



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 06:48 PM EST

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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

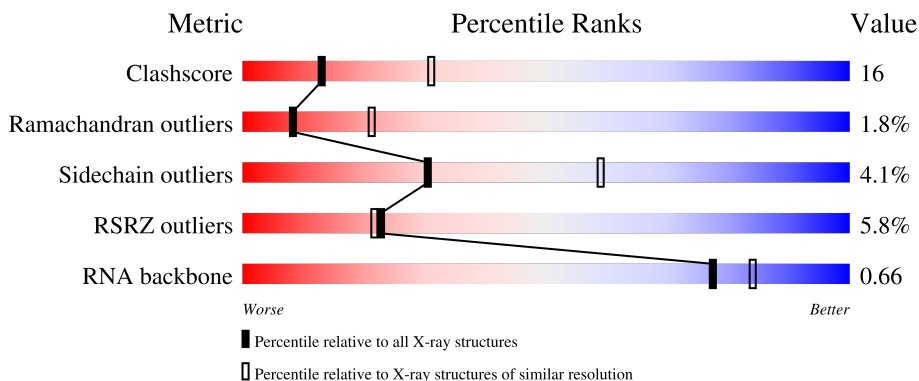
1 Overall quality at a glance

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (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 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 $\leq 5\%$. 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	 3% 58% 31% 5% 6%
2	9	122	 4% 51% 41% 7%
3	4	3	 67% 33%
4	5	6	 50% 33% 17%
5	A	240	 3% 55% 40% 2%




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Mol	Chain	Length	Quality of chain
6	B	338	2% 46% 49% .
7	C	246	% 57% 39% .
8	D	177	36% 33% 43% . 21%
9	E	178	12% 49% 45% . .
10	F	120	18% 60% 35% . .
11	G	348	5% 92%
12	H	171	6% 58% 32% . 6%
13	J	145	59% 35% . .
14	K	132	2% 63% 36% .
15	L	165	13% 50% 36% . 12%
16	M	194	66% 31% .
17	N	187	10% 48% 48% . .
18	O	116	66% 32% . .
19	P	149	4% 64% 29% . .
20	Q	96	3% 74% 21% . .
21	R	155	% 62% 32% . .
22	S	85	4% 61% 33% . 5%
23	T	120	5% 58% 35% 7% .
24	U	66	6% 39% 41% 20%
25	V	71	27% 45% 44% . 8%
26	W	154	50% 46% .
27	X	92	17% 41% 41% 7% 11%
28	Y	241	3% 37% 20% . 41%
29	Z	83	10% 46% 36% 6% 12%
30	1	57	67% 32% .

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Mol	Chain	Length	Quality of chain
31	2	50	
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 [i](#)

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
			Total	C	N	O	P			
1	0	2754	59021	26350	10878	19048	2745	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
15	L	145	1118	670	222	226		0	0	0

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

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

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
			Total	C	N	O	S			
17	N	186	1445	895	262	286	2	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S			
30	1	56	431	258	86	83	4	0	0	0

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

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

- 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	9	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	A	2	Total	Mg	0	0
			2	2		
34	B	2	Total	Mg	0	0
			2	2		
34	K	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	Y	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	9	2	Total Na 2 2	0	0
36	A	1	Total Na 1 1	0	0
36	C	1	Total Na 1 1	0	0
36	H	1	Total Na 1 1	0	0
36	J	1	Total Na 1 1	0	0
36	L	1	Total Na 1 1	0	0
36	M	1	Total Na 1 1	0	0
36	Q	1	Total Na 1 1	0	0
36	R	3	Total Na 3 3	0	0
36	S	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	8	Total Cl 8 8	0	0
37	A	1	Total Cl 1 1	0	0
37	B	1	Total Cl 1 1	0	0
37	J	3	Total Cl 3 3	0	0
37	K	1	Total Cl 1 1	0	0
37	L	1	Total Cl 1 1	0	0
37	M	1	Total Cl 1 1	0	0
37	N	1	Total Cl 1 1	0	0
37	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	R	1	Total Cl 1 1	0	0
37	Y	2	Total Cl 2 2	0	0
37	3	1	Total Cl 1 1	0	0

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

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

- Molecule 39 is water.

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

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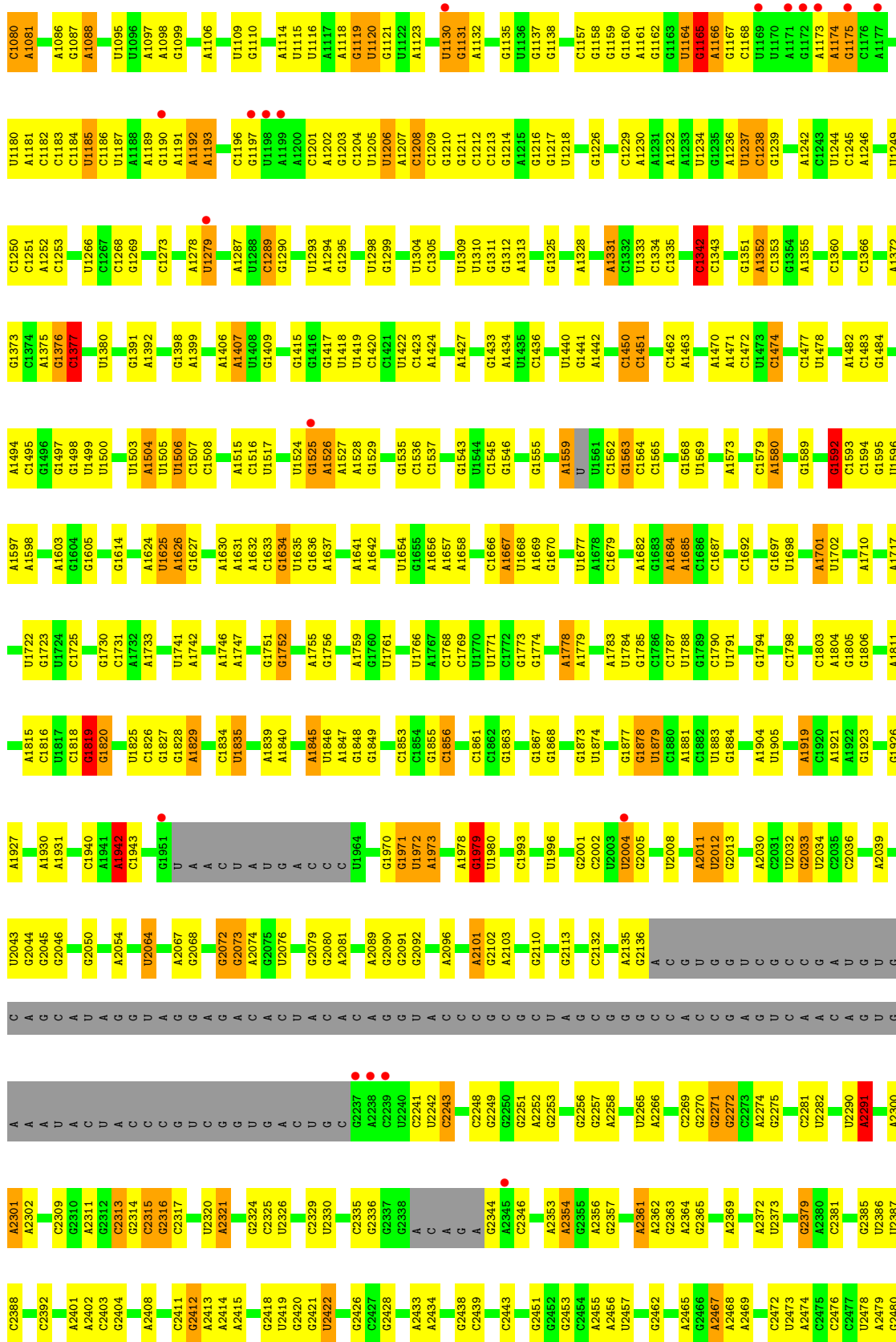
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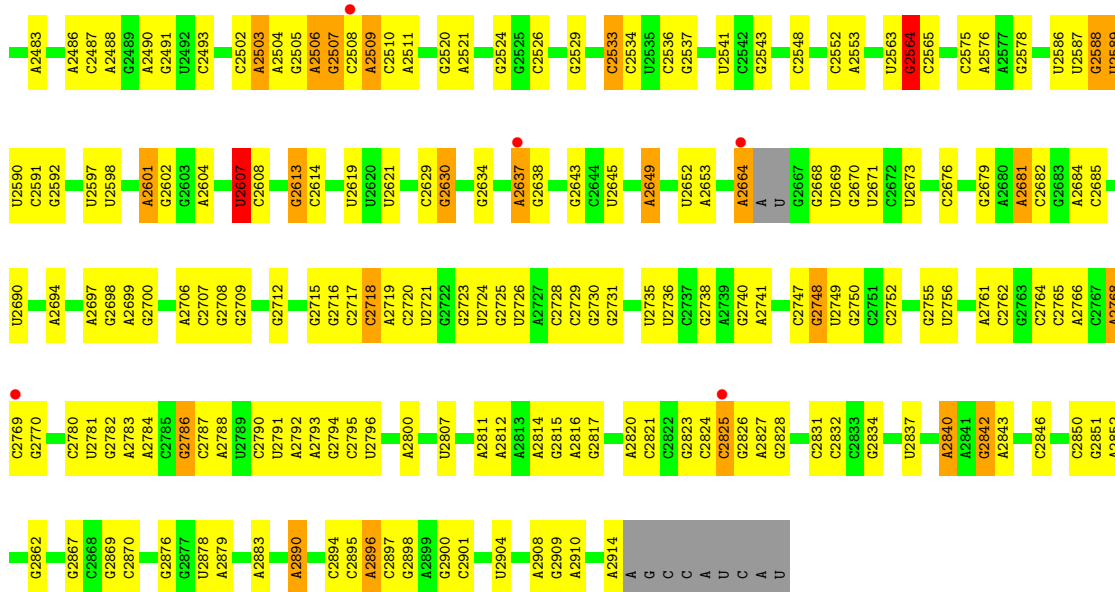
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	F	23	Total O 23 23	0	0
39	G	16	Total O 16 16	0	0
39	H	68	Total O 68 68	0	0
39	J	50	Total O 50 50	0	0
39	K	55	Total O 55 55	0	0
39	L	89	Total O 89 89	0	0
39	M	125	Total O 125 125	0	0
39	N	64	Total O 64 64	0	0
39	O	42	Total O 42 42	0	0
39	P	63	Total O 63 63	0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

