



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 04:10 PM EST

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 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

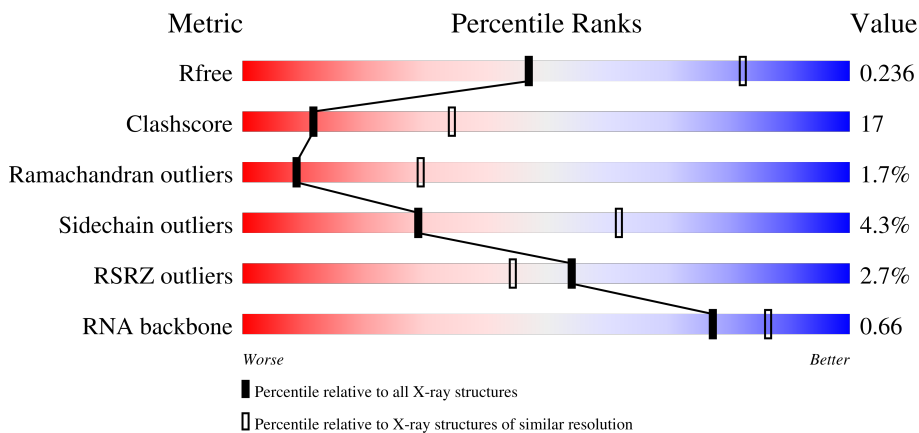
1 Overall quality at a glance i

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.



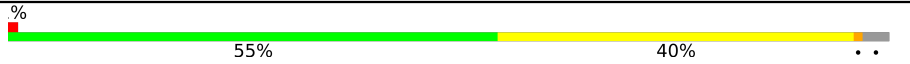

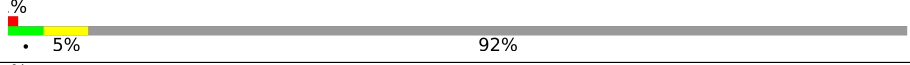

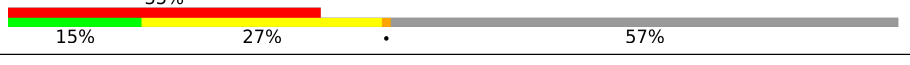
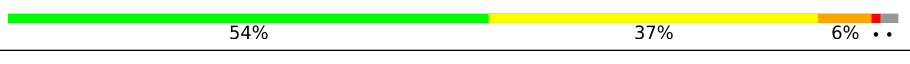
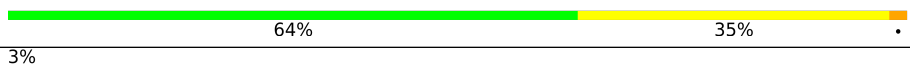
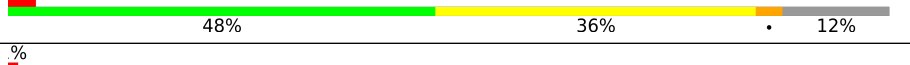
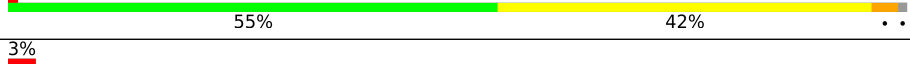


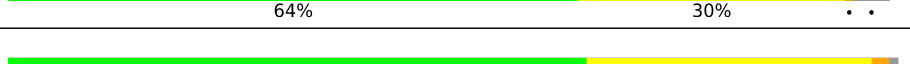
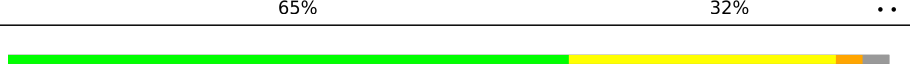


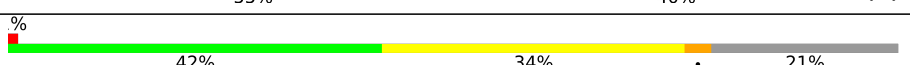
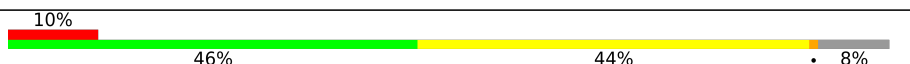
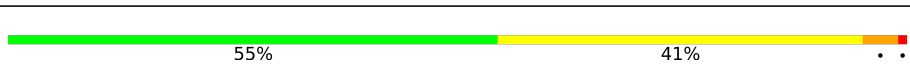
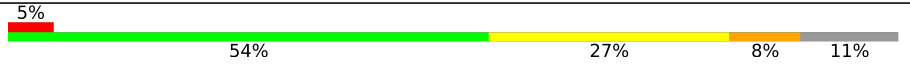
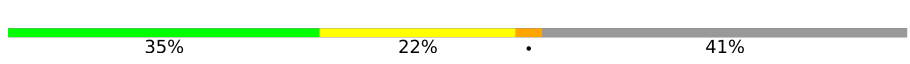
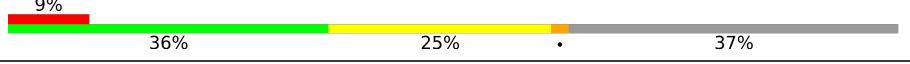
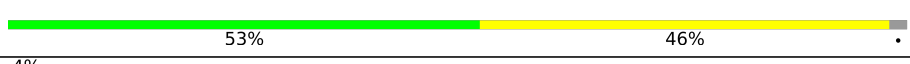



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (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 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	A	240	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 54% 41% ..</p>
2	B	338	<div style="display: flex; align-items: center;"> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 51%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">46% 51% .</p>
3	C	246	<div style="display: flex; align-items: center;"> <div style="width: 62%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">62% 33% 5%</p>
4	D	177	<div style="display: flex; align-items: center;"> <div style="width: 13%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">13% 28% 46% .. 21%</p>

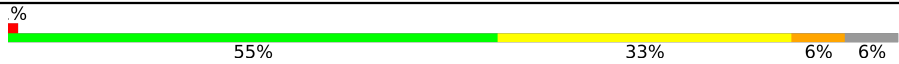

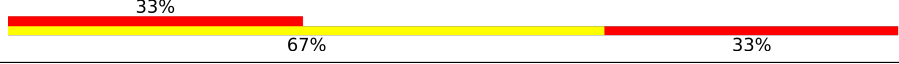
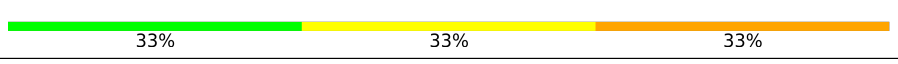
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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	240	
26	Z	116	
27	1	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
			Total	C	N	O	S			
1	A	237	1752	1072	351	324	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	A	2	Total	Mg	0	0
			2	2		
34	B	1	Total	Mg	0	0
			1	1		
34	C	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	K	1	Total Mg 1 1	0	0
34	T	1	Total Mg 1 1	0	0
34	Y	1	Total Mg 1 1	0	0
34	2	1	Total Mg 1 1	0	0
34	0	84	Total Mg 84 84	0	0
34	9	1	Total Mg 1 1	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	6	Total 6	Cl 6	0	0

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

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

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

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	D	1	Total 1	Na 1	0	0
37	J	1	Total 1	Na 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	L	1	Total Na 1 1	0	0
37	M	1	Total Na 1 1	0	0
37	Q	1	Total Na 1 1	0	0
37	R	2	Total Na 2 2	0	0
37	S	1	Total Na 1 1	0	0
37	0	64	Total Na 64 64	0	0
37	9	1	Total Na 1 1	0	0

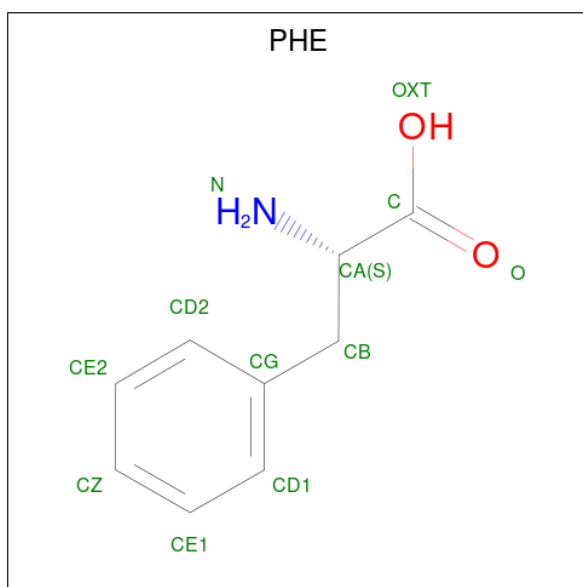
- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

