



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:07 AM GMT

PDB ID : 3CME
Title : The Structure of CA 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 : 2.95 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

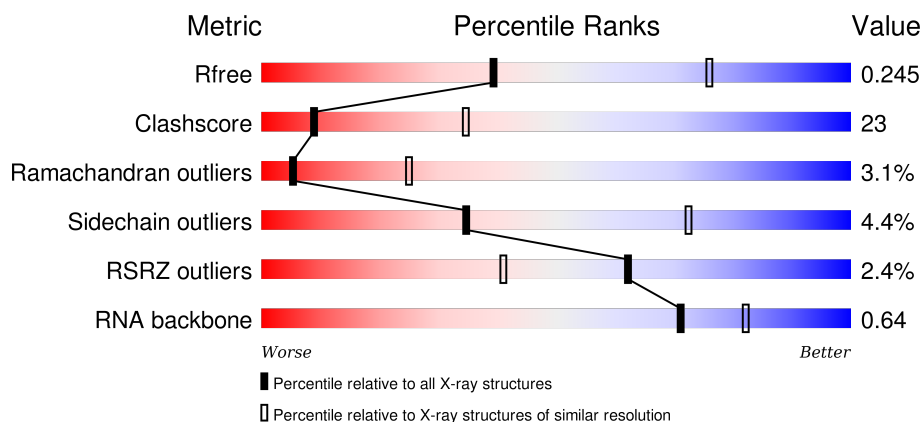
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)
RNA backbone	2183	1010 (3.36-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>2%</div> <div> <div>43%</div> <div>48%</div> <div>7%</div> </div> </div>
2	B	338	<div> <div>41%</div> <div>53%</div> <div>6%</div> </div>
3	C	246	<div> <div>43%</div> <div>51%</div> <div>6%</div> </div>
4	D	177	<div> <div>18%</div> <div>25%</div> <div>46%</div> <div>7%</div> <div>21%</div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	MG	0	8002	-	-	-	X
35	MG	0	8003	-	-	-	X
35	MG	0	8004	-	-	-	X
35	MG	0	8006	-	-	-	X
35	MG	0	8008	-	-	-	X
35	MG	0	8009	-	-	-	X
35	MG	0	8010	-	-	-	X
35	MG	0	8014	-	-	-	X
35	MG	0	8015	-	-	-	X
35	MG	0	8028	-	-	-	X
35	MG	0	8029	-	-	-	X
35	MG	0	8034	-	-	-	X
35	MG	0	8041	-	-	-	X
35	MG	0	8047	-	-	-	X
35	MG	0	8050	-	-	-	X
35	MG	0	8062	-	-	-	X
35	MG	0	8071	-	-	-	X
35	MG	0	8076	-	-	-	X
35	MG	0	8079	-	-	-	X
35	MG	0	8087	-	-	-	X
35	MG	A	8025	-	-	-	X
35	MG	A	8051	-	-	-	X
35	MG	B	8043	-	-	-	X
35	MG	C	8012	-	-	-	X
36	NA	0	8504	-	-	-	X
36	NA	0	8507	-	-	-	X
36	NA	0	8512	-	-	-	X
36	NA	0	8513	-	-	-	X
36	NA	0	8517	-	-	-	X
36	NA	0	8519	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	8520	-	-	-	X
36	NA	0	8521	-	-	-	X
36	NA	0	8523	-	-	-	X
36	NA	0	8527	-	-	-	X
36	NA	0	8528	-	-	-	X
36	NA	0	8530	-	-	-	X
36	NA	0	8533	-	-	-	X
36	NA	0	8534	-	-	-	X
36	NA	0	8535	-	-	-	X
36	NA	0	8542	-	-	-	X
36	NA	0	8547	-	-	-	X
36	NA	0	8550	-	-	-	X
36	NA	0	8552	-	-	-	X
36	NA	0	8553	-	-	-	X
36	NA	0	8556	-	-	-	X
36	NA	0	8557	-	-	-	X
36	NA	0	8559	-	-	-	X
36	NA	0	8560	-	-	-	X
36	NA	0	8562	-	-	-	X
36	NA	0	8563	-	-	-	X
36	NA	0	8565	-	-	-	X
36	NA	0	8567	-	-	-	X
36	NA	0	8568	-	-	-	X
36	NA	0	8569	-	-	-	X
36	NA	9	8572	-	-	-	X
36	NA	C	8503	-	-	-	X
37	SR	0	8904	-	-	-	X
37	SR	0	8910	-	-	-	X
37	SR	0	8948	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8981	-	-	-	X
37	SR	1	8913	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
37	SR	R	8912	-	-	-	X
38	CL	J	8801	-	-	X	-
38	CL	L	8814	-	-	X	-
39	K	0	8401	-	-	-	X
39	K	0	8402	-	-	-	X

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 99194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 30 is a RNA chain called 50S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26345	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
			2595	1156	471	847	121			

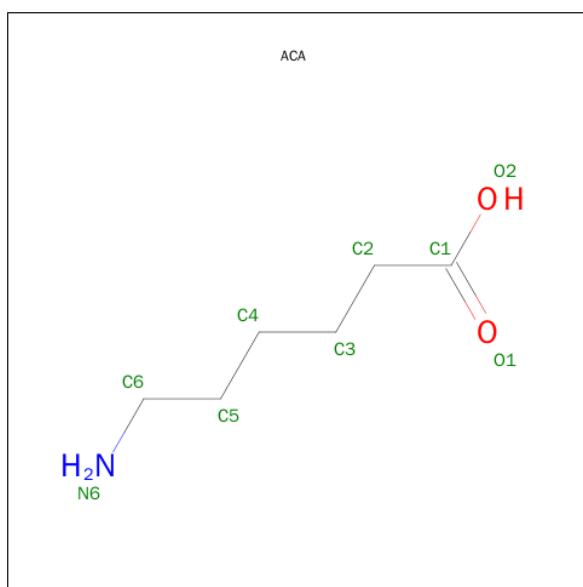
- Molecule 32 is a RNA chain called RNA (5'-R(*C*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	2	Total	C	N	O	P	0	0	0
			39	19	8	11	1			

- 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 PHENYLALANINE (three-letter code: ACA, PHE) (formula: C₆H₁₃NO₂, C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	6	2	Total	C	N	O	0	0
			19	15	2	2		

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total	Mg	0	0
			82	82		
35	Y	1	Total	Mg	0	0
			1	1		
35	K	1	Total	Mg	0	0
			1	1		
35	B	2	Total	Mg	0	0
			2	2		
35	C	1	Total	Mg	0	0
			1	1		
35	A	3	Total	Mg	0	0
			3	3		
35	T	1	Total	Mg	0	0
			1	1		
35	2	1	Total	Mg	0	0
			1	1		
35	9	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	65	Total Na 65 65	0	0
36	J	1	Total Na 1 1	0	0
36	Q	1	Total Na 1 1	0	0
36	H	1	Total Na 1 1	0	0
36	C	1	Total Na 1 1	0	0
36	R	1	Total Na 1 1	0	0
36	9	3	Total Na 3 3	0	0
36	S	1	Total Na 1 1	0	0
36	M	1	Total Na 1 1	0	0

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	87	Total Sr 87 87	0	0
37	Y	1	Total Sr 1 1	0	0
37	H	2	Total Sr 2 2	0	0
37	B	2	Total Sr 2 2	0	0
37	1	2	Total Sr 2 2	0	0
37	A	3	Total Sr 3 3	0	0
37	T	2	Total Sr 2 2	0	0
37	R	1	Total Sr 1 1	0	0
37	9	3	Total Sr 3 3	0	0
37	L	1	Total Sr 1 1	0	0
37	3	3	Total Sr 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	6	Total	Cl	0	0
			6	6		
38	J	4	Total	Cl	0	0
			4	4		
38	Q	1	Total	Cl	0	0
			1	1		
38	B	1	Total	Cl	0	0
			1	1		
38	A	1	Total	Cl	0	0
			1	1		
38	N	1	Total	Cl	0	0
			1	1		
38	O	1	Total	Cl	0	0
			1	1		
38	R	1	Total	Cl	0	0
			1	1		
38	Y	2	Total	Cl	0	0
			2	2		
38	L	2	Total	Cl	0	0
			2	2		
38	3	1	Total	Cl	0	0
			1	1		
38	M	1	Total	Cl	0	0
			1	1		

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

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

- Molecule 40 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	O	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	Z	1	Total	Cd	0	0
			1	1		
40	1	1	Total	Cd	0	0
			1	1		
40	3	1	Total	Cd	0	0
			1	1		
40	U	1	Total	Cd	0	0
			1	1		

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	9	138	Total	O	0	0
			138	138		
41	A	134	Total	O	0	0
			134	134		
41	B	156	Total	O	0	0
			156	156		
41	C	168	Total	O	0	0
			168	168		
41	D	49	Total	O	0	0
			49	49		
41	E	49	Total	O	0	0
			49	49		
41	F	31	Total	O	0	0
			31	31		
41	G	20	Total	O	0	0
			20	20		
41	H	78	Total	O	0	0
			78	78		
41	I	11	Total	O	0	0
			11	11		
41	J	58	Total	O	0	0
			58	58		
41	K	57	Total	O	0	0
			57	57		
41	L	91	Total	O	0	0
			91	91		
41	M	129	Total	O	0	0
			129	129		
41	N	68	Total	O	0	0
			68	68		

