



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1Q82
Title : Crystal Structure of CC-Puromycin bound to the A-site of the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 2.98 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

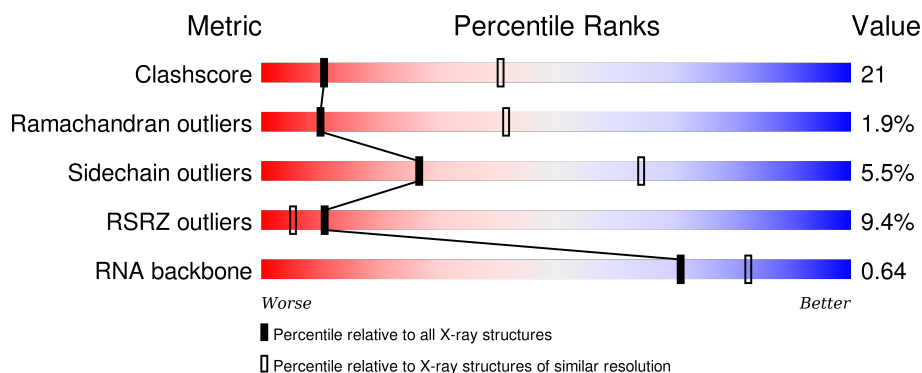
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)
RNA backbone	2183	1001 (3.36-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div>3%</div> <div>50%</div> <div>36%</div> <div>7%</div> <div>6%</div> </div>
2	B	122	<div> <div>4%</div> <div>51%</div> <div>35%</div> <div>10%</div> <div>.</div> </div>
3	5	2	<div> <div>50%</div> <div>50%</div> </div>
4	C	239	<div> <div>11%</div> <div>54%</div> <div>40%</div> <div>5%</div> <div>.</div> </div>
5	D	337	<div> <div>2%</div> <div>48%</div> <div>46%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	

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Mol	Chain	Length	Quality of chain
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	1	8105	-	-	-	X
32	MG	A	8011	-	-	X	-
32	MG	A	8053	-	-	-	X
32	MG	A	8060	-	-	-	X
32	MG	A	8064	-	-	-	X
32	MG	A	8112	-	-	-	X
33	K	A	8201	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8320	-	-	-	X
34	NA	A	8321	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8325	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8327	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8335	-	-	-	X
34	NA	A	8353	-	-	-	X
34	NA	A	8356	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8362	-	-	-	X
34	NA	A	8364	-	-	-	X
34	NA	A	8365	-	-	-	X
34	NA	A	8366	-	-	-	X
34	NA	A	8368	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8373	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8378	-	-	-	X
34	NA	A	8379	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	A	8505	-	-	-	X
35	CL	A	8515	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	D	8519	-	-	-	X
35	CL	M	8510	-	-	-	X
35	CL	N	8518	-	-	X	-
36	PPU	5	76	-	-	-	X
37	CD	4	8404	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98593 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

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

- Molecule 3 is a RNA chain called CC-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	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	G	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	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 15 is a protein called L15 Ribosomal Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	119	Total	C	N	O			
			949	568	180	201		0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	109	Total Mg 109 109	0	0
32	4	1	Total Mg 1 1	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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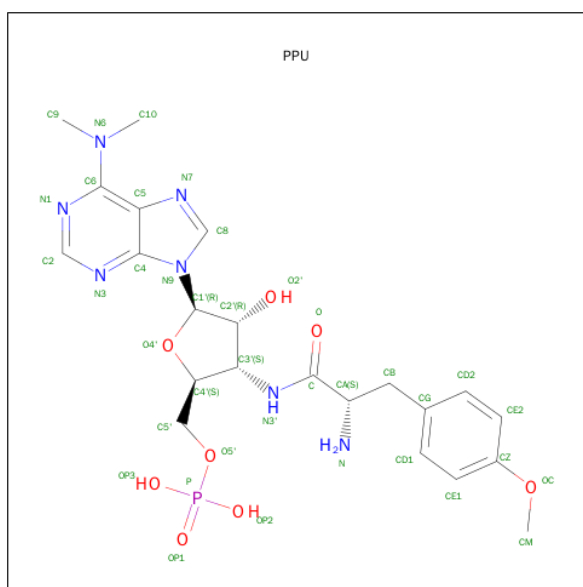
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	4	Total 4	Cl 4	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	A	7	Total 7	Cl 7	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: C₂₂H₃₀N₇O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	5	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	1	Total	Cd	0	0
			1	1		
37	2	1	Total	Cd	0	0
			1	1		
37	1	1	Total	Cd	0	0
			1	1		
37	4	1	Total	Cd	0	0
			1	1		
37	V	1	Total	Cd	0	0
			1	1		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	5860	Total	O	0	0
			5860	5860		
38	B	146	Total	O	0	0
			146	146		
38	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	140	Total 140	O 140	0	0
38	D	146	Total 146	O 146	0	0
38	E	176	Total 176	O 176	0	0
38	F	52	Total 52	O 52	0	0
38	G	45	Total 45	O 45	0	0
38	H	32	Total 32	O 32	0	0
38	I	22	Total 22	O 22	0	0
38	J	78	Total 78	O 78	0	0
38	K	54	Total 54	O 54	0	0
38	L	64	Total 64	O 64	0	0
38	M	86	Total 86	O 86	0	0
38	N	138	Total 138	O 138	0	0
38	O	64	Total 64	O 64	0	0
38	P	44	Total 44	O 44	0	0
38	Q	70	Total 70	O 70	0	0
38	R	57	Total 57	O 57	0	0
38	S	83	Total 83	O 83	0	0
38	T	36	Total 36	O 36	0	0
38	U	38	Total 38	O 38	0	0
38	V	22	Total 22	O 22	0	0
38	W	16	Total 16	O 16	0	0

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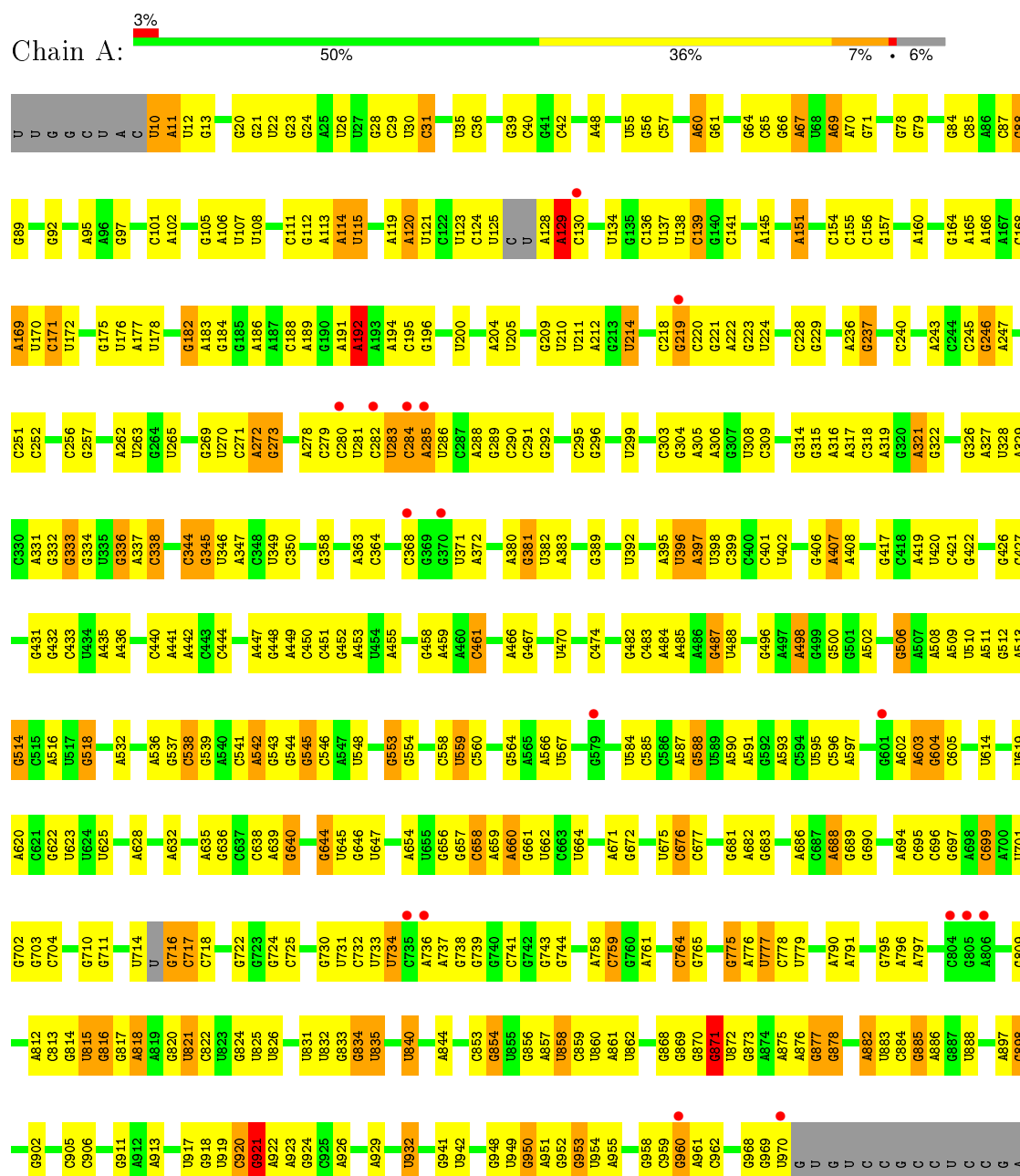
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	67	Total 67	O 67	0	0
38	Y	28	Total 28	O 28	0	0
38	Z	100	Total 100	O 100	0	0
38	1	36	Total 36	O 36	0	0
38	2	58	Total 58	O 58	0	0
38	3	37	Total 37	O 37	0	0
38	4	70	Total 70	O 70	0	0

