



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:22 AM GMT

PDB ID : 1VQ9
Title : The structure of CCA-PHE-CAP-BIO and the antibiotic sparsomycin bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 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>

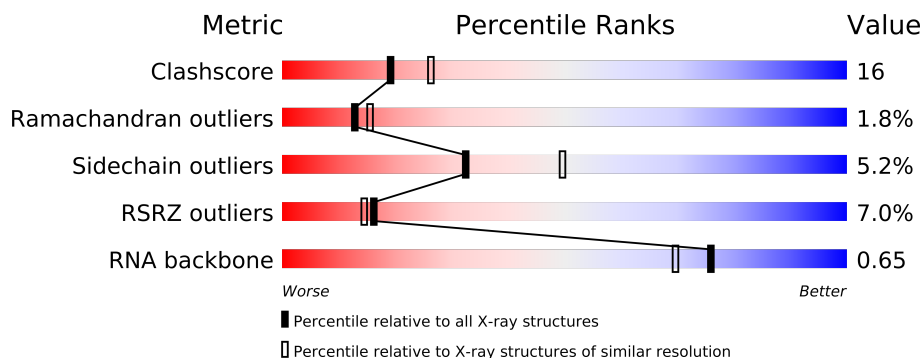
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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	0	2922	
2	9	122	
3	4	5	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

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

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8001	-	X
33	MG	0	8008	-	X
33	MG	0	8012	-	X
33	MG	0	8013	-	X
33	MG	0	8014	-	X
33	MG	0	8021	-	X
33	MG	0	8022	-	X
33	MG	0	8024	-	X
33	MG	0	8025	-	X
33	MG	0	8026	-	X
33	MG	0	8027	-	X
33	MG	0	8029	-	X
33	MG	0	8038	-	X
33	MG	0	8046	-	X
33	MG	0	8047	-	X
33	MG	0	8050	-	X
33	MG	0	8051	-	X
33	MG	0	8052	-	X
33	MG	0	8057	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8058	-	X
33	MG	0	8059	-	X
33	MG	0	8060	-	X
33	MG	0	8070	-	X
33	MG	0	8082	-	X
33	MG	0	8083	-	X
33	MG	0	8084	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8097	-	X
33	MG	0	8099	-	X
33	MG	0	8101	-	X
33	MG	0	8103	-	X
33	MG	0	8104	-	X
33	MG	0	8107	-	X
33	MG	0	8108	-	X
33	MG	0	8110	-	X
33	MG	0	8114	-	X
33	MG	4	8118	-	X
33	MG	9	8095	-	X
33	MG	B	8055	-	X
33	MG	B	8056	-	X
33	MG	K	8069	-	X
34	K	0	9001	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X
35	NA	0	9110	-	X
35	NA	0	9113	-	X
35	NA	0	9114	-	X
35	NA	0	9115	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9122	-	X
35	NA	0	9125	-	X
35	NA	0	9127	-	X
35	NA	0	9128	-	X
35	NA	0	9129	-	X
35	NA	0	9131	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9132	-	X
35	NA	0	9135	-	X
35	NA	0	9136	-	X
35	NA	0	9140	-	X
35	NA	0	9150	-	X
35	NA	0	9154	-	X
35	NA	0	9156	-	X
35	NA	0	9157	-	X
35	NA	0	9158	-	X
35	NA	0	9159	-	X
35	NA	0	9160	-	X
35	NA	0	9163	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9166	-	X
35	NA	0	9167	-	X
35	NA	0	9168	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	X
35	NA	0	9174	-	X
35	NA	0	9175	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9181	-	X
35	NA	0	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	3	9169	-	X
35	NA	9	9152	-	X
35	NA	9	9183	-	X
35	NA	B	9161	-	X
35	NA	R	9186	-	X
35	NA	S	9112	-	X
36	CL	0	9316	-	X
36	CL	0	9322	-	X
36	CL	B	9319	-	X
37	SR	0	9406	-	X
37	SR	0	9407	-	X
37	SR	0	9408	-	X
37	SR	0	9410	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	0	9411	-	X
37	SR	0	9415	-	X
37	SR	0	9420	-	X
37	SR	0	9424	-	X
37	SR	0	9427	-	X
37	SR	0	9429	-	X
37	SR	0	9432	-	X
37	SR	0	9433	-	X
37	SR	0	9434	-	X
37	SR	0	9451	-	X
37	SR	0	9456	-	X
37	SR	0	9482	-	X
37	SR	0	9484	-	X
37	SR	0	9488	-	X
37	SR	0	9500	-	X
37	SR	0	9501	-	X
37	SR	0	9530	-	X
37	SR	0	9539	-	X
37	SR	0	9547	-	X
37	SR	0	9601	-	X
37	SR	0	9626	-	X
37	SR	1	9419	-	X
37	SR	B	9521	-	X
37	SR	S	9470	-	X
39	CD	O	9205	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98979 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 RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	5	Total	C	N	O	P	0	0	0
			74	40	12	20	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 5 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 6 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 8 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	O	115	Total	C	N	O	0	0	0
			865	529	161	175			

- Molecule 18 is a protein called 50S ribosomal protein L19E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	143	Total	C	N	O	0	0	0
			1136	683	229	224			

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	95	Total	C	N	O	0	0	0
			735	450	141	144			

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	119	Total	C	N	O	0	0	0
			950	568	180	202			

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	62	Total	Na	0	0
			62	62		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	D	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	C	1	Total 1	Na 1	0	0
35	3	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

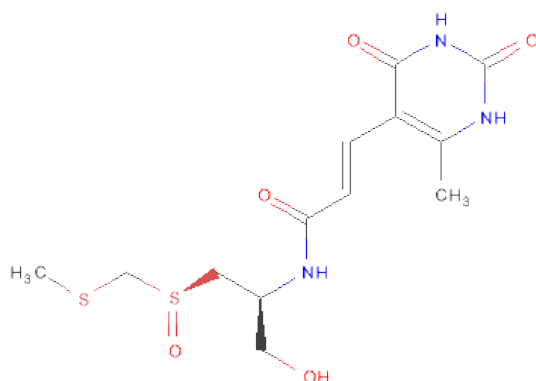
- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: CL).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	J	3	Total 3	Cl 3	0	0
36	K	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	97	Total 97	Sr 97	0	0
37	1	2	Total 2	Sr 2	0	0
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	4	Total 4	Sr 4	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	3	Total 3	Sr 3	0	0
37	L	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

- Molecule 38 is SPARSOMYCIN (three-letter code: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	4	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total	Cd	0	0
			1	1		
39	Z	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	3	1	Total	Cd	0	0
			1	1		
39	U	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5630	Total	O	0	0
			5630	5630		
40	9	130	Total	O	0	0
			130	130		
40	4	1	Total	O	0	0
			1	1		
40	A	132	Total	O	0	0
			132	132		
40	B	137	Total	O	0	0
			137	137		
40	C	175	Total	O	0	0
			175	175		
40	D	43	Total	O	0	0
			43	43		
40	E	42	Total	O	0	0
			42	42		
40	F	25	Total	O	0	0
			25	25		
40	G	16	Total	O	0	0
			16	16		
40	H	77	Total	O	0	0
			77	77		
40	J	52	Total	O	0	0
			52	52		

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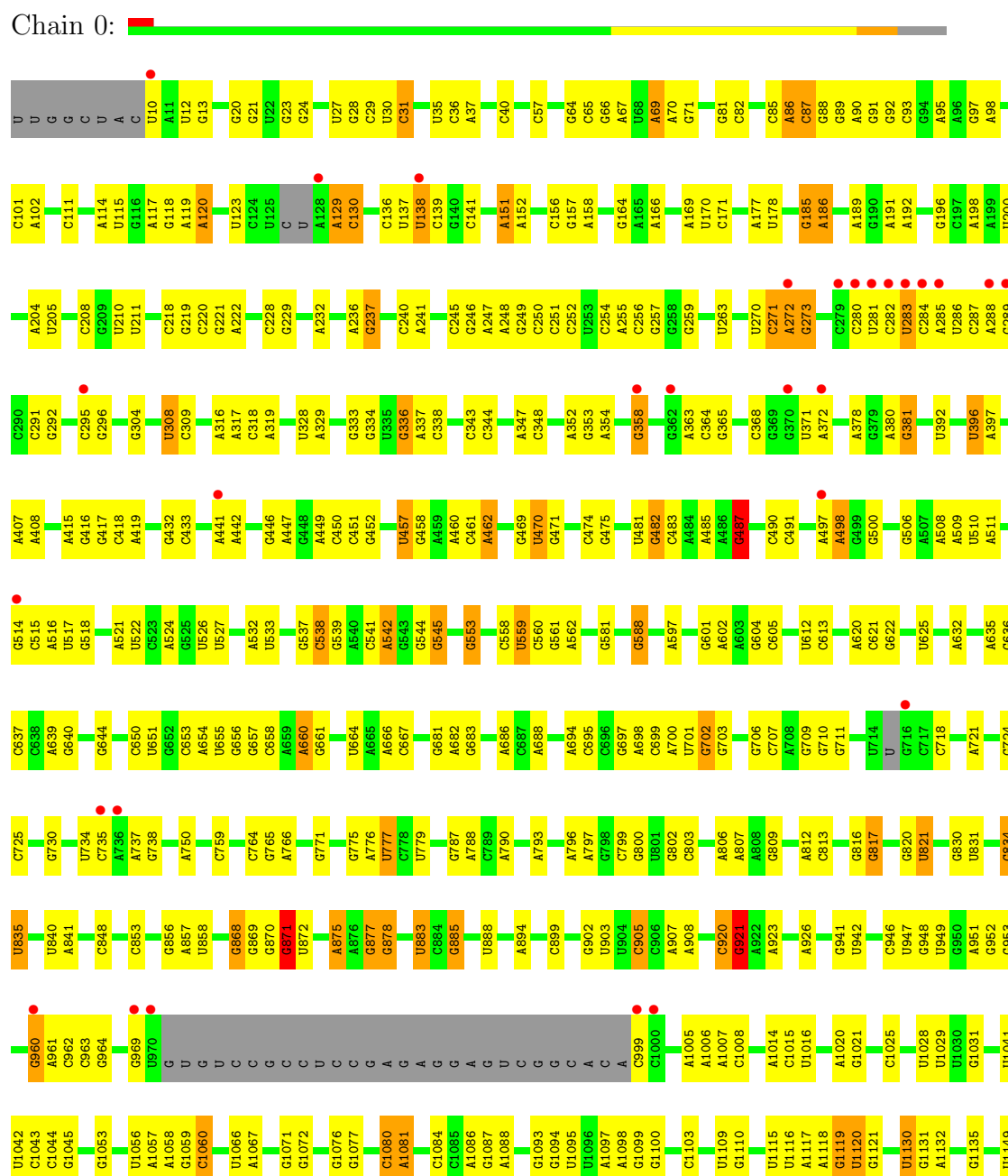
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	K	61	Total 61	O 61	0	0
40	L	93	Total 93	O 93	0	0
40	M	133	Total 133	O 133	0	0
40	N	66	Total 66	O 66	0	0
40	O	42	Total 42	O 42	0	0
40	P	68	Total 68	O 68	0	0
40	Q	53	Total 53	O 53	0	0
40	R	93	Total 93	O 93	0	0
40	S	35	Total 35	O 35	0	0
40	T	40	Total 40	O 40	0	0
40	U	28	Total 28	O 28	0	0
40	V	13	Total 13	O 13	0	0
40	W	70	Total 70	O 70	0	0
40	X	23	Total 23	O 23	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	30	Total 30	O 30	0	0
40	1	60	Total 60	O 60	0	0
40	2	46	Total 46	O 46	0	0
40	3	70	Total 70	O 70	0	0
40	I	9	Total 9	O 9	0	0

