wwPDB X-ray Structure Validation Summary Report (i)

Feb 11, 2024 – 04:19 PM EST

PDB ID	:	3CC2
Title	:	The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors	:	Gurel, G.; Blaha, G.
Deposited on	:	2008-02-23
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*
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:

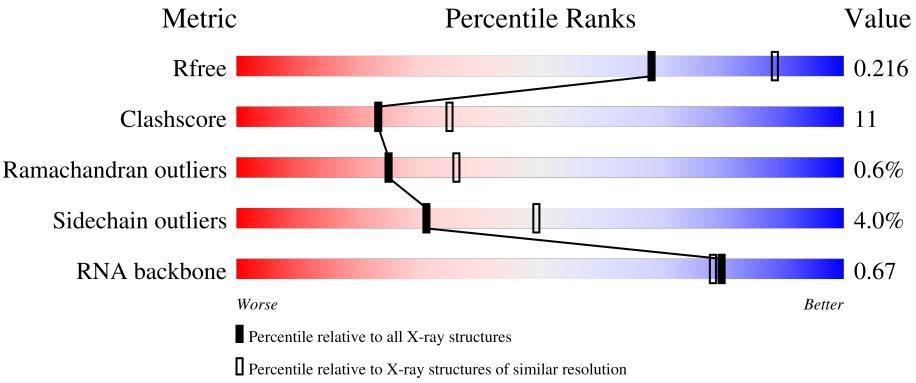
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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)
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 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%

Mol	Chain	Length	Quality of chain
1	A	240	70% 26% • •
2	B	338	71% 25% •
3	C	246	75% 21% •
4	D	177	47% 29% • 21%
5	E	178	69% 28% • •
6	F	120	72% 26% ••

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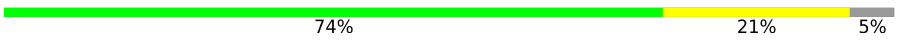
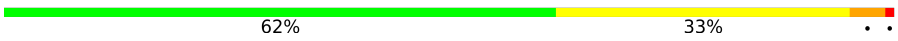
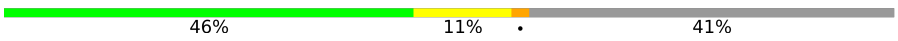
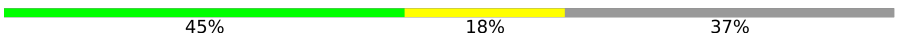
Mol	Chain	Length	Quality of chain
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	
30	0	2923	
31	9	122	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 99049 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	246	1860	1130	345	384	1	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	H	1	Total Na 1 1	0	0
33	J	1	Total Na 1 1	0	0
33	L	1	Total Na 1 1	0	0
33	M	1	Total Na 1 1	0	0
33	Q	1	Total Na 1 1	0	0
33	R	2	Total Na 2 2	0	0
33	S	1	Total Na 1 1	0	0
33	0	73	Total Na 73 73	0	0
33	9	3	Total Na 3 3	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	3	1	Total Cl 1 1	0	0
34	0	10	Total Cl 10 10	0	0

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

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

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	2	Total K 2 2	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	A	117	Total O 117 117	0	0
37	B	146	Total O 146 146	0	0
37	C	170	Total O 170 170	0	0
37	D	47	Total O 47 47	0	0
37	E	42	Total O 42 42	0	0
37	F	24	Total O 24 24	0	0
37	G	19	Total O 19 19	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	H	72	Total O 72 72	0	0
37	I	9	Total O 9 9	0	0
37	J	51	Total O 51 51	0	0
37	K	56	Total O 56 56	0	0
37	L	72	Total O 72 72	0	0
37	M	119	Total O 119 119	0	0
37	N	65	Total O 65 65	0	0
37	O	39	Total O 39 39	0	0
37	P	63	Total O 63 63	0	0
37	Q	52	Total O 52 52	0	0
37	R	80	Total O 80 80	0	0
37	S	33	Total O 33 33	0	0
37	T	38	Total O 38 38	0	0
37	U	27	Total O 27 27	0	0
37	V	14	Total O 14 14	0	0
37	W	66	Total O 66 66	0	0
37	X	29	Total O 29 29	0	0
37	Y	94	Total O 94 94	0	0
37	Z	26	Total O 26 26	0	0
37	1	53	Total O 53 53	0	0
37	2	40	Total O 40 40	0	0

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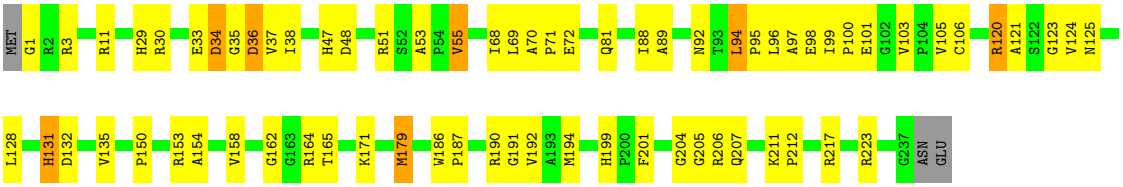
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	3	72	Total O 72 72	0	0
37	0	5949	Total O 5949 5949	0	0
37	9	139	Total O 139 139	0	0

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. 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. 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.