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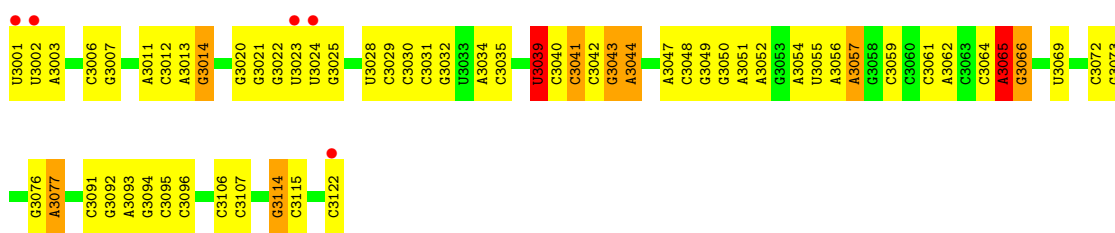
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	2	42	Total O 42 42	0	0
39	3	71	Total O 71 71	0	0
39	I	10	Total O 10 10	0	0

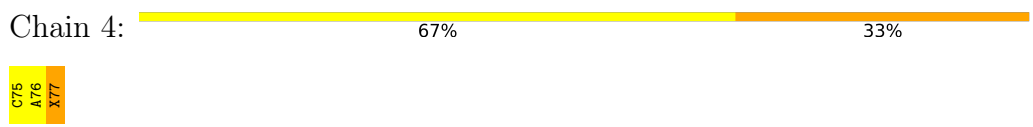




• Molecule 2: 5S ribosomal RNA



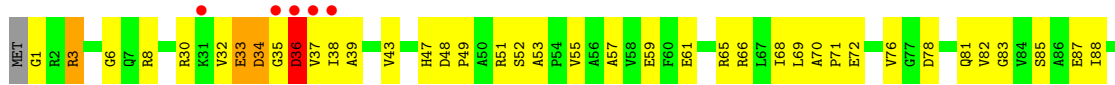
• Molecule 3: 5'-R(*CP*(5AA)*(HFA))-3'

