wwPDB X-ray Structure Validation Summary Report (i)

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

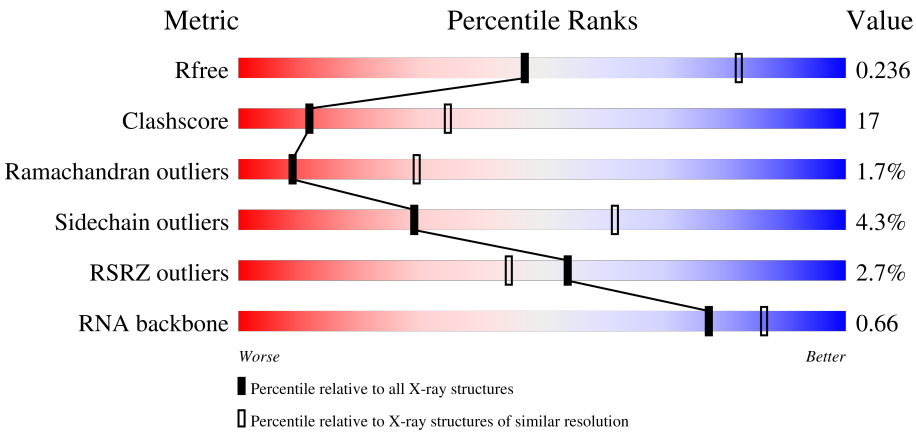
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 <=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	2%, 54%, 41%, • •
2	B	338	46%, 51%, •
3	C	246	62%, 33%, 5%
4	D	177	13%, 28%, 46%, • •, 21%

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Mol	Chain	Length	Quality of chain
5	E	178	%, 55%, 40%
6	F	120	3%, 46%, 49%
7	G	348	%, 5%, 92%
8	H	177	%, 54%, 34%, 10%
9	I	162	35%, 15%, 27%, 57%
10	J	145	54%, 37%, 6%
11	K	132	64%, 35%
12	L	165	3%, 48%, 36%, 12%
13	M	196	%, 55%, 42%
14	N	187	3%, 48%, 47%, 5%
15	O	116	66%, 31%
16	P	149	64%, 30%
17	Q	96	65%, 32%
18	R	155	63%, 30%
19	S	85	%, 51%, 45%, 5%
20	T	120	3%, 55%, 40%
21	U	67	%, 42%, 34%, 21%
22	V	71	10%, 46%, 44%, 8%
23	W	154	55%, 41%
24	X	92	5%, 54%, 27%, 8%, 11%
25	Y	240	35%, 22%, 41%
26	Z	116	9%, 36%, 25%, 37%
27	1	57	53%, 46%
28	2	50	4%, 44%, 48%, 8%
29	3	92	2%, 61%, 36%

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Mol	Chain	Length	Quality of chain
30	0	2923	%, 55%, 33%, 6%, 6%
31	9	122	3%, 48%, 43%, 8%
32	5	3	33%, 67%, 33%
33	6	3	33%, 33%, 33%

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
			Total	C	N	O	S			
21	U	53	410	244	75	86	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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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
			Total	Cl		
35	0	6	6	6	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
37	B	1	1	1	0	0
			Total	Na		
37	C	1	1	1	0	0
			Total	Na		
37	D	1	1	1	0	0
			Total	Na		
37	J	1	1	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

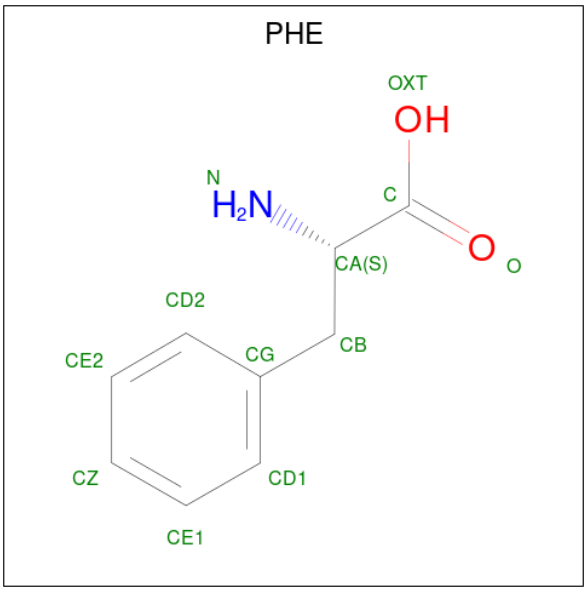
- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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).

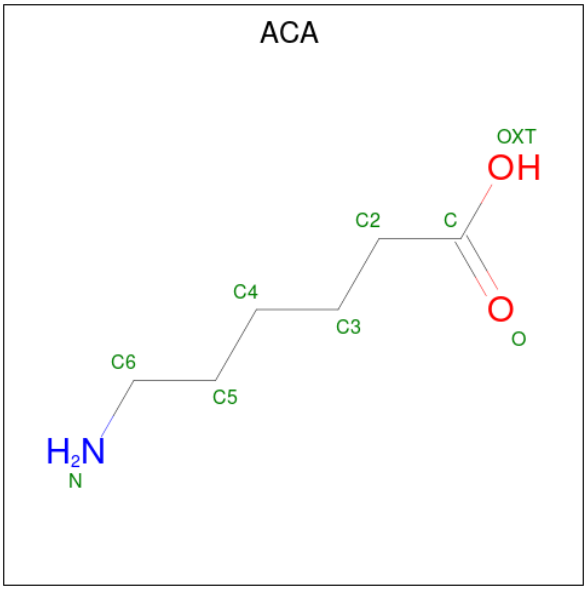
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	2	Total K 2 2	0	0

- Molecule 40 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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: $C_6H_{13}NO_2$).