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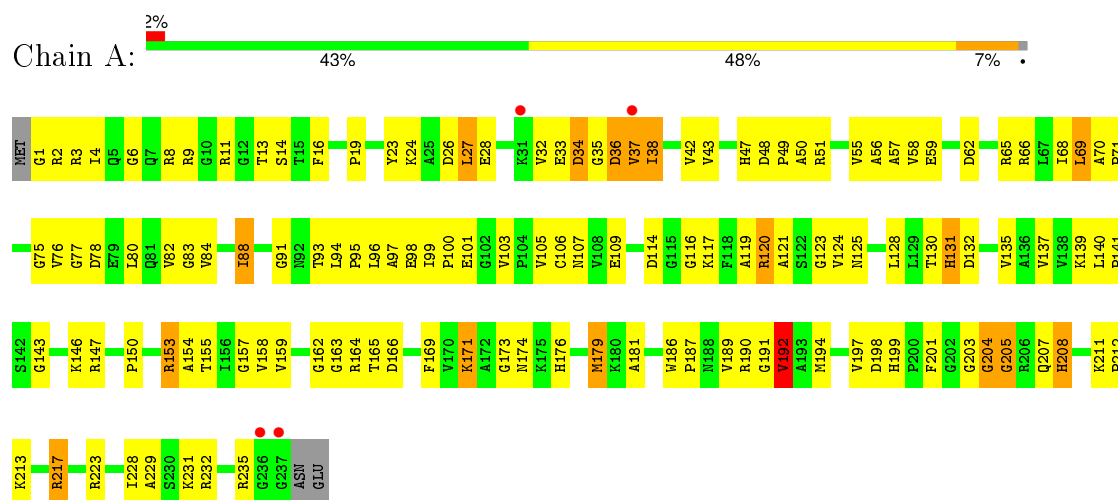
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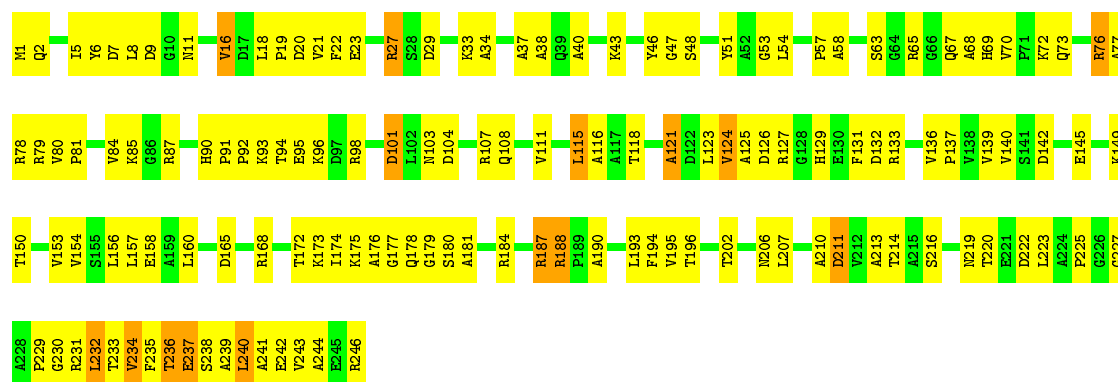
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	46	Total 46	O 46	0	0
41	P	72	Total 72	O 72	0	0
41	Q	52	Total 52	O 52	0	0
41	R	89	Total 89	O 89	0	0
41	S	35	Total 35	O 35	0	0
41	T	42	Total 42	O 42	0	0
41	U	29	Total 29	O 29	0	0
41	V	16	Total 16	O 16	0	0
41	W	75	Total 75	O 75	0	0
41	X	31	Total 31	O 31	0	0
41	Y	105	Total 105	O 105	0	0
41	Z	25	Total 25	O 25	0	0
41	0	5775	Total 5775	O 5775	0	0
41	1	57	Total 57	O 57	0	0
41	2	50	Total 50	O 50	0	0
41	3	66	Total 66	O 66	0	0
41	6	6	Total 6	O 6	0	0

3 Residue-property plots

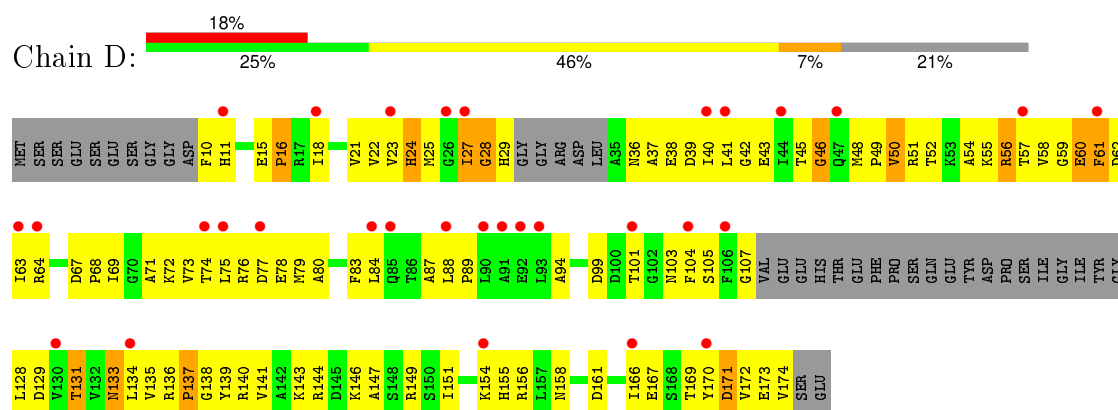
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

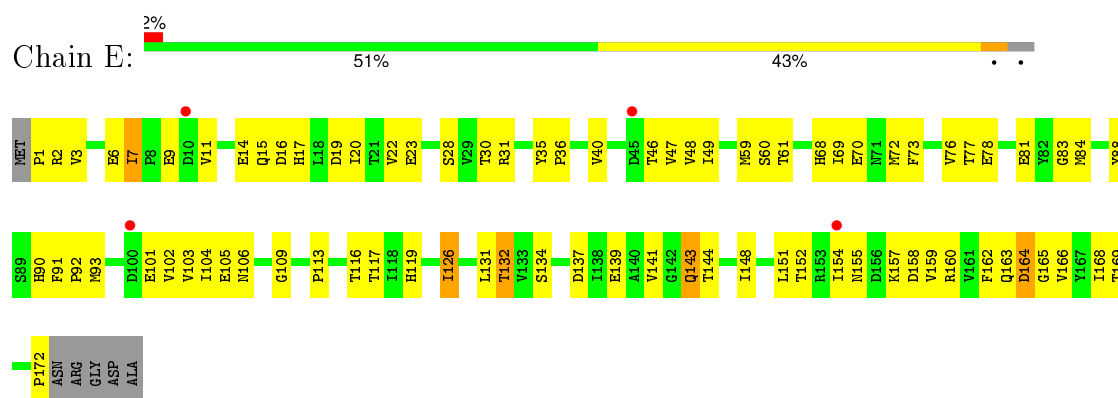




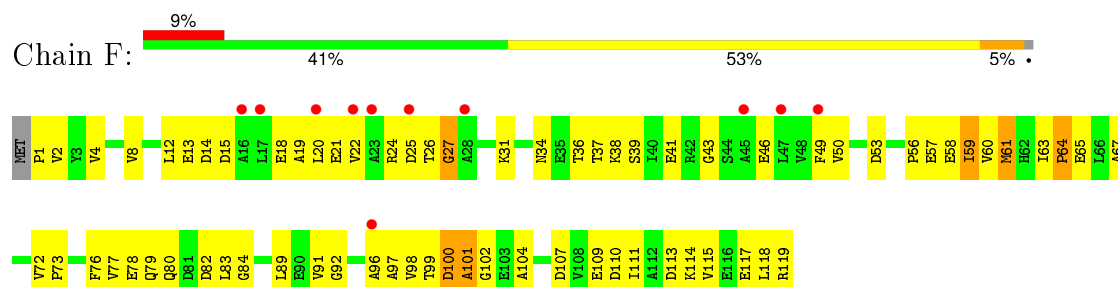
• Molecule 4: 50S ribosomal protein L5P



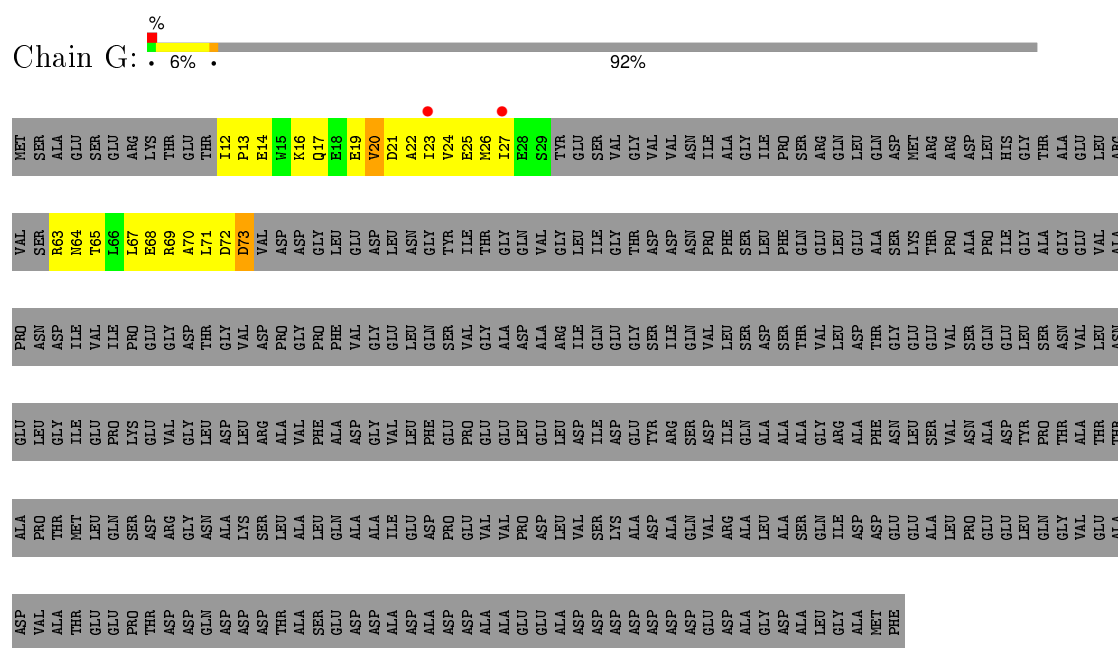
• Molecule 5: 50S ribosomal protein L6P



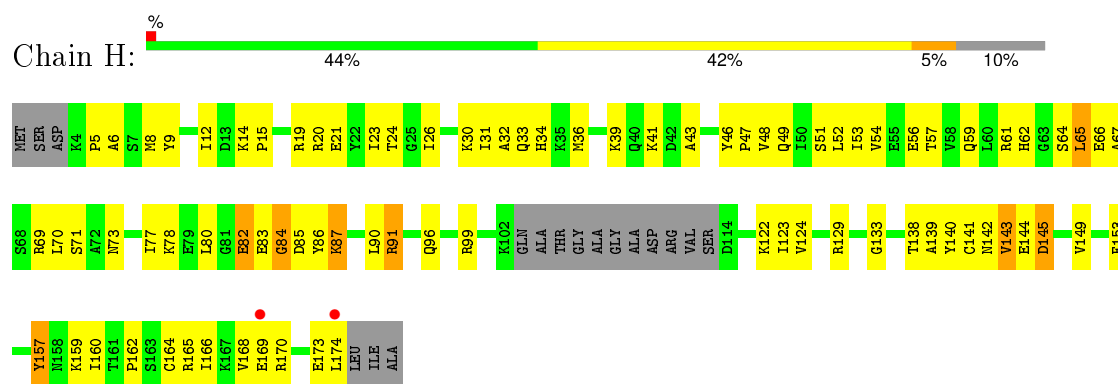
• Molecule 6: 50S ribosomal protein L7Ae