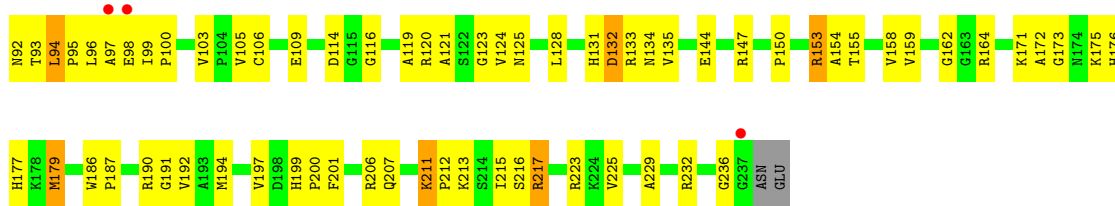


• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

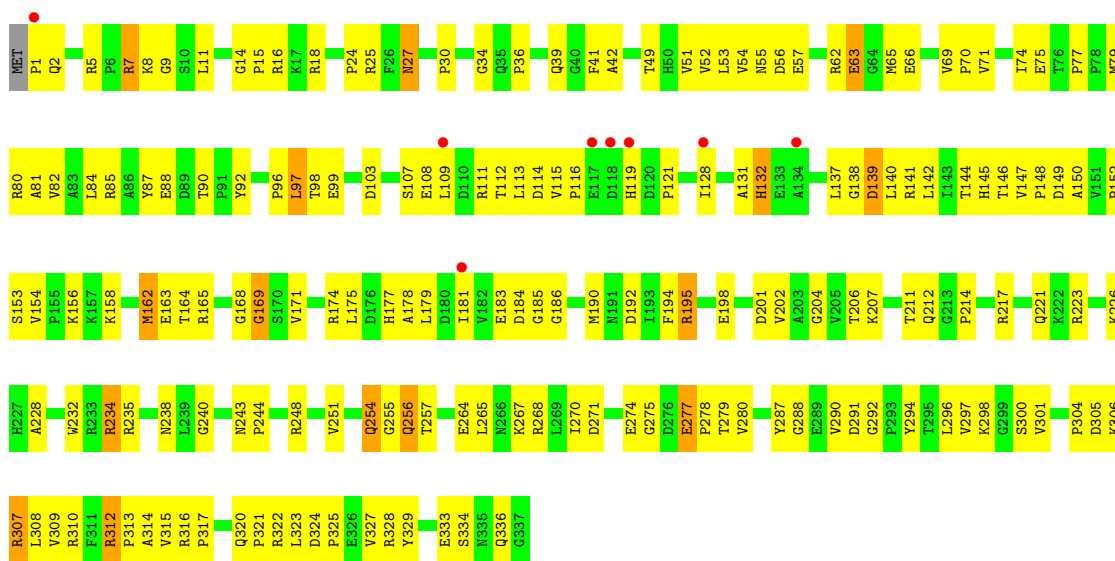


• Molecule 5: 50S ribosomal protein L2P

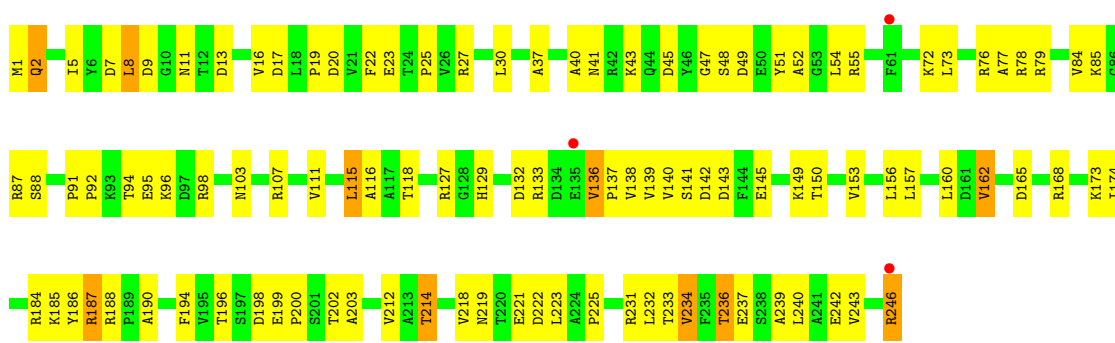




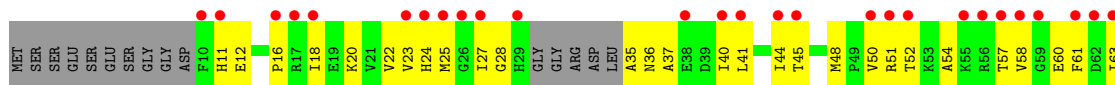
● Molecule 6: 50S ribosomal protein L3P

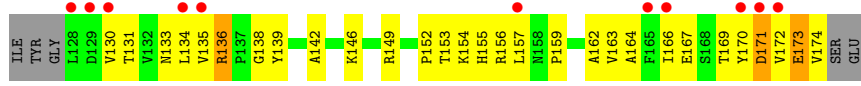
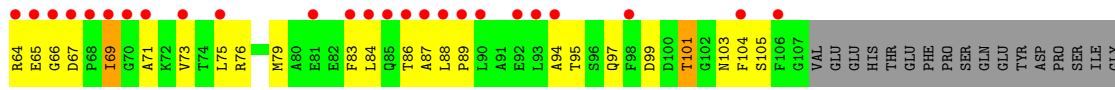


● Molecule 7: 50S ribosomal protein L4E

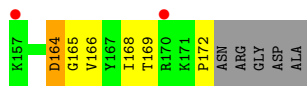
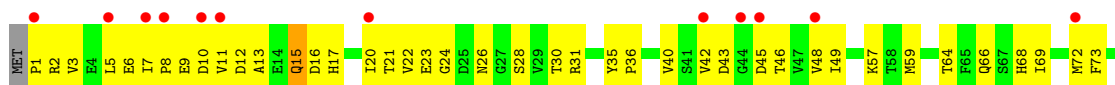


● Molecule 8: 50S ribosomal protein L5P

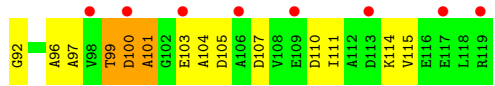
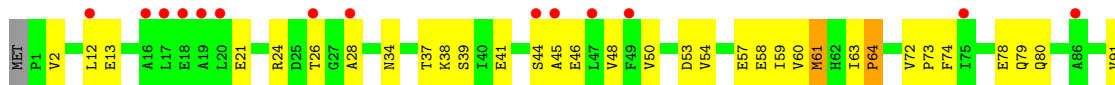




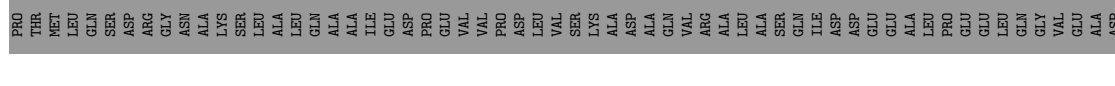
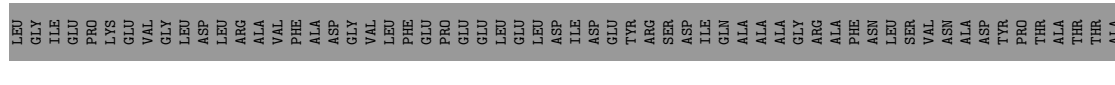
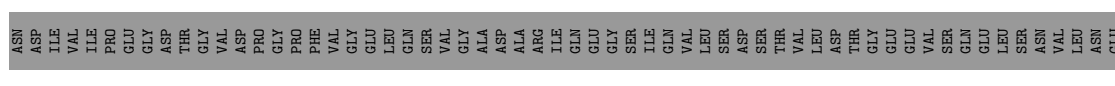
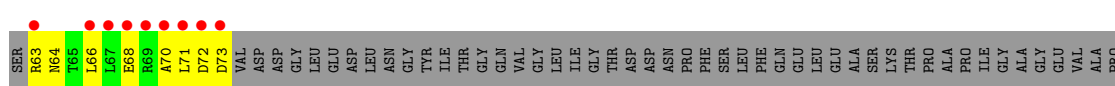
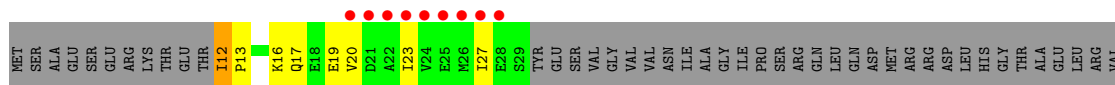
● Molecule 9: 50S ribosomal protein L6P



