



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 07:35 am BST

PDB ID : 3CMA
Title : The structure of CCA and CCA-Phe-Cap-Bio bound to the large ribosomal subunit of *Haloarcula marismortui*
Authors : Simonovic, M.; Steitz, T.A.
Deposited on : 2008-03-21
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

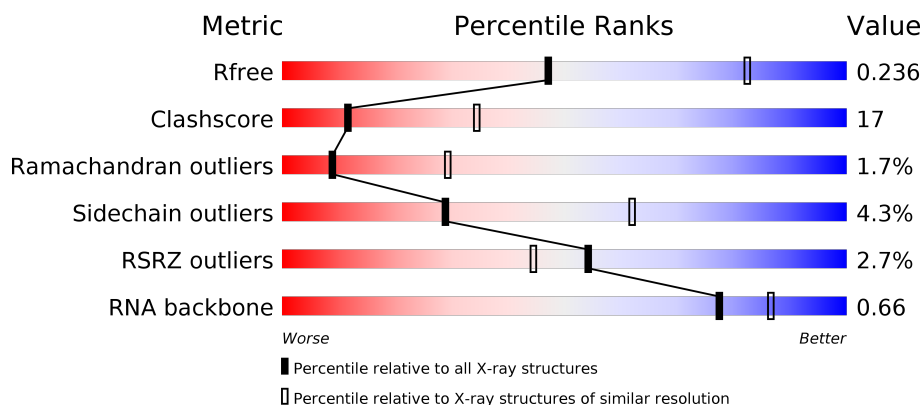
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



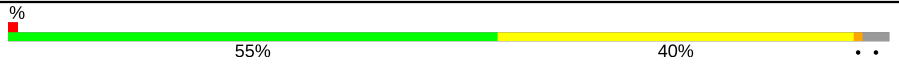

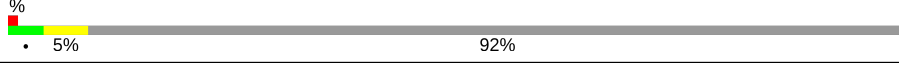

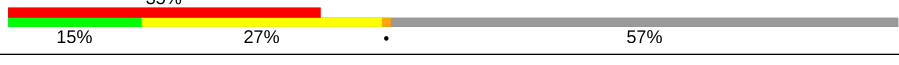
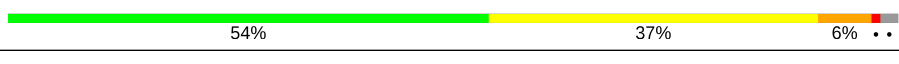
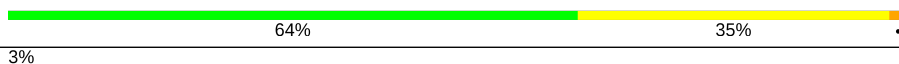
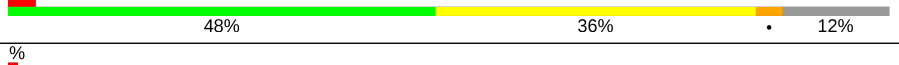
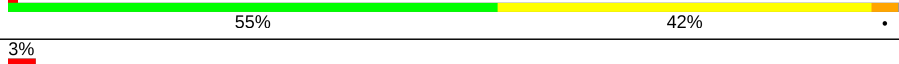


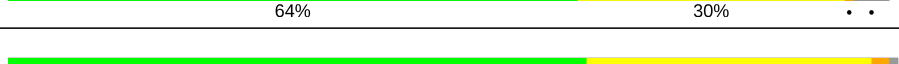



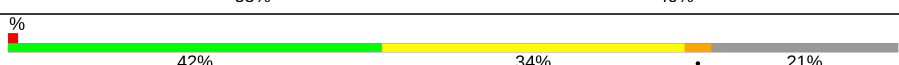
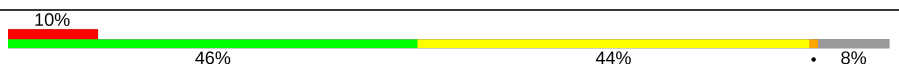
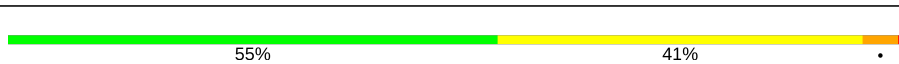
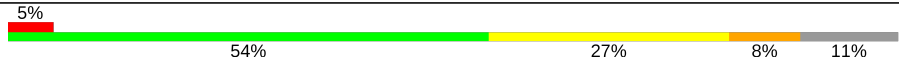
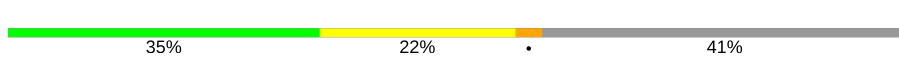
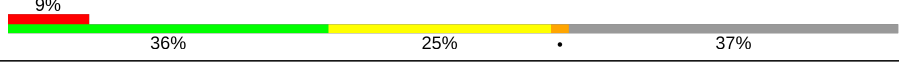
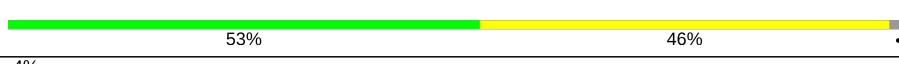



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 ≥ 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	A	240	<div> <div>3%</div> <div>54%</div> <div>41%</div> <div>..</div> </div>
2	B	338	<div> <div>46%</div> <div>51%</div> <div>.</div> </div>
3	C	246	<div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
4	D	177	<div> <div>13%</div> <div>28%</div> <div>46%</div> <div>..</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	240	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	
32	5	3	
33	6	3	

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
34	MG	0	8016	-	-	-	X
34	MG	0	8038	-	-	-	X
34	MG	0	8046	-	-	-	X
34	MG	0	8047	-	-	-	X
34	MG	0	8050	-	-	-	X
34	MG	0	8063	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8078	-	-	-	X
34	MG	0	8087	-	-	-	X
34	MG	0	8090	-	-	-	X
36	SR	0	8920	-	-	-	X
36	SR	0	8933	-	-	-	X
36	SR	0	9006	-	-	-	X
36	SR	0	9007	-	-	-	X
36	SR	B	8987	-	-	-	X
37	NA	0	8509	-	-	-	X
37	NA	0	8519	-	-	-	X
37	NA	0	8547	-	-	-	X
37	NA	0	8560	-	-	-	X
37	NA	0	8567	-	-	-	X
37	NA	0	8571	-	-	-	X
37	NA	0	8573	-	-	-	X
40	PHE	6	77	-	-	-	X

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 99205 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1752	1072	351	324	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2624	1616	492	511	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1859	1130	344	384	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1093	685	194	210	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1356	840	223	289	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			889	551	140	197	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1281	798	239	238	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			518	323	80	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1119	696	198	222	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			993	609	188	192	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O		0	0	0
			1117	670	221	226				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1557	943	332	281	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1444	895	261	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			864	529	160	175				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1135	683	228	224				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			734	450	140	144				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1148	713	208	223	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			640	389	110	138	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			949	568	179	202				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1195	737	208	244	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			653	402	128	122	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			572	343	112	112	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			754	458	152	137	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59018	26346	10873	19054	2745			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2596	1157	471	847	121			

- Molecule 32 is a RNA chain called RNA (5'-R(*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 33 is a RNA chain called RNA (5'-R(*CP*CP*(8AN))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	84	Total	Mg	0	0
			84	84		
34	9	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	B	1	Total 1	Mg 1	0	0
34	C	1	Total 1	Mg 1	0	0
34	A	2	Total 2	Mg 2	0	0
34	T	1	Total 1	Mg 1	0	0
34	2	1	Total 1	Mg 1	0	0
34	Y	1	Total 1	Mg 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	6	Total 6	Cl 6	0	0
35	J	3	Total 3	Cl 3	0	0
35	Q	1	Total 1	Cl 1	0	0
35	K	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	A	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	2	Total 2	Cl 2	0	0
35	2	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	M	1	Total	Cl	0	0
			1	1		

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	86	Total	Sr	0	0
			86	86		
36	9	3	Total	Sr	0	0
			3	3		
36	1	2	Total	Sr	0	0
			2	2		
36	H	2	Total	Sr	0	0
			2	2		
36	B	2	Total	Sr	0	0
			2	2		
36	3	3	Total	Sr	0	0
			3	3		
36	A	3	Total	Sr	0	0
			3	3		
36	T	2	Total	Sr	0	0
			2	2		
36	R	1	Total	Sr	0	0
			1	1		
36	Y	1	Total	Sr	0	0
			1	1		
36	S	1	Total	Sr	0	0
			1	1		
36	F	1	Total	Sr	0	0
			1	1		

- Molecule 37 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	64	Total	Na	0	0
			64	64		
37	J	1	Total	Na	0	0
			1	1		
37	Q	1	Total	Na	0	0
			1	1		
37	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	B	1	Total 1	Na 1	0	0
37	C	1	Total 1	Na 1	0	0
37	R	2	Total 2	Na 2	0	0
37	9	1	Total 1	Na 1	0	0
37	L	1	Total 1	Na 1	0	0
37	S	1	Total 1	Na 1	0	0
37	M	1	Total 1	Na 1	0	0

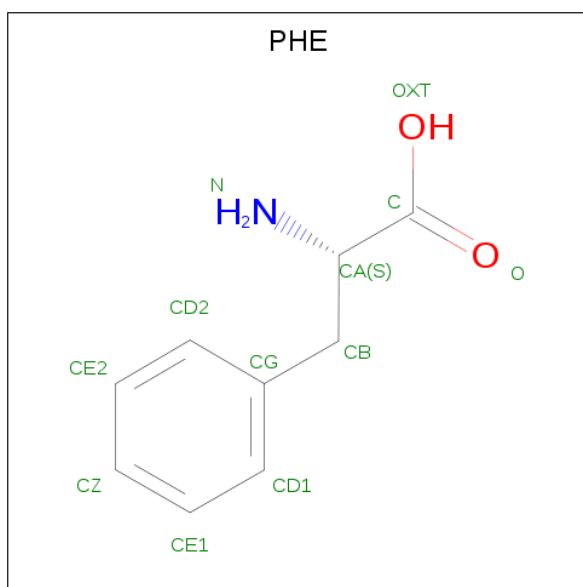
- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 39 is POTASSIUM ION (three-letter code: K) (formula: K).

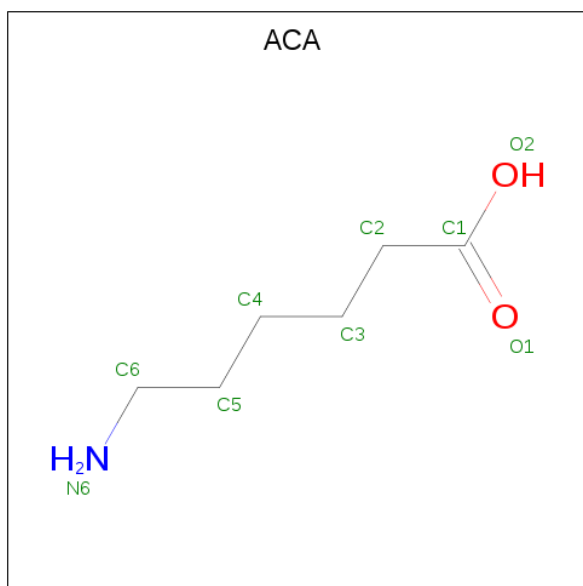
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total 2	K 2	0	0

- Molecule 40 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
40	6	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 41 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
41	6	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	128	Total 128	O 128	0	0
42	B	165	Total 165	O 165	0	0
42	C	170	Total 170	O 170	0	0
42	D	49	Total 49	O 49	0	0
42	E	48	Total 48	O 48	0	0
42	F	31	Total 31	O 31	0	0
42	G	19	Total 19	O 19	0	0
42	H	77	Total 77	O 77	0	0
42	I	11	Total 11	O 11	0	0
42	J	63	Total 63	O 63	0	0
42	K	54	Total 54	O 54	0	0
42	L	92	Total 92	O 92	0	0
42	M	136	Total 136	O 136	0	0
42	N	64	Total 64	O 64	0	0
42	O	43	Total 43	O 43	0	0
42	P	69	Total 69	O 69	0	0
42	Q	51	Total 51	O 51	0	0
42	R	87	Total 87	O 87	0	0
42	S	33	Total 33	O 33	0	0
42	T	40	Total 40	O 40	0	0
42	U	30	Total 30	O 30	0	0
42	V	16	Total 16	O 16	0	0

