



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 06:39 pm GMT

PDB ID : 1VQ6  
Title : The structure of c-hpmn and CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

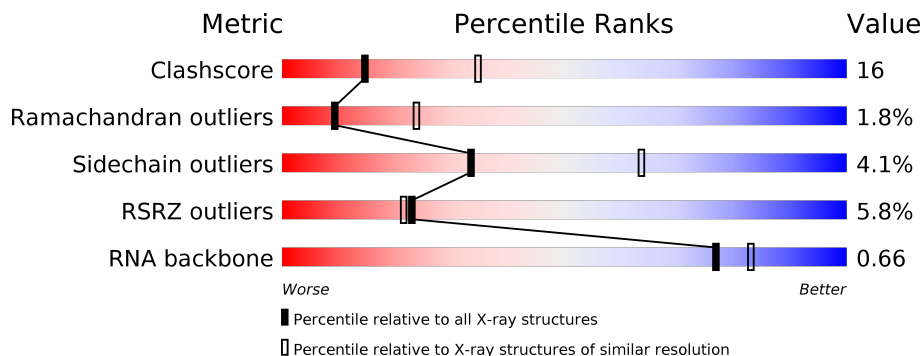
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>31%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>41%</div> <div>7%</div> <div>.</div> </div> </div>
3	4	3	<div> <div>100%</div> </div>
4	5	6	<div> <div>50%</div> <div>50%</div> </div>
5	A	240	<div> <div>3%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>.</div> <div>.</div> </div> </div>
6	B	338	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>49%</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

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Mol	Chain	Length	Quality of chain
32	3	92	
33	I	162	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	9175	-	-	-	X
36	NA	0	9184	-	-	-	X
36	NA	R	9186	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99029 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
			59021	26350	10878	19048	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(\*CP\*(5AA)\*(HFA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			52	30	9	12	1			

- Molecule 4 is a RNA chain called 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA)\*(BTN))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	0	0	0
			82	46	13	21	2			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

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

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	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 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.



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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	107	Total	Mg	0	0
			107	107		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	B	2	Total	Mg	0	0
			2	2		
34	A	2	Total	Mg	0	0
			2	2		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		
34	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	73	Total	Na	0	0
			73	73		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	J	1	Total 1	Na 1	0	0
36	Q	1	Total 1	Na 1	0	0
36	H	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	A	1	Total 1	Na 1	0	0
36	R	3	Total 3	Na 3	0	0
36	9	2	Total 2	Na 2	0	0
36	L	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	8	Total 8	Cl 8	0	0
37	J	3	Total 3	Cl 3	0	0
37	K	1	Total 1	Cl 1	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	2	Total 2	Cl 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	L	1	Total	Cl	0	0
			1	1		
37	3	1	Total	Cl	0	0
			1	1		
37	M	1	Total	Cl	0	0
			1	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5764	Total	O	0	0
			5764	5764		
39	9	135	Total	O	0	0
			135	135		
39	4	1	Total	O	0	0
			1	1		
39	5	1	Total	O	0	0
			1	1		
39	A	120	Total	O	0	0
			120	120		
39	B	156	Total	O	0	0
			156	156		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	49	Total	O	0	0
			49	49		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	F	23	Total 23	O 23	0	0
39	G	16	Total 16	O 16	0	0
39	H	68	Total 68	O 68	0	0
39	J	50	Total 50	O 50	0	0
39	K	55	Total 55	O 55	0	0
39	L	89	Total 89	O 89	0	0
39	M	125	Total 125	O 125	0	0
39	N	64	Total 64	O 64	0	0
39	O	42	Total 42	O 42	0	0
39	P	63	Total 63	O 63	0	0
39	Q	50	Total 50	O 50	0	0
39	R	81	Total 81	O 81	0	0
39	S	35	Total 35	O 35	0	0
39	T	35	Total 35	O 35	0	0
39	U	29	Total 29	O 29	0	0
39	V	13	Total 13	O 13	0	0
39	W	70	Total 70	O 70	0	0
39	X	25	Total 25	O 25	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	30	Total 30	O 30	0	0
39	1	59	Total 59	O 59	0	0

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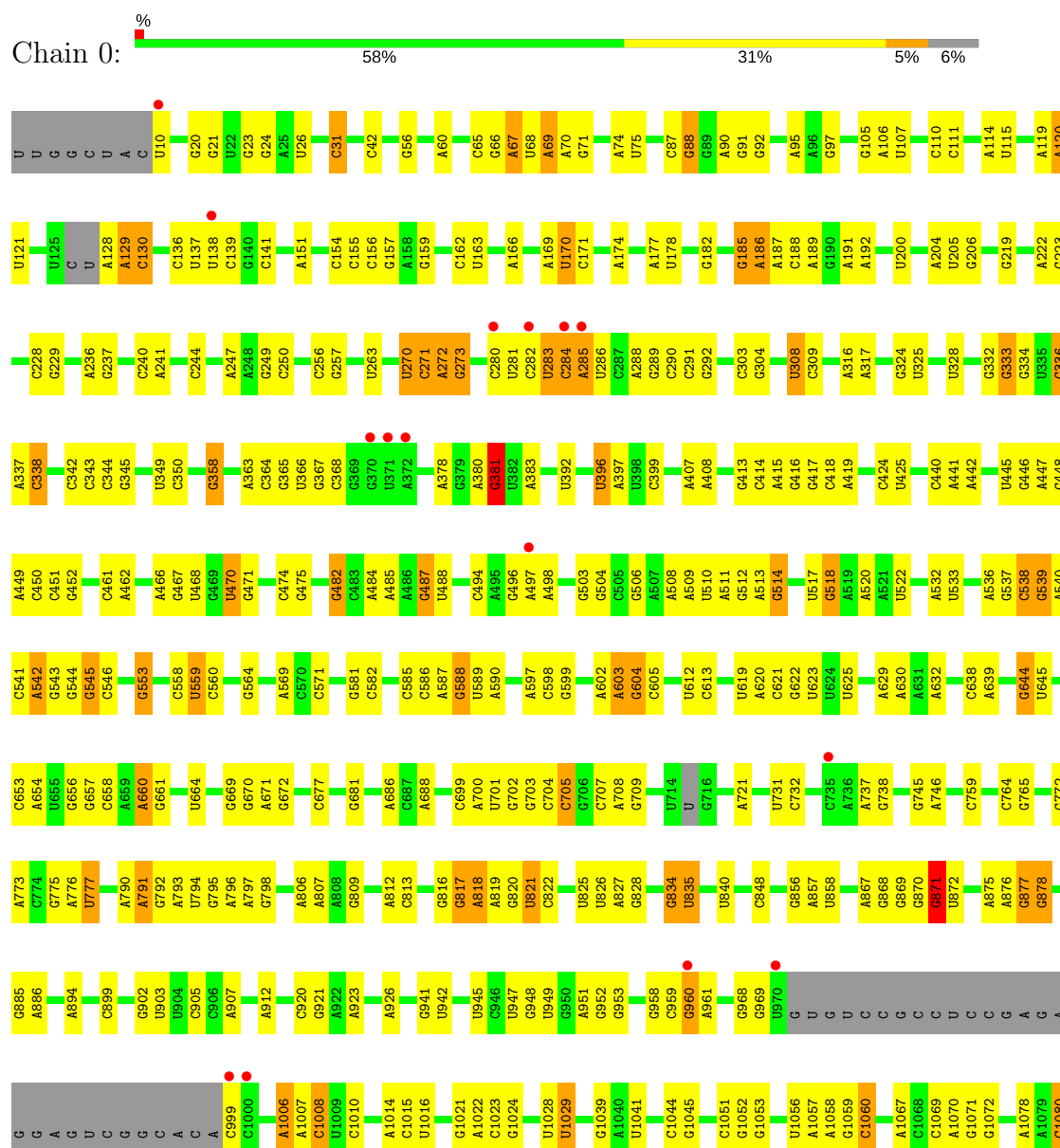
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	2	42	Total 42	O 42	0	0
39	3	71	Total 71	O 71	0	0
39	I	10	Total 10	O 10	0	0

### 3 Residue-property plots

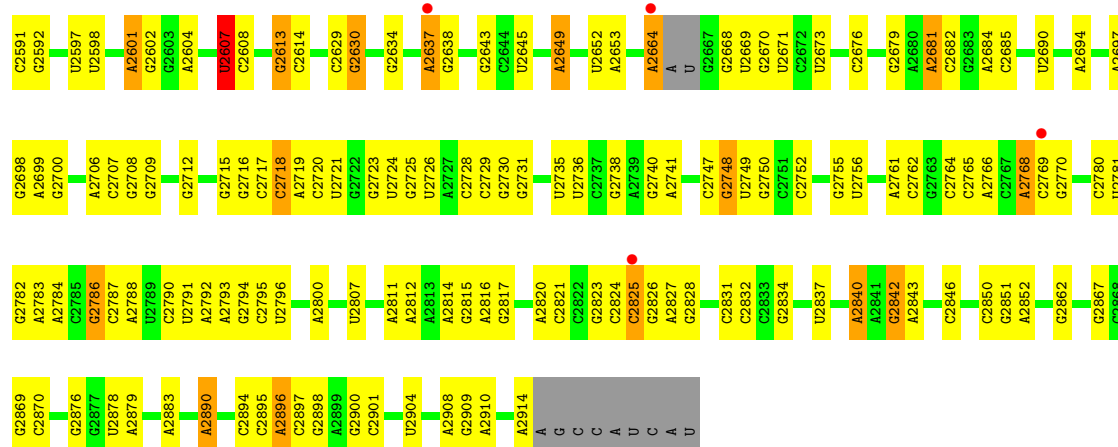
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: 23S ribosomal rna