● Molecule 10: 50S ribosomal protein L7AE

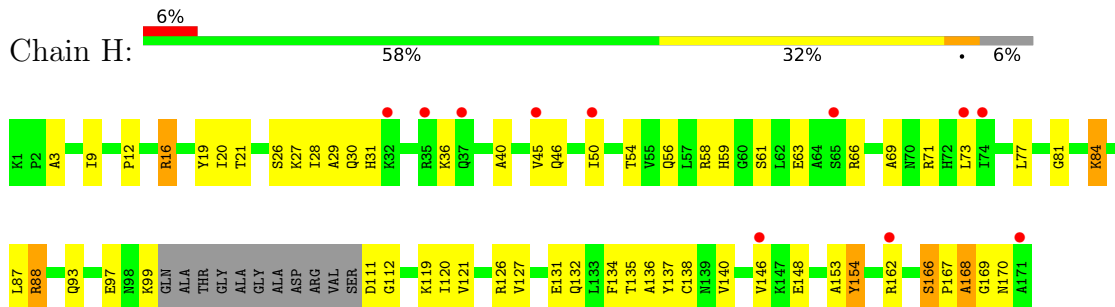


● Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

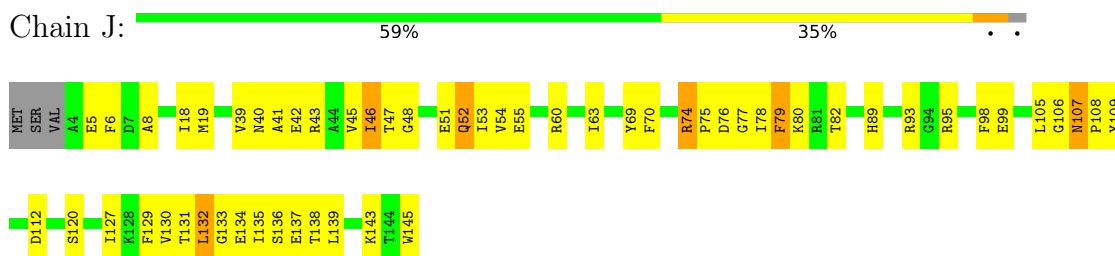


VAL
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GLU
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ALA
ALA
GLU
ALA
ASP
ASP
ASP
ASP
GLU
ASP
ALA
GLY
ALA
GLY
MET
PHE

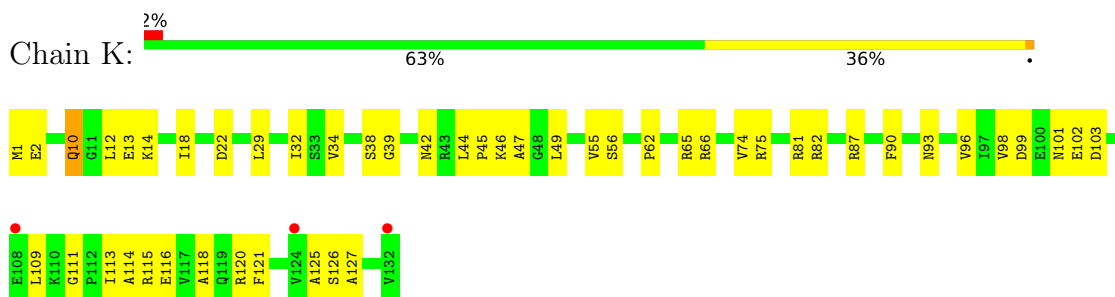
• Molecule 12: 50S RIBOSOMAL PROTEIN L10E



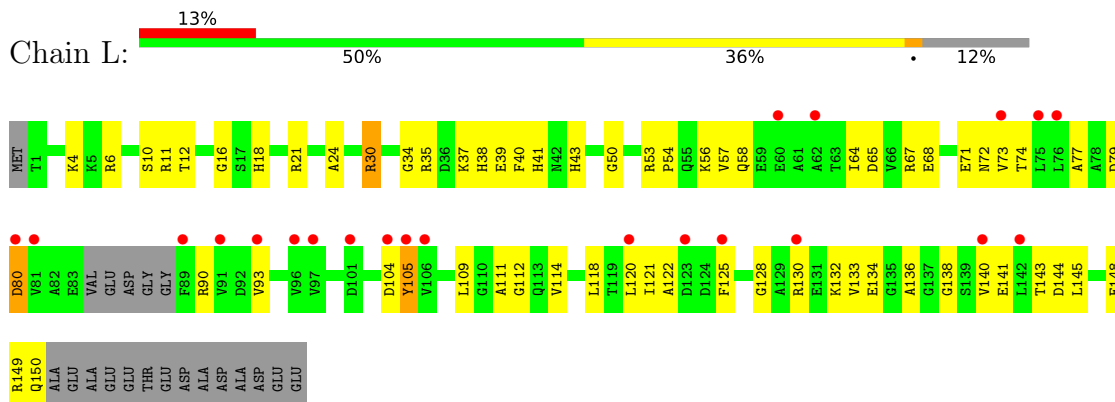
• Molecule 13: 50S ribosomal protein L13P



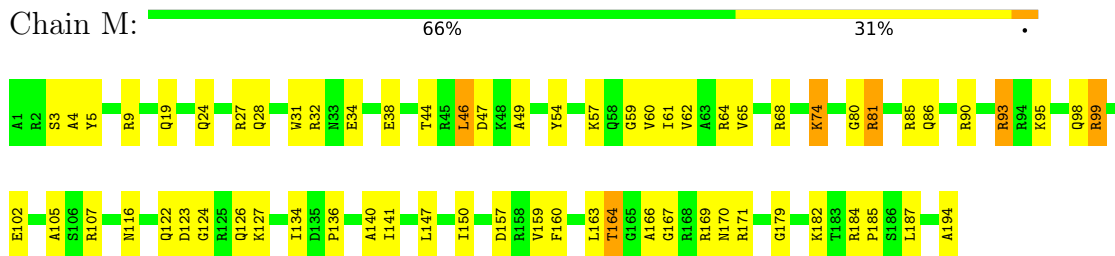
• Molecule 14: 50S ribosomal protein L14P



• Molecule 15: 50S ribosomal protein L15P



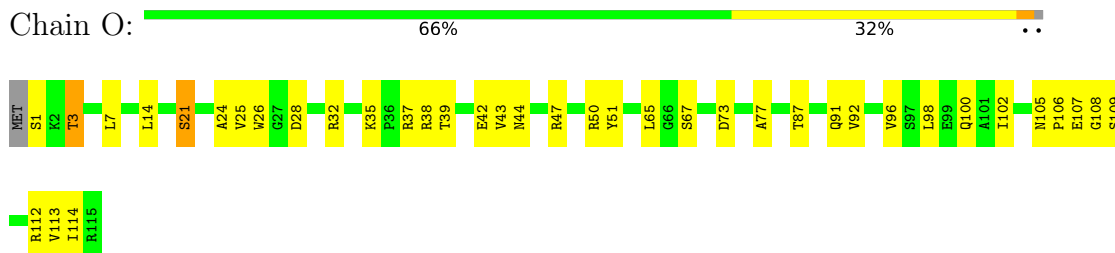
• Molecule 16: 50S Ribosomal Protein L15E



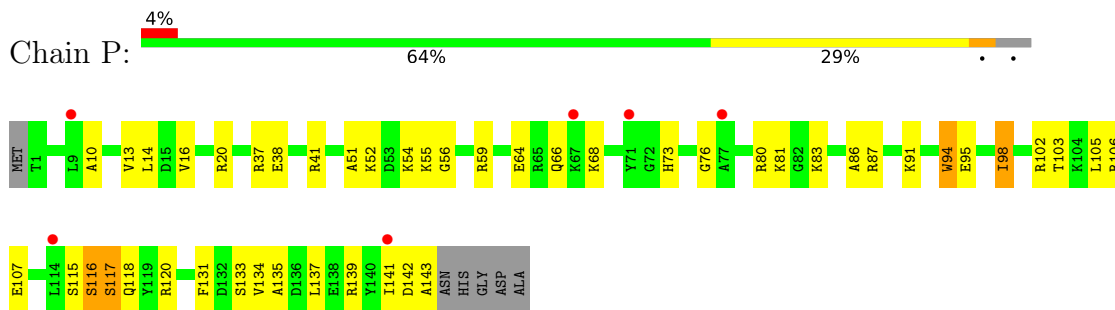
- Molecule 17: 50S ribosomal protein L18P



