1	Mg 1	0	0
33	Y	1	Total 1	Mg 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	74	Total Na 74 74	0	0
35	9	2	Total Na 2 2	0	0
35	A	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	L	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	3	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5842	Total O 5842 5842	0	0
38	1	60	Total O 60 60	0	0
38	2	49	Total O 49 49	0	0
38	3	69	Total O 69 69	0	0
38	4	2	Total O 2 2	0	0
38	9	143	Total O 143 143	0	0
38	A	123	Total O 123 123	0	0
38	B	146	Total O 146 146	0	0
38	C	185	Total O 185 185	0	0
38	D	49	Total O 49 49	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	20	Total O 20 20	0	0
38	H	69	Total O 69 69	0	0
38	I	9	Total O 9 9	0	0
38	J	55	Total O 55 55	0	0
38	K	59	Total O 59 59	0	0
38	L	82	Total O 82 82	0	0
38	M	129	Total O 129 129	0	0
38	N	60	Total O 60 60	0	0
38	O	42	Total O 42 42	0	0
38	P	72	Total O 72 72	0	0
38	Q	48	Total O 48 48	0	0
38	R	85	Total O 85 85	0	0
38	S	30	Total O 30 30	0	0
38	T	39	Total O 39 39	0	0
38	U	29	Total O 29 29	0	0
38	V	13	Total O 13 13	0	0
38	W	69	Total O 69 69	0	0
38	X	26	Total O 26 26	0	0
38	Y	101	Total O 101 101	0	0

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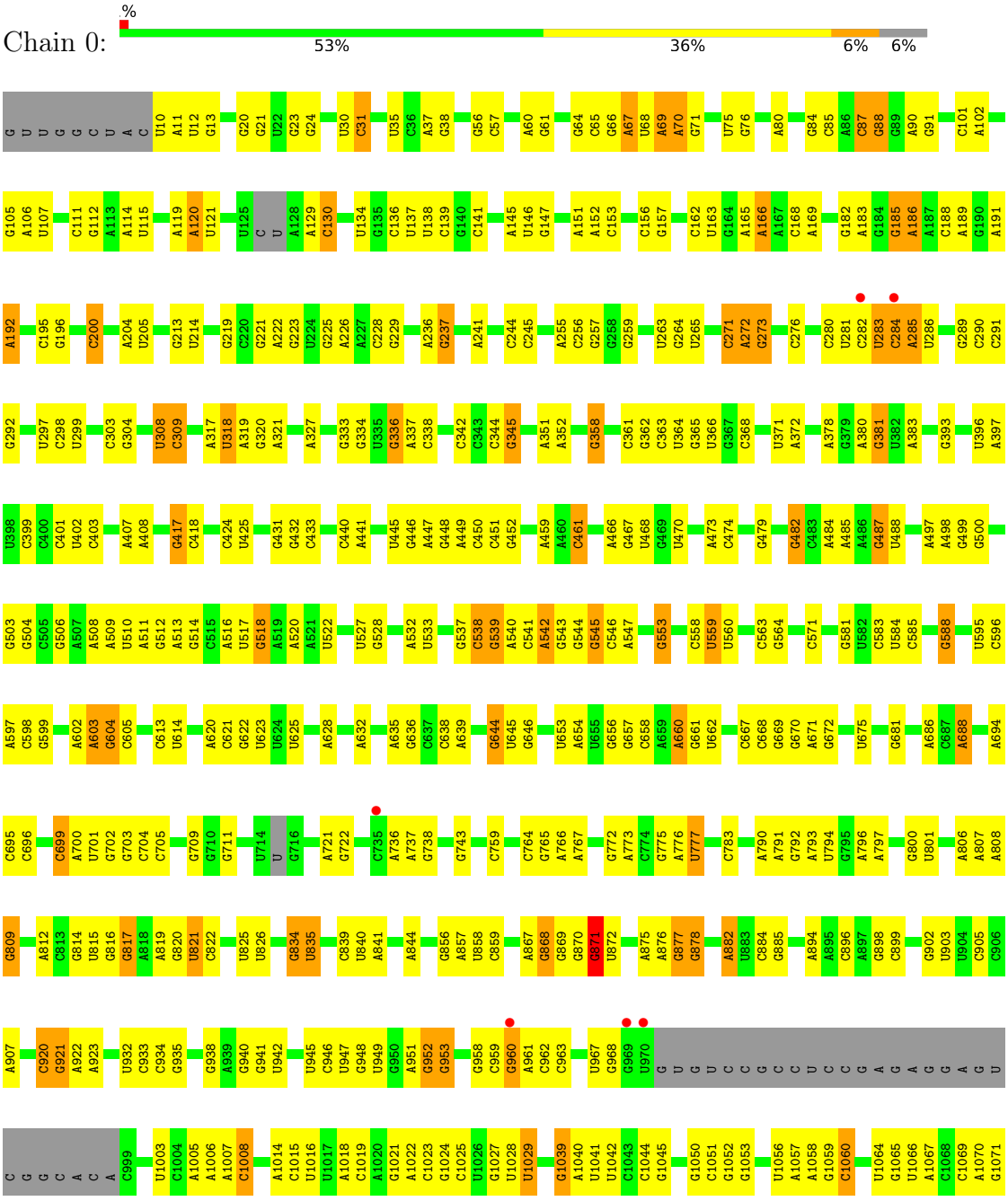
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	Z	37	Total O 37 37	0	0

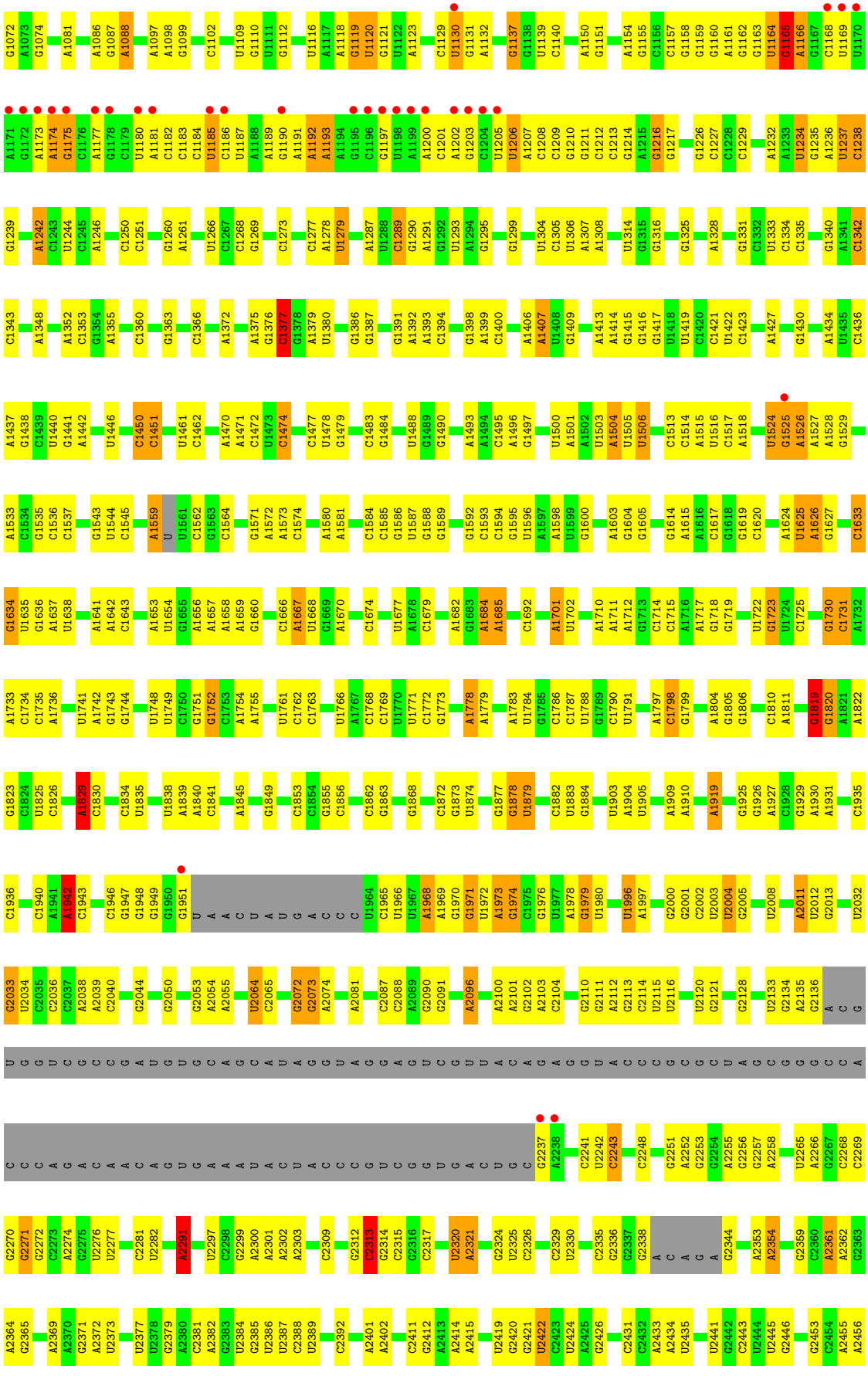
3 Residue-property plots (i)