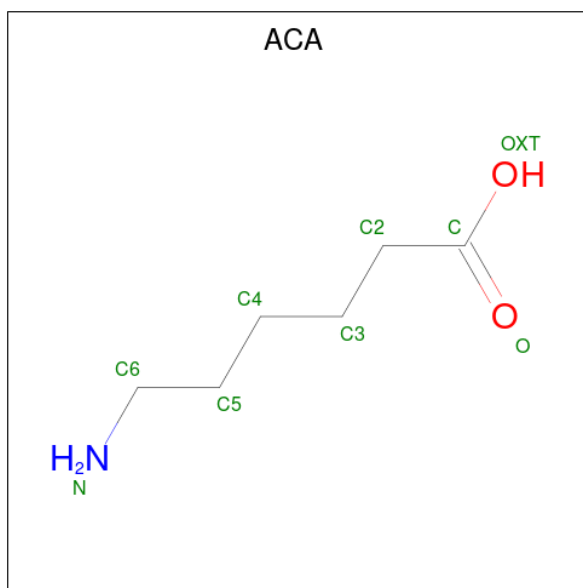
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	2	Total K 2 2	0	0

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



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

- Molecule 41 is 6-AMINOHEXANOIC ACID (three-letter code: ACA) (formula: C₆H₁₃NO₂).



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

- 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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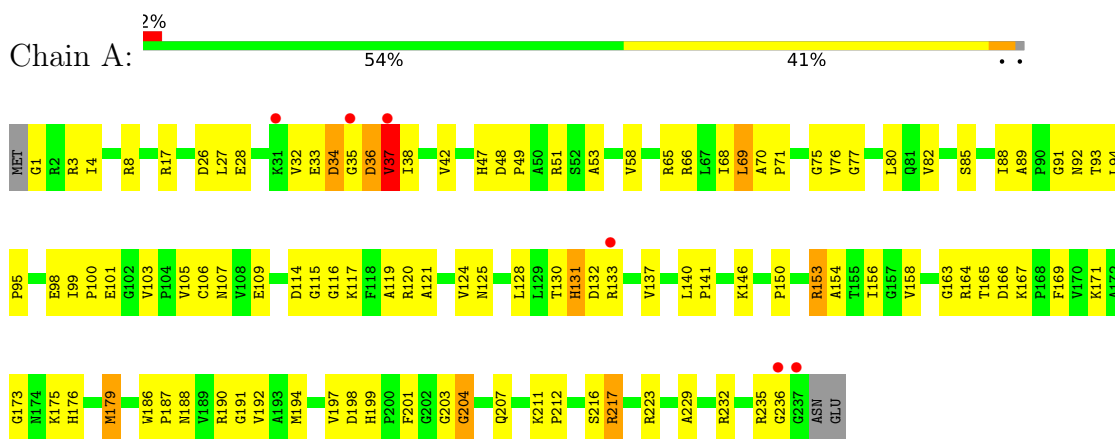
Continued from previous page...

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

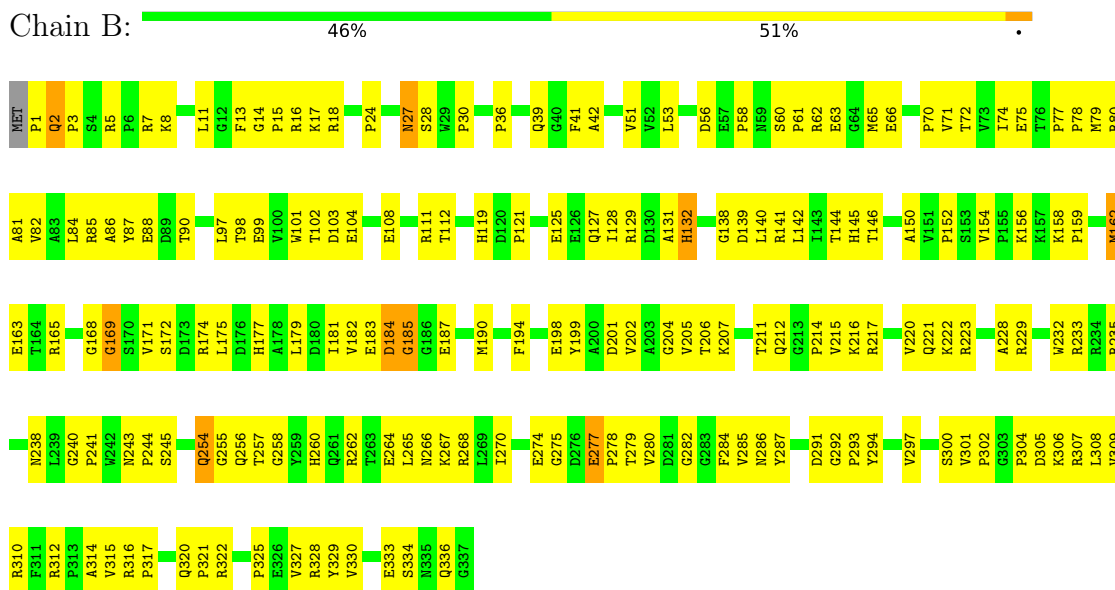
3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L2P