- Molecule 18: 50S ribosomal protein L18e

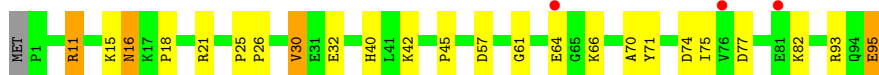


- Molecule 19: 50S ribosomal protein L19E

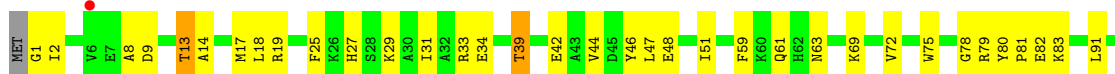


- Molecule 20: 50S ribosomal protein L21e





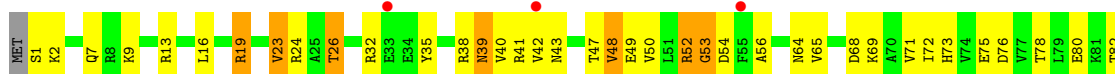
- Molecule 21: 50S ribosomal protein L22P



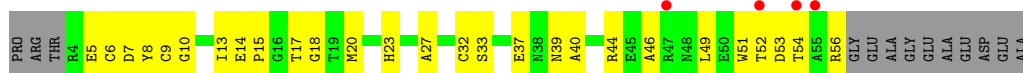
- Molecule 22: 50S ribosomal protein L23P



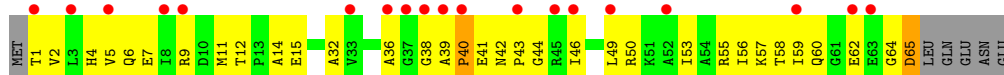
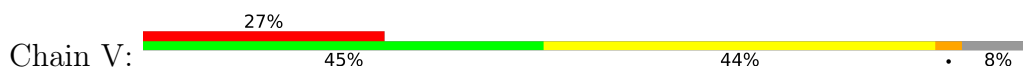
- Molecule 23: 50S ribosomal protein L24P



- Molecule 24: 50S ribosomal protein L24E

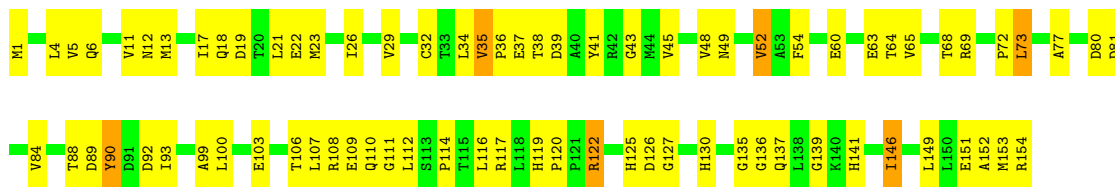


- Molecule 25: 50S ribosomal protein L29P

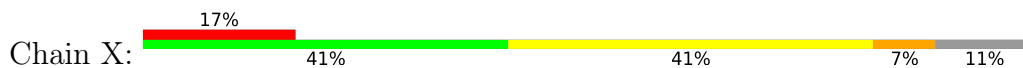


- Molecule 26: 50S ribosomal protein L30P

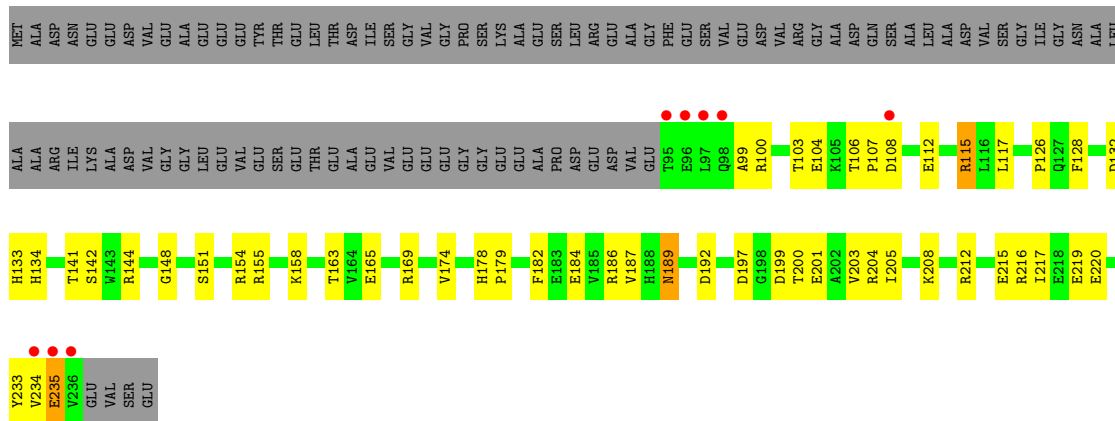




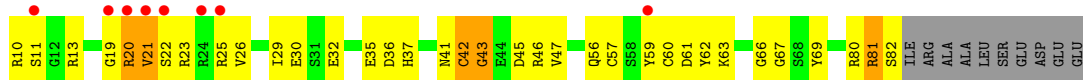
• Molecule 27: 50S ribosomal protein L31e



• Molecule 28: 50S ribosomal protein L32E



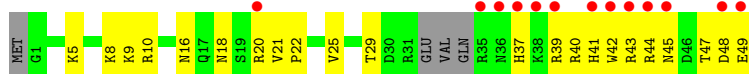
• Molecule 29: 50S ribosomal protein L37Ae



• Molecule 30: 50S ribosomal protein L37e



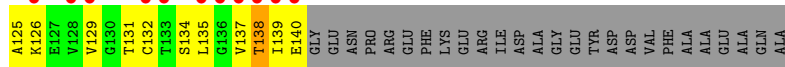
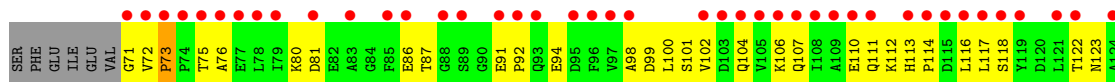
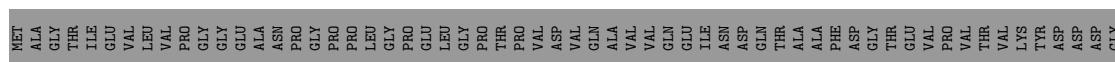
• Molecule 31: 50S ribosomal protein L39e