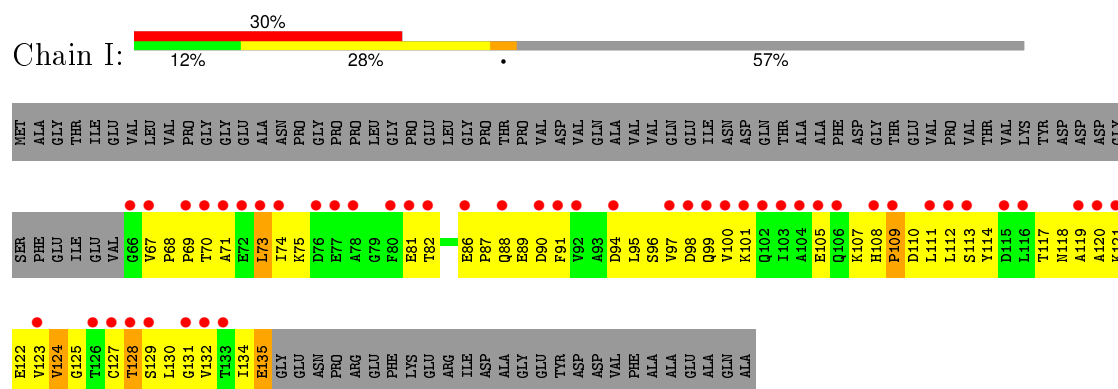
• Molecule 7: 50S ribosomal protein L10E



- Molecule 8: 50S ribosomal protein L10e

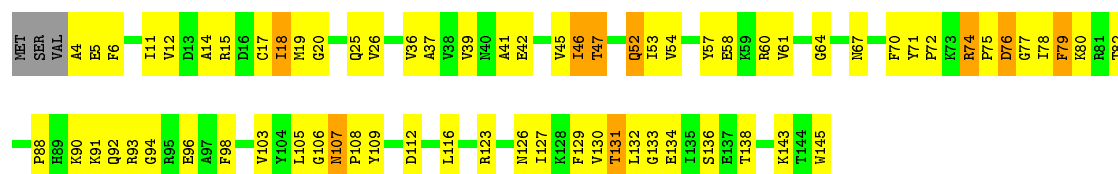


- Molecule 9: 50S ribosomal protein L11P



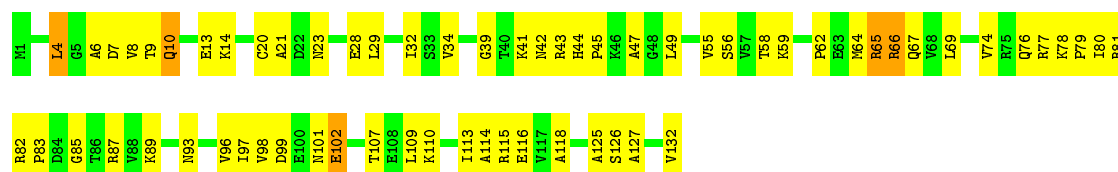
- Molecule 10: 50S ribosomal protein L13P





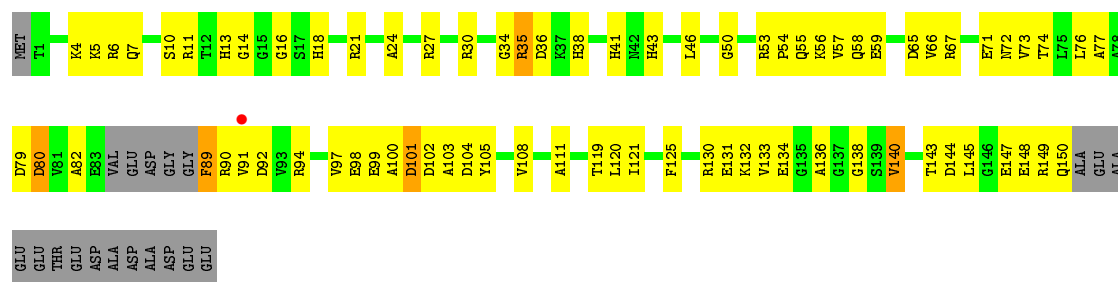
• Molecule 11: 50S ribosomal protein L14P

Chain K: 52% 45%



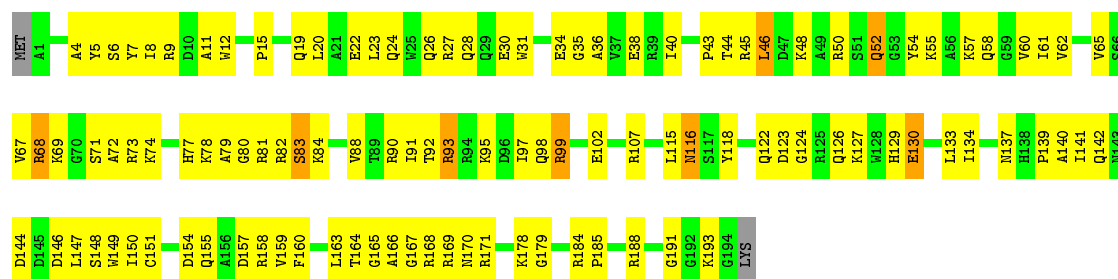
• Molecule 12: 50S ribosomal protein L15P

Chain L: 42% 43% 12%



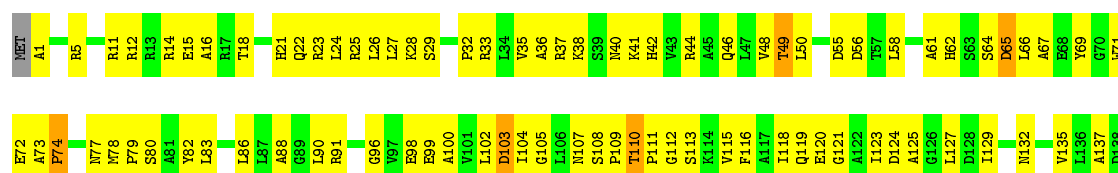
• Molecule 13: 50S ribosomal protein L15e

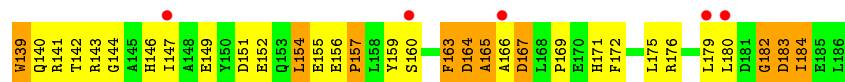
Chain M: 42% 53%



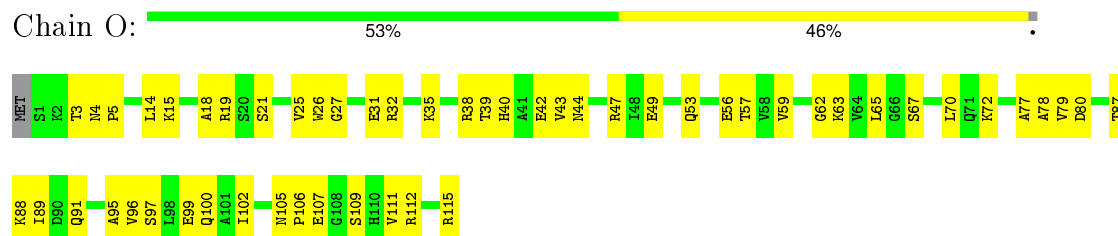
• Molecule 14: 50S ribosomal protein L18P

Chain N: 37% 54% 8%

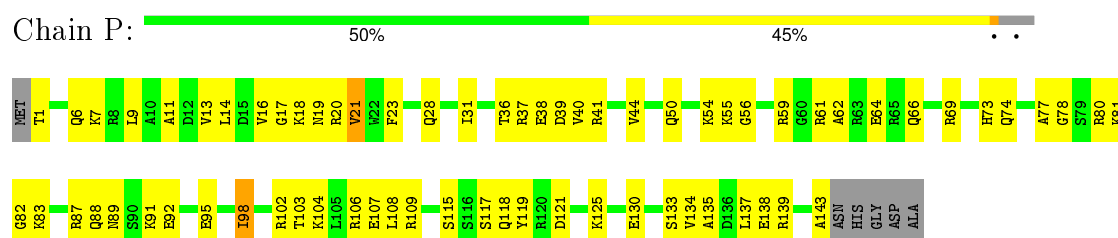




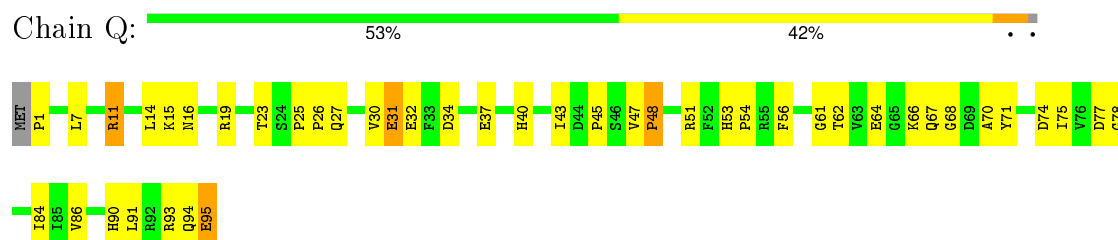
- Molecule 15: 50S ribosomal protein L18e



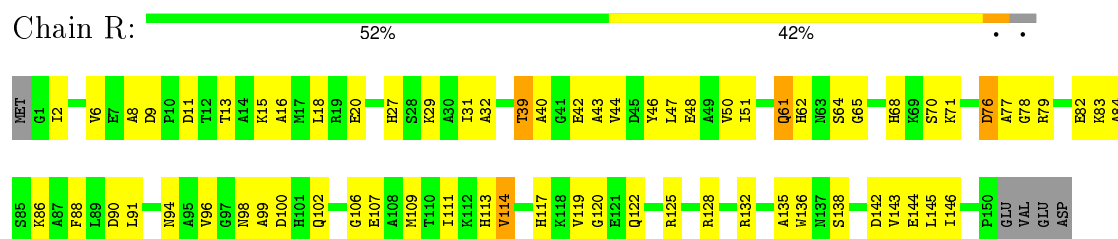
- Molecule 16: 50S ribosomal protein L19e



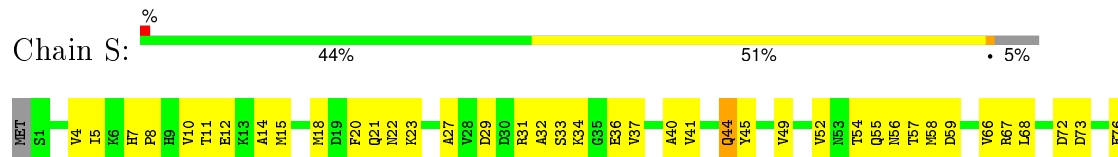
- Molecule 17: 50S ribosomal protein L21e

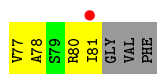


- Molecule 18: 50S ribosomal protein L22P

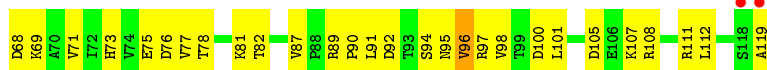
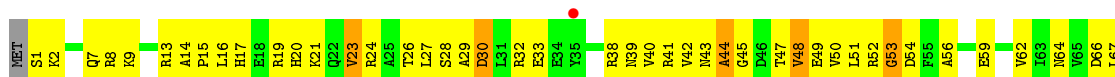