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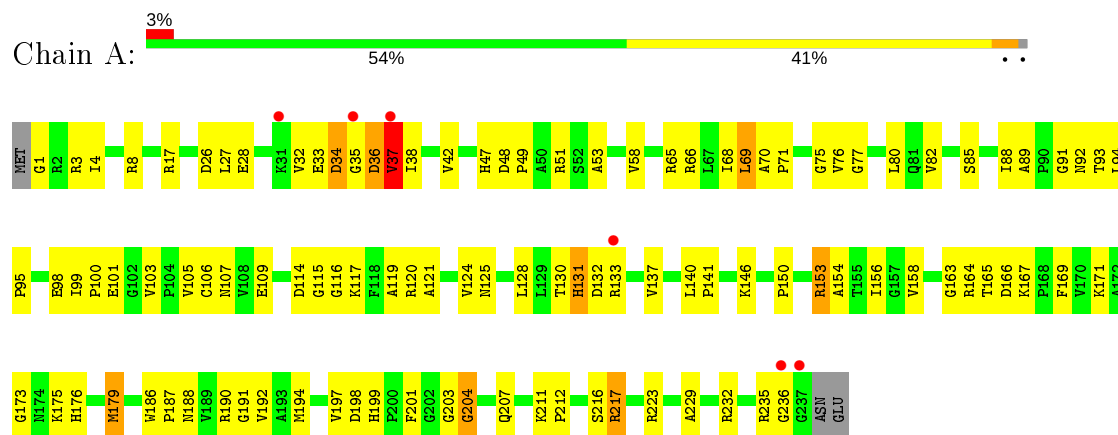
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	W	72	Total 72	O 72	0	0
42	X	25	Total 25	O 25	0	0
42	Y	108	Total 108	O 108	0	0
42	Z	30	Total 30	O 30	0	0
42	1	53	Total 53	O 53	0	0
42	2	42	Total 42	O 42	0	0
42	3	66	Total 66	O 66	0	0
42	0	5771	Total 5771	O 5771	0	0
42	9	148	Total 148	O 148	0	0
42	5	4	Total 4	O 4	0	0
42	6	3	Total 3	O 3	0	0

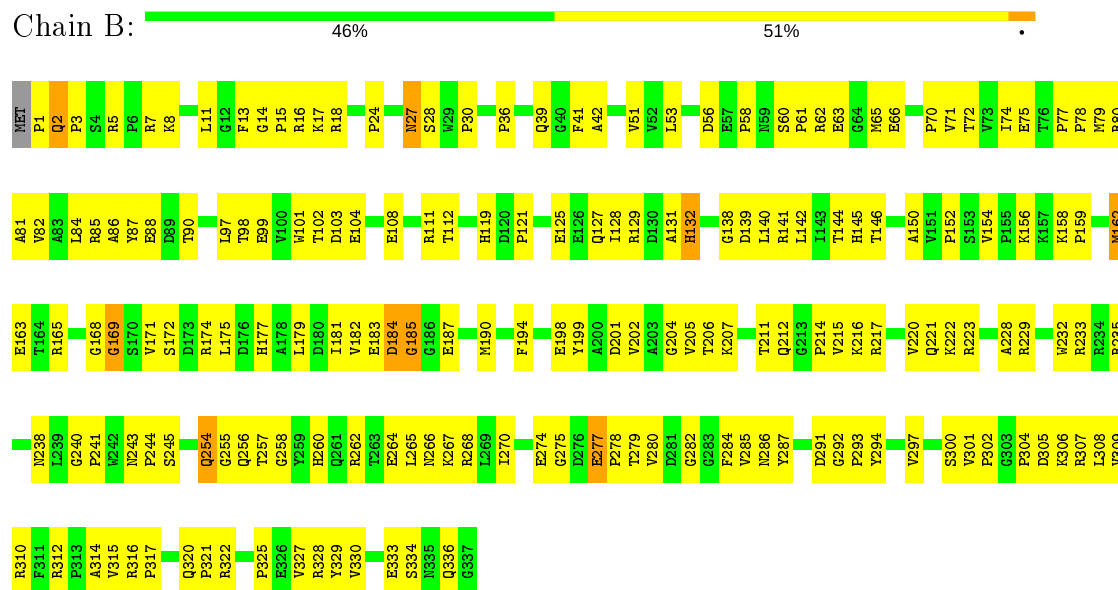
3 Residue-property plots [i](#)

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: 50S ribosomal protein L2P

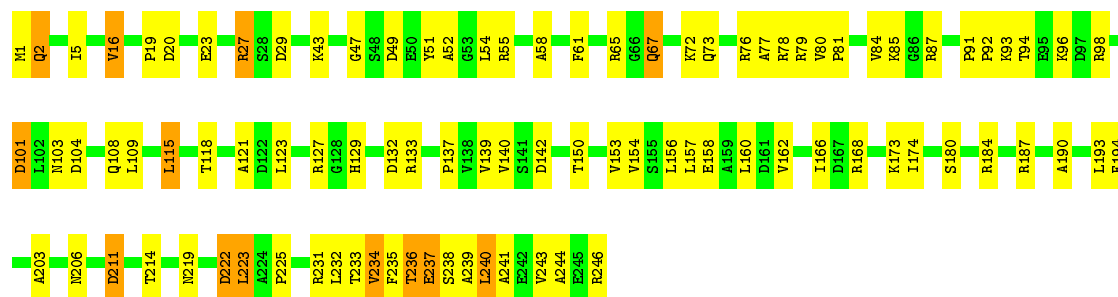


- Molecule 2: 50S ribosomal protein L3P

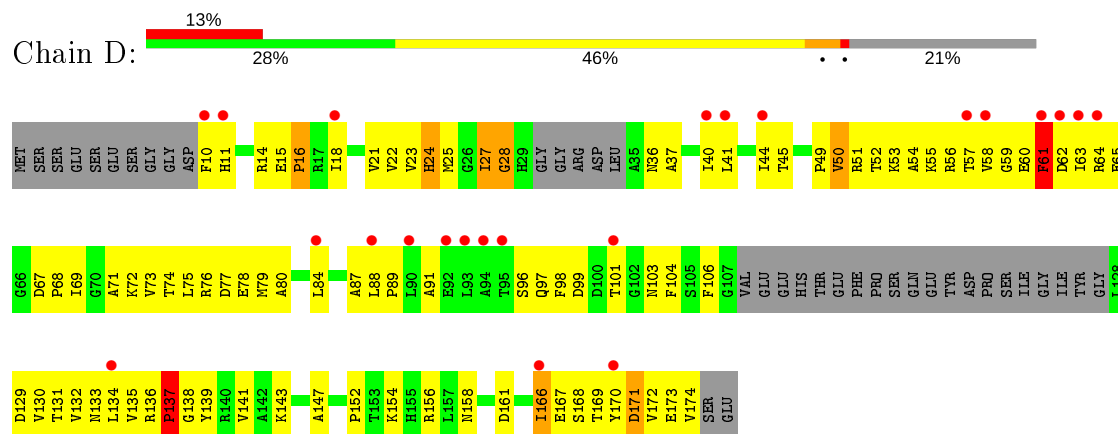


- Molecule 3: 50S ribosomal protein L4P

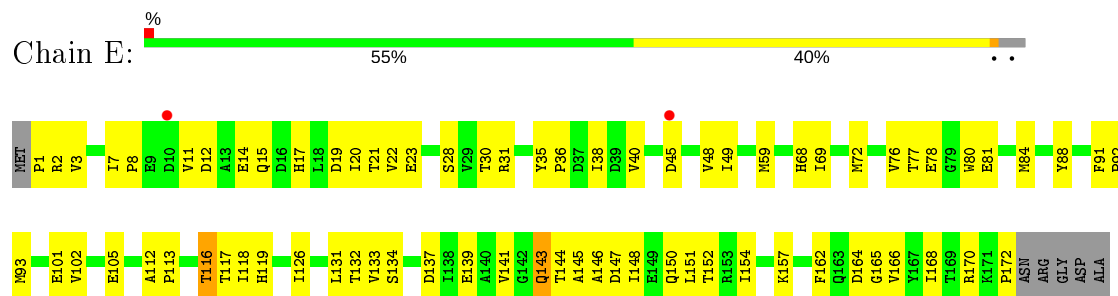




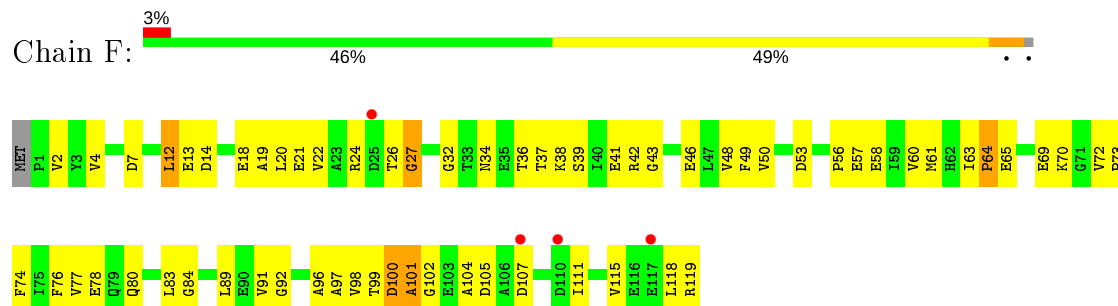
• Molecule 4: 50S ribosomal protein L5P



• Molecule 5: 50S ribosomal protein L6P

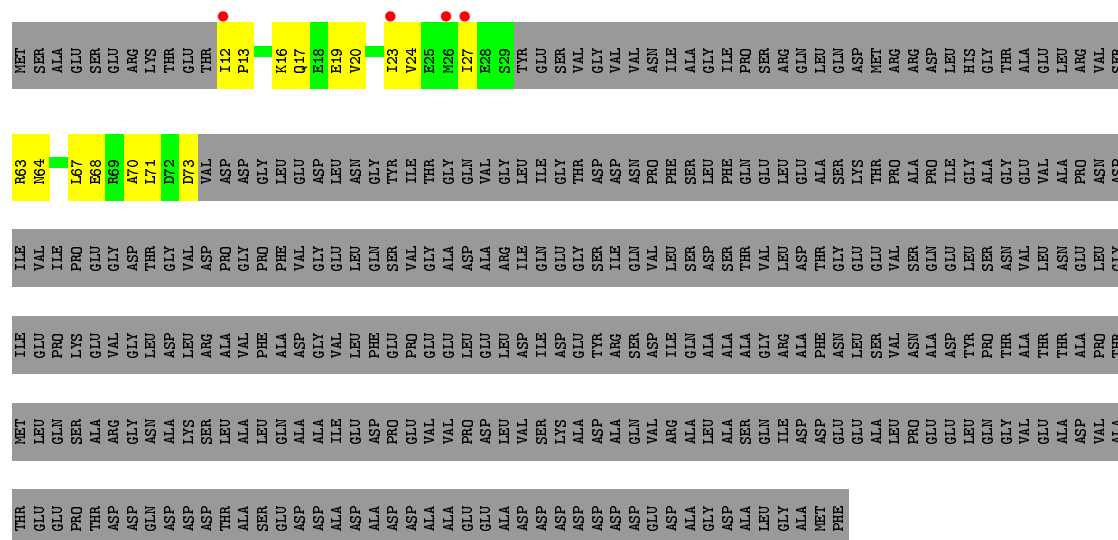


• Molecule 6: 50S ribosomal protein L7Ae

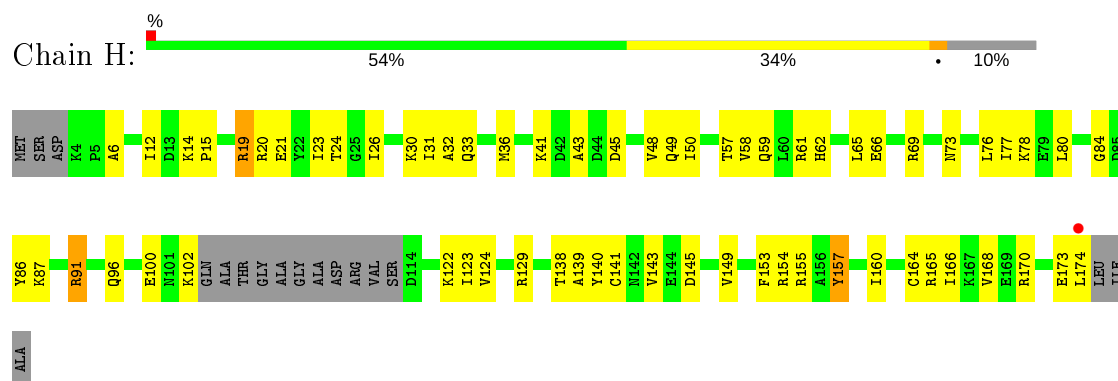


• Molecule 7: 50S ribosomal protein L10E

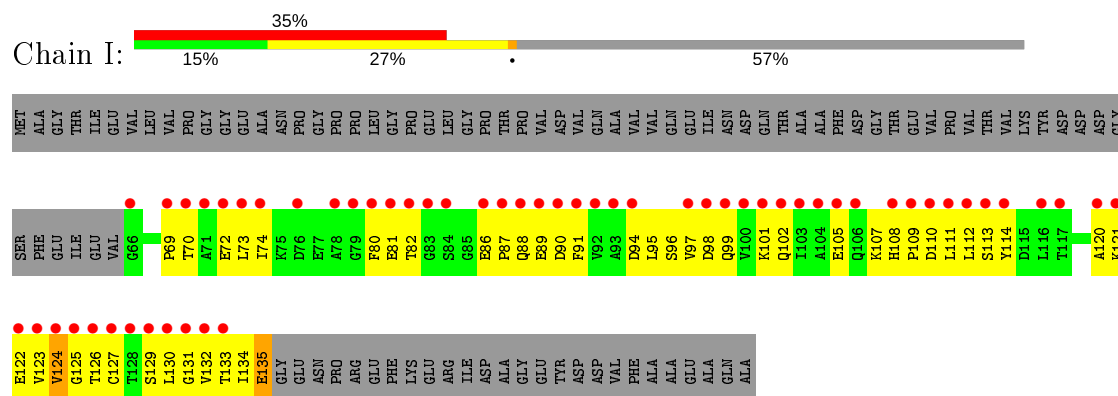




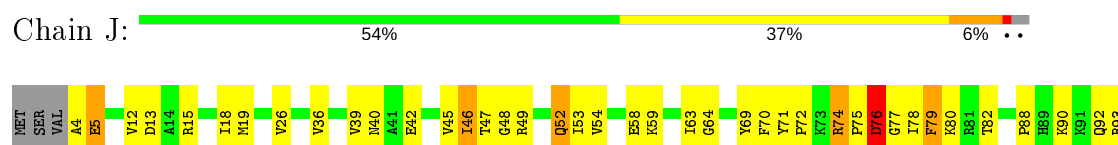
• Molecule 8: 50S ribosomal protein L10e