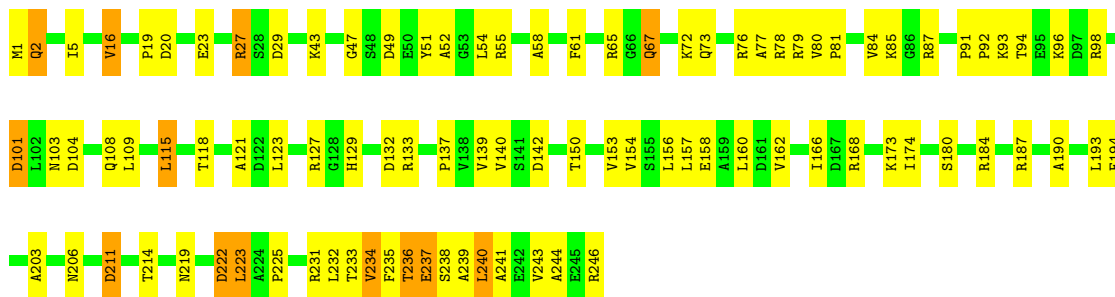


- Molecule 2: 50S ribosomal protein L3P

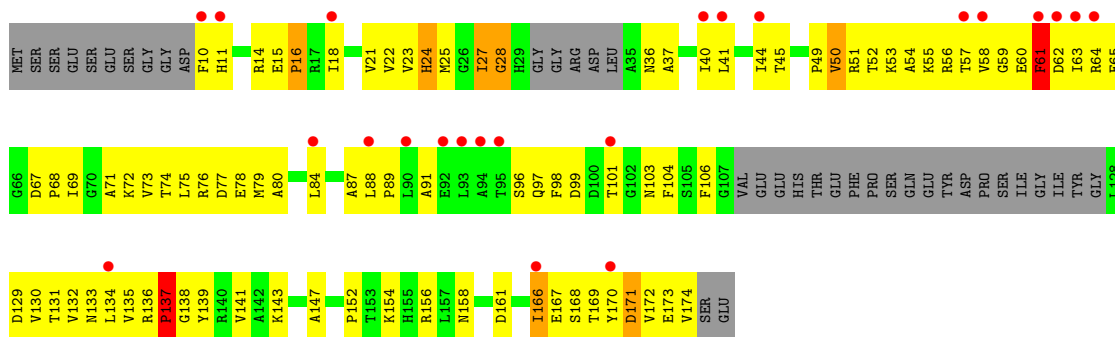


- Molecule 3: 50S ribosomal protein L4P

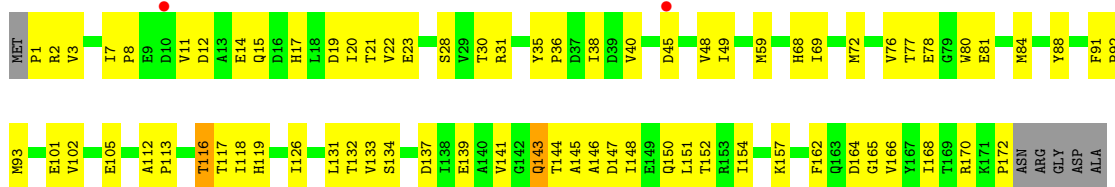




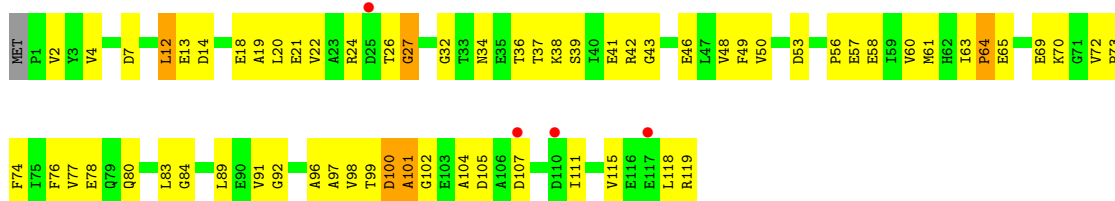
• Molecule 4: 50S ribosomal protein L5P



• Molecule 5: 50S ribosomal protein L6P

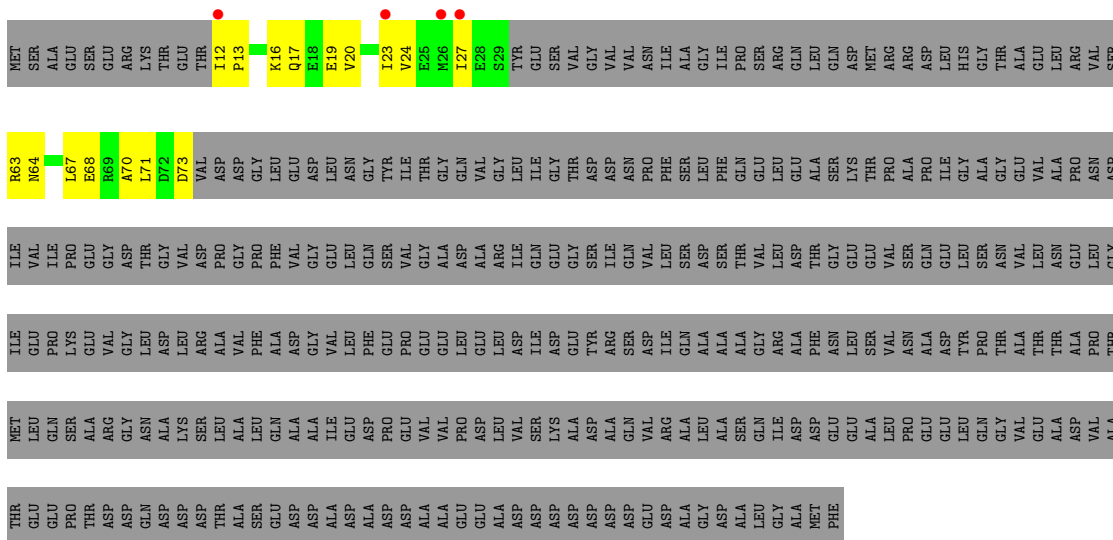


• Molecule 6: 50S ribosomal protein L7Ae



• Molecule 7: 50S ribosomal protein L10E

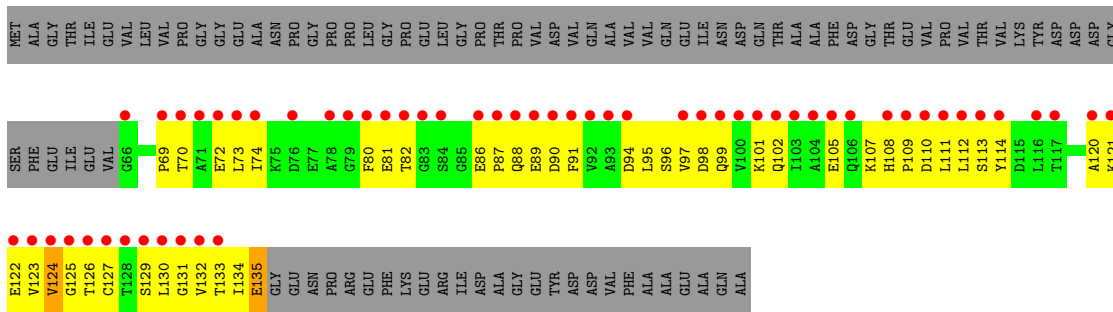




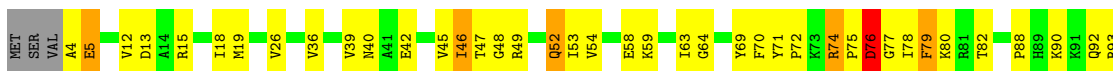
• Molecule 8: 50S ribosomal protein L10e



• Molecule 9: 50S ribosomal protein L11P

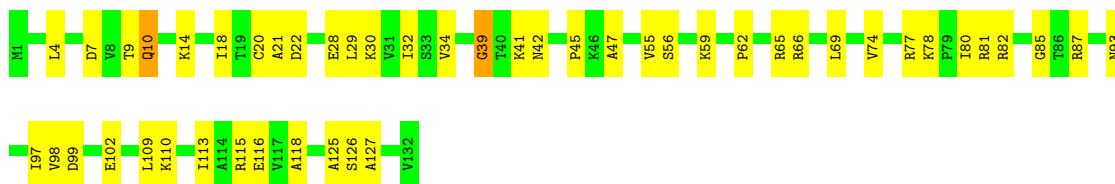


• Molecule 10: 50S ribosomal protein L13P

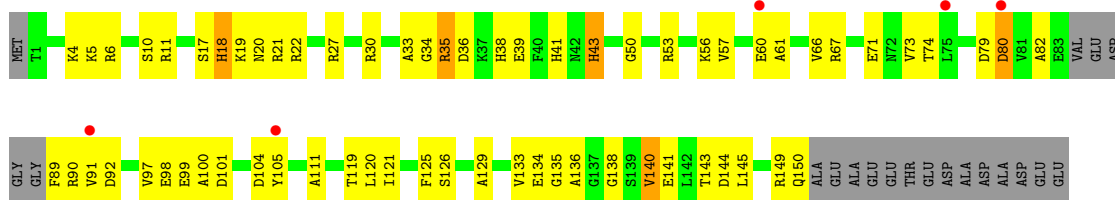




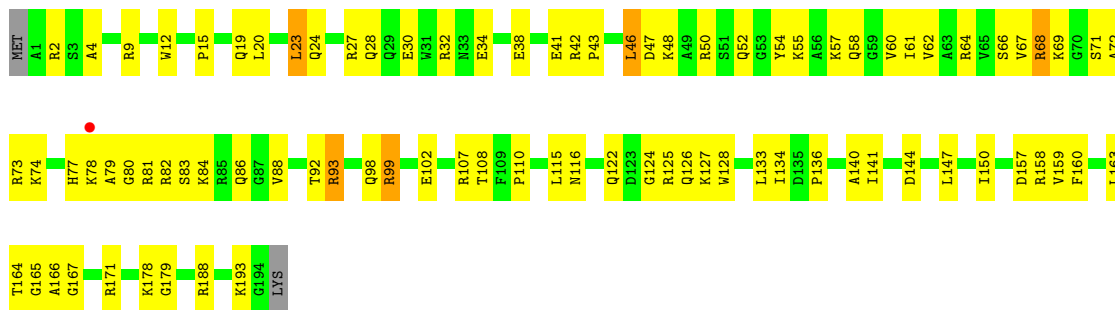
- Molecule 11: 50S ribosomal protein L14P



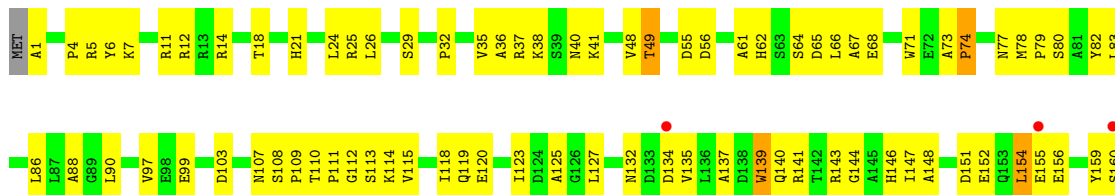
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e



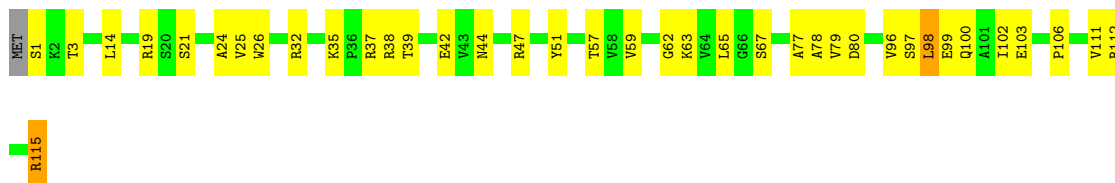
- Molecule 14: 50S ribosomal protein L18P





- Molecule 15: 50S ribosomal protein L18e

Chain O: 66% 31% ..