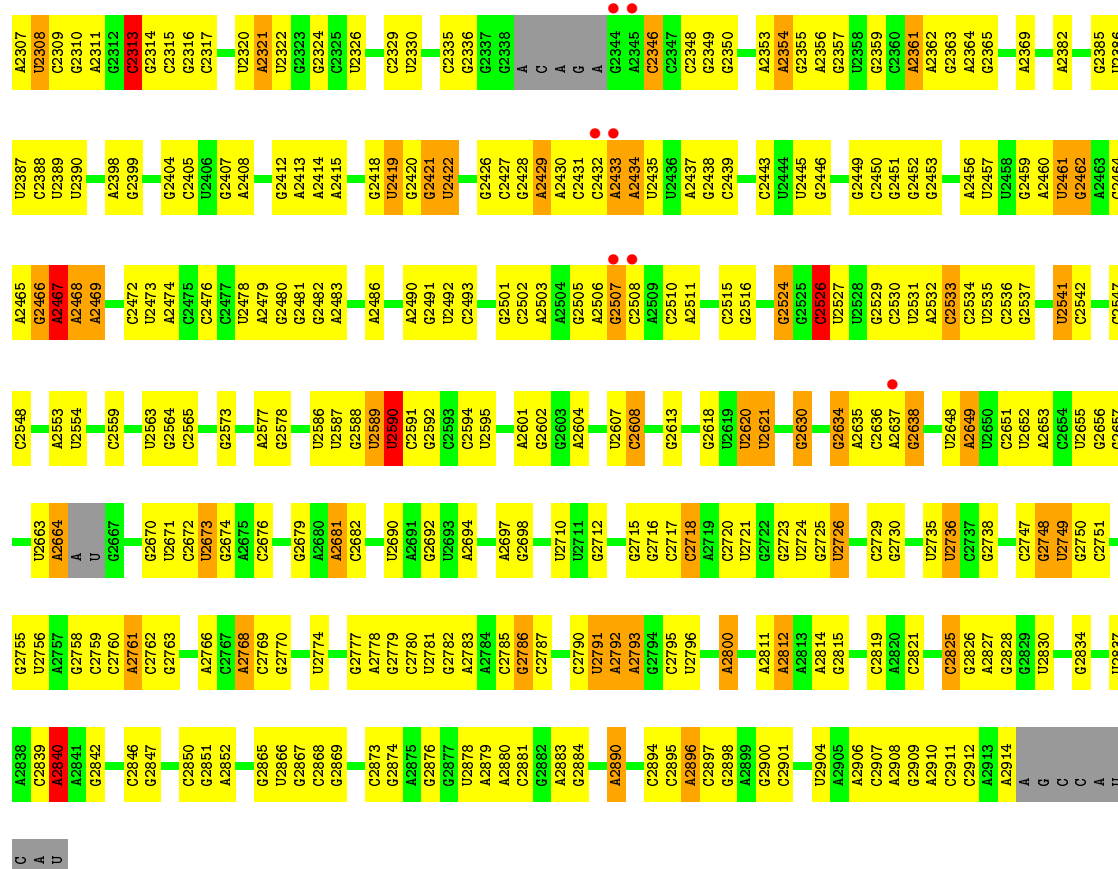
3 Residue-property plots

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.

