



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:52 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 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/ValidationPDFNotes.html>

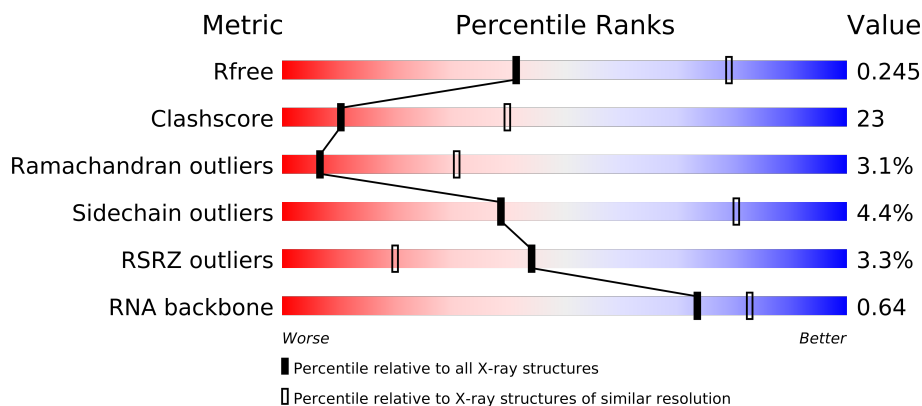
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
34	PHE	6	77	-	X
34	ACA	6	78	-	X
35	MG	0	8001	-	X
35	MG	0	8002	-	X
35	MG	0	8004	-	X
35	MG	0	8005	-	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	8016	-	X
35	MG	0	8018	-	X
35	MG	0	8020	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	MG	0	8022	-	X
35	MG	0	8023	-	X
35	MG	0	8024	-	X
35	MG	0	8027	-	X
35	MG	0	8028	-	X
35	MG	0	8029	-	X
35	MG	0	8034	-	X
35	MG	0	8036	-	X
35	MG	0	8037	-	X
35	MG	0	8039	-	X
35	MG	0	8040	-	X
35	MG	0	8041	-	X
35	MG	0	8045	-	X
35	MG	0	8046	-	X
35	MG	0	8047	-	X
35	MG	0	8048	-	X
35	MG	0	8049	-	X
35	MG	0	8050	-	X
35	MG	0	8055	-	X
35	MG	0	8056	-	X
35	MG	0	8058	-	X
35	MG	0	8059	-	X
35	MG	0	8061	-	X
35	MG	0	8062	-	X
35	MG	0	8063	-	X
35	MG	0	8064	-	X
35	MG	0	8065	-	X
35	MG	0	8066	-	X
35	MG	0	8067	-	X
35	MG	0	8070	-	X
35	MG	0	8071	-	X
35	MG	0	8072	-	X
35	MG	0	8076	-	X
35	MG	0	8078	-	X
35	MG	0	8079	-	X
35	MG	0	8081	-	X
35	MG	0	8085	-	X
35	MG	0	8087	-	X
35	MG	0	8088	-	X
35	MG	0	8090	-	X
35	MG	0	8092	-	X
35	MG	2	8060	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	MG	9	8074	-	X
35	MG	A	8025	-	X
35	MG	A	8051	-	X
35	MG	B	8042	-	X
35	MG	B	8043	-	X
35	MG	C	8012	-	X
35	MG	K	8054	-	X
35	MG	Y	8086	-	X
36	NA	0	8501	-	X
36	NA	0	8502	-	X
36	NA	0	8505	-	X
36	NA	0	8507	-	X
36	NA	0	8509	-	X
36	NA	0	8511	-	X
36	NA	0	8512	-	X
36	NA	0	8513	-	X
36	NA	0	8514	-	X
36	NA	0	8516	-	X
36	NA	0	8519	-	X
36	NA	0	8520	-	X
36	NA	0	8521	-	X
36	NA	0	8523	-	X
36	NA	0	8524	-	X
36	NA	0	8525	-	X
36	NA	0	8527	-	X
36	NA	0	8528	-	X
36	NA	0	8530	-	X
36	NA	0	8531	-	X
36	NA	0	8533	-	X
36	NA	0	8534	-	X
36	NA	0	8535	-	X
36	NA	0	8536	-	X
36	NA	0	8541	-	X
36	NA	0	8545	-	X
36	NA	0	8546	-	X
36	NA	0	8547	-	X
36	NA	0	8548	-	X
36	NA	0	8550	-	X
36	NA	0	8552	-	X
36	NA	0	8553	-	X
36	NA	0	8554	-	X
36	NA	0	8555	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	NA	0	8556	-	X
36	NA	0	8557	-	X
36	NA	0	8558	-	X
36	NA	0	8559	-	X
36	NA	0	8560	-	X
36	NA	0	8561	-	X
36	NA	0	8562	-	X
36	NA	0	8563	-	X
36	NA	0	8565	-	X
36	NA	0	8566	-	X
36	NA	0	8567	-	X
36	NA	0	8568	-	X
36	NA	0	8569	-	X
36	NA	0	8570	-	X
36	NA	0	8571	-	X
36	NA	0	8573	-	X
36	NA	0	8574	-	X
36	NA	9	8544	-	X
36	NA	9	8572	-	X
36	NA	H	8518	-	X
36	NA	S	8510	-	X
37	SR	0	8901	-	X
37	SR	0	8903	-	X
37	SR	0	8904	-	X
37	SR	0	8905	-	X
37	SR	0	8906	-	X
37	SR	0	8908	-	X
37	SR	0	8909	-	X
37	SR	0	8910	-	X
37	SR	0	8914	-	X
37	SR	0	8917	-	X
37	SR	0	8918	-	X
37	SR	0	8920	-	X
37	SR	0	8923	-	X
37	SR	0	8924	-	X
37	SR	0	8925	-	X
37	SR	0	8926	-	X
37	SR	0	8927	-	X
37	SR	0	8931	-	X
37	SR	0	8933	-	X
37	SR	0	8936	-	X
37	SR	0	8937	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	0	8938	-	X
37	SR	0	8941	-	X
37	SR	0	8942	-	X
37	SR	0	8944	-	X
37	SR	0	8946	-	X
37	SR	0	8948	-	X
37	SR	0	8949	-	X
37	SR	0	8954	-	X
37	SR	0	8958	-	X
37	SR	0	8961	-	X
37	SR	0	8963	-	X
37	SR	0	8965	-	X
37	SR	0	8966	-	X
37	SR	0	8974	-	X
37	SR	0	8976	-	X
37	SR	0	8979	-	X
37	SR	0	8983	-	X
37	SR	0	8984	-	X
37	SR	0	8985	-	X
37	SR	0	8989	-	X
37	SR	0	8990	-	X
37	SR	0	8994	-	X
37	SR	0	8996	-	X
37	SR	0	8998	-	X
37	SR	0	9000	-	X
37	SR	0	9001	-	X
37	SR	0	9006	-	X
37	SR	0	9007	-	X
37	SR	0	9008	-	X
37	SR	1	8913	-	X
37	SR	1	8952	-	X
37	SR	B	8950	-	X
37	SR	B	8987	-	X
37	SR	L	8969	-	X
37	SR	T	8939	-	X
38	CL	0	8822	-	X
38	CL	J	8816	-	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 hydrogen and 0 are deuterium.

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	S	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			

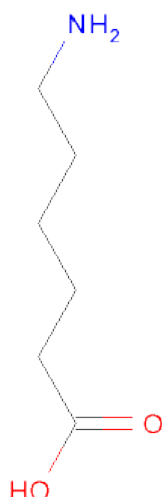
- Molecule 32 is a RNA chain called RNA (5'-R(*C*CP*A)-3').

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 1	Cd 1	0	0
40	1	1	Total 1	Cd 1	0	0
40	3	1	Total 1	Cd 1	0	0
40	U	1	Total 1	Cd 1	0	0

- Molecule 41 is water.

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

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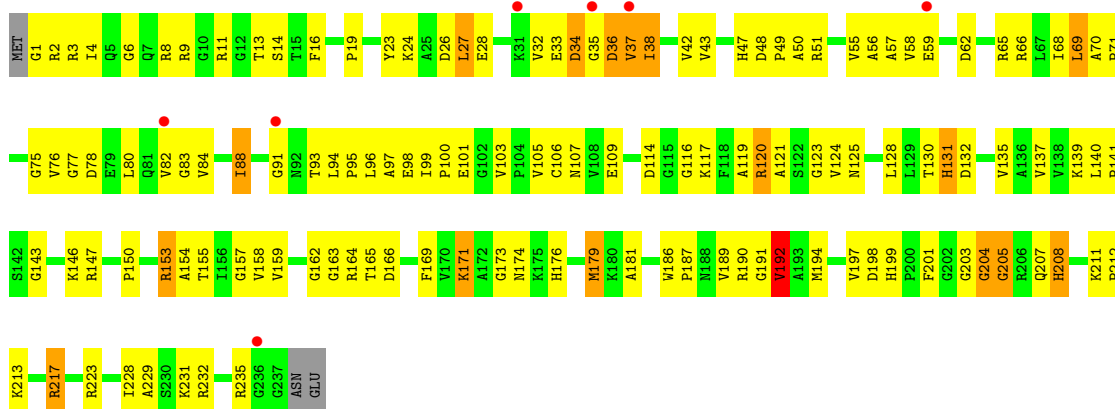
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	O	46	Total 46	O 46	0	0
41	P	72	Total 72	O 72	0	0
41	Q	52	Total 52	O 52	0	0
41	R	89	Total 89	O 89	0	0
41	S	35	Total 35	O 35	0	0
41	T	42	Total 42	O 42	0	0
41	U	29	Total 29	O 29	0	0
41	V	16	Total 16	O 16	0	0
41	W	75	Total 75	O 75	0	0
41	X	31	Total 31	O 31	0	0
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.