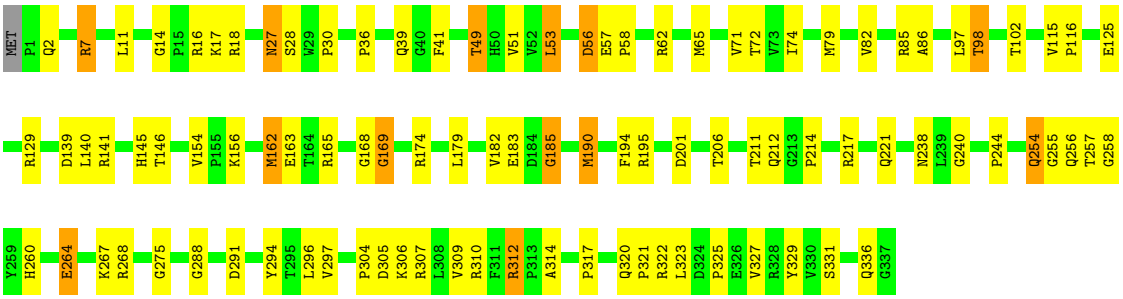
• Molecule 1: 50S ribosomal protein L2P

Chain A:



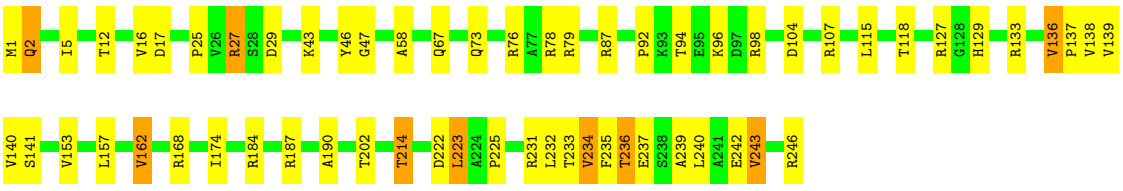
• Molecule 2: 50S ribosomal protein L3P

Chain B:



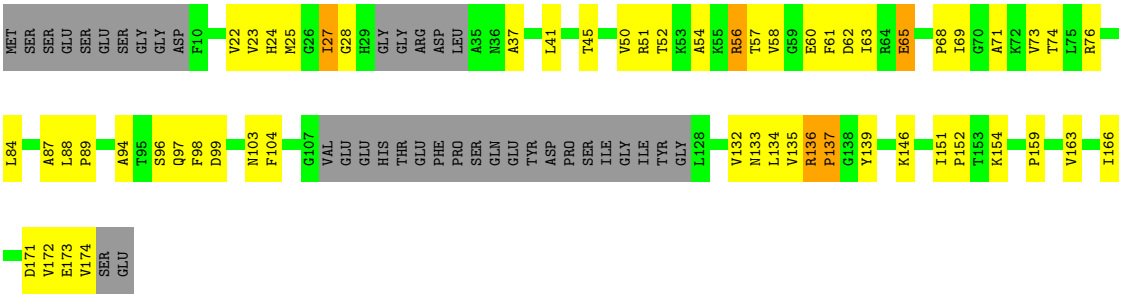
• Molecule 3: 50S ribosomal protein L4P

Chain C:



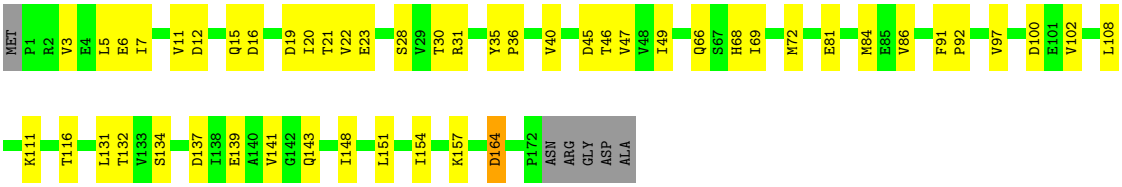
• Molecule 4: 50S ribosomal protein L5P

Chain D:



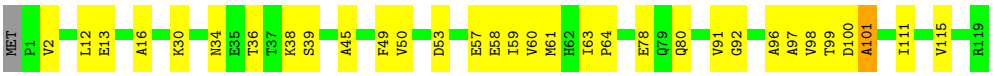
• Molecule 5: 50S ribosomal protein L6P

Chain E:



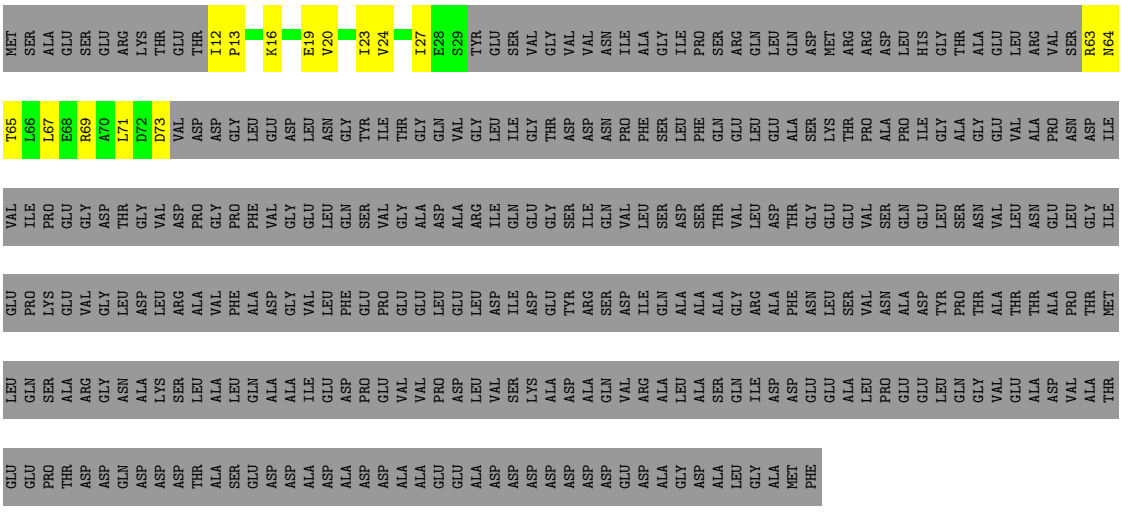
• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



• Molecule 7: 50S ribosomal protein L10E

Chain G:

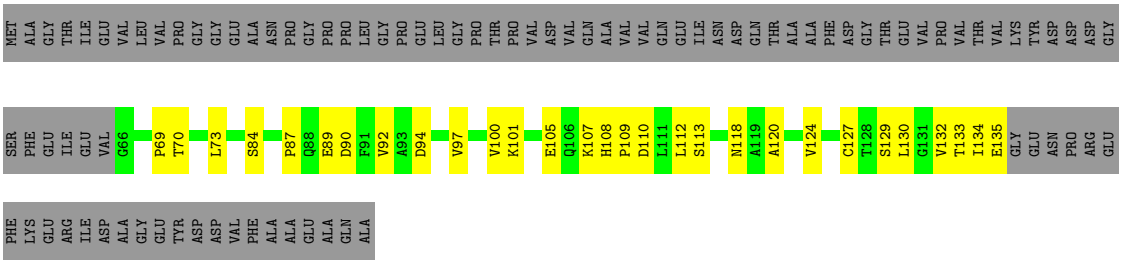


• Molecule 8: 50S ribosomal protein L10e

Chain H:

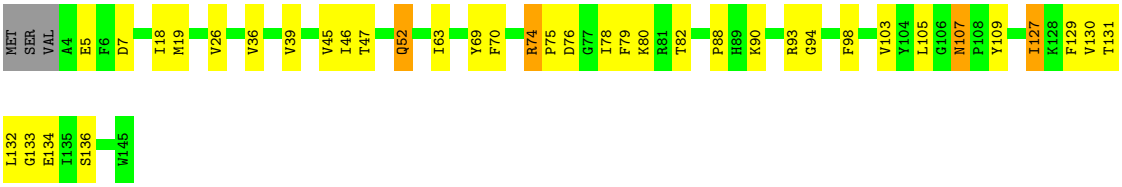
• Molecule 9: 50S ribosomal protein L11P

Chain I:



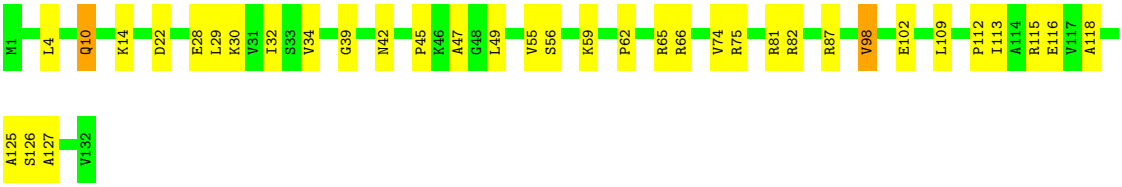
• Molecule 10: 50S ribosomal protein L13P

Chain J:



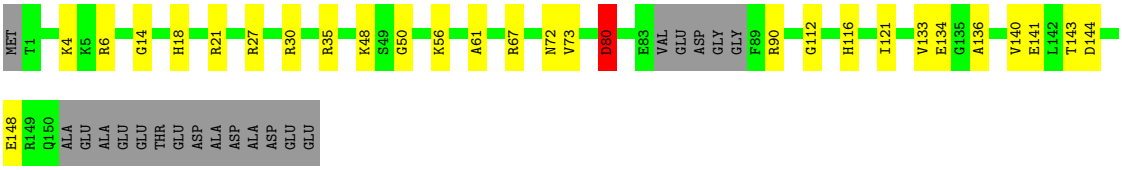
• Molecule 11: 50S ribosomal protein L14P

Chain K:



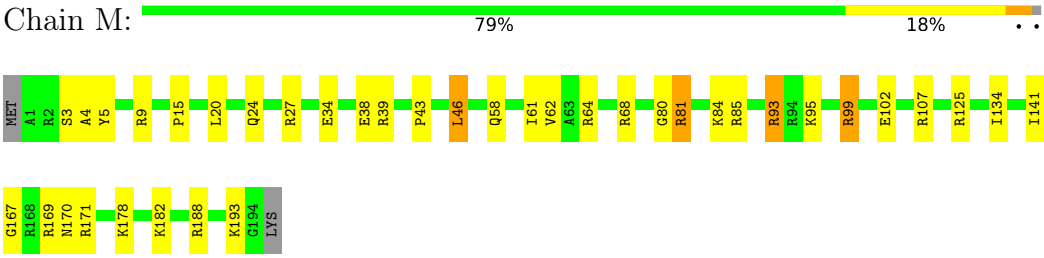
• Molecule 12: 50S ribosomal protein L15P

Chain L:



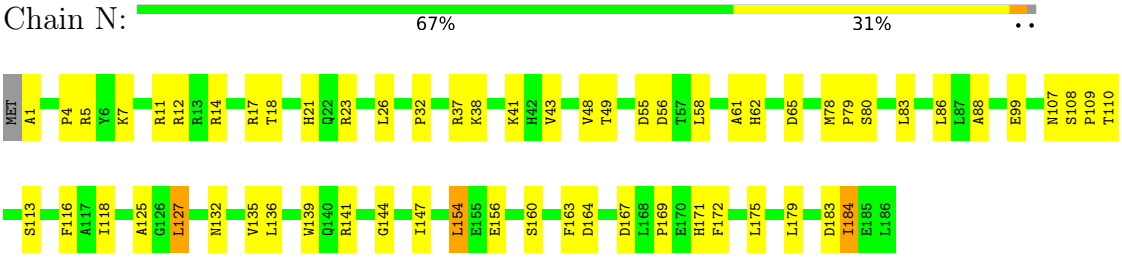
• Molecule 13: 50S ribosomal protein L15e

Chain M:



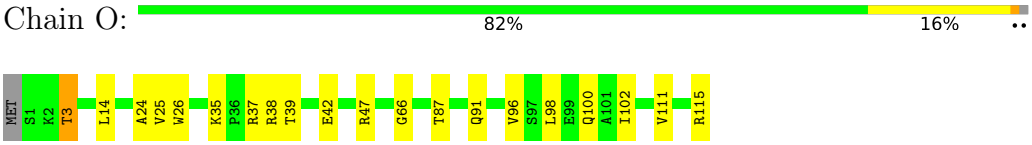
• Molecule 14: 50S ribosomal protein L18P

Chain N:



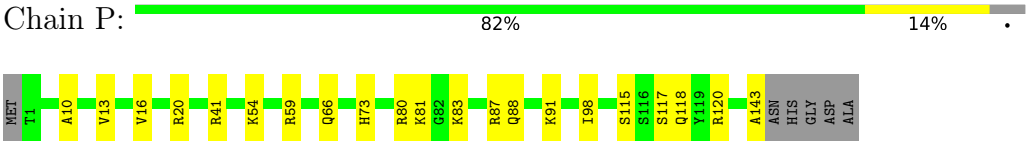
• Molecule 15: 50S ribosomal protein L18e

Chain O:



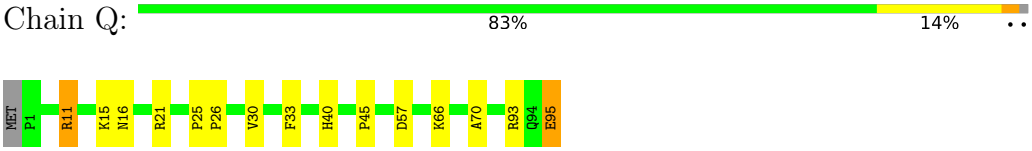
• Molecule 16: 50S ribosomal protein L19e

Chain P:



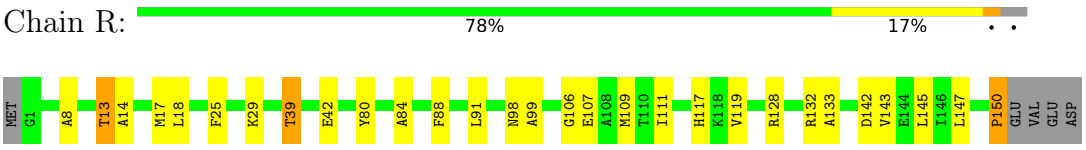
• Molecule 17: 50S ribosomal protein L21e

Chain Q:



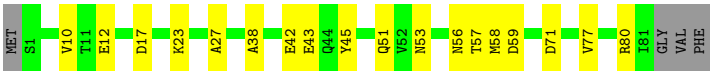
• Molecule 18: 50S ribosomal protein L22P

Chain R:



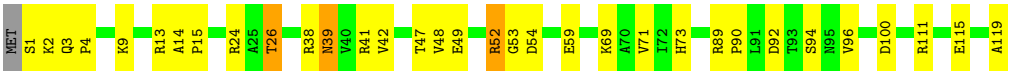
• Molecule 19: 50S ribosomal protein L23P

Chain S:



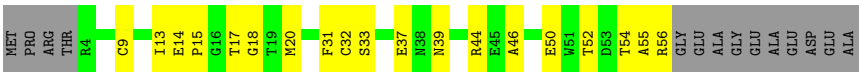
• Molecule 20: 50S ribosomal protein L24P

Chain T:



• Molecule 21: 50S ribosomal protein L24e

Chain U:

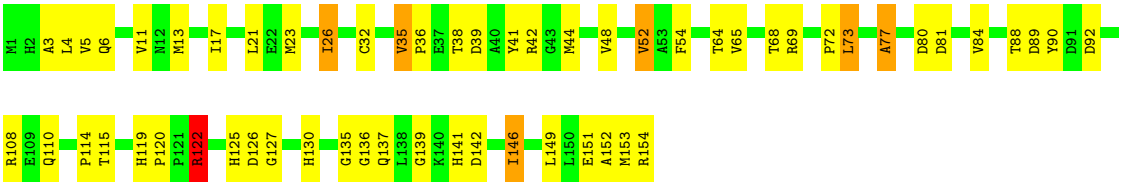


• Molecule 22: 50S ribosomal protein L29P

Chain V:

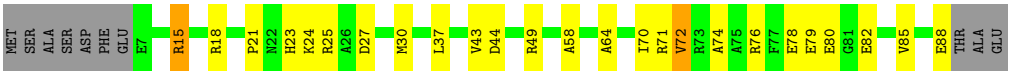
• Molecule 23: 50S ribosomal protein L30P

Chain W:



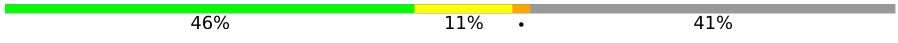
• Molecule 24: 50S ribosomal protein L31e

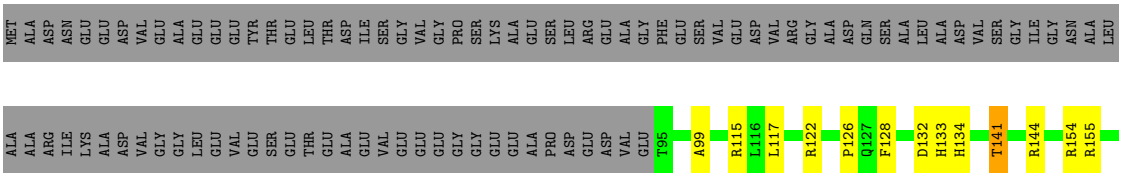
Chain X:



• Molecule 25: 50S ribosomal protein L32e

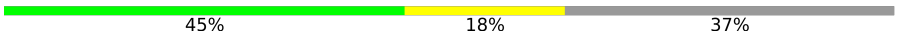
Chain Y:





• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:

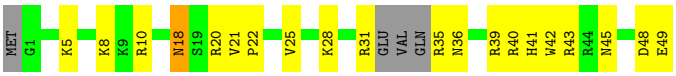


• Molecule 27: 50S ribosomal protein L37e

Chain 1:

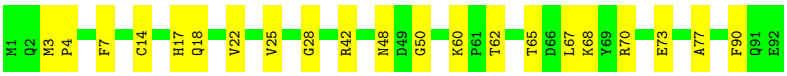
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