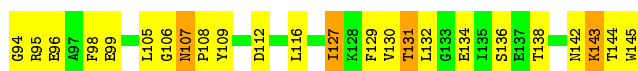


• Molecule 9: 50S ribosomal protein L11P



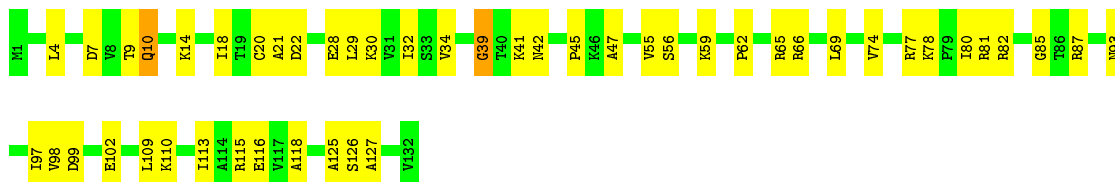
• Molecule 10: 50S ribosomal protein L13P





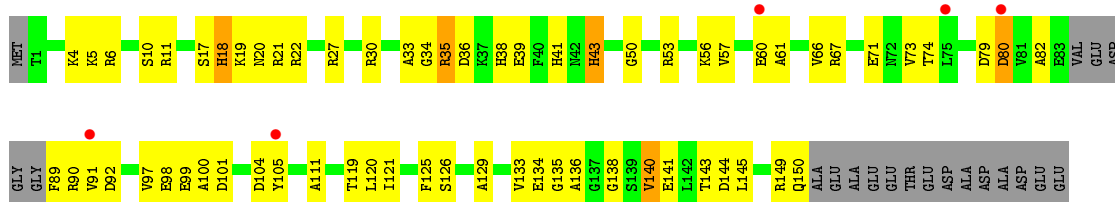
- Molecule 11: 50S ribosomal protein L14P

Chain K: 64% 35%



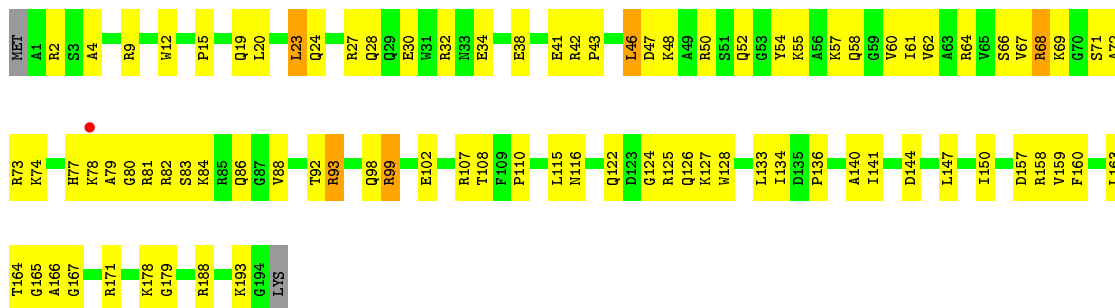
- Molecule 12: 50S ribosomal protein L15P

Chain L: 3% 48% 36% 12%



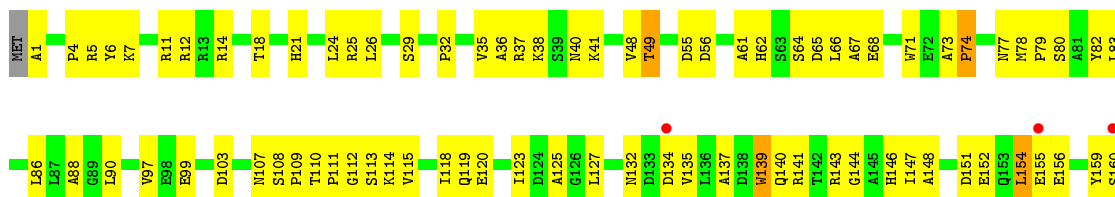
- Molecule 13: 50S ribosomal protein L15e

Chain M: % 55% 42%



- Molecule 14: 50S ribosomal protein L18P

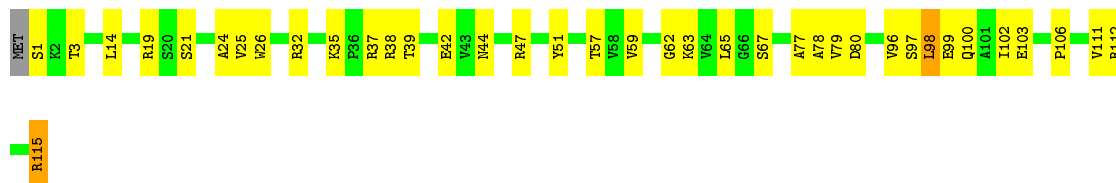
Chain N: 3% 48% 47% 5%





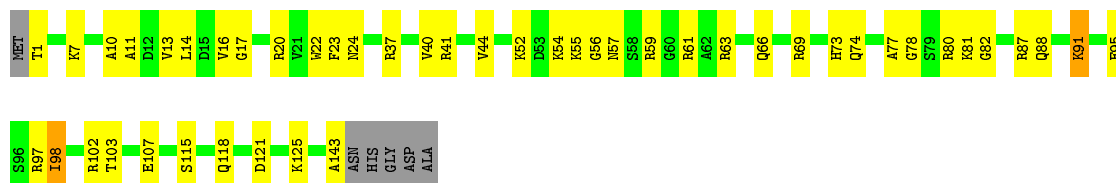
- Molecule 15: 50S ribosomal protein L18e

Chain O: 66% 31% ..



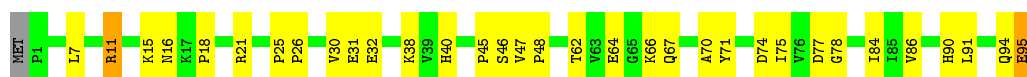
- Molecule 16: 50S ribosomal protein L19e

Chain P: 64% 30% ..



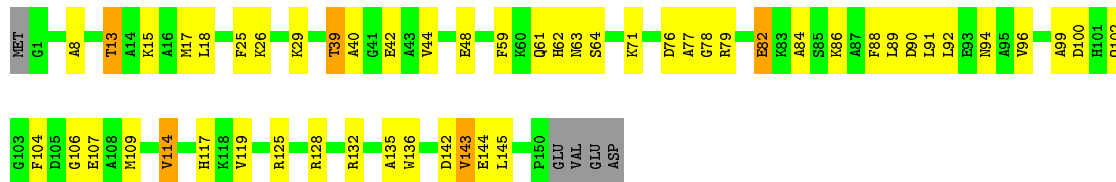
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 65% 32% ..



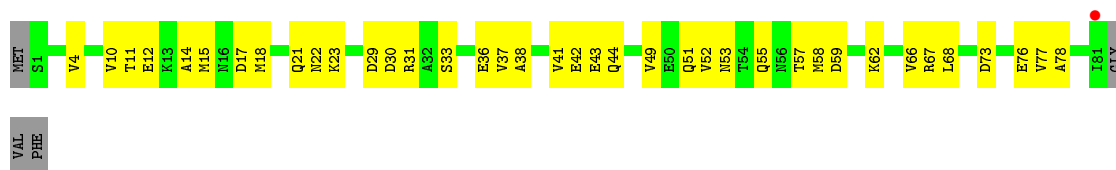
- Molecule 18: 50S ribosomal protein L22P

Chain R: 63% 30% ..

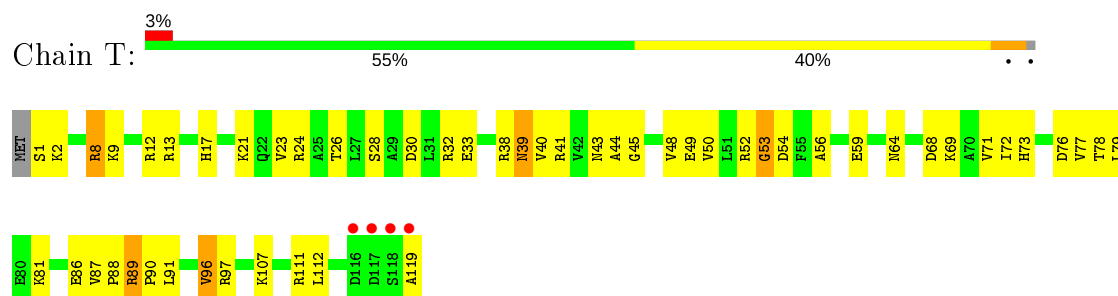


- Molecule 19: 50S ribosomal protein L23P

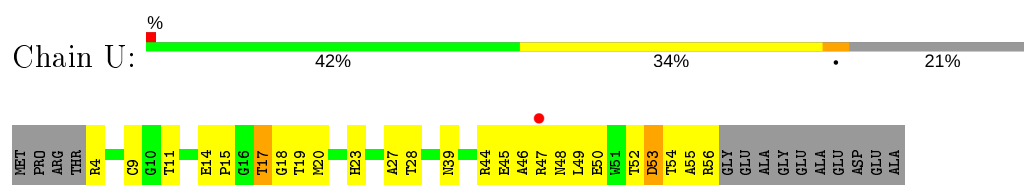
Chain S: 51% 45% 5%



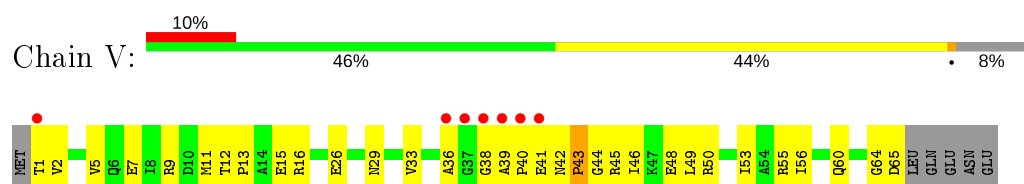
- Molecule 20: 50S ribosomal protein L24P



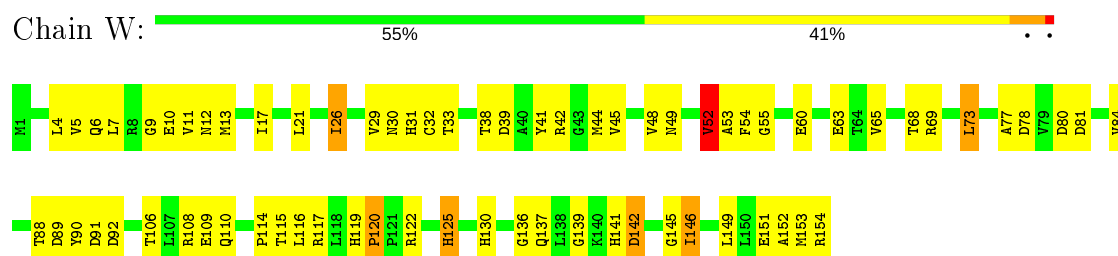
- Molecule 21: 50S ribosomal protein L24e



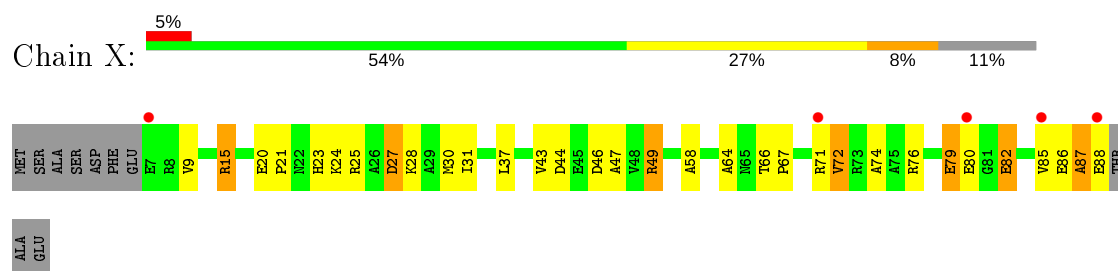
- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