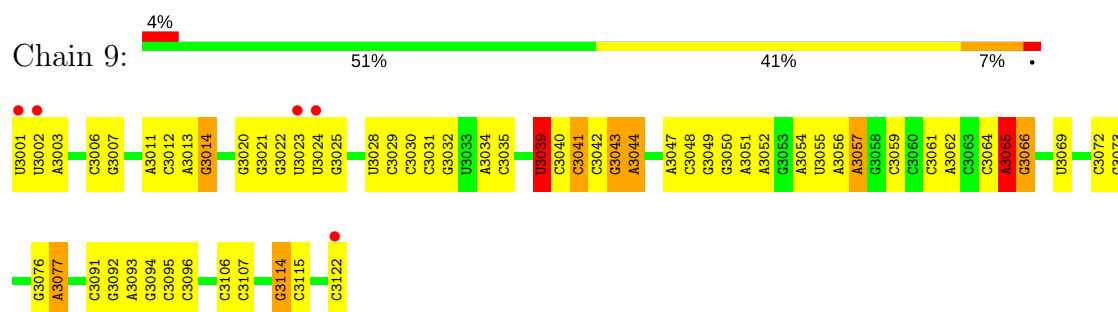




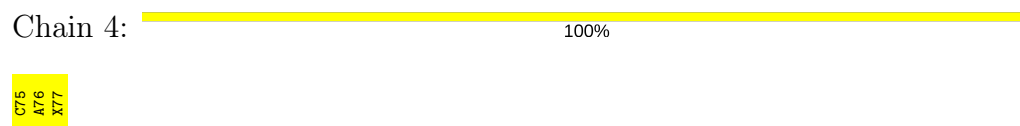




• Molecule 2: 5S ribosomal RNA



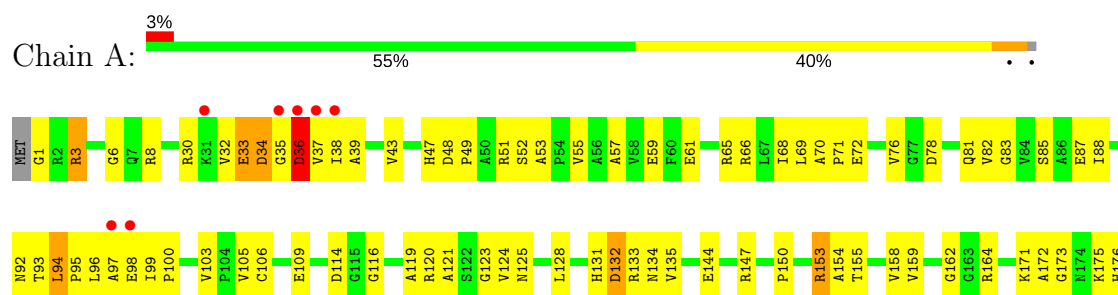
• Molecule 3: 5'-R(\*CP\*(5AA)\*(HFA))-3'



• Molecule 4: 5'-R(\*CP\*CP\*AP\*(PHE)\*(ACA)\*(BTN))-3'