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtrriage
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 ²)	56.1	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99029	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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 [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	59021	0	29810	904	0
2	9	2600	0	1326	60	0
3	4	52	0	36	2	0
4	5	82	0	50	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	59983	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 [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	
5	A	235/240 (98%)	205 (87%)	24 (10%)	6 (3%)	5	13
6	B	335/338 (99%)	295 (88%)	33 (10%)	7 (2%)	7	18
7	C	244/246 (99%)	215 (88%)	28 (12%)	1 (0%)	34	60
8	D	134/177 (76%)	94 (70%)	33 (25%)	7 (5%)	2	3
9	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
10	F	117/120 (98%)	104 (89%)	7 (6%)	6 (5%)	2	3
11	G	25/348 (7%)	24 (96%)	0	1 (4%)	3	6
12	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	8	20
13	J	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	7	18
14	K	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	10	26
15	L	141/165 (86%)	122 (86%)	17 (12%)	2 (1%)	11	28
16	M	192/194 (99%)	176 (92%)	16 (8%)	0	100	100
17	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	5	12
18	O	113/116 (97%)	109 (96%)	2 (2%)	2 (2%)	8	21
19	P	141/149 (95%)	131 (93%)	7 (5%)	3 (2%)	7	18
20	Q	93/96 (97%)	84 (90%)	9 (10%)	0	100	100
21	R	148/155 (96%)	135 (91%)	11 (7%)	2 (1%)	11	28
22	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
23	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17	40
24	U	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	7	19
25	V	63/71 (89%)	54 (86%)	7 (11%)	2 (3%)	4	9
26	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	46
27	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	5	14
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	55 (78%)	9 (13%)	7 (10%)	0	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%)	14	34
33	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	2	5
All	All	3705/4430 (84%)	3316 (90%)	321 (9%)	68 (2%)	8	21

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 [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	
5	A	179/182 (98%)	170 (95%)	9 (5%)	24	51
6	B	282/283 (100%)	267 (95%)	15 (5%)	22	48
7	C	193/193 (100%)	180 (93%)	13 (7%)	16	37
8	D	117/148 (79%)	112 (96%)	5 (4%)	29	57
9	E	152/156 (97%)	147 (97%)	5 (3%)	38	67
10	F	93/94 (99%)	90 (97%)	3 (3%)	39	68
11	G	27/283 (10%)	26 (96%)	1 (4%)	34	63
12	H	132/138 (96%)	126 (96%)	6 (4%)	27	55
13	J	118/121 (98%)	110 (93%)	8 (7%)	16	36
14	K	106/106 (100%)	104 (98%)	2 (2%)	57	82
15	L	113/127 (89%)	110 (97%)	3 (3%)	44	74
16	M	158/158 (100%)	150 (95%)	8 (5%)	24	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	149/150 (99%)	145 (97%)	4 (3%)	44	74
18	O	93/94 (99%)	91 (98%)	2 (2%)	52	79
19	P	113/117 (97%)	108 (96%)	5 (4%)	28	56
20	Q	79/80 (99%)	74 (94%)	5 (6%)	18	40
21	R	117/122 (96%)	113 (97%)	4 (3%)	37	66
22	S	71/74 (96%)	70 (99%)	1 (1%)	67	86
23	T	105/106 (99%)	98 (93%)	7 (7%)	16	37
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	55	81
26	W	130/130 (100%)	125 (96%)	5 (4%)	33	62
27	X	66/74 (89%)	61 (92%)	5 (8%)	13	30
28	Y	120/196 (61%)	114 (95%)	6 (5%)	24	51
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%)	25	53
32	3	79/79 (100%)	77 (98%)	2 (2%)	47	76
33	I	58/130 (45%)	57 (98%)	1 (2%)	60	84
All	All	3093/3611 (86%)	2965 (96%)	128 (4%)	30	59

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

Mol	Chain	Res	Type
27	X	72	VAL
28	Y	163	THR
10	F	99	THR
10	F	12	LEU
28	Y	203	VAL

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

Mol	Chain	Res	Type
23	T	43	ASN
28	Y	189	ASN
24	U	39	ASN
26	W	119	HIS

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Mol	Chain	Res	Type
31	2	16	ASN

5.3.3 RNA [i](#)

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	2718	C
1	0	1563	G
1	0	2791	U
1	0	2467	A

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

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	36,1	19,22,23	0.33	0	26,31,34	0.37	0
3	5AA	4	76	1,3	18,26,27	0.78	0	15,38,41	1.01	0
1	UR3	0	2619	1	19,22,23	0.51	0	26,32,35	0.64	1 (3%)
4	ACA	5	78	4	7,7,8	1.83	1 (14%)	6,6,8	0.84	0
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	22,30,33	1.30	3 (13%)
1	OMG	0	2588	1,3	18,26,27	1.05	3 (16%)	19,38,41	0.72	1 (5%)
3	HFA	4	77	3	10,11,12	1.15	1 (10%)	12,13,15	0.65	0
1	1MA	0	628	36,1	16,25,26	1.31	3 (18%)	18,37,40	1.14	2 (11%)

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	36,1	-	0/9/27/28	0/2/2/2
3	5AA	4	76	1,3	-	0/7/29/30	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
4	ACA	5	78	4	-	2/4/5/6	-
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
3	HFA	4	77	3	-	0/5/6/8	0/1/1/1
1	1MA	0	628	36,1	-	0/3/25/26	0/3/3/3

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	C2-N1	4.94	1.43	1.36
4	5	78	ACA	C3-C2	-4.53	1.34	1.52
1	0	628	1MA	C2-N3	3.29	1.33	1.29
3	4	77	HFA	OA-CA	3.10	1.49	1.43
1	0	2621	PSU	C6-C5	3.03	1.38	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.40	120.58	118.20
1	0	2621	PSU	C6-N1-C2	-3.08	119.53	122.68
1	0	628	1MA	N1-C2-N3	2.82	129.31	126.02
1	0	2621	PSU	O2-C2-N1	2.62	125.68	122.79
1	0	628	1MA	C5-C6-N1	2.47	117.59	113.90

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	5	78	ACA	C2-C3-C4-C5
4	5	78	ACA	C4-C5-C6-N

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
3	4	76	5AA	1	0
4	5	78	ACA	1	0
1	0	2588	OMG	1	0
3	4	77	HFA	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	76:A	O3'	77:PHE	C	1.60