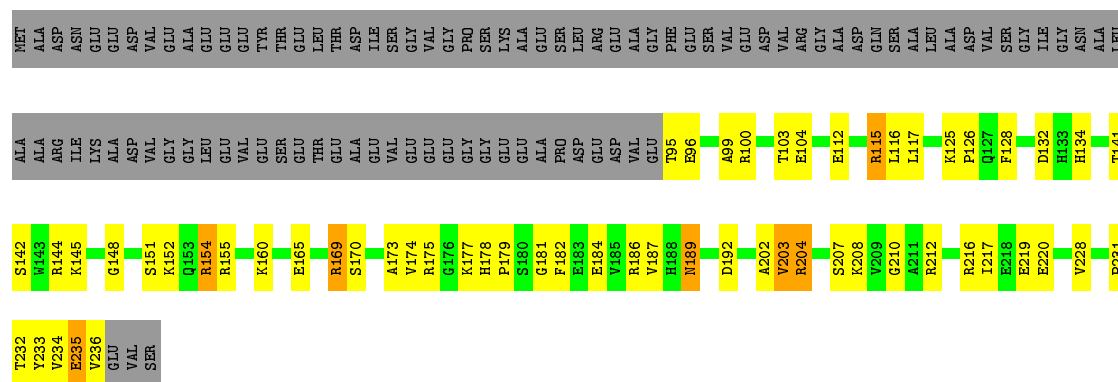


- Molecule 24: 50S ribosomal protein L31e

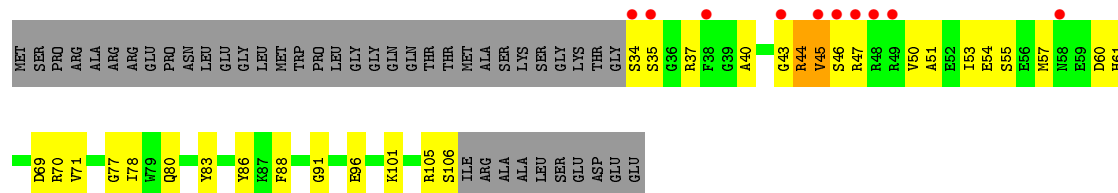


- Molecule 25: 50S ribosomal protein L32e





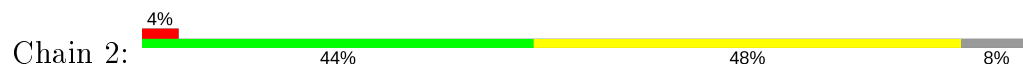
• Molecule 26: 50S ribosomal protein L37Ae



• Molecule 27: 50S ribosomal protein L37e



• Molecule 28: 50S ribosomal protein L39e



• Molecule 29: 50S ribosomal protein L44E



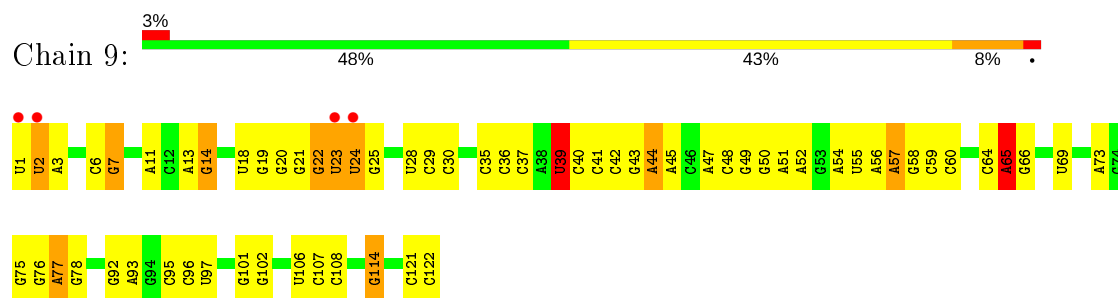
• Molecule 30: 23S RIBOSOMAL RNA



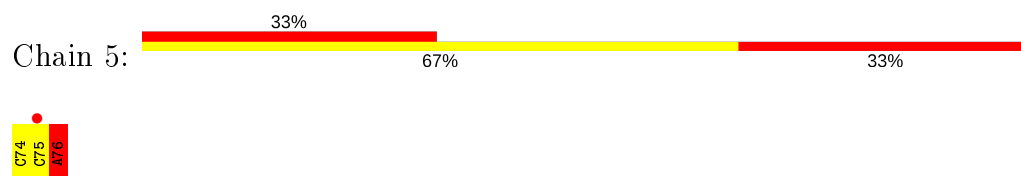
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A1522	G1405	U1405	U1406	G1310	U1309	G1131	A1014	A922	G809	G707	G607	G503	U396	C303	A191	C101
U1524	G1312	G1311	A1407	G1310	C1015	A1132	C1015	A923	A812	A708	A608	G504	A397	G304	A192	A102
G1525	A1313	U1218	U1219	C1019	U1021	C1140	C1019	A926	G814	G709	U612	G505	U398	A305	A198	G105
A1526	U1314	U1313	U1314	A1020	G1021	G1151	A1020	U932	U815	G710	U614	A507	C399	G307	C200	U107
A1527	G1315	G1315	C1229	A1022	A1022	G1158	A1022	C933	G816	U714	A620	A508	A407	U308	U109	U108
A1528	G1316	A1230	C1229	U1029	U1029	G1159	U1029	G944	G817	U	G716	A509	A408	C309	C110	U109
A1529	G1325	A1159	C1230	U1029	U1029	G1160	U1029	U945	G820	A721	U625	A511	A415	G314	C111	C111
A1533	G1326	A1161	U1234	G1039	G1039	A1161	G1039	C946	U821	G722	U625	G514	G416	G315	A114	A114
C1534	G1327	G1162	G1235	A1040	A1040	G1163	A1040	U947	C822	G722	A629	G518	G417	A316	U115	U115
C1545	A1328	G1163	U1236	U1041	U1041	G1164	U1041	G948	U823	G730	A630	A519	C418	A317	A119	A119
G1546	U1418	U1237	U1237	U1042	U1042	G1165	U1042	U949	U824	U731	A631	A520	A419	U318	A120	A120
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G1552	U1422	G1239	G1239	G1045	G1045	G1167	G1045	G953	U831	C735	G636	U522	G426	U325	A226	A226
G1555	C1342	A1242	A1242	C1168	C1168	G1168	C1168	G958	G834	A736	A639	C523	C427	G326	G237	U125
A1559	C1343	U1243	U1243	U1169	U1169	G1169	U1169	C959	U835	A737	A640	C524	C440	A329	A241	C
U1561	G1344	C1245	C1245	A1171	A1171	G1171	A1057	G960	U840	G738	U640	C530	A441	G333	A242	U
C1562	U1440	A1246	A1246	G1172	G1172	A1172	A1058	A961	A841	C741	G644	C531	A442	U335	A243	A129
G1565	U1350	U1249	U1249	A1173	A1173	G1173	G1059	C962	U855	G744	U645	C532	U445	G336	C244	C130
C1566	G1351	C1250	C1250	A1174	A1174	G1174	C1060	G969	G856	G745	G656	C533	G446	A337	A248	C136
G1567	A1352	G1251	G1251	C1176	C1176	G1176	A1067	U970	A857	A746	G657	C534	A447	C338	G249	U137
C1573	G1353	U1252	U1252	A1177	A1177	G1177	U1066	G	U858	G747	U664	C535	G448	A339	U138	U138
C1574	A1355	C1253	C1253	U1180	U1180	G1180	A1067	U	C959	A750	G661	C536	A449	A340	C251	C139
G1588	A1356	G1260	G1260	A1181	A1181	G1181	G1072	G	U860	G757	U662	C537	C450	C341	G140	G140
G1589	C1357	U1266	U1266	C1182	C1182	G1182	A1073	C	A861	C757	U663	C538	C451	C342	C141	C141
U1595	C1358	C1267	C1267	C1183	C1183	G1183	G1074	C	U867	A758	U664	C539	C452	C343	A148	A148
G1596	C1359	U1276	U1276	U1185	U1185	G1185	A1078	G	G868	C759	U665	C540	G458	C344	G257	G257
A1597	A1372	C1277	C1277	C1186	C1186	G1186	C1080	C	G870	G764	U666	C541	A459	A347	G259	A151
A1598	A1375	U1278	U1278	U1187	U1187	G1187	A1081	C	G871	G765	U667	C542	A460	G358	G264	A152
A1603	G1376	A1287	A1287	A1188	A1188	G1188	C1081	U	U872	A766	U668	C543	C461	U359	U285	C153
G1604	C1377	U1288	U1288	C1189	C1189	G1189	A1086	C	A875	G767	U669	C544	A462	G360	G269	C155
G1605	G1378	C1289	C1289	U1190	U1190	G1190	G1087	G	G876	A767	U670	C545	A463	A360	U270	G156
A1606	A1379	G1290	G1290	A1191	A1191	G1191	A1088	A	G877	C770	U671	C546	G464	C361	C271	G157
A1607	U1380	U1291	U1291	U1192	U1192	G1192	A1088	G	G878	G771	U672	C547	A466	U364	A272	A158
A1615	C1384	U1292	U1292	A1193	A1193	G1193	A1097	C	G879	G772	U681	C548	C467	G365	G273	G159
A1616	G1385	G1293	G1293	C1194	C1194	G1194	A1098	G	C879	A773	U686	C549	U470	C368	G274	G164
C1617	G1386	A1294	A1294	G1195	G1195	G1195	G1099	A	C880	C774	A687	C550	G471	G369	A278	A165
A1625	U1298	U1298	U1298	C1196	C1196	G1196	A1116	C	C881	G775	U688	C551	A486	U371	C282	U177
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U1627	U1304	U1304	U1304	U1198	U1198	G1198	C1104	U	U883	U777	U690	C553	G488	U372	C284	A285
A1630	C1394	U1502	U1502	A1199	A1199	G1199	A1118	A	G884	C778	U691	C554	C494	G381	U286	G185
A1631	C1395	U1503	U1503	U1200	U1200	G1200	G1119	C999	A907	A796	U692	C555	A495	U382	A186	A186
A1632	C1396	U1504	U1504	U1201	U1201	G1201	U1120	A	G902	A797	U693	C556	C496	U391	A187	C188
A1633	C1397	U1505	U1505	U1202	U1202	G1202	U1121	A1006	U903	A806	U701	C557	A497	U392	G292	A189
A1634	C1398	U1506	U1506	U1203	U1203	G1203	U1122	A1007	U904	A807	G702	C558	G498	U393	G293	A190
A1635	C1399	U1507	U1507	U1204	U1204	G1204	U1123	A1008	C905	A808	U702	C559	G499	U394	G294	A191
A1636	C1400	U1508	U1508	U1205	U1205	G1205	U1124	A1009	C906	A809	U703	C560	G500	U395	G295	A192
A1637	C1401	U1509	U1509	U1206	U1206	G1206	U1125	A1010	A907	A810	U704	C561	G501	U396	G296	A193
A1638	C1402	U1510	U1510	U1207	U1207	G1207	U1126	A1011	A912	A811	U705	C562	G502	U397	G297	A194
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A1641	C1405	U1513	U1513	U1210	U1210	G1210	U1129	A1014	C922	A814	U708	C565	G505	U400	G300	A197
A1642	C1406	U1514	U1514	U1211	U1211	G1211	U1130	A1015	C923	A815	U709	C566	G506	U401	G301	A198
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A1649	C1413	U1521	U1521	U1218	U1218	G1218	U1137	A1022	C930	A822	U716	C573	G513	U408	G308	A205
A1650	C1414	U1522	U1522	U1219	U1219	G1219	U1138	A1023	C931	A823	U717	C574	G514	U409	G309	A206
A1651	C1415	U1523	U1523	U1220	U1220	G1220	U1139	A1024	C932	A824	U718	C575	G515	U410	G310	A207
A1652	C1416	U1524	U1524	U1221	U1221	G1221	U1140	A1025	C933	A825	U719	C576	G516	U411	G311	A208
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A1654	C1418	U1526	U1526	U1223	U1223	G1223	U1142	A1027	C935	A827	U721	C578	G518	U413	G313	A210
A1655	C1419	U1527	U1527	U1224	U1224	G1224	U1143	A1028	C936	A828	U722	C579	G519	U414	G314	A211
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A1663	C1427	U1535	U1535	U1232	U1232	G1232	U1151	A1036	C944	A836	U730	C587	G527	U422	G322	A219
A1664	C1428	U1536	U1536	U1233	U1233	G1233	U1152	A1037	C945	A837	U731	C588	G528	U423	G323	A220
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A1667	C1431	U1539	U1539	U1236	U1236	G1236	U1155	A1040	C948	A840	U734	C591	G531	U426	G326	A223
A1668	C1432	U1540	U1540	U1237	U1237	G1237	U1156	A1041	C949	A841	U735	C592	G532	U427	G327	A224
A1669																