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

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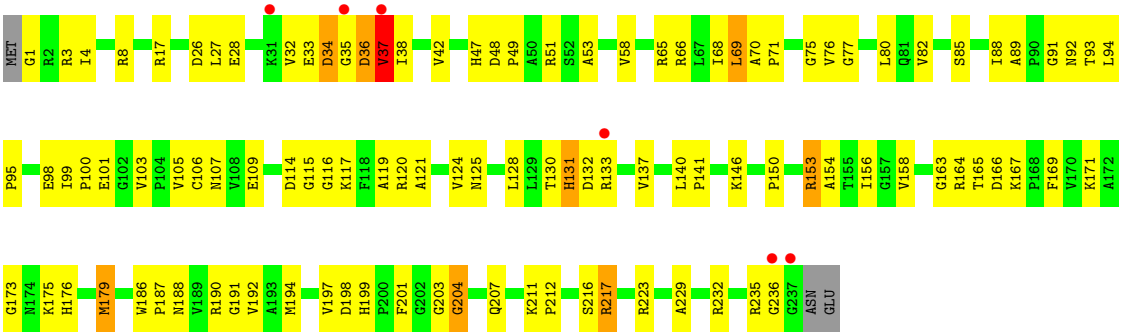
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	W	72	Total O 72 72	0	0
42	X	25	Total O 25 25	0	0
42	Y	108	Total O 108 108	0	0
42	Z	30	Total O 30 30	0	0
42	1	53	Total O 53 53	0	0
42	2	42	Total O 42 42	0	0
42	3	66	Total O 66 66	0	0
42	0	5771	Total O 5771 5771	0	0
42	9	148	Total O 148 148	0	0
42	5	4	Total O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

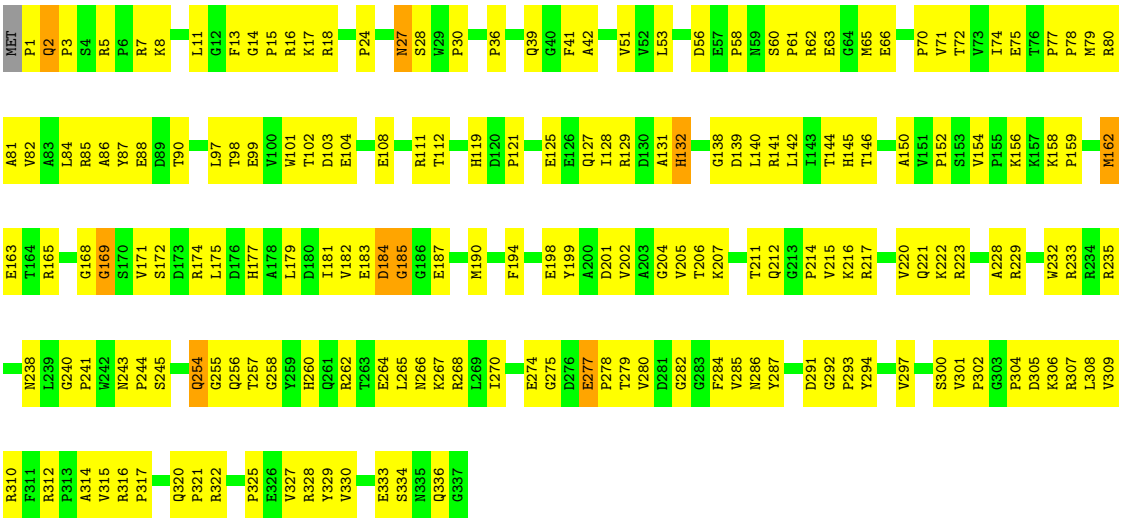
• Molecule 1: 50S ribosomal protein L2P

Chain A: 2% 54% 41%



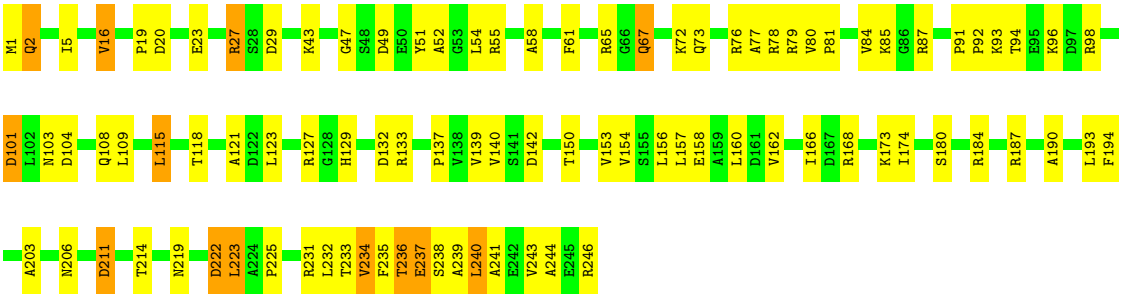
• Molecule 2: 50S ribosomal protein L3P

Chain B: 46% 51%



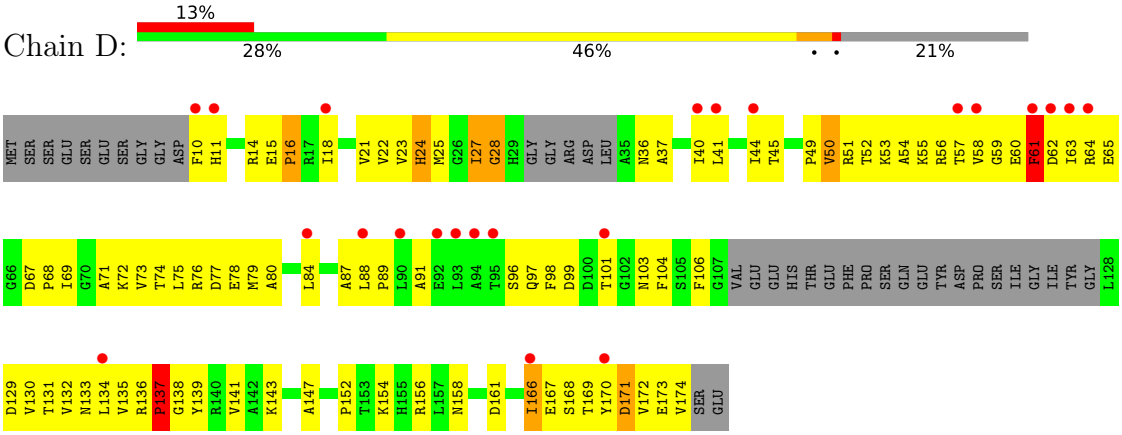
• Molecule 3: 50S ribosomal protein L4P

Chain C: 62% 33% 5%



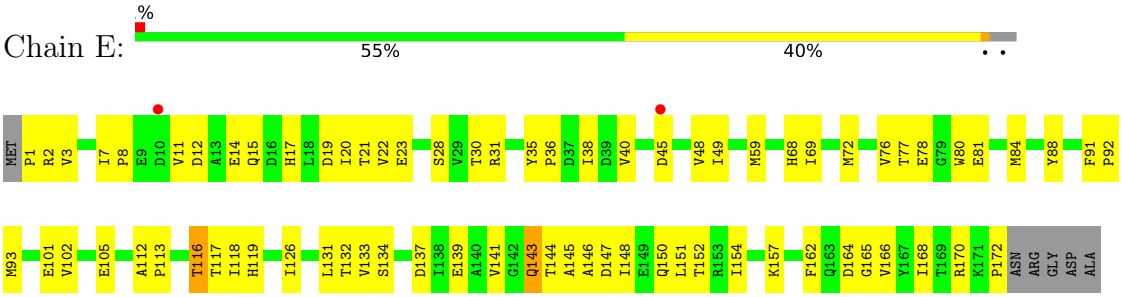
- Molecule 4: 50S ribosomal protein L5P

Chain D:



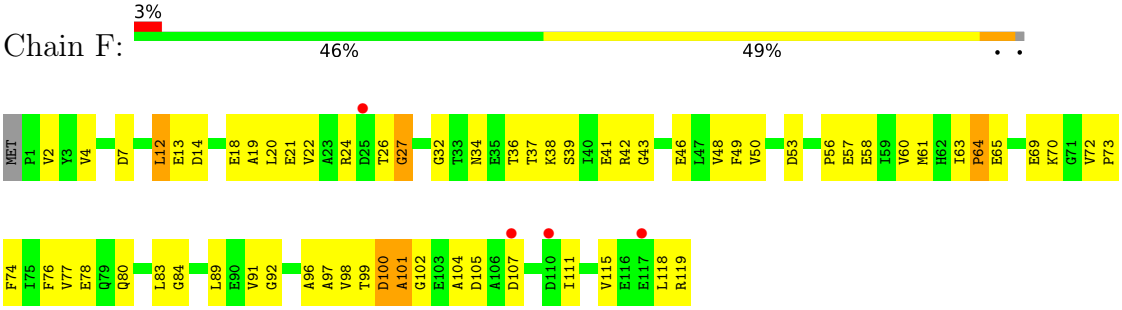
- Molecule 5: 50S ribosomal protein L6P

Chain E:



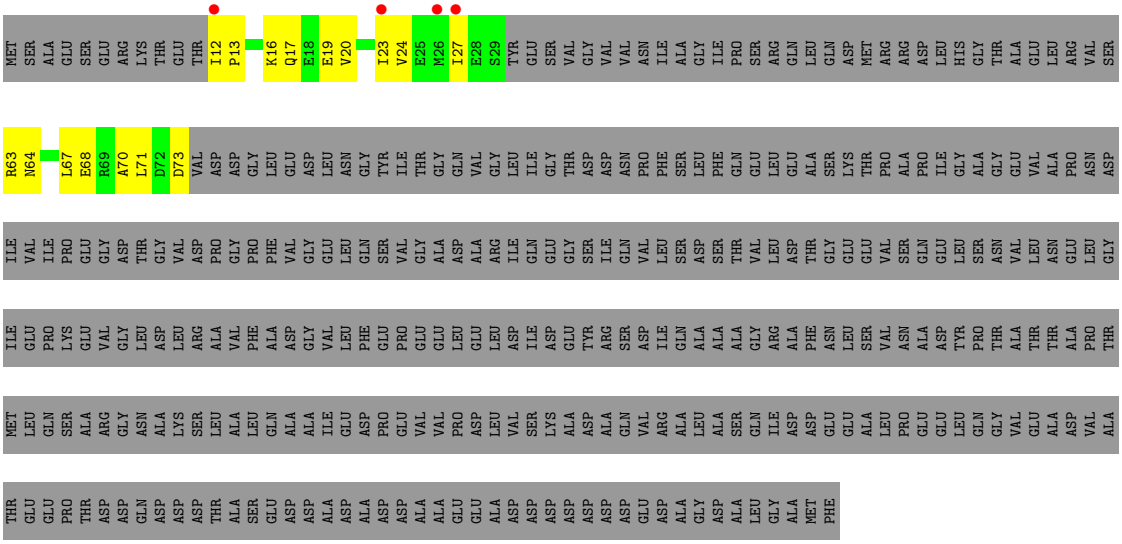
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



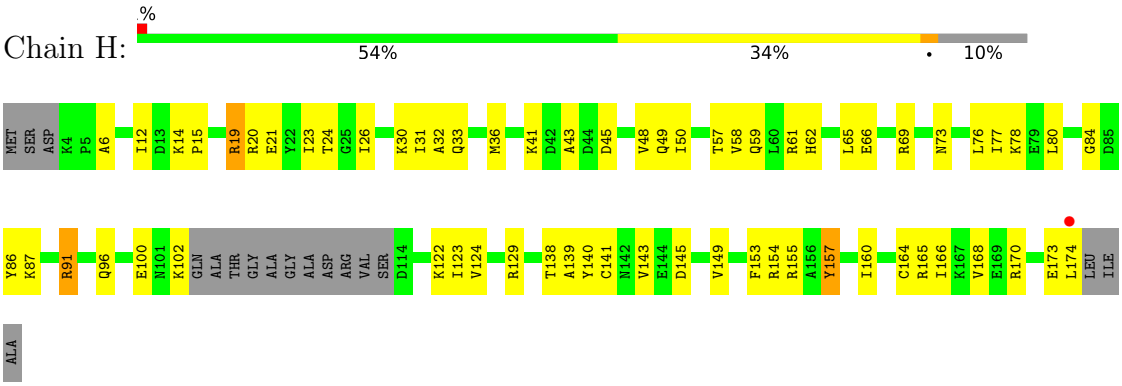
- Molecule 7: 50S ribosomal protein L10E

Chain G:



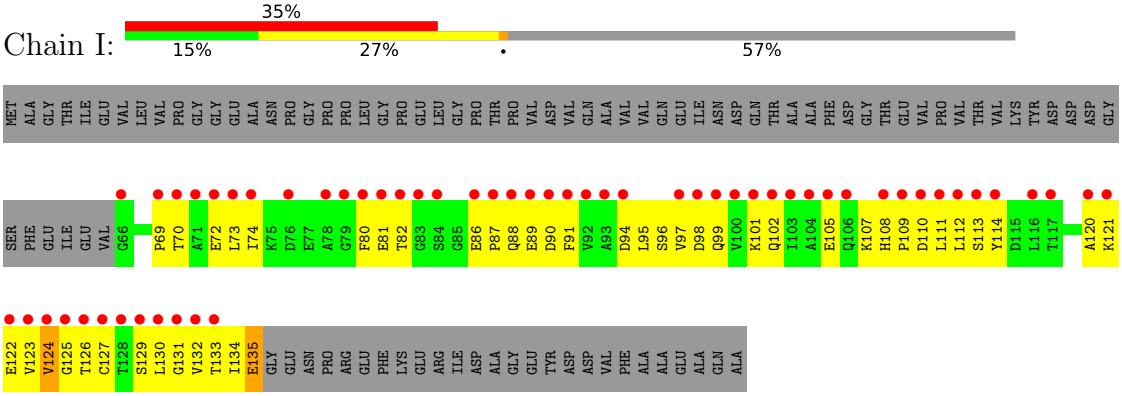
• Molecule 8: 50S ribosomal protein L10e

Chain H:



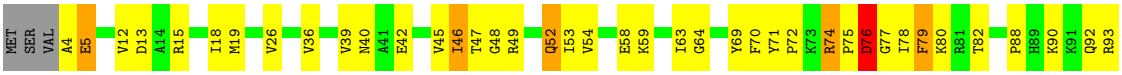
• Molecule 9: 50S ribosomal protein L11P

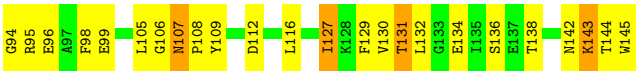
Chain I:



• Molecule 10: 50S ribosomal protein L13P

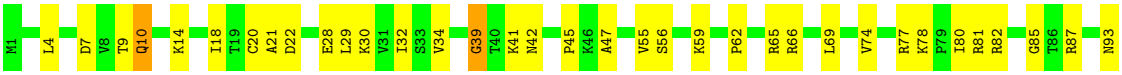
Chain J:

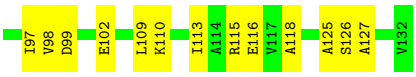




• Molecule 11: 50S ribosomal protein L14P

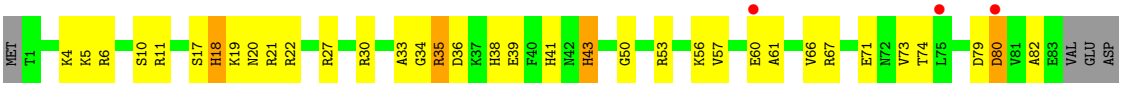
Chain K:

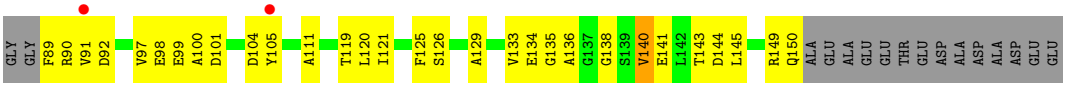




• Molecule 12: 50S ribosomal protein L15P

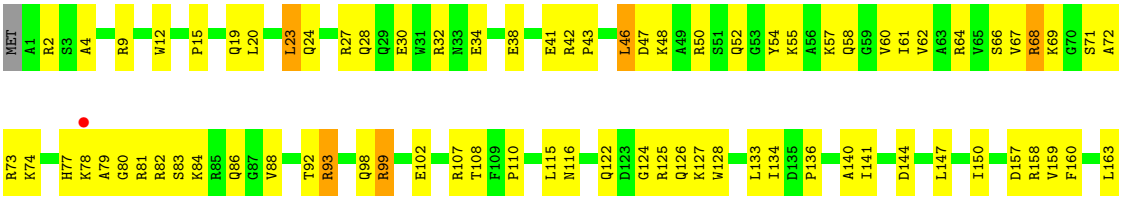
Chain L:

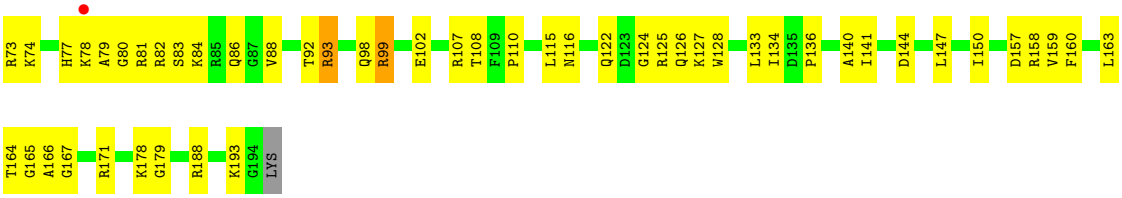




• Molecule 13: 50S ribosomal protein L15e

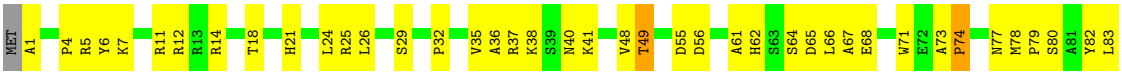
Chain M:

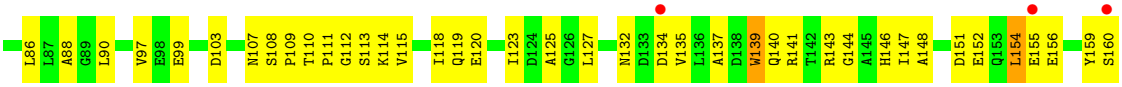


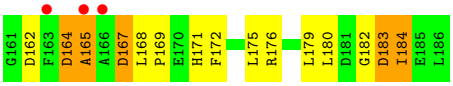


• Molecule 14: 50S ribosomal protein L18P

Chain N:

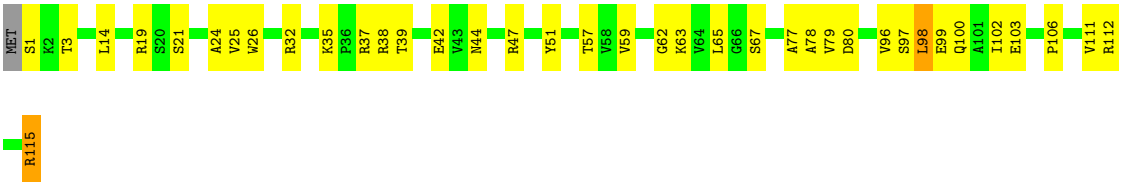






- Molecule 15: 50S ribosomal protein L18e

Chain O:

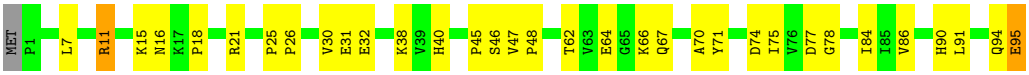


- Molecule 16: 50S ribosomal protein L19e

Chain P:

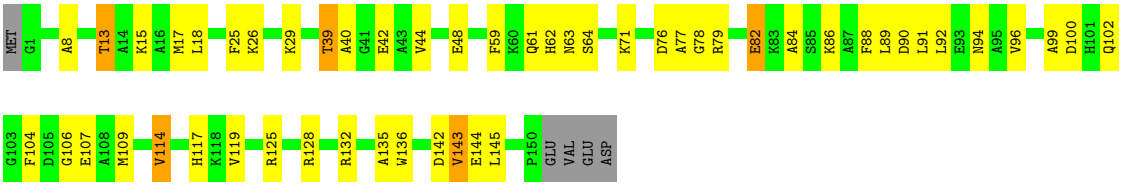
- Molecule 17: 50S ribosomal protein L21e

Chain Q:



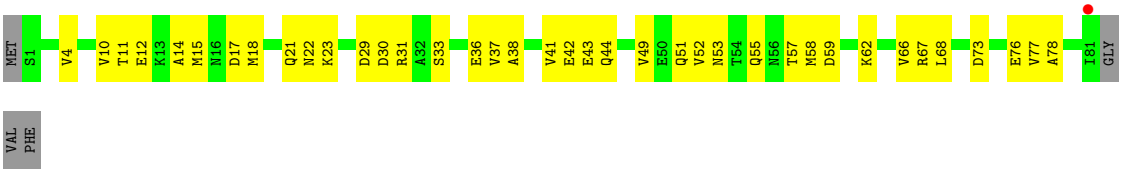
- Molecule 18: 50S ribosomal protein L22P

Chain R:



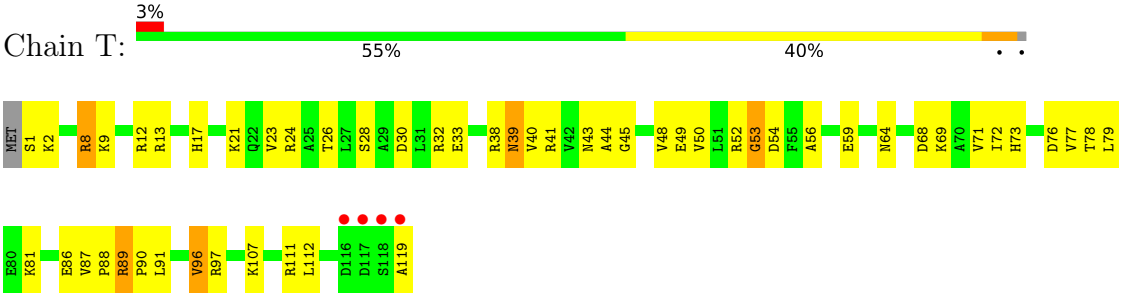
- Molecule 19: 50S ribosomal protein L23P

Chain S:



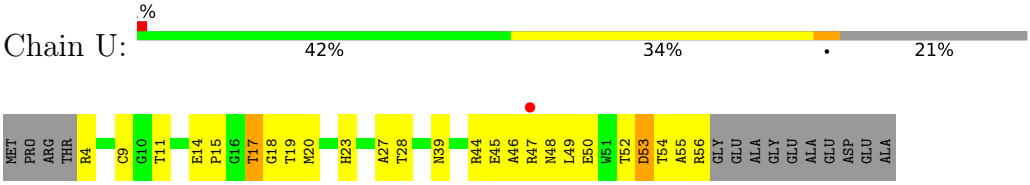
• Molecule 20: 50S ribosomal protein L24P

Chain T:



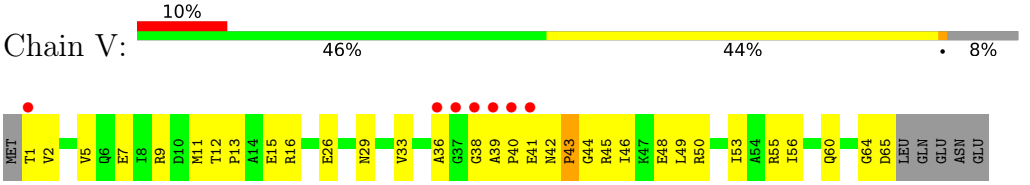
• Molecule 21: 50S ribosomal protein L24e

Chain U:



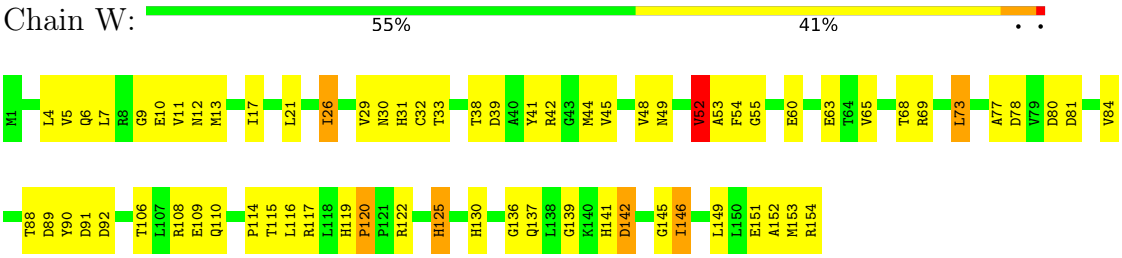
• Molecule 22: 50S ribosomal protein L29P

Chain V:



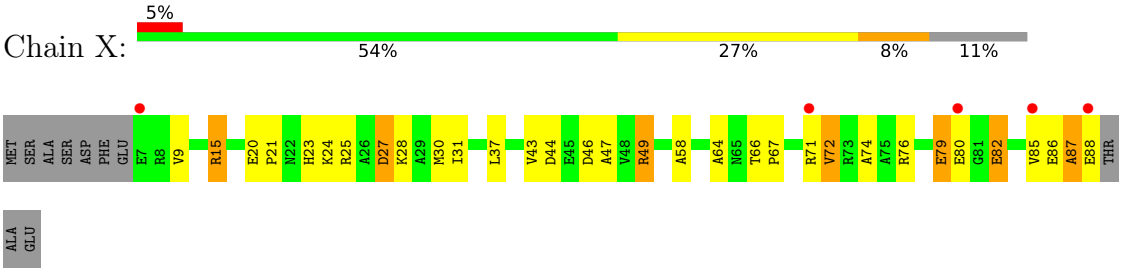
• Molecule 23: 50S ribosomal protein L30P