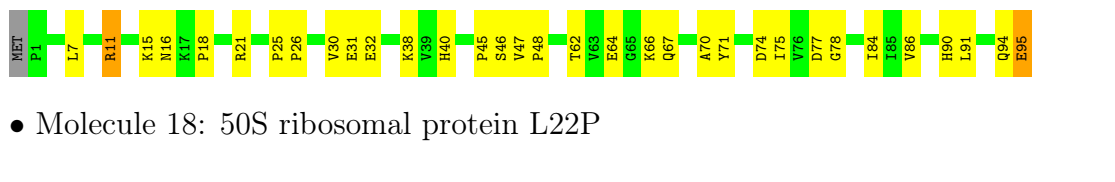
- Molecule 16: 50S ribosomal protein L19e

Chain P: 64% 30% ..



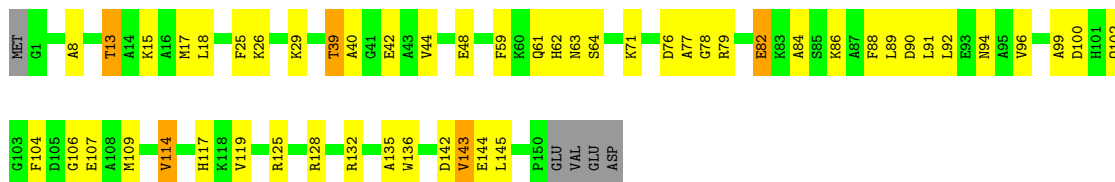
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 65% 32% ..



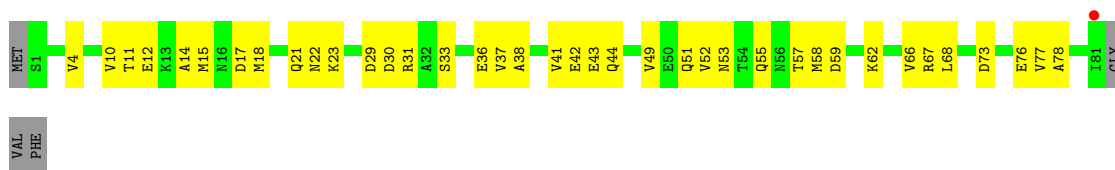
- Molecule 18: 50S ribosomal protein L22P

Chain R: 63% 30% ..

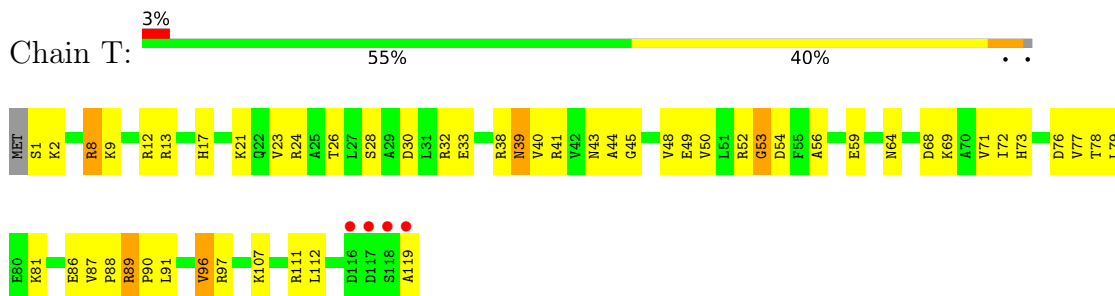


- Molecule 19: 50S ribosomal protein L23P

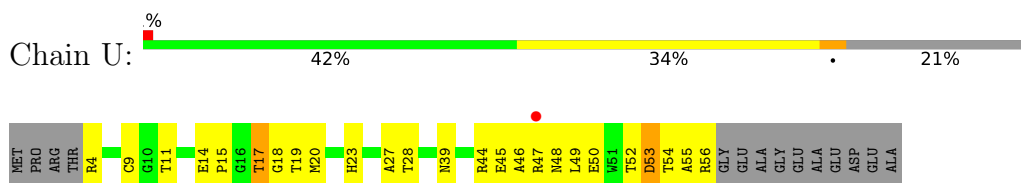
Chain S: 51% 45% 5%



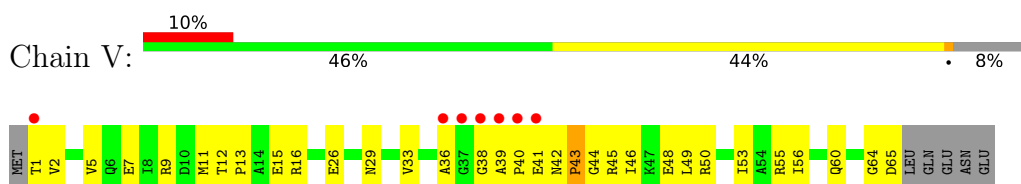
- Molecule 20: 50S ribosomal protein L24P



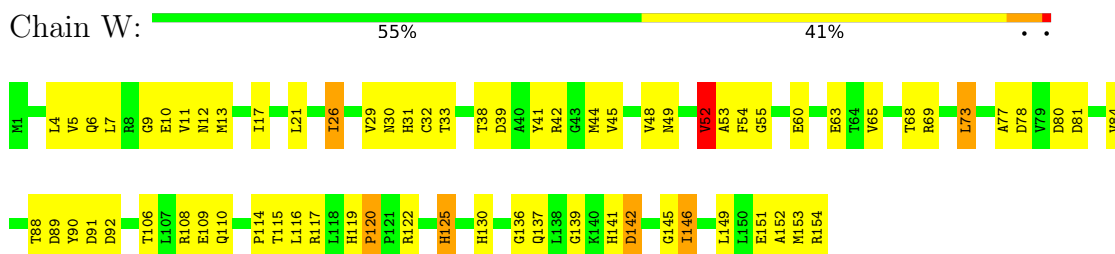
- Molecule 21: 50S ribosomal protein L24e



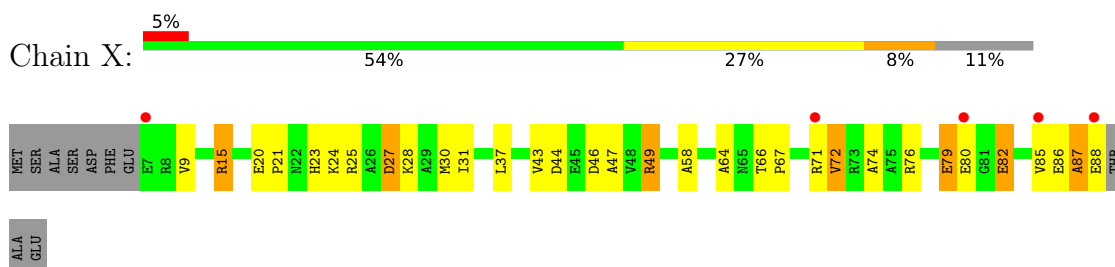
- Molecule 22: 50S ribosomal protein L29P



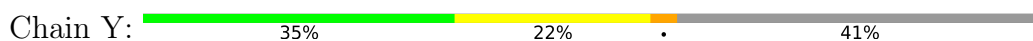
- Molecule 23: 50S ribosomal protein L30P