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U2889	U2796	G2896	A2599	A2513	G2421	G2323	C	U	A2101	A2007	G1926	U1817	G1730	A1632
A2890	A2799	G2897	A2600	G2514	U2422	U2324	U	A	G2102	U2008	A1927	C1818	C1731	C1633
C2894	A2800	G2898	A2601	C2515	C2423	U2325	G	C	U2103	G2009	A1930	U1819	A1732	C1634
C2895	G2806	A2899	G2602	A2517	U2424	C2326	C	A	A2104	A2010	A1931	G1820	A1733	U1635
A2896	U2807	G2904	G2603	C2518	G2425	G2327	G	A	C2105	A2011	G1932	U1829	A1734	A1637
G2897	G2807	U2705	G2604	C2519	G2426	A2328	A	A	C2106	U2012	C1936	A1829	A1735	
G2898	G2808	G2712	U2607	A2521	C2427	C2329	U	G	G2110	G2013	U1936	A1830	A1736	
C2903	A2811	G2713	C2608	G2524	U2428	U2330	G	U	G2111	U2016	C1937	A1831	A1737	A1641
A2906	A2812	G2714	G2525	G2526	A2429	G2338	A	U	C2114	U2017	U1939	U1832	C1738	A1642
C2907	A2813	G2715	G2527	U2528	C2432	A	C	C	A2115	A2018	C1940	C1834	G1739	
A2908	G2814	G2716	A2611	C2529	A2433	C	A	C	U2116	A2019	A1941	U1835	U1740	G1649
G2909	G2815	G2717	A2612	U2531	A2434	A	G	C	C2119	U2032	A1942	U1836	U1741	
A2910	G2816	G2718	G2613	U2532	U2435	G2344	A	G	C2120	G2033	C1943	U1837	U1742	U1654
	G2817	A2719	C2614	A2533	U2436	A2345	A	C	C2121	U2034	C1944	A1840	A1743	G1655
	A2820	C2720	C2615	U2534	U2437	C2346	C	C	C2122	A2038	G1945	A1841	A1744	G1656
	C2821	U2721	G2616	U2535	C2443	C2347	U	U	G2123	A2039	G1946	A1842	U1745	A1657
	A2822	G2722	G2617	U2536	G2453	C2348	G	A	C2124	U2042	U1950	U1843	A1752	A1658
	C2823	G2723	U2619	C2537	A2456	C2349	C	C	C2125	U2043	G1951	C1853	G1753	A1659
	G2824	U2724	U2620	A2538	U2457	G2350	U	G	A2135	G2044	U	C1854	A1754	A1660
	G2825	G2725	C2626	U2539	A2462	G2351	G	C	A2136	G2045	A	G1855	G1755	C1666
	C2826	C2726	G2627	A2540	A2463	A2352	C	C	A	G2046	A	C1856	C1762	U1668
	A2827	U2727	G2630	U2541	G2464	A2353	U	G	C	C2047	U	C1857	G1763	G1675
	G2828	G2728	U2631	C2542	A2465	A2354	C	C	C	C2048	U	G1858	G1764	U1677
	C2829	U2729	G2632	G2543	G2466	A2355	C	C	C	C2049	U	C1859	C1765	A1678
	G2830	C2730	G2633	U2544	A2467	G2356	U	U	C	G2050	G	G1860	U1766	C1679
	C2831	U2731	U2634	U2545	A2468	A2357	C	C	C	G2051	A	C1861	U1767	C1680
	C2832	G2732	A2637	U2546	C2472	G2358	C	C	C	G2052	C	G1862	U1771	G1681
	G2833	U2733	G2638	U2547	G2473	A2359	C	C	C	G2053	C	U1874	C1772	A1682
	A2834	G2734	U2639	C2548	A2474	A2360	U	U	C	A2054	C	G1875	G1773	G1683
	C2835	U2735	G2640	U2549	A2475	A2361	C	C	C	A2055	C	G1876	G1774	A1684
	G2836	C2736	U2641	U2550	A2476	A2362	C	C	C	G2056	U	G1877	U1964	G1685
	U2837	G2737	A2642	C2551	A2477	A2363	C	C	C	G2057	U	G1878	C1965	A1686
	C2838	U2738	G2643	U2552	A2478	A2364	C	C	C	G2058	U	U1879	U1966	C1687
	A2839	G2739	U2644	U2553	A2479	A2365	C	C	C	U2059	U	C1884	A1778	A1688
	G2840	C2740	A2645	U2554	G2480	A2366	C	C	C	U2060	U	A1885	A1779	C1689
	C2841	U2741	U2646	U2555	A2481	A2367	C	C	C	U2061	U	G1886	U1783	C1690
	A2842	G2742	U2647	U2556	A2482	A2368	C	C	C	U2062	U	U1887	G1785	G1695
	C2843	U2743	G2648	U2557	A2483	A2369	C	C	C	U2063	U	C1888	C1786	U1696
	G2844	C2744	A2649	U2558	U2484	A2370	C	C	C	U2064	U	U1889	G1787	U1697
	U2845	G2745	U2650	U2559	A2485	A2371	C	C	C	U2065	U	C1890	U1788	U1698
	C2846	U2746	C2651	U2560	G2486	U2372	C	C	C	G2066	U	C1891	G1789	C1699
	A2847	G2747	U2652	U2561	A2487	U2373	C	C	C	U2067	U	A1701	C1790	G1700
	C2848	U2748	U2653	U2562	A2488	U2374	C	C	C	U2068	U	G1902	U1791	U1702
	G2849	C2749	A2654	U2563	A2489	U2375	C	C	C	U2069	U	U1903	G1792	A1710
	U2850	G2750	C2655	U2564	G2490	U2376	C	C	C	U2070	U	A1909	C1803	C1714
	C2851	U2751	U2656	U2565	A2491	U2377	C	C	C	G2071	U	C1910	C1715	C1716
	A2852	G2752	U2657	U2566	G2492	U2378	C	C	C	C2072	U	G1911	G1805	A1717
	G2853	U2753	A2658	U2567	U2493	U2379	C	C	C	G2073	U	A1919	G1806	
	C2854	C2754	U2659	U2568	C2494	U2380	C	C	C	A2074	U	C1920	U1722	U1724
	A2855	U2755	A2660	U2569	U2495	U2381	C	C	C	G2075	U	U1921	G1809	
	G2856	G2756	C2661	U2570	C2496	U2382	C	C	C	G2076	U	C1922	C1810	
	U2857	U2757	U2662	U2571	U2497	U2383	C	C	C	G2077	U	A1923	G1723	
	C2858	C2758	A2663	U2572	G2498	U2384	C	C	C	G2078	U	U1924	U1724	
	G2859	U2759	U2664	U2573	C2500	U2385	C	C	C	U2079	U	C1925	U1725	
	A2860	C2760	A	U	G2501	U2386	C	C	C	A2080	U	U1926	G1726	
	C2861	U2761	U2665	U2574	U2502	U2387	C	C	C	G2081	U	C1927	U1727	
	G2862	G2762	U2666	U2575	G2503	U2388	C	C	C	G2082	U	U1928	U1728	
	U2863	C2763	A2667	U2576	A2504	U2389	C	C	C	A2083	U	A1929	G1729	
	C2864	U2764	U2668	U2577	G2505	U2390	C	C	C	C2084	U	C1930	C1803	
	A2865	G2765	U2669	U2578	A2506	U2391	C	C	C	G2085	U	C1931	C1715	
	G2866	U2766	A	U	G2507	U2392	C	C	C	C2086	U	G1932	G1805	
	C2867	C2767	U2670	U2579	U2508	U2393	C	C	C	G2087	U	U1933	G1806	
	U2868	G2768	U2671	U2580	A2509	U2394	C	C	C	C2088	U	C1934	U1729	
	G2869	U2769	U2672	U2581	G2510	U2395	C	C	C	G2089	U	G1935	G1807	
	A2870	C2770	U2673	U2582	U2511	U2396	C	C	C	G2090	U	U1936	G1808	
	C2871	U2771	U2674	U2583		U2397	C	C	C	G2091	U	C1937	U1730	
	G2872	G2772	A2675	U2584		U2398	C	C	C	G2092	U	A1938	G1809	
	U2873	C2773	U2676	U2585		U2399	C	C	C	A2093	U	C1939	C1810	
	A2874	U2774	U2677	U2586		U2400	C	C	C	C2094	U	U1940	G1723	
	C2875	G2775	A2678	U2587		A2401	C	C	C	G2095	U	C1941	U1724	
	G2876	U2776	U2679	U2588		C2402	C	C	C	C2096	U	U1942	U1725	
	U2877	C2777	U2680	U2589		U2403	C	C	C	G2097	U	C1943	U1726	
	C2878	U2778	A2681	U2590		A2404	C	C	C	C2098	U	A1944	G1805	
	A2879	G2779	U2682	U2591		G2405	C	C	C	G2099	U	G1945	G1806	
	C2880	U2780	U2683	U2592		G2406	C	C	C	G2100	U	U1946	U1727	
	G2881	C2781	U2684	U2593		G2407	C	C	C	C2101	U	C1947	U1728	
	A2882	U2782	U2685	U2594		U2408	C	C	C	G2102	U	A1948	G1807	
	C2883	G2783	U2686	U2595		A2409	C	C	C	A2094	U	C1949	U1729	
	G2884	U2784	A2687	U2596		G2410	C	C	C	C2095	U	U1950	C1808	
	U2885	C2785	U2688	U2597		G2411	C	C	C	G2096	U	G1951	G1809	
	A2886	U2786	U2689	U2598		G2412	C	C	C	G2097	U	U1952	U1730	
	C2887	G2787	U2690	U2599		G2413	C	C	C	C2098	U	C1953	C1810	
	U2888	U2788	U2691	U2600		G2414	C	C	C	G2099	U	U1954	G1723	
	G2889	C2789	U2692	U2601		G2415	C	C	C	G2100	U	G1955	U1724	
	A2890	U2790	U2693	U2602		G2416	C	C	C	G2101	U	U1956	U1725	
	C2891	G2791	U2694	U2603		U2417	C	C	C	C2102	U	C1957	U1726	
	G2892	U2792	U2695	U2604		U2418	C	C	C	A2095	U	A1958	U1727	
	A2893	C2793	U2696	U2605		U2419	C	C	C	G2096	U	C1959	G1805	
	C2894	U2794	U2697	U2606		U2420	C	C	C	G2097	U	U1960	G1806	
	G2895	G2795	U2698	U2607		U2421	C	C	C	G2098	U	A1961	U1728	
	A2896	U2796	U2699	U2608		U2422	C	C	C	A2099	U	C1962	C1807	
	C2897	C2797	U2700	U2609		U2423	C	C	C	C2100	U	U1963	G1808	
	G2898	U2798	U2701	U2610		U2424	C	C	C	G2101	U	G1964	U1729	
	A2899	G2799	U2702	U2611		U2425	C	C	C	U2092	U	A1965	U1730	
	C2900	U2800	U2703	U2612		U2426	C	C	C	U2093	U	C1966	C1809	
	G2901	A2801	U2704	U2613		U2427	C	C	C	U2094	U	U1967	G1810	
	A2902	C2802	U2705	U2614		U2428	C	C	C	U2095	U	U1968	U1723	
	C2903	U2803	U2706	U2615		U2429	C	C	C	U2096	U	A1969	G1724	
	G2904	A2804	U2707	U2616		U2430	C	C	C	U2097	U	C1970	U1725	
	A2905	C2805	U2708	U2617		U2431	C	C	C	U2098	U	U1971	C1805	
	C2906	U2806	U2709	U2618		U2432	C	C	C	U2099	U	G1972	G1806	
	G2907	A2807												

- Molecule 31: 5S RIBOSOMAL RNA



- Molecule 32: RNA (5'-R(*CP*CP*A)-3')



- Molecule 33: RNA (5'-R(*CP*CP*(8AN))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.32Å 297.90Å 573.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 2.80 85.22 – 2.39	Depositor EDS
% Data completeness (in resolution range)	91.2 (49.79-2.80) 90.7 (85.22-2.39)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.194 , 0.245 0.184 , 0.236	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99205	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACA, OMG, 8AN, CL, SR, NA, K, MG, CD, OMU, UR3, 1MA, 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	A	0.33	0/1784	0.64	0/2403
2	B	0.35	0/2687	0.66	0/3644
3	C	0.37	0/1883	0.62	0/2547
4	D	0.31	0/1109	0.56	0/1493
5	E	0.33	0/1380	0.61	0/1875
6	F	0.32	0/899	0.56	0/1219
7	G	0.29	0/241	0.47	0/324
8	H	0.34	0/1300	0.64	0/1738
9	I	0.27	0/524	0.50	0/711
10	J	0.36	0/1134	0.60	0/1525
11	K	0.36	0/1002	0.68	0/1346
12	L	0.33	0/1128	0.63	0/1504
13	M	0.36	0/1580	0.60	0/2111
14	N	0.29	0/1472	0.61	0/1994
15	O	0.33	0/872	0.60	0/1176
16	P	0.35	0/1145	0.54	0/1524
17	Q	0.35	0/747	0.67	0/1001
18	R	0.37	0/1170	0.63	0/1574
19	S	0.33	0/646	0.56	0/870
20	T	0.33	0/956	0.62	0/1284
21	U	0.34	0/417	0.60	0/562
22	V	0.28	0/502	0.53	0/675
23	W	0.54	1/1217 (0.1%)	1.06	2/1650 (0.1%)
24	X	0.33	0/662	0.59	0/890
25	Y	0.36	0/1146	0.65	0/1536
26	Z	0.34	0/582	0.59	0/776
27	1	0.40	0/438	0.63	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.38	0/769	0.58	0/1019
30	0	0.39	0/65951	0.69	20/102855 (0.0%)
31	9	0.35	0/2897	0.71	1/4512 (0.0%)
32	5	0.64	0/65	1.28	2/99 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.38	0/40	0.60	0/60
All	All	0.38	1/98746 (0.0%)	0.68	25/147604 (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
30	0	0	47
31	9	0	2
32	5	0	1
All	All	0	50

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	52	VAL	CB-CG2	-14.55	1.22	1.52

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	30.26	159.32	110.90
23	W	52	VAL	CA-CB-CG2	-16.79	85.72	110.90
30	0	1979	G	C2'-C3'-O3'	7.10	125.13	109.50
30	0	1942	A	C5'-C4'-C3'	7.05	127.28	116.00
30	0	2313	C	C5'-C4'-O4'	7.00	117.50	109.10

There are no chirality outliers.