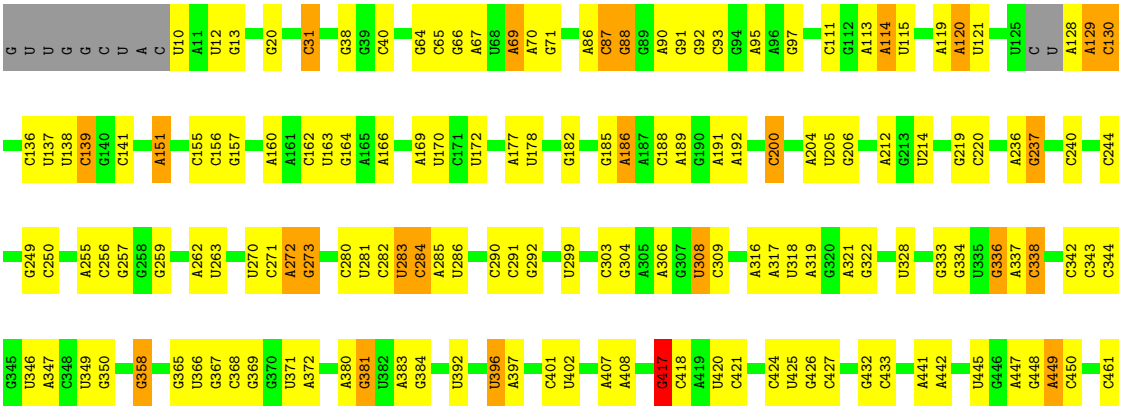
• Molecule 29: 50S ribosomal protein L44E

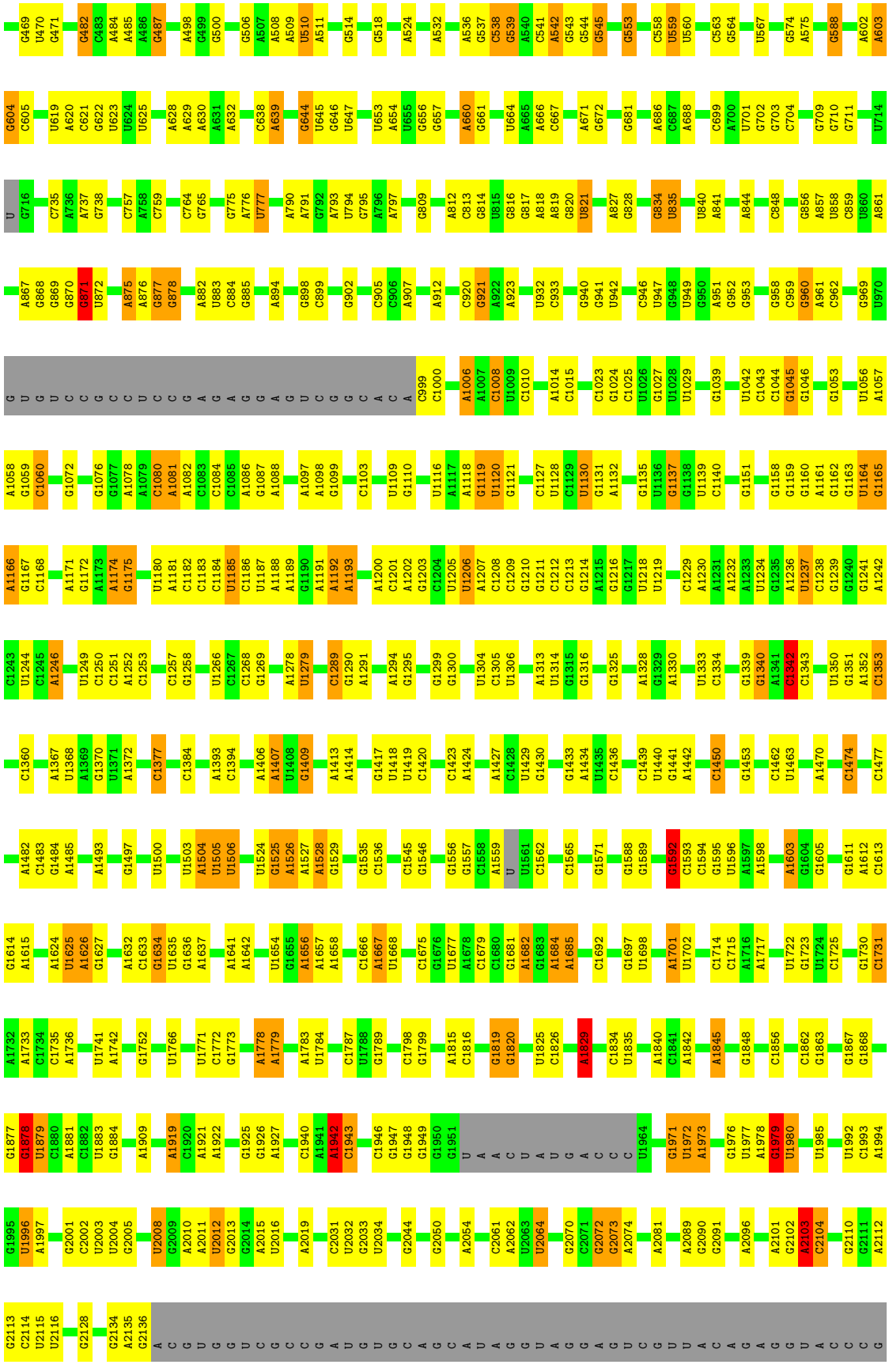
Chain 3:

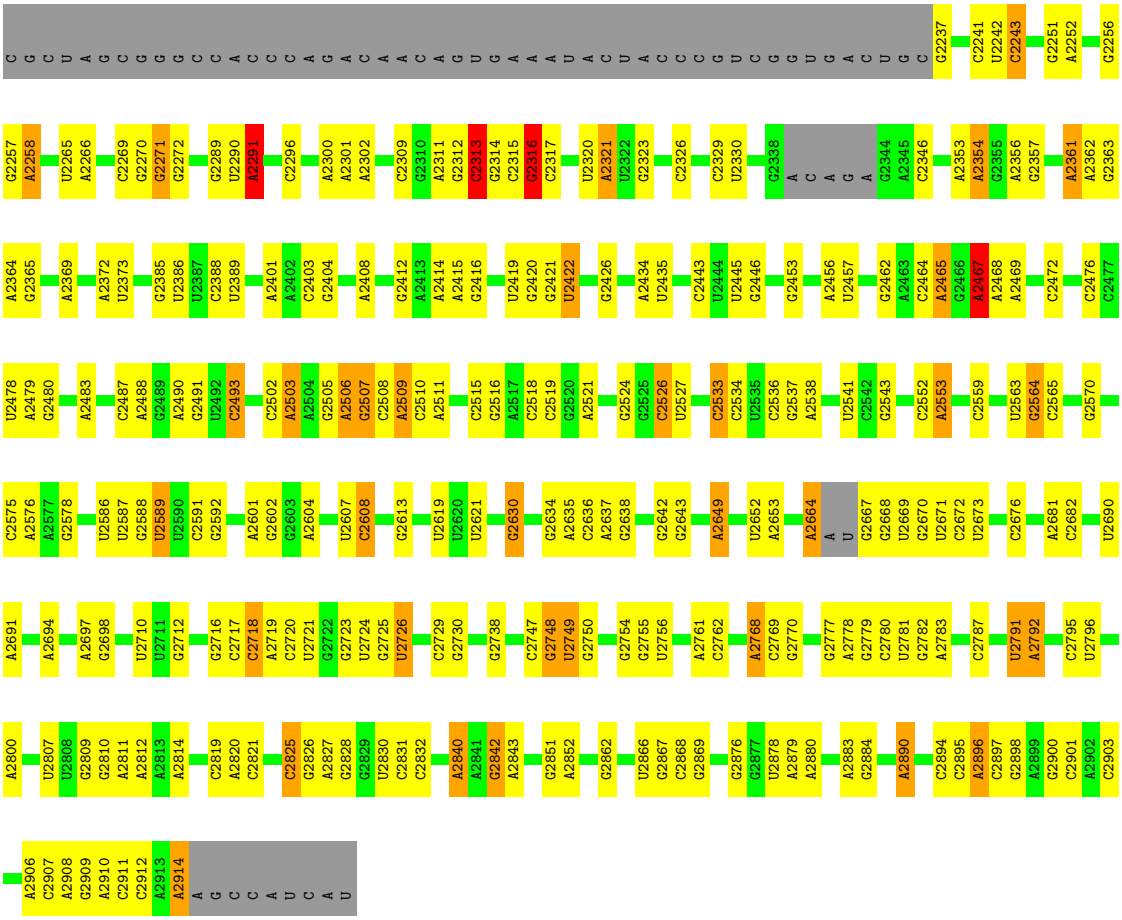


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

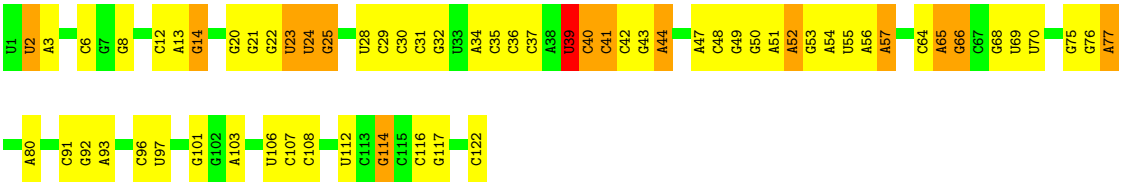






• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.231 0.184 , 0.216	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.4	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	0.90	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

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

[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: NA, UR3, OMG, OMU, CL, PSU, MG, K, 1MA, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	270	U	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	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	A	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	73	0	0	0	0
33	9	3	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	1	0	0	0	0
33	J	1	0	0	0	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	2	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	3	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	J	3	0	0	1	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	O	1	0	0	0	0
34	R	1	0	0	0	0
34	Y	1	0	0	0	0
35	1	1	0	0	0	0
35	3	1	0	0	0	0
35	O	1	0	0	0	0
35	U	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	2	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	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 11.