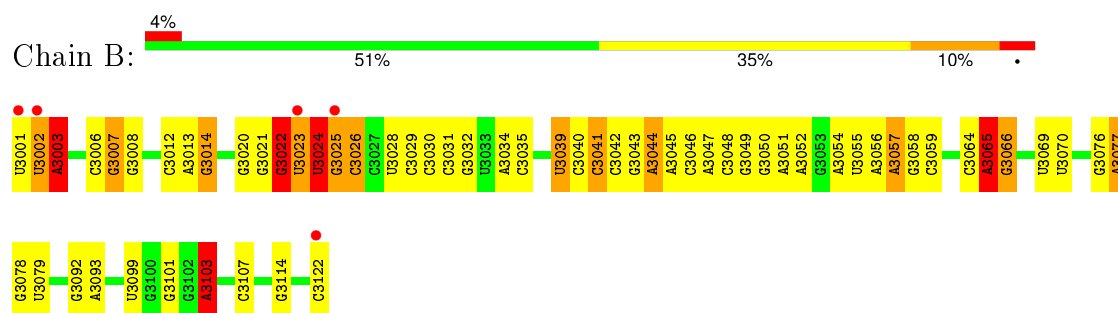
- Molecule 1: 23S ribosomal rna



G	C2104	G2005	U1645	U	C1467	C1253	C1184	A1081	G
A	C2105	C2006	G1646	U1561	C1467	C1360	U1185	A1086	A
C	C2106	A2007	G1647	C1562	A1471	C1261	U1186	A1087	C
U	U2107	U1915	A1733	G1563	U1472	U1362	U1187	A1088	G
C	A2108	G2009	C1651	C1564	C1473	U1368	A1188		A
C	U2109	A2010	U1654	C1565	U1474	U1265	A1189		G
C	G2110	A2011	U1655	C1566	C1474	U1266	A1190	A1097	C
A	G2111	U2012	G1656	U1567	U1477	U1267	U1191		U
G	C2112	C2013	A1657	G1568	U1478	C1268	A1192	U1109	G
A	G2113	A1921	A1658	U1569	U1478	U1269	A1193	G1110	C
U	C2114	G1923	A1659	U1572	G1483	U1270	A1194		G
C	U2115	A1924	G1660	A1573	G1484	U1279	U1195	U1116	A
C	U2116	G1925		C1574	A1485	U1380	G1196	A1117	C
C		G1926	G1665	A1580	U1488		G1197	A1118	A
C	C2119	A2022	C1666	A1580	U1488	U1383	U1198	G1119	C
G	U2120	A1847	C1667	A1589	U1494	U1297	A1199	U1120	G
C	G2121	G1848	U1668	G1599	A1494	U1298	C1201	G1121	C
G	C2122	G1849	G1752	G1599	U1494	U1298	C1201	U1122	G
C	A2123	U1850	C1753	G1599	U1494	U1298	C1201	U1123	C
U	G2124	G1851	A1754	G1599	U1494	U1298	C1201	U1124	A
C		A1852	U1755	G1599	U1494	U1298	C1201	U1125	C
C	G2128	G1855	A1759	G1599	U1494	U1298	C1201	U1126	A
G	G2134	C1856	C1762	G1599	U1494	U1298	C1201	U1127	C
G	G2136	A1859	U1766	G1599	U1494	U1298	C1201	U1128	G
C	A	U1860	A1767	G1599	U1494	U1298	C1201	U1129	C
C	C	C1861	G1768	G1599	U1494	U1298	C1201	U1130	A
C	G	C1862	C1769	G1599	U1494	U1298	C1201	U1131	C
C	U	C1863	U1770	G1599	U1494	U1298	C1201	U1132	G
C	U	C1864	U1771	G1599	U1494	U1298	C1201	U1133	C
C	U	C1865	U1772	G1599	U1494	U1298	C1201	U1134	A
C	U	C1866	U1773	G1599	U1494	U1298	C1201	U1135	C
C	U	C1867	U1774	G1599	U1494	U1298	C1201	U1136	G
C	U	C1868	U1775	G1599	U1494	U1298	C1201	U1137	C
C	U	C1869	U1776	G1599	U1494	U1298	C1201	U1138	A
C	U	C1870	U1777	G1599	U1494	U1298	C1201	U1139	C
C	U	C1871	U1778	G1599	U1494	U1298	C1201	U1140	G
C	U	C1872	U1779	G1599	U1494	U1298	C1201	U1141	C
C	U	C1873	U1780	G1599	U1494	U1298	C1201	U1142	A
C	U	U1874	U1781	G1599	U1494	U1298	C1201	U1143	C
C	U	U1875	U1782	G1599	U1494	U1298	C1201	U1144	A
C	U	U1876	U1783	G1599	U1494	U1298	C1201	U1145	C
C	U	U1877	U1784	G1599	U1494	U1298	C1201	U1146	G
C	U	U1878	U1785	G1599	U1494	U1298	C1201	U1147	A
C	U	U1879	U1786	G1599	U1494	U1298	C1201	U1148	C
C	U	U1880	U1787	G1599	U1494	U1298	C1201	U1149	A
C	U	U1881	U1788	G1599	U1494	U1298	C1201	U1150	C
C	U	U1882	U1789	G1599	U1494	U1298	C1201	U1151	G
C	U	U1883	U1790	G1599	U1494	U1298	C1201	U1152	A
C	U	U1884	U1791	G1599	U1494	U1298	C1201	U1153	C
C	U	U1885	U1792	G1599	U1494	U1298	C1201	U1154	A
C	U	U1886	U1793	G1599	U1494	U1298	C1201	U1155	C
C	U	U1887	U1794	G1599	U1494	U1298	C1201	U1156	G
C	U	U1888	U1795	G1599	U1494	U1298	C1201	U1157	A
C	U	U1889	U1796	G1599	U1494	U1298	C1201	U1158	C
C	U	U1890	U1797	G1599	U1494	U1298	C1201	U1159	A
C	U	U1891	U1798	G1599	U1494	U1298	C1201	U1160	C
C	U	U1892	U1799	G1599	U1494	U1298	C1201	U1161	A
C	U	U1893	U1800	G1599	U1494	U1298	C1201	U1162	C
C	U	U1894	U1801	G1599	U1494	U1298	C1201	U1163	A
C	U	U1895	U1802	G1599	U1494	U1298	C1201	U1164	C
C	U	U1896	U1803	G1599	U1494	U1298	C1201	U1165	A
C	U	U1897	U1804	G1599	U1494	U1298	C1201	U1166	C
C	U	U1898	U1805	G1599	U1494	U1298	C1201	U1167	A
C	U	U1899	U1806	G1599	U1494	U1298	C1201	U1168	C
C	U	U1900	U1807	G1599	U1494	U1298	C1201	U1169	A
C	U	U1901	U1808	G1599	U1494	U1298	C1201	U1170	C
C	U	U1902	U1809	G1599	U1494	U1298	C1201	U1171	A
C	U	U1903	U1810	G1599	U1494	U1298	C1201	U1172	C
C	U	U1904	U1811	G1599	U1494	U1298	C1201	U1173	A
C	U	U1905	U1812	G1599	U1494	U1298	C1201	U1174	C
C	U	U1906	U1813	G1599	U1494	U1298	C1201	U1175	A
C	U	U1907	U1814	G1599	U1494	U1298	C1201	U1176	C
C	U	U1908	U1815	G1599	U1494	U1298	C1201	U1177	A
C	U	U1909	U1816	G1599	U1494	U1298	C1201	U1178	C
C	U	U1910	U1817	G1599	U1494	U1298	C1201	U1179	A
C	U	U1911	U1818	G1599	U1494	U1298	C1201	U1180	C
C	U	U1912	U1819	G1599	U1494	U1298	C1201	U1181	A
C	U	U1913	U1820	G1599	U1494	U1298	C1201	U1182	C
C	U	U1914	U1821	G1599	U1494	U1298	C1201	U1183	A
C	U	U1915	U1822	G1599	U1494	U1298	C1201	U1184	C
C	U	U1916	U1823	G1599	U1494	U1298	C1201	U1185	A
C	U	U1917	U1824	G1599	U1494	U1298	C1201	U1186	C
C	U	U1918	U1825	G1599	U1494	U1298	C1201	U1187	A
C	U	U1919	U1826	G1599	U1494	U1298	C1201	U1188	C
C	U	U1920	U1827	G1599	U1494	U1298	C1201	U1189	A
C	U	U1921	U1828	G1599	U1494	U1298	C1201	U1190	C
C	U	U1922	U1829	G1599	U1494	U1298	C1201	U1191	A
C	U	U1923	U1830	G1599	U1494	U1298	C1201	U1192	C
C	U	U1924	U1831	G1599	U1494	U1298	C1201	U1193	A
C	U	U1925	U1832	G1599	U1494	U1298	C1201	U1194	C
C	U	U1926	U1833	G1599	U1494	U1298	C1201	U1195	A
C	U	U1927	U1834	G1599	U1494	U1298	C1201	U1196	C
C	U	U1928	U1835	G1599	U1494	U1298	C1201	U1197	A
C	U	U1929	U1836	G1599	U1494	U1298	C1201	U1198	C
C	U	U1930	U1837	G1599	U1494	U1298	C1201	U1199	A
C	U	U1931	U1838	G1599	U1494	U1298	C1201	U1200	C
C	U	U1932	U1839	G1599	U1494	U1298	C1201	U1201	A
C	U	U1933	U1840	G1599	U1494	U1298	C1201	U1202	C
C	U	U1934	U1841	G1599	U1494	U1298	C1201	U1203	A
C	U	U1935	U1842	G1599	U1494	U1298	C1201	U1204	C
C	U	U1936	U1843	G1599	U1494	U1298	C1201	U1205	A
C	U	U1937	U1844	G1599	U1494	U1298	C1201	U1206	C
C	U	U1938	U1845	G1599	U1494	U1298	C1201	U1207	A
C	U	U1939	U1846	G1599	U1494	U1298	C1201	U1208	C
C	U	U1940	U1847	G1599	U1494	U1298	C1201	U1209	A
C	U	U1941	U1848	G1599	U1494	U1298	C1201	U1210	C
C	U	U1942	U1849	G1599	U1494	U1298	C1201	U1211	A
C	U	U1943	U1850	G1599	U1494	U1298	C1201	U1212	C
C	U	U1944	U1851	G1599	U1494	U1298	C1201	U1213	A
C	U	U1945	U1852	G1599	U1494	U1298	C1201	U1214	C
C	U	U1946	U1853	G1599	U1494	U1298	C1201	U1215	A
C	U	U1947	U1854	G1599	U1494	U1298	C1201	U1216	C
C	U	U1948	U1855	G1599	U1494	U1298	C1201	U1217	A
C	U	U1949	U1856	G1599	U1494	U1298	C1201	U1218	C
C	U	U1950	U1857	G1599	U1494	U1298	C1201	U1219	A
C	U	U1951	U1858	G1599	U1494	U1298	C1201	U1220	C
C	U	U1952	U1859	G1599	U1494	U1298	C1201	U1221	A
C	U	U1953	U1860	G1599	U1494	U1298	C1201	U1222	C
C	U	U1954	U1861	G1599	U1494	U1298	C1201	U1223	A
C	U	U1955	U1862	G1599	U1494	U1298	C1201	U1224	C
C	U	U1956	U1863	G1599	U1494	U1298	C1201	U1225	A
C	U	U1957	U1864	G1599	U1494	U1298	C1201	U1226	C
C	U	U1958	U1865	G1599	U1494	U1298	C1201	U1227	A
C	U	U1959	U1866	G1599	U1494	U1298	C1201	U1228	C
C	U	U1960	U1867	G1599	U1494	U1298	C1201	U1229	A
C	U	U1961	U1868	G1599	U1494	U1298	C1201	U1230	C
C	U	U1962	U1869	G1599	U1494	U1298	C1201	U1231	A
C	U	U1963	U1870	G1599	U1494	U1298	C1201	U1232	C
C	U	U1964	U1871	G1599	U1494	U1298	C1201	U1233	A
C	U	U1965	U1872	G1599	U1494	U1298	C1201	U1234	C
C	U	U1966	U1873	G1599	U1494	U1298	C1201	U1235	A
C	U	U1967	U1874	G1599	U1494	U1298	C1201	U1236	C
C	U	U1968	U1875	G1599	U1494	U1298	C1201	U1237	A
C	U	U1969	U1876	G1599	U1494	U1298	C1201	U1238	C
C	U	U1970	U1877	G1599	U1494	U1298	C1201	U1239	A
C	U	U1971	U1878	G1599	U1494	U1298	C1201	U1240	C
C	U	U1972	U1879	G1599	U1494	U1298	C1201	U1241	A
C	U	U1973	U1880	G1599	U1494	U1298	C1201	U1242	C
C									