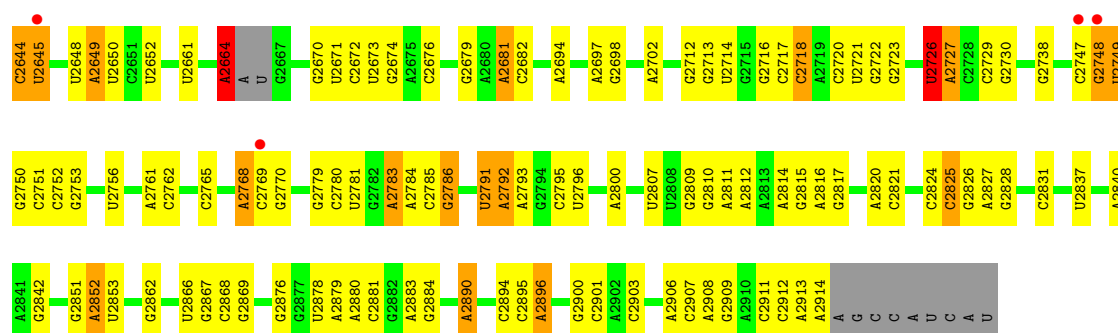
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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: 23S ribosomal rna



U2541	G2453	G	C2241	U1985	A1881	A1797	A1701	G1592	C1474	C1342	U1219	A1150
U2545	A2456	A	U2242	C1993	C1882	C1798	U1702	C1593	G1475	C143	C1229	G1151
U2546	A2345	C	C2243	G1884	G1883	G1799	A1710	C1594	A1476	A1352		G1159
C2547	C2346	C		U1996	A1886	A1804	G1714	C1595	U1477	C1353	U1235	G1160
C2548	A2353	C	A2251	U2003	A1890	A1805	C1715	A1597	A1482	C1360	G1236	A1161
C2552	A2354	C	G2252	U2004	U1890	G1806	A1716	U1598	C1483	C1361	U1237	G1162
A2553	A2361	C	U2253	G2006	G1902	G1809	G1717	A1600	A1486	U1362	G1239	U1163
A2563	A2362	A	U2107	A2007	G1903	A1815	U1722	A1603	A1487	C1366	A1242	G1167
A2564	G2363	C	U2108	G2008	U1902	G1816	G1723	G1604	U1488	C1243	U1244	C1168
C2565	A2364	C	U2109	G2009	C1919	U1817	U1724	G1605	G1489	A1372		U1169
A2568	A2369	C	G2111	A2010	C1920	C1818	C1725	A1615	C1495			U1170
A2569	C2471	C	G2112	U2011	A1921	C1819	G1730	U1624	G1496	C1376	A1246	G1171
A2577	C2472	C	G2113	G2012	U1922	G1820	C1731	A1626	U1500	C1378	A1262	G1172
A2578	C2473	C	U2114	G2013	C1926	C1826	A1736	G1627	U1503		C1253	G1173
A2579	C2474	C	U2115	U2016	A1927	G1827	U1748	U1630	U1504	C1384	U1264	G1174
C2580	C2475	C	U2116	U2017	C1928	G1828	G1739	A1630	U1505	C1391		G1175
U2581	C2476	C	U2117	U2018	C1929	A1829	U1741	A1630	U1506	A1392	C1268	C1176
C2582	C2477	C	U2118	U2019	C1940	C1834	U1741	C1633	C1507		G1269	A1177
A2586	C2478	C	U2119	U2020	C1941	U1835	G1745	G1634	U1516	G1398		U1180
C2587	C2479	C	U2120	U2021	A1942	A1836	G1745	U1635	C1516	A1399	U1279	C1181
C2588	C2480	C	U2121	U2022	C1943	A1837	U1748	U1636	U1524	C1400		C1182
C2589	C2481	C	U2122	U2023	C1944	U1838	U1748	U1637	G1525			C1183
C2590	C2482	C	U2123	U2024	C1945	U1839	G1752	U1638	A1526	A1406	A1287	C1184
C2591	C2483	C	U2124	U2025	C1946	A1840	C1752	U1667	A1527	A1407	C1289	U1185
C2592	C2484	C	U2125	U2026	C1947	A1841	C1752	U1668	A1527	U1408		C1186
A2599	C2485	C	U2126	U2027	C1948	A1842	A1755	U1669	A1528	G1409	U1293	A1188
A2600	C2486	C	U2127	U2028	C1949	U1843	A1755	G1670	U1529	A1414	A1294	A1189
A2601	C2487	C	U2128	U2029	C1950	U1844	G1756	U1677	G1534		G1295	A1190
C2602	C2488	C	U2129	U2030	C1951	U1845	A1759	U1678	C1537	U1419	U1298	A1191
C2608	C2489	C	U2130	U2031	C1952	U1846	A1759	U1679	U1537	U1420	G1299	A1192
C2611	C2490	C	U2131	U2032	C1953	U1847	A1759	U1680	C1545	C1421	U1299	A1193
A2612	C2491	C	U2132	U2033	C1954	U1848	G1764	U1681	G1546	U1422	G1300	A1194
C2613	C2492	C	U2133	U2034	C1955	U1849	G1765	U1682	U1554	C1423	C1305	G1195
C2614	C2493	C	U2134	U2035	C1956	U1850	U1766	U1683	G1552			C1196
C2615	C2494	C	U2135	U2036	C1957	U1851	G1769	U1684	C1553	C1426	U1309	U1197
C2616	C2495	C	U2136	U2037	C1958	U1852	U1770	U1685	U1554	A1427	U1310	U1198
U2619	C2496	C	U2137	U2038	C1959	U1853	G1773	U1686	G1555			A1199
U2620	C2497	C	U2138	U2039	C1960	U1854	G1777	U1687	U1555	G1430	U1314	C1201
C2626	C2498	C	U2139	U2040	C1961	U1855	A1778	U1688	U1559	U1435	G1315	A1202
C2627	C2499	C	U2140	U2041	C1962	U1856	A1778	U1689	U1561	U1440	G1316	G1203
C2630	C2500	C	U2141	U2042	C1963	U1857	A1778	U1690	C1562	U1446	G1325	U1204
U2631	C2501	C	U2142	U2043	C1964	U1858	A1778	U1691	C1563		A1328	U1205
C2632	C2502	C	U2143	U2044	C1965	U1859	A1778	U1692	C1564	C1461	A1331	C1209
C2633	C2503	C	U2144	U2045	C1966	U1860	A1778	U1693	C1565	C1458	C1332	G1210
C2634	C2504	C	U2145	U2046	C1967	U1861	A1778	U1694	C1566	A1573	C1333	C1211
A2637	C2505	C	U2146	U2047	C1968	U1862	A1778	U1695	C1567	C1574	C1335	C1212
C2643	C2506	C	U2147	U2048	C1969	U1863	A1778	U1696	C1568	C1462		G1216
	C2507	C	U2148	U2049	C1970	U1864	A1778	U1697	U1569	A1463	G1340	G1217
	C2508	C	U2149	U2050	C1971	U1865	A1778	U1698	U1570	U1473	A1341	U1218
	C2509	C	U2150	U2051	C1972	U1866	A1778	U1699	U1571			
	C2510	C	U2151	U2052	C1973	U1867	A1778	U1700	U1572			
	C2511	C	U2152	U2053	C1974	U1868	A1778	U1701	U1573			
	C2512	C	U2153	U2054	C1975	U1869	A1778	U1702	U1574			
	C2513	C	U2154	U2055	C1976	U1870	A1778	U1703	U1575			
	C2514	C	U2155	U2056	C1977	U1871	A1778	U1704	U1576			
	C2515	C	U2156	U2057	C1978	U1872	A1778	U1705	U1577			
	C2516	C	U2157	U2058	C1979	U1873	A1778	U1706	U1578			
	C2517	C	U2158	U2059	C1980	U1874	A1778	U1707	U1579			
	C2518	C	U2159	U2060	C1981	U1875	A1778	U1708	U1580			
	C2519	C	U2160	U2061	C1982	U1876	A1778	U1709	U1581			
	C2520	C	U2161	U2062	C1983	U1877	A1778	U1710	U1582			
	C2521	C	U2162	U2063	C1984	U1878	A1778	U1711	U1583			
	C2522	C	U2163	U2064	C1985	U1879	A1778	U1712	U1584			
	C2523	C	U2164	U2065	C1986	U1880	A1778	U1713	U1585			
	C2524	C	U2165	U2066	C1987	U1881	A1778	U1714	U1586			
	C2525	C	U2166	U2067	C1988	U1882	A1778	U1715	U1587			
	C2526	C	U2167	U2068	C1989	U1883	A1778	U1716	U1588			
	C2527	C	U2168	U2069	C1990	U1884	A1778	U1717	U1589			
	C2528	C	U2169	U2070	C1991	U1885	A1778	U1718	U1590			
	C2529	C	U2170	U2071	C1992	U1886	A1778	U1719	U1591			
	C2530	C	U2171	U2072	C1993	U1887	A1778	U1720	U1592			
	C2531	C	U2172	U2073	C1994	U1888	A1778	U1721	U1593			
	C2532	C	U2173	U2074	C1995	U1889	A1778	U1722	U1594			
	C2533	C	U2174	U2075	C1996	U1890	A1778	U1723	U1595			
	C2534	C	U2175	U2076	C1997	U1891	A1778	U1724	U1596			
	C2535	C	U2176	U2077	C1998	U1892	A1778	U1725	U1597			
	C2536	C	U2177	U2078	C1999	U1893	A1778	U1726	U1598			
	C2537	C	U2178	U2079	C2000	U1894	A1778	U1727	U1599			
	C2538	C	U2179	U2080	C2001	U1895	A1778	U1728	U1600			
	C2539	C	U2180	U2081	C2002	U1896	A1778	U1729	U1601			
	C2540	C	U2181	U2082	C2003	U1897	A1778	U1730	U1602			
	C2541	C	U2182	U2083	C2004	U1898	A1778	U1731	U1603			
	C2542	C	U2183	U2084	C2005	U1899	A1778	U1732	U1604			
	C2543	C	U2184	U2085	C2006	U1900	A1778	U1733	U1605			
	C2544	C	U2185	U2086	C2007	U1901	A1778	U1734	U1606			
	C2545	C	U2186	U2087	C2008	U1902	A1778	U1735	U1607			
	C2546	C	U2187	U2088	C2009	U1903	A1778	U1736	U1608			
	C2547	C	U2188	U2089	C2010	U1904	A1778	U1737	U1609			
	C2548	C	U2189	U2090	C2011	U1905	A1778	U1738	U1610			
	C2549	C	U2190	U2091	C2012	U1906	A1778	U1739	U1611			
	C2550	C	U2191	U2092	C2013	U1907	A1778	U1740	U1612			
	C2551	C	U2192	U2093	C2014	U1908	A1778	U1741	U1613			
	C2552	C	U2193	U2094	C2015	U1909	A1778	U1742	U1614			
	C2553	C	U2194	U2095	C2016	U1910	A1778	U1743	U1615			
	C2554	C	U2195	U2096	C2017	U1911	A1778	U1744	U1616			
	C2555	C	U2196	U2097	C2018	U1912	A1778	U1745	U1617			
	C2556	C	U2197	U2098	C2019	U1913	A1778	U1746	U1618			
	C2557	C	U2198	U2099	C2020	U1914	A1778	U1747	U1619			
	C2558	C	U2199	U2100	C2021	U1915	A1778	U1748	U1620			
	C2559	C	U2200	U2101	C2022	U1916	A1778	U1749	U1621			
	C2560	C	U2201	U2102	C2023	U1917	A1778	U1750	U1622			
	C2561	C	U2202	U2103	C2024	U1918	A1778	U1751	U1623			
	C2562	C	U2203	U2104	C2025	U1919	A1778	U1752	U1624			
	C2563	C	U2204	U2105	C2026	U1920	A1778	U1753	U1625			
	C2564	C	U2205	U2106	C2027	U1921	A1778	U1754	U1626			
	C2565	C	U2206	U2107	C2028	U1922	A1778	U1755	U1627			
	C2566	C	U2207	U2108	C2029	U1923	A1778	U1756	U1628			
	C2567	C	U2208	U2109	C2030	U1924	A1778	U1757	U1629			
	C2568	C	U2209	U2110	C2031	U1925	A1778	U1758	U1630			
	C2569	C	U2210	U2111	C2032	U1926	A1778	U1759	U1631			
	C2570	C	U2211	U2112	C2033	U1927	A1778	U1760	U1632			
	C2571	C	U2212	U2113	C2034	U1928	A1778	U1761	U1633			