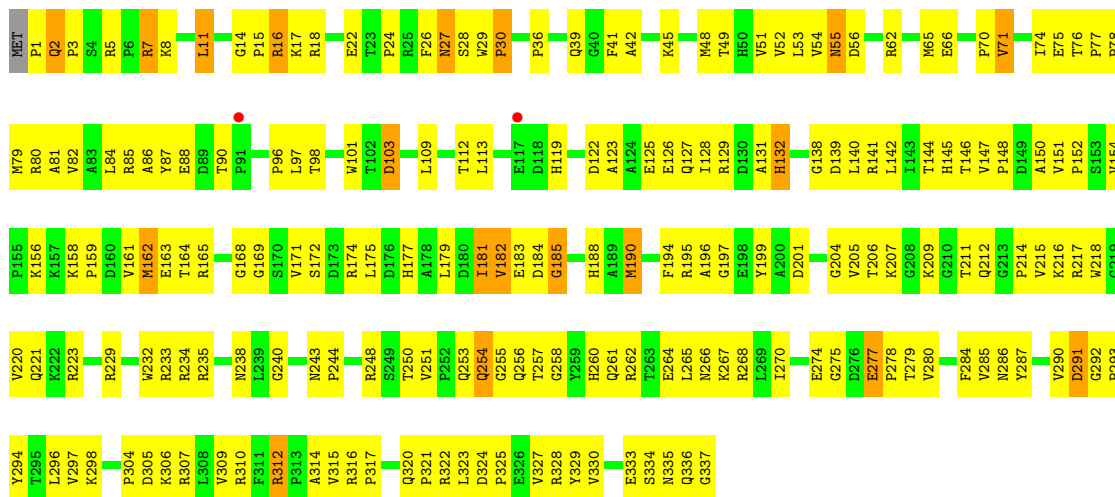
• Molecule 1: 50S ribosomal protein L2P

Chain A: 



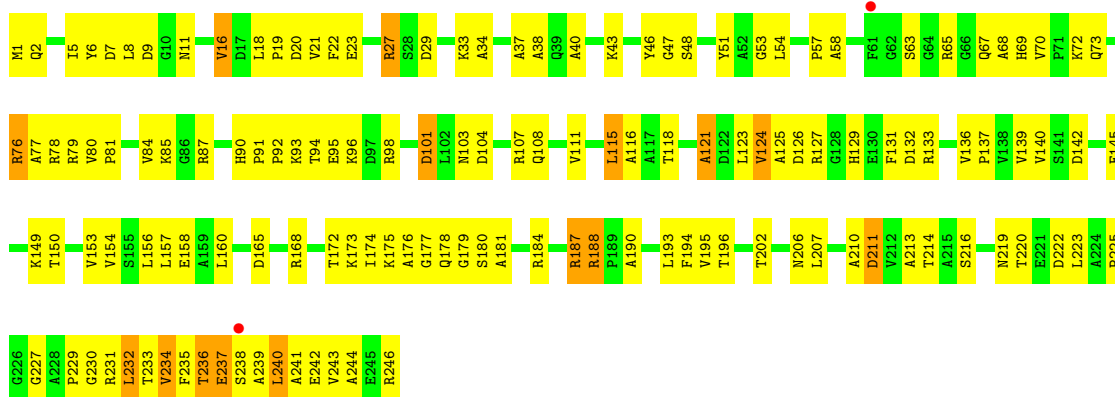
• Molecule 2: 50S ribosomal protein L3P

Chain B: 



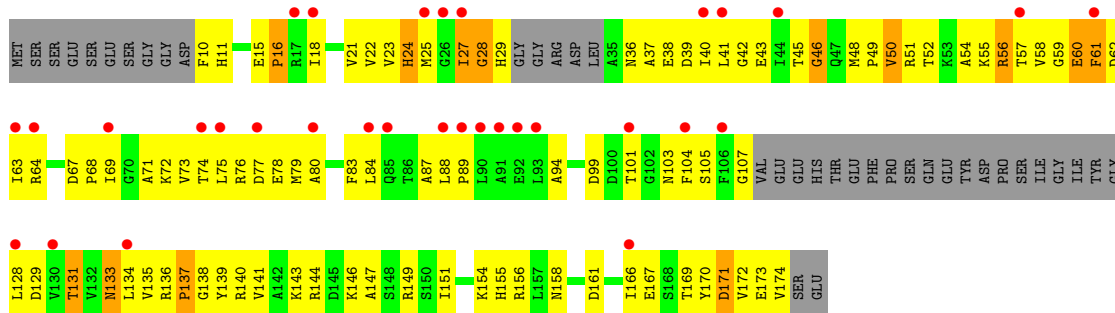
• Molecule 3: 50S ribosomal protein L4P

Chain C: 



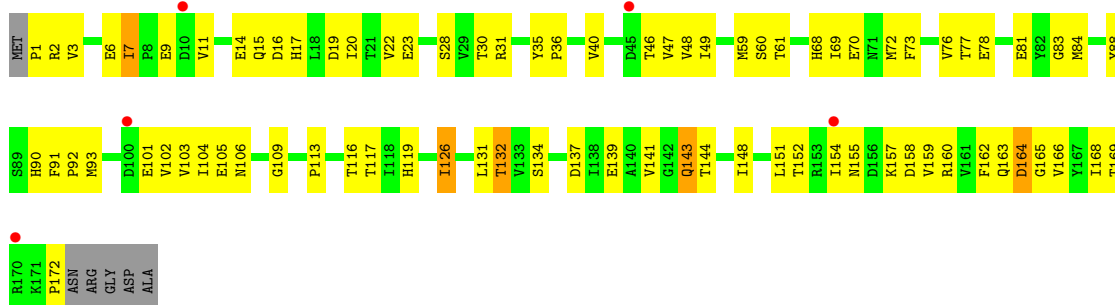
• Molecule 4: 50S ribosomal protein L5P

Chain D:



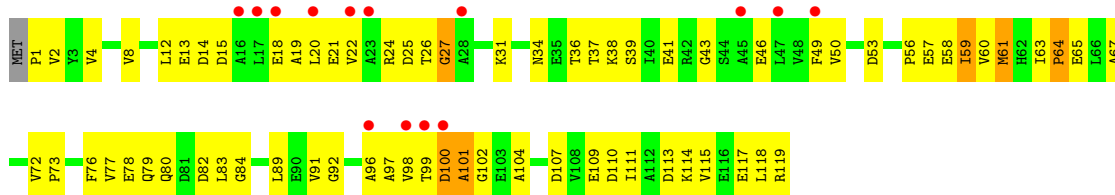
• Molecule 5: 50S ribosomal protein L6P

Chain E:



• Molecule 6: 50S ribosomal protein L7Ae

Chain F:



• Molecule 7: 50S ribosomal protein L10E

Age Group	Percentage
18-24	28%
25-34	22%
35-44	18%
45-54	15%
55-64	10%
65-74	8%
75-84	5%
85+	4%

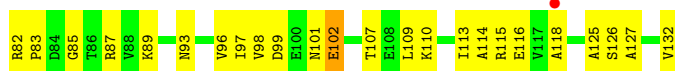
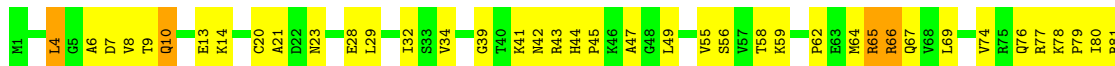
Age Group	Percentage
18-24	5%
25-34	45%
35-44	35%
45-54	5%
55-64	10%
65-74	0%
75-84	0%
85+	0%

Age Group	Percentage
18-24	10%
25-34	45%
35-44	30%
45-54	10%
55-64	5%
65-74	2%
75-84	1%
85+	1%



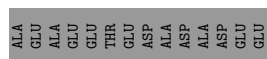
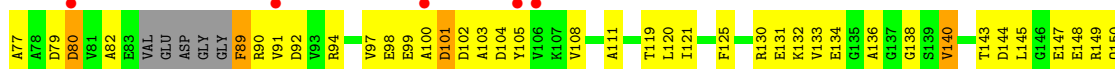
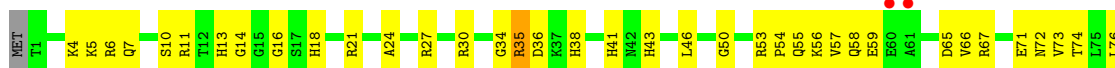
• Molecule 11: 50S ribosomal protein L14P