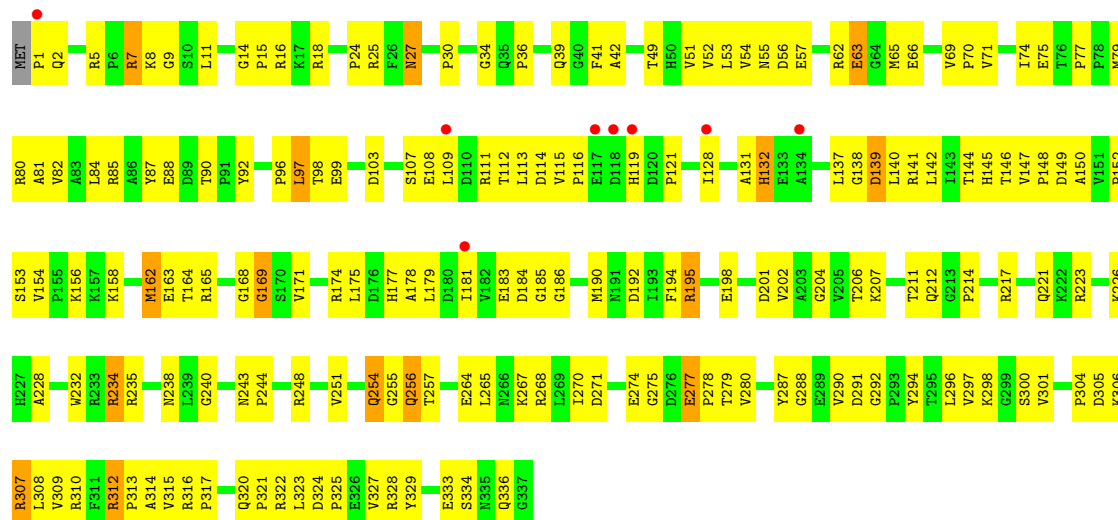


• Molecule 5: 50S ribosomal protein L2P

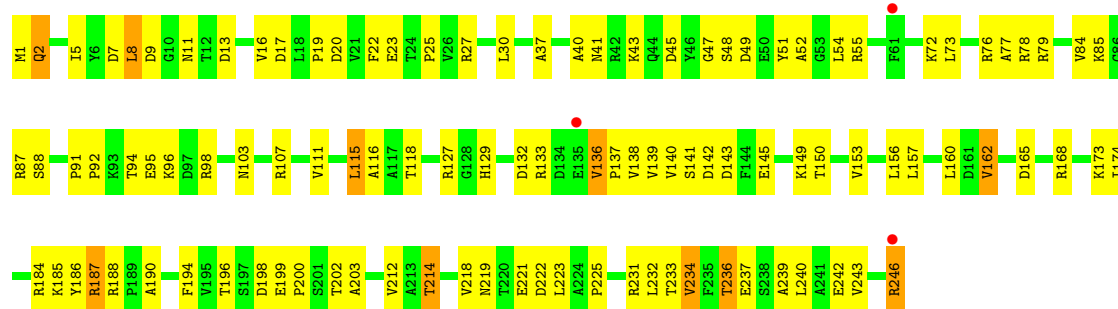




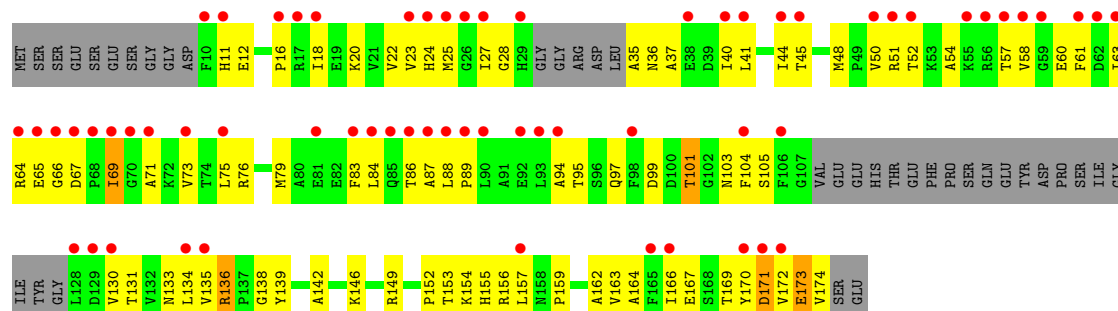
• Molecule 6: 50S ribosomal protein L3P



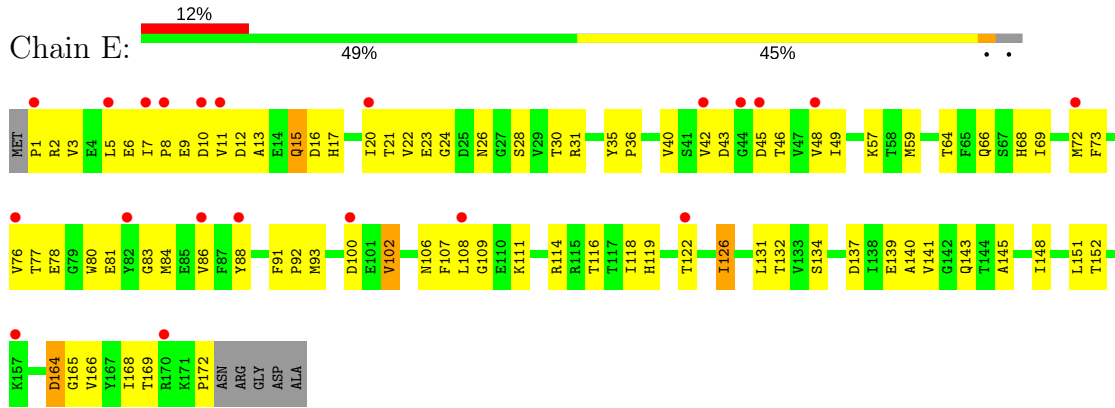
• Molecule 7: 50S ribosomal protein L4E



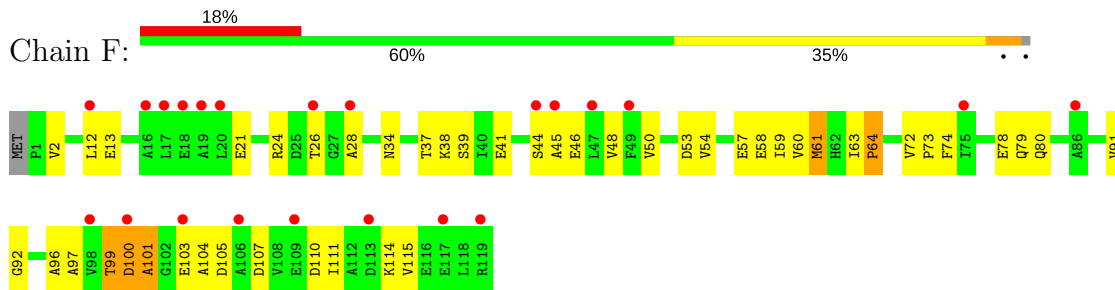
• Molecule 8: 50S ribosomal protein L5P



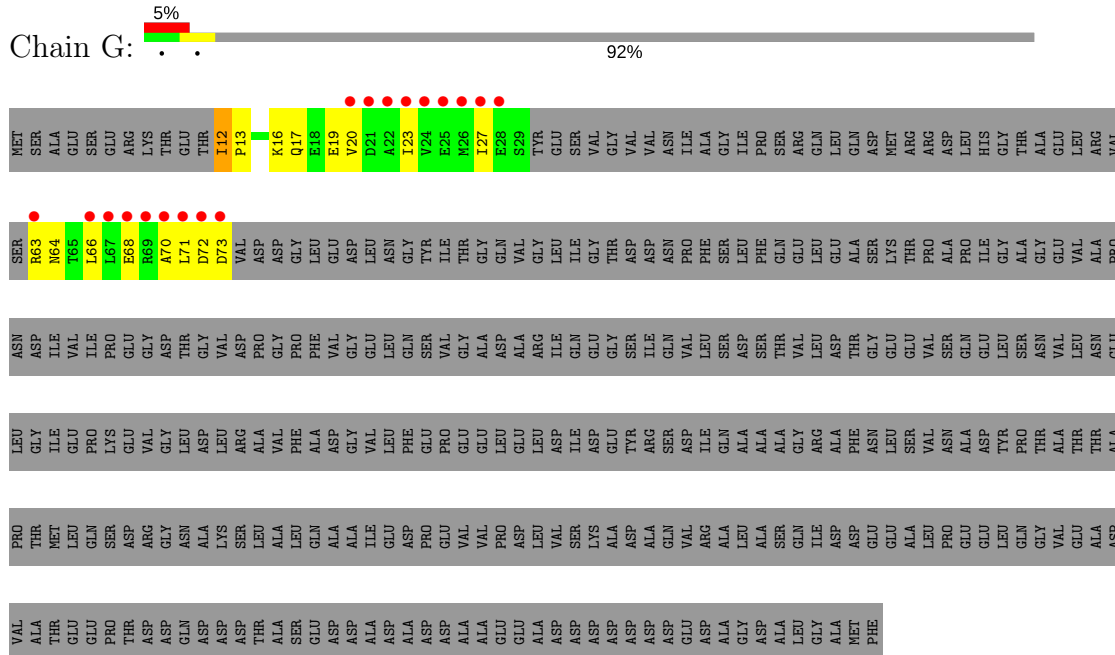
- Molecule 9: 50S ribosomal protein L6P



- Molecule 10: 50S ribosomal protein L7AE

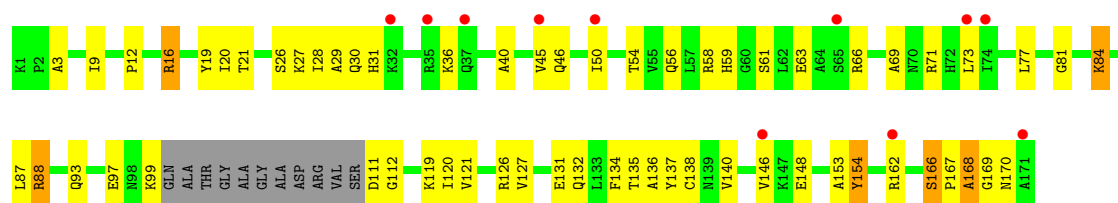


- Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



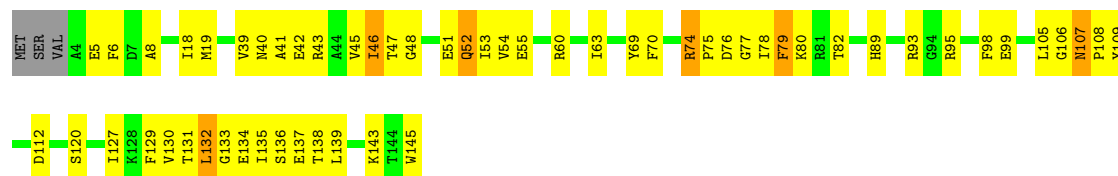
- Molecule 12: 50S RIBOSOMAL PROTEIN L10E





• Molecule 13: 50S ribosomal protein L13P

Chain J: 59% 35%



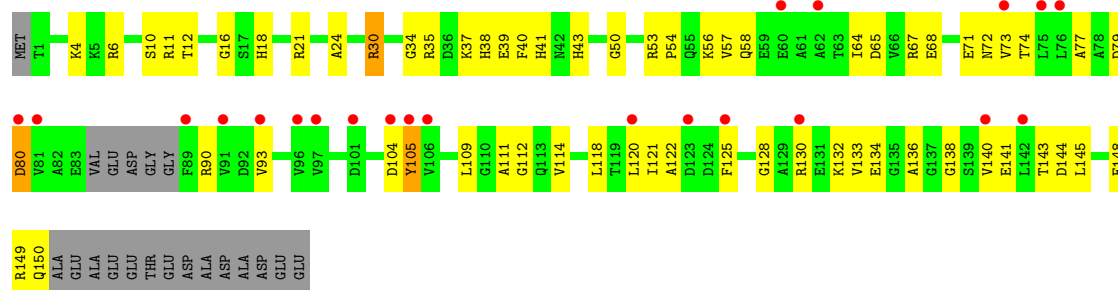
• Molecule 14: 50S ribosomal protein L14P

Chain K: 2% 63% 36%



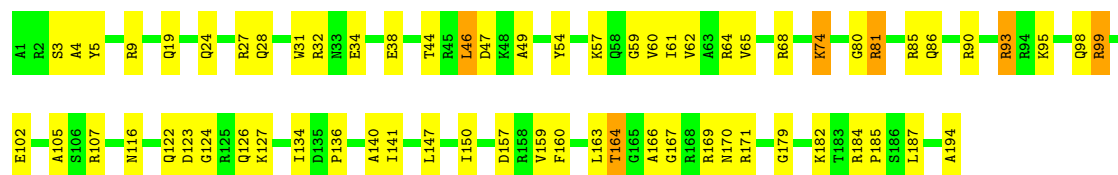
• Molecule 15: 50S ribosomal protein L15P

Chain L: 13% 50% 36% 12%

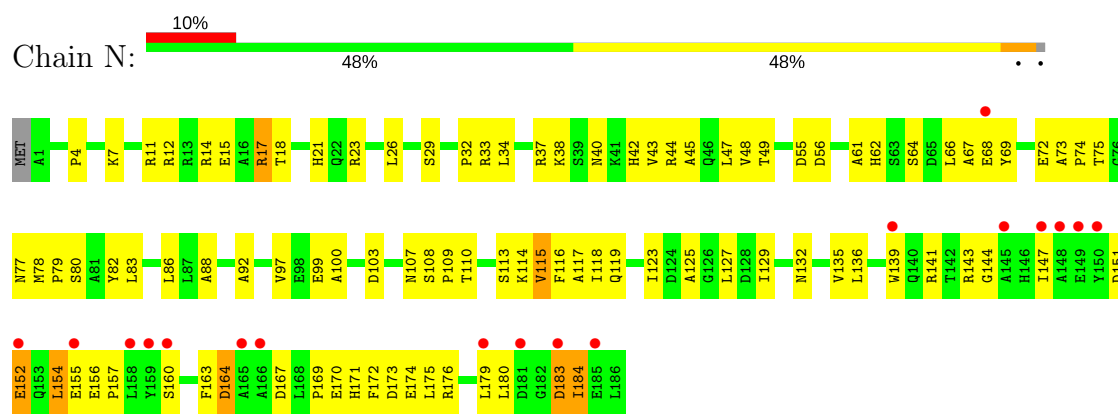


• Molecule 16: 50S Ribosomal Protein L15E

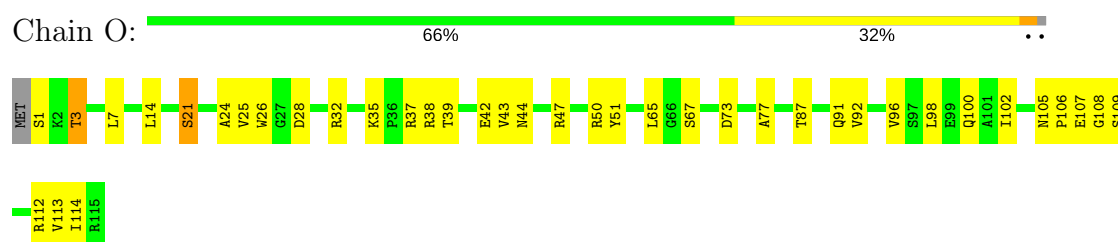
Chain M: 66% 31%



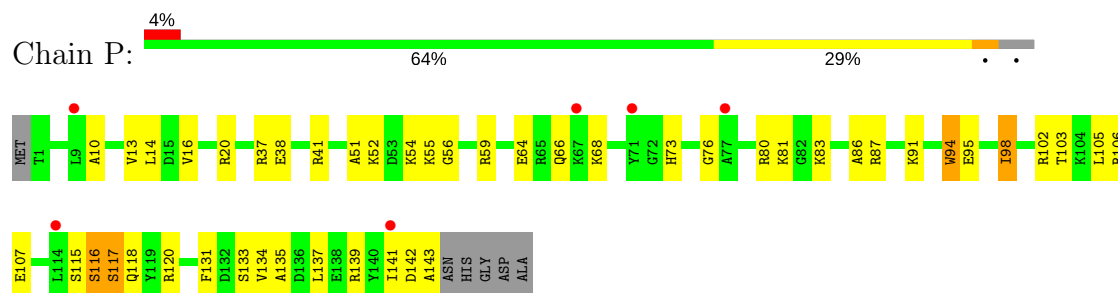
• Molecule 17: 50S ribosomal protein L18P