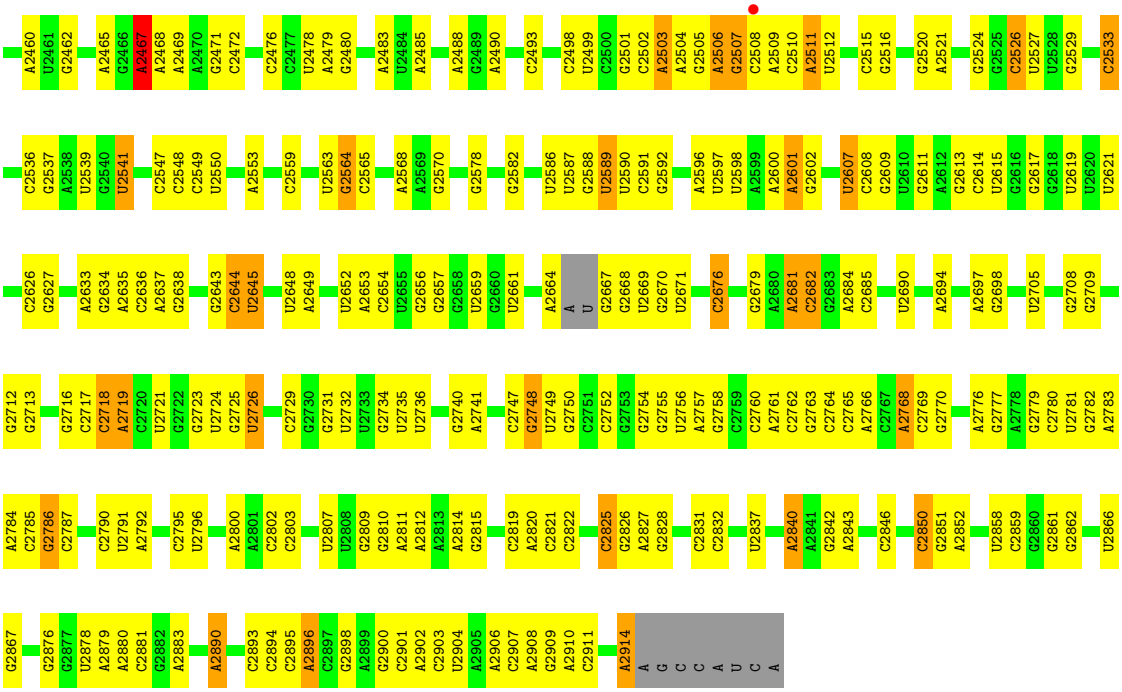
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S RIBOSOMAL RNA

Chain 0:





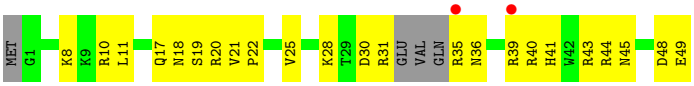


• Molecule 2: 50S ribosomal protein L37e

Chain 1:

• Molecule 3: 50S ribosomal protein L39e

Chain 2:



• Molecule 4: 50S ribosomal protein L44e

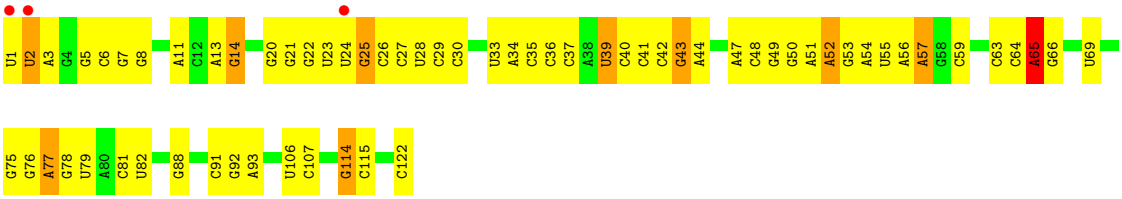
Chain 3:

• Molecule 5: QUINUPRISTIN

Chain 4:

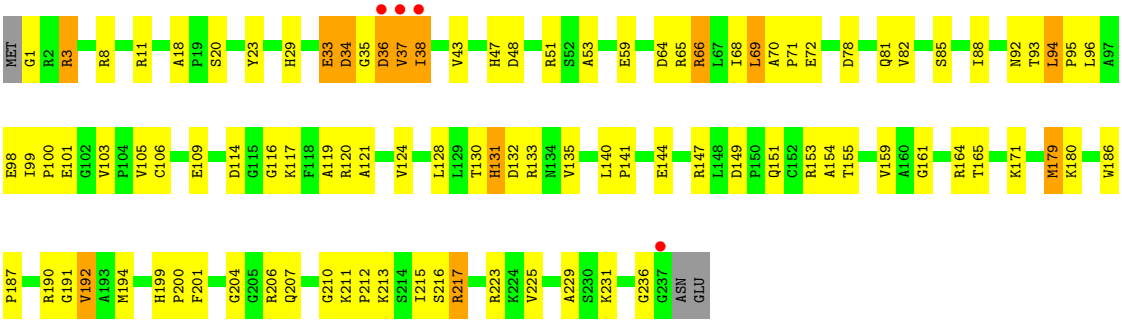
• Molecule 6: 5S RIBOSOMAL RNA

Chain 9:



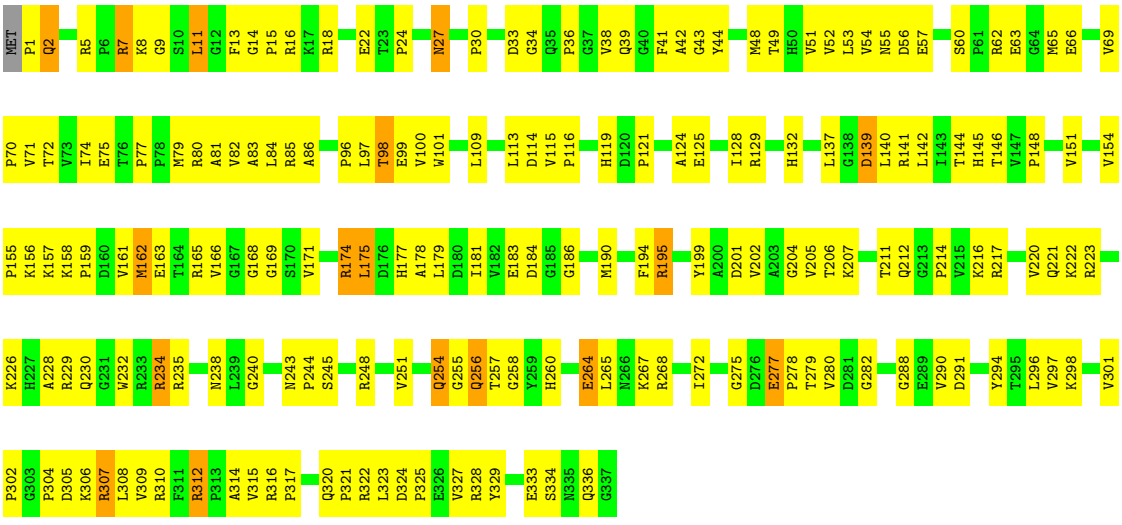
• Molecule 7: 50S ribosomal protein L2

Chain A:



• Molecule 8: 50S ribosomal protein L3

Chain B:

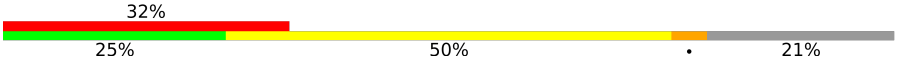


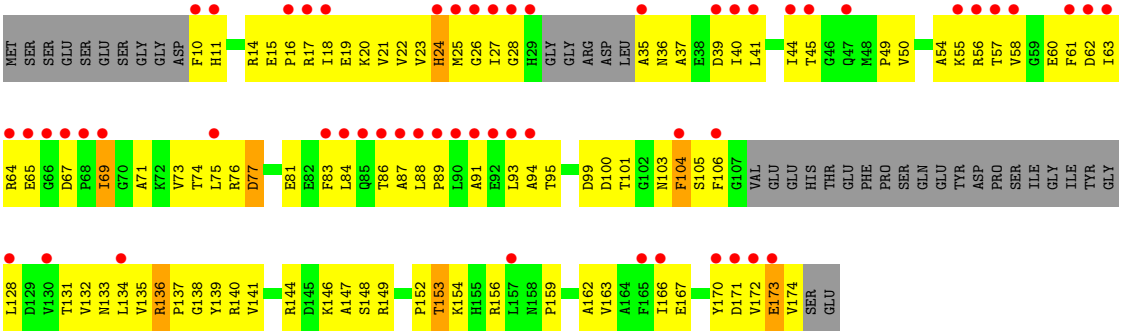
• Molecule 9: 50S ribosomal protein L4

Chain C:

• Molecule 10: 50S ribosomal protein L5

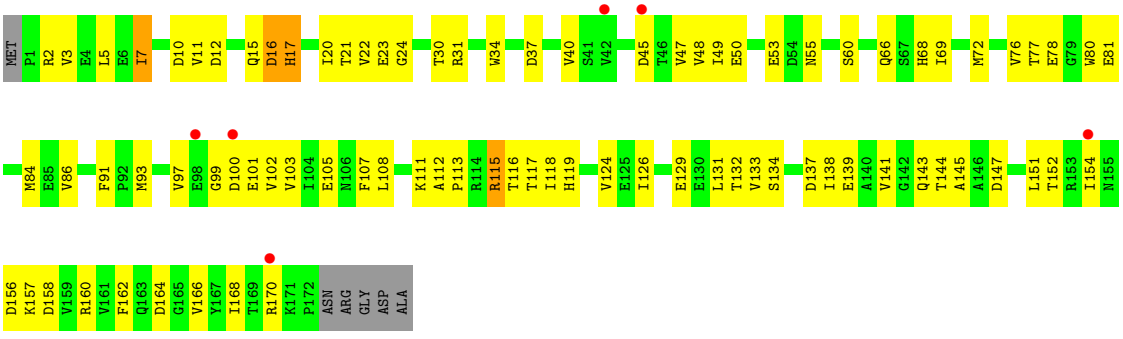
Chain D:





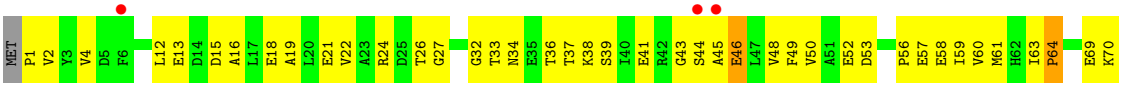
• Molecule 11: 50S ribosomal protein L6

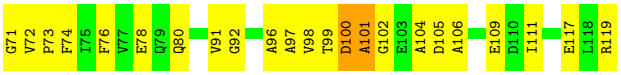
Chain E:



• Molecule 12: 50S ribosomal protein L7Ae

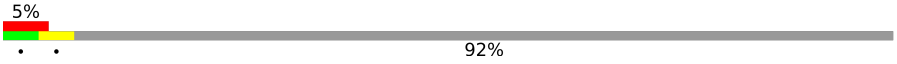
Chain F:

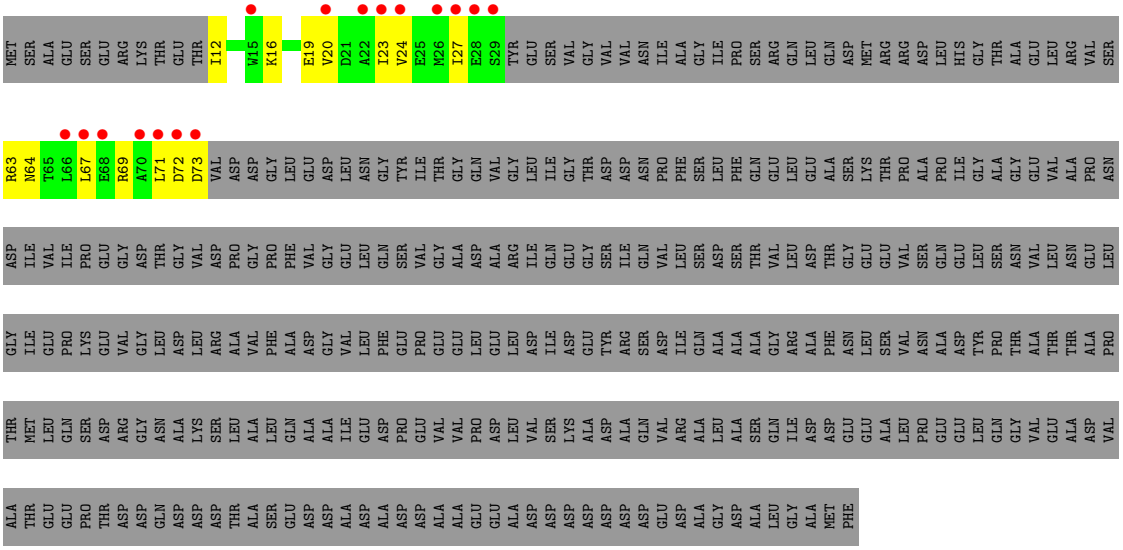




• Molecule 13: 50S ribosomal protein L10

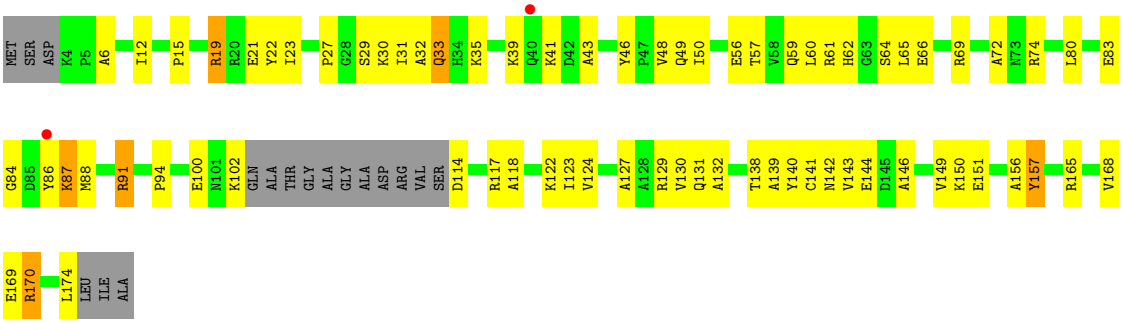
Chain G:





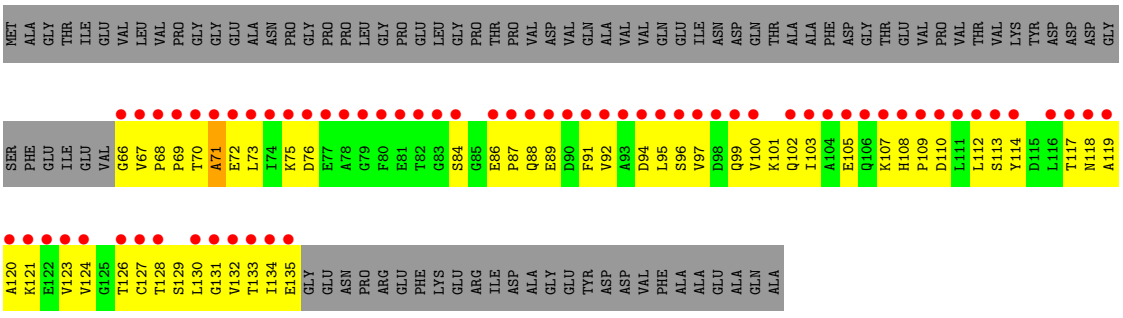
• Molecule 14: 50S ribosomal protein L10e

Chain H:



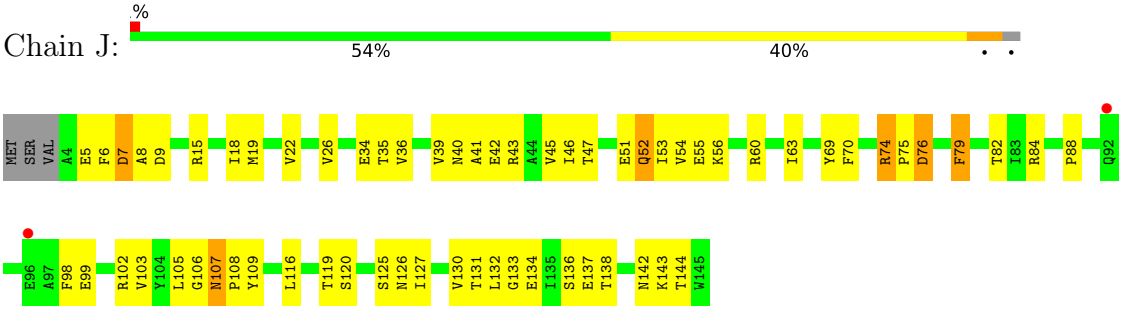
• Molecule 15: 50S ribosomal protein L11

Chain I:



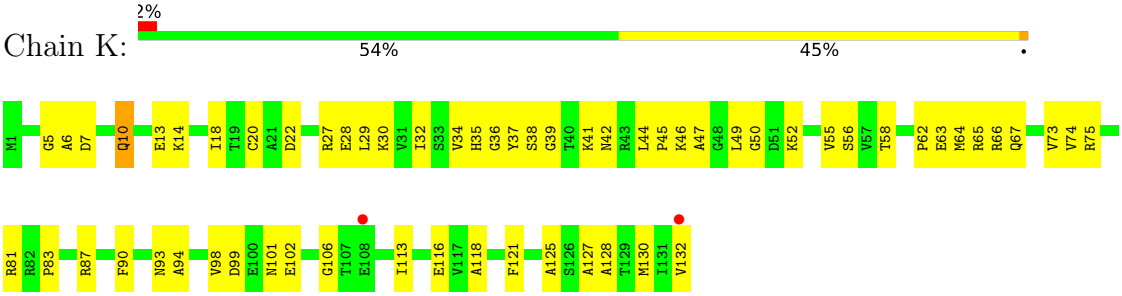
• Molecule 16: 50S ribosomal protein L13