Chain K:



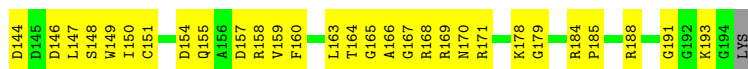
• Molecule 12: 50S ribosomal protein L15P

Chain L:



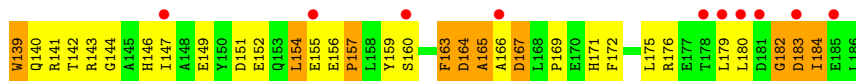
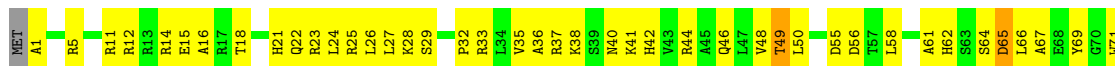
• Molecule 13: 50S ribosomal protein L15e

Chain M:



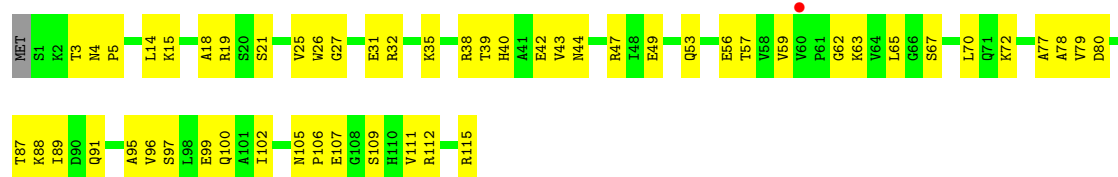
• Molecule 14: 50S ribosomal protein L18P

Chain N:



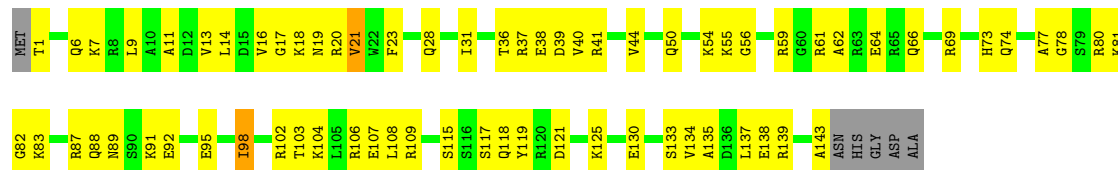
• Molecule 15: 50S ribosomal protein L18e

Chain O: 



- Molecule 16: 50S ribosomal protein L19e

Chain P: 



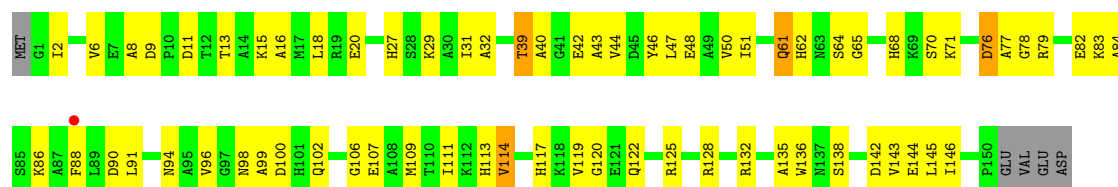
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 



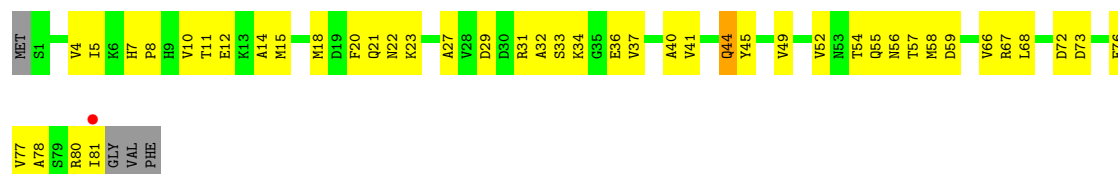
- Molecule 18: 50S ribosomal protein L22P

Chain R: 



- Molecule 19: 50S ribosomal protein L23P

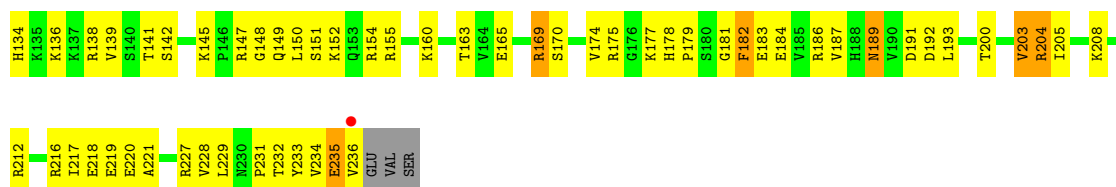
Chain S: 



- Molecule 20: 50S ribosomal protein L24P

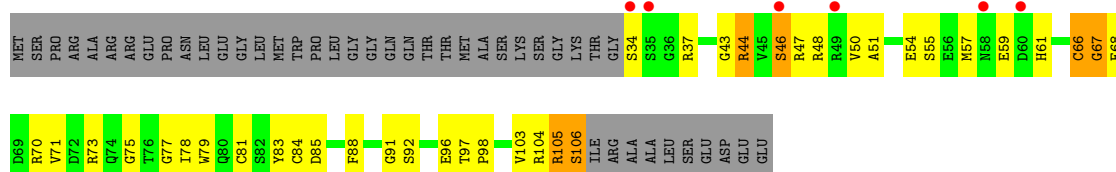
Chain T: 





- Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 27: 50S ribosomal protein L37e

Chain 1:



- Molecule 28: 50S ribosomal protein L39e

Chain 2:



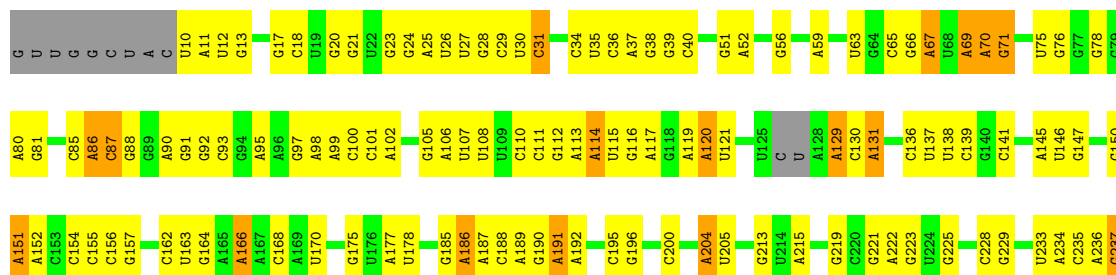
- Molecule 29: 50S ribosomal protein L44E

Chain 3:



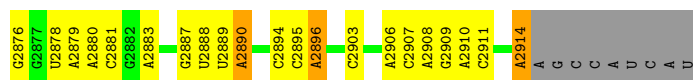
- Molecule 30: 50S RIBOSOMAL RNA

Chain 0:



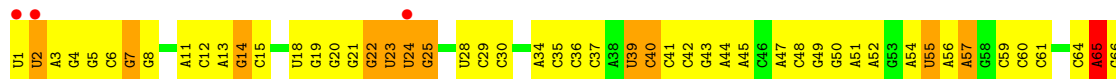
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G1520	G1416	C1332	U1249	C1179	U1096	G	C920	U823	G727	G646	U567	A484	U991	G315	A241
A1522	U1417	U1333	C1250	A1180	A1097	C	9921	G524	G728	G652	G568	A486	U391	A316	
G1523	G1419	C1334		A1181	A1098	A	A922	G830	G729	U653		G487	U392	A317	
U1524	C1420	G1182	G1258	C1182	G1099	C	A923	G834	G730		A575	C491	G393	U318	A247
G1525	C1421	C1183	A1259	C1184	G1100	A	G924	U835	U731	G656	C578	C492	U396	C233	G249
A1526	U1422	U1185	A1261	U1185	C1103	C1000	G925	C839	G732	G657	G579	U493	A397	G324	
A1527	C1423	C1186	C1262	C1187	C1104	U1001	A926	U840	C735	G658	A580	C494	U398	U325	C254
A1528	A1424	U1187	C1263	U1188	U1002	G1002	C936	C839	A736	A659	G581	A495	C399	A326	A255
G1529		U1188	U1264	U1188	U1003	U1003	C937	A841	A737	A660	U582	C496	C400	A327	C256
	G1433	A1189		A1189	U1110		G938		G738	U662	C583	A497	C401	U328	G257
A1533		C1190	C1267	A1190				A844		C663	U584	A498	A407	A329	G258
C1534	G1445	A1191	C1268	A1191	A1114	A1006	G941		C741	U664		C499	A408		G259
	U1446	A1192	G1269	A1192	U1115	C1007	U942	G854		A665	G588	C500	A408	G383	U263
U1447	U1447	A1193	U1270	A1193	U1116	C1008	U943	G854	G744	A666	U589	G500	A408	G334	U263
C1545					U1117	G1021	U944	G856	G745	C667	U590	G506	C412	U335	U264
A1547	C1451	G1351	A1276	C1196	A1118	A1022	U945	G857	A746	C668	A591	A507	C413	G336	U265
U1548	G1452	C1352	U1277	U1197	A1119	G1022	U946	U858	G747	G669	G592	A508	G417	A337	G266
		C1353	C1277	U1198	U1120	G1025	U947	C859		U671	A593	A509	C418	C338	G267
G1552	C1456	A1355	A1278	U1200	G1121		U948	C859	A750		G600	U510	C419	A339	U268
U1457	U1457	A1356	U1279	U1200	U1130	U1029	U949	U862	U751	C677	G601	A511	U420	C342	G269
A1458	A1458	A1357	A1280	U1201	U1131	G1031	U950	G863	G752	G678	A602	A512	C421	C343	C271
				A1202	A1132	C1032	A951	G868			A603	A513		C344	A272
U1461	U1461	A1358	A1287	G1203	A1133	C1033	G952	G868	C757	C681	U604	G514	U425	G345	G273
C1462	C1463	C1360	U1288	C1204	G1135	G1034	G953	G869	A758		C605		G426	U346	
U1463	U1463	C1361	U1289	U1205	U1136			G870	C759			G518	G431	A347	C280
A1559		C1362	G1290	U1206	U1137	U1041	G956	G871	A760	A686	U611	A519	G432	C348	U281
U		G1363	A1291	A1207	U1139	U1042	A957	U872	G764	C687	U612	A521	C433	U349	C282
U1561	C1471	G1364	G1292	C1208	C1043	C1043	G958	A875	G765	A688	C613	U522		U283	U283
C1562	A1472	C1365	U1293	C1209	U1140	C1044	G959	A876		A689	U614		A437	A351	C284
G1563	U1473	C1366	A1294	G1210	U1141	G1044	G960	A877	G772	U690	G615	C530		A352	A285
C1566	C1474	A1367	G1295	G1211	C1142	G1045	A961	G878	A773		U616	A532	A441	G353	U286
G1567		U1368		G1212			C962	G878	G775	C695			A442	A354	C287
A1573	A1476	C1370	U1298	C1213	U1149	C1051	G969	A882	A776	A694	U619	G536	U445	C355	A288
C1574	C1477	G1371	G1300	A1215	A1150	G1052	U970	U883		C696	A620	U530	U445	G358	C290
G1575		U1372	C1301	G1216	A1152	G1053	G	C884	U777	A698	C621	A536	G446	U359	C291
U1577			G1302	G1217	C1153	U1056	U	G885	A790	C699	G622	G537	A447	A360	G292
	G1586	C1377	C1303	U1218	G1158	A1057	U	A886	A791	U700	U623	C538	G448	C361	A293
U1587	U1587	U1378	U1304	G1219	G1159	A1058	G	G887	G792	U701	U624	U539	A449	G362	C294
G1588	G1588	U1379	C1305	U1220	G1059	G1059	U	U888	A793	G702	U625	C540	C450	C363	C295
G1589		U1380	U1306	G1221	C1060	C1060	C	C889		G703	U626	C541	C451	U364	G296
A1590	A1496		A1307	G1161			C	C890	A797	G704	G627	A542	G452	G365	U297
	G1497	U1383	A1308	C1228	G1065	G1065	G	C891		C705	A628	G543	U459	U366	U300
A1591	A1501	C1384	C1309	C1229	U1066	U1066	C	G892	A806	G706	A629	G544	A459	G367	C301
C1592	U1502	U1385	U1310	A1230	A1067	A1067	C	C893	A807	C707	A630	G545	C461	C368	A302
G1593	U1503	A1165	G1165	U1234	G1072	G1072	U	A894	A808	A708	A631		A462	G370	C303
A1594	A1504	G1166	G1167				C	A895	G809	G709	A632	G553	A463	U371	G304
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U1596	U1506	U1169	U1169	U1238	A1078	A1078	A	G902	C813	U711	A635	C558	U465	C376	A306
A1597	C1507	C1238	U1170	U1239	A1079	A1079	G	U903	G816	U714	G636	U559	U470	C376	G307
U1598	C1508	U1239	A1171	G1239	C1080	C1080	A	U904	G817	U	C637	U560	G471	A378	U308
		A1242	A1172		A1081	A1081	G	C905	G817	G716	C638	G561	G471	C378	C309
C1602	A1603	C1243	A1173				C	C906	A818		G640	A562	A477	G379	U310
A1603	G1604	U1244	A1174	U1244	A1086	A1086	A	A907	A819	C719	G641	C563	A477	A380	C311
G1605	G1605	C1245	G1175	G1175	G1087	G1087	G	A907	A819			G564	A477	G381	U312
U1606	U1516	A1246	C1176	A1247	A1088	A1088	U		U821	G722	G644	A565	G482	U382	U313
A1607							C	A912							

G2794	G2698	G2616	G2540	A2311	C2105	G2023	C1946	C1853	G1773	C1687	G1608
C2795	A2699	G2617	U2541	G2312	C2106	C2029	G1947	C1854	G1774	G1688	
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A2799	U2705	U2620	G2543	C2314	A2108	G2031	G1949	C1856	A1776	C1692	
A2800	G2712	G2626	U2544	G2315	U2109	U2032	G1950	G1863	G1777	G1695	
A2801		G2627		G2316	G2110	G2033	G1951	C1864	A1778	G1618	
A2802	G2715		C2548	C2317	G2111	U2034	U	A1865	A1779	G1619	
C2803	G2716	G2634	C2549	C2318	G2112		A	A1866		C1700	
C2807	G2717	A2635	U2550	G2319	G2113	A2039	A	G1867	A1783	A1701	
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	A2719	A2637	U2552	G2403	U2115	U2042	U	C1869	G1785	U1702	
	C2720	G2638	U2553	G2404	G2116	U2242	A	C1870	C1786	G1705	
A2811			U2554			C2243	U	C1871	C1787		
A2812	G2721			C2247	U2120	U2043	U	G1872	U1788	A1710	
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A2815		U2645	G2561	G2250		G2046	C	C1876	U1791	C1715	
A2816	U2626	G2646	G2562	G2251	G2128	C2047	C	G1877	C1792	A1716	
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	C2747	G2651	G2567	G2256	C	C2056		A1882	C1803	U1724	
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C2826	G2750	G2656	G2570	G2259	C	G2059		A1885	G1806	C1643	
C2827	C2751	G2657		G2260	C	A2060		A1886		C1644	
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C2831	C2753		G2574	G2262	C	U2064		U1888	C1810	G1646	
C2832	U2754	U2661		G2263	C	C2065		U1889	A1811	G1647	
	G2755		G2578	G2264	C	C2066		U1900	C1816	G1648	
C2836	G2758	A2664	A2583	G2265	C	C2067		A1901	U1817	C1735	
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		G2670	G2588	G2270	C			A1906	A1822		
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A2843	G2765	G2672	U2589	G2272	C	G2079		A1908	G1827	A1746	
C2846	A2766	G2673	G2590	G2273	C	G2080		U1909	C1828	U1747	
C2847	G2767	G2674	G2591	G2274	C	A2081		A1910	A1829	U1748	
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	U2781	C2685		G2281	C	G2090		A1917	A1836		
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C2862	A2783	G2687	C2608	G2283	C	A2092		A1919	U1838	U1766	
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C2868		G2613	G2612	G2287	C	A2096		A1923	U1939	G1683	
G2869	U2790	G2614	G2613	G2288	C	A2097		A1924	U1940	C1769	
C2870	U2791	A2615	G2614	G2289	C	A2101		A1925	A1941	U1770	
			G2615	G2290	C	A2102		A1926	A1942	A1684	
				G2291	C	A2103		A1927	C1943	A1685	
				G2292	C	A2104		A1928	U1846	C1686	
				G2293	C			A1929			
				G2294	C			A1930			
				G2295	C			A1931			
				G2296	C			A1932			
				G2297	C			A1933			
				G2298	C			A1934			
				G2299	C			A1935			
				G2300	C			A1936			
				G2301	C			A1937			
				G2302	C			A1938			
				G2303	C			A1939			
				G2304	C			A1940			
				G2305	C			A1941			
				G2306	C			A1942			
				G2307	C			A1943			
				G2308	C			A1944			
				G2309	C			A1945			
				G2310	C			A1946			
				G2311	C			A1947			
				G2312	C			A1948			
				G2313	C			A1949			
				G2314	C			A1950			
				G2315	C			A1951			
				G2316	C			A1952			
				G2317	C			A1953			
				G2318	C			A1954			
				G2319	C			A1955			
				G2320	C			A1956			
				G2321	C			A1957			
				G2322	C			A1958			
				G2323	C			A1959			
				G2324	C			A1960			
				G2325	C			A1961			
				G2326	C			A1962			
				G2327	C			A1963			
				G2328	C			A1964			
				G2329	C			A1965			
				G2330	C			A1966			
				G2331	C			A1967			
				G2332	C			A1968			
				G2333	C			A1969			
				G2334	C			A1970			
				G2335	C			A1971			
				G2336	C			A1972			
				G2337	C			A1973			
				G2338	C			A1974			
				G2339	C			A1975			
				G2340	C			A1976			
				G2341	C			A1977			
				G2342	C			A1978			
				G2343	C			A1979			
				G2344	C			A1980			
				G2345	C			A1981			
				G2346	C			A1982			
				G2347	C			A1983			
				G2348	C			A1984			
				G2349	C			A1985			
				G2350	C			A1986			
				G2351	C			A1987			
				G2352	C			A1988			
				G2353	C			A1989			
				G2354	C			A1990			
				G2355	C			A1991			
				G2356	C			A1992			
				G2357	C			A1993			
				G2358	C			A1994			
				G2359	C			A1995			
				G2360	C			A1996			
				G2361	C			A1997			
				G2362	C			A1998			
				G2363	C			A1999			
				G2364	C			A2000			
				G2365	C			A2001			
				G2366	C			A2002			
				G2367	C			A2003			
				G2368	C			A2004			
				G2369	C			A2005			
				G2370	C			A2006			
				G2371	C			A2007			
				G2372	C			A2008			
				G2373	C			A2009			
				G2374	C			A2010			
				G2375	C			A2011			
				G2376	C			A2012			
				G2377	C			A2013			
				G2378	C			A2014			
				G2379	C			A2015			
				G2380	C			A2016			
				G2381	C			A2017			
				G2382	C			A2018			
				G2383	C			A2019			
				G2384	C			A2020			
				G2385	C			A2021			
				G2386	C			A2022			