- Molecule 19: 50S ribosomal protein L23P

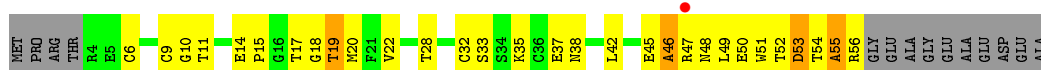




- Molecule 20: 50S ribosomal protein L24P



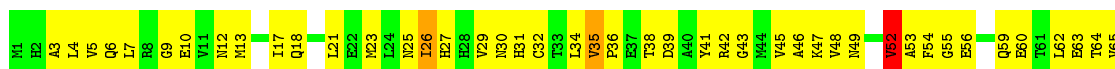
- Molecule 21: 50S ribosomal protein L24e



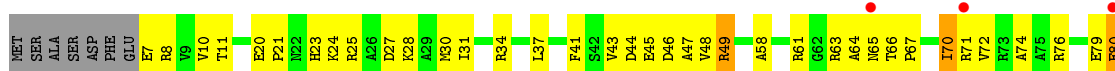
- Molecule 22: 50S ribosomal protein L29P

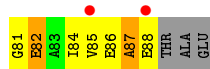


- Molecule 23: 50S ribosomal protein L30P

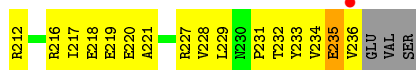
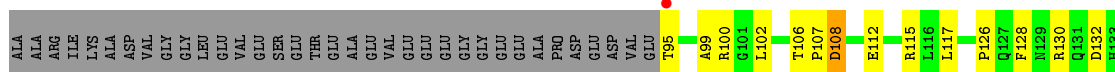
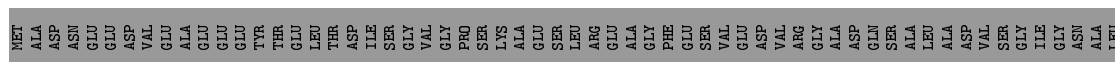
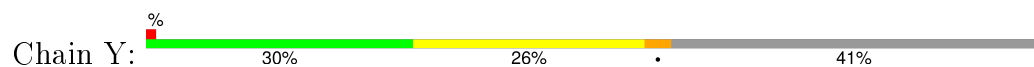


- Molecule 24: 50S ribosomal protein L31e

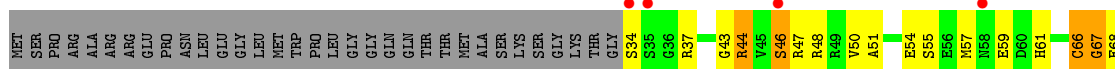
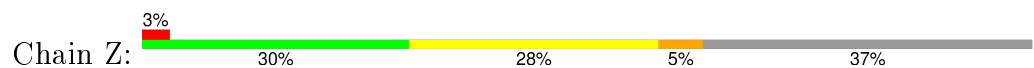




- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae



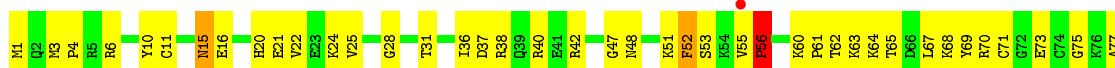
- Molecule 27: 50S ribosomal protein L37e

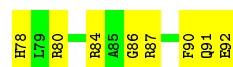


- Molecule 28: 50S ribosomal protein L39e

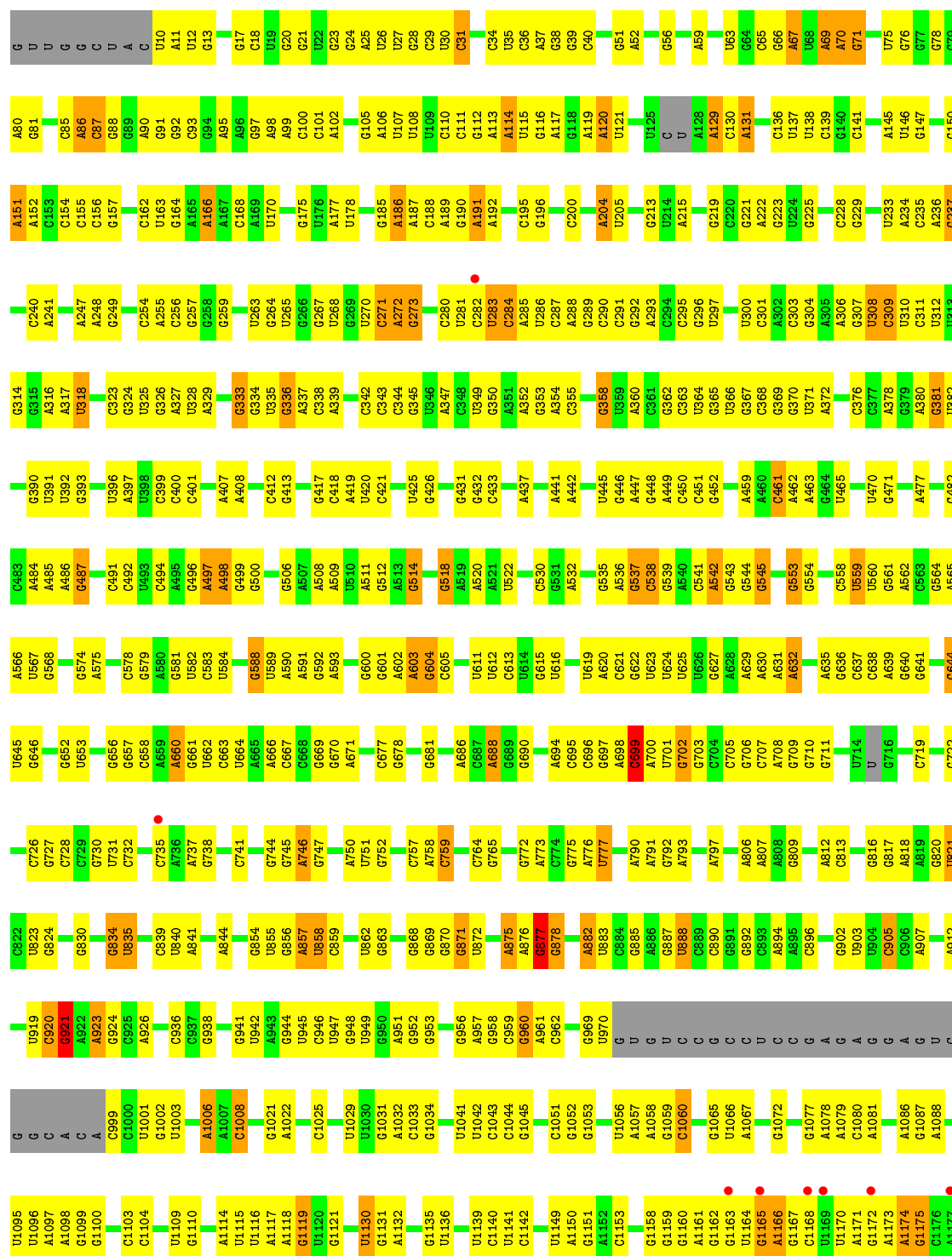


- Molecule 29: 50S ribosomal protein L44E

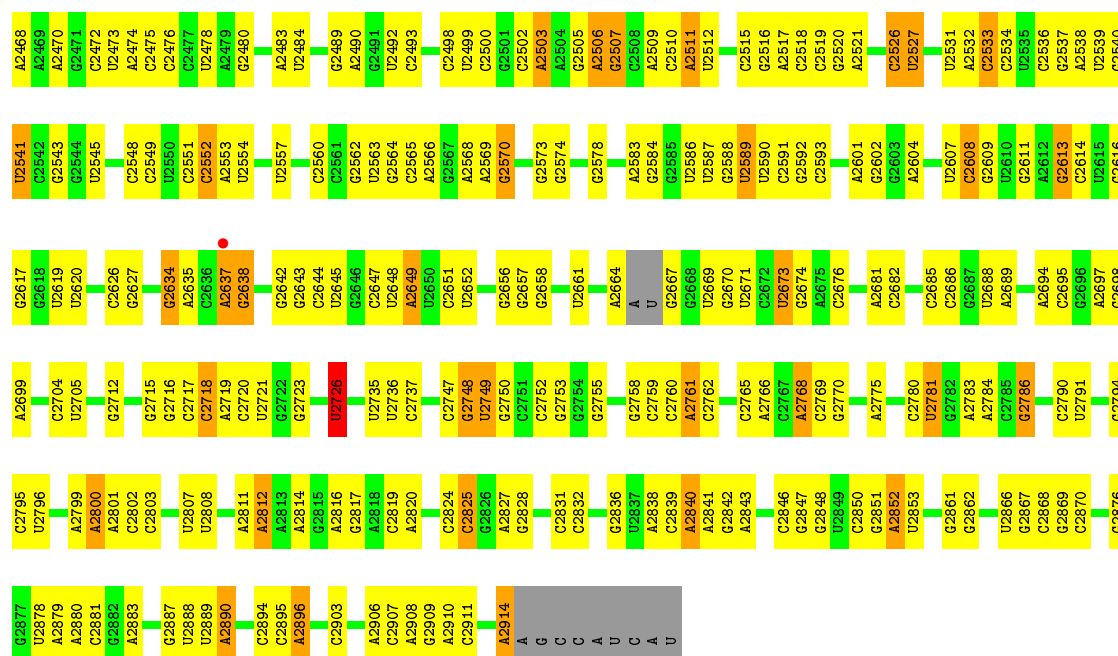




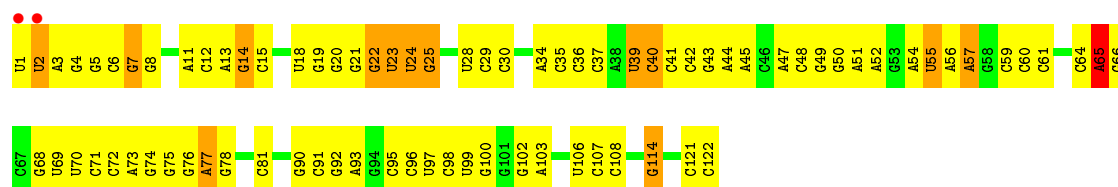
• Molecule 30: 50S RIBOSOMAL RNA







• Molecule 31: 5S RIBOSOMAL RNA



• Molecule 32: RNA (5'-R(*C*CP*A)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	210.79Å 297.78Å 572.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.95 85.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.82-2.95) 90.2 (85.07-2.39)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.198 , 0.255 0.193 , 0.245	Depositor DCC
R_{free} test set	3661 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 667135 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99194	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.37	0/1784	0.67	0/2403
2	B	0.36	0/2687	0.68	0/3644
3	C	0.38	0/1883	0.65	0/2547
4	D	0.33	0/1109	0.58	0/1493
5	E	0.35	0/1380	0.61	0/1875
6	F	0.36	0/899	0.60	0/1219
7	G	0.30	0/241	0.51	0/324
8	H	0.36	0/1300	0.67	0/1738
9	I	0.29	0/524	0.54	0/711
10	J	0.38	0/1134	0.62	0/1525
11	K	0.39	0/1002	0.68	0/1346
12	L	0.34	0/1128	0.65	0/1504
13	M	0.38	0/1580	0.61	0/2111
14	N	0.31	0/1472	0.66	1/1994 (0.1%)
15	O	0.35	0/872	0.64	0/1176
16	P	0.37	0/1145	0.56	0/1524
17	Q	0.36	0/747	0.68	0/1001
18	R	0.39	0/1170	0.66	0/1574
19	S	0.37	0/646	0.60	1/870 (0.1%)
20	T	0.35	0/956	0.64	0/1284
21	U	0.36	0/417	0.64	0/562
22	V	0.29	0/502	0.57	0/675
23	W	0.39	0/1217	1.24	2/1650 (0.1%)
24	X	0.35	0/662	0.61	0/890
25	Y	0.37	0/1146	0.65	0/1536
26	Z	0.36	0/582	0.62	0/776
27	1	0.41	0/438	0.62	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.40	0/769	0.61	0/1019
30	0	0.42	1/65948 (0.0%)	0.69	18/102852 (0.0%)
31	9	0.37	0/2894	0.71	0/4509
32	5	0.45	0/43	0.61	0/65