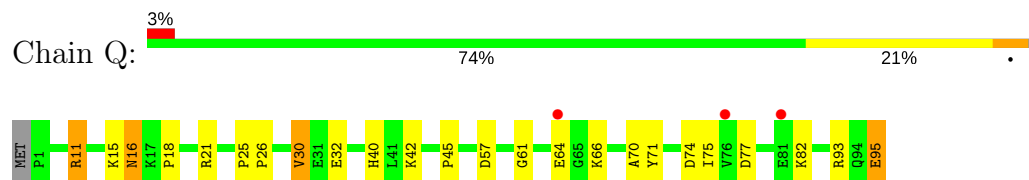
• Molecule 18: 50S ribosomal protein L18e



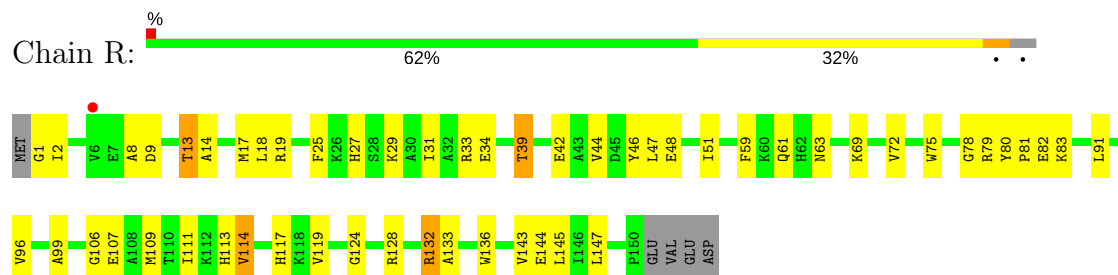
• Molecule 19: 50S ribosomal protein L19E



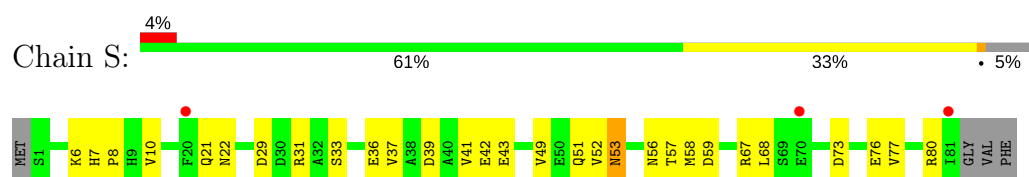
• Molecule 20: 50S ribosomal protein L21e



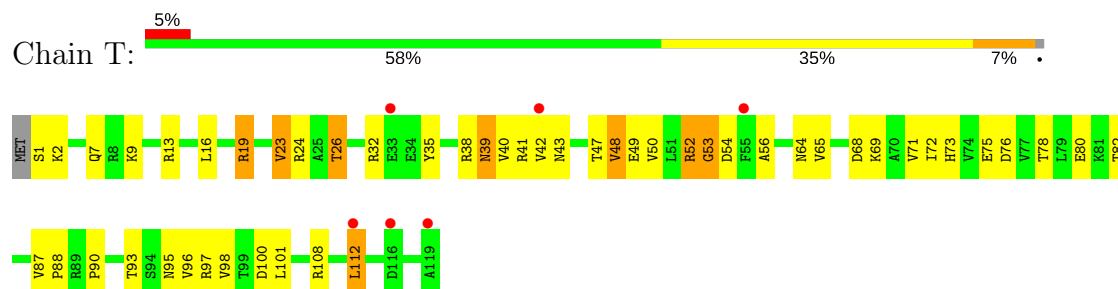
• Molecule 21: 50S ribosomal protein L22P



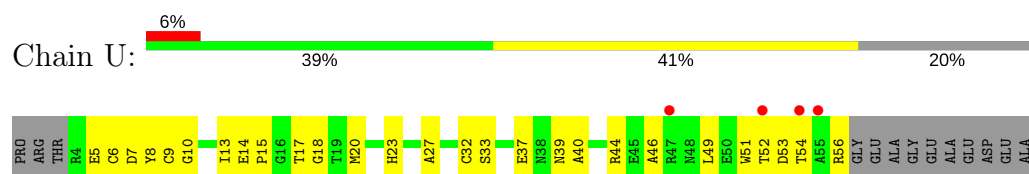
• Molecule 22: 50S ribosomal protein L23P



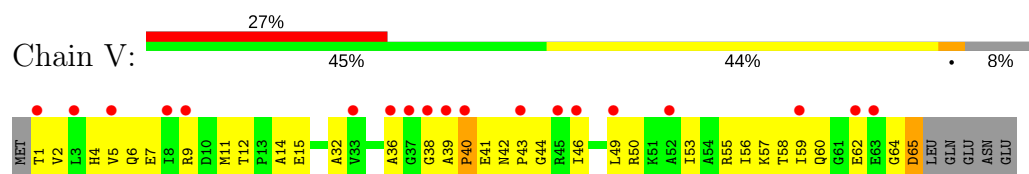
- Molecule 23: 50S ribosomal protein L24P



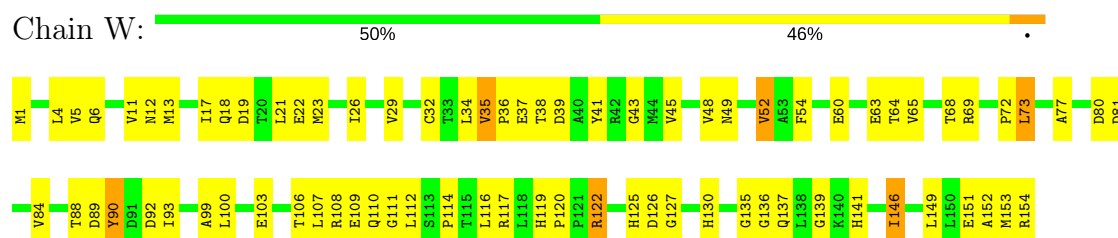
- Molecule 24: 50S ribosomal protein L24E



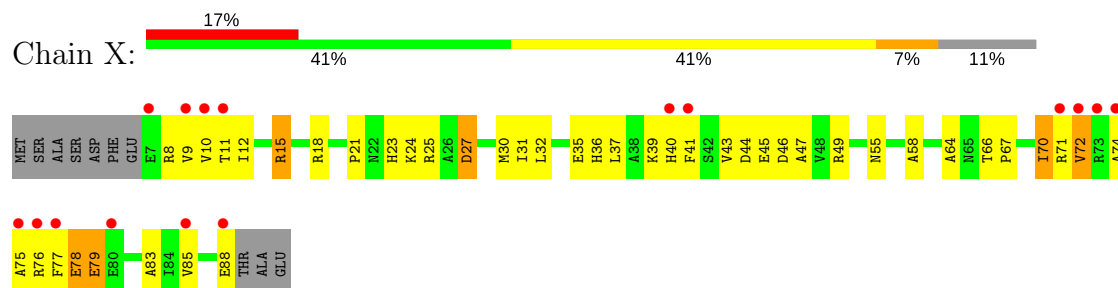
- Molecule 25: 50S ribosomal protein L29P



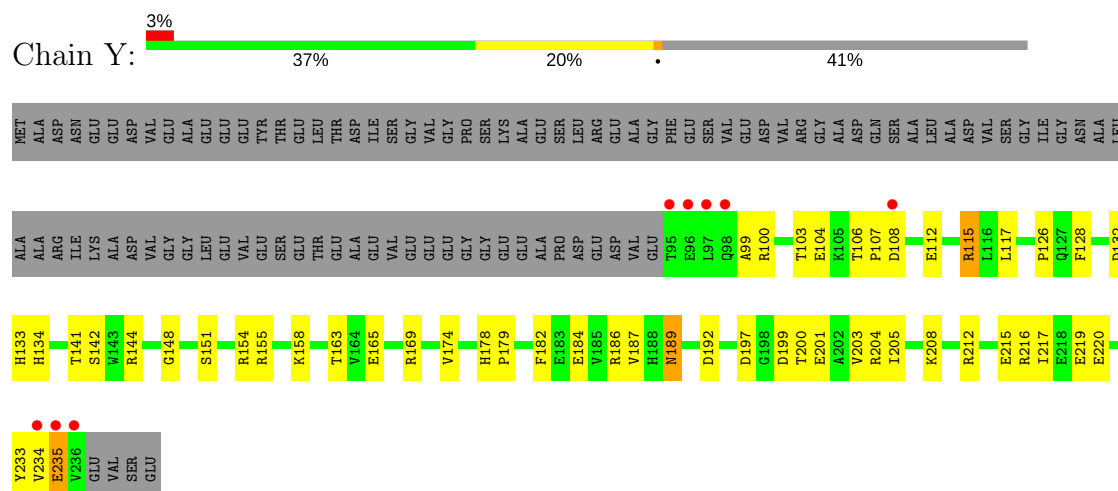
- Molecule 26: 50S ribosomal protein L30P