The worst 5 of 1694 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)
18:R:150:PRO:CD	18:R:150:PRO:CG	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5"	1.61	1.14
30:0:871:G:H5'	30:0:871:G:C8	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08

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
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	17 25
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	17 25
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100 100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	4 3
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100 100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	9 11
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100 100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100 100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100 100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	22 32
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19 29
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	22 32
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100 100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	9 13
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100 100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100 100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100 100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100 100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100 100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100 100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	7 9
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	9 13
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22 32
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	12 17
25	Y	140/241 (58%)	140 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	5 4
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100 100
28	2	42/50 (84%)	42 (100%)	0	0	100 100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100 100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	25 36

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU

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
1	A	179/182 (98%)	171 (96%)	8 (4%)	27 44
2	B	282/283 (100%)	268 (95%)	14 (5%)	24 40
3	C	193/193 (100%)	179 (93%)	14 (7%)	14 22
4	D	117/148 (79%)	112 (96%)	5 (4%)	29 46
5	E	152/156 (97%)	148 (97%)	4 (3%)	46 66
6	F	93/94 (99%)	92 (99%)	1 (1%)	73 87
7	G	27/282 (10%)	26 (96%)	1 (4%)	34 53
8	H	134/145 (92%)	129 (96%)	5 (4%)	34 53
9	I	58/130 (45%)	57 (98%)	1 (2%)	60 78
10	J	118/121 (98%)	110 (93%)	8 (7%)	16 25
11	K	106/106 (100%)	103 (97%)	3 (3%)	43 63
12	L	113/127 (89%)	110 (97%)	3 (3%)	44 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
13	M	158/160 (99%)	152 (96%)	6 (4%)	33 51
14	N	149/150 (99%)	146 (98%)	3 (2%)	55 74
15	O	93/94 (99%)	90 (97%)	3 (3%)	39 59
16	P	113/117 (97%)	111 (98%)	2 (2%)	59 76
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24 39
18	R	117/122 (96%)	115 (98%)	2 (2%)	60 78
19	S	71/74 (96%)	69 (97%)	2 (3%)	43 63
20	T	105/106 (99%)	98 (93%)	7 (7%)	16 26
21	U	44/53 (83%)	44 (100%)	0	100 100
22	V	51/57 (90%)	49 (96%)	2 (4%)	32 50
23	W	130/130 (100%)	123 (95%)	7 (5%)	22 36
24	X	66/74 (89%)	60 (91%)	6 (9%)	9 14
25	Y	120/196 (61%)	112 (93%)	8 (7%)	16 26
26	Z	60/94 (64%)	58 (97%)	2 (3%)	38 57
27	1	46/47 (98%)	46 (100%)	0	100 100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49 68
29	3	79/79 (100%)	78 (99%)	1 (1%)	69 84
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	31 49

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	74	ARG
24	X	88	GLU
13	M	99	ARG
24	X	82	GLU
25	Y	220	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
23	W	125	HIS
29	3	2	GLN
24	X	23	HIS
27	1	16	HIS

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Mol	Chain	Res	Type
8	H	73	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	32 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	240 (8%)	33 (1%)

5 of 240 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	2718	C
30	0	2726	U
31	9	65	A
30	0	1237	U
30	0	1232	A

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

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	$\#\|Z\|>2$
30	1MA	0	628	30,33	16,25,26	1.32	3 (18%)	18,37,40	1.01	2 (11%)
30	PSU	0	2621	30	18,21,22	1.38	2 (11%)	22,30,33	1.18	3 (13%)
30	UR3	0	2619	30	19,22,23	0.36	0	26,32,35	0.66	1 (3%)
30	OMG	0	2588	30	18,26,27	1.03	2 (11%)	19,38,41	0.73	1 (5%)
30	OMU	0	2587	30	19,22,23	0.24	0	26,31,34	0.35	0

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
30	1MA	0	628	30,33	-	0/3/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.76	1.43	1.36
30	0	628	1MA	C2-N3	3.42	1.33	1.29
30	0	2588	OMG	C5-C6	-2.67	1.42	1.47
30	0	628	1MA	C6-N6	2.45	1.33	1.27
30	0	2588	OMG	C8-N7	-2.43	1.30	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	0	2621	PSU	C6-C5-C4	3.08	120.35	118.20
30	0	628	1MA	N1-C2-N3	2.75	129.23	126.02
30	0	2621	PSU	O2-C2-N1	2.69	125.76	122.79
30	0	628	1MA	C5-C6-N1	2.54	117.68	113.90
30	0	2621	PSU	C6-N1-C2	-2.51	120.12	122.68

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
30	0	2587	OMU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.