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.38	0/40	0.60	0/60
All	All	0.40	1/98718 (0.0%)	0.69	22/147564 (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
23	W	0	1
30	0	0	39
31	9	0	2
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	1942	A	O3'-P	-6.61	1.53	1.61

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	36.02	168.52	110.90
23	W	52	VAL	CA-CB-CG2	-23.54	75.59	110.90
30	0	1942	A	C5'-C4'-C3'	7.03	127.25	116.00
30	0	1942	A	OP2-P-O3'	6.73	120.00	105.20
30	0	1942	A	C5'-C4'-O4'	6.64	117.07	109.10

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	333	G	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
30	0	63	U	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1752	0	1764	160	0
2	B	2624	0	2530	225	0
3	C	1859	0	1811	154	0
4	D	1093	0	1083	102	0
5	E	1356	0	1264	81	0
6	F	889	0	841	68	0
7	G	240	0	231	30	0
8	H	1281	0	1290	86	0
9	I	518	0	495	67	0
10	J	1119	0	1096	87	0
11	K	993	0	1025	77	0
12	L	1117	0	1071	85	0
13	M	1557	0	1571	130	0
14	N	1444	0	1399	140	0
15	O	864	0	868	60	0
16	P	1135	0	1120	68	0
17	Q	734	0	726	50	0
18	R	1148	0	1119	81	0
19	S	640	0	600	36	0
20	T	949	0	922	88	0
21	U	410	0	364	38	0
22	V	499	0	511	49	0
23	W	1195	0	1135	118	0
24	X	653	0	651	50	0
25	Y	1130	0	1133	82	0
26	Z	572	0	529	35	0
27	1	431	0	426	43	0
28	2	396	0	413	30	0
29	3	754	0	726	58	0
30	0	59017	0	29809	1406	0
31	9	2595	0	1322	96	0
32	5	39	0	24	3	0
33	6	59	0	35	6	0
34	6	19	0	20	0	0
35	0	82	0	0	0	0
35	2	1	0	0	0	0
35	9	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	3	0	0	0	0
35	B	2	0	0	0	0
35	C	1	0	0	0	0
35	K	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	65	0	0	0	0
36	9	3	0	0	0	0
36	C	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	87	0	0	1	0
37	1	2	0	0	0	0
37	3	3	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	2	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	T	2	0	0	0	0
37	Y	1	0	0	0	0
38	0	6	0	0	1	0
38	3	1	0	0	0	0
38	A	1	0	0	0	0
38	B	1	0	0	0	0
38	J	4	0	0	4	0
38	L	2	0	0	2	0
38	M	1	0	0	1	0
38	N	1	0	0	0	0
38	O	1	0	0	1	0
38	Q	1	0	0	1	0
38	R	1	0	0	0	0
38	Y	2	0	0	0	0
39	0	2	0	0	0	0
40	1	1	0	0	0	0
40	3	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	O	1	0	0	0	0
40	U	1	0	0	0	0
40	Z	1	0	0	0	0
41	0	5775	0	0	197	0
41	1	57	0	0	3	0
41	2	50	0	0	2	0
41	3	66	0	0	7	0
41	6	6	0	0	4	0
41	9	138	0	0	12	0
41	A	134	0	0	19	0
41	B	156	0	0	21	0
41	C	168	0	0	21	0
41	D	49	0	0	6	0
41	E	49	0	0	5	0
41	F	31	0	0	3	0
41	G	20	0	0	2	0
41	H	78	0	0	9	0
41	I	11	0	0	3	0
41	J	58	0	0	2	0
41	K	57	0	0	3	0
41	L	91	0	0	11	0
41	M	129	0	0	5	0
41	N	68	0	0	14	0
41	O	46	0	0	6	0
41	P	72	0	0	7	0
41	Q	52	0	0	3	0
41	R	89	0	0	5	0
41	S	35	0	0	1	0
41	T	42	0	0	5	0
41	U	29	0	0	3	0
41	V	16	0	0	2	0
41	W	75	0	0	10	0
41	X	31	0	0	5	0
41	Y	105	0	0	5	0
41	Z	25	0	0	6	0
All	All	99194	0	59924	3515	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 23.

The worst 5 of 3515 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)
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.27	1.15
3:C:236:THR:HG22	3:C:239:ALA:H	1.00	1.13
37:O:8979:SR:SR	41:O:4399:HOH:O	0.84	1.13
14:N:37:ARG:HH12	31:9:6:C:H5''	1.10	1.09
30:O:870:G:H2'	30:O:871:G:H5''	1.30	1.08

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%)	198 (85%)	25 (11%)	10 (4%)	3	16
2	B	333/338 (98%)	285 (86%)	41 (12%)	7 (2%)	9	37
3	C	242/246 (98%)	202 (84%)	32 (13%)	8 (3%)	5	23
4	D	132/177 (75%)	87 (66%)	35 (26%)	10 (8%)	1	5
5	E	168/178 (94%)	150 (89%)	17 (10%)	1 (1%)	30	70
6	F	115/120 (96%)	94 (82%)	15 (13%)	6 (5%)	2	12
7	G	25/348 (7%)	15 (60%)	7 (28%)	3 (12%)	0	1
8	H	154/177 (87%)	125 (81%)	23 (15%)	6 (4%)	4	19
9	I	66/162 (41%)	43 (65%)	18 (27%)	5 (8%)	1	5
10	J	138/145 (95%)	120 (87%)	15 (11%)	3 (2%)	8	35
11	K	128/132 (97%)	115 (90%)	8 (6%)	5 (4%)	4	19
12	L	139/165 (84%)	106 (76%)	27 (19%)	6 (4%)	3	16
13	M	190/196 (97%)	170 (90%)	16 (8%)	4 (2%)	9	37
14	N	182/187 (97%)	153 (84%)	19 (10%)	10 (6%)	2	11
15	O	111/116 (96%)	92 (83%)	19 (17%)	0	100	100
16	P	139/149 (93%)	129 (93%)	8 (6%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Q	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	3	16
18	R	146/155 (94%)	131 (90%)	12 (8%)	3 (2%)	9	37
19	S	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	15	51
20	T	115/120 (96%)	95 (83%)	17 (15%)	3 (3%)	7	30
21	U	51/67 (76%)	45 (88%)	4 (8%)	2 (4%)	4	19
22	V	63/71 (89%)	53 (84%)	9 (14%)	1 (2%)	12	45
23	W	150/154 (97%)	131 (87%)	19 (13%)	0	100	100
24	X	78/92 (85%)	68 (87%)	7 (9%)	3 (4%)	4	19
25	Y	140/240 (58%)	128 (91%)	11 (8%)	1 (1%)	26	67
26	Z	69/116 (60%)	51 (74%)	13 (19%)	5 (7%)	1	6
27	1	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	10	40
28	2	42/50 (84%)	34 (81%)	8 (19%)	0	100	100
29	3	88/92 (96%)	77 (88%)	9 (10%)	2 (2%)	8	34
All	All	3659/4471 (82%)	3087 (84%)	460 (13%)	112 (3%)	5	25

5 of 112 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL
1	A	208	HIS
2	B	181	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	167 (94%)	11 (6%)	23	58
2	B	281/283 (99%)	266 (95%)	15 (5%)	28	65
3	C	192/193 (100%)	179 (93%)	13 (7%)	20	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	116/148 (78%)	111 (96%)	5 (4%)	35	73
5	E	151/156 (97%)	144 (95%)	7 (5%)	33	71
6	F	92/94 (98%)	92 (100%)	0	100	100
7	G	27/283 (10%)	26 (96%)	1 (4%)	41	77
8	H	133/145 (92%)	127 (96%)	6 (4%)	34	72
9	I	58/130 (45%)	57 (98%)	1 (2%)	68	90
10	J	117/121 (97%)	109 (93%)	8 (7%)	20	54
11	K	105/106 (99%)	102 (97%)	3 (3%)	50	82
12	L	113/127 (89%)	108 (96%)	5 (4%)	35	72
13	M	157/160 (98%)	149 (95%)	8 (5%)	29	67
14	N	148/150 (99%)	143 (97%)	5 (3%)	44	79
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	66	89
17	Q	79/80 (99%)	77 (98%)	2 (2%)	55	85
18	R	117/122 (96%)	112 (96%)	5 (4%)	35	73
19	S	71/74 (96%)	69 (97%)	2 (3%)	51	83
20	T	104/106 (98%)	99 (95%)	5 (5%)	31	69
21	U	44/53 (83%)	42 (96%)	2 (4%)	34	72
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	27	64
24	X	65/74 (88%)	58 (89%)	7 (11%)	8	28
25	Y	120/195 (62%)	111 (92%)	9 (8%)	17	49
26	Z	59/94 (63%)	56 (95%)	3 (5%)	29	67
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	40 (95%)	2 (5%)	31	69
29	3	78/79 (99%)	76 (97%)	2 (3%)	54	84
All	All	3079/3646 (84%)	2943 (96%)	136 (4%)	35	72

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	52	GLN
13	M	52	GLN

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Mol	Chain	Res	Type
25	Y	203	VAL
10	J	79	PHE
11	K	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	52	GLN
16	P	66	GLN
27	1	16	HIS
13	M	58	GLN
14	N	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	240 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	2 (1%)
32	5	1/3 (33%)	0	0
33	6	1/3 (33%)	0	0
All	All	2868/3051 (94%)	258 (8%)	32 (1%)