Chain J:



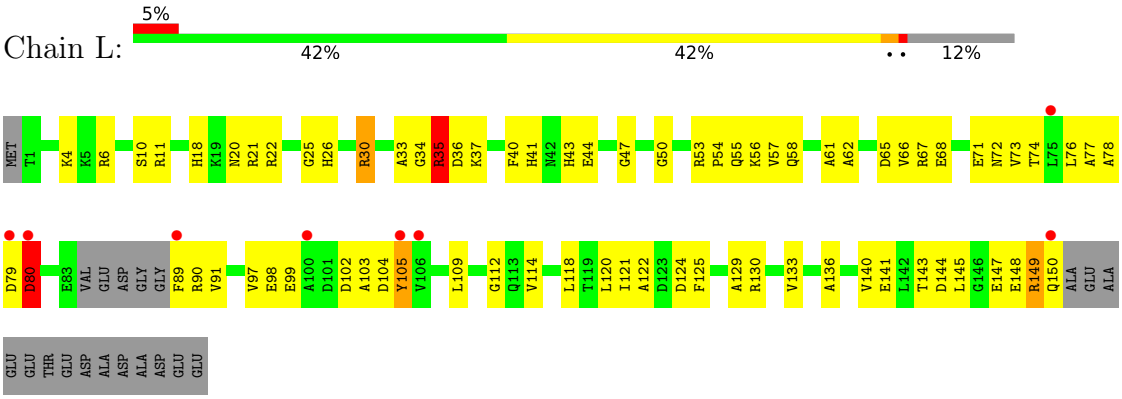
• Molecule 17: 50S ribosomal protein L14

Chain K:



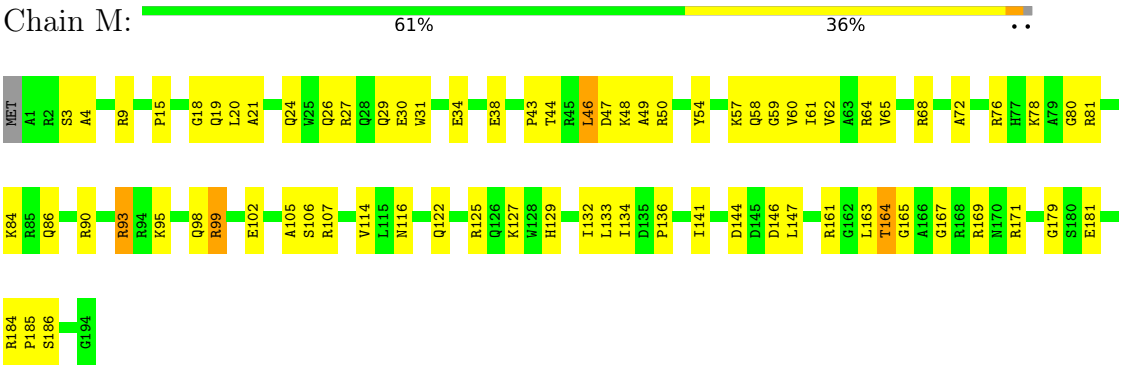
• Molecule 18: 50S ribosomal protein L15

Chain L:



• Molecule 19: 50S ribosomal protein L15e

Chain M:

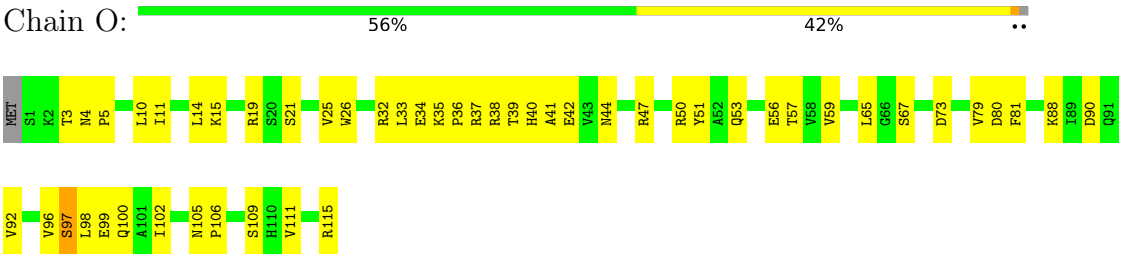


• Molecule 20: 50S ribosomal protein L18

Chain N:

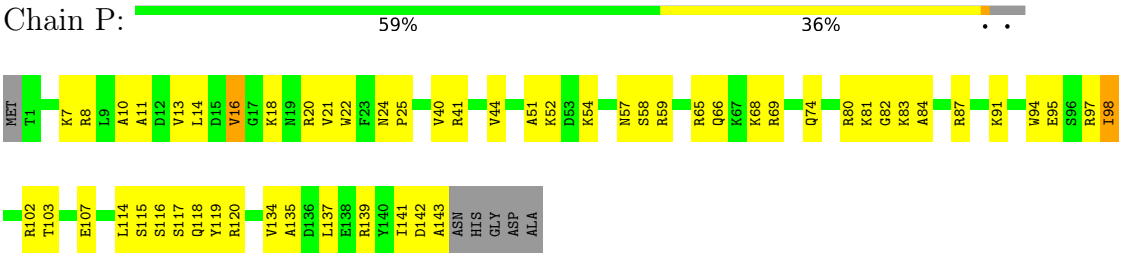
• Molecule 21: 50S ribosomal protein L18e

Chain O:



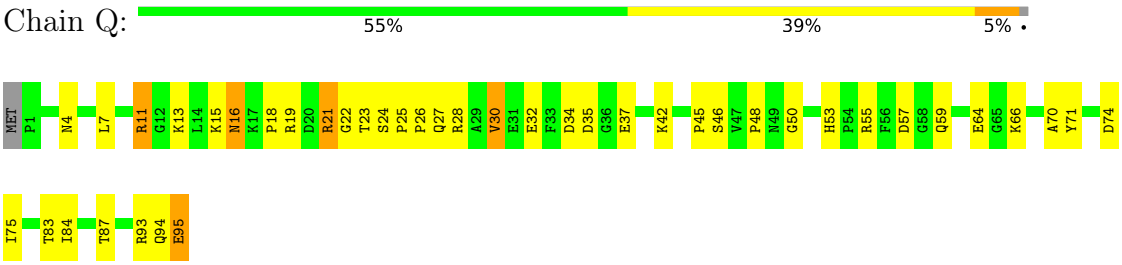
• Molecule 22: 50S ribosomal protein L19e

Chain P:



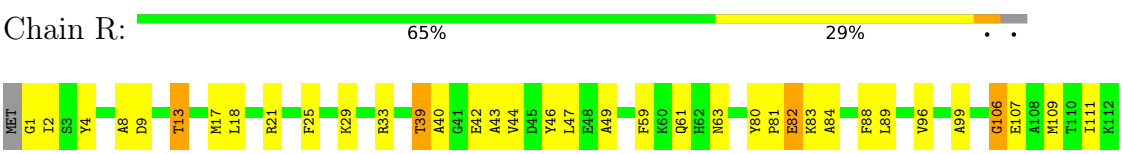
• Molecule 23: 50S ribosomal protein L21e

Chain Q:



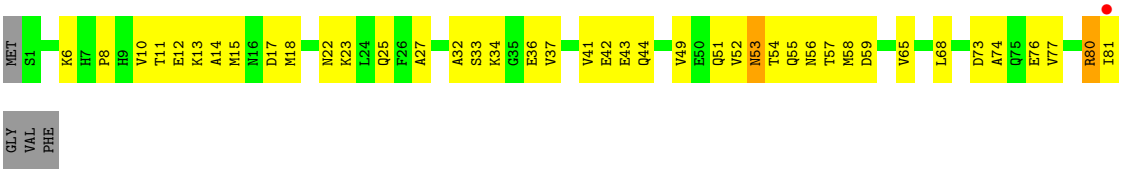
• Molecule 24: 50S ribosomal protein L22

Chain R:



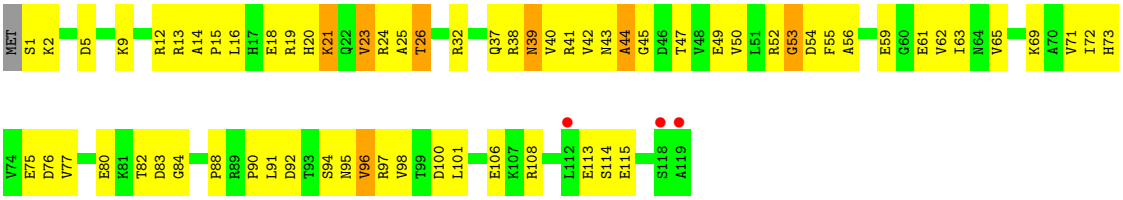
• Molecule 25: 50S ribosomal protein L23

Chain S:



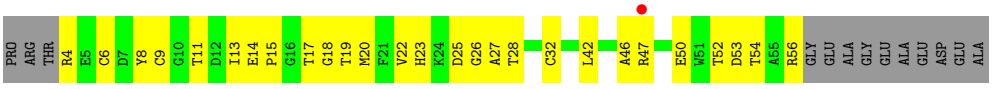
• Molecule 26: 50S ribosomal protein L24

Chain T:



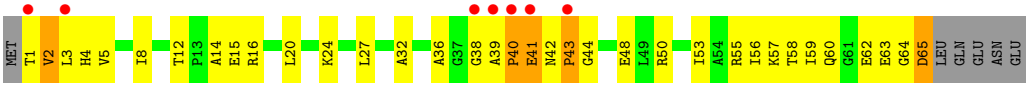
• Molecule 27: 50S ribosomal protein L24e

Chain U:



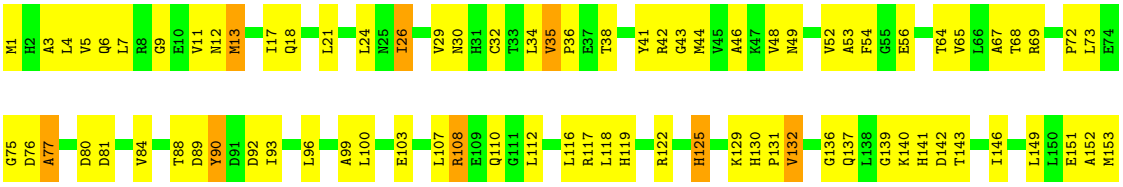
• Molecule 28: 50S ribosomal protein L29

Chain V:

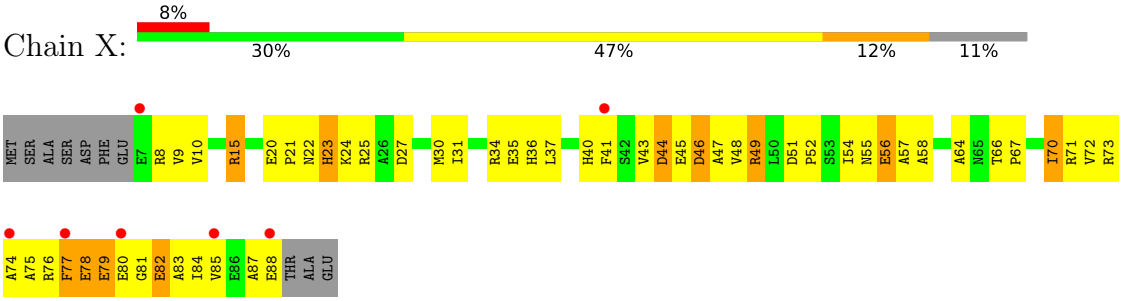


• Molecule 29: 50S ribosomal protein L30

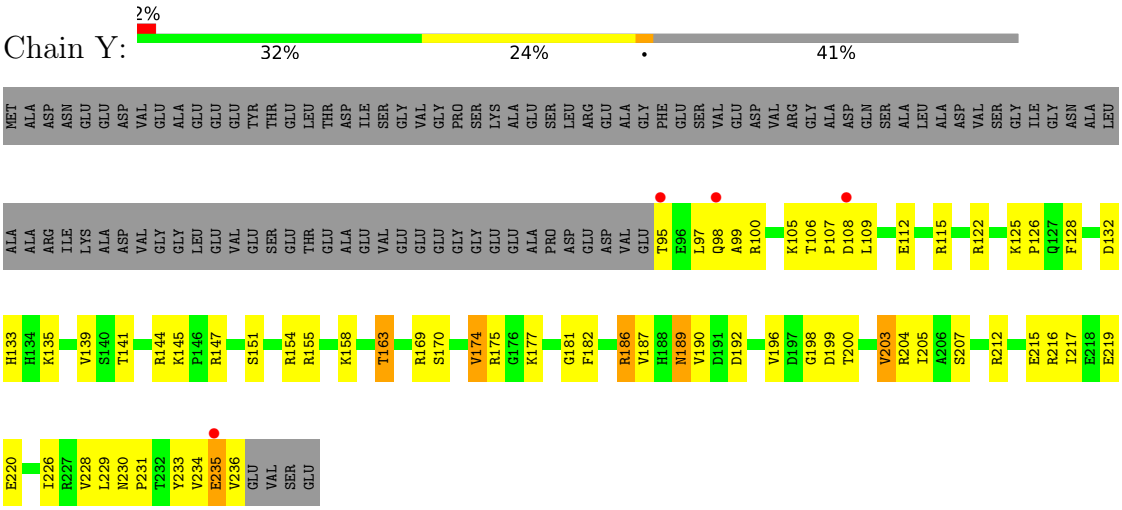
Chain W:



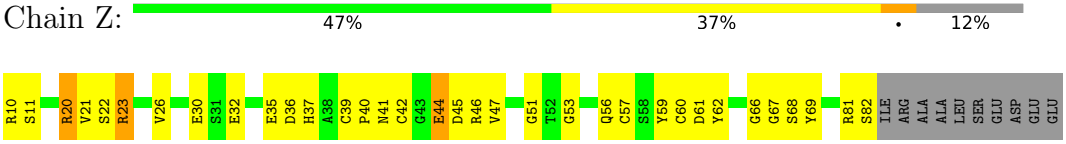
• Molecule 30: 50S ribosomal protein L31e



• Molecule 31: 50S ribosomal protein L32e



• Molecule 32: 50S ribosomal protein L37Ae



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.69Å 299.78Å 573.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.90 49.95 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.98-2.90) 83.4 (49.95-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.223 0.171 , 0.219	Depositor DCC
R_{free} test set	3279 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	43.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	99111	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MHV, MHW, OMG, MG, PSU, CD, 1MA, NA, UR3, OMU, 004, MHT, K, MHU, CL, DBB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	0	0.37	0/65957	0.69	13/102867 (0.0%)
2	1	0.38	0/438	0.61	0/578
3	2	0.34	0/401	0.56	0/529
4	3	0.37	0/771	0.57	0/1024
5	4	1.63	0/13	1.38	0/15
6	9	0.35	0/2904	0.69	1/4526 (0.0%)
7	A	0.33	0/1786	0.65	0/2408
8	B	0.33	0/2690	0.63	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.32	0/1111	0.56	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.33	0/901	0.57	0/1224
13	G	0.30	0/241	0.48	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.31	0/526	0.55	0/716
16	J	0.35	0/1136	0.59	0/1530
17	K	0.35	0/1001	0.67	0/1347
18	L	0.32	0/1130	0.63	0/1509
19	M	0.34	0/1582	0.60	0/2117
20	N	0.30	0/1474	0.64	0/1999
21	O	0.34	0/874	0.60	0/1181
22	P	0.33	0/1147	0.54	0/1528
23	Q	0.35	0/749	0.66	0/1005
24	R	0.34	0/1172	0.63	0/1578
25	S	0.34	0/648	0.59	0/875
26	T	0.32	0/958	0.61	0/1289
27	U	0.32	0/417	0.58	0/562
28	V	0.29	0/502	0.55	0/675
29	W	0.36	0/1219	0.62	0/1655
30	X	0.33	0/664	0.61	0/895
31	Y	0.35	0/1146	0.62	0/1536
32	Z	0.35	0/589	0.67	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
All	All	0.36	0/98715	0.67	14/147603 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	20
6	9	0	1
29	W	0	1
All	All	0	22

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	0	1504	A	C1'-O4'-C4'	-6.45	104.74	109.90
1	0	1942	A	C5'-C4'-C3'	6.01	125.61	116.00
1	0	871	G	C5'-C4'-O4'	-5.83	102.10	109.10
1	0	2291	A	N9-C1'-C2'	5.68	121.39	114.00
1	0	2726	U	N1-C1'-C2'	5.63	121.33	114.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain

5.2 Too-close contacts (i)

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	59020	0	29811	1125	0
2	1	431	0	426	27	0
3	2	396	0	413	30	0
4	3	755	0	728	38	0
5	4	73	0	64	1	0
6	9	2599	0	1325	72	0
7	A	1753	0	1766	116	0
8	B	2625	0	2533	203	0
9	C	1859	0	1816	140	0
10	D	1094	0	1085	111	0
11	E	1357	0	1266	79	0
12	F	890	0	843	56	0
13	G	240	0	231	19	0
14	H	1282	0	1292	88	0
15	I	519	0	500	62	0
16	J	1120	0	1098	75	0
17	K	992	0	1031	72	0
18	L	1118	0	1076	82	0
19	M	1558	0	1566	82	0
20	N	1445	0	1401	145	0
21	O	865	0	873	48	0
22	P	1136	0	1123	57	0
23	Q	735	0	729	45	0
24	R	1149	0	1122	59	0
25	S	641	0	605	39	0
26	T	950	0	923	71	0
27	U	410	0	364	35	0
28	V	499	0	511	43	0
29	W	1196	0	1137	116	0
30	X	654	0	653	59	0
31	Y	1130	0	1133	69	0
32	Z	578	0	539	24	0
33	0	109	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	74	0	0	0	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	2	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5842	0	0	196	0
38	1	60	0	0	8	0
38	2	49	0	0	5	0
38	3	69	0	0	11	0
38	4	2	0	0	0	0
38	9	143	0	0	9	0
38	A	123	0	0	19	0
38	B	146	0	0	20	0
38	C	185	0	0	37	0
38	D	49	0	0	22	0
38	E	42	0	0	11	0
38	F	26	0	0	5	0
38	G	20	0	0	2	0
38	H	69	0	0	15	0
38	I	9	0	0	3	0
38	J	55	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	K	59	0	0	11	0
38	L	82	0	0	21	0
38	M	129	0	0	12	0
38	N	60	0	0	11	0
38	O	42	0	0	7	0
38	P	72	0	0	5	0
38	Q	48	0	0	7	0
38	R	85	0	0	6	0
38	S	30	0	0	5	0
38	T	39	0	0	8	0
38	U	29	0	0	3	0
38	V	13	0	0	3	0
38	W	69	0	0	12	0
38	X	26	0	0	6	0
38	Y	101	0	0	16	0
38	Z	37	0	0	2	0
All	All	99111	0	59983	2986	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 20.