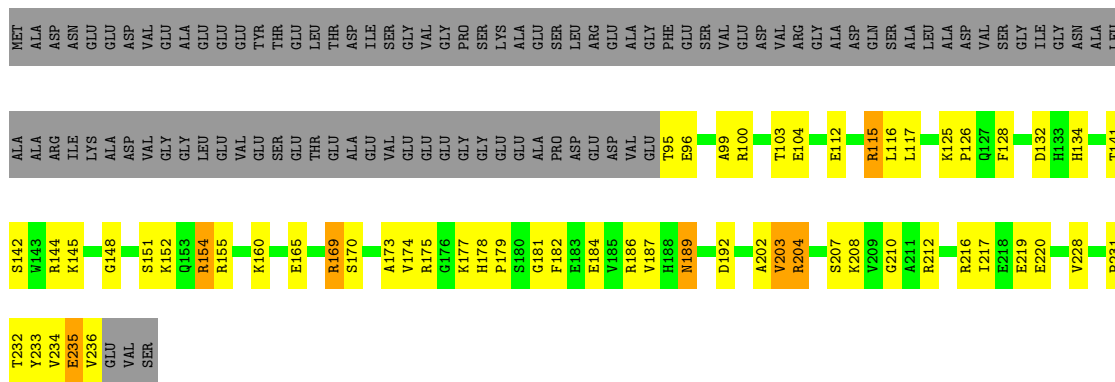


- Molecule 24: 50S ribosomal protein L31e

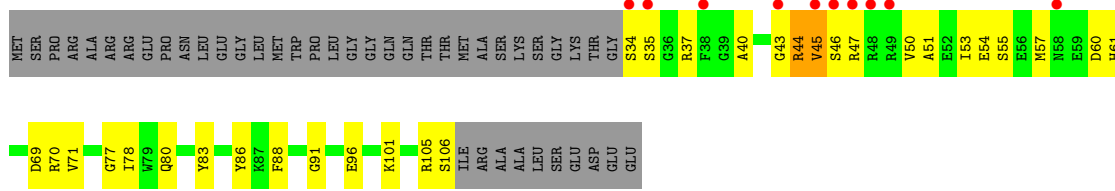


- Molecule 25: 50S ribosomal protein L32e





● Molecule 26: 50S ribosomal protein L37Ae



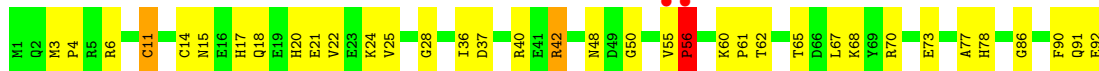
● Molecule 27: 50S ribosomal protein L37e