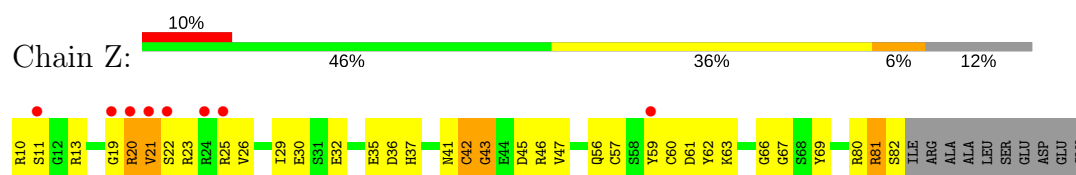
- Molecule 27: 50S ribosomal protein L31e



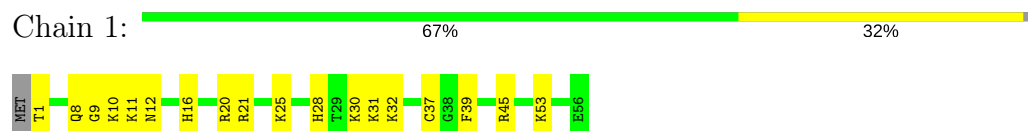
## • Molecule 28: 50S ribosomal protein L32E



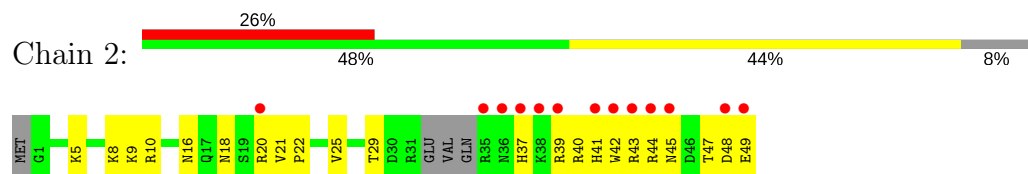
## • Molecule 29: 50S ribosomal protein L37Ae



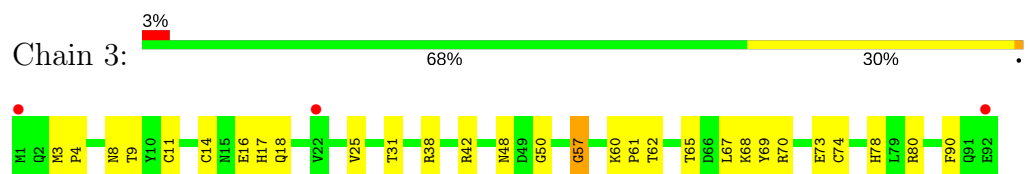
## • Molecule 30: 50S ribosomal protein L37e



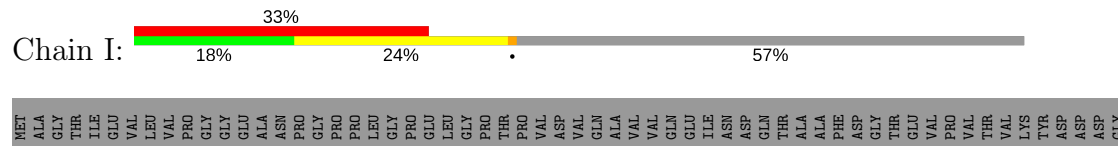
## • Molecule 31: 50S ribosomal protein L39e

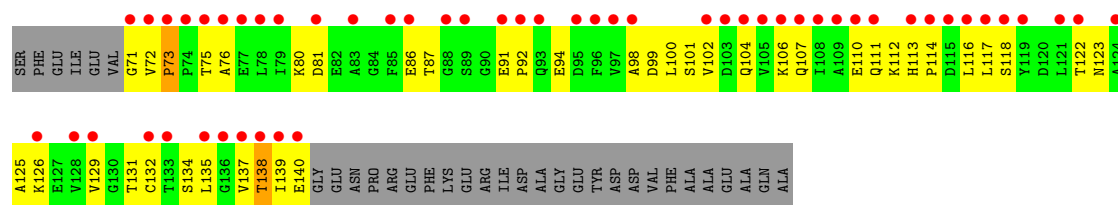


## • Molecule 32: 50S ribosomal protein L44E



## • Molecule 33: 50S RIBOSOMAL PROTEIN L11P







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.05Å 300.19Å 573.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 48.36 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.70) 93.2 (48.36-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.194 , 0.233 0.184 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99029	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, NA, K, ACA, CD, HFA, OMU, UR3, 5AA, 1MA, BTN, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.38	0/65959	0.69	19/102870 (0.0%)
2	9	0.35	0/2905	0.70	1/4528 (0.0%)
3	4	0.30	0/18	0.52	0/26
4	5	0.53	0/76	0.91	1/112 (0.9%)
5	A	0.32	0/1786	0.64	0/2408
6	B	0.33	0/2690	0.64	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.30	0/1111	0.53	0/1498
9	E	0.32	0/1382	0.57	0/1880
10	F	0.31	0/901	0.56	0/1224
11	G	0.29	0/241	0.46	0/324
12	H	0.33	0/1287	0.64	1/1725 (0.1%)
13	J	0.36	0/1136	0.61	0/1530
14	K	0.35	0/1001	0.69	0/1347
15	L	0.33	0/1130	0.66	0/1509
16	M	0.35	0/1584	0.61	0/2119
17	N	0.29	0/1474	0.62	0/1999
18	O	0.33	0/874	0.60	0/1181
19	P	0.34	0/1147	0.55	0/1528
20	Q	0.36	0/749	0.70	0/1005
21	R	0.35	0/1172	0.64	0/1578
22	S	0.33	0/648	0.60	0/875
23	T	0.33	0/958	0.63	1/1289 (0.1%)
24	U	0.34	0/417	0.60	0/562
25	V	0.29	0/502	0.53	0/675
26	W	0.34	0/1219	0.64	0/1655
27	X	0.34	0/664	0.58	0/895
28	Y	0.36	0/1146	0.65	0/1536
29	Z	0.36	0/589	0.64	0/787
30	1	0.42	0/438	0.64	0/578
31	2	0.33	0/401	0.53	0/529
32	3	0.40	0/771	0.60	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	I	0.30	0/526	0.56	0/716
All	All	0.37	0/98786	0.67	23/147715 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	49
2	9	0	2
26	W	0	1
All	All	1	52

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.66	130.76	109.50
1	0	871	G	C5'-C4'-O4'	-7.33	100.30	109.10
1	0	1942	A	C5'-C4'-C3'	7.21	127.54	116.00
2	9	3039	U	N1-C1'-C2'	6.70	122.70	114.00
1	0	2467	A	C1'-O4'-C4'	-6.33	104.84	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	26	U	Sidechain
1	0	270	U	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	904	0
2	9	2600	0	1326	60	0
3	4	52	0	36	2	0
4	5	82	0	55	3	0
5	A	1753	0	1766	128	0
6	B	2625	0	2533	202	0
7	C	1859	0	1816	113	0
8	D	1094	0	1085	84	0
9	E	1357	0	1266	86	0
10	F	890	0	843	45	0
11	G	240	0	231	15	0
12	H	1266	0	1268	66	0
13	J	1120	0	1098	69	0
14	K	992	0	1031	63	0
15	L	1118	0	1076	59	0
16	M	1560	0	1568	64	0
17	N	1445	0	1401	104	0
18	O	865	0	873	39	0
19	P	1136	0	1123	50	0
20	Q	735	0	729	20	0
21	R	1149	0	1122	56	0
22	S	641	0	605	22	0
23	T	950	0	923	54	0
24	U	410	0	364	31	0
25	V	499	0	511	34	0
26	W	1196	0	1137	100	0
27	X	654	0	653	51	0
28	Y	1130	0	1133	63	0
29	Z	578	0	539	27	0
30	1	431	0	426	24	0
31	2	396	0	413	31	0
32	3	755	0	728	27	0
33	I	519	0	500	46	0
34	0	107	0	0	0	0
34	3	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	2	0	0	0	0
36	0	73	0	0	0	0
36	9	2	0	0	0	0
36	A	1	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	3	0	0	0	0
36	S	1	0	0	0	0
37	0	8	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	J	3	0	0	0	0
37	K	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	2	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5764	0	0	115	0
39	1	59	0	0	2	0
39	2	42	0	0	1	0
39	3	71	0	0	5	0
39	4	1	0	0	0	0
39	5	1	0	0	0	0
39	9	135	0	0	2	0
39	A	120	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	156	0	0	21	0
39	C	168	0	0	18	0
39	D	45	0	0	8	0
39	E	49	0	0	8	0
39	F	23	0	0	3	0
39	G	16	0	0	1	0
39	H	68	0	0	6	0
39	I	10	0	0	2	0
39	J	50	0	0	2	0
39	K	55	0	0	8	0
39	L	89	0	0	15	0
39	M	125	0	0	3	0
39	N	64	0	0	8	0
39	O	42	0	0	7	0
39	P	63	0	0	3	0
39	Q	50	0	0	6	0
39	R	81	0	0	4	0
39	S	35	0	0	2	0
39	T	35	0	0	3	0
39	U	29	0	0	1	0
39	V	13	0	0	1	0
39	W	70	0	0	4	0
39	X	25	0	0	6	0
39	Y	95	0	0	8	0
39	Z	30	0	0	1	0
All	All	99029	0	59988	2476	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 16.