The worst 5 of 2986 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)
6:9:6:C:H5"	20:N:37:ARG:NH1	1.59	1.16
1:0:156:C:H5"	19:M:171:ARG:HD3	1.25	1.15
6:9:6:C:H5"	20:N:37:ARG:HH12	0.97	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.07
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.06

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	
2	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
4	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	14	42
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	9	31
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	10	34
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	7	27
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	6	24
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	25	58
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	2	10
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	11
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	8	28
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	4	18
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	7	26
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	5	19
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	2	8
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	17	48
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	14	42
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	22	54
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	5	20
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	1	4
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	22	54
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	1	4
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	8 29

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
7	A	37	VAL
8	B	184	ASP
9	C	8	LEU
10	D	173	GLU

5.3.2 Protein sidechains (i)

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
2	1	46/47 (98%)	46 (100%)	0	100 100
3	2	42/46 (91%)	41 (98%)	1 (2%)	49 79
4	3	79/79 (100%)	79 (100%)	0	100 100
5	4	2/2 (100%)	2 (100%)	0	100 100
7	A	179/182 (98%)	168 (94%)	11 (6%)	18 48
8	B	282/283 (100%)	264 (94%)	18 (6%)	17 45
9	C	193/193 (100%)	181 (94%)	12 (6%)	18 47
10	D	117/148 (79%)	109 (93%)	8 (7%)	16 42
11	E	152/156 (97%)	146 (96%)	6 (4%)	32 66
12	F	93/94 (99%)	90 (97%)	3 (3%)	39 73
13	G	27/283 (10%)	27 (100%)	0	100 100
14	H	134/145 (92%)	128 (96%)	6 (4%)	27 61
15	I	58/130 (45%)	58 (100%)	0	100 100
16	J	118/121 (98%)	110 (93%)	8 (7%)	16 42
17	K	106/106 (100%)	105 (99%)	1 (1%)	78 93
18	L	113/127 (89%)	107 (95%)	6 (5%)	22 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
20	N	149/150 (99%)	144 (97%)	5 (3%)	37	71
21	O	93/94 (99%)	90 (97%)	3 (3%)	39	73
22	P	113/117 (97%)	109 (96%)	4 (4%)	36	70
23	Q	79/80 (99%)	74 (94%)	5 (6%)	18	46
24	R	117/122 (96%)	113 (97%)	4 (3%)	37	71
25	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
26	T	105/106 (99%)	98 (93%)	7 (7%)	16	43
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	55	82
29	W	130/130 (100%)	122 (94%)	8 (6%)	18	47
30	X	66/74 (89%)	58 (88%)	8 (12%)	5	15
31	Y	120/196 (61%)	114 (95%)	6 (5%)	24	57
32	Z	60/68 (88%)	56 (93%)	4 (7%)	16	43
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	26	59

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	T	39	ASN
32	Z	44	GLU
29	W	13	MET
30	X	46	ASP
10	D	149	ARG

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

Mol	Chain	Res	Type
20	N	40	ASN
24	R	123	GLN
20	N	107	ASN
23	Q	40	HIS
26	T	43	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	23 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	261 (9%)	24 (0%)

5 of 261 RNA backbone outliers are listed below:

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

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1856	C
1	0	2467	A
1	0	2313	C
1	0	2526	C
1	0	871	G

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

10 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	OMG	0	2588	1	18,26,27	1.03	2 (11%)	19,38,41	0.69	1 (5%)
5	MHV	4	6	5	7,9,10	2.05	2 (28%)	7,11,13	1.72	2 (28%)
1	OMU	0	2587	35,1	19,22,23	0.22	0	26,31,34	0.42	0
5	DBB	4	3	5	4,5,6	1.05	0	1,5,7	0.24	0
5	MHU	4	5	5	14,15,16	2.86	8 (57%)	18,19,21	1.65	5 (27%)
5	004	4	7	5	9,10,11	2.92	3 (33%)	9,12,14	2.09	3 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	1MA	0	628	35,1	16,25,26	1.40	3 (18%)	18,37,40	1.13	2 (11%)
1	PSU	0	2621	1	18,21,22	1.45	2 (11%)	22,30,33	1.26	3 (13%)
1	UR3	0	2619	1	19,22,23	0.45	0	26,32,35	0.63	1 (3%)
5	MHW	4	1	33,5	9,9,10	2.56	4 (44%)	10,11,13	1.22	1 (10%)

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	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
5	MHV	4	6	5	-	0/1/12/14	0/1/1/1
1	OMU	0	2587	35,1	-	0/9/27/28	0/2/2/2
5	DBB	4	3	5	-	0/3/4/6	-
5	MHU	4	5	5	-	0/9/12/14	0/1/1/1
5	004	4	7	5	-	2/4/6/8	0/1/1/1
1	1MA	0	628	35,1	-	0/3/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
5	MHW	4	1	33,5	-	0/2/2/4	0/1/1/1

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	004	CB-CA	7.09	1.60	1.52
1	0	2621	PSU	C2-N1	4.62	1.43	1.36
5	4	1	MHW	CA-N	4.54	1.42	1.35
5	4	5	MHU	CA-N	4.52	1.55	1.47
5	4	6	MHV	CB-CG	4.38	1.57	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	4	7	004	CG2-CB-CA	3.82	126.81	120.65
5	4	5	MHU	CB-CA-N	3.45	116.00	110.65
5	4	7	004	CB-CA-N	-3.42	104.21	112.40
1	0	2621	PSU	C6-C5-C4	3.21	120.44	118.20
5	4	5	MHU	O-C-CA	-3.19	116.43	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	7	004	C-CA-CB-CG1
5	4	7	004	C-CA-CB-CG2

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 232 ligands modelled in this entry, 232 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	2749/2922 (94%)	-0.23	37 (1%) 77 77	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.56	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.10	2 (4%) 35 31	24, 56, 82, 96	0
4	3	92/92 (100%)	0.02	1 (1%) 80 80	30, 48, 61, 79	0
5	4	2/8 (25%)	-0.11	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.14	3 (2%) 57 55	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.11	4 (1%) 70 69	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.13	0 100 100	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.32	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	1.73	56 (40%) 0 0	47, 94, 117, 125	0
11	E	172/178 (96%)	0.47	6 (3%) 44 38	41, 61, 83, 88	0
12	F	119/120 (99%)	0.35	3 (2%) 57 55	41, 63, 88, 104	0
13	G	29/348 (8%)	2.33	16 (55%) 0 0	71, 87, 95, 96	0
14	H	160/177 (90%)	0.10	2 (1%) 77 77	36, 52, 88, 105	0
15	I	70/162 (43%)	4.05	65 (92%) 0 0	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.08	2 (1%) 75 75	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.22	2 (1%) 73 73	26, 46, 65, 75	0
18	L	145/165 (87%)	0.38	8 (5%) 25 21	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.48	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.05	5 (2%) 54 50	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.13	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.03	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.15	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.20	0 100 100	28, 40, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	S	81/85 (95%)	0.01	1 (1%) 79 79	37, 52, 71, 79	0
26	T	119/120 (99%)	0.21	3 (2%) 57 55	35, 51, 80, 94	0
27	U	53/66 (80%)	0.08	1 (1%) 66 65	39, 51, 67, 78	0
28	V	65/71 (91%)	0.69	7 (10%) 5 4	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.17	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	0.36	7 (8%) 10 8	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.10	4 (2%) 53 49	24, 40, 62, 81	0
32	Z	73/83 (87%)	-0.19	0 100 100	39, 53, 69, 87	0
All	All	6648/7489 (88%)	-0.03	235 (3%) 44 38	18, 46, 91, 148	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	88	GLN	8.5
15	I	132	VAL	8.5
15	I	128	THR	7.7
15	I	70	THR	7.4
15	I	66	GLY	7.1