5 of 258 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 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1856	C
30	0	2011	A
30	0	2852	A
30	0	1979	G
30	0	2103	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	OMU	0	2587	30	12,22,23	0.97	2 (16%)	19,31,34	3.17	2 (10%)
30	OMG	0	2588	32,30	17,26,27	1.03	1 (5%)	21,38,41	2.65	3 (14%)
30	UR3	0	2619	30	12,22,23	0.84	1 (8%)	16,32,35	0.74	0
30	PSU	0	2621	30	13,21,22	1.69	2 (15%)	18,30,33	6.17	4 (22%)
30	1MA	0	628	30,36	14,25,26	1.01	1 (7%)	15,37,40	1.21	1 (6%)
33	8AN	6	76	33,30	15,24,25	1.02	1 (6%)	11,35,38	1.99	3 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	32,30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,36	-	0/3/25/26	0/3/3/3
33	8AN	6	76	33,30	-	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	C5-C1'	-5.05	1.47	1.52
30	0	2587	OMU	C6-C5	-2.21	1.33	1.38
30	0	2619	UR3	C6-C5	-2.18	1.33	1.38
33	6	76	8AN	C3'-N3'	-2.15	1.44	1.47
30	0	2587	OMU	C4-N3	2.18	1.37	1.33

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-21.73	114.47	128.33
30	0	2588	OMG	C5-C6-N1	-8.92	111.39	123.59
30	0	628	1MA	C2-N3-C4	-3.76	110.58	116.40
30	0	2587	OMU	C5-C4-N3	-3.38	114.44	123.12
30	0	2588	OMG	N3-C2-N1	-2.62	123.45	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2588	OMG	2	0
30	0	2619	UR3	1	0
33	6	76	8AN	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 305 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
34	PHE	6	77	-	10,11,12	1.26	2 (20%)	10,13,15	0.66	0
34	ACA	6	78	-	7,7,8	1.87	2 (28%)	5,6,8	1.61	1 (20%)

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
34	PHE	6	77	-	-	0/4/6/8	0/1/1/1
34	ACA	6	78	-	-	0/4/5/6	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	6	78	ACA	C3-C2	-4.17	1.36	1.52
34	6	77	PHE	CA-N	-2.05	1.41	1.47
34	6	78	ACA	C5-C6	2.23	1.62	1.51
34	6	77	PHE	CE1-CD1	2.57	1.44	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	6	78	ACA	C5-C4-C3	-2.32	102.56	114.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.33	4 (1%) 73 53	24, 46, 80, 105	0
2	B	337/338 (99%)	-0.53	1 (0%) 94 87	26, 49, 75, 88	0
3	C	246/246 (100%)	-0.45	0 100 100	24, 45, 69, 80	0
4	D	140/177 (79%)	1.01	31 (22%) 1 1	64, 93, 124, 135	0
5	E	172/178 (96%)	-0.16	4 (2%) 64 43	41, 62, 84, 92	0
6	F	119/120 (99%)	0.42	11 (9%) 11 6	50, 73, 100, 114	0
7	G	29/348 (8%)	0.83	2 (6%) 20 10	75, 95, 109, 113	0
8	H	160/177 (90%)	-0.12	2 (1%) 79 61	39, 58, 93, 99	0
9	I	70/162 (43%)	3.48	48 (68%) 0 0	141, 152, 166, 168	0
10	J	142/145 (97%)	-0.46	0 100 100	35, 47, 66, 86	0
11	K	132/132 (100%)	-0.67	0 100 100	28, 41, 63, 73	0
12	L	145/165 (87%)	-0.08	1 (0%) 89 76	22, 67, 105, 121	0
13	M	194/196 (98%)	-0.48	0 100 100	25, 46, 68, 82	0
14	N	186/187 (99%)	-0.11	5 (2%) 58 37	42, 63, 116, 124	0
15	O	115/116 (99%)	-0.36	0 100 100	39, 55, 67, 75	0
16	P	143/149 (95%)	-0.47	0 100 100	35, 51, 62, 68	0
17	Q	95/96 (98%)	-0.38	0 100 100	35, 49, 66, 75	0
18	R	150/155 (96%)	-0.56	0 100 100	22, 42, 62, 69	0
19	S	81/85 (95%)	-0.29	1 (1%) 81 63	44, 56, 81, 94	0
20	T	119/120 (99%)	-0.16	3 (2%) 61 39	38, 54, 84, 116	0
21	U	53/67 (79%)	-0.32	1 (1%) 70 50	38, 49, 73, 86	0
22	V	65/71 (91%)	0.93	10 (15%) 3 1	55, 78, 115, 122	0
23	W	154/154 (100%)	-0.37	1 (0%) 90 78	37, 48, 72, 86	0
24	X	82/92 (89%)	-0.19	5 (6%) 25 13	39, 55, 80, 103	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/240 (59%)	-0.53	2 (1%) 78 59	25, 44, 64, 90	0
26	Z	73/116 (62%)	0.12	4 (5%) 29 16	48, 67, 87, 96	0
27	1	56/57 (98%)	-0.59	0 100 100	22, 32, 39, 51	0
28	2	46/50 (92%)	-0.14	2 (4%) 39 23	29, 61, 76, 89	0
29	3	92/92 (100%)	-0.25	1 (1%) 82 65	33, 58, 71, 81	0
30	0	2749/2923 (94%)	-0.50	17 (0%) 90 78	16, 45, 92, 179	0
31	9	122/122 (100%)	-0.56	2 (1%) 74 55	36, 65, 92, 148	0
32	5	2/3 (66%)	2.15	1 (50%) 0 0	100, 100, 100, 102	0
33	6	2/3 (66%)	1.75	1 (50%) 0 0	96, 96, 96, 104	0
All	All	6650/7522 (88%)	-0.32	160 (2%) 62 41	16, 50, 99, 179	0

The worst 5 of 160 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	66	GLY	16.5
22	V	40	PRO	8.9
9	I	113	SER	8.1
9	I	72	GLU	7.6
9	I	132	VAL	7.4