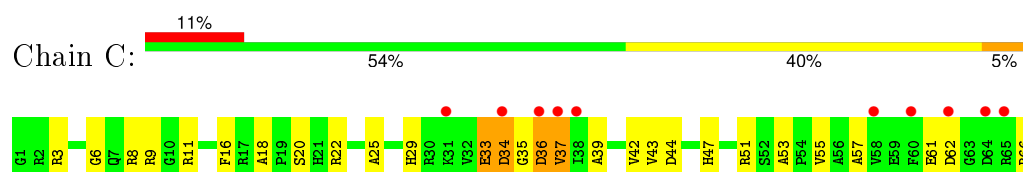
• Molecule 2: 5S ribosomal RNA

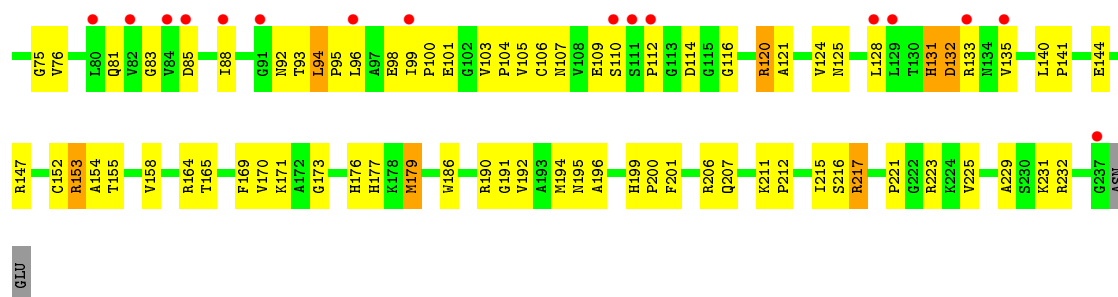


• Molecule 3: CC-puromycin

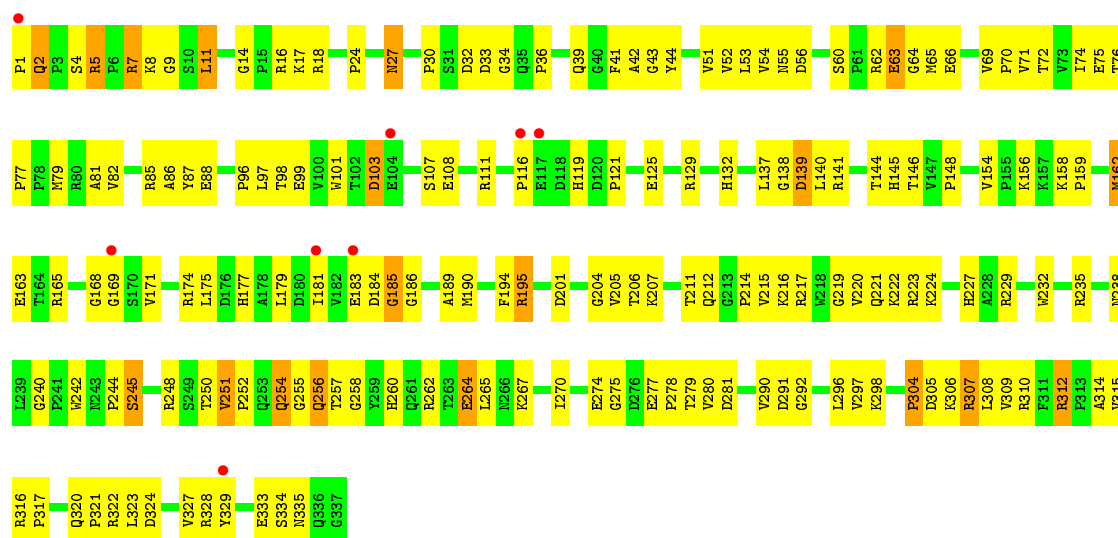


• Molecule 4: 50S ribosomal protein L2P

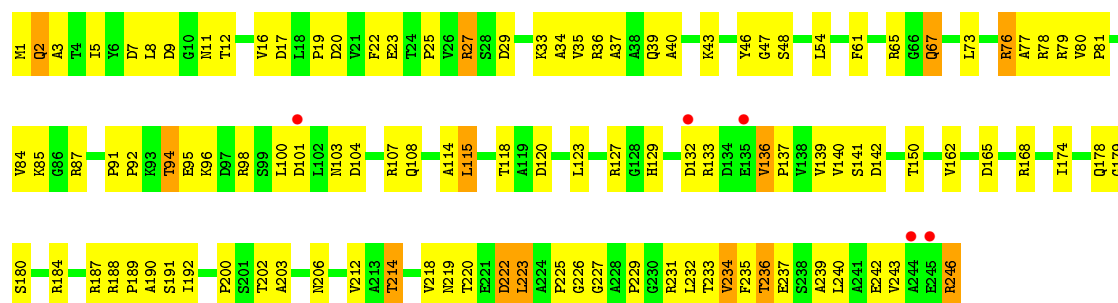




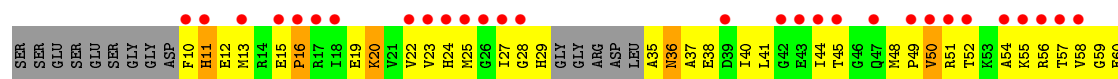
• Molecule 5: 50S ribosomal protein L3P

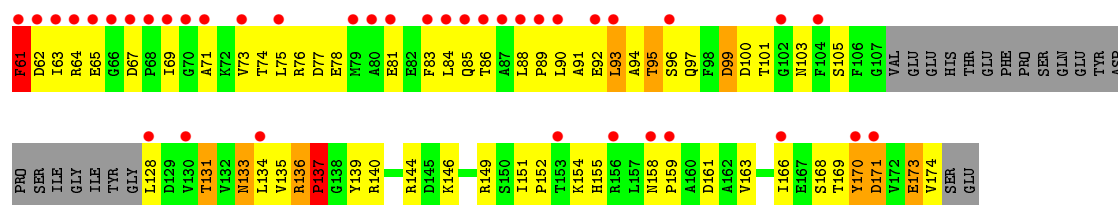


• Molecule 6: 50S ribosomal protein L4E

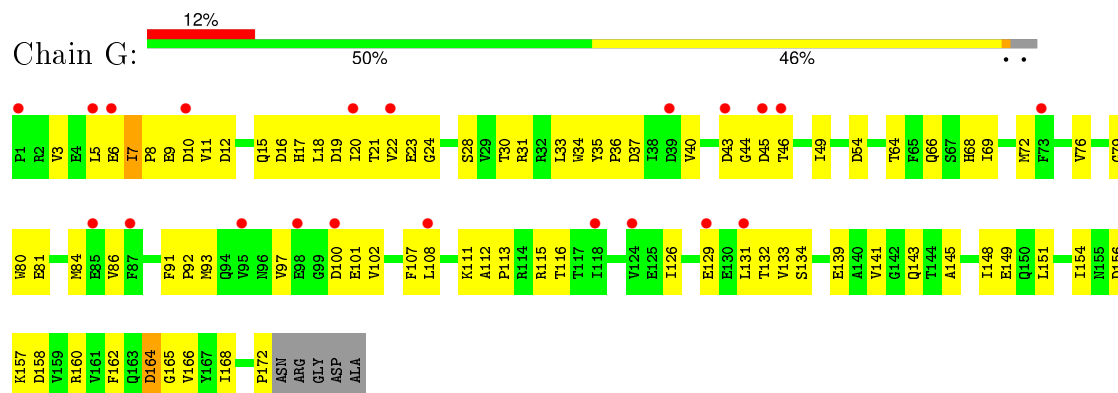


• Molecule 7: 50S ribosomal protein L5P

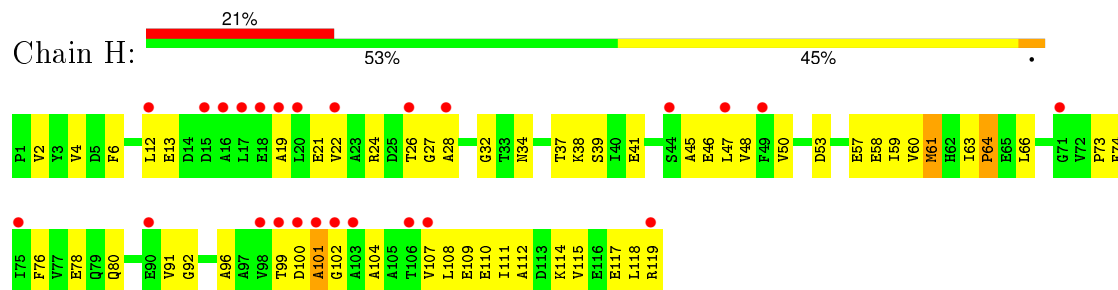




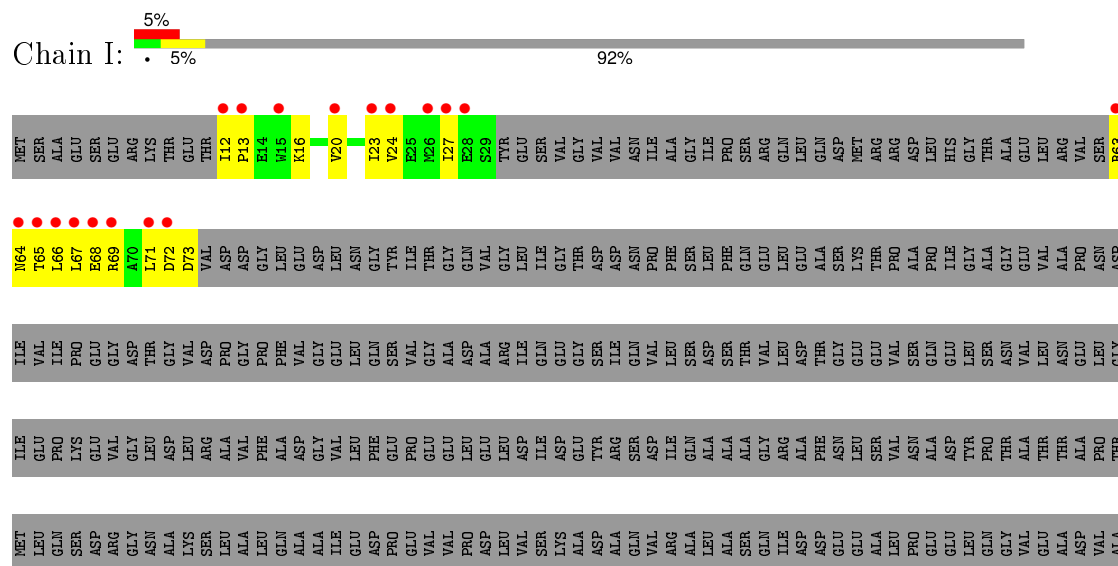
• Molecule 8: 50S ribosomal protein L6P



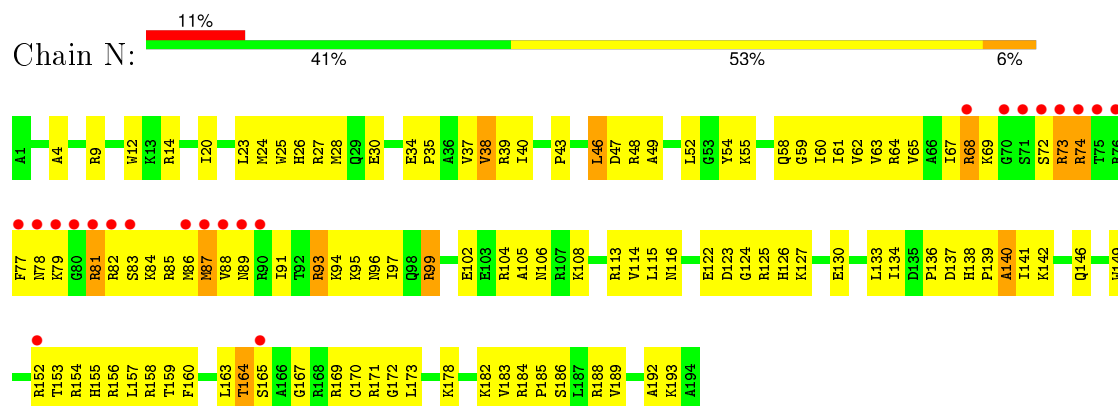
• Molecule 9: 50S ribosomal protein L7Ae



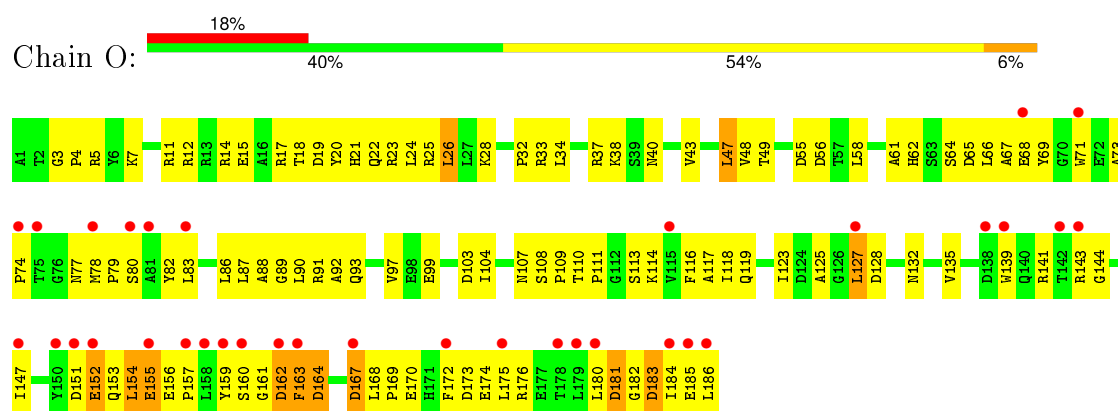
• Molecule 10: Acidic ribosomal protein P0 homolog