● Molecule 28: 50S ribosomal protein L39e

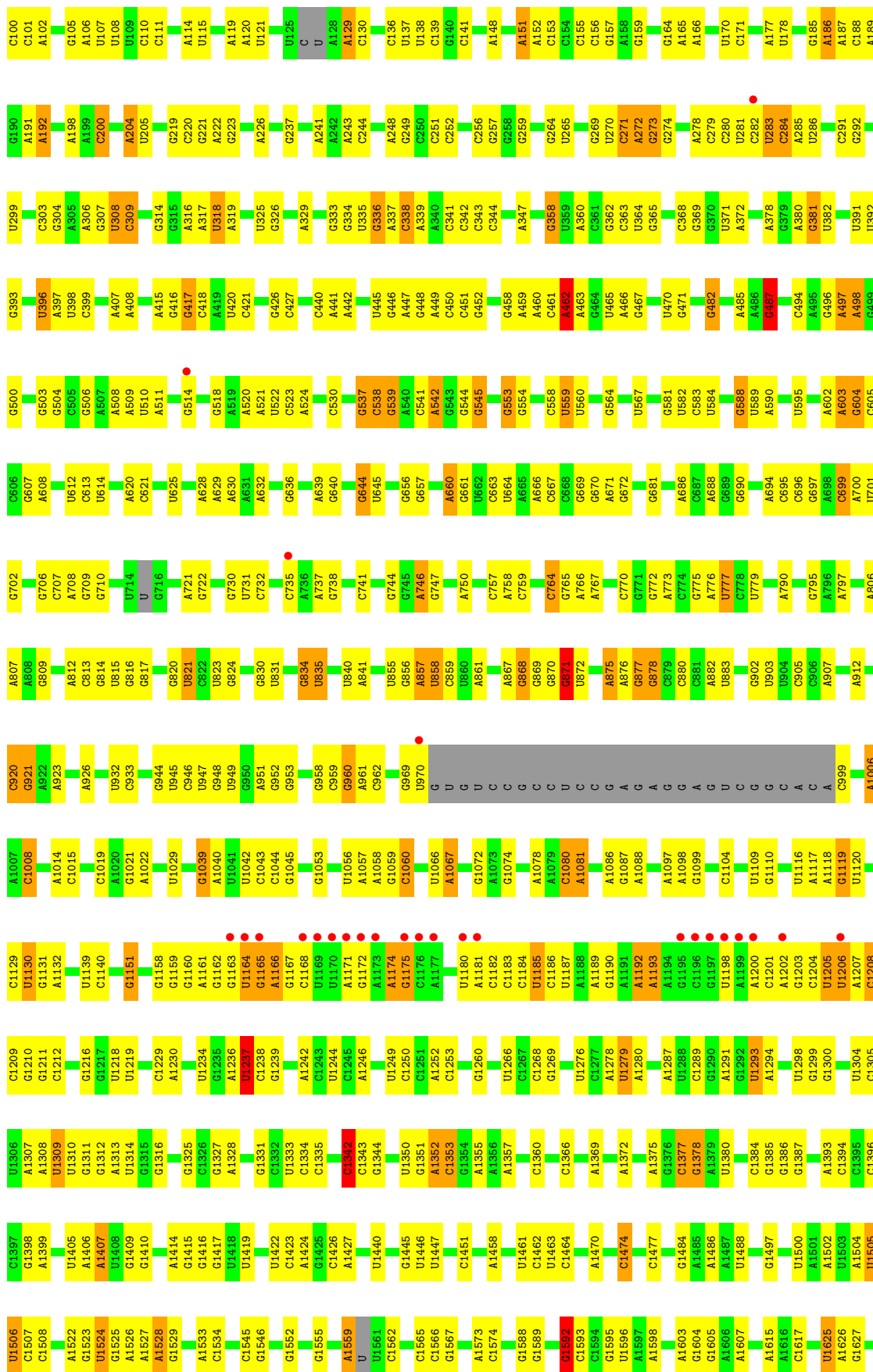


● Molecule 29: 50S ribosomal protein L44E



● Molecule 30: 23S RIBOSOMAL RNA

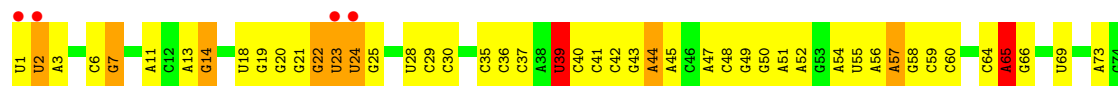




G2887	A2782	G2592	A2511	U2419	A2321	A2095	G2005	G1925	A1811	U1724	A1690
U2888	C2796	C2593	U2512	G2420	U2322	A2096	C2006	G1926	C1816	C1725	A1691
U2889	G2795	A2599	A2513	G2421	G2324	A2101	U2007	G1927	U1817	G1730	C1632
A2890	U2796	A2599	U2514	U2422	G2325	A2102	U2008	C1633	C1818	C1731	C1634
C2894	A2799	A2601	C2515	U2423	U2326	A2103	A2009	U1635	G1819	A1732	U1636
C2895	A2800	G2602	A2517	U2424	G2327	C2104	A2011	A1931	G1820	A1733	G1637
A2896	C2806	G2606	C2516	G2426	C2329	C2105	U2012	G1932	A1829	A1736	A1641
C2898	U2807	U2607	A2521	C2427	U2330	C2106	G2013	C1936	C1830	A1737	A1642
C2903	G2811	C2609	G2524	A2428	G2338	G2110	U2016	U1939	U1833	C1738	A1644
A2906	U2812	C2609	G2525	A2429	A	C2114	U2017	C1940	U1834	U1740	G1649
C2907	A2813	G2611	C2526	C2430	C	U2115	A2018	A1941	C1834	U1741	
C2908	U2814	A2612	U2527	A2433	A	U2116	A2019	A1942	U1835	U1741	
A2909	C2815	G2613	G2528	A2434	G	C2119	U2032	C1943	U1838	U1748	U1654
G2909	U2816	C2614	U2531	U2435	G2344	C2120	U2033	C1946	A1839	G1752	G1655
A2910	C2817	C2614	A2532	U2436	A2345	C2121	U2034	G1947	A1840	A1757	A1657
A2914	U2721	G2618	C2533	C2443	G2346	C2122	A2038	G1948	A1845	A1754	A1658
A	G2722	U2619	U2534	G2443	C2347	C2123	A2039	G1949	U1846	A1755	A1659
G	U2723	U2620	U2535	G2443	C2348	C2131	U2042	G1950	A1847	G1756	G1660
C	U2724	U2621	G2536	U2457	C2349	C2132	U2043	G1951	A1847	G1756	C1666
C	G2725	G2626	U2537	A2456	C2351	G2135	U2044	U	A1853	A1759	A1667
A	U2726	G2627	A2538	U2457	C2352	G2136	G2044	A	C1854	G1760	U1668
A	U2735	G2630	U2541	G2462	A2354	C	G2045	A	G1855	U1761	
U	U2736	G2631	C2542	A2465	G2355	A	G2046	C	C1856	U1762	C1675
U	C2737	G2634	G2543	A2466	G2357	C	C2047	C	G1857	G1763	G1676
C	G2738	G2634	U2545	A2467	G2357	C	C2048	A	U1677	C1764	A1677
C	U2739	A2637	U2545	A2468	G2361	C	G2049	A	A1678	G1765	A1678
U	U2748	G2638	C2549	A2468	A2362	C	G2050	C	G1868	U1766	C1679
A	U2749	G2642	U2550	C2472	A2363	C	G2053	C	G1873	U1771	C1680
A	G2750	G2643	C2551	U2476	G2364	A	A2054	C	U1874	C1772	G1681
A	G2751	G2644	C2552	C2476	G2365	C	A2055	C	U1874	G1773	A1682
A	G2752	U2645	U2554	G2480	A2369	C	G2058	C	G1877	G1774	A1683
A	U2753	U2648	U2557	A2483	A2372	C	U2063	C	U1877	A1778	A1684
A	U2754	A2649	U2558	U2484	U2373	C	U2064	C	G1884	A1779	C1686
A	U2755	U2650	U2559	A2484	U2377	C	G2070	C	A1885	U1783	C1692
A	U2756	C2651	G2564	A2488	U2378	C	C2071	C	A1886	U1784	G1695
A	U2757	A2653	G2565	G2489	G2379	C	G2072	C	U1887	G1785	U1696
A	U2758	G2661	G2566	A2491	U2381	C	G2073	C	C1888	C1786	U1696
A	U2759	U2664	U2569	G2492	A2388	A	A2074	C	C1889	C1787	G1697
A	U2760	A2664	C2570	C2493	U2389	C	G2079	C	U1890	U1788	U1698
A	U2761	A	U2578	U2499	A2401	C	G2080	C	C1894	G1789	C1700
A	U2762	U	G2578	C2500	A2402	C	A2081	C	U1902	U1791	A1701
A	U2763	G2667	G2582	G2501	C2403	C	G2082	C	G1903	U1791	U1702
A	U2764	G2670	A2583	C2502	A2408	C	A2083	C	U1903	C1798	A1710
A	U2765	U2671	U2584	A2503	G2413	C	C2087	C	A1909	G1799	A1710
A	U2766	C2672	U2586	A2504	G2415	C	C2088	C	A1910	C1803	C1714
A	U2767	U2676	U2587	G2506	G2417	C	A2089	C	C1911	U1804	C1715
A	U2768	U2676	G2588	C2507	A2414	C	G2090	C	A1919	G1805	A1716
A	U2769	U2681	U2590	C2508	G2415	C	G2091	C	C1920	G1806	A1717
A	U2770	C2682	C2591	A2509	G2416	C	G2094	C	U1921	U1722	U1722
A	U2771	G2687	G2591	C2510	G2416	C		C	A1922	G1810	G1723

- Molecule 31: 5S RIBOSOMAL RNA

Chain 9: 



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

Chain 5: 



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

Chain 6: 



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)	Xtrriage
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	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 8AN, MG, OMU, UR3, SR, 1MA, NA, PSU, K, ACA, CD, CL, OMG

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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	6	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	59934	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:H5'	30:0:871:G:H8	1.20	1.06
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.41	1.03
14:N:37:ARG:NH1	31:9:6:C:H5''	1.72	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	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
25	Y	115	ARG
25	Y	203	VAL
29	3	40	ARG
8	H	87	LYS
8	H	21	GLU

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

Mol	Chain	Res	Type
16	P	88	GLN
20	T	39	ASN
17	Q	16	ASN
18	R	117	HIS
21	U	48	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	2726	U
30	0	1942	A
30	0	2852	A
30	0	2637	A

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

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	OMG	0	2588	30,32	18,26,27	1.00	2 (11%)	19,38,41	0.75	1 (5%)
30	UR3	0	2619	30	19,22,23	0.55	0	26,32,35	0.73	1 (3%)
33	8AN	6	76	33	19,24,25	1.15	1 (5%)	13,35,38	1.79	3 (23%)
30	PSU	0	2621	30	18,21,22	1.57	2 (11%)	22,30,33	1.25	3 (13%)
30	OMU	0	2587	30	19,22,23	0.35	0	26,31,34	0.41	0
30	1MA	0	628	30	16,25,26	1.36	3 (18%)	18,37,40	1.32	3 (16%)

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	OMG	0	2588	30,32	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
33	8AN	6	76	33	-	3/3/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	1MA	0	628	30	-	0/3/25/26	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	C2-N1	5.51	1.44	1.36
30	0	628	1MA	C2-N3	3.52	1.33	1.29
33	6	76	8AN	C3'-N3'	-2.63	1.43	1.47
30	0	2621	PSU	C6-C5	2.61	1.38	1.35
30	0	2588	OMG	C5-C6	-2.51	1.42	1.47

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	76	8AN	O2'-C2'-C3'	3.74	121.22	111.47
33	6	76	8AN	O4'-C4'-C3'	3.51	109.19	104.15
30	0	2621	PSU	C6-C5-C4	3.27	120.48	118.20
30	0	628	1MA	CM1-N1-C6	2.94	124.72	120.27
30	0	2621	PSU	O2-C2-N1	2.79	125.87	122.79

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	2588	OMG	2	0
30	0	2619	UR3	1	0
33	6	76	8AN	1	0
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PHE	6	77	-	10,11,12	1.89	3 (30%)	10,13,15	1.00	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
41	ACA	6	78	-	-	1/4/5/6	-
40	PHE	6	77	-	-	5/5/6/8	0/1/1/1

All (5) 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
40	6	77	PHE	CE2-CD2	3.27	1.45	1.38
40	6	77	PHE	CE1-CD1	2.36	1.43	1.38
40	6	77	PHE	CB-CG	2.11	1.56	1.51
41	6	78	ACA	O-C	2.00	1.31	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	6	77	PHE	CB-CA-C	2.45	116.06	111.47

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	6	77	PHE	O-C-CA-CB
40	6	77	PHE	C-CA-CB-CG
41	6	78	ACA	C2-C3-C4-C5
40	6	77	PHE	N-CA-CB-CG
40	6	77	PHE	CA-CB-CG-CD1