5 of 50 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	148	A	Sidechain
30	0	26	U	Sidechain
30	0	270	U	Sidechain
30	0	396	U	Sidechain
30	0	458	G	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	A	1752	0	1764	129	0
2	B	2624	0	2530	190	0
3	C	1859	0	1811	97	0
4	D	1093	0	1083	96	0
5	E	1356	0	1264	77	0
6	F	889	0	841	63	0
7	G	240	0	231	17	0
8	H	1281	0	1290	63	0
9	I	518	0	495	49	0
10	J	1119	0	1096	74	0
11	K	993	0	1025	57	0
12	L	1117	0	1071	69	0
13	M	1557	0	1571	86	0
14	N	1444	0	1399	101	0
15	O	864	0	868	51	0
16	P	1135	0	1120	46	0
17	Q	734	0	726	29	0
18	R	1148	0	1119	51	0
19	S	640	0	600	30	0
20	T	949	0	922	54	0
21	U	410	0	364	32	0
22	V	499	0	511	41	0
23	W	1195	0	1135	89	0
24	X	653	0	651	34	0
25	Y	1130	0	1133	63	0
26	Z	572	0	529	25	0
27	1	431	0	426	35	0
28	2	396	0	413	27	0
29	3	754	0	727	33	0
30	0	59018	0	29811	1006	0
31	9	2596	0	1324	76	0
32	5	59	0	35	10	0
33	6	59	0	35	1	0
34	0	84	0	0	0	0
34	2	1	0	0	0	0
34	9	1	0	0	0	0
34	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	1	0	0	0	0
34	C	1	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	6	0	0	0	0
35	2	1	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	K	1	0	0	1	0
35	L	2	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	86	0	0	0	0
36	1	2	0	0	0	0
36	3	3	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	2	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
36	T	2	0	0	0	0
36	Y	1	0	0	0	0
37	0	64	0	0	0	0
37	9	1	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	D	1	0	0	0	0
37	J	1	0	0	0	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	2	0	0	0	0
37	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0	0	0	0
40	6	11	0	8	0	0
41	6	8	0	12	0	0
42	0	5771	0	0	145	0
42	1	53	0	0	6	0
42	2	42	0	0	1	0
42	3	66	0	0	6	0
42	5	4	0	0	2	0
42	6	3	0	0	0	0
42	9	148	0	0	10	0
42	A	128	0	0	21	0
42	B	165	0	0	19	0
42	C	170	0	0	14	0
42	D	49	0	0	7	0
42	E	48	0	0	3	0
42	F	31	0	0	4	0
42	G	19	0	0	0	0
42	H	77	0	0	10	0
42	I	11	0	0	1	0
42	J	63	0	0	1	0
42	K	54	0	0	4	0
42	L	92	0	0	10	0
42	M	136	0	0	5	0
42	N	64	0	0	8	0
42	O	43	0	0	5	0
42	P	69	0	0	2	0
42	Q	51	0	0	0	0
42	R	87	0	0	5	0
42	S	33	0	0	4	0
42	T	40	0	0	3	0
42	U	30	0	0	2	0
42	V	16	0	0	4	0
42	W	72	0	0	8	0
42	X	25	0	0	4	0
42	Y	108	0	0	6	0
42	Z	30	0	0	4	0
All	All	99205	0	59940	2631	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 17.

The worst 5 of 2631 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)
3:C:236:THR:HG22	3:C:239:ALA:H	1.02	1.12
31:9:76:G:H3'	31:9:77:A:H5''	1.31	1.12
30:0:871:G:H8	30:0:871:G:H5'	1.20	1.06
14:N:37:ARG:NH1	31:9:6:C:H5''	1.72	1.03
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.41	1.03

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/240 (97%)	197 (84%)	31 (13%)	5 (2%)	7	23
2	B	333/338 (98%)	300 (90%)	29 (9%)	4 (1%)	13	39
3	C	242/246 (98%)	215 (89%)	25 (10%)	2 (1%)	19	49
4	D	132/177 (75%)	98 (74%)	23 (17%)	11 (8%)	1	2
5	E	168/178 (94%)	159 (95%)	9 (5%)	0	100	100
6	F	115/120 (96%)	97 (84%)	13 (11%)	5 (4%)	2	8
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	154/177 (87%)	131 (85%)	21 (14%)	2 (1%)	12	36
9	I	66/162 (41%)	45 (68%)	19 (29%)	2 (3%)	4	15
10	J	138/145 (95%)	126 (91%)	9 (6%)	3 (2%)	6	22
11	K	128/132 (97%)	117 (91%)	9 (7%)	2 (2%)	9	31
12	L	139/165 (84%)	115 (83%)	19 (14%)	5 (4%)	3	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	190/196 (97%)	171 (90%)	17 (9%)	2 (1%)	14	41
14	N	182/187 (97%)	156 (86%)	18 (10%)	8 (4%)	2	8
15	O	111/116 (96%)	103 (93%)	8 (7%)	0	100	100
16	P	139/149 (93%)	133 (96%)	6 (4%)	0	100	100
17	Q	91/96 (95%)	82 (90%)	8 (9%)	1 (1%)	14	41
18	R	146/155 (94%)	132 (90%)	13 (9%)	1 (1%)	22	53
19	S	77/85 (91%)	73 (95%)	4 (5%)	0	100	100
20	T	115/120 (96%)	109 (95%)	4 (4%)	2 (2%)	9	29
21	U	51/67 (76%)	46 (90%)	4 (8%)	1 (2%)	7	24
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	9	31
23	W	150/154 (97%)	140 (93%)	9 (6%)	1 (1%)	22	53
24	X	78/92 (85%)	70 (90%)	7 (9%)	1 (1%)	12	36
25	Y	140/240 (58%)	135 (96%)	5 (4%)	0	100	100
26	Z	69/116 (60%)	60 (87%)	6 (9%)	3 (4%)	2	8
27	1	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
28	2	42/50 (84%)	36 (86%)	6 (14%)	0	100	100
29	3	88/92 (96%)	83 (94%)	4 (4%)	1 (1%)	14	41
All	All	3659/4471 (82%)	3256 (89%)	340 (9%)	63 (2%)	9	29

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL
4	D	27	ILE
4	D	171	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	168 (94%)	10 (6%)	21	51
2	B	281/283 (99%)	271 (96%)	10 (4%)	35	69
3	C	192/193 (100%)	176 (92%)	16 (8%)	11	32
4	D	116/148 (78%)	111 (96%)	5 (4%)	29	62
5	E	151/156 (97%)	147 (97%)	4 (3%)	46	79
6	F	92/94 (98%)	91 (99%)	1 (1%)	73	92
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	133/145 (92%)	129 (97%)	4 (3%)	41	75
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	87
10	J	117/121 (97%)	108 (92%)	9 (8%)	13	35
11	K	105/106 (99%)	103 (98%)	2 (2%)	57	85
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
13	M	157/160 (98%)	150 (96%)	7 (4%)	27	60
14	N	148/150 (99%)	144 (97%)	4 (3%)	44	78
15	O	93/94 (99%)	91 (98%)	2 (2%)	52	83
16	P	113/117 (97%)	110 (97%)	3 (3%)	44	78
17	Q	79/80 (99%)	77 (98%)	2 (2%)	47	80
18	R	117/122 (96%)	111 (95%)	6 (5%)	24	55
19	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
20	T	104/106 (98%)	100 (96%)	4 (4%)	33	67
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	60
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	22	53
24	X	65/74 (88%)	58 (89%)	7 (11%)	6	19
25	Y	120/195 (62%)	111 (92%)	9 (8%)	13	37
26	Z	59/94 (63%)	58 (98%)	1 (2%)	60	87
27	1	46/47 (98%)	45 (98%)	1 (2%)	52	83
28	2	42/46 (91%)	40 (95%)	2 (5%)	25	58
29	3	78/79 (99%)	73 (94%)	5 (6%)	17	45
All	All	3079/3645 (84%)	2946 (96%)	133 (4%)	29	62

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	131	THR
13	M	116	ASN
25	Y	231	PRO
11	K	7	ASP
12	L	140	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	66	GLN
27	1	28	HIS
13	M	129	HIS
14	N	40	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	248 (9%)	30 (1%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
32	5	2/3 (66%)	1 (50%)	0
33	6	1/3 (33%)	0	0
All	All	2869/3051 (94%)	265 (9%)	31 (1%)

5 of 265 RNA backbone outliers are listed below:

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

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1685	A
30	0	1942	A
30	0	2791	U
30	0	1692	C
30	0	1979	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
30	OMU	0	2587	30	14,22,23	0.96	1 (7%)	14,31,34	1.18	1 (7%)
30	UR3	0	2619	30	14,22,23	0.89	1 (7%)	15,32,35	0.76	0
30	PSU	0	2621	30	17,21,22	1.67	3 (17%)	20,30,33	5.43	4 (20%)
33	8AN	6	76	33	19,24,25	1.15	1 (5%)	13,35,38	1.79	3 (23%)
30	1MA	0	628	30	15,25,26	0.78	0	15,37,40	1.44	1 (6%)
30	OMG	0	2588	32,30	18,26,27	1.03	2 (11%)	20,38,41	2.59	5 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
33	8AN	6	76	33	-	3/3/25/26	0/3/3/3
30	1MA	0	628	30	-	0/3/25/26	0/3/3/3
30	OMG	0	2588	32,30	-	0/5/27/28	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.92	1.48	1.52
30	0	2588	OMG	C6-N1	3.29	1.38	1.33
30	0	2621	PSU	C4-N3	3.06	1.38	1.33
30	0	2621	PSU	C2-N1	3.04	1.44	1.38
33	6	76	8AN	C3'-N3'	-2.63	1.43	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.58	114.45	128.43
30	0	2621	PSU	C4-N3-C2	13.94	126.92	115.14
30	0	2588	OMG	C5-C6-N1	-8.75	111.46	123.43
30	0	2621	PSU	C5-C4-N3	-7.90	115.18	125.36
30	0	2588	OMG	C6-N1-C2	5.77	125.10	115.93

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	6	76	8AN	O4'-C4'-C5'-O5'
33	6	76	8AN	C4'-C5'-O5'-P
33	6	76	8AN	C3'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2619	UR3	1	0
33	6	76	8AN	1	0
30	0	2588	OMG	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 304 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
41	ACA	6	78	-	7,7,8	1.80	2 (28%)	6,6,8	0.78	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
41	ACA	6	78	-	-	1/4/5/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	78	ACA	C3-C2	-3.83	1.37	1.52
41	6	78	ACA	O1-C1	2.00	1.31	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
41	6	78	ACA	C2-C3-C4-C5