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



• Molecule 32: RNA (5'-R(*C*CP*A)-3')

Chain 5:



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

Chain 6:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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	3262 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	2	1	0	0	0	0
35	9	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	1	1	0	0	0	0
40	3	1	0	0	0	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 3515 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

5.3.1 Protein backbone ⓘ

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%)	4	21
2	B	333/338 (98%)	285 (86%)	41 (12%)	7 (2%)	11	45
3	C	242/246 (98%)	202 (84%)	32 (13%)	8 (3%)	6	29
4	D	132/177 (75%)	87 (66%)	35 (26%)	10 (8%)	2	6
5	E	168/178 (94%)	150 (89%)	17 (10%)	1 (1%)	33	79
6	F	115/120 (96%)	94 (82%)	15 (13%)	6 (5%)	3	16
7	G	25/348 (7%)	15 (60%)	7 (28%)	3 (12%)	1	2
8	H	154/177 (87%)	125 (81%)	23 (15%)	6 (4%)	5	23
9	I	66/162 (41%)	43 (65%)	18 (27%)	5 (8%)	2	6
10	J	138/145 (95%)	120 (87%)	15 (11%)	3 (2%)	10	43
11	K	128/132 (97%)	115 (90%)	8 (6%)	5 (4%)	5	23
12	L	139/165 (84%)	106 (76%)	27 (19%)	6 (4%)	4	21
13	M	190/196 (97%)	170 (90%)	16 (8%)	4 (2%)	11	45
14	N	182/187 (97%)	153 (84%)	19 (10%)	10 (6%)	3	14
15	O	111/116 (96%)	92 (83%)	19 (17%)	0	100	100
16	P	139/149 (93%)	129 (93%)	8 (6%)	2 (1%)	16	58
17	Q	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	4	20
18	R	146/155 (94%)	131 (90%)	12 (8%)	3 (2%)	11	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	18	60
20	T	115/120 (96%)	95 (83%)	17 (15%)	3 (3%)	8	37
21	U	51/67 (76%)	45 (88%)	4 (8%)	2 (4%)	5	23
22	V	63/71 (89%)	53 (84%)	9 (14%)	1 (2%)	14	54
23	W	150/154 (97%)	131 (87%)	19 (13%)	0	100	100
24	X	78/92 (85%)	68 (87%)	7 (9%)	3 (4%)	5	24
25	Y	140/240 (58%)	128 (91%)	11 (8%)	1 (1%)	30	76
26	Z	69/116 (60%)	51 (74%)	13 (19%)	5 (7%)	2	7
27	1	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	12	49
28	2	42/50 (84%)	34 (81%)	8 (19%)	0	100	100
29	3	88/92 (96%)	77 (88%)	9 (10%)	2 (2%)	10	41
All	All	3659/4471 (82%)	3087 (84%)	460 (13%)	112 (3%)	7	31

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%)	26	66
2	B	281/283 (99%)	266 (95%)	15 (5%)	32	73
3	C	192/193 (100%)	179 (93%)	13 (7%)	22	61
4	D	116/148 (78%)	111 (96%)	5 (4%)	40	81
5	E	151/156 (97%)	144 (95%)	7 (5%)	37	79
6	F	92/94 (98%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/283 (10%)	26 (96%)	1 (4%)	45	85
8	H	133/145 (92%)	127 (96%)	6 (4%)	38	80
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	94
10	J	117/121 (97%)	109 (93%)	8 (7%)	22	61
11	K	105/106 (99%)	102 (97%)	3 (3%)	55	89
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	80
13	M	157/160 (98%)	149 (95%)	8 (5%)	33	75
14	N	148/150 (99%)	143 (97%)	5 (3%)	49	86
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	77 (98%)	2 (2%)	60	91
18	R	117/122 (96%)	112 (96%)	5 (4%)	40	81
19	S	71/74 (96%)	69 (97%)	2 (3%)	56	90
20	T	104/106 (98%)	99 (95%)	5 (5%)	35	77
21	U	44/53 (83%)	42 (96%)	2 (4%)	38	80
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	129/130 (99%)	122 (95%)	7 (5%)	31	72
24	X	65/74 (88%)	58 (89%)	7 (11%)	9	33
25	Y	120/195 (62%)	111 (92%)	9 (8%)	19	56
26	Z	59/94 (63%)	56 (95%)	3 (5%)	33	75
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	40 (95%)	2 (5%)	35	77
29	3	78/79 (99%)	76 (97%)	2 (3%)	59	91
All	All	3079/3646 (84%)	2943 (96%)	136 (4%)	39	80

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

Mol	Chain	Res	Type
10	J	52	GLN
13	M	52	GLN
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	20,22,23	0.76	1 (5%)	24,31,34	0.77	0
30	OMG	0	2588	32,30	24,26,27	0.90	1 (4%)	32,38,41	5.10	4 (12%)
30	UR3	0	2619	30	20,22,23	0.79	1 (5%)	23,32,35	0.83	0
30	PSU	0	2621	30	19,21,22	1.20	3 (15%)	23,30,33	1.12	2 (8%)
30	1MA	0	628	30,36	23,25,26	0.88	1 (4%)	32,37,40	1.15	2 (6%)
33	8AN	6	76	33,30	24,24,25	1.02	1 (4%)	34,35,38	1.88	6 (17%)

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	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	32,30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30,36	-	1/8/25/26	0/1/3/3
33	8AN	6	76	33,30	-	0/9/25/26	0/1/3/3

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	3.24	1.43	1.37
30	0	2621	PSU	C6-N1	2.48	1.34	1.32
30	0	2587	OMU	P-OP1	2.39	1.49	1.46
30	0	2588	OMG	P-OP1	2.18	1.49	1.46
30	0	2619	UR3	P-OP1	2.15	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.17	130.35	134.14
33	6	76	8AN	C4'-C3'-N3'	-5.54	101.69	113.46
33	6	76	8AN	C2'-C3'-N3'	-5.05	102.55	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	76	8AN	O2'-C2'-C3'	4.01	121.22	110.90
30	0	2588	OMG	C6-N1-C2	3.52	125.67	119.51

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

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	-	11,11,12	5.52	3 (27%)	11,13,15	2.92	1 (9%)
34	ACA	6	78	-	7,7,8	8.85	3 (42%)	4,6,8	1.41	1 (25%)