The worst 5 of 2476 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)
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.27	1.14
1:O:1160:G:H5'	1:O:1161:A:H5'	1.18	1.10
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.30	1.08
1:O:1242:A:H5'	13:J:82:THR:HG23	1.37	1.07
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.40	1.04

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	A	235/240 (98%)	205 (87%)	24 (10%)	6 (3%)	6	15
6	B	335/338 (99%)	295 (88%)	33 (10%)	7 (2%)	8	20
7	C	244/246 (99%)	215 (88%)	28 (12%)	1 (0%)	36	64
8	D	134/177 (76%)	94 (70%)	33 (25%)	7 (5%)	2	4
9	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
10	F	117/120 (98%)	104 (89%)	7 (6%)	6 (5%)	2	4
11	G	25/348 (7%)	24 (96%)	0	1 (4%)	3	7
12	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	9	22
13	J	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	8	20
14	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	11	29
15	L	141/165 (86%)	122 (86%)	17 (12%)	2 (1%)	12	31
16	M	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
17	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	5	14
18	O	113/116 (97%)	109 (96%)	2 (2%)	2 (2%)	9	24
19	P	141/149 (95%)	131 (93%)	7 (5%)	3 (2%)	8	20
20	Q	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
21	R	148/155 (96%)	135 (91%)	11 (7%)	2 (1%)	12	31
22	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
23	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	19	44
24	U	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	8	21
25	V	63/71 (89%)	54 (86%)	7 (11%)	2 (3%)	4	10
26	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	24	50
27	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	6	16
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	55 (78%)	9 (13%)	7 (10%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
32	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	16	38
33	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	3	6
All	All	3705/4430 (84%)	3316 (90%)	321 (9%)	68 (2%)	9	24

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	139	ASP
6	B	184	ASP
10	F	101	ALA
12	H	166	SER
12	H	168	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	A	179/182 (98%)	170 (95%)	9 (5%)	27	55
6	B	282/283 (100%)	267 (95%)	15 (5%)	25	52
7	C	193/193 (100%)	180 (93%)	13 (7%)	18	40
8	D	117/148 (79%)	112 (96%)	5 (4%)	32	61
9	E	152/156 (97%)	147 (97%)	5 (3%)	41	71
10	F	93/94 (99%)	90 (97%)	3 (3%)	42	73
11	G	27/283 (10%)	26 (96%)	1 (4%)	37	67
12	H	132/138 (96%)	126 (96%)	6 (4%)	30	60
13	J	118/121 (98%)	110 (93%)	8 (7%)	17	40
14	K	106/106 (100%)	104 (98%)	2 (2%)	60	85
15	L	113/127 (89%)	110 (97%)	3 (3%)	48	78
16	M	158/158 (100%)	150 (95%)	8 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	149/150 (99%)	145 (97%)	4 (3%)	48	78
18	O	93/94 (99%)	91 (98%)	2 (2%)	55	83
19	P	113/117 (97%)	108 (96%)	5 (4%)	31	60
20	Q	79/80 (99%)	74 (94%)	5 (6%)	20	44
21	R	117/122 (96%)	113 (97%)	4 (3%)	40	71
22	S	71/74 (96%)	70 (99%)	1 (1%)	69	89
23	T	105/106 (99%)	98 (93%)	7 (7%)	18	40
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	58	84
26	W	130/130 (100%)	125 (96%)	5 (4%)	36	66
27	X	66/74 (89%)	61 (92%)	5 (8%)	14	33
28	Y	120/196 (61%)	114 (95%)	6 (5%)	27	55
29	Z	60/68 (88%)	60 (100%)	0	100	100
30	1	46/47 (98%)	46 (100%)	0	100	100
31	2	42/46 (91%)	40 (95%)	2 (5%)	28	57
32	3	79/79 (100%)	77 (98%)	2 (2%)	50	80
33	I	58/130 (45%)	57 (98%)	1 (2%)	63	87
All	All	3093/3611 (86%)	2965 (96%)	128 (4%)	33	63

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	J	46	ILE
16	M	68	ARG
28	Y	141	THR
13	J	74	ARG
14	K	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
16	M	58	GLN
20	Q	40	HIS
31	2	41	HIS
17	N	40	ASN

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Mol	Chain	Res	Type
19	P	50	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	30 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
3	4	0/3	-	-
4	5	2/6 (33%)	0	0
All	All	2868/3053 (93%)	251 (8%)	31 (1%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1563	G
1	0	2726	U
1	0	1450	C
1	0	1667	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	0	2587	1,36	14,22,23	0.95	1 (7%)	18,31,34	3.73	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.01	2 (10%)	22,38,41	2.45	4 (18%)
1	UR3	0	2619	1	13,22,23	0.81	1 (7%)	15,32,35	0.71	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	5.41	4 (20%)
1	1MA	0	628	1,36	16,25,26	1.01	1 (6%)	12,37,40	1.23	1 (8%)
3	5AA	4	76	1,3	17,26,27	0.70	0	16,38,41	1.26	1 (6%)
3	HFA	4	77	3	11,11,12	1.20	1 (9%)	13,13,15	0.76	0
4	ACA	5	78	4	7,7,8	2.01	1 (14%)	5,6,8	0.87	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
1	OMU	0	2587	1,36	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1
4	ACA	5	78	4	-	0/4/5/6	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.92	1.48	1.52
4	5	78	ACA	C3-C2	-4.70	1.34	1.52
1	0	2588	OMG	C8-N7	-2.09	1.30	1.34
1	0	2619	UR3	C6-C5	-2.03	1.33	1.38
1	0	2587	OMU	C4-N3	2.24	1.37	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.05	114.71	128.41
1	0	2621	PSU	C5-C4-N3	-8.35	114.60	125.36
1	0	2588	OMG	C5-C6-N1	-8.34	111.61	123.47
1	0	628	1MA	C2-N3-C4	-3.70	110.85	116.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2587	OMU	C5-C4-N3	-3.61	114.78	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0
3	4	76	5AA	1	0
3	4	77	HFA	1	0
4	5	78	ACA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.40	39 (1%) 75 76	30, 57, 102, 163	0
2	9	122/122 (100%)	-0.26	5 (4%) 37 35	51, 72, 98, 158	0
3	4	1/3 (33%)	0.19	0 100 100	75, 75, 75, 75	0
4	5	4/6 (66%)	0.16	0 100 100	63, 63, 71, 81	0
5	A	237/240 (98%)	0.33	8 (3%) 45 44	37, 61, 97, 120	0
6	B	337/338 (99%)	0.20	8 (2%) 59 59	38, 68, 95, 104	0
7	C	246/246 (100%)	-0.03	3 (1%) 79 80	32, 55, 81, 89	0
8	D	140/177 (79%)	1.97	63 (45%) 0 0	67, 111, 136, 143	0
9	E	172/178 (96%)	0.84	21 (12%) 4 3	58, 83, 108, 116	0
10	F	119/120 (99%)	0.89	22 (18%) 1 1	58, 84, 112, 127	0
11	G	29/348 (8%)	2.41	18 (62%) 0 0	78, 96, 110, 112	0
12	H	160/171 (93%)	0.42	11 (6%) 17 15	46, 66, 98, 104	0
13	J	142/145 (97%)	0.04	0 100 100	49, 63, 82, 103	0
14	K	132/132 (100%)	0.20	3 (2%) 60 61	41, 67, 88, 94	0
15	L	145/165 (87%)	0.67	22 (15%) 2 1	34, 77, 120, 133	0
16	M	194/194 (100%)	-0.06	0 100 100	38, 51, 68, 77	0
17	N	186/187 (99%)	0.53	18 (9%) 8 6	47, 72, 120, 126	0
18	O	115/116 (99%)	0.12	0 100 100	47, 66, 83, 96	0
19	P	143/149 (95%)	0.41	6 (4%) 36 34	47, 68, 83, 91	0
20	Q	95/96 (98%)	0.22	3 (3%) 47 47	45, 54, 68, 87	0
21	R	150/155 (96%)	-0.04	1 (0%) 87 88	42, 55, 73, 84	0
22	S	81/85 (95%)	0.22	3 (3%) 41 40	52, 68, 87, 94	0
23	T	119/120 (99%)	0.62	6 (5%) 29 27	48, 67, 99, 115	0
24	U	53/66 (80%)	0.39	4 (7%) 14 12	52, 67, 84, 92	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	V	65/71 (91%)	1.53	19 (29%) 0 0	62, 85, 123, 128	0
26	W	154/154 (100%)	-0.01	0 100 100	46, 61, 81, 92	0
27	X	82/92 (89%)	0.75	16 (19%) 1 0	53, 69, 89, 106	0
28	Y	142/241 (58%)	0.20	8 (5%) 24 23	35, 56, 79, 97	0
29	Z	73/83 (87%)	0.43	8 (10%) 5 4	54, 72, 84, 105	0
30	1	56/57 (98%)	-0.32	0 100 100	37, 42, 48, 60	0
31	2	46/50 (92%)	1.31	13 (28%) 0 0	42, 71, 124, 132	0
32	3	92/92 (100%)	0.23	3 (3%) 46 46	42, 62, 77, 89	0
33	I	70/162 (43%)	3.64	53 (75%) 0 0	118, 134, 156, 158	0
All	All	6651/7483 (88%)	0.10	384 (5%) 23 21	30, 62, 110, 163	0