Chain W:



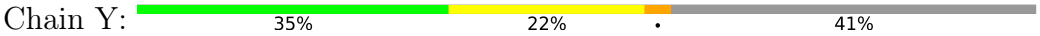
• Molecule 24: 50S ribosomal protein L31e

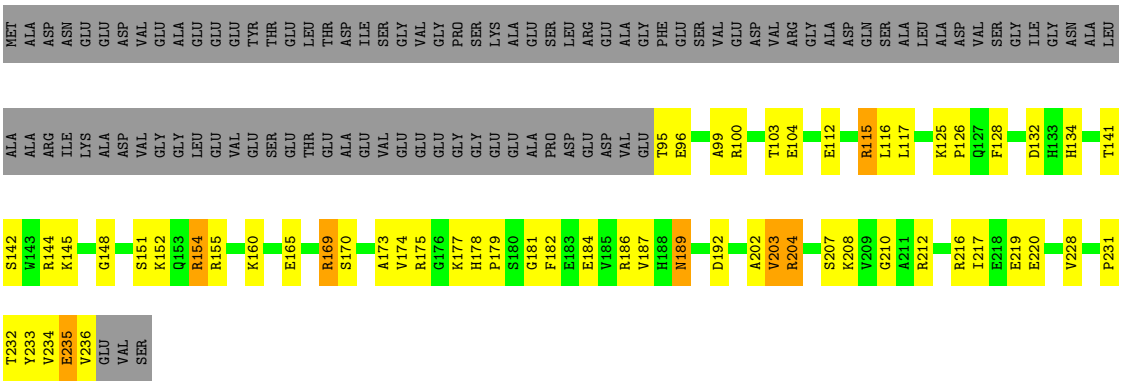
Chain X:



• Molecule 25: 50S ribosomal protein L32e

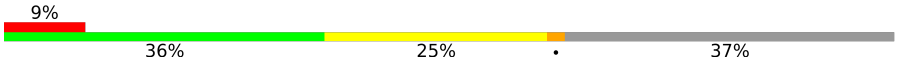
Chain Y:

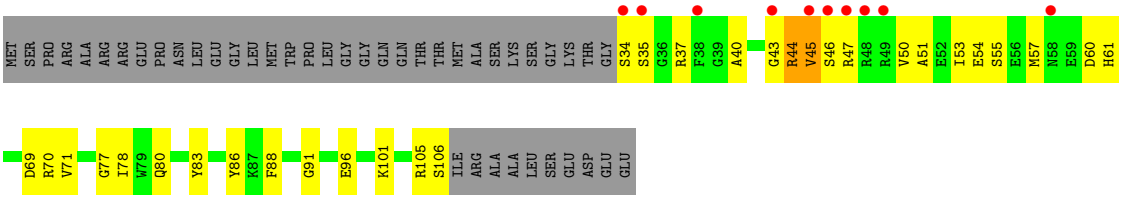




• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



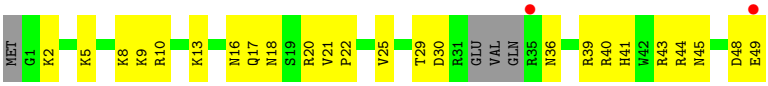


• Molecule 27: 50S ribosomal protein L37e

Chain 1:

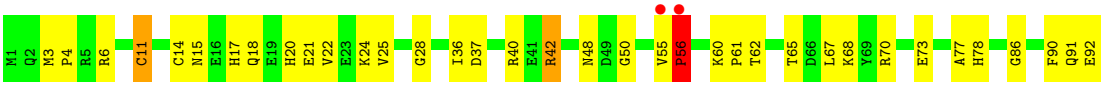
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



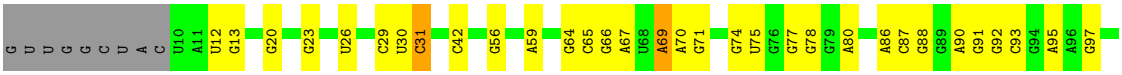
• Molecule 29: 50S ribosomal protein L44E