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

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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	6	78	ACA	O1-C1	23.03	1.27	1.11
34	6	77	PHE	O-C	17.45	1.23	1.11
34	6	77	PHE	CA-C	4.57	1.57	1.48
34	6	78	ACA	C3-C2	-3.33	1.36	1.51
34	6	77	PHE	CE1-CD1	2.24	1.44	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	6	77	PHE	C-CA-N	9.45	123.27	113.83
34	6	78	ACA	C5-C4-C3	-2.23	102.56	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.26	7 (2%) 48 21	24, 46, 80, 105	0
2	B	337/338 (99%)	-0.48	2 (0%) 86 47	26, 49, 75, 88	0
3	C	246/246 (100%)	-0.42	2 (0%) 83 42	24, 45, 69, 80	0
4	D	140/177 (79%)	1.21	32 (22%) 1 1	64, 93, 124, 135	0
5	E	172/178 (96%)	-0.08	5 (2%) 49 22	41, 62, 84, 92	0
6	F	119/120 (99%)	0.58	14 (11%) 5 3	50, 73, 100, 114	0
7	G	29/348 (8%)	1.26	5 (17%) 2 2	75, 95, 109, 113	0
8	H	160/177 (90%)	-0.08	3 (1%) 64 28	39, 58, 93, 99	0
9	I	70/162 (43%)	3.72	51 (72%) 0 0	141, 152, 166, 168	0
10	J	142/145 (97%)	-0.42	1 (0%) 84 44	35, 47, 66, 86	0
11	K	132/132 (100%)	-0.70	1 (0%) 83 42	28, 41, 63, 73	0
12	L	145/165 (87%)	0.03	7 (4%) 29 15	22, 67, 105, 121	0
13	M	194/196 (98%)	-0.42	1 (0%) 88 50	25, 46, 68, 82	0
14	N	186/187 (99%)	0.03	10 (5%) 25 12	42, 63, 116, 124	0
15	O	115/116 (99%)	-0.24	1 (0%) 81 39	39, 55, 67, 75	0
16	P	143/149 (95%)	-0.49	0 100 100	35, 51, 62, 68	0
17	Q	95/96 (98%)	-0.32	1 (1%) 77 36	35, 49, 66, 75	0
18	R	150/155 (96%)	-0.49	1 (0%) 84 44	22, 42, 62, 69	0
19	S	81/85 (95%)	-0.15	1 (1%) 75 36	44, 56, 81, 94	0
20	T	119/120 (99%)	-0.12	1 (0%) 83 42	38, 54, 84, 116	0
21	U	53/67 (79%)	-0.28	1 (1%) 64 28	38, 49, 73, 86	0
22	V	65/71 (91%)	1.05	10 (15%) 3 2	55, 78, 115, 122	0
23	W	154/154 (100%)	-0.25	1 (0%) 86 47	37, 48, 72, 86	0
24	X	82/92 (89%)	-0.06	6 (7%) 15 8	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%)	-0.48	2 (1%) 72 34	25, 44, 64, 90	0
26	Z	73/116 (62%)	0.26	6 (8%) 12 6	48, 67, 87, 96	0
27	1	56/57 (98%)	-0.62	0 100 100	22, 32, 39, 51	0
28	2	46/50 (92%)	-0.03	2 (4%) 34 16	29, 61, 76, 89	0
29	3	92/92 (100%)	-0.19	0 100 100	33, 58, 71, 81	0
30	0	2754/2923 (94%)	-0.38	35 (1%) 74 35	16, 45, 92, 179	0
31	9	122/122 (100%)	-0.39	4 (3%) 44 20	36, 65, 92, 148	0
32	5	2/3 (66%)	2.75	2 (100%) 0 0	100, 100, 100, 102	0
33	6	3/3 (100%)	1.71	1 (33%) 1 0	92, 92, 96, 104	0
All	All	6656/7522 (88%)	-0.22	216 (3%) 44 20	16, 50, 99, 179	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	66	GLY	14.4
22	V	40	PRO	10.9
9	I	113	SER	9.7
9	I	132	VAL	9.5
9	I	72	GLU	7.9