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
33	8AN	6	76	22/23	0.86	0.29	-	87,92,94,95	0
30	1MA	0	628	23/24	0.98	0.17	-	36,40,42,42	0
30	UR3	0	2619	21/22	0.98	0.14	-	40,41,44,47	0
30	OMU	0	2587	21/22	0.97	0.12	-	30,33,38,38	0
30	PSU	0	2621	20/21	0.98	0.15	-	36,38,42,42	0
30	OMG	0	2588	24/25	0.97	0.12	-	30,34,35,37	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
36	NA	0	8547	1/1	0.79	0.62	78.08	78,78,78,78	0
36	NA	0	8519	1/1	0.62	0.83	59.37	71,71,71,71	0
35	MG	0	8087	1/1	0.13	0.81	57.94	107,107,107,107	0
36	NA	0	8535	1/1	0.56	0.87	57.55	75,75,75,75	0
36	NA	0	8527	1/1	0.78	0.44	26.79	73,73,73,73	0
35	MG	0	8050	1/1	0.96	0.32	26.41	152,152,152,152	0
35	MG	0	8079	1/1	0.80	0.38	22.86	64,64,64,64	0
39	K	0	8401	1/1	0.49	0.82	21.78	82,82,82,82	0
35	MG	0	8071	1/1	0.93	0.41	18.66	88,88,88,88	0
36	NA	0	8562	1/1	0.84	0.36	18.19	55,55,55,55	0
39	K	0	8402	1/1	-0.03	0.91	17.71	117,117,117,117	0
37	SR	L	8969	1/1	0.75	0.45	17.24	175,175,175,175	0
36	NA	0	8523	1/1	0.95	0.23	15.16	61,61,61,61	0
35	MG	0	8010	1/1	0.47	0.42	14.06	78,78,78,78	0
36	NA	0	8521	1/1	0.95	0.34	13.52	51,51,51,51	0
36	NA	0	8512	1/1	0.94	0.44	13.19	46,46,46,46	0
35	MG	0	8076	1/1	0.96	0.28	11.92	72,72,72,72	0
36	NA	9	8572	1/1	0.60	0.25	11.87	96,96,96,96	0
35	MG	A	8051	1/1	0.94	0.98	11.85	82,82,82,82	0
36	NA	0	8520	1/1	0.90	0.23	11.80	58,58,58,58	0
36	NA	0	8556	1/1	0.89	0.80	11.57	75,75,75,75	0
36	NA	0	8567	1/1	0.72	0.34	10.87	61,61,61,61	0
35	MG	0	8029	1/1	0.92	0.24	10.86	83,83,83,83	0
35	MG	0	8009	1/1	0.98	0.32	10.63	1,1,1,1	0
36	NA	0	8568	1/1	0.91	0.43	10.33	18,18,18,18	0
36	NA	0	8565	1/1	0.88	0.37	10.03	48,48,48,48	0
36	NA	0	8533	1/1	0.96	0.28	9.74	64,64,64,64	0
36	NA	0	8507	1/1	0.95	0.26	9.64	29,29,29,29	0
35	MG	0	8028	1/1	0.96	0.22	8.99	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8563	1/1	0.94	0.30	8.43	51,51,51,51	0
35	MG	0	8047	1/1	0.87	0.26	8.07	92,92,92,92	0
37	SR	B	8987	1/1	0.86	0.39	7.43	199,199,199,199	0
36	NA	0	8553	1/1	0.88	0.25	7.30	100,100,100,100	0
36	NA	0	8552	1/1	0.89	0.26	7.25	86,86,86,86	0
35	MG	0	8062	1/1	0.93	0.30	7.22	41,41,41,41	0
36	NA	0	8550	1/1	0.88	0.25	6.56	51,51,51,51	0
36	NA	0	8557	1/1	0.14	0.21	6.52	82,82,82,82	0
35	MG	0	8002	1/1	1.00	0.28	5.81	19,19,19,19	0
36	NA	0	8559	1/1	0.85	0.16	5.75	64,64,64,64	0
37	SR	0	8949	1/1	0.99	0.16	5.51	62,62,62,62	0
35	MG	0	8041	1/1	0.94	0.19	5.39	33,33,33,33	0
35	MG	0	8014	1/1	0.94	0.18	5.37	16,16,16,16	0
36	NA	0	8560	1/1	0.82	0.34	4.99	134,134,134,134	0
35	MG	C	8012	1/1	0.98	0.28	4.98	17,17,17,17	0
36	NA	0	8530	1/1	0.90	0.24	4.90	49,49,49,49	0
35	MG	A	8025	1/1	0.98	0.22	4.87	39,39,39,39	0
37	SR	0	8904	1/1	0.98	0.21	4.87	55,55,55,55	0
36	NA	0	8513	1/1	0.91	0.25	4.77	53,53,53,53	0
35	MG	0	8008	1/1	0.89	0.17	4.26	9,9,9,9	0
36	NA	0	8504	1/1	0.93	0.23	4.08	31,31,31,31	0
35	MG	0	8015	1/1	0.93	0.17	3.71	41,41,41,41	0
36	NA	0	8569	1/1	0.82	0.22	3.70	32,32,32,32	0
37	SR	0	8948	1/1	0.97	0.17	3.69	65,65,65,65	0
36	NA	0	8534	1/1	0.95	0.32	3.45	68,68,68,68	0
36	NA	0	8517	1/1	0.95	0.20	3.29	36,36,36,36	0
36	NA	0	8528	1/1	0.91	0.16	3.22	55,55,55,55	0
37	SR	1	8913	1/1	0.99	0.20	2.86	54,54,54,54	0
36	NA	C	8503	1/1	0.89	0.27	2.66	31,31,31,31	0
35	MG	0	8006	1/1	0.97	0.18	2.65	8,8,8,8	0
37	SR	0	8910	1/1	0.99	0.16	2.43	47,47,47,47	0
35	MG	B	8043	1/1	0.98	0.17	2.40	29,29,29,29	0
35	MG	0	8004	1/1	0.97	0.20	2.40	21,21,21,21	0
35	MG	0	8034	1/1	0.92	0.20	2.33	30,30,30,30	0
37	SR	R	8912	1/1	1.00	0.20	2.25	64,64,64,64	0
37	SR	0	8981	1/1	0.97	0.18	2.18	117,117,117,117	0
36	NA	0	8542	1/1	0.95	0.20	2.13	31,31,31,31	0
35	MG	0	8003	1/1	0.93	0.18	2.07	14,14,14,14	0
35	MG	K	8054	1/1	0.97	0.15	1.83	15,15,15,15	0
36	NA	0	8515	1/1	0.98	0.22	1.67	26,26,26,26	0
37	SR	0	8964	1/1	0.97	0.15	1.53	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8935	1/1	0.98	0.14	1.09	73,73,73,73	0
35	MG	0	8011	1/1	0.97	0.18	1.02	4,4,4,4	0
37	SR	0	8922	1/1	1.00	0.17	1.00	61,61,61,61	0
37	SR	3	8932	1/1	0.95	0.17	0.97	74,74,74,74	0
35	MG	0	8052	1/1	0.85	0.14	0.86	42,42,42,42	0
36	NA	0	8575	1/1	0.92	0.16	0.69	44,44,44,44	0
37	SR	0	8943	1/1	0.99	0.12	0.44	88,88,88,88	0
38	CL	O	8808	1/1	0.92	0.16	0.23	75,75,75,75	0
36	NA	M	8539	1/1	0.97	0.14	0.21	33,33,33,33	0
35	MG	0	8088	1/1	0.96	0.14	0.21	40,40,40,40	0
38	CL	J	8816	1/1	0.93	0.14	0.21	80,80,80,80	0
37	SR	0	8985	1/1	0.89	0.11	0.15	142,142,142,142	0
38	CL	J	8821	1/1	0.92	0.17	0.12	64,64,64,64	0
38	CL	0	8812	1/1	0.97	0.13	0.12	50,50,50,50	0
36	NA	0	8522	1/1	0.97	0.11	0.08	72,72,72,72	0
37	SR	0	8957	1/1	0.91	0.13	-0.06	124,124,124,124	0
40	CD	1	8702	1/1	0.99	0.12	-0.20	57,57,57,57	0
38	CL	M	8818	1/1	0.94	0.12	-0.57	46,46,46,46	0
36	NA	J	8538	1/1	0.99	0.12	-0.68	31,31,31,31	0
36	NA	0	8564	1/1	0.86	0.09	-0.68	35,35,35,35	0
35	MG	0	8084	1/1	0.94	0.10	-0.70	27,27,27,27	0
35	MG	0	8007	1/1	0.98	0.15	-0.75	30,30,30,30	0
36	NA	Q	8540	1/1	0.92	0.11	-0.88	66,66,66,66	0
36	NA	0	8537	1/1	0.95	0.09	-0.96	21,21,21,21	0
40	CD	Z	8703	1/1	0.99	0.10	-0.97	55,55,55,55	0
35	MG	T	8057	1/1	0.97	0.17	-1.01	31,31,31,31	0
35	MG	A	8044	1/1	0.61	0.08	-1.06	51,51,51,51	0
40	CD	U	8701	1/1	0.99	0.09	-1.07	57,57,57,57	0
37	SR	A	8929	1/1	0.95	0.09	-1.27	114,114,114,114	0
37	SR	H	8972	1/1	0.82	0.09	-1.50	132,132,132,132	0
38	CL	L	8810	1/1	0.89	0.08	-1.62	56,56,56,56	0
40	CD	3	8704	1/1	0.99	0.08	-1.70	52,52,52,52	0
37	SR	0	8962	1/1	0.60	0.11	-1.74	104,104,104,104	0
35	MG	0	8021	1/1	0.96	0.09	-1.77	24,24,24,24	0
37	SR	0	8970	1/1	0.98	0.08	-1.97	99,99,99,99	0
35	MG	0	8075	1/1	0.90	0.08	-2.02	38,38,38,38	0
38	CL	B	8819	1/1	0.92	0.11	-2.24	62,62,62,62	0
38	CL	3	8804	1/1	0.92	0.11	-2.44	60,60,60,60	0
37	SR	0	8945	1/1	0.95	0.09	-2.65	104,104,104,104	0
37	SR	0	8975	1/1	0.95	0.06	-2.78	125,125,125,125	0
37	SR	0	8992	1/1	0.90	0.05	-3.35	122,122,122,122	0
38	CL	0	8805	1/1	0.95	0.07	-5.12	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8013	1/1	0.98	0.04	-9.12	20,20,20,20	0
35	MG	Y	8086	1/1	0.95	0.05	-9.12	48,48,48,48	0
35	MG	0	8001	1/1	0.99	0.23	-	7,7,7,7	0
37	SR	0	9001	1/1	0.41	0.37	-	190,190,190,190	0
35	MG	0	8027	1/1	0.94	0.15	-	28,28,28,28	0
37	SR	0	8991	1/1	0.87	0.10	-	148,148,148,148	0
37	SR	0	8963	1/1	0.98	0.14	-	74,74,74,74	0
36	NA	0	8524	1/1	0.97	0.13	-	52,52,52,52	0
35	MG	0	8061	1/1	0.97	0.25	-	17,17,17,17	0
36	NA	0	8502	1/1	0.97	0.34	-	60,60,60,60	0
37	SR	0	8937	1/1	0.97	0.22	-	69,69,69,69	0
35	MG	0	8049	1/1	0.95	0.98	-	103,103,103,103	0
35	MG	0	8064	1/1	0.88	0.24	-	53,53,53,53	0
35	MG	0	8032	1/1	0.95	0.04	-	21,21,21,21	0
36	NA	0	8508	1/1	0.87	0.12	-	27,27,27,27	0
35	MG	0	8089	1/1	0.90	0.10	-	31,31,31,31	0
37	SR	0	8947	1/1	0.96	0.15	-	91,91,91,91	0
36	NA	0	8545	1/1	0.80	0.34	-	64,64,64,64	0
37	SR	0	8995	1/1	0.91	0.15	-	98,98,98,98	0
36	NA	0	8506	1/1	0.83	0.07	-	50,50,50,50	0
35	MG	9	8074	1/1	0.98	0.23	-	52,52,52,52	0
35	MG	0	8016	1/1	0.85	0.38	-	131,131,131,131	0
40	CD	O	8705	1/1	0.89	0.05	-	111,111,111,111	0
37	SR	0	8936	1/1	0.95	0.18	-	67,67,67,67	0
35	MG	0	8035	1/1	0.86	0.14	-	84,84,84,84	0
37	SR	0	8934	1/1	0.98	0.17	-	71,71,71,71	0
35	MG	0	8072	1/1	0.88	0.17	-	55,55,55,55	0
38	CL	0	8813	1/1	0.93	0.09	-	63,63,63,63	0
37	SR	3	8953	1/1	0.98	0.16	-	110,110,110,110	0
36	NA	0	8570	1/1	0.94	0.15	-	48,48,48,48	0
37	SR	0	8906	1/1	0.99	0.21	-	56,56,56,56	0
37	SR	Y	9002	1/1	0.91	0.11	-	124,124,124,124	0
37	SR	3	8999	1/1	1.00	0.13	-	69,69,69,69	0
35	MG	0	8005	1/1	0.94	0.25	-	25,25,25,25	0