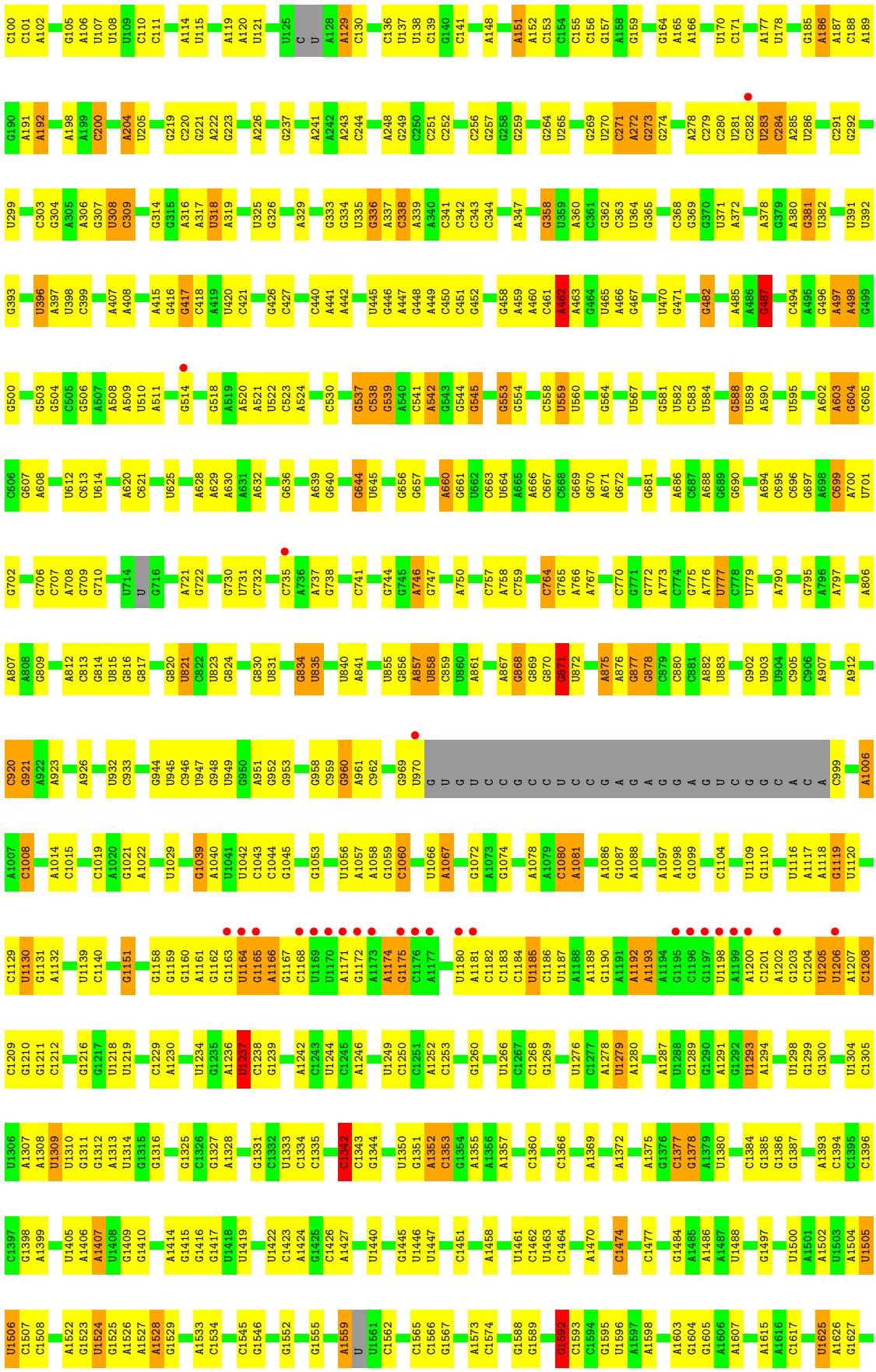
Chain 3:

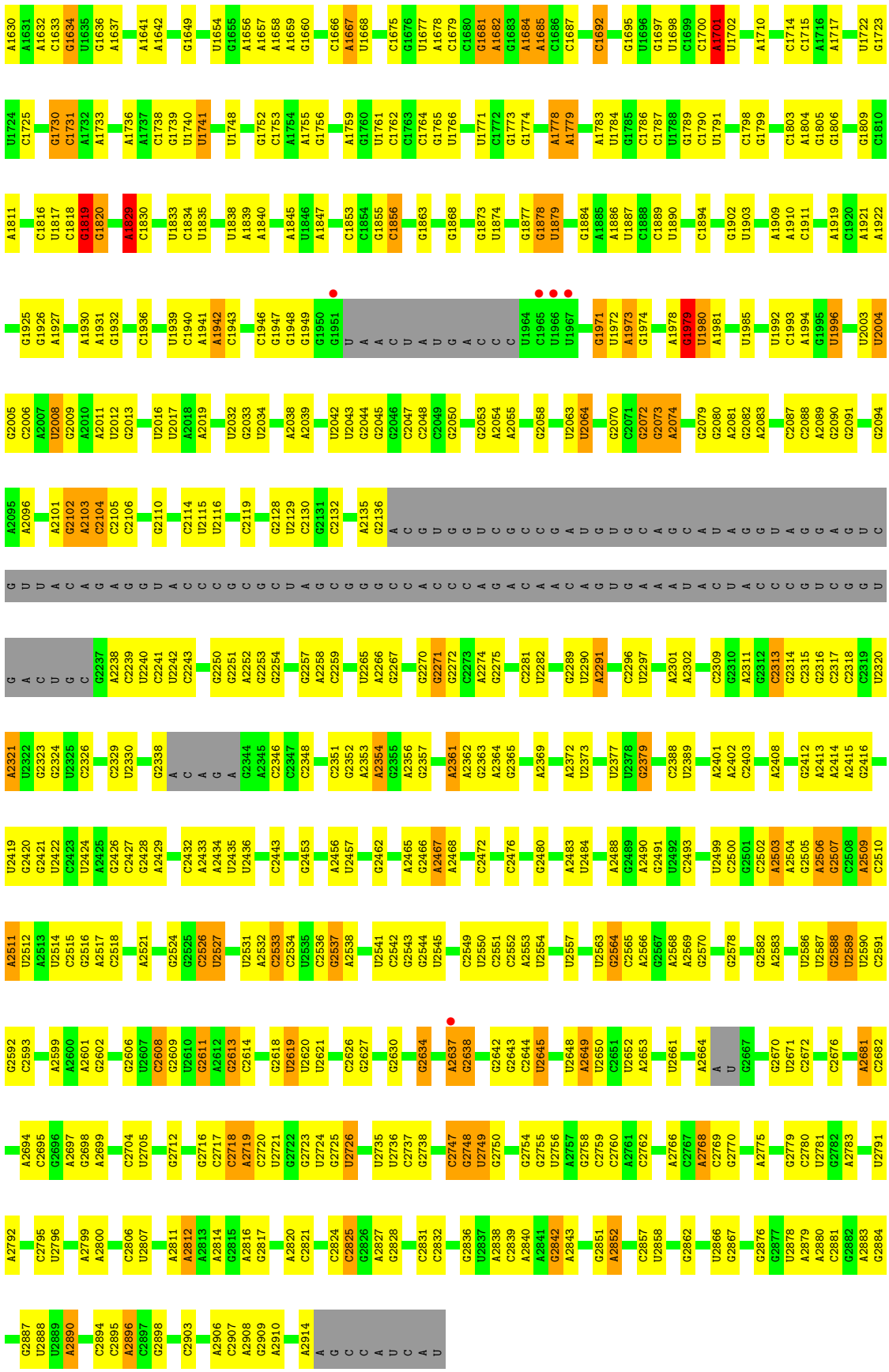


• Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

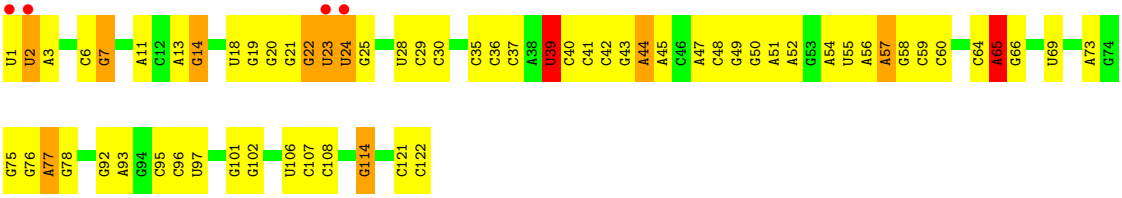



C100 C101 A102 G105 A106 U107 U108 U109 C110 C111 A114 U115 A119 A120 U121 U125 C U A128 A129 C130 C136 U137 U138 C139 G140 C141 A148 A151 A152 C153 C154 C155 C156 G157 A158 G159 G164 A165 A166 U170 C171 A177 U178 G185 A186 A187 C188 A189
G190 A191 A192 A198 A199 C200 A204 U205 G219 C220 G221 A222 G223 A226 G237 A241 A242 A243 C244 A248 G249 C250 C251 C252 C256 G257 G258 G259 G264 U265 G269 U270 C271 A272 G273 G274 A278 C279 C280 U281 C282 U283 C284 A285 U286 C291 G292
U299 C303 G304 A305 A306 G307 U308 C309 G314 G315 A316 A317 U318 A319 U325 G326 A329 G333 G334 U335 G336 A337 C338 A339 A340 C341 C342 C343 C344 A347 G358 U359 A360 C361 G362 C363 U364 G365 C368 G369 G370 U371 A372 A378 G379 A380 G381 U382 U391 U392
G393 U396 A397 U398 C399 A407 A408 A415 G416 G417 C418 A419 U420 C421 G426 C427 C440 A441 A442 U445 G446 A447 G448 A449 C450 C451 G452 G458 A459 A460 C461 A462 A463 G464 U465 A466 G467 U470 G471 G482 A485 A486 G487 C494 A495 G496 A497 A498 G499
G500 G503 G504 C505 G506 A507 A508 A509 U510 A511 G514 G518 A519 A520 A521 U522 C523 A524 C530 G537 C538 G539 A540 C541 A542 G543 G544 G545 G553 G554 C558 U559 U560 G564 U567 G581 U582 C583 U584 G588 U589 A590 U595 A602 A603 G604 C605
C606 G607 A608 U612 C613 U614 A620 C621 U625 A628 A629 A630 A631 A632 G636 A639 G640 G644 U645 G656 G657 A660 G661 U662 C663 U664 A665 A666 C667 C668 G669 G670 A671 G672 G681 A686 C687 A688 G689 G690 A694 C695 C696 G697 A698 C699 A700 U701
G702 G706 C707 A708 G709 G710 U714 U G716 A721 G722 G730 U731 C732 C735 A736 A737 G738 C741 G744 G745 A746 G747 A750 C757 A758 C759 C764 G765 A766 A767 C770 G771 G772 A773 C774 G775 A776 U777 C778 U779 A790 G795 A796 A797 A806
A807 A808 G809 A812 C813 G814 U815 C816 G817 G820 U821 C822 U823 G824 G830 U831 G834 U835 U840 A841 U855 G856 A857 U858 C859 U860 A861 A867 G868 G869 G870 G871 U872 A875 A876 G877 G878 C879 C880 C881 A882 U883 G902 U903 U904 C905 C906 A907 A912
C920 G921 A922 A923 A926 U932 C933 G944 U945 C946 U947 G948 U949 G950 A951 G952 G953 G958 C959 G960 A961 C962 G969 U970 G U G U C C G C C U C C G A G G A G A G U U C G G C C A C A C999 A1006
A1007 C1008 A1014 C1015 C1019 A1020 G1021 A1022 U1029 G1039 A1040 U1041 U1042 C1043 C1044 G1045 G1053 U1056 A1057 A1058 G1059 C1060 U1066 A1067 G1072 A1073 G1074 A1078 A1079 C1080 A1081 A1086 G1087 A1088 A1097 A1098 G1099 C1104 U1109 G1110 U1116 A1117 A1118 G1119 U1120
C1129 U1130 G1131 A1132 U1139 C1140 G1151 G1158 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171 G1172 A1173 A1174 G1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 A1194 G1195 C1196 G1197 U1198 A1199 A1200 C1201 A1202 G1203 C1204 U1205 U1206 A1207 C1208
C1209 G1210 G1211 C1212 G1216 G1217 U1218 U1219 C1229 A1230 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243 U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 G1260 U1266 C1267 C1268 G1269 U1276 C1277 A1278 U1279 A1280 A1287 U1288 C1289 G1290 A1291 G1292 U1293 A1294 U1298 G1299 G1300 U1304 C1305
U1306 A1307 A1308 U1309 U1310 G1311 G1312 A1313 U1314 G1315 G1316 G1325 C1326 G1327 A1328 G1331 C1332 U1333 C1334 C1335 C1342 C1343 G1344 U1350 G1351 A1352 C1353 G1354 A1355 A1356 A1357 C1360 C1366 A1369 A1372 A1375 G1376 C1377 G1378 A1379 U1380 C1384 G1385 G1386 G1387 A1393 C1394 C1395 C1396
C1397 G1398 A1399 U1405 A1406 A1407 U1408 G1409 G1410 A1414 G1415 G1416 G1417 U1418 U1419 U1422 C1423 A1424 G1425 C1426 A1427 U1440 G1445 U1446 U1447 C1451 A1458 U1461 C1462 U1463 C1464 A1470 C1474 C1477 G1484 A1485 A1486 A1487 U1488 G1497 U1500 A1501 A1502 U1503 A1504 U1505
U1506 C1507 C1508 A1522 G1523 U1524 G1525 A1526 A1527 A1528 G1529 A1533 C1534 C1545 G1546 G1552 G1555 A1559 U U1561 C1562 C1565 C1566 G1567 A1573 C1574 G1588 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 A1603 G1604 G1605 A1606 A1607 A1615 A1616 C1617 U1625 A1626 G1627



- Molecule 31: 5S RIBOSOMAL RNA

Chain 9:

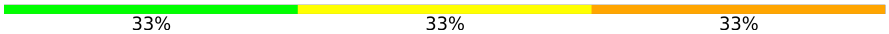


- Molecule 32: RNA (5'-R(*CP*CP*A)-3')

Chain 5:

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

Chain 6:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(Å^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(Å^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(Å^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(Å^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(Å^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.