The worst 5 of 384 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	V	1	THR	11.3
33	I	71	GLY	9.2
33	I	96	PHE	8.9
33	I	93	GLN	8.9
33	I	133	THR	8.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACA	5	78	8/9	0.89	0.30	77,82,89,90	0
3	HFA	4	77	11/12	0.91	0.31	86,86,87,88	0
3	5AA	4	76	24/25	0.94	0.21	77,82,86,87	0
1	OMG	0	2588	24/25	0.98	0.15	38,40,45,46	0
1	UR3	0	2619	21/22	0.98	0.16	40,46,49,54	0
1	PSU	0	2621	20/21	0.99	0.13	34,37,42,43	0
1	1MA	0	628	23/24	0.99	0.16	39,41,42,44	0
1	OMU	0	2587	21/22	0.99	0.15	41,43,46,49	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
36	NA	0	9184	1/1	0.54	0.79	103,103,103,103	0
36	NA	0	9129	1/1	0.69	0.19	68,68,68,68	0
34	MG	0	8114	1/1	0.74	0.24	62,62,62,62	0
34	MG	0	8113	1/1	0.75	0.22	56,56,56,56	0
36	NA	R	9186	1/1	0.75	0.50	80,80,80,80	0
36	NA	0	9171	1/1	0.75	0.29	74,74,74,74	0
36	NA	S	9112	1/1	0.76	0.36	74,74,74,74	0
36	NA	0	9108	1/1	0.78	0.15	57,57,57,57	0
36	NA	0	9107	1/1	0.79	0.28	55,55,55,55	0
36	NA	0	9175	1/1	0.79	0.82	61,61,61,61	0
36	NA	0	9152	1/1	0.80	0.73	76,76,76,76	0
36	NA	0	9126	1/1	0.80	0.20	51,51,51,51	0
36	NA	0	9185	1/1	0.81	0.56	61,61,61,61	0
36	NA	9	9151	1/1	0.81	0.13	80,80,80,80	0
36	NA	0	9172	1/1	0.81	0.34	64,64,64,64	0
34	MG	0	8024	1/1	0.82	0.14	61,61,61,61	0
38	CD	O	9205	1/1	0.82	0.07	146,146,146,146	0
34	MG	0	8087	1/1	0.82	0.13	53,53,53,53	0
34	MG	0	8046	1/1	0.82	0.14	68,68,68,68	0
34	MG	T	8073	1/1	0.82	0.06	68,68,68,68	0
36	NA	H	9122	1/1	0.83	0.23	75,75,75,75	0
34	MG	0	8085	1/1	0.83	0.14	68,68,68,68	0
36	NA	0	9155	1/1	0.84	0.51	80,80,80,80	0
34	MG	0	8090	1/1	0.84	0.41	77,77,77,77	0
36	NA	0	9166	1/1	0.84	0.12	71,71,71,71	0
36	NA	0	9177	1/1	0.85	0.32	78,78,78,78	0
34	MG	0	8082	1/1	0.86	0.23	72,72,72,72	0
34	MG	0	8045	1/1	0.86	0.30	87,87,87,87	0
34	MG	0	8049	1/1	0.87	0.29	93,93,93,93	0
36	NA	0	9169	1/1	0.87	0.30	65,65,65,65	0
36	NA	0	9163	1/1	0.87	0.34	75,75,75,75	0
36	NA	0	9110	1/1	0.87	0.22	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8106	1/1	0.88	0.11	57,57,57,57	0
34	MG	0	8092	1/1	0.88	0.55	102,102,102,102	0
36	NA	0	9168	1/1	0.88	0.15	69,69,69,69	0
36	NA	0	9182	1/1	0.89	0.34	78,78,78,78	0
34	MG	0	8043	1/1	0.89	0.10	55,55,55,55	0
34	MG	0	8053	1/1	0.89	0.15	57,57,57,57	0
36	NA	0	9121	1/1	0.89	0.46	69,69,69,69	0
34	MG	0	8076	1/1	0.89	0.10	68,68,68,68	0
34	MG	0	8088	1/1	0.89	0.06	41,41,41,41	0
36	NA	0	9161	1/1	0.90	0.22	62,62,62,62	0
36	NA	0	9181	1/1	0.90	0.17	69,69,69,69	0
34	MG	5	8118	1/1	0.90	0.18	47,47,47,47	0
37	CL	J	9302	1/1	0.90	0.16	86,86,86,86	0
36	NA	0	9150	1/1	0.90	0.18	46,46,46,46	0
37	CL	N	9307	1/1	0.90	0.23	74,74,74,74	0
36	NA	C	9104	1/1	0.91	0.09	43,43,43,43	0
34	MG	0	8089	1/1	0.91	0.07	65,65,65,65	0
36	NA	J	9146	1/1	0.91	0.12	41,41,41,41	0
36	NA	0	9136	1/1	0.91	0.09	68,68,68,68	0
34	MG	0	8102	1/1	0.91	0.08	64,64,64,64	0
36	NA	0	9142	1/1	0.91	0.21	45,45,45,45	0
36	NA	0	9141	1/1	0.91	0.12	52,52,52,52	0
34	MG	0	8050	1/1	0.91	0.09	86,86,86,86	0
36	NA	0	9164	1/1	0.91	0.34	55,55,55,55	0
34	MG	0	8044	1/1	0.92	0.12	52,52,52,52	0
36	NA	0	9159	1/1	0.92	0.35	62,62,62,62	0
36	NA	L	9180	1/1	0.92	0.55	61,61,61,61	0
37	CL	R	9306	1/1	0.92	0.19	67,67,67,67	0
36	NA	0	9111	1/1	0.92	0.18	71,71,71,71	0
37	CL	3	9304	1/1	0.92	0.12	67,67,67,67	0
36	NA	0	9132	1/1	0.92	0.08	34,34,34,34	0
35	K	0	9001	1/1	0.92	0.40	70,70,70,70	0
36	NA	R	9137	1/1	0.92	0.07	47,47,47,47	0
37	CL	0	9315	1/1	0.93	0.60	89,89,89,89	0
36	NA	0	9140	1/1	0.93	0.27	53,53,53,53	0
34	MG	0	8096	1/1	0.93	0.19	63,63,63,63	0
34	MG	0	8041	1/1	0.93	0.36	87,87,87,87	0
37	CL	J	9301	1/1	0.93	0.20	69,69,69,69	0
36	NA	9	9183	1/1	0.93	0.19	63,63,63,63	0
34	MG	0	8097	1/1	0.93	0.12	46,46,46,46	0
34	MG	0	8104	1/1	0.93	0.23	59,59,59,59	0
36	NA	0	9127	1/1	0.93	0.13	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	NA	0	9117	1/1	0.93	0.12	62,62,62,62	0
37	CL	0	9322	1/1	0.93	0.76	90,90,90,90	0
34	MG	0	8016	1/1	0.94	0.19	40,40,40,40	0
34	MG	0	8099	1/1	0.94	0.10	55,55,55,55	0
34	MG	0	8057	1/1	0.94	0.14	49,49,49,49	0
36	NA	0	9176	1/1	0.94	0.24	49,49,49,49	0
34	MG	0	8051	1/1	0.94	0.18	87,87,87,87	0
34	MG	0	8002	1/1	0.94	0.10	48,48,48,48	0
34	MG	0	8062	1/1	0.94	0.15	64,64,64,64	0
34	MG	0	8047	1/1	0.94	0.18	85,85,85,85	0
36	NA	0	9128	1/1	0.94	0.12	43,43,43,43	0
36	NA	0	9170	1/1	0.94	0.70	85,85,85,85	0
36	NA	0	9153	1/1	0.94	0.14	35,35,35,35	0
36	NA	0	9101	1/1	0.94	0.15	47,47,47,47	0
34	MG	0	8067	1/1	0.94	0.09	52,52,52,52	0
34	MG	0	8080	1/1	0.95	0.11	43,43,43,43	0
34	MG	0	8068	1/1	0.95	0.04	75,75,75,75	0
37	CL	Y	9320	1/1	0.95	0.14	55,55,55,55	0
36	NA	0	9119	1/1	0.95	0.13	45,45,45,45	0
37	CL	L	9310	1/1	0.95	0.14	72,72,72,72	0
34	MG	K	8069	1/1	0.95	0.12	48,48,48,48	0
36	NA	0	9106	1/1	0.95	0.75	49,49,49,49	0
36	NA	0	9124	1/1	0.95	0.16	69,69,69,69	0
34	MG	0	8014	1/1	0.95	0.12	50,50,50,50	0
36	NA	0	9158	1/1	0.95	0.37	122,122,122,122	0
37	CL	Y	9317	1/1	0.95	0.13	72,72,72,72	0
34	MG	0	8101	1/1	0.95	0.15	74,74,74,74	0
34	MG	0	8012	1/1	0.95	0.15	43,43,43,43	0
34	MG	0	8063	1/1	0.95	0.08	68,68,68,68	0
36	NA	0	9135	1/1	0.95	0.17	55,55,55,55	0
36	NA	0	9114	1/1	0.95	0.22	44,44,44,44	0
36	NA	0	9165	1/1	0.95	0.32	45,45,45,45	0
34	MG	0	8013	1/1	0.95	0.19	43,43,43,43	0
34	MG	0	8103	1/1	0.95	0.12	66,66,66,66	0
36	NA	0	9133	1/1	0.95	0.13	38,38,38,38	0
34	MG	0	8070	1/1	0.95	0.17	66,66,66,66	0