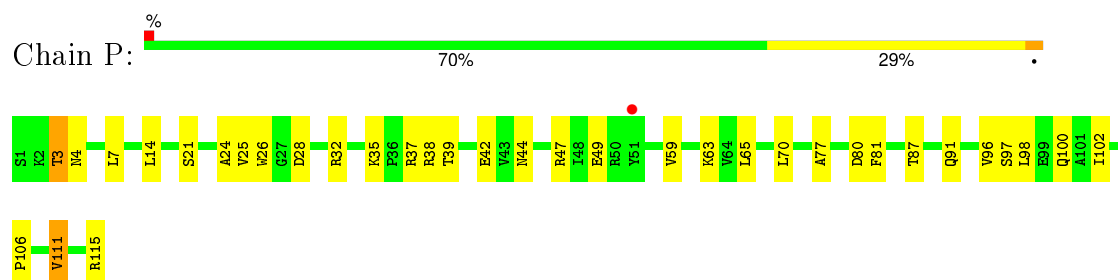
- Molecule 15: L15 Ribosomal Protein



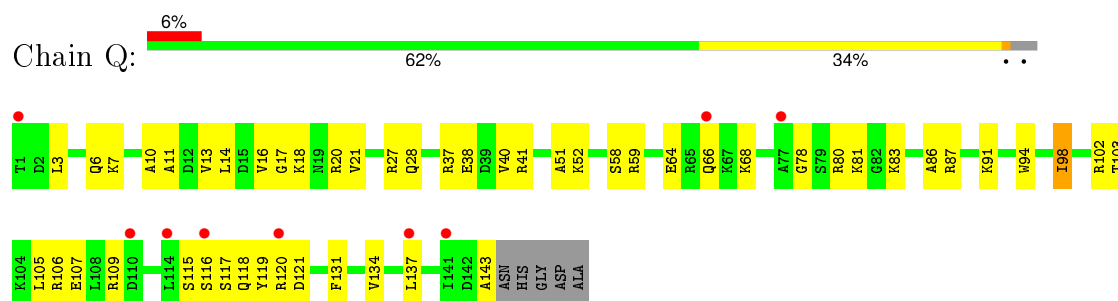
- Molecule 16: 50S ribosomal protein L18P



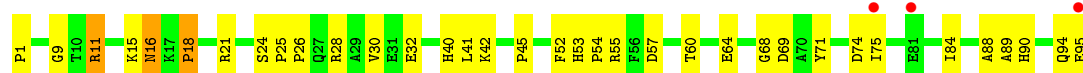
- Molecule 17: 50S ribosomal protein L18e



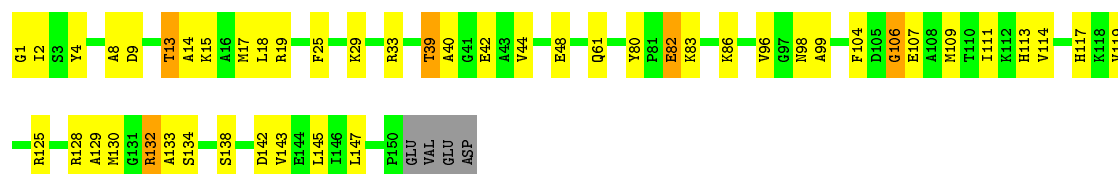
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



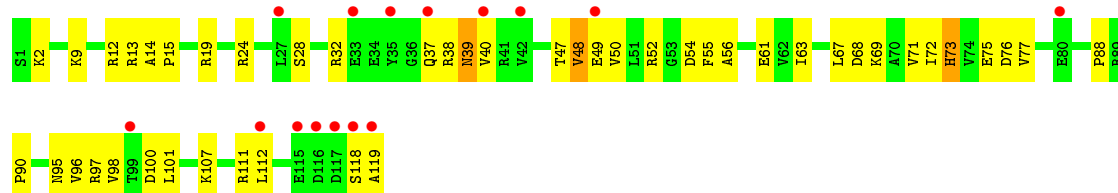
- Molecule 20: 50S ribosomal protein L22P



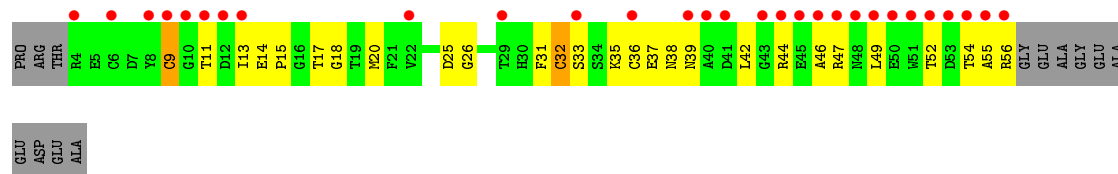
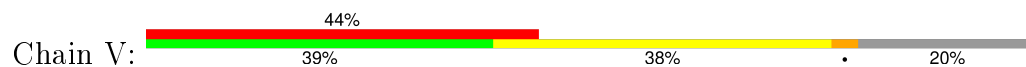
- Molecule 21: 50S ribosomal protein L23P



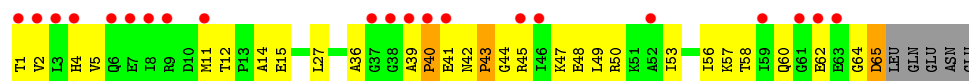
- Molecule 22: 50S ribosomal protein L24P



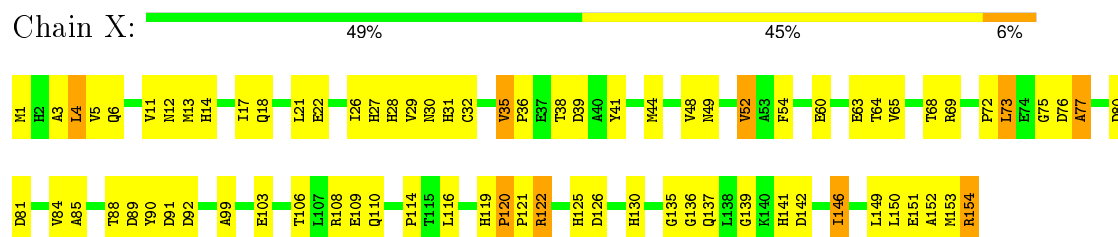
- Molecule 23: 50S ribosomal protein L24E



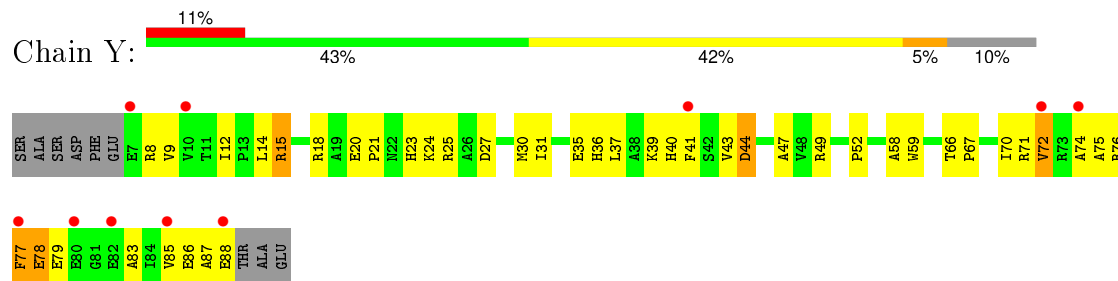
- Molecule 24: 50S ribosomal protein L29P



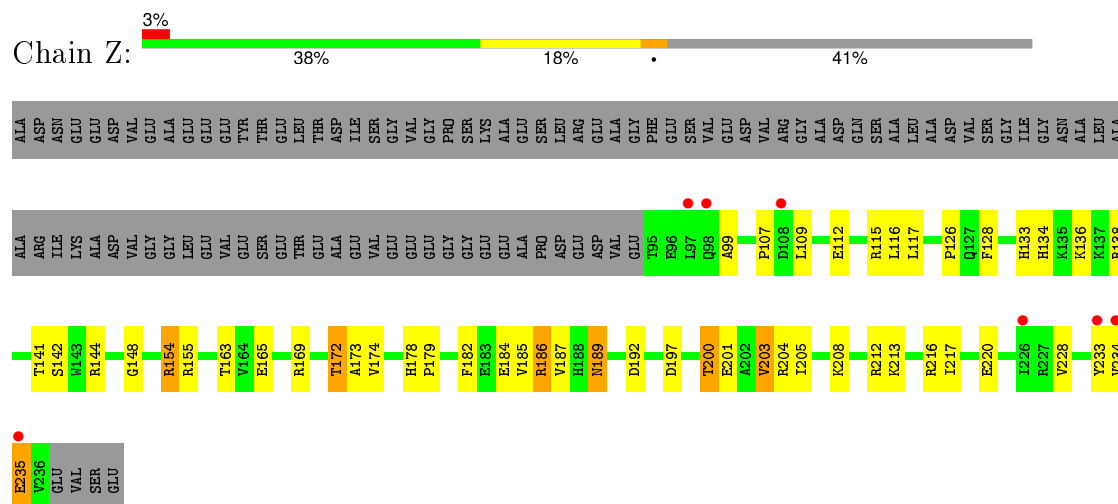
- Molecule 25: 50S ribosomal protein L30P



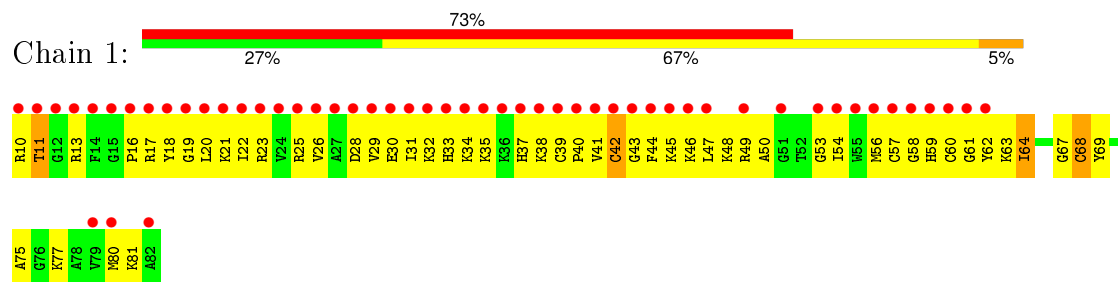
- Molecule 26: 50S ribosomal protein L31e