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	8AN	6	76	22/23	0.27	1.10	87,92,94,95	0
30	UR3	0	2619	21/22	0.14	0.57	40,41,44,47	0
30	1MA	0	628	23/24	0.15	0.44	36,40,42,42	0
30	OMU	0	2587	21/22	0.11	-0.61	30,33,38,38	0
30	OMG	0	2588	24/25	0.12	-0.67	30,34,35,37	0
30	PSU	0	2621	20/21	0.13	-1.46	36,38,42,42	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	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	8979	1/1	1.70	1060.33	184,184,184,184	0
37	SR	0	8920	1/1	0.92	826.00	200,200,200,200	0
37	SR	0	9000	1/1	0.28	295.00	147,147,147,147	0
37	SR	0	9006	1/1	0.47	109.20	198,198,198,198	0
35	MG	0	8087	1/1	0.96	91.38	107,107,107,107	0
35	MG	0	8049	1/1	0.97	90.42	103,103,103,103	0
35	MG	0	8081	1/1	0.55	85.70	91,91,91,91	0
37	SR	0	8994	1/1	0.98	82.82	200,200,200,200	0
36	NA	0	8547	1/1	0.58	76.81	78,78,78,78	0
35	MG	0	8056	1/1	0.38	61.64	94,94,94,94	0
35	MG	0	8045	1/1	0.65	59.75	119,119,119,119	0
35	MG	0	8066	1/1	0.79	53.87	98,98,98,98	0
36	NA	0	8558	1/1	1.00	53.64	67,67,67,67	0
36	NA	0	8505	1/1	0.52	53.43	29,29,29,29	0
36	NA	0	8519	1/1	0.71	49.43	71,71,71,71	0
36	NA	0	8535	1/1	0.81	49.29	75,75,75,75	0
35	MG	0	8018	1/1	0.24	48.78	3,3,3,3	0
35	MG	0	8078	1/1	0.75	45.72	115,115,115,115	0
38	CL	0	8822	1/1	0.32	45.22	66,66,66,66	0
35	MG	0	8092	1/1	0.54	43.80	76,76,76,76	0
36	NA	0	8571	1/1	0.29	43.00	85,85,85,85	0
35	MG	0	8085	1/1	0.67	39.66	92,92,92,92	0
36	NA	9	8544	1/1	0.52	38.88	73,73,73,73	0
35	MG	0	8079	1/1	0.33	33.77	64,64,64,64	0
35	MG	0	8050	1/1	0.32	32.20	152,152,152,152	0
35	MG	0	8047	1/1	0.47	32.18	92,92,92,92	0
36	NA	0	8514	1/1	0.29	31.41	83,83,83,83	0
39	K	0	8402	1/1	1.51	29.78	117,117,117,117	0
36	NA	0	8566	1/1	0.50	27.46	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8065	1/1	0.39	25.73	102,102,102,102	0
36	NA	0	8516	1/1	0.46	25.00	65,65,65,65	0
37	SR	0	8925	1/1	0.17	24.37	70,70,70,70	0
35	MG	0	8016	1/1	0.48	23.14	131,131,131,131	0
35	MG	0	8090	1/1	0.89	23.12	130,130,130,130	0
37	SR	0	9007	1/1	0.48	23.05	195,195,195,195	0
36	NA	0	8527	1/1	0.43	21.47	73,73,73,73	0
36	NA	0	8555	1/1	0.37	19.78	52,52,52,52	0
37	SR	0	8990	1/1	0.56	19.07	177,177,177,177	0
35	MG	0	8071	1/1	0.47	18.79	88,88,88,88	0
36	NA	0	8509	1/1	0.37	18.46	80,80,80,80	0
36	NA	0	8523	1/1	0.25	17.84	61,61,61,61	0
36	NA	0	8562	1/1	0.32	17.62	55,55,55,55	0
39	K	0	8401	1/1	0.58	17.21	82,82,82,82	0
37	SR	L	8969	1/1	0.50	16.66	175,175,175,175	0
35	MG	0	8010	1/1	0.56	16.09	78,78,78,78	0
37	SR	0	9001	1/1	0.33	14.32	190,190,190,190	0
36	NA	0	8512	1/1	0.40	14.14	46,46,46,46	0
35	MG	0	8046	1/1	0.42	14.10	72,72,72,72	0
35	MG	0	8028	1/1	0.23	14.10	1,1,1,1	0
35	MG	0	8076	1/1	0.32	13.87	72,72,72,72	0
35	MG	0	8029	1/1	0.28	13.65	83,83,83,83	0
36	NA	0	8520	1/1	0.22	13.60	58,58,58,58	0
36	NA	0	8548	1/1	0.18	13.12	26,26,26,26	0
36	NA	9	8572	1/1	0.27	12.77	96,96,96,96	0
36	NA	0	8546	1/1	0.73	12.59	97,97,97,97	0
37	SR	0	8917	1/1	0.18	12.55	67,67,67,67	0
35	MG	0	8009	1/1	0.32	12.51	1,1,1,1	0
36	NA	0	8502	1/1	0.23	12.28	60,60,60,60	0
35	MG	0	8058	1/1	0.20	11.82	1,1,1,1	0
36	NA	0	8574	1/1	0.31	11.79	43,43,43,43	0
36	NA	0	8528	1/1	0.25	11.58	55,55,55,55	0
35	MG	0	8036	1/1	0.15	11.57	50,50,50,50	0
36	NA	0	8507	1/1	0.24	11.57	29,29,29,29	0
34	ACA	6	78	8/9	0.43	11.49	88,90,91,91	0
36	NA	S	8510	1/1	0.61	11.10	80,80,80,80	0
36	NA	0	8553	1/1	0.26	10.99	100,100,100,100	0
35	MG	0	8001	1/1	0.23	10.83	7,7,7,7	0
36	NA	0	8521	1/1	0.33	10.82	51,51,51,51	0
37	SR	0	8989	1/1	0.29	10.61	200,200,200,200	0
36	NA	0	8556	1/1	0.79	10.34	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8064	1/1	0.26	10.03	53,53,53,53	0
35	MG	0	8072	1/1	0.20	10.00	55,55,55,55	0
37	SR	0	8927	1/1	0.19	9.82	70,70,70,70	0
36	NA	0	8557	1/1	0.22	9.75	82,82,82,82	0
35	MG	A	8025	1/1	0.28	9.75	39,39,39,39	0
36	NA	0	8533	1/1	0.29	9.74	64,64,64,64	0
37	SR	0	8905	1/1	0.25	9.66	61,61,61,61	0
35	MG	A	8051	1/1	1.00	9.60	82,82,82,82	0
37	SR	0	8926	1/1	0.17	9.36	87,87,87,87	0
36	NA	0	8568	1/1	0.39	9.32	18,18,18,18	0
35	MG	0	8037	1/1	0.18	9.26	64,64,64,64	0
36	NA	0	8550	1/1	0.27	9.22	51,51,51,51	0
35	MG	0	8040	1/1	0.26	9.09	70,70,70,70	0
35	MG	9	8074	1/1	0.22	9.09	52,52,52,52	0
37	SR	0	8942	1/1	0.30	8.90	155,155,155,155	0
36	NA	0	8536	1/1	0.18	8.86	63,63,63,63	0
36	NA	0	8567	1/1	0.28	8.81	61,61,61,61	0
36	NA	0	8545	1/1	0.27	8.68	64,64,64,64	0
36	NA	0	8561	1/1	0.23	8.55	66,66,66,66	0
37	SR	T	8939	1/1	0.14	8.22	70,70,70,70	0
38	CL	J	8816	1/1	0.31	8.21	80,80,80,80	0
35	MG	0	8063	1/1	0.31	8.14	69,69,69,69	0
35	MG	0	8048	1/1	0.27	7.98	49,49,49,49	0
36	NA	0	8525	1/1	0.17	7.91	53,53,53,53	0
35	MG	0	8024	1/1	0.33	7.80	69,69,69,69	0
37	SR	B	8987	1/1	0.39	7.71	199,199,199,199	0
37	SR	0	8949	1/1	0.16	7.69	62,62,62,62	0
35	MG	0	8061	1/1	0.23	7.67	17,17,17,17	0
37	SR	0	8937	1/1	0.21	7.47	69,69,69,69	0
37	SR	0	8903	1/1	0.21	7.39	55,55,55,55	0
36	NA	0	8559	1/1	0.18	7.37	64,64,64,64	0
37	SR	0	8983	1/1	0.22	7.31	169,169,169,169	0
36	NA	0	8541	1/1	0.23	7.17	103,103,103,103	0
37	SR	0	8958	1/1	0.15	7.17	77,77,77,77	0
35	MG	0	8023	1/1	0.24	7.11	25,25,25,25	0
36	NA	0	8531	1/1	0.14	7.09	41,41,41,41	0
37	SR	0	8976	1/1	0.21	7.07	117,117,117,117	0
35	MG	0	8002	1/1	0.27	7.01	19,19,19,19	0
36	NA	0	8552	1/1	0.27	7.00	86,86,86,86	0
37	SR	0	8914	1/1	0.26	6.83	88,88,88,88	0
37	SR	0	9008	1/1	0.22	6.73	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	MG	0	8059	1/1	0.17	6.68	88,88,88,88	0
37	SR	0	8961	1/1	0.15	6.48	185,185,185,185	0
36	NA	0	8511	1/1	0.16	6.35	35,35,35,35	0
35	MG	0	8014	1/1	0.20	6.34	16,16,16,16	0
35	MG	0	8062	1/1	0.29	6.22	41,41,41,41	0
37	SR	0	8938	1/1	0.14	6.20	95,95,95,95	0
37	SR	0	8901	1/1	0.19	6.15	48,48,48,48	0
35	MG	0	8020	1/1	0.20	6.10	24,24,24,24	0
37	SR	0	8944	1/1	0.18	5.84	155,155,155,155	0
35	MG	0	8022	1/1	0.21	5.76	11,11,11,11	0
34	PHE	6	77	11/12	0.34	5.72	88,88,90,90	0
36	NA	0	8569	1/1	0.23	5.64	32,32,32,32	0
37	SR	0	8931	1/1	0.18	5.59	80,80,80,80	0
36	NA	0	8563	1/1	0.22	5.57	51,51,51,51	0
37	SR	0	8904	1/1	0.21	5.43	55,55,55,55	0
35	MG	0	8055	1/1	0.27	5.43	26,26,26,26	0
35	MG	0	8041	1/1	0.20	5.19	33,33,33,33	0
35	MG	0	8070	1/1	0.19	5.09	63,63,63,63	0
35	MG	C	8012	1/1	0.27	5.08	17,17,17,17	0
35	MG	0	8015	1/1	0.17	4.92	41,41,41,41	0
35	MG	B	8042	1/1	0.28	4.90	103,103,103,103	0
37	SR	0	8923	1/1	0.20	4.73	72,72,72,72	0
36	NA	0	8534	1/1	0.35	4.68	68,68,68,68	0
36	NA	H	8518	1/1	0.28	4.48	69,69,69,69	0
37	SR	0	8924	1/1	0.22	4.37	80,80,80,80	0
37	SR	0	8933	1/1	0.28	4.34	126,126,126,126	0
35	MG	2	8060	1/1	0.21	4.23	45,45,45,45	0
37	SR	0	8998	1/1	0.23	4.22	113,113,113,113	0
37	SR	1	8952	1/1	0.19	4.16	67,67,67,67	0
37	SR	0	8966	1/1	0.15	3.99	85,85,85,85	0
36	NA	0	8560	1/1	0.32	3.82	134,134,134,134	0
36	NA	0	8565	1/1	0.20	3.80	48,48,48,48	0
37	SR	0	8948	1/1	0.17	3.79	65,65,65,65	0
36	NA	0	8573	1/1	0.36	3.55	79,79,79,79	0
35	MG	0	8034	1/1	0.21	3.55	30,30,30,30	0
36	NA	0	8570	1/1	0.15	3.50	48,48,48,48	0
35	MG	Y	8086	1/1	0.16	3.45	48,48,48,48	0
36	NA	0	8530	1/1	0.18	3.43	49,49,49,49	0
37	SR	0	8946	1/1	0.19	3.41	98,98,98,98	0