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.40	39 (1%) 75 77	30, 56, 102, 163	0
2	9	122/122 (100%)	-0.26	5 (4%) 37 36	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 45	37, 61, 97, 120	0
6	B	337/338 (99%)	0.20	8 (2%) 59 60	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%) 16 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 62	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%) 7 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 35	47, 68, 83, 91	0
20	Q	95/96 (98%)	0.22	3 (3%) 47 48	45, 54, 68, 87	0
21	R	150/155 (96%)	-0.04	1 (0%) 87 89	42, 55, 73, 84	0
22	S	81/85 (95%)	0.22	3 (3%) 41 41	52, 68, 87, 94	0
23	T	119/120 (99%)	0.62	6 (5%) 28 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 ²)	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 22	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 [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
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	UR3	0	2619	21/22	0.98	0.16	40,46,49,54	0
1	OMG	0	2588	24/25	0.98	0.15	38,40,45,46	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
1	PSU	0	2621	20/21	0.99	0.13	34,37,42,43	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, 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
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
36	NA	0	9171	1/1	0.75	0.29	74,74,74,74	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	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	9175	1/1	0.79	0.82	61,61,61,61	0
36	NA	0	9107	1/1	0.79	0.28	55,55,55,55	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	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
36	NA	0	9185	1/1	0.81	0.56	61,61,61,61	0
34	MG	0	8024	1/1	0.82	0.14	61,61,61,61	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
34	MG	0	8087	1/1	0.82	0.13	53,53,53,53	0
38	CD	O	9205	1/1	0.82	0.07	146,146,146,146	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
36	NA	0	9166	1/1	0.84	0.12	71,71,71,71	0
34	MG	0	8090	1/1	0.84	0.41	77,77,77,77	0
36	NA	0	9177	1/1	0.85	0.32	78,78,78,78	0
34	MG	0	8045	1/1	0.86	0.30	87,87,87,87	0
34	MG	0	8082	1/1	0.86	0.23	72,72,72,72	0
36	NA	0	9169	1/1	0.87	0.30	65,65,65,65	0
36	NA	0	9110	1/1	0.87	0.22	44,44,44,44	0
36	NA	0	9163	1/1	0.87	0.34	75,75,75,75	0
34	MG	0	8049	1/1	0.87	0.29	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	MG	0	8092	1/1	0.88	0.55	102,102,102,102	0
34	MG	0	8106	1/1	0.88	0.11	57,57,57,57	0
36	NA	0	9168	1/1	0.88	0.15	69,69,69,69	0
34	MG	0	8043	1/1	0.89	0.10	55,55,55,55	0
36	NA	0	9121	1/1	0.89	0.46	69,69,69,69	0
34	MG	0	8053	1/1	0.89	0.15	57,57,57,57	0
34	MG	0	8076	1/1	0.89	0.10	68,68,68,68	0
36	NA	0	9182	1/1	0.89	0.34	78,78,78,78	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
34	MG	5	8118	1/1	0.90	0.18	47,47,47,47	0
36	NA	0	9150	1/1	0.90	0.18	46,46,46,46	0
37	CL	J	9302	1/1	0.90	0.16	86,86,86,86	0
37	CL	N	9307	1/1	0.90	0.23	74,74,74,74	0
36	NA	0	9181	1/1	0.90	0.17	69,69,69,69	0
36	NA	0	9136	1/1	0.91	0.09	68,68,68,68	0
36	NA	C	9104	1/1	0.91	0.09	43,43,43,43	0
36	NA	0	9141	1/1	0.91	0.12	52,52,52,52	0
36	NA	J	9146	1/1	0.91	0.12	41,41,41,41	0
36	NA	0	9164	1/1	0.91	0.34	55,55,55,55	0
36	NA	0	9142	1/1	0.91	0.21	45,45,45,45	0
34	MG	0	8102	1/1	0.91	0.08	64,64,64,64	0
34	MG	0	8050	1/1	0.91	0.09	86,86,86,86	0
34	MG	0	8089	1/1	0.91	0.07	65,65,65,65	0
36	NA	L	9180	1/1	0.92	0.55	61,61,61,61	0
36	NA	R	9137	1/1	0.92	0.07	47,47,47,47	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	0	9111	1/1	0.92	0.18	71,71,71,71	0
36	NA	0	9132	1/1	0.92	0.08	34,34,34,34	0
37	CL	R	9306	1/1	0.92	0.19	67,67,67,67	0
37	CL	3	9304	1/1	0.92	0.12	67,67,67,67	0
35	K	0	9001	1/1	0.92	0.40	70,70,70,70	0
34	MG	0	8097	1/1	0.93	0.12	46,46,46,46	0
36	NA	0	9117	1/1	0.93	0.12	62,62,62,62	0
36	NA	0	9140	1/1	0.93	0.27	53,53,53,53	0
37	CL	0	9315	1/1	0.93	0.60	89,89,89,89	0
37	CL	0	9322	1/1	0.93	0.76	90,90,90,90	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	8041	1/1	0.93	0.36	87,87,87,87	0
34	MG	0	8104	1/1	0.93	0.23	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	NA	0	9127	1/1	0.93	0.13	46,46,46,46	0
34	MG	0	8096	1/1	0.93	0.19	63,63,63,63	0
34	MG	0	8016	1/1	0.94	0.19	40,40,40,40	0
34	MG	0	8051	1/1	0.94	0.18	87,87,87,87	0
36	NA	0	9153	1/1	0.94	0.14	35,35,35,35	0
36	NA	0	9176	1/1	0.94	0.24	49,49,49,49	0
34	MG	0	8099	1/1	0.94	0.10	55,55,55,55	0
36	NA	0	9128	1/1	0.94	0.12	43,43,43,43	0
36	NA	0	9101	1/1	0.94	0.15	47,47,47,47	0
34	MG	0	8047	1/1	0.94	0.18	85,85,85,85	0
34	MG	0	8057	1/1	0.94	0.14	49,49,49,49	0
34	MG	0	8062	1/1	0.94	0.15	64,64,64,64	0
34	MG	0	8067	1/1	0.94	0.09	52,52,52,52	0
34	MG	0	8002	1/1	0.94	0.10	48,48,48,48	0
36	NA	0	9170	1/1	0.94	0.70	85,85,85,85	0
36	NA	0	9133	1/1	0.95	0.13	38,38,38,38	0
36	NA	0	9135	1/1	0.95	0.17	55,55,55,55	0
34	MG	Y	8109	1/1	0.95	0.20	62,62,62,62	0
34	MG	0	8013	1/1	0.95	0.19	43,43,43,43	0
34	MG	0	8084	1/1	0.95	0.10	47,47,47,47	0
36	NA	0	9102	1/1	0.95	0.14	54,54,54,54	0
36	NA	0	9106	1/1	0.95	0.75	49,49,49,49	0
34	MG	0	8063	1/1	0.95	0.08	68,68,68,68	0
34	MG	0	8101	1/1	0.95	0.15	74,74,74,74	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
34	MG	0	8103	1/1	0.95	0.12	66,66,66,66	0
36	NA	0	9114	1/1	0.95	0.22	44,44,44,44	0
34	MG	0	8068	1/1	0.95	0.04	75,75,75,75	0
36	NA	0	9119	1/1	0.95	0.13	45,45,45,45	0