- Molecule 27: 50S ribosomal protein L32E

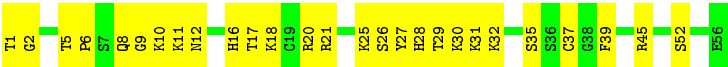


- Molecule 28: L37Ae 50S ribosomal protein

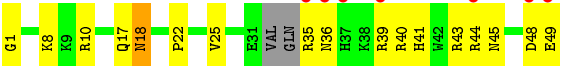


- Molecule 29: 50S ribosomal protein L37e

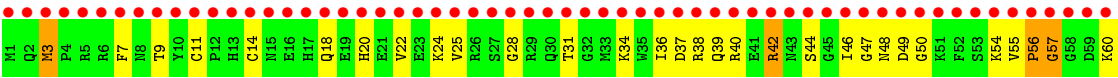




• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16 Å 301.29 Å 575.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.98 49.62 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.8 (49.62-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 2.96 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.251 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 370643 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, PPU

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	0.58	2/66076 (0.0%)	0.76	28/103052 (0.0%)
2	B	0.54	0/2905	0.82	4/4528 (0.1%)
3	5	2.09	1/43 (2.3%)	1.94	0/64
4	C	0.45	0/1787	0.75	0/2409
5	D	0.44	0/2689	0.70	0/3652
6	E	0.48	0/1883	0.72	0/2551
7	F	0.40	0/1111	0.63	0/1498
8	G	0.45	0/1382	0.65	0/1880
9	H	0.39	0/896	0.62	0/1219
10	I	0.38	0/241	0.56	0/324
11	J	0.48	0/1246	0.81	2/1686 (0.1%)
12	K	0.49	0/1135	0.70	0/1530
13	L	0.46	0/1003	0.76	0/1351
14	M	0.49	0/1126	0.76	0/1504
15	N	0.61	0/1633	0.83	2/2180 (0.1%)
16	O	0.40	0/1473	0.71	0/1999
17	P	0.47	0/873	0.70	0/1181
18	Q	0.44	0/1143	0.62	0/1521
19	R	0.44	0/748	0.75	1/1005 (0.1%)
20	S	0.49	0/1172	0.73	0/1578
21	T	0.41	0/648	0.65	0/875
22	U	0.39	0/957	0.70	0/1289
23	V	0.58	0/417	0.74	1/562 (0.2%)
24	W	0.38	0/502	0.60	0/675
25	X	0.50	0/1218	0.72	0/1655
26	Y	0.46	0/664	0.71	0/895
27	Z	0.48	0/1146	0.71	0/1536
28	1	0.77	0/575	0.84	0/763
29	2	0.55	0/437	0.77	0/578
30	3	0.44	0/398	0.61	0/527
31	4	0.93	0/771	0.80	0/1024
All	All	0.56	3/98298 (0.0%)	0.75	38/147091 (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	A	1	143
2	B	1	4
All	All	2	147

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1206	U	N1-C2	5.33	1.43	1.38
1	A	1206	U	C3'-O3'	-5.24	1.34	1.42
3	5	75	C	C4'-C3'	-5.04	1.47	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-18.53	64.43	105.20
1	A	1164	U	OP2-P-O3'	-18.53	64.44	105.20
1	A	1165	G	O5'-P-OP1	-11.90	94.99	105.70
2	B	3024	U	C2'-C3'-O3'	9.55	130.52	109.50
1	A	1563	G	C2'-C3'-O3'	9.10	129.51	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 147 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	26	U	Sidechain
1	A	28	G	Sidechain
1	A	48	A	Sidechain
1	A	55	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29798	1217	0
2	B	2600	0	1326	82	0
3	5	40	0	22	5	0
4	C	1754	0	1763	125	0
5	D	2624	0	2533	189	0
6	E	1858	0	1816	137	0
7	F	1094	0	1085	137	0
8	G	1357	0	1266	83	0
9	H	885	0	854	57	0
10	I	240	0	231	25	0
11	J	1215	0	1215	155	0
12	K	1119	0	1098	70	0
13	L	993	0	1027	67	0
14	M	1114	0	1072	67	0
15	N	1605	0	1676	179	0
16	O	1444	0	1401	142	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	60	0
19	R	734	0	728	28	0
20	S	1149	0	1122	56	0
21	T	641	0	605	28	0
22	U	949	0	923	49	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	99	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	63	0
28	1	563	0	601	80	0
29	2	430	0	426	39	0
30	3	393	0	406	30	0
31	4	755	0	732	62	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	36	0	0	13	0
38	2	58	0	0	4	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	268	0
38	B	146	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	20	0
38	G	45	0	0	11	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	20	0
38	K	54	0	0	4	0
38	L	64	0	0	16	0
38	M	86	0	0	15	0
38	N	138	0	0	27	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	4	0
38	S	83	0	0	10	0
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	6	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 3185 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10
1:A:1751:G:H2'	1:A:1752:G:H5''	1.30	1.10

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	
4	C	235/239 (98%)	202 (86%)	29 (12%)	4 (2%)	11	44
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	7	34
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	39	79
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	1	4
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	30	71
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	7	32
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4	19
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	5	24
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	4	22
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	13	48
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	26	68
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	34	75
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	3	18
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	26	68
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	5	25
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	26	68
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	25
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	15	52
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	4	20
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	8	36
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	10	41

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
7	F	173	GLU

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	C	179/181 (99%)	167 (93%)	12 (7%)	20	56
5	D	282/282 (100%)	264 (94%)	18 (6%)	22	58
6	E	193/193 (100%)	176 (91%)	17 (9%)	12	41
7	F	117/147 (80%)	107 (92%)	10 (8%)	13	43
8	G	152/155 (98%)	148 (97%)	4 (3%)	54	84
9	H	92/92 (100%)	91 (99%)	1 (1%)	80	94
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	110 (90%)	12 (10%)	10	35
12	K	118/121 (98%)	107 (91%)	11 (9%)	11	38
13	L	106/106 (100%)	103 (97%)	3 (3%)	51	83
14	M	112/126 (89%)	108 (96%)	4 (4%)	42	78
15	N	166/166 (100%)	157 (95%)	9 (5%)	27	65
16	O	149/149 (100%)	143 (96%)	6 (4%)	38	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	93/93 (100%)	89 (96%)	4 (4%)	35	74
18	Q	113/116 (97%)	110 (97%)	3 (3%)	52	84
19	R	79/79 (100%)	75 (95%)	4 (5%)	29	67
20	S	117/121 (97%)	113 (97%)	4 (3%)	44	80
21	T	71/73 (97%)	70 (99%)	1 (1%)	74	92
22	U	105/105 (100%)	102 (97%)	3 (3%)	50	83
23	V	44/52 (85%)	42 (96%)	2 (4%)	34	72
24	W	51/56 (91%)	49 (96%)	2 (4%)	39	76
25	X	130/130 (100%)	121 (93%)	9 (7%)	19	55
26	Y	66/73 (90%)	61 (92%)	5 (8%)	16	49
27	Z	120/195 (62%)	112 (93%)	8 (7%)	20	56
28	1	56/56 (100%)	50 (89%)	6 (11%)	8	29
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	57	86
31	4	79/79 (100%)	73 (92%)	6 (8%)	16	49
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	27	64

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	K	46	ILE
15	N	38	VAL
28	1	11	THR
12	K	74	ARG
12	K	127	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
15	N	58	GLN
18	Q	66	GLN
30	3	16	ASN
15	N	89	ASN
16	O	119	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	36 (1%)
2	B	121/122 (99%)	18 (14%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	266 (9%)	41 (1%)

5 of 266 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
1	A	1685	A
2	B	3024	U
1	A	1377	C
1	A	1450	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 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	$\# Z > 2$
36	PPU	5	76	3	30,40,41	2.25	12 (40%)	37,57,60	1.81	9 (24%)