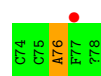
• Molecule 2: 5S ribosomal RNA

Chain 9:



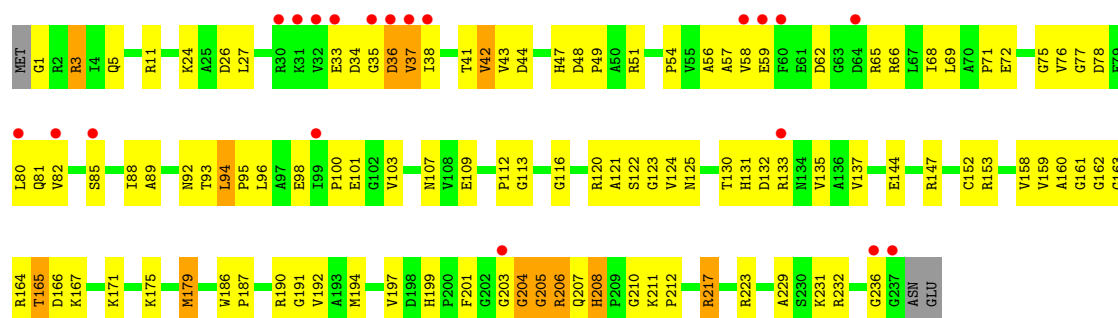
• Molecule 3: 5'-R(*CP*CP*AP*(PHE)*(ACA))-3'

Chain 4:



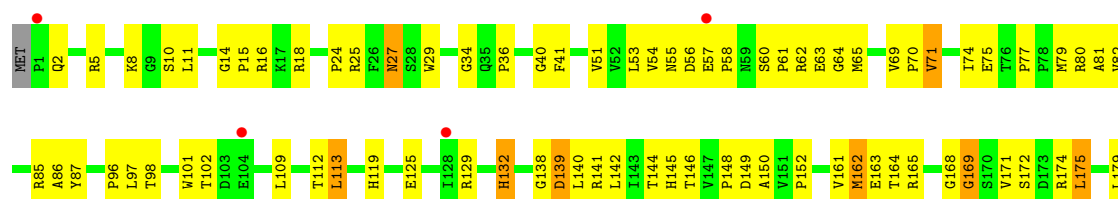
• Molecule 4: 50S ribosomal protein L2P

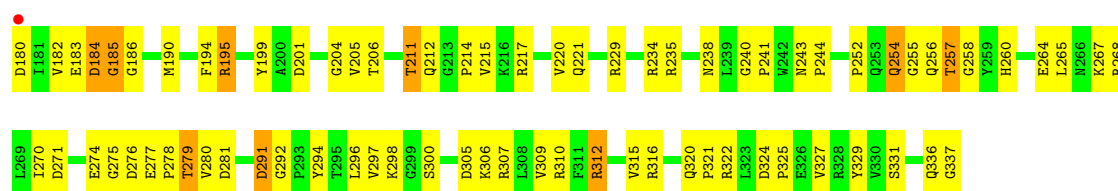
Chain A:



• Molecule 5: 50S ribosomal protein L3P

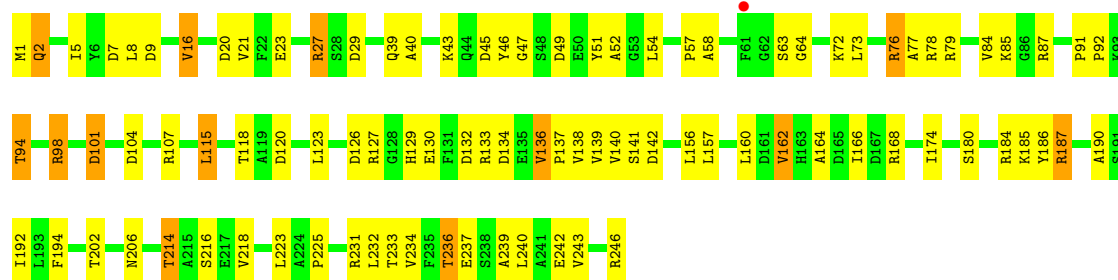
Chain B:





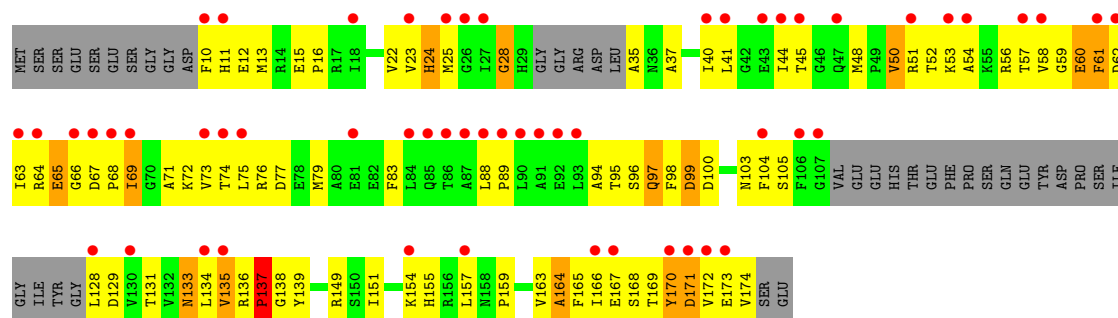
• Molecule 6: 50S ribosomal protein L4E

Chain C:



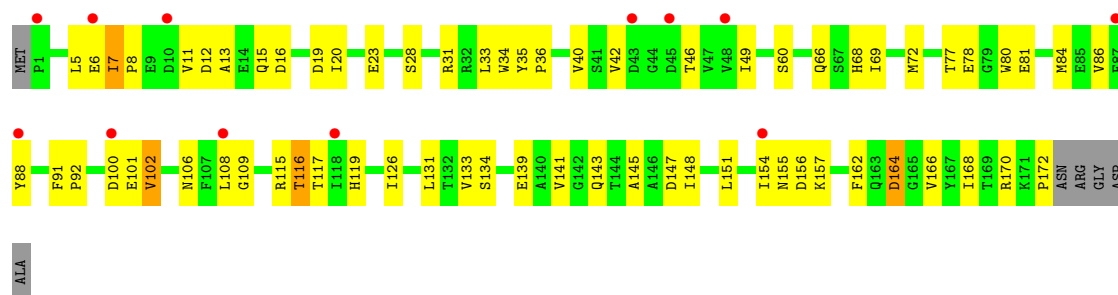
• Molecule 7: 50S ribosomal protein L5P

Chain D:



• Molecule 8: 50S ribosomal protein L6P

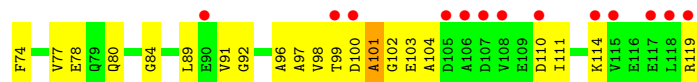
Chain E:



• Molecule 9: 50S ribosomal protein L7AE

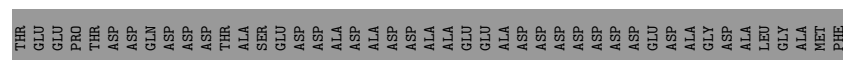
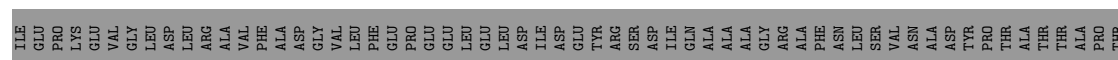
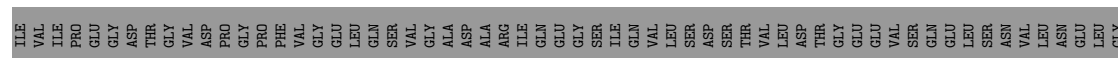
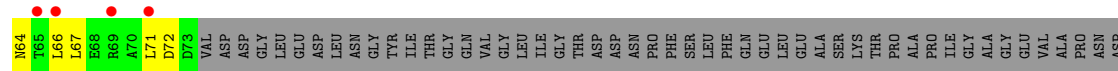
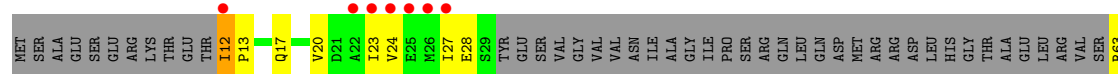
Chain F:





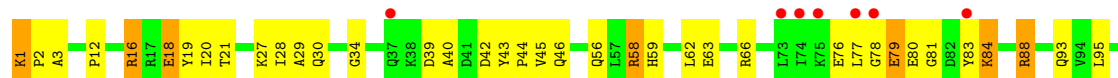
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



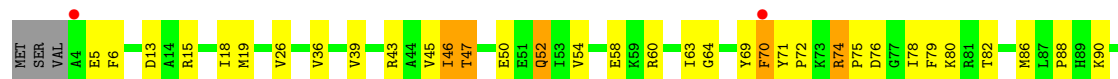
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



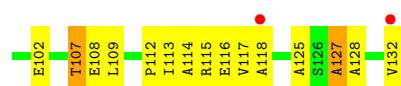
• Molecule 12: 50S ribosomal protein L13P

Chain J:



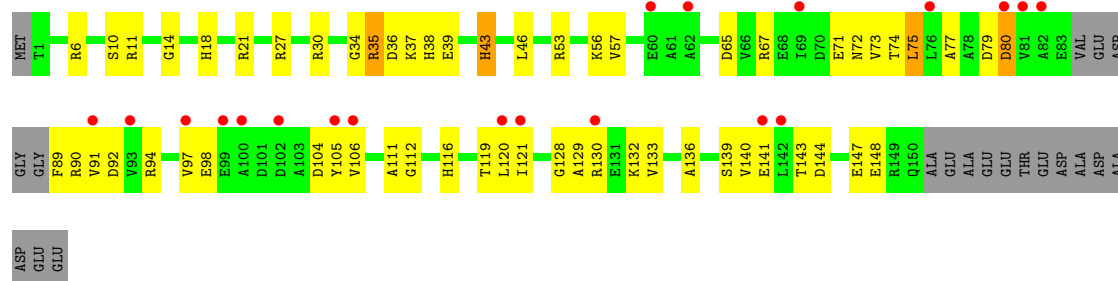
• Molecule 13: 50S ribosomal protein L14P

Chain K:



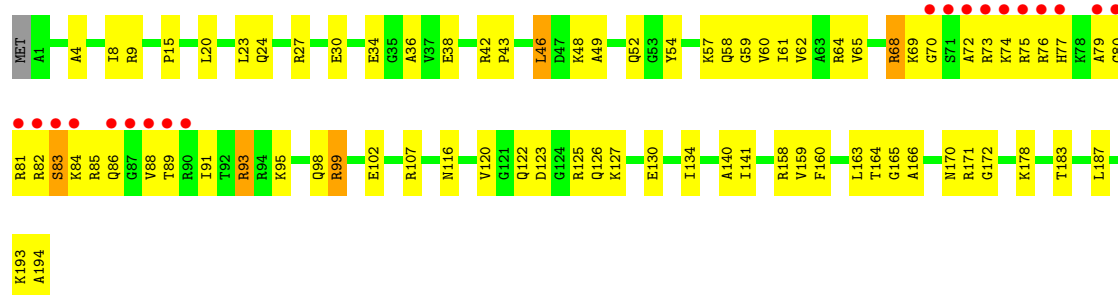
• Molecule 14: 50S ribosomal protein L15P

Chain L:



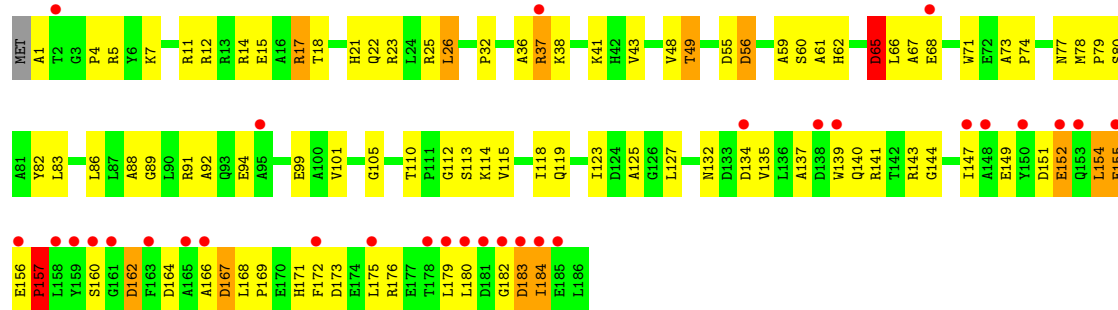
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



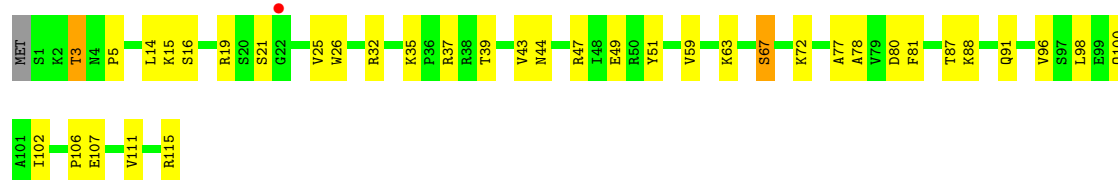
• Molecule 16: 50S ribosomal protein L18P

Chain N:



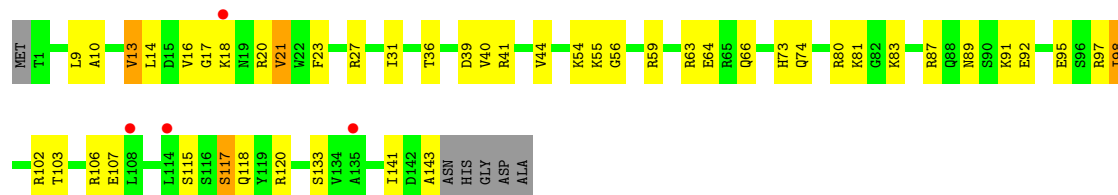
• Molecule 17: 50S ribosomal protein L18e

Chain O:



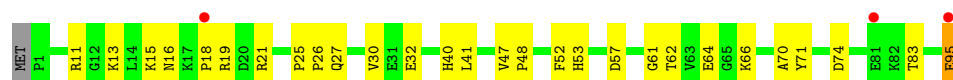
- Molecule 18: 50S ribosomal protein L19E

Chain P:



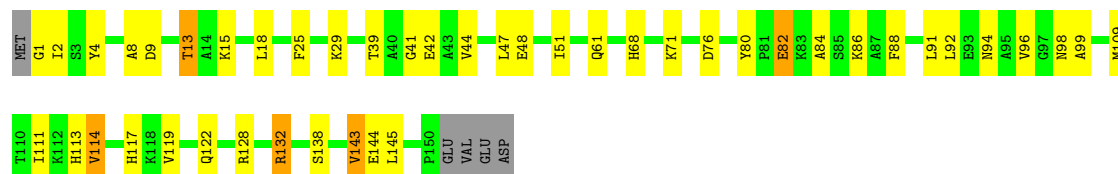
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



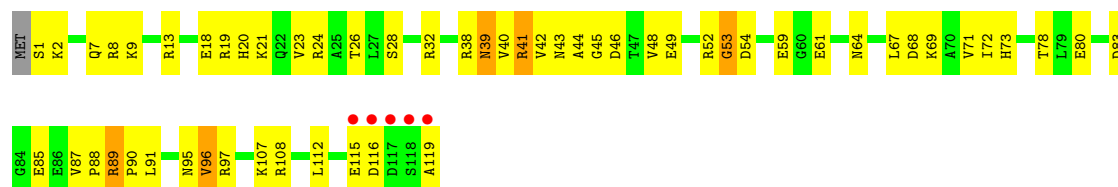
- Molecule 21: 50S ribosomal protein L23P

Chain S:



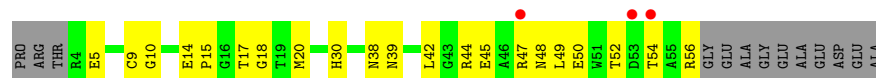
- Molecule 22: 50S ribosomal protein L24P

Chain T:



- Molecule 23: 50S ribosomal protein L24E

Chain U:



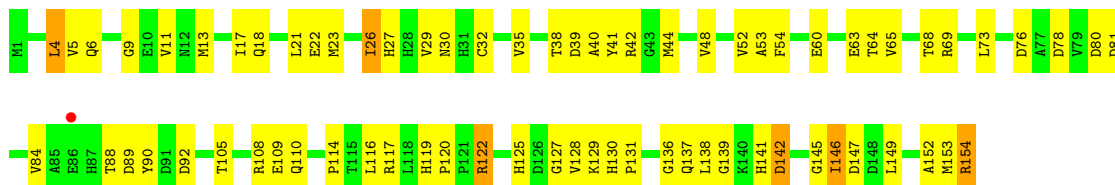
- Molecule 24: 50S ribosomal protein L29P

Chain V:



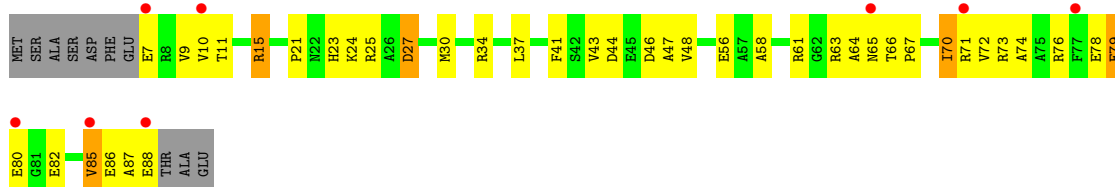
• Molecule 25: 50S ribosomal protein L30P

Chain W:



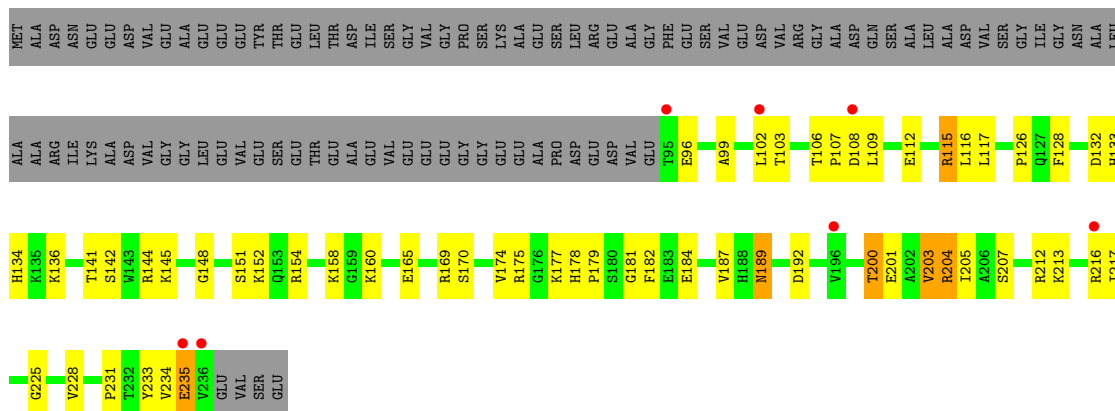
• Molecule 26: 50S ribosomal protein L31e