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, 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	A	237/240 (98%)	-0.52	6 (2%) 57 47	22, 45, 81, 106	0
2	B	337/338 (99%)	-0.75	0 100 100	20, 45, 72, 88	0
3	C	246/246 (100%)	-0.63	0 100 100	17, 41, 65, 82	0
4	D	140/177 (79%)	0.81	23 (16%) 1 1	54, 93, 129, 137	0
5	E	172/178 (96%)	-0.47	2 (1%) 79 73	38, 60, 81, 91	0
6	F	119/120 (99%)	0.28	4 (3%) 45 35	41, 70, 106, 115	0
7	G	29/348 (8%)	0.78	4 (13%) 2 1	66, 93, 107, 109	0
8	H	160/177 (90%)	-0.28	1 (0%) 89 86	34, 56, 93, 104	0
9	I	70/162 (43%)	3.97	57 (81%) 0 0	143, 158, 174, 175	0
10	J	142/145 (97%)	-0.71	0 100 100	28, 44, 63, 81	0
11	K	132/132 (100%)	-0.83	0 100 100	25, 39, 60, 72	0
12	L	145/165 (87%)	0.02	5 (3%) 45 35	20, 61, 109, 127	0
13	M	194/196 (98%)	-0.69	1 (0%) 91 88	24, 40, 63, 74	0
14	N	186/187 (99%)	-0.23	6 (3%) 47 37	37, 60, 119, 126	0
15	O	115/116 (99%)	-0.51	0 100 100	33, 53, 68, 74	0
16	P	143/149 (95%)	-0.75	0 100 100	30, 45, 58, 67	0
17	Q	95/96 (98%)	-0.64	0 100 100	30, 42, 60, 74	0
18	R	150/155 (96%)	-0.72	0 100 100	23, 37, 59, 70	0
19	S	81/85 (95%)	-0.28	1 (1%) 79 73	37, 53, 74, 95	0
20	T	119/120 (99%)	-0.33	4 (3%) 45 35	36, 51, 80, 121	0
21	U	53/67 (79%)	-0.45	1 (1%) 66 59	32, 47, 71, 81	0
22	V	65/71 (91%)	0.99	7 (10%) 5 3	44, 74, 117, 125	0
23	W	154/154 (100%)	-0.70	0 100 100	30, 45, 66, 80	0
24	X	82/92 (89%)	-0.32	5 (6%) 21 13	37, 52, 83, 106	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/240 (59%)	-0.73	0 100 100	18, 39, 62, 85	0
26	Z	73/116 (62%)	0.55	10 (13%) 3 1	44, 82, 99, 108	0
27	1	56/57 (98%)	-0.81	0 100 100	21, 28, 36, 43	0
28	2	46/50 (92%)	-0.45	2 (4%) 35 25	30, 52, 68, 86	0
29	3	92/92 (100%)	-0.42	2 (2%) 62 52	34, 53, 71, 80	0
30	0	2749/2923 (94%)	-0.70	31 (1%) 80 75	17, 40, 89, 186	0
31	9	122/122 (100%)	-0.74	4 (3%) 46 36	33, 61, 86, 151	0
32	5	3/3 (100%)	1.88	1 (33%) 0 0	81, 81, 83, 86	0
33	6	2/3 (66%)	0.85	0 100 100	96, 96, 96, 104	0
All	All	6651/7522 (88%)	-0.49	177 (2%) 54 44	17, 46, 98, 186	0