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
36	PPU	5	76	3	-	0/21/43/44	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	C10-N6	-3.82	1.36	1.45
36	5	76	PPU	CE2-CD2	-3.79	1.31	1.38
36	5	76	PPU	CD1-CG	-3.54	1.31	1.38
36	5	76	PPU	C9-N6	-3.37	1.37	1.45
36	5	76	PPU	CE1-CD1	-3.04	1.33	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	PPU	C3'-N3'-C	-3.87	117.09	123.18
36	5	76	PPU	CG-CB-CA	-3.54	105.98	114.31
36	5	76	PPU	C2'-C1'-N9	-2.37	110.67	114.29
36	5	76	PPU	CE2-CZ-CE1	-2.05	116.86	120.20
36	5	76	PPU	CA-C-N3'	-2.01	110.28	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	0.12	75 (2%) 58 35	19, 45, 94, 144	0
2	B	122/122 (100%)	0.47	5 (4%) 41 22	33, 67, 97, 147	0
3	5	2/2 (100%)	2.18	1 (50%) 0 0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.61	26 (10%) 7 4	30, 62, 97, 109	0
5	D	337/337 (100%)	0.20	8 (2%) 62 39	22, 50, 77, 89	0
6	E	246/246 (100%)	0.07	5 (2%) 68 46	20, 44, 69, 78	0
7	F	140/176 (79%)	2.20	68 (48%) 0 0	65, 101, 122, 128	0
8	G	172/177 (97%)	0.97	21 (12%) 5 3	38, 62, 84, 89	0
9	H	119/119 (100%)	0.98	25 (21%) 1 1	51, 76, 99, 107	0
10	I	29/348 (8%)	2.42	18 (62%) 0 0	66, 87, 95, 99	0
11	J	156/167 (93%)	0.78	18 (11%) 6 3	35, 59, 82, 89	0
12	K	142/145 (97%)	0.09	2 (1%) 78 57	32, 44, 67, 78	0
13	L	132/132 (100%)	0.28	2 (1%) 76 56	33, 49, 75, 82	0
14	M	145/164 (88%)	1.32	40 (27%) 1 0	26, 79, 106, 111	0
15	N	194/194 (100%)	0.65	22 (11%) 7 3	28, 47, 106, 118	0
16	O	186/186 (100%)	1.13	34 (18%) 2 1	46, 73, 112, 125	0
17	P	115/115 (100%)	0.27	1 (0%) 85 69	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.58	9 (6%) 23 11	34, 53, 76, 85	0
19	R	95/95 (100%)	0.22	3 (3%) 51 30	36, 47, 63, 82	0
20	S	150/154 (97%)	0.01	0 100 100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.54	4 (4%) 33 18	44, 62, 82, 88	0
22	U	119/119 (100%)	0.85	15 (12%) 5 2	40, 55, 84, 104	0
23	V	53/66 (80%)	2.41	29 (54%) 0 0	77, 92, 100, 108	0
24	W	65/70 (92%)	1.46	21 (32%) 1 0	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	0.09	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.73	10 (12%) 5 3	37, 53, 77, 91	0
27	Z	142/240 (59%)	0.19	7 (4%) 33 18	25, 41, 64, 82	0
28	1	73/73 (100%)	5.68	53 (72%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.23	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.90	7 (15%) 3 1	34, 63, 96, 105	0
31	4	92/92 (100%)	9.00	92 (100%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.59	621 (9%) 11 5	19, 52, 105, 147	0