Chain X:



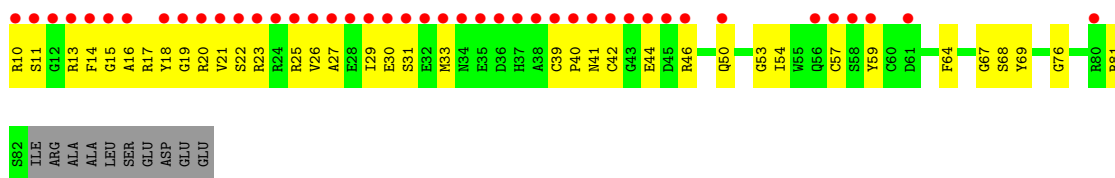
• Molecule 27: 50S ribosomal protein L32E

Chain Y:



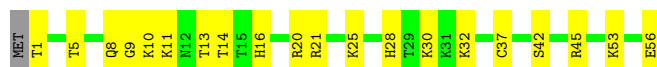
• Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



• Molecule 29: 50S ribosomal protein L37e

Chain 1:



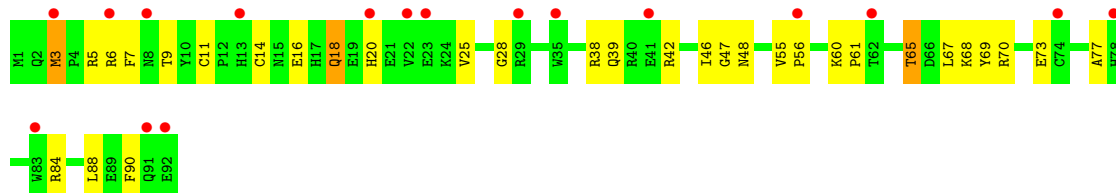
- Molecule 30: 50S ribosomal protein L39e

Chain 2:



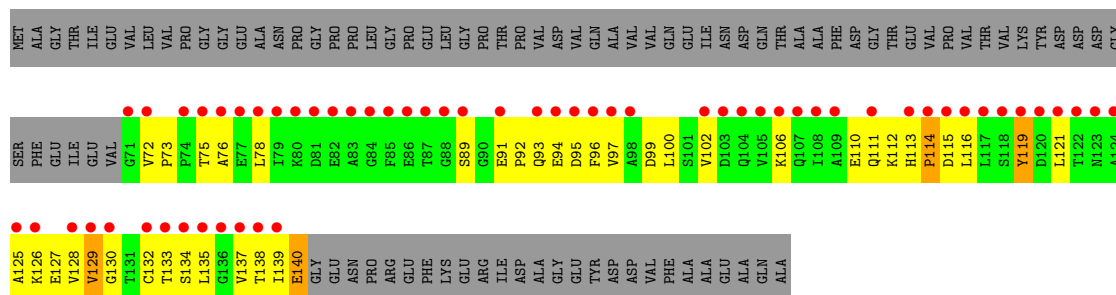
- Molecule 31: 50S ribosomal protein L44E

Chain 3:



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.82Å 298.60Å 574.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.40) 89.6 (49.68-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.255 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 698193 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98979	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.81% 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, CL, SR, NA, K, SPS, 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	0	0.42	0/65959	0.71	23/102870 (0.0%)
2	9	0.39	0/2905	0.73	1/4528 (0.0%)
3	4	0.50	0/76	0.74	0/112
4	A	0.34	0/1786	0.64	0/2408
5	B	0.36	0/2690	0.67	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.34	0/1111	0.57	0/1498
8	E	0.37	0/1382	0.61	0/1880
9	F	0.36	0/901	0.57	0/1224
10	G	0.33	0/241	0.49	0/324
11	H	0.37	0/1287	0.66	0/1725
12	J	0.38	0/1136	0.64	0/1530
13	K	0.38	0/1001	0.68	0/1347
14	L	0.36	0/1130	0.66	0/1509
15	M	0.38	0/1584	0.61	0/2119
16	N	0.32	0/1474	0.63	0/1999
17	O	0.35	0/874	0.62	0/1181
18	P	0.36	0/1147	0.59	0/1528
19	Q	0.36	0/749	0.68	0/1005
20	R	0.37	0/1172	0.68	0/1578
21	S	0.37	0/648	0.60	0/875
22	T	0.34	0/958	0.63	0/1289
23	U	0.38	0/417	0.56	0/562
24	V	0.31	0/502	0.56	0/675
25	W	0.37	0/1219	0.64	0/1655
26	X	0.38	0/664	0.63	0/895
27	Y	0.39	0/1146	0.68	0/1536
28	Z	0.36	0/589	0.58	0/787
29	1	0.45	0/438	0.68	0/578
30	2	0.38	0/401	0.63	0/529
31	3	0.36	0/771	0.55	0/1024
32	I	0.32	0/526	0.55	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.40	0/98768	0.69	24/147689 (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
1	0	1	44
2	9	0	1
All	All	1	45

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.83	131.13	109.50
1	0	871	G	C5'-C4'-O4'	-7.12	100.56	109.10
2	9	3039	U	N1-C1'-C2'	7.04	123.15	114.00
1	0	1979	G	C2'-C3'-O3'	6.99	124.88	113.70
1	0	883	U	N1-C1'-C2'	6.65	122.64	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	460	A	Sidechain
1	0	462	A	Sidechain
1	0	469	G	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	0	59021	0	29809	911	0
2	9	2600	0	1326	55	0
3	4	74	0	44	1	0
4	A	1753	0	1765	133	0
5	B	2625	0	2531	156	0
6	C	1859	0	1816	118	0
7	D	1094	0	1085	94	0
8	E	1357	0	1266	67	0
9	F	890	0	843	62	0
10	G	240	0	231	14	0
11	H	1266	0	1268	62	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	60	0
14	L	1118	0	1076	65	0
15	M	1560	0	1567	91	0
16	N	1445	0	1401	96	0
17	O	865	0	873	46	0
18	P	1136	0	1123	44	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	47	0
21	S	641	0	605	24	0
22	T	950	0	923	73	0
23	U	410	0	364	24	0
24	V	499	0	511	38	0
25	W	1196	0	1137	99	0
26	X	654	0	653	35	0
27	Y	1130	0	1133	67	0
28	Z	578	0	542	42	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	43	0
32	I	519	0	500	40	0
33	0	86	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	9	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	K	1	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	97	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	4	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	4	23	0	19	3	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	0	5630	0	0	126	0
40	1	60	0	0	3	0
40	2	46	0	0	1	0
40	3	70	0	0	6	0
40	4	1	0	0	0	0
40	9	130	0	0	5	0
40	A	132	0	0	13	0
40	B	137	0	0	22	0
40	C	175	0	0	20	0
40	D	43	0	0	8	0
40	E	42	0	0	2	0
40	F	25	0	0	4	0
40	G	16	0	0	2	0
40	H	77	0	0	4	0
40	I	9	0	0	0	0
40	J	52	0	0	1	0
40	K	61	0	0	7	1
40	L	93	0	0	11	0
40	M	133	0	0	8	0
40	N	66	0	0	5	0
40	O	42	0	0	5	0
40	P	68	0	0	3	0
40	Q	53	0	0	2	0
40	R	93	0	0	5	0
40	S	35	0	0	2	0
40	T	40	0	0	4	0
40	U	28	0	0	2	0
40	V	13	0	0	1	0
40	W	70	0	0	4	0
40	X	23	0	0	3	0
40	Y	93	0	0	9	0
40	Z	30	0	0	5	0
All	All	98979	0	59958	2476	1

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 16.

The worst 5 of 2476 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.29	1.15
1:O:1160:G:H5'	1:O:1161:A:H5'	1.27	1.13
15:M:68:ARG:HH21	15:M:73:ARG:HD3	1.12	1.13

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:C:236:THR:HG22	6:C:239:ALA:H	1.06	1.12
9:F:91:VAL:HG12	9:F:92:GLY:H	1.12	1.11

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
40:K:6344:HOH:O	40:K:6344:HOH:O[3_655]	2.05	0.15

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	
4	A	235/240 (98%)	208 (88%)	20 (8%)	7 (3%)	7	5
5	B	335/338 (99%)	296 (88%)	32 (10%)	7 (2%)	11	12
6	C	244/246 (99%)	221 (91%)	22 (9%)	1 (0%)	43	61
7	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
8	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
9	F	117/120 (98%)	102 (87%)	12 (10%)	3 (3%)	8	8
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	136 (87%)	15 (10%)	5 (3%)	6	5
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	16	22
13	K	130/132 (98%)	118 (91%)	11 (8%)	1 (1%)	27	39
14	L	141/165 (86%)	115 (82%)	25 (18%)	1 (1%)	30	43
15	M	192/195 (98%)	179 (93%)	11 (6%)	2 (1%)	22	32
16	N	184/187 (98%)	158 (86%)	17 (9%)	9 (5%)	3	2
17	O	113/116 (97%)	105 (93%)	8 (7%)	0	100	100
18	P	141/149 (95%)	136 (96%)	5 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	21	29
20	R	148/155 (96%)	137 (93%)	10 (7%)	1 (1%)	30	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	8	8
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	14	18
25	W	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
26	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	18	24
27	Y	140/241 (58%)	135 (96%)	5 (4%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	9 (13%)	4 (6%)	3	1
29	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
30	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	9	9
31	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
32	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	2	1
All	All	3705/4431 (84%)	3338 (90%)	302 (8%)	65 (2%)	13	15

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	139	ASP
5	B	169	GLY
7	D	164	ALA