The worst 5 of 177 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	40	PRO	13.2
9	I	66	GLY	11.4
9	I	74	ILE	9.9
22	V	1	THR	8.5
4	D	57	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, 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
33	8AN	6	76	22/23	0.87	0.28	84,92,94,95	0
30	PSU	0	2621	20/21	0.97	0.14	29,31,38,39	0
30	UR3	0	2619	21/22	0.97	0.14	33,35,40,41	0
30	1MA	0	628	23/24	0.97	0.15	25,28,29,30	0
30	OMG	0	2588	24/25	0.97	0.11	24,29,31,33	0
30	OMU	0	2587	21/22	0.98	0.09	24,28,32,33	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, 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	SR	0	8942	1/1	-0.19	0.23	186,186,186,186	0
34	MG	0	8063	1/1	-0.06	0.42	87,87,87,87	0
36	SR	0	8933	1/1	0.01	0.41	168,168,168,168	0
34	MG	0	8038	1/1	0.08	2.39	112,112,112,112	0
34	MG	0	8090	1/1	0.17	1.00	126,126,126,126	0
37	NA	0	8573	1/1	0.27	0.99	107,107,107,107	0
34	MG	0	8087	1/1	0.28	1.17	106,106,106,106	0
37	NA	0	8560	1/1	0.34	0.62	107,107,107,107	0
36	SR	0	8996	1/1	0.47	0.11	148,148,148,148	0
34	MG	0	8016	1/1	0.48	0.87	98,98,98,98	0
37	NA	0	8547	1/1	0.48	0.40	66,66,66,66	0
37	NA	0	8571	1/1	0.49	0.69	131,131,131,131	0
34	MG	0	8079	1/1	0.50	0.34	64,64,64,64	0
36	SR	0	9007	1/1	0.51	0.72	200,200,200,200	0
36	SR	0	8920	1/1	0.52	0.70	200,200,200,200	0
37	NA	0	8567	1/1	0.52	0.44	75,75,75,75	0
39	K	0	8402	1/1	0.52	0.22	81,81,81,81	0
36	SR	0	9006	1/1	0.55	0.57	199,199,199,199	0
36	SR	0	8959	1/1	0.60	0.06	131,131,131,131	0
40	PHE	6	77	11/12	0.62	0.45	72,73,77,80	0
36	SR	0	8969	1/1	0.63	0.20	154,154,154,154	0
36	SR	B	8987	1/1	0.65	0.42	200,200,200,200	0
37	NA	0	8525	1/1	0.65	0.32	63,63,63,63	0
34	MG	0	8065	1/1	0.66	0.41	84,84,84,84	0
37	NA	Q	8540	1/1	0.66	0.10	48,48,48,48	0
37	NA	0	8559	1/1	0.66	0.36	75,75,75,75	0
37	NA	0	8506	1/1	0.67	0.20	65,65,65,65	0
35	CL	3	8804	1/1	0.67	0.09	88,88,88,88	0
34	MG	0	8030	1/1	0.69	0.15	188,188,188,188	0
34	MG	T	8057	1/1	0.69	0.13	65,65,65,65	0
37	NA	0	8522	1/1	0.70	0.15	64,64,64,64	0
34	MG	0	8078	1/1	0.71	0.88	104,104,104,104	0
36	SR	0	8976	1/1	0.72	0.22	124,124,124,124	0
34	MG	0	8046	1/1	0.72	0.82	99,99,99,99	0
36	SR	0	8998	1/1	0.73	0.20	159,159,159,159	0
34	MG	0	8085	1/1	0.73	0.34	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	NA	0	8546	1/1	0.74	0.25	79,79,79,79	0
37	NA	0	8541	1/1	0.74	0.39	80,80,80,80	0
37	NA	9	8572	1/1	0.75	0.09	85,85,85,85	0
41	ACA	6	78	8/9	0.75	0.37	74,74,81,82	0
34	MG	0	8050	1/1	0.76	0.58	162,162,162,162	0
34	MG	0	8005	1/1	0.76	0.33	30,30,30,30	0
36	SR	0	9001	1/1	0.77	0.09	155,155,155,155	0
34	MG	0	8047	1/1	0.77	0.88	89,89,89,89	0
37	NA	0	8507	1/1	0.77	0.37	88,88,88,88	0
37	NA	0	8509	1/1	0.79	0.41	83,83,83,83	0
37	NA	0	8511	1/1	0.79	0.19	48,48,48,48	0
34	MG	0	8092	1/1	0.80	0.12	48,48,48,48	0
37	NA	0	8519	1/1	0.80	0.54	53,53,53,53	0
34	MG	0	8037	1/1	0.80	0.14	70,70,70,70	0
37	NA	0	8564	1/1	0.80	0.08	68,68,68,68	0
34	MG	0	8053	1/1	0.80	0.11	54,54,54,54	0
36	SR	S	8961	1/1	0.80	0.08	189,189,189,189	0
36	SR	A	8929	1/1	0.81	0.06	105,105,105,105	0
37	NA	0	8516	1/1	0.81	0.19	42,42,42,42	0
36	SR	0	8974	1/1	0.81	0.19	110,110,110,110	0
39	K	0	8401	1/1	0.81	0.24	66,66,66,66	0
34	MG	0	8059	1/1	0.81	0.13	58,58,58,58	0
37	NA	0	8536	1/1	0.82	0.15	69,69,69,69	0
37	NA	0	8569	1/1	0.82	0.21	44,44,44,44	0
37	NA	0	8565	1/1	0.82	0.32	59,59,59,59	0
34	MG	0	8048	1/1	0.82	0.16	43,43,43,43	0
37	NA	0	8557	1/1	0.83	0.10	57,57,57,57	0
37	NA	0	8542	1/1	0.83	0.22	38,38,38,38	0
37	NA	0	8535	1/1	0.83	0.39	64,64,64,64	0
34	MG	0	8056	1/1	0.83	0.17	69,69,69,69	0
34	MG	0	8081	1/1	0.83	0.52	103,103,103,103	0
37	NA	M	8539	1/1	0.83	0.11	33,33,33,33	0
34	MG	0	8069	1/1	0.83	0.25	88,88,88,88	0
37	NA	0	8555	1/1	0.83	0.72	64,64,64,64	0
34	MG	0	8040	1/1	0.84	0.20	75,75,75,75	0
37	NA	0	8556	1/1	0.84	0.17	39,39,39,39	0
37	NA	0	8566	1/1	0.84	0.24	39,39,39,39	0
37	NA	D	8543	1/1	0.84	0.07	60,60,60,60	0
37	NA	0	8549	1/1	0.84	0.34	61,61,61,61	0
34	MG	0	8089	1/1	0.84	0.15	35,35,35,35	0
37	NA	J	8538	1/1	0.84	0.21	31,31,31,31	0
34	MG	0	8082	1/1	0.85	0.31	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8076	1/1	0.85	0.52	81,81,81,81	0
34	MG	B	8042	1/1	0.85	0.11	92,92,92,92	0
37	NA	0	8508	1/1	0.85	0.12	31,31,31,31	0
37	NA	B	8552	1/1	0.85	0.45	69,69,69,69	0
34	MG	0	8024	1/1	0.85	0.25	80,80,80,80	0
37	NA	0	8504	1/1	0.85	0.20	20,20,20,20	0
34	MG	0	8064	1/1	0.85	0.18	51,51,51,51	0
34	MG	0	8091	1/1	0.85	0.10	59,59,59,59	0
34	MG	0	8062	1/1	0.86	0.60	76,76,76,76	0
34	MG	A	8051	1/1	0.86	0.39	58,58,58,58	0
34	MG	0	8033	1/1	0.86	0.09	59,59,59,59	0
36	SR	0	8951	1/1	0.86	0.09	107,107,107,107	0
36	SR	0	8955	1/1	0.86	0.09	115,115,115,115	0
36	SR	0	8994	1/1	0.86	0.53	200,200,200,200	0
37	NA	0	8528	1/1	0.86	0.10	42,42,42,42	0
37	NA	0	8518	1/1	0.86	0.21	68,68,68,68	0
34	MG	0	8010	1/1	0.87	0.34	103,103,103,103	0
36	SR	0	8944	1/1	0.87	0.13	113,113,113,113	0
36	SR	0	9000	1/1	0.88	0.18	137,137,137,137	0
37	NA	0	8531	1/1	0.88	0.21	37,37,37,37	0
34	MG	0	8023	1/1	0.88	0.14	21,21,21,21	0
37	NA	0	8521	1/1	0.88	0.39	61,61,61,61	0
37	NA	0	8558	1/1	0.88	0.65	56,56,56,56	0
34	MG	0	8049	1/1	0.88	0.55	141,141,141,141	0
36	SR	9	8980	1/1	0.89	0.05	155,155,155,155	0
34	MG	0	8001	1/1	0.89	0.24	22,22,22,22	0
37	NA	0	8551	1/1	0.89	0.28	53,53,53,53	0
36	SR	9	8968	1/1	0.89	0.09	105,105,105,105	0
35	CL	0	8813	1/1	0.90	0.08	53,53,53,53	0
37	NA	S	8510	1/1	0.90	0.15	58,58,58,58	0
37	NA	0	8517	1/1	0.90	0.41	40,40,40,40	0
37	NA	0	8530	1/1	0.90	0.23	38,38,38,38	0
34	MG	0	8075	1/1	0.90	0.08	35,35,35,35	0
34	MG	0	8039	1/1	0.91	0.22	32,32,32,32	0
36	SR	9	9003	1/1	0.91	0.06	127,127,127,127	0
34	MG	0	8077	1/1	0.91	0.09	37,37,37,37	0
37	NA	0	8505	1/1	0.91	0.40	29,29,29,29	0
37	NA	0	8570	1/1	0.91	0.15	53,53,53,53	0
34	MG	0	8002	1/1	0.91	0.42	62,62,62,62	0
37	NA	0	8523	1/1	0.91	0.19	49,49,49,49	0
36	SR	0	8971	1/1	0.91	0.07	157,157,157,157	0
34	MG	0	8027	1/1	0.91	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8988	1/1	0.91	0.06	110,110,110,110	0
37	NA	0	8515	1/1	0.91	0.15	20,20,20,20	0
36	SR	0	8993	1/1	0.91	0.05	126,126,126,126	0
37	NA	0	8520	1/1	0.92	0.17	43,43,43,43	0
34	MG	0	8032	1/1	0.92	0.07	44,44,44,44	0
36	SR	0	8919	1/1	0.92	0.12	82,82,82,82	0
34	MG	0	8029	1/1	0.92	0.27	87,87,87,87	0
37	NA	0	8545	1/1	0.92	0.15	40,40,40,40	0
37	NA	0	8501	1/1	0.92	0.32	100,100,100,100	0
34	MG	0	8021	1/1	0.92	0.07	24,24,24,24	0
36	SR	H	8972	1/1	0.92	0.11	119,119,119,119	0
37	NA	0	8514	1/1	0.92	0.40	53,53,53,53	0
36	SR	0	8995	1/1	0.92	0.15	86,86,86,86	0
36	SR	0	8983	1/1	0.92	0.23	195,195,195,195	0
36	SR	Y	9002	1/1	0.93	0.11	118,118,118,118	0
37	NA	0	8575	1/1	0.93	0.15	59,59,59,59	0
34	MG	0	8067	1/1	0.93	0.29	48,48,48,48	0
36	SR	0	8982	1/1	0.93	0.12	105,105,105,105	0
36	SR	0	8986	1/1	0.93	0.12	114,114,114,114	0
36	SR	0	8956	1/1	0.93	0.12	105,105,105,105	0
34	MG	0	8080	1/1	0.93	0.16	62,62,62,62	0
36	SR	0	9004	1/1	0.93	0.16	107,107,107,107	0
35	CL	J	8821	1/1	0.93	0.17	61,61,61,61	0
34	MG	0	8073	1/1	0.93	0.09	62,62,62,62	0
36	SR	0	8957	1/1	0.93	0.12	122,122,122,122	0
34	MG	0	8017	1/1	0.93	0.66	80,80,80,80	0
37	NA	0	8527	1/1	0.94	0.20	40,40,40,40	0
34	MG	0	8008	1/1	0.94	0.12	13,13,13,13	0
36	SR	0	8916	1/1	0.94	0.13	65,65,65,65	0
36	SR	0	8975	1/1	0.94	0.04	115,115,115,115	0
37	NA	0	8554	1/1	0.94	0.46	53,53,53,53	0
34	MG	0	8004	1/1	0.94	0.21	13,13,13,13	0
37	NA	R	8533	1/1	0.94	0.14	42,42,42,42	0
37	NA	0	8512	1/1	0.94	0.43	43,43,43,43	0
34	MG	0	8013	1/1	0.94	0.04	28,28,28,28	0
34	MG	0	8044	1/1	0.94	0.08	47,47,47,47	0
37	NA	0	8550	1/1	0.94	0.20	43,43,43,43	0
34	MG	0	8036	1/1	0.94	0.15	47,47,47,47	0
34	MG	0	8068	1/1	0.94	0.24	74,74,74,74	0
36	SR	F	9005	1/1	0.94	0.12	85,85,85,85	0
34	MG	Y	8086	1/1	0.94	0.19	46,46,46,46	0
37	NA	0	8562	1/1	0.94	0.46	61,61,61,61	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	0.94	0.18	94,94,94,94	0
35	CL	O	8808	1/1	0.94	0.10	63,63,63,63	0
36	SR	0	8966	1/1	0.94	0.13	86,86,86,86	0
37	NA	0	8544	1/1	0.94	0.34	67,67,67,67	0
36	SR	0	8967	1/1	0.95	0.11	92,92,92,92	0
35	CL	Q	8811	1/1	0.95	0.06	68,68,68,68	0
35	CL	0	8822	1/1	0.95	0.15	53,53,53,53	0
35	CL	A	8809	1/1	0.95	0.07	57,57,57,57	0
36	SR	0	8941	1/1	0.95	0.14	71,71,71,71	0
36	SR	0	8928	1/1	0.95	0.08	87,87,87,87	0
34	MG	0	8014	1/1	0.95	0.21	9,9,9,9	0
34	MG	0	8043	1/1	0.95	0.15	37,37,37,37	0
36	SR	0	8936	1/1	0.95	0.16	59,59,59,59	0
36	SR	0	8985	1/1	0.95	0.07	116,116,116,116	0
35	CL	N	8807	1/1	0.95	0.06	62,62,62,62	0
36	SR	0	8962	1/1	0.95	0.09	96,96,96,96	0
35	CL	J	8801	1/1	0.95	0.10	58,58,58,58	0
34	MG	0	8055	1/1	0.95	0.29	30,30,30,30	0
36	SR	B	8950	1/1	0.95	0.17	89,89,89,89	0
37	NA	0	8524	1/1	0.95	0.09	37,37,37,37	0
37	NA	0	8502	1/1	0.95	0.21	55,55,55,55	0
37	NA	0	8553	1/1	0.95	0.51	100,100,100,100	0
35	CL	0	8805	1/1	0.96	0.07	46,46,46,46	0
36	SR	0	9008	1/1	0.96	0.14	80,80,80,80	0
37	NA	0	8563	1/1	0.96	0.24	55,55,55,55	0
35	CL	J	8802	1/1	0.96	0.06	66,66,66,66	0
34	MG	0	8066	1/1	0.96	0.24	32,32,32,32	0
37	NA	L	8568	1/1	0.96	0.18	30,30,30,30	0
34	MG	0	8041	1/1	0.96	0.26	31,31,31,31	0
35	CL	L	8814	1/1	0.96	0.07	49,49,49,49	0
37	NA	0	8537	1/1	0.96	0.04	22,22,22,22	0
36	SR	0	8938	1/1	0.96	0.07	101,101,101,101	0
37	NA	0	8529	1/1	0.96	0.04	20,20,20,20	0
36	SR	0	8923	1/1	0.96	0.17	66,66,66,66	0
35	CL	Y	8820	1/1	0.96	0.05	35,35,35,35	0
36	SR	A	8977	1/1	0.96	0.10	95,95,95,95	0
34	MG	0	8007	1/1	0.96	0.12	37,37,37,37	0
34	MG	0	8083	1/1	0.96	0.09	36,36,36,36	0
34	MG	0	8071	1/1	0.96	0.49	98,98,98,98	0
36	SR	0	8917	1/1	0.96	0.17	61,61,61,61	0
36	SR	0	8960	1/1	0.96	0.08	98,98,98,98	0
36	SR	0	8984	1/1	0.96	0.10	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8031	1/1	0.96	0.12	48,48,48,48	0
36	SR	0	8997	1/1	0.96	0.05	116,116,116,116	0
34	MG	0	8052	1/1	0.96	0.07	37,37,37,37	0
34	MG	0	8093	1/1	0.97	0.12	25,25,25,25	0
38	CD	O	8705	1/1	0.97	0.03	103,103,103,103	0
36	SR	0	8922	1/1	0.97	0.14	62,62,62,62	0
34	MG	C	8012	1/1	0.97	0.22	13,13,13,13	0
37	NA	0	8574	1/1	0.97	0.44	48,48,48,48	0
35	CL	M	8818	1/1	0.97	0.08	33,33,33,33	0
37	NA	0	8513	1/1	0.97	0.15	29,29,29,29	0
37	NA	R	8532	1/1	0.97	0.09	29,29,29,29	0
34	MG	0	8028	1/1	0.97	0.26	1,1,1,1	0
36	SR	0	8965	1/1	0.97	0.11	88,88,88,88	0
36	SR	0	8958	1/1	0.97	0.11	68,68,68,68	0
35	CL	0	8817	1/1	0.97	0.06	42,42,42,42	0
35	CL	2	8803	1/1	0.97	0.07	51,51,51,51	0
36	SR	0	8954	1/1	0.97	0.12	67,67,67,67	0
36	SR	0	8945	1/1	0.97	0.13	89,89,89,89	0
36	SR	0	8943	1/1	0.97	0.13	65,65,65,65	0
37	NA	0	8526	1/1	0.97	0.12	47,47,47,47	0
36	SR	0	8964	1/1	0.97	0.07	92,92,92,92	0
37	NA	0	8534	1/1	0.97	0.69	78,78,78,78	0
36	SR	0	8991	1/1	0.97	0.10	147,147,147,147	0
34	MG	9	8074	1/1	0.97	0.24	53,53,53,53	0
36	SR	0	8906	1/1	0.97	0.17	49,49,49,49	0
36	SR	0	8947	1/1	0.97	0.17	84,84,84,84	0
35	CL	0	8816	1/1	0.98	0.11	60,60,60,60	0
34	MG	0	8011	1/1	0.98	0.20	17,17,17,17	0
37	NA	0	8548	1/1	0.98	0.20	27,27,27,27	0
36	SR	0	8973	1/1	0.98	0.10	91,91,91,91	0
34	MG	0	8018	1/1	0.98	0.26	9,9,9,9	0
36	SR	A	8930	1/1	0.98	0.13	72,72,72,72	0
34	MG	0	8003	1/1	0.98	0.17	18,18,18,18	0
37	NA	C	8503	1/1	0.98	0.23	22,22,22,22	0
36	SR	0	8978	1/1	0.98	0.16	60,60,60,60	0
35	CL	L	8810	1/1	0.98	0.05	52,52,52,52	0
36	SR	1	8952	1/1	0.98	0.15	60,60,60,60	0
34	MG	0	8019	1/1	0.98	0.19	9,9,9,9	0
36	SR	0	8934	1/1	0.98	0.18	67,67,67,67	0
34	MG	0	8084	1/1	0.98	0.11	31,31,31,31	0
36	SR	3	8999	1/1	0.98	0.12	70,70,70,70	0
34	MG	0	8088	1/1	0.98	0.18	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	8015	1/1	0.98	0.18	45,45,45,45	0
34	MG	0	8020	1/1	0.98	0.20	24,24,24,24	0
34	MG	0	8045	1/1	0.98	0.56	147,147,147,147	0
36	SR	0	8946	1/1	0.98	0.17	86,86,86,86	0
36	SR	0	8963	1/1	0.98	0.16	70,70,70,70	0
34	MG	0	8034	1/1	0.98	0.12	31,31,31,31	0
34	MG	0	8006	1/1	0.98	0.15	6,6,6,6	0
37	NA	0	8561	1/1	0.98	0.33	89,89,89,89	0
36	SR	0	8914	1/1	0.98	0.22	75,75,75,75	0
36	SR	0	8935	1/1	0.98	0.11	64,64,64,64	0
36	SR	0	8992	1/1	0.98	0.07	102,102,102,102	0
34	MG	2	8060	1/1	0.98	0.12	42,42,42,42	0
36	SR	0	8903	1/1	0.98	0.16	44,44,44,44	0
34	MG	A	8025	1/1	0.98	0.06	40,40,40,40	0
36	SR	0	8931	1/1	0.98	0.13	74,74,74,74	0
34	MG	0	8070	1/1	0.98	0.22	62,62,62,62	0
36	SR	0	8908	1/1	0.99	0.13	66,66,66,66	0
36	SR	0	8905	1/1	0.99	0.22	49,49,49,49	0
36	SR	0	8937	1/1	0.99	0.19	59,59,59,59	0
36	SR	0	8904	1/1	0.99	0.16	39,39,39,39	0
35	CL	B	8819	1/1	0.99	0.34	56,56,56,56	0
35	CL	K	8812	1/1	0.99	0.06	43,43,43,43	0
36	SR	0	8901	1/1	0.99	0.13	44,44,44,44	0
36	SR	0	8949	1/1	0.99	0.13	49,49,49,49	0
36	SR	0	8924	1/1	0.99	0.18	65,65,65,65	0
36	SR	0	8918	1/1	0.99	0.14	41,41,41,41	0
38	CD	Z	8703	1/1	0.99	0.08	62,62,62,62	0
36	SR	0	8940	1/1	0.99	0.12	53,53,53,53	0
34	MG	0	8061	1/1	0.99	0.20	17,17,17,17	0
36	SR	0	8921	1/1	0.99	0.13	51,51,51,51	0
34	MG	0	8009	1/1	0.99	0.30	1,1,1,1	0
34	MG	K	8054	1/1	0.99	0.17	18,18,18,18	0
36	SR	3	8953	1/1	0.99	0.12	103,103,103,103	0
36	SR	3	8932	1/1	0.99	0.15	68,68,68,68	0
36	SR	0	8902	1/1	0.99	0.17	32,32,32,32	0
36	SR	0	8925	1/1	0.99	0.15	66,66,66,66	0
36	SR	0	8915	1/1	0.99	0.10	73,73,73,73	0
36	SR	R	8912	1/1	0.99	0.18	64,64,64,64	0
36	SR	0	8989	1/1	0.99	0.11	71,71,71,71	0
36	SR	0	8948	1/1	0.99	0.16	57,57,57,57	0
34	MG	0	8058	1/1	0.99	0.20	1,1,1,1	0
34	MG	0	8072	1/1	0.99	0.14	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	R	8806	1/1	0.99	0.08	36,36,36,36	0
36	SR	1	8913	1/1	0.99	0.15	42,42,42,42	0
36	SR	T	8939	1/1	0.99	0.09	70,70,70,70	0
36	SR	0	8970	1/1	0.99	0.05	88,88,88,88	0
36	SR	0	8927	1/1	0.99	0.17	67,67,67,67	0
38	CD	1	8702	1/1	0.99	0.09	50,50,50,50	0
34	MG	0	8026	1/1	0.99	0.14	35,35,35,35	0
36	SR	0	8990	1/1	0.99	0.17	39,39,39,39	0
36	SR	0	8981	1/1	0.99	0.15	107,107,107,107	0
34	MG	0	8022	1/1	0.99	0.19	12,12,12,12	0
36	SR	0	8926	1/1	1.00	0.16	81,81,81,81	0
36	SR	H	8907	1/1	1.00	0.15	41,41,41,41	0
35	CL	0	8815	1/1	1.00	0.06	61,61,61,61	0
36	SR	0	8909	1/1	1.00	0.17	59,59,59,59	0
36	SR	T	8911	1/1	1.00	0.10	52,52,52,52	0
38	CD	3	8704	1/1	1.00	0.09	54,54,54,54	0
38	CD	U	8701	1/1	1.00	0.11	50,50,50,50	0
36	SR	0	8910	1/1	1.00	0.12	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.