36	NA	0	9165	1/1	0.95	0.32	45,45,45,45	0
34	MG	0	8070	1/1	0.95	0.17	66,66,66,66	0
36	NA	0	9124	1/1	0.95	0.16	69,69,69,69	0
34	MG	0	8012	1/1	0.95	0.15	43,43,43,43	0
37	CL	L	9310	1/1	0.95	0.14	72,72,72,72	0
34	MG	0	8091	1/1	0.95	0.12	74,74,74,74	0
34	MG	0	8080	1/1	0.95	0.11	43,43,43,43	0
37	CL	Y	9317	1/1	0.95	0.13	72,72,72,72	0
37	CL	Y	9320	1/1	0.95	0.14	55,55,55,55	0
34	MG	K	8069	1/1	0.95	0.12	48,48,48,48	0
34	MG	0	8094	1/1	0.95	0.14	80,80,80,80	0
34	MG	0	8117	1/1	0.96	0.06	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
36	NA	0	9113	1/1	0.96	0.20	71,71,71,71	0
34	MG	9	8095	1/1	0.96	0.09	73,73,73,73	0
36	NA	0	9115	1/1	0.96	0.15	41,41,41,41	0
34	MG	0	8072	1/1	0.96	0.27	56,56,56,56	0
36	NA	0	9157	1/1	0.96	0.05	75,75,75,75	0
34	MG	A	8065	1/1	0.96	0.20	54,54,54,54	0
34	MG	B	8055	1/1	0.96	0.16	60,60,60,60	0
36	NA	0	9160	1/1	0.96	0.51	48,48,48,48	0
34	MG	0	8100	1/1	0.96	0.21	79,79,79,79	0
34	MG	0	8075	1/1	0.96	0.09	48,48,48,48	0
36	NA	R	9138	1/1	0.96	0.10	67,67,67,67	0
34	MG	0	8042	1/1	0.96	0.10	47,47,47,47	0
34	MG	3	8078	1/1	0.96	0.07	41,41,41,41	0
37	CL	0	9303	1/1	0.96	0.19	63,63,63,63	0
34	MG	0	8018	1/1	0.96	0.19	49,49,49,49	0
36	NA	0	9167	1/1	0.96	0.08	56,56,56,56	0
36	NA	0	9131	1/1	0.96	0.15	35,35,35,35	0
34	MG	0	8033	1/1	0.96	0.14	44,44,44,44	0
37	CL	J	9321	1/1	0.96	0.17	60,60,60,60	0
34	MG	0	8040	1/1	0.96	0.15	55,55,55,55	0
34	MG	0	8112	1/1	0.96	0.09	43,43,43,43	0
34	MG	0	8019	1/1	0.96	0.08	35,35,35,35	0
36	NA	0	9174	1/1	0.96	0.49	74,74,74,74	0
36	NA	0	9139	1/1	0.96	0.15	30,30,30,30	0
34	MG	0	8054	1/1	0.96	0.16	35,35,35,35	0
34	MG	0	8116	1/1	0.96	0.30	67,67,67,67	0
34	MG	0	8052	1/1	0.97	0.08	51,51,51,51	0
36	NA	A	9145	1/1	0.97	0.10	41,41,41,41	0
34	MG	0	8098	1/1	0.97	0.12	46,46,46,46	0
34	MG	0	8086	1/1	0.97	0.07	58,58,58,58	0
34	MG	0	8039	1/1	0.97	0.12	50,50,50,50	0
34	MG	0	8007	1/1	0.97	0.10	25,25,25,25	0
36	NA	M	9147	1/1	0.97	0.16	32,32,32,32	0
34	MG	A	8066	1/1	0.97	0.07	67,67,67,67	0
34	MG	0	8010	1/1	0.97	0.10	42,42,42,42	0
36	NA	0	9116	1/1	0.97	0.16	48,48,48,48	0
36	NA	0	9143	1/1	0.97	0.09	38,38,38,38	0
36	NA	0	9149	1/1	0.97	0.13	43,43,43,43	0
37	CL	0	9311	1/1	0.97	0.14	58,58,58,58	0
36	NA	0	9173	1/1	0.97	0.39	62,62,62,62	0
34	MG	0	8015	1/1	0.97	0.09	37,37,37,37	0
37	CL	A	9309	1/1	0.97	0.23	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8032	1/1	0.97	0.13	47,47,47,47	0
34	MG	0	8064	1/1	0.97	0.13	38,38,38,38	0
34	MG	0	8108	1/1	0.97	0.12	58,58,58,58	0
36	NA	0	9178	1/1	0.97	0.54	75,75,75,75	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
37	CL	O	9308	1/1	0.97	0.14	81,81,81,81	0
34	MG	0	8093	1/1	0.97	0.16	65,65,65,65	0
34	MG	0	8083	1/1	0.97	0.13	45,45,45,45	0
34	MG	0	8004	1/1	0.97	0.07	38,38,38,38	0
36	NA	0	9105	1/1	0.97	0.12	45,45,45,45	0
34	MG	0	8115	1/1	0.97	0.20	54,54,54,54	0
36	NA	0	9154	1/1	0.98	0.16	38,38,38,38	0
34	MG	0	8038	1/1	0.98	0.18	33,33,33,33	0
36	NA	0	9156	1/1	0.98	0.35	57,57,57,57	0
36	NA	0	9120	1/1	0.98	0.20	35,35,35,35	0
34	MG	0	8006	1/1	0.98	0.09	43,43,43,43	0
36	NA	0	9123	1/1	0.98	0.17	47,47,47,47	0
34	MG	0	8026	1/1	0.98	0.14	31,31,31,31	0
36	NA	0	9125	1/1	0.98	0.22	62,62,62,62	0
34	MG	0	8107	1/1	0.98	0.08	49,49,49,49	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	8111	1/1	0.98	0.11	59,59,59,59	0
36	NA	0	9130	1/1	0.98	0.22	49,49,49,49	0
37	CL	0	9305	1/1	0.98	0.13	62,62,62,62	0
34	MG	0	8029	1/1	0.98	0.17	39,39,39,39	0
37	CL	0	9313	1/1	0.98	0.14	64,64,64,64	0
37	CL	0	9314	1/1	0.98	0.13	57,57,57,57	0
36	NA	0	9103	1/1	0.98	0.08	48,48,48,48	0
37	CL	0	9316	1/1	0.98	0.25	75,75,75,75	0
34	MG	0	8074	1/1	0.98	0.10	38,38,38,38	0
36	NA	0	9134	1/1	0.98	0.07	46,46,46,46	0
37	CL	B	9319	1/1	0.98	0.24	57,57,57,57	0
34	MG	0	8030	1/1	0.98	0.15	36,36,36,36	0
34	MG	0	8017	1/1	0.98	0.07	31,31,31,31	0
34	MG	0	8020	1/1	0.98	0.09	33,33,33,33	0
34	MG	0	8081	1/1	0.98	0.16	59,59,59,59	0
34	MG	0	8059	1/1	0.98	0.08	52,52,52,52	0
34	MG	0	8060	1/1	0.98	0.22	45,45,45,45	0
34	MG	0	8034	1/1	0.98	0.12	38,38,38,38	0
36	NA	0	9144	1/1	0.98	0.10	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8035	1/1	0.98	0.10	49,49,49,49	0
34	MG	0	8037	1/1	0.98	0.08	47,47,47,47	0
34	MG	B	8056	1/1	0.98	0.16	57,57,57,57	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
34	MG	0	8025	1/1	0.99	0.12	45,45,45,45	0
34	MG	0	8003	1/1	0.99	0.13	36,36,36,36	0
34	MG	0	8027	1/1	0.99	0.14	48,48,48,48	0
36	NA	0	9109	1/1	0.99	0.11	35,35,35,35	0
34	MG	0	8077	1/1	0.99	0.07	28,28,28,28	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
36	NA	0	9162	1/1	0.99	0.27	61,61,61,61	0
34	MG	0	8058	1/1	0.99	0.16	48,48,48,48	0
34	MG	0	8001	1/1	0.99	0.06	37,37,37,37	0
34	MG	0	8008	1/1	0.99	0.09	31,31,31,31	0
34	MG	0	8061	1/1	0.99	0.12	36,36,36,36	0
37	CL	K	9312	1/1	0.99	0.10	60,60,60,60	0
34	MG	0	8031	1/1	0.99	0.08	29,29,29,29	0
34	MG	0	8009	1/1	0.99	0.13	35,35,35,35	0
34	MG	0	8021	1/1	0.99	0.16	33,33,33,33	0
34	MG	0	8022	1/1	0.99	0.09	39,39,39,39	0
36	NA	Q	9148	1/1	0.99	0.19	46,46,46,46	0
34	MG	0	8110	1/1	0.99	0.07	36,36,36,36	0
34	MG	0	8048	1/1	0.99	0.12	63,63,63,63	0
34	MG	0	8023	1/1	0.99	0.22	53,53,53,53	0
34	MG	0	8036	1/1	0.99	0.16	32,32,32,32	0
38	CD	U	9201	1/1	0.99	0.07	78,78,78,78	0
38	CD	Z	9203	1/1	0.99	0.09	76,76,76,76	0
34	MG	0	8005	1/1	0.99	0.10	38,38,38,38	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.