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	
4	A	179/182 (98%)	169 (94%)	10 (6%)	30	45
5	B	282/283 (100%)	266 (94%)	16 (6%)	29	44
6	C	193/193 (100%)	176 (91%)	17 (9%)	14	21
7	D	117/148 (79%)	108 (92%)	9 (8%)	18	28
8	E	152/156 (97%)	144 (95%)	8 (5%)	32	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	94
10	G	27/283 (10%)	25 (93%)	2 (7%)	20	30
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	57
12	J	118/121 (98%)	106 (90%)	12 (10%)	11	15
13	K	106/106 (100%)	99 (93%)	7 (7%)	24	35
14	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
15	M	158/159 (99%)	153 (97%)	5 (3%)	51	72
16	N	149/150 (99%)	138 (93%)	11 (7%)	20	30
17	O	93/94 (99%)	89 (96%)	4 (4%)	40	59
18	P	113/117 (97%)	109 (96%)	4 (4%)	48	69
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	65
20	R	117/122 (96%)	113 (97%)	4 (3%)	49	70
21	S	71/74 (96%)	70 (99%)	1 (1%)	78	92
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	65
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	48 (94%)	3 (6%)	28	42
25	W	130/130 (100%)	122 (94%)	8 (6%)	26	39
26	X	66/74 (89%)	59 (89%)	7 (11%)	10	14
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	29
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	40 (95%)	2 (5%)	35	53
31	3	79/79 (100%)	76 (96%)	3 (4%)	44	65
32	I	58/130 (45%)	56 (97%)	2 (3%)	49	70
All	All	3093/3612 (86%)	2932 (95%)	161 (5%)	32	49

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	52	GLN
14	L	75	LEU
27	Y	189	ASN
12	J	74	ARG
13	K	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	126	GLN
18	P	89	ASN
30	2	41	HIS
15	M	137	ASN
16	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	249 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
3	4	2/5 (40%)	1 (50%)	0
All	All	2868/3049 (94%)	268 (9%)	34 (1%)

5 of 268 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1563	G
1	0	1856	C
1	0	2791	U
1	0	1685	A
1	0	699	C

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

5 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
1	OMU	0	2587	1	20,22,23	0.86	1 (5%)	24,31,34	0.76	0
1	OMG	0	2588	1	24,26,27	0.92	1 (4%)	32,38,41	5.05	3 (9%)
1	UR3	0	2619	1	20,22,23	0.84	0	23,32,35	0.84	0
1	PSU	0	2621	1	19,21,22	1.34	3 (15%)	23,30,33	1.06	1 (4%)
1	1MA	0	628	1,35	23,25,26	0.96	2 (8%)	32,37,40	1.03	1 (3%)

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
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1,35	-	1/8/25/26	0/1/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C6-N1	3.27	1.35	1.32
1	0	2621	PSU	C2-N1	3.13	1.43	1.37
1	0	2587	OMU	P-OP1	2.96	1.50	1.46
1	0	2588	OMG	P-OP1	2.72	1.49	1.46
1	0	2621	PSU	P-OP1	2.54	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.01	130.37	134.14
1	0	2588	OMG	C6-N1-C2	3.28	125.25	119.51
1	0	628	1MA	C2-N3-C4	-3.16	110.83	116.23
1	0	2621	PSU	C5-C4-N3	-2.36	114.56	118.86
1	0	2588	OMG	C2-N3-C4	-2.22	111.97	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 313 ligands modelled in this entry, 312 are monoatomic - leaving 1 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$
38	SPS	4	9701	33	23,23,23	1.42	4 (17%)	25,30,30	2.16	3 (12%)

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
38	SPS	4	9701	33	-	1/17/18/18	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	9701	SPS	C1-C6	3.72	1.53	1.43
38	4	9701	SPS	C9-C10	-2.88	1.41	1.48
38	4	9701	SPS	C16-S15	-2.21	1.79	1.82
38	4	9701	SPS	O15-S15	-2.11	1.43	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	4	9701	SPS	C7-C5-C6	-7.88	121.38	126.94
38	4	9701	SPS	C6-C5-N4	4.51	119.42	117.31
38	4	9701	SPS	C1-N2-C3	-2.06	121.19	125.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	4	9701	SPS	S15-C16-S17-C18

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	0	2754/2922 (94%)	-0.14	80 (2%)	49	47	19, 43, 80, 130	0
2	9	122/122 (100%)	0.16	5 (4%)	35	33	35, 59, 79, 129	0
3	4	5/5 (100%)	0.34	1 (20%)	2	1	44, 46, 53, 57	0
4	A	237/240 (98%)	0.50	20 (8%)	11	10	28, 51, 79, 92	0
5	B	337/338 (99%)	0.07	5 (1%)	70	69	25, 46, 66, 77	0
6	C	246/246 (100%)	-0.03	1 (0%)	90	90	24, 43, 61, 72	0
7	D	140/177 (79%)	1.74	55 (39%)	1	0	53, 76, 103, 111	0
8	E	172/178 (96%)	0.47	12 (6%)	16	14	37, 55, 69, 73	0
9	F	119/120 (99%)	0.99	21 (17%)	2	1	45, 64, 88, 91	0
10	G	29/348 (8%)	2.13	11 (37%)	1	0	60, 77, 82, 85	0
11	H	160/171 (93%)	0.44	11 (6%)	17	15	39, 54, 80, 84	0
12	J	142/145 (97%)	0.02	2 (1%)	72	71	32, 43, 59, 75	0
13	K	132/132 (100%)	-0.20	2 (1%)	70	69	30, 42, 59, 67	0
14	L	145/165 (87%)	0.71	20 (13%)	4	3	26, 60, 92, 101	0
15	M	194/195 (99%)	0.62	19 (9%)	8	7	31, 42, 80, 85	0
16	N	186/187 (99%)	0.83	31 (16%)	2	2	43, 58, 93, 98	0
17	O	115/116 (99%)	-0.01	1 (0%)	81	81	36, 49, 61, 67	0
18	P	143/149 (95%)	0.16	4 (2%)	50	48	35, 47, 58, 66	0
19	Q	95/96 (98%)	0.13	3 (3%)	45	43	39, 46, 59, 65	0
20	R	150/155 (96%)	-0.14	0	100	100	27, 39, 56, 67	0
21	S	81/85 (95%)	0.24	3 (3%)	39	38	39, 52, 69, 84	0
22	T	119/120 (99%)	0.41	5 (4%)	35	32	35, 50, 72, 96	0
23	U	53/66 (80%)	0.45	3 (5%)	23	21	39, 50, 66, 72	0
24	V	65/71 (91%)	1.58	15 (23%)	1	1	47, 65, 94, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.08	1 (0%) 86 86	31, 44, 58, 68	0
26	X	82/92 (89%)	0.44	8 (9%) 8 7	37, 49, 69, 85	0
27	Y	142/241 (58%)	0.18	7 (4%) 28 26	24, 41, 57, 76	0
28	Z	73/83 (87%)	3.69	43 (58%) 0 0	63, 85, 94, 98	0
29	1	56/57 (98%)	-0.31	0 100 100	25, 31, 38, 47	0
30	2	46/50 (92%)	0.43	3 (6%) 18 17	32, 51, 65, 70	0
31	3	92/92 (100%)	1.32	17 (18%) 2 1	48, 65, 72, 81	0
32	I	70/162 (43%)	4.78	59 (84%) 0 0	92, 106, 120, 121	0
All	All	6656/7480 (88%)	0.25	468 (7%) 16 14	19, 47, 85, 130	0

The worst 5 of 468 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	15.2
28	Z	22	SER	14.8
28	Z	11	SER	13.0
24	V	1	THR	12.9
15	M	70	GLY	11.9