34	MG	Y	8109	1/1	0.95	0.20	62,62,62,62	0
34	MG	0	8091	1/1	0.95	0.12	74,74,74,74	0
36	NA	0	9102	1/1	0.95	0.14	54,54,54,54	0
34	MG	0	8084	1/1	0.95	0.10	47,47,47,47	0
34	MG	0	8094	1/1	0.95	0.14	80,80,80,80	0
34	MG	B	8055	1/1	0.96	0.16	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8019	1/1	0.96	0.08	35,35,35,35	0
34	MG	0	8075	1/1	0.96	0.09	48,48,48,48	0
34	MG	0	8100	1/1	0.96	0.21	79,79,79,79	0
36	NA	0	9115	1/1	0.96	0.15	41,41,41,41	0
34	MG	0	8054	1/1	0.96	0.16	35,35,35,35	0
34	MG	9	8095	1/1	0.96	0.09	73,73,73,73	0
34	MG	A	8065	1/1	0.96	0.20	54,54,54,54	0
34	MG	0	8018	1/1	0.96	0.19	49,49,49,49	0
34	MG	0	8117	1/1	0.96	0.06	34,34,34,34	0
34	MG	0	8112	1/1	0.96	0.09	43,43,43,43	0
36	NA	R	9138	1/1	0.96	0.10	67,67,67,67	0
36	NA	0	9160	1/1	0.96	0.51	48,48,48,48	0
34	MG	0	8042	1/1	0.96	0.10	47,47,47,47	0
36	NA	0	9139	1/1	0.96	0.15	30,30,30,30	0
36	NA	0	9157	1/1	0.96	0.05	75,75,75,75	0
36	NA	0	9113	1/1	0.96	0.20	71,71,71,71	0
37	CL	0	9303	1/1	0.96	0.19	63,63,63,63	0
34	MG	0	8040	1/1	0.96	0.15	55,55,55,55	0
36	NA	0	9167	1/1	0.96	0.08	56,56,56,56	0
34	MG	0	8072	1/1	0.96	0.27	56,56,56,56	0
34	MG	0	8116	1/1	0.96	0.30	67,67,67,67	0
37	CL	J	9321	1/1	0.96	0.17	60,60,60,60	0
36	NA	0	9131	1/1	0.96	0.15	35,35,35,35	0
34	MG	3	8078	1/1	0.96	0.07	41,41,41,41	0
36	NA	0	9174	1/1	0.96	0.49	74,74,74,74	0
34	MG	0	8033	1/1	0.96	0.14	44,44,44,44	0
34	MG	0	8032	1/1	0.97	0.13	47,47,47,47	0
34	MG	0	8098	1/1	0.97	0.12	46,46,46,46	0
34	MG	A	8066	1/1	0.97	0.07	67,67,67,67	0
37	CL	M	9318	1/1	0.97	0.11	45,45,45,45	0
36	NA	0	9179	1/1	0.97	0.18	72,72,72,72	0
34	MG	0	8108	1/1	0.97	0.12	58,58,58,58	0
37	CL	0	9311	1/1	0.97	0.14	58,58,58,58	0
36	NA	0	9105	1/1	0.97	0.12	45,45,45,45	0
36	NA	M	9147	1/1	0.97	0.16	32,32,32,32	0
34	MG	0	8064	1/1	0.97	0.13	38,38,38,38	0
36	NA	A	9145	1/1	0.97	0.10	41,41,41,41	0
34	MG	0	8115	1/1	0.97	0.20	54,54,54,54	0
36	NA	0	9178	1/1	0.97	0.54	75,75,75,75	0
36	NA	0	9143	1/1	0.97	0.09	38,38,38,38	0
34	MG	0	8039	1/1	0.97	0.12	50,50,50,50	0
34	MG	0	8093	1/1	0.97	0.16	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8052	1/1	0.97	0.08	51,51,51,51	0
34	MG	0	8004	1/1	0.97	0.07	38,38,38,38	0
37	CL	A	9309	1/1	0.97	0.23	72,72,72,72	0
34	MG	0	8007	1/1	0.97	0.10	25,25,25,25	0
34	MG	0	8086	1/1	0.97	0.07	58,58,58,58	0
37	CL	O	9308	1/1	0.97	0.14	81,81,81,81	0
34	MG	0	8015	1/1	0.97	0.09	37,37,37,37	0
36	NA	0	9149	1/1	0.97	0.13	43,43,43,43	0
34	MG	0	8010	1/1	0.97	0.10	42,42,42,42	0
36	NA	0	9173	1/1	0.97	0.39	62,62,62,62	0
34	MG	0	8083	1/1	0.97	0.13	45,45,45,45	0
36	NA	0	9116	1/1	0.97	0.16	48,48,48,48	0
34	MG	0	8030	1/1	0.98	0.15	36,36,36,36	0
37	CL	0	9313	1/1	0.98	0.14	64,64,64,64	0
36	NA	0	9154	1/1	0.98	0.16	38,38,38,38	0
34	MG	B	8056	1/1	0.98	0.16	57,57,57,57	0
34	MG	0	8037	1/1	0.98	0.08	47,47,47,47	0
34	MG	0	8035	1/1	0.98	0.10	49,49,49,49	0
37	CL	0	9305	1/1	0.98	0.13	62,62,62,62	0
36	NA	0	9156	1/1	0.98	0.35	57,57,57,57	0
36	NA	0	9134	1/1	0.98	0.07	46,46,46,46	0
36	NA	0	9120	1/1	0.98	0.20	35,35,35,35	0
34	MG	0	8060	1/1	0.98	0.22	45,45,45,45	0
34	MG	0	8017	1/1	0.98	0.07	31,31,31,31	0
36	NA	0	9130	1/1	0.98	0.22	49,49,49,49	0
37	CL	0	9316	1/1	0.98	0.25	75,75,75,75	0
34	MG	0	8026	1/1	0.98	0.14	31,31,31,31	0
34	MG	0	8020	1/1	0.98	0.09	33,33,33,33	0
36	NA	0	9144	1/1	0.98	0.10	37,37,37,37	0
34	MG	0	8071	1/1	0.98	0.10	62,62,62,62	0
35	K	0	9002	1/1	0.98	0.10	47,47,47,47	0
34	MG	0	8029	1/1	0.98	0.17	39,39,39,39	0
34	MG	0	8111	1/1	0.98	0.11	59,59,59,59	0
36	NA	0	9103	1/1	0.98	0.08	48,48,48,48	0
36	NA	0	9125	1/1	0.98	0.22	62,62,62,62	0
37	CL	B	9319	1/1	0.98	0.24	57,57,57,57	0
36	NA	0	9123	1/1	0.98	0.17	47,47,47,47	0
34	MG	0	8059	1/1	0.98	0.08	52,52,52,52	0
34	MG	0	8034	1/1	0.98	0.12	38,38,38,38	0
37	CL	0	9314	1/1	0.98	0.13	57,57,57,57	0
34	MG	0	8107	1/1	0.98	0.08	49,49,49,49	0
34	MG	0	8038	1/1	0.98	0.18	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	MG	0	8006	1/1	0.98	0.09	43,43,43,43	0
34	MG	0	8074	1/1	0.98	0.10	38,38,38,38	0
34	MG	0	8081	1/1	0.98	0.16	59,59,59,59	0
36	NA	0	9118	1/1	0.98	0.17	54,54,54,54	0
38	CD	3	9204	1/1	0.98	0.06	64,64,64,64	0
36	NA	0	9162	1/1	0.99	0.27	61,61,61,61	0
38	CD	Z	9203	1/1	0.99	0.09	76,76,76,76	0
34	MG	0	8021	1/1	0.99	0.16	33,33,33,33	0
34	MG	0	8009	1/1	0.99	0.13	35,35,35,35	0
36	NA	0	9109	1/1	0.99	0.11	35,35,35,35	0
34	MG	0	8036	1/1	0.99	0.16	32,32,32,32	0
36	NA	Q	9148	1/1	0.99	0.19	46,46,46,46	0
34	MG	0	8022	1/1	0.99	0.09	39,39,39,39	0
37	CL	K	9312	1/1	0.99	0.10	60,60,60,60	0
34	MG	0	8027	1/1	0.99	0.14	48,48,48,48	0
34	MG	0	8001	1/1	0.99	0.06	37,37,37,37	0
34	MG	0	8061	1/1	0.99	0.12	36,36,36,36	0
34	MG	0	8023	1/1	0.99	0.22	53,53,53,53	0
38	CD	U	9201	1/1	0.99	0.07	78,78,78,78	0
34	MG	0	8031	1/1	0.99	0.08	29,29,29,29	0
34	MG	0	8003	1/1	0.99	0.13	36,36,36,36	0
34	MG	0	8110	1/1	0.99	0.07	36,36,36,36	0
34	MG	0	8025	1/1	0.99	0.12	45,45,45,45	0
34	MG	0	8008	1/1	0.99	0.09	31,31,31,31	0
34	MG	0	8048	1/1	0.99	0.12	63,63,63,63	0
34	MG	0	8079	1/1	0.99	0.15	34,34,34,34	0
34	MG	0	8028	1/1	0.99	0.12	43,43,43,43	0
34	MG	0	8058	1/1	0.99	0.16	48,48,48,48	0
34	MG	0	8005	1/1	0.99	0.10	38,38,38,38	0
34	MG	0	8077	1/1	0.99	0.07	28,28,28,28	0
38	CD	1	9202	1/1	1.00	0.05	65,65,65,65	0
34	MG	0	8011	1/1	1.00	0.16	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.