37	SR	0	8996	1/1	0.21	3.37	158,158,158,158	0
35	MG	0	8039	1/1	0.20	3.36	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	8985	1/1	0.15	3.25	142,142,142,142	0
35	MG	B	8043	1/1	0.17	3.11	29,29,29,29	0
35	MG	0	8067	1/1	0.29	3.09	33,33,33,33	0
37	SR	0	8918	1/1	0.19	3.02	53,53,53,53	0
36	NA	0	8501	1/1	0.16	3.01	107,107,107,107	0
35	MG	K	8054	1/1	0.17	2.99	15,15,15,15	0
36	NA	0	8554	1/1	0.20	2.96	42,42,42,42	0
37	SR	0	8936	1/1	0.17	2.92	67,67,67,67	0
35	MG	0	8008	1/1	0.16	2.90	9,9,9,9	0
36	NA	0	8513	1/1	0.20	2.89	53,53,53,53	0
35	MG	0	8004	1/1	0.20	2.82	21,21,21,21	0
37	SR	0	8954	1/1	0.16	2.82	82,82,82,82	0
37	SR	0	8941	1/1	0.20	2.81	77,77,77,77	0
35	MG	0	8027	1/1	0.12	2.71	28,28,28,28	0
37	SR	0	8906	1/1	0.21	2.69	56,56,56,56	0
35	MG	0	8005	1/1	0.22	2.58	25,25,25,25	0
35	MG	0	8006	1/1	0.17	2.52	8,8,8,8	0
37	SR	0	8963	1/1	0.15	2.45	74,74,74,74	0
37	SR	0	8984	1/1	0.14	2.38	92,92,92,92	0
35	MG	0	8088	1/1	0.17	2.36	40,40,40,40	0
37	SR	0	8910	1/1	0.16	2.27	47,47,47,47	0
37	SR	0	8908	1/1	0.15	2.18	64,64,64,64	0
37	SR	1	8913	1/1	0.19	2.17	54,54,54,54	0
36	NA	0	8524	1/1	0.13	2.12	52,52,52,52	0
37	SR	0	8909	1/1	0.16	2.07	56,56,56,56	0
37	SR	0	8965	1/1	0.14	2.04	95,95,95,95	0
37	SR	B	8950	1/1	0.16	2.01	98,98,98,98	0
37	SR	0	8974	1/1	0.21	2.00	125,125,125,125	0
37	SR	0	8916	1/1	0.14	1.91	64,64,64,64	0
38	CL	A	8809	1/1	0.16	1.85	51,51,51,51	0
35	MG	0	8003	1/1	0.18	1.81	14,14,14,14	0
37	SR	0	8964	1/1	0.14	1.67	102,102,102,102	0
37	SR	R	8912	1/1	0.18	1.57	64,64,64,64	0
35	MG	0	8030	1/1	0.23	1.57	167,167,167,167	0
37	SR	0	8915	1/1	0.14	1.57	84,84,84,84	0
36	NA	0	8522	1/1	0.13	1.35	72,72,72,72	0
37	SR	0	8928	1/1	0.11	1.34	92,92,92,92	0
37	SR	0	8978	1/1	0.14	1.33	71,71,71,71	0
37	SR	0	8922	1/1	0.17	1.31	61,61,61,61	0
35	MG	0	8011	1/1	0.18	1.29	4,4,4,4	0
37	SR	0	8902	1/1	0.18	1.25	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	8504	1/1	0.16	1.23	31,31,31,31	0
36	NA	0	8517	1/1	0.16	1.23	36,36,36,36	0
37	SR	0	8981	1/1	0.17	1.21	117,117,117,117	0
36	NA	C	8503	1/1	0.19	1.17	31,31,31,31	0
37	SR	3	8932	1/1	0.17	1.16	74,74,74,74	0
37	SR	0	8921	1/1	0.14	1.13	58,58,58,58	0
37	SR	A	8930	1/1	0.17	0.99	78,78,78,78	0
37	SR	0	8935	1/1	0.14	0.97	73,73,73,73	0
37	SR	H	8907	1/1	0.13	0.88	48,48,48,48	0
38	CL	Y	8817	1/1	0.16	0.80	55,55,55,55	0
35	MG	0	8035	1/1	0.14	0.76	84,84,84,84	0
37	SR	0	8973	1/1	0.11	0.74	98,98,98,98	0
35	MG	0	8068	1/1	0.14	0.73	50,50,50,50	0
35	MG	0	8077	1/1	0.17	0.67	41,41,41,41	0
37	SR	0	8934	1/1	0.16	0.65	71,71,71,71	0
37	SR	Y	9002	1/1	0.11	0.64	124,124,124,124	0
35	MG	0	8017	1/1	0.19	0.58	123,123,123,123	0
38	CL	Q	8811	1/1	0.21	0.57	86,86,86,86	0
36	NA	R	8532	1/1	0.12	0.55	25,25,25,25	0
38	CL	J	8801	1/1	0.15	0.54	62,62,62,62	0
36	NA	0	8515	1/1	0.16	0.49	26,26,26,26	0
35	MG	0	8052	1/1	0.14	0.43	42,42,42,42	0
36	NA	0	8549	1/1	0.15	0.43	36,36,36,36	0
37	SR	0	8943	1/1	0.12	0.40	88,88,88,88	0
37	SR	0	8940	1/1	0.17	0.39	51,51,51,51	0
35	MG	0	8053	1/1	0.15	0.26	33,33,33,33	0
38	CL	O	8808	1/1	0.17	0.20	75,75,75,75	0
37	SR	T	8911	1/1	0.11	0.08	58,58,58,58	0
37	SR	0	8947	1/1	0.14	0.07	91,91,91,91	0
36	NA	0	8575	1/1	0.14	0.07	44,44,44,44	0
38	CL	J	8821	1/1	0.15	0.04	64,64,64,64	0
35	MG	0	8019	1/1	0.15	-0.03	1,1,1,1	0
37	SR	9	8968	1/1	0.11	-0.05	117,117,117,117	0
35	MG	A	8044	1/1	0.13	-0.05	51,51,51,51	0
37	SR	0	8956	1/1	0.14	-0.14	111,111,111,111	0
38	CL	L	8814	1/1	0.14	-0.15	62,62,62,62	0
36	NA	0	8542	1/1	0.15	-0.16	31,31,31,31	0
37	SR	0	8919	1/1	0.15	-0.19	92,92,92,92	0
37	SR	0	9004	1/1	0.16	-0.22	121,121,121,121	0
37	SR	3	8953	1/1	0.16	-0.24	110,110,110,110	0
36	NA	0	8564	1/1	0.09	-0.29	35,35,35,35	0
37	SR	A	8977	1/1	0.16	-0.32	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8986	1/1	0.11	-0.43	108,108,108,108	0
37	SR	0	8957	1/1	0.11	-0.44	124,124,124,124	0
38	CL	0	8812	1/1	0.11	-0.44	50,50,50,50	0
35	MG	0	8069	1/1	0.16	-0.44	120,120,120,120	0
36	NA	J	8538	1/1	0.12	-0.64	31,31,31,31	0
35	MG	0	8084	1/1	0.10	-0.66	27,27,27,27	0
37	SR	A	8929	1/1	0.12	-0.68	114,114,114,114	0
36	NA	Q	8540	1/1	0.12	-0.81	66,66,66,66	0
37	SR	0	8951	1/1	0.10	-0.83	105,105,105,105	0
37	SR	F	9005	1/1	0.11	-0.84	98,98,98,98	0
37	SR	0	8967	1/1	0.09	-0.88	103,103,103,103	0
38	CL	0	8815	1/1	0.10	-0.88	69,69,69,69	0
38	CL	M	8818	1/1	0.12	-0.90	46,46,46,46	0
36	NA	0	8508	1/1	0.11	-0.92	27,27,27,27	0
35	MG	0	8083	1/1	0.09	-0.95	29,29,29,29	0
37	SR	0	8995	1/1	0.12	-0.97	98,98,98,98	0
35	MG	0	8080	1/1	0.07	-1.00	45,45,45,45	0
40	CD	1	8702	1/1	0.11	-1.01	57,57,57,57	0
40	CD	Z	8703	1/1	0.10	-1.02	55,55,55,55	0
37	SR	0	8962	1/1	0.13	-1.02	104,104,104,104	0
37	SR	0	8993	1/1	0.04	-1.10	146,146,146,146	0
36	NA	0	8537	1/1	0.09	-1.11	21,21,21,21	0
36	NA	0	8529	1/1	0.07	-1.16	24,24,24,24	0
36	NA	M	8539	1/1	0.10	-1.22	33,33,33,33	0
35	MG	T	8057	1/1	0.15	-1.26	31,31,31,31	0
35	MG	0	8082	1/1	0.12	-1.27	70,70,70,70	0
40	CD	U	8701	1/1	0.08	-1.37	57,57,57,57	0
36	NA	9	8543	1/1	0.13	-1.38	65,65,65,65	0
37	SR	0	8960	1/1	0.09	-1.40	98,98,98,98	0
37	SR	3	8999	1/1	0.12	-1.43	69,69,69,69	0
37	SR	0	8955	1/1	0.09	-1.47	127,127,127,127	0
36	NA	0	8551	1/1	0.10	-1.50	32,32,32,32	0
38	CL	L	8810	1/1	0.07	-1.50	56,56,56,56	0
37	SR	0	8991	1/1	0.09	-1.64	148,148,148,148	0
35	MG	0	8073	1/1	0.08	-1.70	58,58,58,58	0
37	SR	0	8970	1/1	0.08	-1.72	99,99,99,99	0
35	MG	0	8007	1/1	0.14	-1.79	30,30,30,30	0
35	MG	0	8075	1/1	0.09	-1.79	38,38,38,38	0
37	SR	0	8945	1/1	0.09	-1.80	104,104,104,104	0
37	SR	H	8972	1/1	0.08	-1.83	132,132,132,132	0
35	MG	0	8033	1/1	0.09	-1.96	44,44,44,44	0
38	CL	J	8802	1/1	0.08	-2.06	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
40	CD	3	8704	1/1	0.08	-2.15	52,52,52,52	0
38	CL	Y	8820	1/1	0.06	-2.16	48,48,48,48	0
38	CL	B	8819	1/1	0.10	-2.17	62,62,62,62	0
35	MG	0	8026	1/1	0.09	-2.18	43,43,43,43	0
37	SR	0	8959	1/1	0.06	-2.20	120,120,120,120	0
36	NA	0	8506	1/1	0.07	-2.23	50,50,50,50	0
40	CD	O	8705	1/1	0.04	-2.27	111,111,111,111	0
37	SR	0	8988	1/1	0.09	-2.41	114,114,114,114	0
38	CL	N	8807	1/1	0.07	-2.58	70,70,70,70	0
38	CL	R	8806	1/1	0.11	-2.83	44,44,44,44	0
35	MG	0	8021	1/1	0.07	-2.93	24,24,24,24	0
37	SR	0	8992	1/1	0.06	-3.06	122,122,122,122	0
37	SR	0	8975	1/1	0.04	-3.25	125,125,125,125	0
38	CL	0	8805	1/1	0.08	-3.28	60,60,60,60	0
38	CL	3	8804	1/1	0.10	-3.62	60,60,60,60	0
38	CL	0	8813	1/1	0.08	-4.07	63,63,63,63	0
38	CL	0	8803	1/1	0.05	-4.47	51,51,51,51	0
35	MG	0	8032	1/1	0.04	-4.86	21,21,21,21	0
35	MG	0	8093	1/1	0.06	-6.07	27,27,27,27	0
37	SR	0	8982	1/1	0.08	-6.33	116,116,116,116	0
35	MG	0	8013	1/1	0.04	-6.84	20,20,20,20	0
37	SR	9	8980	1/1	0.08	-7.33	132,132,132,132	0
36	NA	0	8526	1/1	0.10	-7.87	55,55,55,55	0
37	SR	9	9003	1/1	0.04	-8.00	144,144,144,144	0
35	MG	0	8089	1/1	0.09	-9.07	31,31,31,31	0
37	SR	0	8997	1/1	0.06	-9.25	116,116,116,116	0
35	MG	0	8031	1/1	0.05	-9.61	41,41,41,41	0
35	MG	0	8091	1/1	0.14	-	76,76,76,76	0
35	MG	0	8038	1/1	0.25	-	97,97,97,97	0
37	SR	0	8971	1/1	0.12	-	191,191,191,191	0

6.5 Other polymers ⓘ

There are no such residues in this entry.