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
1	OMU	0	2587	21/22	0.12	0.73	31,34,36,38	0
1	UR3	0	2619	21/22	0.14	0.27	30,33,37,40	0
1	PSU	0	2621	20/21	0.13	-0.86	32,35,39,40	0
1	1MA	0	628	23/24	0.13	-1.04	27,30,32,32	0
1	OMG	0	2588	24/25	0.11	-2.12	31,32,34,36	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	9601	1/1	0.57	224.50	196,196,196,196	0
33	MG	0	8047	1/1	0.69	76.16	92,92,92,92	0
35	NA	0	9179	1/1	0.75	69.66	94,94,94,94	0
35	NA	B	9161	1/1	0.64	59.98	73,73,73,73	0
35	NA	0	9106	1/1	0.34	50.31	39,39,39,39	0
33	MG	0	8082	1/1	0.33	46.33	80,80,80,80	0
35	NA	0	9125	1/1	0.63	46.33	93,93,93,93	0
33	MG	0	8108	1/1	0.57	45.63	88,88,88,88	0
37	SR	0	9500	1/1	1.23	42.03	196,196,196,196	0
36	CL	0	9322	1/1	0.18	40.66	53,53,53,53	0
37	SR	0	9501	1/1	0.21	36.07	193,193,193,193	0
35	NA	0	9102	1/1	0.43	34.82	68,68,68,68	0
35	NA	0	9178	1/1	0.48	32.95	44,44,44,44	0
37	SR	0	9482	1/1	0.50	30.98	175,175,175,175	0
35	NA	0	9174	1/1	0.46	29.41	67,67,67,67	0
35	NA	0	9156	1/1	0.40	28.56	57,57,57,57	0
35	NA	0	9164	1/1	0.46	28.09	56,56,56,56	0
33	MG	0	8085	1/1	0.32	26.46	69,69,69,69	0
35	NA	0	9185	1/1	0.60	25.98	53,53,53,53	0
33	MG	0	8013	1/1	0.39	22.95	10,10,10,10	0
35	NA	0	9107	1/1	0.38	22.12	52,52,52,52	0
35	NA	0	9177	1/1	0.51	21.91	76,76,76,76	0
33	MG	0	8094	1/1	0.24	21.87	65,65,65,65	0
33	MG	0	8014	1/1	0.31	21.69	74,74,74,74	0
35	NA	0	9172	1/1	0.70	20.87	76,76,76,76	0
33	MG	0	8024	1/1	0.77	20.35	87,87,87,87	0
35	NA	0	9158	1/1	0.36	20.22	46,46,46,46	0
33	MG	0	8099	1/1	0.26	18.69	77,77,77,77	0
33	MG	0	8084	1/1	0.38	18.13	107,107,107,107	0
35	NA	0	9122	1/1	0.37	18.05	75,75,75,75	0
35	NA	0	9175	1/1	0.21	17.96	42,42,42,42	0
33	MG	0	8025	1/1	0.28	17.90	19,19,19,19	0
35	NA	0	9168	1/1	0.21	17.89	74,74,74,74	0
33	MG	0	8083	1/1	0.18	17.86	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8027	1/1	0.22	17.81	31,31,31,31	0
33	MG	0	8090	1/1	0.34	17.42	67,67,67,67	0
35	NA	0	9135	1/1	0.28	17.27	42,42,42,42	0
35	NA	9	9152	1/1	0.27	16.75	59,59,59,59	0
35	NA	0	9132	1/1	0.46	15.92	77,77,77,77	0
37	SR	B	9521	1/1	0.59	15.47	196,196,196,196	0
35	NA	0	9184	1/1	1.36	14.90	87,87,87,87	0
35	NA	0	9154	1/1	0.35	14.82	54,54,54,54	0
35	NA	0	9127	1/1	0.32	14.41	75,75,75,75	0
37	SR	0	9406	1/1	0.22	14.40	45,45,45,45	0
37	SR	0	9420	1/1	0.16	14.18	74,74,74,74	0
33	MG	0	8052	1/1	0.29	14.08	75,75,75,75	0
33	MG	0	8092	1/1	0.45	13.83	68,68,68,68	0
33	MG	0	8022	1/1	0.50	12.91	67,67,67,67	0
37	SR	0	9539	1/1	0.41	12.26	173,173,173,173	0
37	SR	0	9410	1/1	0.20	11.89	46,46,46,46	0
37	SR	0	9411	1/1	0.20	11.80	49,49,49,49	0
35	NA	0	9140	1/1	0.31	10.95	65,65,65,65	0
35	NA	0	9110	1/1	0.24	10.42	39,39,39,39	0
35	NA	0	9114	1/1	0.23	10.09	56,56,56,56	0
35	NA	0	9159	1/1	0.42	10.07	56,56,56,56	0
33	MG	0	8012	1/1	0.25	9.70	26,26,26,26	0
37	SR	0	9626	1/1	0.25	9.60	146,146,146,146	0
33	MG	0	8051	1/1	0.20	8.78	24,24,24,24	0
37	SR	0	9408	1/1	0.22	8.53	48,48,48,48	0
35	NA	0	9165	1/1	0.37	8.05	37,37,37,37	0
33	MG	0	8038	1/1	0.23	8.05	16,16,16,16	0
33	MG	0	8059	1/1	0.22	7.84	46,46,46,46	0
33	MG	0	8114	1/1	0.22	7.76	74,74,74,74	0
34	K	0	9001	1/1	0.34	7.45	101,101,101,101	0
33	MG	0	8029	1/1	0.25	7.36	22,22,22,22	0
35	NA	0	9157	1/1	0.18	7.17	35,35,35,35	0
33	MG	0	8058	1/1	0.28	7.10	34,34,34,34	0
33	MG	0	8110	1/1	0.23	6.99	40,40,40,40	0
35	NA	0	9118	1/1	0.19	6.96	43,43,43,43	0
33	MG	0	8057	1/1	0.23	6.95	64,64,64,64	0
37	SR	0	9547	1/1	0.21	6.89	175,175,175,175	0
37	SR	0	9407	1/1	0.19	6.61	50,50,50,50	0
33	MG	9	8095	1/1	0.24	6.58	46,46,46,46	0
39	CD	O	9205	1/1	0.39	6.43	196,196,196,196	0
35	NA	0	9150	1/1	0.20	6.30	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8101	1/1	0.16	6.22	68,68,68,68	0
35	NA	0	9170	1/1	0.21	6.20	92,92,92,92	0
35	NA	0	9129	1/1	0.24	6.15	74,74,74,74	0
33	MG	0	8026	1/1	0.17	5.90	25,25,25,25	0
37	SR	0	9433	1/1	0.16	5.87	74,74,74,74	0
35	NA	0	9128	1/1	0.17	5.87	40,40,40,40	0
35	NA	0	9160	1/1	0.20	5.84	45,45,45,45	0
35	NA	9	9183	1/1	0.22	5.82	84,84,84,84	0
33	MG	0	8050	1/1	0.26	5.67	91,91,91,91	0
37	SR	1	9419	1/1	0.17	5.50	47,47,47,47	0
33	MG	0	8089	1/1	0.17	5.39	54,54,54,54	0
36	CL	B	9319	1/1	0.18	5.38	54,54,54,54	0
37	SR	0	9432	1/1	0.16	5.28	65,65,65,65	0
33	MG	0	8001	1/1	0.21	5.12	17,17,17,17	0
35	NA	0	9181	1/1	0.18	5.10	58,58,58,58	0
33	MG	0	8021	1/1	0.18	5.07	49,49,49,49	0
33	MG	0	8046	1/1	0.16	4.99	37,37,37,37	0
35	NA	0	9113	1/1	0.18	4.89	67,67,67,67	0
37	SR	0	9415	1/1	0.15	4.70	57,57,57,57	0
35	NA	0	9115	1/1	0.19	4.48	42,42,42,42	0
36	CL	0	9316	1/1	0.29	4.33	74,74,74,74	0
33	MG	0	8097	1/1	0.19	4.15	65,65,65,65	0
37	SR	0	9434	1/1	0.17	4.01	61,61,61,61	0
35	NA	0	9120	1/1	0.15	3.96	59,59,59,59	0
33	MG	B	8056	1/1	0.23	3.85	46,46,46,46	0
33	MG	0	8060	1/1	0.19	3.81	88,88,88,88	0
37	SR	0	9424	1/1	0.20	3.60	49,49,49,49	0
37	SR	0	9427	1/1	0.15	3.45	55,55,55,55	0
33	MG	0	8070	1/1	0.14	3.38	26,26,26,26	0
37	SR	0	9484	1/1	0.13	3.35	148,148,148,148	0
33	MG	4	8118	1/1	0.21	3.26	29,29,29,29	0
35	NA	0	9166	1/1	0.17	3.14	76,76,76,76	0
33	MG	0	8008	1/1	0.16	3.08	15,15,15,15	0
37	SR	0	9429	1/1	0.14	3.05	67,67,67,67	0
35	NA	0	9171	1/1	0.14	2.91	67,67,67,67	0
35	NA	3	9169	1/1	0.40	2.80	84,84,84,84	0
35	NA	0	9182	1/1	0.19	2.69	68,68,68,68	0
35	NA	0	9131	1/1	0.15	2.68	51,51,51,51	0
35	NA	S	9112	1/1	0.20	2.62	71,71,71,71	0
35	NA	0	9167	1/1	0.13	2.61	59,59,59,59	0
35	NA	0	9163	1/1	0.18	2.60	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9451	1/1	0.18	2.59	57,57,57,57	0
33	MG	K	8069	1/1	0.18	2.58	20,20,20,20	0
37	SR	0	9530	1/1	0.17	2.57	107,107,107,107	0
33	MG	0	8107	1/1	0.21	2.55	61,61,61,61	0
33	MG	0	8104	1/1	0.20	2.54	58,58,58,58	0
37	SR	S	9470	1/1	0.15	2.47	98,98,98,98	0
37	SR	0	9488	1/1	0.14	2.45	80,80,80,80	0
33	MG	0	8103	1/1	0.14	2.43	53,53,53,53	0
33	MG	B	8055	1/1	0.21	2.32	85,85,85,85	0
35	NA	R	9186	1/1	0.19	2.22	75,75,75,75	0
35	NA	0	9136	1/1	0.15	2.20	32,32,32,32	0
37	SR	0	9456	1/1	0.13	2.12	69,69,69,69	0
33	MG	0	8020	1/1	0.18	1.66	37,37,37,37	0
35	NA	0	9173	1/1	0.15	1.64	57,57,57,57	0
36	CL	0	9314	1/1	0.18	1.58	52,52,52,52	0
33	MG	0	8040	1/1	0.30	1.58	73,73,73,73	0
37	SR	0	9447	1/1	0.13	1.55	62,62,62,62	0
33	MG	0	8045	1/1	0.19	1.54	73,73,73,73	0
35	NA	0	9155	1/1	0.21	1.52	65,65,65,65	0
35	NA	0	9124	1/1	0.20	1.51	52,52,52,52	0
35	NA	0	9116	1/1	0.15	1.50	51,51,51,51	0
35	NA	0	9162	1/1	0.15	1.33	43,43,43,43	0
37	SR	0	9412	1/1	0.14	1.29	51,51,51,51	0
33	MG	0	8065	1/1	0.25	1.25	92,92,92,92	0
33	MG	0	8074	1/1	0.20	1.11	15,15,15,15	0
37	SR	R	9418	1/1	0.17	1.09	58,58,58,58	0
37	SR	0	9413	1/1	0.15	1.01	50,50,50,50	0
37	SR	0	9416	1/1	0.14	0.89	48,48,48,48	0
37	SR	0	9430	1/1	0.16	0.83	48,48,48,48	0
36	CL	0	9317	1/1	0.15	0.80	58,58,58,58	0
33	MG	0	8076	1/1	0.14	0.75	57,57,57,57	0
37	SR	0	9425	1/1	0.13	0.67	151,151,151,151	0
37	SR	0	9462	1/1	0.15	0.64	67,67,67,67	0
37	SR	0	9457	1/1	0.13	0.62	50,50,50,50	0
34	K	0	9002	1/1	0.27	0.62	91,91,91,91	0
33	MG	A	8066	1/1	0.18	0.61	57,57,57,57	0
36	CL	M	9318	1/1	0.19	0.61	40,40,40,40	0
37	SR	0	9534	1/1	0.14	0.54	113,113,113,113	0
33	MG	0	8102	1/1	0.17	0.52	94,94,94,94	0