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

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DBB	4	3	6/7	0.94	0.18	51,51,52,53	0
5	MHV	4	6	9/10	0.94	0.18	53,55,59,59	0
5	MHU	4	5	15/16	0.95	0.17	56,59,62,63	0
5	004	4	7	10/11	0.95	0.20	45,48,49,51	0
5	MHW	4	1	9/10	0.96	0.20	46,47,49,50	0
1	1MA	0	628	23/24	0.98	0.15	25,28,31,32	0
1	OMU	0	2587	21/22	0.98	0.15	29,32,37,38	0
1	OMG	0	2588	24/25	0.98	0.14	28,31,34,35	0
1	UR3	0	2619	21/22	0.98	0.13	30,35,39,42	0
1	PSU	0	2621	20/21	0.98	0.14	33,35,37,38	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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^{th} 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^2)	Q<0.9
35	NA	0	3183	1/1	0.09	0.92	81,81,81,81	0
35	NA	0	3174	1/1	0.53	0.47	75,75,75,75	0
35	NA	R	202	1/1	0.60	0.59	75,75,75,75	0
35	NA	0	3134	1/1	0.61	0.61	72,72,72,72	0
35	NA	0	3175	1/1	0.71	0.45	54,54,54,54	0
35	NA	9	203	1/1	0.73	0.70	85,85,85,85	0
35	NA	0	3140	1/1	0.74	0.35	47,47,47,47	0
35	NA	0	3137	1/1	0.76	0.30	81,81,81,81	0
33	MG	0	3105	1/1	0.77	0.26	47,47,47,47	0
35	NA	0	3120	1/1	0.80	0.52	36,36,36,36	0
35	NA	0	3121	1/1	0.80	0.30	50,50,50,50	0
35	NA	0	3141	1/1	0.81	0.12	37,37,37,37	0
35	NA	C	301	1/1	0.82	0.25	32,32,32,32	0
35	NA	0	3117	1/1	0.83	0.43	56,56,56,56	0
35	NA	0	3170	1/1	0.83	0.35	72,72,72,72	0
35	NA	9	202	1/1	0.84	0.13	31,31,31,31	0
35	NA	0	3147	1/1	0.84	0.25	44,44,44,44	0
33	MG	0	3063	1/1	0.85	0.39	37,37,37,37	0
35	NA	0	3165	1/1	0.85	0.33	60,60,60,60	0
35	NA	0	3156	1/1	0.86	0.28	55,55,55,55	0
33	MG	0	3082	1/1	0.86	0.18	46,46,46,46	0
33	MG	0	3071	1/1	0.87	0.08	55,55,55,55	0
35	NA	0	3184	1/1	0.87	0.15	45,45,45,45	0
33	MG	0	3097	1/1	0.87	0.44	79,79,79,79	0
36	CL	0	3192	1/1	0.87	0.43	88,88,88,88	0
35	NA	0	3173	1/1	0.88	0.23	53,53,53,53	0
35	NA	0	3122	1/1	0.88	0.17	47,47,47,47	0
35	NA	0	3164	1/1	0.88	0.34	75,75,75,75	0
33	MG	0	3050	1/1	0.88	0.19	72,72,72,72	0
35	NA	0	3118	1/1	0.88	0.15	39,39,39,39	0
36	CL	0	3194	1/1	0.88	0.18	58,58,58,58	0
33	MG	0	3108	1/1	0.89	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	NA	0	3161	1/1	0.89	0.48	54,54,54,54	0
33	MG	0	3093	1/1	0.89	0.16	45,45,45,45	0
35	NA	0	3138	1/1	0.89	0.31	41,41,41,41	0
33	MG	0	3092	1/1	0.90	0.16	42,42,42,42	0
33	MG	0	3047	1/1	0.90	0.20	62,62,62,62	0
35	NA	H	201	1/1	0.90	0.15	38,38,38,38	0
35	NA	0	3166	1/1	0.90	0.14	35,35,35,35	0
35	NA	0	3160	1/1	0.90	0.47	48,48,48,48	0
33	MG	0	3049	1/1	0.90	0.25	58,58,58,58	0
35	NA	0	3159	1/1	0.91	0.07	49,49,49,49	0
35	NA	0	3171	1/1	0.91	0.36	65,65,65,65	0
35	NA	0	3132	1/1	0.91	0.21	39,39,39,39	0
33	MG	T	201	1/1	0.91	0.11	45,45,45,45	0
33	MG	0	3034	1/1	0.91	0.09	29,29,29,29	0
35	NA	0	3154	1/1	0.91	0.36	40,40,40,40	0
33	MG	0	3051	1/1	0.91	0.12	58,58,58,58	0
36	CL	A	303	1/1	0.91	0.19	58,58,58,58	0
35	NA	0	3167	1/1	0.92	0.51	43,43,43,43	0
35	NA	0	3185	1/1	0.92	0.32	38,38,38,38	0
33	MG	0	3084	1/1	0.92	0.11	49,49,49,49	0
33	MG	0	3066	1/1	0.92	0.07	34,34,34,34	0
35	NA	0	3125	1/1	0.92	0.25	39,39,39,39	0
33	MG	0	3061	1/1	0.92	0.06	52,52,52,52	0
35	NA	R	201	1/1	0.92	0.10	33,33,33,33	0
33	MG	0	3077	1/1	0.92	0.17	58,58,58,58	0
35	NA	0	3179	1/1	0.92	0.23	64,64,64,64	0
35	NA	0	3181	1/1	0.92	0.31	46,46,46,46	0
33	MG	0	3046	1/1	0.92	0.11	52,52,52,52	0
35	NA	0	3145	1/1	0.93	0.06	55,55,55,55	0
33	MG	0	3101	1/1	0.93	0.08	73,73,73,73	0
35	NA	0	3148	1/1	0.93	0.13	29,29,29,29	0
33	MG	0	3069	1/1	0.93	0.08	56,56,56,56	0
33	MG	0	3087	1/1	0.93	0.29	75,75,75,75	0
35	NA	0	3157	1/1	0.93	0.56	71,71,71,71	0
33	MG	0	3089	1/1	0.93	0.13	47,47,47,47	0
34	K	0	3111	1/1	0.93	0.12	62,62,62,62	0
35	NA	0	3176	1/1	0.93	0.63	60,60,60,60	0
35	NA	0	3114	1/1	0.93	0.20	50,50,50,50	0
35	NA	0	3143	1/1	0.93	0.26	47,47,47,47	0
35	NA	0	3182	1/1	0.93	0.16	40,40,40,40	0
33	MG	0	3086	1/1	0.94	0.05	41,41,41,41	0
33	MG	9	201	1/1	0.94	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	K	201	1/1	0.94	0.07	46,46,46,46	0
35	NA	0	3144	1/1	0.94	0.13	44,44,44,44	0
33	MG	0	3060	1/1	0.94	0.08	27,27,27,27	0
35	NA	0	3168	1/1	0.94	0.20	40,40,40,40	0
33	MG	0	3073	1/1	0.94	0.07	28,28,28,28	0
35	NA	0	3130	1/1	0.94	0.42	61,61,61,61	0
33	MG	0	3103	1/1	0.94	0.08	60,60,60,60	0
35	NA	L	201	1/1	0.94	0.71	61,61,61,61	0
35	NA	Q	101	1/1	0.94	0.09	33,33,33,33	0
35	NA	0	3115	1/1	0.94	0.11	29,29,29,29	0
35	NA	0	3135	1/1	0.94	0.31	60,60,60,60	0
35	NA	0	3116	1/1	0.94	0.41	33,33,33,33	0
35	NA	0	3177	1/1	0.94	0.30	58,58,58,58	0
36	CL	0	3195	1/1	0.94	0.27	88,88,88,88	0
33	MG	0	3076	1/1	0.94	0.10	50,50,50,50	0
36	CL	O	202	1/1	0.94	0.18	74,74,74,74	0
33	MG	0	3001	1/1	0.95	0.07	30,30,30,30	0
33	MG	0	3083	1/1	0.95	0.07	25,25,25,25	0
35	NA	0	3139	1/1	0.95	0.17	62,62,62,62	0
35	NA	J	201	1/1	0.95	0.09	61,61,61,61	0
35	NA	0	3123	1/1	0.95	0.12	27,27,27,27	0
33	MG	0	3106	1/1	0.95	0.24	42,42,42,42	0
35	NA	0	3126	1/1	0.95	0.10	28,28,28,28	0
35	NA	0	3127	1/1	0.95	0.17	26,26,26,26	0
36	CL	0	3187	1/1	0.95	0.19	57,57,57,57	0
33	MG	0	3094	1/1	0.95	0.10	73,73,73,73	0
33	MG	0	3041	1/1	0.95	0.20	38,38,38,38	0
33	MG	0	3098	1/1	0.95	0.20	48,48,48,48	0
35	NA	0	3150	1/1	0.95	0.09	42,42,42,42	0
36	CL	J	203	1/1	0.95	0.14	63,63,63,63	0
36	CL	L	202	1/1	0.95	0.11	46,46,46,46	0
33	MG	0	3090	1/1	0.95	0.08	41,41,41,41	0
35	NA	A	302	1/1	0.96	0.16	38,38,38,38	0
33	MG	0	3085	1/1	0.96	0.18	41,41,41,41	0
35	NA	0	3112	1/1	0.96	0.14	21,21,21,21	0
33	MG	0	3035	1/1	0.96	0.05	50,50,50,50	0