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 [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	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, 46, 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 [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
33	8AN	6	76	22/23	0.87	0.28	84,92,94,95	0
30	OMG	0	2588	24/25	0.97	0.11	24,29,31,33	0
30	UR3	0	2619	21/22	0.97	0.14	33,35,40,41	0
30	PSU	0	2621	20/21	0.97	0.14	29,31,38,39	0
30	1MA	0	628	23/24	0.97	0.15	25,28,29,30	0
30	OMU	0	2587	21/22	0.98	0.09	24,28,32,33	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	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
37	NA	0	8525	1/1	0.65	0.32	63,63,63,63	0
36	SR	B	8987	1/1	0.65	0.42	200,200,200,200	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
34	MG	0	8085	1/1	0.73	0.34	91,91,91,91	0
36	SR	0	8998	1/1	0.73	0.20	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	NA	0	8541	1/1	0.74	0.39	80,80,80,80	0
37	NA	0	8546	1/1	0.74	0.25	79,79,79,79	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
37	NA	0	8507	1/1	0.77	0.37	88,88,88,88	0
34	MG	0	8047	1/1	0.77	0.88	89,89,89,89	0
36	SR	0	9001	1/1	0.77	0.09	155,155,155,155	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
36	SR	S	8961	1/1	0.80	0.08	189,189,189,189	0
37	NA	0	8519	1/1	0.80	0.54	53,53,53,53	0
34	MG	0	8092	1/1	0.80	0.12	48,48,48,48	0
34	MG	0	8053	1/1	0.80	0.11	54,54,54,54	0
37	NA	0	8564	1/1	0.80	0.08	68,68,68,68	0
34	MG	0	8037	1/1	0.80	0.14	70,70,70,70	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
36	SR	A	8929	1/1	0.81	0.06	105,105,105,105	0
34	MG	0	8059	1/1	0.81	0.13	58,58,58,58	0
37	NA	0	8516	1/1	0.81	0.19	42,42,42,42	0
37	NA	0	8569	1/1	0.82	0.21	44,44,44,44	0
37	NA	0	8536	1/1	0.82	0.15	69,69,69,69	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
34	MG	0	8081	1/1	0.83	0.52	103,103,103,103	0
37	NA	0	8555	1/1	0.83	0.72	64,64,64,64	0
37	NA	0	8557	1/1	0.83	0.10	57,57,57,57	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	8069	1/1	0.83	0.25	88,88,88,88	0
37	NA	0	8542	1/1	0.83	0.22	38,38,38,38	0
37	NA	M	8539	1/1	0.83	0.11	33,33,33,33	0
37	NA	D	8543	1/1	0.84	0.07	60,60,60,60	0
37	NA	J	8538	1/1	0.84	0.21	31,31,31,31	0
37	NA	0	8549	1/1	0.84	0.34	61,61,61,61	0
34	MG	0	8040	1/1	0.84	0.20	75,75,75,75	0
37	NA	0	8566	1/1	0.84	0.24	39,39,39,39	0
37	NA	0	8556	1/1	0.84	0.17	39,39,39,39	0
34	MG	0	8089	1/1	0.84	0.15	35,35,35,35	0
34	MG	0	8076	1/1	0.85	0.52	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8064	1/1	0.85	0.18	51,51,51,51	0
37	NA	0	8504	1/1	0.85	0.20	20,20,20,20	0
34	MG	B	8042	1/1	0.85	0.11	92,92,92,92	0
34	MG	0	8024	1/1	0.85	0.25	80,80,80,80	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	8091	1/1	0.85	0.10	59,59,59,59	0
34	MG	0	8082	1/1	0.85	0.31	64,64,64,64	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
36	SR	0	8951	1/1	0.86	0.09	107,107,107,107	0
37	NA	0	8518	1/1	0.86	0.21	68,68,68,68	0
36	SR	0	8994	1/1	0.86	0.53	200,200,200,200	0
36	SR	0	8955	1/1	0.86	0.09	115,115,115,115	0
34	MG	0	8033	1/1	0.86	0.09	59,59,59,59	0
37	NA	0	8528	1/1	0.86	0.10	42,42,42,42	0
36	SR	0	8944	1/1	0.87	0.13	113,113,113,113	0
34	MG	0	8010	1/1	0.87	0.34	103,103,103,103	0
34	MG	0	8049	1/1	0.88	0.55	141,141,141,141	0
34	MG	0	8023	1/1	0.88	0.14	21,21,21,21	0
37	NA	0	8531	1/1	0.88	0.21	37,37,37,37	0
37	NA	0	8558	1/1	0.88	0.65	56,56,56,56	0
37	NA	0	8521	1/1	0.88	0.39	61,61,61,61	0
36	SR	0	9000	1/1	0.88	0.18	137,137,137,137	0
36	SR	9	8968	1/1	0.89	0.09	105,105,105,105	0
37	NA	0	8551	1/1	0.89	0.28	53,53,53,53	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
34	MG	0	8075	1/1	0.90	0.08	35,35,35,35	0
37	NA	S	8510	1/1	0.90	0.15	58,58,58,58	0
37	NA	0	8530	1/1	0.90	0.23	38,38,38,38	0
35	CL	0	8813	1/1	0.90	0.08	53,53,53,53	0
37	NA	0	8517	1/1	0.90	0.41	40,40,40,40	0
36	SR	9	9003	1/1	0.91	0.06	127,127,127,127	0
36	SR	0	8971	1/1	0.91	0.07	157,157,157,157	0
37	NA	0	8523	1/1	0.91	0.19	49,49,49,49	0
34	MG	0	8077	1/1	0.91	0.09	37,37,37,37	0
37	NA	0	8570	1/1	0.91	0.15	53,53,53,53	0
34	MG	0	8027	1/1	0.91	0.13	44,44,44,44	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8039	1/1	0.91	0.22	32,32,32,32	0
34	MG	0	8002	1/1	0.91	0.42	62,62,62,62	0
37	NA	0	8505	1/1	0.91	0.40	29,29,29,29	0
36	SR	0	8919	1/1	0.92	0.12	82,82,82,82	0
37	NA	0	8514	1/1	0.92	0.40	53,53,53,53	0
37	NA	0	8501	1/1	0.92	0.32	100,100,100,100	0
34	MG	0	8029	1/1	0.92	0.27	87,87,87,87	0
36	SR	0	8983	1/1	0.92	0.23	195,195,195,195	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	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
37	NA	0	8545	1/1	0.92	0.15	40,40,40,40	0
36	SR	0	8995	1/1	0.92	0.15	86,86,86,86	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	Y	9002	1/1	0.93	0.11	118,118,118,118	0
36	SR	0	8982	1/1	0.93	0.12	105,105,105,105	0
36	SR	0	9004	1/1	0.93	0.16	107,107,107,107	0
34	MG	0	8067	1/1	0.93	0.29	48,48,48,48	0
37	NA	0	8575	1/1	0.93	0.15	59,59,59,59	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
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
34	MG	0	8080	1/1	0.93	0.16	62,62,62,62	0
34	MG	0	8036	1/1	0.94	0.15	47,47,47,47	0
34	MG	0	8004	1/1	0.94	0.21	13,13,13,13	0
37	NA	0	8527	1/1	0.94	0.20	40,40,40,40	0
34	MG	0	8013	1/1	0.94	0.04	28,28,28,28	0
36	SR	F	9005	1/1	0.94	0.12	85,85,85,85	0
37	NA	0	8562	1/1	0.94	0.46	61,61,61,61	0
34	MG	Y	8086	1/1	0.94	0.19	46,46,46,46	0
37	NA	0	8512	1/1	0.94	0.43	43,43,43,43	0
34	MG	0	8008	1/1	0.94	0.12	13,13,13,13	0
34	MG	0	8068	1/1	0.94	0.24	74,74,74,74	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	8916	1/1	0.94	0.13	65,65,65,65	0
37	NA	R	8533	1/1	0.94	0.14	42,42,42,42	0
34	MG	0	8044	1/1	0.94	0.08	47,47,47,47	0
35	CL	O	8808	1/1	0.94	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	NA	0	8550	1/1	0.94	0.20	43,43,43,43	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	8035	1/1	0.94	0.18	94,94,94,94	0