33	MG	0	8080	1/1	0.16	0.46	46,46,46,46	0
36	CL	A	9309	1/1	0.19	0.36	70,70,70,70	0
33	MG	0	8017	1/1	0.13	0.33	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	C	9104	1/1	0.16	0.30	26,26,26,26	0
37	SR	9	9588	1/1	0.14	0.25	132,132,132,132	0
37	SR	0	9417	1/1	0.14	0.24	58,58,58,58	0
33	MG	0	8117	1/1	0.13	0.24	40,40,40,40	0
33	MG	0	8072	1/1	0.14	0.08	65,65,65,65	0
37	SR	0	9443	1/1	0.13	0.04	62,62,62,62	0
38	SPS	4	9701	23/23	0.16	0.02	39,45,57,60	0
37	SR	0	9414	1/1	0.14	0.02	56,56,56,56	0
37	SR	F	9595	1/1	0.16	-0.02	92,92,92,92	0
35	NA	0	9111	1/1	0.11	-0.05	46,46,46,46	0
37	SR	0	9509	1/1	0.14	-0.05	86,86,86,86	0
33	MG	0	8002	1/1	0.13	-0.15	33,33,33,33	0
37	SR	0	9452	1/1	0.15	-0.17	94,94,94,94	0
37	SR	0	9445	1/1	0.11	-0.17	62,62,62,62	0
36	CL	L	9310	1/1	0.16	-0.18	51,51,51,51	0
37	SR	0	9421	1/1	0.11	-0.24	68,68,68,68	0
37	SR	0	9474	1/1	0.12	-0.29	68,68,68,68	0
37	SR	0	9423	1/1	0.11	-0.32	56,56,56,56	0
33	MG	0	8115	1/1	0.11	-0.41	58,58,58,58	0
37	SR	H	9486	1/1	0.14	-0.41	121,121,121,121	0
37	SR	0	9428	1/1	0.12	-0.48	51,51,51,51	0
37	SR	0	9422	1/1	0.13	-0.48	57,57,57,57	0
35	NA	M	9147	1/1	0.14	-0.52	33,33,33,33	0
36	CL	O	9308	1/1	0.13	-0.63	56,56,56,56	0
37	SR	0	9529	1/1	0.14	-0.67	123,123,123,123	0
37	SR	0	9490	1/1	0.11	-0.71	129,129,129,129	0
37	SR	L	9409	1/1	0.13	-0.72	46,46,46,46	0
35	NA	0	9139	1/1	0.12	-0.76	61,61,61,61	0
36	CL	0	9303	1/1	0.13	-0.79	47,47,47,47	0
37	SR	A	9537	1/1	0.11	-0.82	159,159,159,159	0
36	CL	J	9321	1/1	0.14	-0.84	65,65,65,65	0
37	SR	0	9508	1/1	0.12	-0.86	87,87,87,87	0
37	SR	A	9497	1/1	0.09	-0.87	99,99,99,99	0
33	MG	0	8079	1/1	0.10	-0.89	29,29,29,29	0
37	SR	A	9437	1/1	0.10	-0.91	70,70,70,70	0
35	NA	0	9138	1/1	0.10	-0.93	56,56,56,56	0
36	CL	0	9311	1/1	0.12	-0.95	66,66,66,66	0
33	MG	0	8041	1/1	0.11	-0.99	52,52,52,52	0
39	CD	U	9201	1/1	0.10	-1.02	61,61,61,61	0
35	NA	0	9126	1/1	0.10	-1.11	49,49,49,49	0
37	SR	1	9460	1/1	0.13	-1.12	52,52,52,52	0
37	SR	0	9465	1/1	0.10	-1.15	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	D	9151	1/1	0.22	-1.16	60,60,60,60	0
37	SR	0	9545	1/1	0.07	-1.18	84,84,84,84	0
37	SR	0	9431	1/1	0.15	-1.25	57,57,57,57	0
37	SR	0	9590	1/1	0.11	-1.27	131,131,131,131	0
37	SR	0	9453	1/1	0.10	-1.28	76,76,76,76	0
37	SR	0	9585	1/1	0.10	-1.31	91,91,91,91	0
35	NA	0	9130	1/1	0.10	-1.31	41,41,41,41	0
35	NA	J	9146	1/1	0.11	-1.32	58,58,58,58	0
37	SR	0	9467	1/1	0.10	-1.40	73,73,73,73	0
37	SR	0	9442	1/1	0.13	-1.40	63,63,63,63	0
36	CL	0	9315	1/1	0.11	-1.41	58,58,58,58	0
37	SR	0	9461	1/1	0.04	-1.44	86,86,86,86	0
37	SR	0	9504	1/1	0.10	-1.46	92,92,92,92	0
33	MG	0	8054	1/1	0.10	-1.47	61,61,61,61	0
37	SR	0	9468	1/1	0.08	-1.61	113,113,113,113	0
36	CL	N	9307	1/1	0.14	-1.61	60,60,60,60	0
39	CD	Z	9203	1/1	0.11	-1.61	155,155,155,155	0
37	SR	0	9449	1/1	0.10	-1.61	61,61,61,61	0
37	SR	0	9455	1/1	0.08	-1.62	66,66,66,66	0
37	SR	0	9444	1/1	0.11	-1.64	52,52,52,52	0
33	MG	T	8073	1/1	0.11	-1.65	34,34,34,34	0
37	SR	0	9477	1/1	0.11	-1.66	79,79,79,79	0
35	NA	R	9137	1/1	0.08	-1.67	23,23,23,23	0
33	MG	0	8037	1/1	0.09	-1.74	42,42,42,42	0
33	MG	Y	8109	1/1	0.12	-1.83	39,39,39,39	0
37	SR	0	9515	1/1	0.09	-1.84	109,109,109,109	0
36	CL	0	9305	1/1	0.10	-1.87	58,58,58,58	0
36	CL	Y	9320	1/1	0.10	-1.91	42,42,42,42	0
36	CL	K	9312	1/1	0.09	-1.92	45,45,45,45	0
33	MG	0	8088	1/1	0.10	-1.92	42,42,42,42	0
37	SR	0	9450	1/1	0.06	-1.94	63,63,63,63	0
37	SR	0	9483	1/1	0.09	-2.05	77,77,77,77	0
37	SR	A	9436	1/1	0.06	-2.07	87,87,87,87	0
37	SR	0	9475	1/1	0.08	-2.07	80,80,80,80	0
37	SR	0	9495	1/1	0.12	-2.09	90,90,90,90	0
33	MG	0	8063	1/1	0.11	-2.11	74,74,74,74	0
33	MG	0	8015	1/1	0.08	-2.17	29,29,29,29	0
35	NA	0	9117	1/1	0.08	-2.21	31,31,31,31	0
37	SR	0	9517	1/1	0.07	-2.23	94,94,94,94	0
35	NA	0	9101	1/1	0.14	-2.32	41,41,41,41	0
33	MG	0	8004	1/1	0.07	-2.32	24,24,24,24	0
35	NA	0	9134	1/1	0.06	-2.36	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	9566	1/1	0.07	-2.37	97,97,97,97	0
37	SR	0	9448	1/1	0.10	-2.42	64,64,64,64	0
33	MG	0	8075	1/1	0.11	-2.45	49,49,49,49	0
37	SR	0	9426	1/1	0.08	-2.50	72,72,72,72	0
33	MG	0	8096	1/1	0.08	-2.55	37,37,37,37	0
37	SR	0	9532	1/1	0.08	-2.55	114,114,114,114	0
37	SR	0	9570	1/1	0.09	-2.67	117,117,117,117	0
37	SR	0	9469	1/1	0.06	-2.69	88,88,88,88	0
36	CL	J	9302	1/1	0.05	-2.72	54,54,54,54	0
39	CD	1	9202	1/1	0.08	-2.76	58,58,58,58	0
35	NA	0	9123	1/1	0.11	-2.77	50,50,50,50	0
37	SR	0	9454	1/1	0.12	-2.78	79,79,79,79	0
33	MG	0	8098	1/1	0.09	-2.79	40,40,40,40	0
37	SR	0	9459	1/1	0.07	-2.79	93,93,93,93	0
37	SR	0	9446	1/1	0.06	-2.80	93,93,93,93	0
37	SR	0	9478	1/1	0.08	-2.80	72,72,72,72	0
36	CL	0	9313	1/1	0.08	-2.88	51,51,51,51	0
37	SR	3	9439	1/1	0.03	-2.98	79,79,79,79	0
33	MG	0	8093	1/1	0.13	-2.99	45,45,45,45	0
33	MG	0	8116	1/1	0.07	-3.02	69,69,69,69	0
37	SR	0	9568	1/1	0.03	-3.03	86,86,86,86	0
36	CL	R	9306	1/1	0.10	-3.06	45,45,45,45	0
37	SR	B	9458	1/1	0.11	-3.08	66,66,66,66	0
36	CL	3	9304	1/1	0.06	-3.18	74,74,74,74	0
33	MG	0	8067	1/1	0.09	-3.25	35,35,35,35	0
35	NA	0	9141	1/1	0.08	-3.25	64,64,64,64	0
36	CL	J	9301	1/1	0.07	-3.36	50,50,50,50	0
35	NA	Q	9148	1/1	0.09	-3.37	48,48,48,48	0
33	MG	0	8042	1/1	0.06	-3.56	50,50,50,50	0
33	MG	0	8031	1/1	0.09	-3.70	48,48,48,48	0
33	MG	0	8106	1/1	0.05	-3.72	39,39,39,39	0
35	NA	0	9108	1/1	0.07	-3.74	31,31,31,31	0
37	SR	9	9481	1/1	0.08	-3.76	86,86,86,86	0
33	MG	0	8061	1/1	0.10	-3.78	78,78,78,78	0
35	NA	T	9143	1/1	0.07	-3.91	37,37,37,37	0
37	SR	0	9489	1/1	0.05	-3.92	101,101,101,101	0
37	SR	0	9506	1/1	0.06	-3.95	108,108,108,108	0
33	MG	0	8028	1/1	0.11	-3.99	31,31,31,31	0
39	CD	3	9204	1/1	0.02	-4.05	70,70,70,70	0
33	MG	0	8003	1/1	0.13	-4.08	24,24,24,24	0
37	SR	0	9440	1/1	0.08	-4.09	60,60,60,60	0
37	SR	0	9560	1/1	0.08	-4.12	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8091	1/1	0.06	-4.14	55,55,55,55	0
37	SR	0	9480	1/1	0.04	-4.17	83,83,83,83	0
37	SR	0	9435	1/1	0.09	-4.21	71,71,71,71	0
37	SR	0	9473	1/1	0.05	-4.36	77,77,77,77	0
33	MG	0	8030	1/1	0.07	-4.70	38,38,38,38	0
33	MG	0	8068	1/1	0.11	-4.70	36,36,36,36	0
37	SR	0	9438	1/1	0.10	-4.84	66,66,66,66	0
37	SR	0	9466	1/1	0.04	-5.22	95,95,95,95	0
33	MG	0	8112	1/1	0.08	-5.28	44,44,44,44	0
37	SR	0	9464	1/1	0.07	-5.51	80,80,80,80	0
37	SR	0	9498	1/1	0.07	-5.70	65,65,65,65	0
37	SR	9	9503	1/1	0.06	-5.75	105,105,105,105	0
33	MG	0	8009	1/1	0.07	-5.80	31,31,31,31	0
33	MG	0	8036	1/1	0.06	-6.02	47,47,47,47	0
33	MG	0	8019	1/1	0.09	-6.06	52,52,52,52	0
33	MG	0	8044	1/1	0.05	-6.15	35,35,35,35	0
35	NA	0	9105	1/1	0.08	-6.21	36,36,36,36	0
33	MG	0	8005	1/1	0.06	-6.63	31,31,31,31	0
33	MG	0	8043	1/1	0.08	-6.68	56,56,56,56	0
33	MG	0	8032	1/1	0.06	-6.69	34,34,34,34	0
37	SR	0	9629	1/1	0.08	-6.71	73,73,73,73	0
37	SR	0	9505	1/1	0.09	-6.73	117,117,117,117	0
37	SR	0	9581	1/1	0.04	-6.86	105,105,105,105	0
37	SR	0	9522	1/1	0.07	-7.18	100,100,100,100	0
33	MG	0	8039	1/1	0.08	-7.23	45,45,45,45	0
37	SR	0	9441	1/1	0.08	-7.30	64,64,64,64	0
35	NA	0	9149	1/1	0.09	-9.63	46,46,46,46	0
37	SR	0	9405	1/1	0.04	-16.35	81,81,81,81	0
33	MG	0	8113	1/1	0.20	-	78,78,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.