33	MG	0	3052	1/1	0.96	0.05	35,35,35,35	0
33	MG	0	3088	1/1	0.96	0.21	48,48,48,48	0
33	MG	0	3008	1/1	0.96	0.04	33,33,33,33	0
33	MG	0	3011	1/1	0.96	0.08	21,21,21,21	0
33	MG	0	3015	1/1	0.96	0.06	38,38,38,38	0
36	CL	0	3191	1/1	0.96	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	3	101	1/1	0.96	0.04	40,40,40,40	0
35	NA	0	3163	1/1	0.96	0.21	44,44,44,44	0
33	MG	0	3033	1/1	0.96	0.09	31,31,31,31	0
35	NA	0	3142	1/1	0.96	0.07	26,26,26,26	0
36	CL	J	202	1/1	0.96	0.18	55,55,55,55	0
33	MG	0	3002	1/1	0.96	0.04	26,26,26,26	0
36	CL	J	204	1/1	0.96	0.11	57,57,57,57	0
33	MG	0	3096	1/1	0.96	0.16	49,49,49,49	0
34	K	0	3110	1/1	0.96	0.20	86,86,86,86	0
33	MG	0	3059	1/1	0.97	0.14	44,44,44,44	0
33	MG	0	3099	1/1	0.97	0.22	53,53,53,53	0
35	NA	0	3158	1/1	0.97	0.53	43,43,43,43	0
33	MG	0	3010	1/1	0.97	0.07	24,24,24,24	0
35	NA	0	3136	1/1	0.97	0.32	50,50,50,50	0
33	MG	0	3027	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	3045	1/1	0.97	0.08	58,58,58,58	0
33	MG	0	3091	1/1	0.97	0.06	26,26,26,26	0
33	MG	0	3107	1/1	0.97	0.09	49,49,49,49	0
35	NA	0	3119	1/1	0.97	0.09	40,40,40,40	0
35	NA	M	201	1/1	0.97	0.13	30,30,30,30	0
33	MG	0	3065	1/1	0.97	0.10	38,38,38,38	0
33	MG	0	3109	1/1	0.97	0.11	20,20,20,20	0
35	NA	0	3169	1/1	0.97	0.14	35,35,35,35	0
33	MG	0	3056	1/1	0.97	0.09	42,42,42,42	0
36	CL	0	3188	1/1	0.97	0.14	57,57,57,57	0
33	MG	0	3067	1/1	0.97	0.11	41,41,41,41	0
35	NA	0	3146	1/1	0.97	0.12	26,26,26,26	0
36	CL	0	3193	1/1	0.97	0.13	56,56,56,56	0
33	MG	B	401	1/1	0.97	0.09	32,32,32,32	0
33	MG	0	3095	1/1	0.97	0.11	49,49,49,49	0
35	NA	0	3149	1/1	0.97	0.12	35,35,35,35	0
33	MG	0	3068	1/1	0.97	0.09	59,59,59,59	0
35	NA	0	3151	1/1	0.97	0.05	30,30,30,30	0
35	NA	0	3180	1/1	0.97	0.38	45,45,45,45	0
35	NA	0	3153	1/1	0.97	0.14	43,43,43,43	0
36	CL	N	201	1/1	0.97	0.13	57,57,57,57	0
33	MG	0	3058	1/1	0.97	0.06	27,27,27,27	0
36	CL	R	203	1/1	0.97	0.15	43,43,43,43	0
33	MG	0	3081	1/1	0.98	0.16	41,41,41,41	0
33	MG	0	3013	1/1	0.98	0.10	37,37,37,37	0
33	MG	0	3053	1/1	0.98	0.13	48,48,48,48	0
33	MG	4	102	1/1	0.98	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	3054	1/1	0.98	0.09	24,24,24,24	0
33	MG	A	301	1/1	0.98	0.08	44,44,44,44	0
33	MG	0	3055	1/1	0.98	0.13	40,40,40,40	0
33	MG	0	3014	1/1	0.98	0.07	31,31,31,31	0
33	MG	0	3057	1/1	0.98	0.08	32,32,32,32	0
33	MG	Y	301	1/1	0.98	0.12	34,34,34,34	0
33	MG	0	3006	1/1	0.98	0.05	46,46,46,46	0
33	MG	0	3038	1/1	0.98	0.08	28,28,28,28	0
33	MG	0	3039	1/1	0.98	0.10	33,33,33,33	0
35	NA	0	3113	1/1	0.98	0.26	44,44,44,44	0
33	MG	0	3040	1/1	0.98	0.14	70,70,70,70	0
33	MG	0	3062	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	3016	1/1	0.98	0.11	23,23,23,23	0
35	NA	0	3152	1/1	0.98	0.11	34,34,34,34	0
33	MG	0	3064	1/1	0.98	0.18	96,96,96,96	0
33	MG	0	3043	1/1	0.98	0.06	35,35,35,35	0
35	NA	0	3155	1/1	0.98	0.20	39,39,39,39	0
33	MG	0	3044	1/1	0.98	0.06	37,37,37,37	0
33	MG	0	3017	1/1	0.98	0.05	26,26,26,26	0
35	NA	S	101	1/1	0.98	0.13	10,10,10,10	0
36	CL	0	3186	1/1	0.98	0.16	43,43,43,43	0
33	MG	0	3018	1/1	0.98	0.09	34,34,34,34	0
33	MG	0	3021	1/1	0.98	0.10	32,32,32,32	0
36	CL	0	3189	1/1	0.98	0.07	39,39,39,39	0
33	MG	0	3100	1/1	0.98	0.05	35,35,35,35	0
35	NA	0	3124	1/1	0.98	0.12	48,48,48,48	0
35	NA	0	3162	1/1	0.98	0.40	49,49,49,49	0
33	MG	0	3048	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	3025	1/1	0.98	0.03	42,42,42,42	0
36	CL	3	103	1/1	0.98	0.08	53,53,53,53	0
33	MG	0	3104	1/1	0.98	0.06	40,40,40,40	0
36	CL	B	402	1/1	0.98	0.12	40,40,40,40	0
35	NA	0	3128	1/1	0.98	0.13	22,22,22,22	0
33	MG	0	3075	1/1	0.98	0.07	38,38,38,38	0
35	NA	0	3131	1/1	0.98	0.12	39,39,39,39	0
33	MG	0	3012	1/1	0.98	0.07	25,25,25,25	0
35	NA	0	3133	1/1	0.98	0.16	50,50,50,50	0
33	MG	0	3032	1/1	0.98	0.07	40,40,40,40	0
35	NA	0	3172	1/1	0.98	0.13	58,58,58,58	0
36	CL	Y	302	1/1	0.98	0.11	30,30,30,30	0
37	CD	3	102	1/1	0.98	0.05	55,55,55,55	0
37	CD	O	201	1/1	0.98	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	MG	0	3102	1/1	0.99	0.08	23,23,23,23	0
33	MG	0	3079	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	3080	1/1	0.99	0.09	65,65,65,65	0
33	MG	0	3004	1/1	0.99	0.07	27,27,27,27	0
33	MG	0	3042	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	3026	1/1	0.99	0.07	19,19,19,19	0
33	MG	0	3009	1/1	0.99	0.07	22,22,22,22	0
33	MG	0	3028	1/1	0.99	0.09	39,39,39,39	0
36	CL	0	3190	1/1	0.99	0.12	46,46,46,46	0
33	MG	0	3029	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	3030	1/1	0.99	0.08	31,31,31,31	0
35	NA	0	3178	1/1	0.99	0.10	29,29,29,29	0
33	MG	0	3031	1/1	0.99	0.08	28,28,28,28	0
35	NA	0	3129	1/1	0.99	0.10	25,25,25,25	0
33	MG	0	3005	1/1	0.99	0.10	27,27,27,27	0
33	MG	0	3019	1/1	0.99	0.05	23,23,23,23	0
33	MG	0	3020	1/1	0.99	0.08	22,22,22,22	0
33	MG	0	3003	1/1	0.99	0.12	31,31,31,31	0
33	MG	0	3070	1/1	0.99	0.06	25,25,25,25	0
33	MG	0	3036	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	3072	1/1	0.99	0.08	47,47,47,47	0
36	CL	M	202	1/1	0.99	0.08	31,31,31,31	0
33	MG	0	3037	1/1	0.99	0.07	44,44,44,44	0
33	MG	0	3074	1/1	0.99	0.10	20,20,20,20	0
33	MG	0	3022	1/1	0.99	0.08	36,36,36,36	0
33	MG	0	3023	1/1	0.99	0.06	34,34,34,34	0
37	CD	1	101	1/1	0.99	0.08	56,56,56,56	0
33	MG	0	3024	1/1	0.99	0.06	12,12,12,12	0
33	MG	0	3078	1/1	0.99	0.04	22,22,22,22	0
33	MG	0	3007	1/1	1.00	0.07	12,12,12,12	0
37	CD	U	8701	1/1	1.00	0.08	60,60,60,60	0
37	CD	Z	101	1/1	1.00	0.11	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.