34	MG	0	8014	1/1	0.95	0.21	9,9,9,9	0
36	SR	0	8985	1/1	0.95	0.07	116,116,116,116	0
35	CL	Q	8811	1/1	0.95	0.06	68,68,68,68	0
34	MG	0	8055	1/1	0.95	0.29	30,30,30,30	0
35	CL	A	8809	1/1	0.95	0.07	57,57,57,57	0
35	CL	0	8822	1/1	0.95	0.15	53,53,53,53	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
36	SR	0	8967	1/1	0.95	0.11	92,92,92,92	0
36	SR	0	8928	1/1	0.95	0.08	87,87,87,87	0
37	NA	0	8502	1/1	0.95	0.21	55,55,55,55	0
36	SR	B	8950	1/1	0.95	0.17	89,89,89,89	0
36	SR	0	8936	1/1	0.95	0.16	59,59,59,59	0
37	NA	0	8553	1/1	0.95	0.51	100,100,100,100	0
37	NA	0	8524	1/1	0.95	0.09	37,37,37,37	0
36	SR	0	8941	1/1	0.95	0.14	71,71,71,71	0
34	MG	0	8043	1/1	0.95	0.15	37,37,37,37	0
35	CL	N	8807	1/1	0.95	0.06	62,62,62,62	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
35	CL	0	8805	1/1	0.96	0.07	46,46,46,46	0
36	SR	0	8997	1/1	0.96	0.05	116,116,116,116	0
34	MG	0	8083	1/1	0.96	0.09	36,36,36,36	0
36	SR	0	8923	1/1	0.96	0.17	66,66,66,66	0
37	NA	0	8529	1/1	0.96	0.04	20,20,20,20	0
34	MG	0	8041	1/1	0.96	0.26	31,31,31,31	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
36	SR	A	8977	1/1	0.96	0.10	95,95,95,95	0
36	SR	0	8938	1/1	0.96	0.07	101,101,101,101	0
37	NA	0	8537	1/1	0.96	0.04	22,22,22,22	0
36	SR	0	9008	1/1	0.96	0.14	80,80,80,80	0
34	MG	0	8007	1/1	0.96	0.12	37,37,37,37	0
35	CL	L	8814	1/1	0.96	0.07	49,49,49,49	0
34	MG	0	8071	1/1	0.96	0.49	98,98,98,98	0
36	SR	0	8984	1/1	0.96	0.10	89,89,89,89	0
34	MG	0	8052	1/1	0.96	0.07	37,37,37,37	0
34	MG	0	8066	1/1	0.96	0.24	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	NA	L	8568	1/1	0.96	0.18	30,30,30,30	0
35	CL	Y	8820	1/1	0.96	0.05	35,35,35,35	0
34	MG	0	8031	1/1	0.96	0.12	48,48,48,48	0
35	CL	0	8817	1/1	0.97	0.06	42,42,42,42	0
34	MG	9	8074	1/1	0.97	0.24	53,53,53,53	0
34	MG	0	8028	1/1	0.97	0.26	1,1,1,1	0
36	SR	0	8958	1/1	0.97	0.11	68,68,68,68	0
36	SR	0	8906	1/1	0.97	0.17	49,49,49,49	0
37	NA	0	8534	1/1	0.97	0.69	78,78,78,78	0
35	CL	2	8803	1/1	0.97	0.07	51,51,51,51	0
37	NA	0	8513	1/1	0.97	0.15	29,29,29,29	0
36	SR	0	8991	1/1	0.97	0.10	147,147,147,147	0
35	CL	M	8818	1/1	0.97	0.08	33,33,33,33	0
36	SR	0	8964	1/1	0.97	0.07	92,92,92,92	0
36	SR	0	8965	1/1	0.97	0.11	88,88,88,88	0
34	MG	C	8012	1/1	0.97	0.22	13,13,13,13	0
36	SR	0	8943	1/1	0.97	0.13	65,65,65,65	0
37	NA	R	8532	1/1	0.97	0.09	29,29,29,29	0
37	NA	0	8574	1/1	0.97	0.44	48,48,48,48	0
34	MG	0	8093	1/1	0.97	0.12	25,25,25,25	0
36	SR	0	8945	1/1	0.97	0.13	89,89,89,89	0
38	CD	O	8705	1/1	0.97	0.03	103,103,103,103	0
36	SR	0	8947	1/1	0.97	0.17	84,84,84,84	0
36	SR	0	8922	1/1	0.97	0.14	62,62,62,62	0
36	SR	0	8954	1/1	0.97	0.12	67,67,67,67	0
37	NA	0	8526	1/1	0.97	0.12	47,47,47,47	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	8914	1/1	0.98	0.22	75,75,75,75	0
34	MG	0	8045	1/1	0.98	0.56	147,147,147,147	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
34	MG	0	8003	1/1	0.98	0.17	18,18,18,18	0
36	SR	0	8963	1/1	0.98	0.16	70,70,70,70	0
35	CL	0	8816	1/1	0.98	0.11	60,60,60,60	0
34	MG	0	8015	1/1	0.98	0.18	45,45,45,45	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	2	8060	1/1	0.98	0.12	42,42,42,42	0
37	NA	0	8561	1/1	0.98	0.33	89,89,89,89	0
36	SR	0	8934	1/1	0.98	0.18	67,67,67,67	0
37	NA	C	8503	1/1	0.98	0.23	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8973	1/1	0.98	0.10	91,91,91,91	0
36	SR	0	8935	1/1	0.98	0.11	64,64,64,64	0
36	SR	A	8930	1/1	0.98	0.13	72,72,72,72	0
34	MG	0	8018	1/1	0.98	0.26	9,9,9,9	0
36	SR	0	8978	1/1	0.98	0.16	60,60,60,60	0
34	MG	0	8084	1/1	0.98	0.11	31,31,31,31	0
35	CL	L	8810	1/1	0.98	0.05	52,52,52,52	0
34	MG	0	8070	1/1	0.98	0.22	62,62,62,62	0
34	MG	0	8019	1/1	0.98	0.19	9,9,9,9	0
34	MG	0	8088	1/1	0.98	0.18	37,37,37,37	0
36	SR	0	8946	1/1	0.98	0.17	86,86,86,86	0
34	MG	0	8020	1/1	0.98	0.20	24,24,24,24	0
36	SR	0	8992	1/1	0.98	0.07	102,102,102,102	0
36	SR	1	8952	1/1	0.98	0.15	60,60,60,60	0
36	SR	3	8999	1/1	0.98	0.12	70,70,70,70	0
36	SR	0	8903	1/1	0.98	0.16	44,44,44,44	0
36	SR	0	8905	1/1	0.99	0.22	49,49,49,49	0
34	MG	0	8061	1/1	0.99	0.20	17,17,17,17	0
36	SR	0	8908	1/1	0.99	0.13	66,66,66,66	0
36	SR	0	8989	1/1	0.99	0.11	71,71,71,71	0
36	SR	0	8990	1/1	0.99	0.17	39,39,39,39	0
34	MG	0	8022	1/1	0.99	0.19	12,12,12,12	0
36	SR	0	8948	1/1	0.99	0.16	57,57,57,57	0
36	SR	0	8949	1/1	0.99	0.13	49,49,49,49	0
36	SR	0	8915	1/1	0.99	0.10	73,73,73,73	0
35	CL	K	8812	1/1	0.99	0.06	43,43,43,43	0
34	MG	0	8009	1/1	0.99	0.30	1,1,1,1	0
36	SR	0	8918	1/1	0.99	0.14	41,41,41,41	0
34	MG	K	8054	1/1	0.99	0.17	18,18,18,18	0
36	SR	R	8912	1/1	0.99	0.18	64,64,64,64	0
36	SR	0	8921	1/1	0.99	0.13	51,51,51,51	0
34	MG	0	8058	1/1	0.99	0.20	1,1,1,1	0
36	SR	T	8939	1/1	0.99	0.09	70,70,70,70	0
36	SR	0	8924	1/1	0.99	0.18	65,65,65,65	0
36	SR	0	8925	1/1	0.99	0.15	66,66,66,66	0
36	SR	0	8927	1/1	0.99	0.17	67,67,67,67	0
34	MG	0	8072	1/1	0.99	0.14	25,25,25,25	0
36	SR	1	8913	1/1	0.99	0.15	42,42,42,42	0
35	CL	B	8819	1/1	0.99	0.34	56,56,56,56	0
36	SR	0	8970	1/1	0.99	0.05	88,88,88,88	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	MG	0	8026	1/1	0.99	0.14	35,35,35,35	0
36	SR	0	8937	1/1	0.99	0.19	59,59,59,59	0
36	SR	0	8901	1/1	0.99	0.13	44,44,44,44	0
36	SR	0	8940	1/1	0.99	0.12	53,53,53,53	0
38	CD	Z	8703	1/1	0.99	0.08	62,62,62,62	0
38	CD	1	8702	1/1	0.99	0.09	50,50,50,50	0
36	SR	0	8981	1/1	0.99	0.15	107,107,107,107	0
36	SR	0	8902	1/1	0.99	0.17	32,32,32,32	0
35	CL	R	8806	1/1	0.99	0.08	36,36,36,36	0
36	SR	0	8904	1/1	0.99	0.16	39,39,39,39	0
38	CD	U	8701	1/1	1.00	0.11	50,50,50,50	0
36	SR	0	8926	1/1	1.00	0.16	81,81,81,81	0
35	CL	0	8815	1/1	1.00	0.06	61,61,61,61	0
38	CD	3	8704	1/1	1.00	0.09	54,54,54,54	0
36	SR	0	8909	1/1	1.00	0.17	59,59,59,59	0
36	SR	0	8910	1/1	1.00	0.12	40,40,40,40	0
36	SR	T	8911	1/1	1.00	0.10	52,52,52,52	0
36	SR	H	8907	1/1	1.00	0.15	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.