37	SR	0	8926	1/1	0.95	0.17	-	87,87,87,87	0
37	SR	1	8952	1/1	0.98	0.20	-	67,67,67,67	0
38	CL	L	8814	1/1	0.96	0.13	-	62,62,62,62	0
36	NA	0	8548	1/1	0.99	0.17	-	26,26,26,26	0
35	MG	0	8018	1/1	1.00	0.26	-	3,3,3,3	0
37	SR	0	8986	1/1	0.91	0.10	-	108,108,108,108	0
37	SR	0	8983	1/1	0.53	0.22	-	169,169,169,169	0
35	MG	0	8031	1/1	0.97	0.05	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	R	8532	1/1	0.89	0.12	-	25,25,25,25	0
36	NA	9	8543	1/1	0.66	0.16	-	65,65,65,65	0
37	SR	0	8961	1/1	-0.02	0.13	-	185,185,185,185	0
37	SR	B	8950	1/1	0.96	0.17	-	98,98,98,98	0
37	SR	0	8965	1/1	0.95	0.13	-	95,95,95,95	0
37	SR	0	8927	1/1	0.98	0.19	-	70,70,70,70	0
37	SR	0	8998	1/1	0.68	0.22	-	113,113,113,113	0
37	SR	F	9005	1/1	0.97	0.10	-	98,98,98,98	0
37	SR	0	8954	1/1	0.98	0.16	-	82,82,82,82	0
37	SR	0	9006	1/1	0.89	0.75	-	198,198,198,198	0
35	MG	0	8070	1/1	0.80	0.23	-	63,63,63,63	0
35	MG	0	8058	1/1	0.99	0.20	-	1,1,1,1	0
37	SR	T	8939	1/1	0.99	0.14	-	70,70,70,70	0
37	SR	9	9003	1/1	0.92	0.04	-	144,144,144,144	0
36	NA	0	8573	1/1	0.46	0.20	-	79,79,79,79	0
37	SR	0	8928	1/1	0.91	0.11	-	92,92,92,92	0
35	MG	0	8065	1/1	0.87	0.39	-	102,102,102,102	0
35	MG	0	8022	1/1	0.99	0.21	-	11,11,11,11	0
37	SR	0	8988	1/1	0.96	0.10	-	114,114,114,114	0
37	SR	0	8940	1/1	0.98	0.17	-	51,51,51,51	0
37	SR	0	8996	1/1	0.80	0.13	-	158,158,158,158	0
36	NA	0	8536	1/1	0.88	0.18	-	63,63,63,63	0
37	SR	0	8923	1/1	0.94	0.21	-	72,72,72,72	0
35	MG	0	8077	1/1	0.92	0.19	-	41,41,41,41	0
38	CL	0	8822	1/1	0.88	0.34	-	66,66,66,66	0
35	MG	0	8038	1/1	0.68	0.24	-	97,97,97,97	0
37	SR	9	8980	1/1	0.87	0.07	-	132,132,132,132	0
37	SR	0	9007	1/1	0.80	0.59	-	195,195,195,195	0
37	SR	0	8931	1/1	1.00	0.20	-	80,80,80,80	0
37	SR	0	8990	1/1	0.93	0.55	-	177,177,177,177	0
35	MG	0	8083	1/1	0.99	0.11	-	29,29,29,29	0
37	SR	0	8951	1/1	0.98	0.09	-	105,105,105,105	0
38	CL	J	8801	1/1	0.93	0.13	-	62,62,62,62	0
37	SR	H	8907	1/1	0.99	0.14	-	48,48,48,48	0
37	SR	9	8968	1/1	0.78	0.10	-	117,117,117,117	0
36	NA	0	8505	1/1	0.99	0.54	-	29,29,29,29	0
35	MG	0	8019	1/1	0.99	0.16	-	1,1,1,1	0
36	NA	0	8561	1/1	0.98	0.19	-	66,66,66,66	0
36	NA	0	8526	1/1	0.69	0.10	-	55,55,55,55	0
36	NA	0	8509	1/1	0.91	0.34	-	80,80,80,80	0
35	MG	0	8069	1/1	0.93	0.17	-	120,120,120,120	0
37	SR	0	8903	1/1	0.98	0.21	-	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8055	1/1	0.99	0.27	-	26,26,26,26	0
38	CL	0	8803	1/1	0.91	0.07	-	51,51,51,51	0
35	MG	0	8067	1/1	0.99	0.33	-	33,33,33,33	0
35	MG	0	8091	1/1	0.90	0.11	-	76,76,76,76	0
37	SR	0	8997	1/1	0.97	0.04	-	116,116,116,116	0
37	SR	0	8967	1/1	0.92	0.07	-	103,103,103,103	0
37	SR	0	8979	1/1	0.82	1.99	-	184,184,184,184	0
35	MG	0	8037	1/1	0.94	0.16	-	64,64,64,64	0
35	MG	0	8048	1/1	0.98	0.26	-	49,49,49,49	0
35	MG	0	8092	1/1	0.81	0.70	-	76,76,76,76	0
37	SR	0	8966	1/1	0.96	0.15	-	85,85,85,85	0
37	SR	0	8955	1/1	0.90	0.08	-	127,127,127,127	0
37	SR	0	8994	1/1	-0.13	0.79	-	200,200,200,200	0
35	MG	0	8053	1/1	0.94	0.15	-	33,33,33,33	0
35	MG	0	8090	1/1	0.56	0.59	-	130,130,130,130	0
37	SR	0	8942	1/1	0.88	0.31	-	155,155,155,155	0
35	MG	0	8093	1/1	0.96	0.07	-	27,27,27,27	0
38	CL	0	8815	1/1	0.90	0.09	-	69,69,69,69	0
37	SR	0	8920	1/1	0.55	0.92	-	200,200,200,200	0
36	NA	0	8549	1/1	0.85	0.16	-	36,36,36,36	0
35	MG	0	8017	1/1	0.38	0.22	-	123,123,123,123	0
37	SR	0	8971	1/1	0.53	0.13	-	191,191,191,191	0
36	NA	0	8525	1/1	0.79	0.18	-	53,53,53,53	0
35	MG	0	8026	1/1	0.96	0.11	-	43,43,43,43	0
37	SR	0	8901	1/1	0.92	0.19	-	48,48,48,48	0
37	SR	0	9004	1/1	0.88	0.18	-	121,121,121,121	0
35	MG	0	8063	1/1	0.72	0.28	-	69,69,69,69	0
38	CL	Y	8817	1/1	0.80	0.13	-	55,55,55,55	0
37	SR	0	8921	1/1	0.98	0.14	-	58,58,58,58	0
35	MG	0	8078	1/1	0.13	0.41	-	115,115,115,115	0
35	MG	0	8030	1/1	0.72	0.25	-	167,167,167,167	0
38	CL	Q	8811	1/1	0.78	0.24	-	86,86,86,86	0
37	SR	0	8958	1/1	0.99	0.15	-	77,77,77,77	0
37	SR	0	8956	1/1	0.95	0.16	-	111,111,111,111	0
35	MG	0	8033	1/1	0.95	0.11	-	44,44,44,44	0
36	NA	0	8529	1/1	0.90	0.08	-	24,24,24,24	0
34	PHE	6	77	11/12	0.86	0.34	-	88,88,90,90	0
36	NA	0	8554	1/1	0.93	0.25	-	42,42,42,42	0
36	NA	9	8544	1/1	0.71	0.54	-	73,73,73,73	0
35	MG	0	8059	1/1	0.84	0.16	-	88,88,88,88	0
36	NA	0	8531	1/1	0.98	0.15	-	41,41,41,41	0
38	CL	N	8807	1/1	0.92	0.07	-	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8511	1/1	0.62	0.18	-	35,35,35,35	0
37	SR	0	8924	1/1	0.99	0.23	-	80,80,80,80	0
35	MG	0	8036	1/1	0.93	0.16	-	50,50,50,50	0
35	MG	0	8068	1/1	0.99	0.13	-	50,50,50,50	0
36	NA	0	8566	1/1	0.87	0.35	-	54,54,54,54	0
37	SR	0	8919	1/1	0.96	0.15	-	92,92,92,92	0
35	MG	0	8082	1/1	0.98	0.14	-	70,70,70,70	0
37	SR	A	8930	1/1	0.97	0.16	-	78,78,78,78	0
37	SR	0	8973	1/1	0.93	0.12	-	98,98,98,98	0
37	SR	0	8989	1/1	0.06	0.29	-	200,200,200,200	0
35	MG	0	8039	1/1	0.90	0.23	-	40,40,40,40	0
37	SR	0	8982	1/1	0.92	0.09	-	116,116,116,116	0
37	SR	0	8925	1/1	0.99	0.17	-	70,70,70,70	0
35	MG	0	8040	1/1	0.62	0.34	-	70,70,70,70	0
35	MG	0	8085	1/1	0.72	0.71	-	92,92,92,92	0
35	MG	0	8073	1/1	0.94	0.13	-	58,58,58,58	0
37	SR	0	8984	1/1	0.96	0.15	-	92,92,92,92	0
35	MG	0	8045	1/1	0.89	0.64	-	119,119,119,119	0
36	NA	0	8574	1/1	0.97	0.35	-	43,43,43,43	0
36	NA	0	8571	1/1	0.78	0.41	-	85,85,85,85	0
38	CL	J	8802	1/1	0.99	0.12	-	69,69,69,69	0
37	SR	0	8909	1/1	0.99	0.16	-	56,56,56,56	0
35	MG	0	8046	1/1	0.93	0.44	-	72,72,72,72	0
35	MG	0	8081	1/1	0.80	0.55	-	91,91,91,91	0
37	SR	0	8946	1/1	0.96	0.20	-	98,98,98,98	0
35	MG	0	8020	1/1	0.96	0.20	-	24,24,24,24	0
37	SR	0	8974	1/1	0.99	0.23	-	125,125,125,125	0
35	MG	0	8023	1/1	0.92	0.23	-	25,25,25,25	0
37	SR	T	8911	1/1	0.98	0.12	-	58,58,58,58	0
35	MG	B	8042	1/1	0.61	0.19	-	103,103,103,103	0
36	NA	0	8555	1/1	0.94	0.39	-	52,52,52,52	0
37	SR	0	8916	1/1	0.96	0.14	-	64,64,64,64	0
37	SR	0	8917	1/1	0.99	0.17	-	67,67,67,67	0
37	SR	0	8918	1/1	0.98	0.19	-	53,53,53,53	0
37	SR	0	8976	1/1	0.85	0.23	-	117,117,117,117	0
37	SR	0	8914	1/1	0.95	0.27	-	88,88,88,88	0
35	MG	2	8060	1/1	0.68	0.21	-	45,45,45,45	0
35	MG	0	8080	1/1	0.93	0.09	-	45,45,45,45	0
37	SR	0	8944	1/1	0.64	0.17	-	155,155,155,155	0
36	NA	0	8558	1/1	0.93	0.91	-	67,67,67,67	0
37	SR	0	8960	1/1	0.99	0.08	-	98,98,98,98	0
36	NA	H	8518	1/1	0.97	0.29	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8978	1/1	0.98	0.17	-	71,71,71,71	0
37	SR	0	9008	1/1	0.96	0.21	-	90,90,90,90	0
37	SR	0	8959	1/1	0.69	0.06	-	120,120,120,120	0
36	NA	0	8551	1/1	0.90	0.10	-	32,32,32,32	0
35	MG	0	8066	1/1	0.68	0.80	-	98,98,98,98	0
36	NA	0	8541	1/1	0.63	0.20	-	103,103,103,103	0
37	SR	0	8941	1/1	0.99	0.22	-	77,77,77,77	0
38	CL	R	8806	1/1	0.97	0.09	-	44,44,44,44	0
34	ACA	6	78	8/9	0.62	0.52	-	88,90,91,91	0
36	NA	0	8516	1/1	0.80	0.54	-	65,65,65,65	0
37	SR	0	9000	1/1	0.84	0.27	-	147,147,147,147	0
37	SR	0	8915	1/1	0.95	0.14	-	84,84,84,84	0
37	SR	0	8993	1/1	0.86	0.04	-	146,146,146,146	0
37	SR	0	8902	1/1	0.99	0.19	-	39,39,39,39	0
36	NA	0	8546	1/1	0.94	0.78	-	97,97,97,97	0
36	NA	0	8501	1/1	0.95	0.16	-	107,107,107,107	0
38	CL	A	8809	1/1	0.95	0.14	-	51,51,51,51	0
37	SR	A	8977	1/1	0.96	0.16	-	95,95,95,95	0
36	NA	0	8514	1/1	0.69	0.24	-	83,83,83,83	0
37	SR	0	8938	1/1	0.97	0.11	-	95,95,95,95	0
38	CL	Y	8820	1/1	0.94	0.06	-	48,48,48,48	0
37	SR	0	8905	1/1	0.93	0.25	-	61,61,61,61	0
35	MG	0	8056	1/1	0.90	0.38	-	94,94,94,94	0
35	MG	0	8024	1/1	0.96	0.37	-	69,69,69,69	0
37	SR	0	8908	1/1	0.99	0.16	-	64,64,64,64	0
36	NA	S	8510	1/1	0.80	0.65	-	80,80,80,80	0
37	SR	0	8933	1/1	0.86	0.30	-	126,126,126,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.