The worst 5 of 621 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	29.1
28	1	11	THR	20.4
31	4	37	ASP	19.4
31	4	83	TRP	19.1
31	4	62	THR	18.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	A	8332	1/1	0.80	0.45	111.27	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	A	8371	1/1	0.53	0.60	32.79	54,54,54,54	0
34	NA	B	8383	1/1	0.69	0.94	27.54	77,77,77,77	0
34	NA	A	8303	1/1	0.84	0.36	27.43	51,51,51,51	0
34	NA	A	8356	1/1	0.85	0.81	27.34	57,57,57,57	0
34	NA	A	8364	1/1	0.89	0.33	25.97	54,54,54,54	0
34	NA	A	8382	1/1	0.48	0.52	21.69	79,79,79,79	0
34	NA	A	8374	1/1	0.82	0.66	20.98	60,60,60,60	0
34	NA	A	8378	1/1	0.84	0.55	19.39	52,52,52,52	0
34	NA	A	8335	1/1	0.90	0.26	14.67	57,57,57,57	0
34	NA	A	8365	1/1	0.55	0.56	14.66	46,46,46,46	0
34	NA	A	8372	1/1	0.66	0.54	14.24	80,80,80,80	0
34	NA	A	8321	1/1	0.94	0.42	14.01	48,48,48,48	0
34	NA	A	8361	1/1	0.94	0.46	11.79	62,62,62,62	0
34	NA	S	8386	1/1	0.62	0.53	11.25	70,70,70,70	0
34	NA	A	8325	1/1	0.95	0.25	11.01	40,40,40,40	0
34	NA	A	8323	1/1	0.94	0.22	9.06	45,45,45,45	0
34	NA	A	8366	1/1	0.90	0.43	8.50	47,47,47,47	0
35	CL	A	8515	1/1	0.91	0.31	8.31	68,68,68,68	0
34	NA	A	8326	1/1	0.76	0.65	8.26	60,60,60,60	0
34	NA	A	8379	1/1	0.96	0.23	7.88	48,48,48,48	0
35	CL	D	8519	1/1	0.81	0.40	7.14	70,70,70,70	0
32	MG	A	8064	1/1	0.88	0.24	6.36	24,24,24,24	0
34	NA	A	8368	1/1	0.79	0.24	6.34	56,56,56,56	0
35	CL	M	8510	1/1	0.41	0.43	5.86	97,97,97,97	0
34	NA	A	8327	1/1	0.77	0.20	5.37	40,40,40,40	0
34	NA	A	8320	1/1	0.95	0.23	5.34	42,42,42,42	0
33	K	A	8201	1/1	0.97	0.24	5.07	71,71,71,71	0
35	CL	A	8505	1/1	0.85	0.26	4.19	74,74,74,74	0
34	NA	A	8362	1/1	0.92	0.20	3.52	74,74,74,74	0
34	NA	A	8373	1/1	0.70	0.27	3.50	54,54,54,54	0
32	MG	A	8060	1/1	0.95	0.18	3.29	44,44,44,44	0
32	MG	A	8053	1/1	0.91	0.19	3.28	41,41,41,41	0
32	MG	A	8112	1/1	0.90	0.20	3.10	57,57,57,57	0
34	NA	A	8353	1/1	0.88	0.22	2.56	53,53,53,53	0
36	PPU	5	76	37/38	0.91	0.27	2.22	60,64,69,71	0
34	NA	A	8350	1/1	0.94	0.16	1.96	37,37,37,37	0
35	CL	K	8521	1/1	0.93	0.24	1.72	60,60,60,60	0
34	NA	S	8337	1/1	0.65	0.26	1.61	52,52,52,52	0
35	CL	P	8508	1/1	0.98	0.31	1.23	82,82,82,82	0
34	NA	A	8376	1/1	0.98	0.17	0.99	79,79,79,79	0
34	NA	A	8324	1/1	0.92	0.25	0.92	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	1	8105	1/1	0.59	0.73	0.90	58,58,58,58	0
32	MG	A	8044	1/1	0.95	0.15	0.30	54,54,54,54	0
34	NA	A	8381	1/1	0.73	0.16	0.21	46,46,46,46	0
34	NA	J	8309	1/1	0.92	0.18	-0.09	42,42,42,42	0
34	NA	R	8348	1/1	0.69	0.21	-0.14	57,57,57,57	0
34	NA	K	8346	1/1	0.86	0.19	-0.29	37,37,37,37	0
32	MG	Z	8109	1/1	0.89	0.15	-0.34	38,38,38,38	0
33	K	A	8202	1/1	0.93	0.15	-0.37	89,89,89,89	0
34	NA	A	8331	1/1	0.92	0.15	-0.43	76,76,76,76	0
32	MG	A	8047	1/1	0.91	0.16	-0.64	31,31,31,31	0
35	CL	N	8518	1/1	0.90	0.18	-0.66	46,46,46,46	0
32	MG	A	8057	1/1	0.94	0.17	-0.86	46,46,46,46	0
34	NA	M	8380	1/1	0.93	0.17	-0.93	65,65,65,65	0
32	MG	A	8086	1/1	0.99	0.09	-1.14	49,49,49,49	0
32	MG	D	8055	1/1	0.82	0.15	-1.18	81,81,81,81	0
32	MG	A	8056	1/1	0.94	0.15	-1.28	56,56,56,56	0
34	NA	E	8304	1/1	0.91	0.14	-1.35	25,25,25,25	0
35	CL	A	8512	1/1	0.97	0.11	-1.48	31,31,31,31	0
32	MG	4	8078	1/1	0.93	0.19	-1.53	74,74,74,74	0
32	MG	C	8065	1/1	0.96	0.12	-1.57	68,68,68,68	0
32	MG	A	8062	1/1	0.94	0.14	-1.70	49,49,49,49	0
32	MG	U	8073	1/1	0.84	0.21	-1.73	48,48,48,48	0
37	CD	1	8403	1/1	0.73	0.31	-1.78	203,203,203,203	0
34	NA	A	8317	1/1	0.95	0.06	-2.06	32,32,32,32	0
34	NA	C	8345	1/1	0.95	0.12	-2.11	35,35,35,35	0
32	MG	A	8008	1/1	0.94	0.08	-2.18	42,42,42,42	0
34	NA	U	8343	1/1	0.95	0.09	-2.21	27,27,27,27	0
32	MG	A	8091	1/1	0.96	0.10	-2.30	67,67,67,67	0
34	NA	A	8314	1/1	0.95	0.10	-2.42	43,43,43,43	0
34	NA	N	8347	1/1	0.90	0.12	-2.47	24,24,24,24	0
37	CD	2	8402	1/1	0.99	0.07	-2.74	57,57,57,57	0
34	NA	A	8333	1/1	0.93	0.08	-3.04	33,33,33,33	0
32	MG	A	8107	1/1	0.98	0.06	-3.10	36,36,36,36	0
32	MG	A	8033	1/1	0.97	0.12	-3.11	25,25,25,25	0
32	MG	A	8027	1/1	0.93	0.05	-3.34	54,54,54,54	0
32	MG	A	8032	1/1	0.97	0.06	-3.43	34,34,34,34	0
34	NA	A	8344	1/1	0.94	0.07	-3.51	27,27,27,27	0
37	CD	V	8401	1/1	0.96	0.15	-3.52	129,129,129,129	0
32	MG	A	8074	1/1	0.97	0.05	-3.52	42,42,42,42	0
32	MG	A	8012	1/1	0.97	0.10	-3.53	44,44,44,44	0
34	NA	A	8338	1/1	0.96	0.09	-3.86	44,44,44,44	0
32	MG	A	8067	1/1	0.96	0.14	-3.97	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8077	1/1	0.94	0.06	-4.24	32,32,32,32	0
32	MG	A	8010	1/1	0.94	0.05	-4.24	30,30,30,30	0
32	MG	A	8059	1/1	0.93	0.10	-4.29	47,47,47,47	0
32	MG	A	8058	1/1	0.96	0.08	-4.48	39,39,39,39	0
37	CD	4	8404	1/1	0.74	0.42	-4.66	203,203,203,203	0
32	MG	A	8021	1/1	0.97	0.11	-4.68	32,32,32,32	0
34	NA	A	8305	1/1	0.98	0.09	-4.81	27,27,27,27	0
34	NA	A	8339	1/1	0.95	0.09	-5.19	30,30,30,30	0
32	MG	A	8006	1/1	0.97	0.09	-5.23	57,57,57,57	0
32	MG	A	8108	1/1	0.92	0.06	-5.30	53,53,53,53	0
32	MG	A	8004	1/1	0.95	0.07	-5.59	53,53,53,53	0
32	MG	A	8071	1/1	0.90	0.07	-5.70	93,93,93,93	0
32	MG	A	8013	1/1	0.94	0.12	-6.15	42,42,42,42	0
32	MG	A	8052	1/1	0.95	0.08	-6.15	51,51,51,51	0
32	MG	A	8080	1/1	0.99	0.06	-6.27	35,35,35,35	0
32	MG	A	8028	1/1	0.96	0.07	-6.35	37,37,37,37	0
32	MG	A	8017	1/1	0.97	0.05	-6.40	35,35,35,35	0
32	MG	A	8001	1/1	0.97	0.09	-6.75	33,33,33,33	0
32	MG	A	8038	1/1	0.97	0.05	-6.85	33,33,33,33	0
32	MG	A	8039	1/1	0.95	0.05	-7.08	51,51,51,51	0
32	MG	A	8015	1/1	0.98	0.05	-7.94	50,50,50,50	0
32	MG	A	8084	1/1	0.98	0.05	-8.13	50,50,50,50	0
32	MG	A	8019	1/1	0.99	0.07	-8.87	30,30,30,30	0
32	MG	A	8018	1/1	0.95	0.08	-9.06	42,42,42,42	0
32	MG	A	8035	1/1	0.94	0.06	-9.25	48,48,48,48	0
32	MG	A	8002	1/1	0.97	0.05	-9.46	36,36,36,36	0
32	MG	A	8020	1/1	0.98	0.05	-9.53	46,46,46,46	0
32	MG	A	8110	1/1	0.97	0.07	-10.71	30,30,30,30	0
32	MG	A	8003	1/1	0.97	0.07	-11.38	23,23,23,23	0
32	MG	A	8034	1/1	0.95	0.05	-12.24	36,36,36,36	0
32	MG	A	8054	1/1	0.97	0.06	-12.45	33,33,33,33	0
32	MG	A	8007	1/1	0.97	0.03	-12.53	28,28,28,28	0
32	MG	A	8096	1/1	0.93	0.07	-13.19	51,51,51,51	0
32	MG	A	8014	1/1	0.97	0.07	-34.59	20,20,20,20	0
34	NA	A	8355	1/1	0.82	0.62	-	64,64,64,64	0
34	NA	A	8306	1/1	0.92	0.61	-	44,44,44,44	0
32	MG	A	8016	1/1	0.92	0.13	-	36,36,36,36	0
32	MG	A	8075	1/1	0.94	0.12	-	45,45,45,45	0
32	MG	A	8100	1/1	0.94	0.13	-	79,79,79,79	0
35	CL	A	8514	1/1	0.94	0.27	-	50,50,50,50	0
32	MG	A	8011	1/1	0.99	0.13	-	24,24,24,24	0
35	CL	A	8503	1/1	0.90	0.24	-	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8092	1/1	0.73	0.47	-	91,91,91,91	0
34	NA	A	8341	1/1	0.87	0.17	-	55,55,55,55	0
34	NA	A	8310	1/1	0.76	0.54	-	40,40,40,40	0
32	MG	A	8090	1/1	0.93	0.19	-	70,70,70,70	0
32	MG	A	8025	1/1	0.99	0.06	-	40,40,40,40	0
32	MG	A	8043	1/1	0.94	0.09	-	32,32,32,32	0
32	MG	A	8099	1/1	0.88	0.24	-	68,68,68,68	0
32	MG	A	8042	1/1	0.94	0.17	-	34,34,34,34	0
32	MG	A	8087	1/1	0.95	0.09	-	49,49,49,49	0
35	CL	K	8516	1/1	0.87	0.27	-	61,61,61,61	0
32	MG	A	8040	1/1	0.96	0.13	-	100,100,100,100	0
34	NA	A	8308	1/1	0.90	0.15	-	63,63,63,63	0
35	CL	R	8511	1/1	0.83	0.38	-	67,67,67,67	0
34	NA	4	8369	1/1	0.79	0.33	-	66,66,66,66	0
32	MG	A	8045	1/1	0.82	0.13	-	50,50,50,50	0
32	MG	A	8089	1/1	0.84	0.22	-	82,82,82,82	0
32	MG	A	8111	1/1	0.98	0.07	-	61,61,61,61	0
32	MG	A	8114	1/1	0.70	1.02	-	124,124,124,124	0
34	NA	A	8316	1/1	0.88	0.21	-	45,45,45,45	0
32	MG	A	8093	1/1	0.80	0.23	-	44,44,44,44	0
34	NA	A	8358	1/1	0.89	0.45	-	105,105,105,105	0
32	MG	A	8116	1/1	0.91	0.16	-	55,55,55,55	0
34	NA	A	8330	1/1	0.94	0.20	-	35,35,35,35	0
35	CL	A	8522	1/1	0.79	0.62	-	83,83,83,83	0
32	MG	A	8022	1/1	0.97	0.05	-	32,32,32,32	0
35	CL	K	8501	1/1	0.91	0.17	-	58,58,58,58	0
32	MG	A	8061	1/1	0.95	0.06	-	45,45,45,45	0
35	CL	4	8504	1/1	0.39	0.37	-	101,101,101,101	0
32	MG	A	8104	1/1	0.92	0.20	-	52,52,52,52	0
32	MG	A	8097	1/1	0.95	0.20	-	32,32,32,32	0
34	NA	A	8311	1/1	0.91	0.13	-	31,31,31,31	0
32	MG	A	8030	1/1	0.95	0.12	-	34,34,34,34	0
34	NA	A	8359	1/1	0.94	0.45	-	60,60,60,60	0
32	MG	A	8072	1/1	0.96	0.07	-	53,53,53,53	0
32	MG	A	8024	1/1	0.37	0.60	-	110,110,110,110	0
35	CL	Z	8517	1/1	0.96	0.31	-	61,61,61,61	0
34	NA	A	8352	1/1	0.78	0.33	-	39,39,39,39	0
32	MG	A	8063	1/1	0.93	0.11	-	85,85,85,85	0
34	NA	A	8363	1/1	0.57	0.78	-	48,48,48,48	0
34	NA	A	8307	1/1	0.77	0.64	-	58,58,58,58	0
34	NA	J	8322	1/1	0.84	0.37	-	72,72,72,72	0
32	MG	A	8037	1/1	0.97	0.09	-	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8117	1/1	0.97	0.08	-	33,33,33,33	0
34	NA	A	8336	1/1	0.93	0.10	-	49,49,49,49	0
32	MG	A	8048	1/1	0.97	0.07	-	33,33,33,33	0
34	NA	A	8357	1/1	0.76	0.10	-	49,49,49,49	0
37	CD	P	8405	1/1	0.94	0.07	-	89,89,89,89	0
32	MG	A	8026	1/1	0.99	0.05	-	33,33,33,33	0
32	MG	A	8102	1/1	0.62	1.13	-	135,135,135,135	0
34	NA	A	8377	1/1	0.85	0.33	-	86,86,86,86	0
35	CL	C	8509	1/1	0.83	0.32	-	86,86,86,86	0
32	MG	A	8101	1/1	0.87	0.10	-	50,50,50,50	0
35	CL	S	8506	1/1	0.91	0.20	-	60,60,60,60	0
32	MG	B	8095	1/1	0.83	0.08	-	72,72,72,72	0
34	NA	A	8328	1/1	0.70	0.57	-	47,47,47,47	0
32	MG	A	8070	1/1	0.95	0.78	-	69,69,69,69	0
32	MG	A	8051	1/1	0.90	0.10	-	86,86,86,86	0
34	NA	A	8375	1/1	0.90	0.25	-	55,55,55,55	0
32	MG	A	8041	1/1	0.92	0.17	-	55,55,55,55	0
34	NA	A	8342	1/1	0.94	0.14	-	28,28,28,28	0
32	MG	A	8023	1/1	0.96	0.12	-	45,45,45,45	0
32	MG	A	8094	1/1	0.93	0.17	-	65,65,65,65	0
34	NA	A	8367	1/1	0.96	0.14	-	43,43,43,43	0
32	MG	A	8031	1/1	0.98	0.04	-	32,32,32,32	0
32	MG	A	8103	1/1	0.89	0.23	-	45,45,45,45	0
32	MG	A	8106	1/1	0.93	0.21	-	76,76,76,76	0
34	NA	A	8315	1/1	0.98	0.16	-	43,43,43,43	0
34	NA	T	8312	1/1	0.39	0.57	-	80,80,80,80	0
32	MG	L	8069	1/1	0.98	0.09	-	81,81,81,81	0
34	NA	A	8385	1/1	0.71	0.34	-	46,46,46,46	0
35	CL	Z	8520	1/1	0.92	0.15	-	35,35,35,35	0
35	CL	K	8502	1/1	0.80	0.19	-	71,71,71,71	0
34	NA	A	8349	1/1	0.93	0.23	-	67,67,67,67	0
34	NA	A	8360	1/1	0.96	0.74	-	61,61,61,61	0
34	NA	A	8370	1/1	0.91	0.32	-	52,52,52,52	0
34	NA	A	8334	1/1	0.94	0.09	-	46,46,46,46	0
34	NA	A	8354	1/1	0.86	0.39	-	51,51,51,51	0
32	MG	A	8082	1/1	0.93	0.16	-	56,56,56,56	0
32	MG	A	8009	1/1	0.98	0.06	-	32,32,32,32	0
34	NA	A	8319	1/1	0.79	0.15	-	44,44,44,44	0
32	MG	A	8076	1/1	0.34	0.17	-	79,79,79,79	0
34	NA	A	8329	1/1	0.53	0.34	-	61,61,61,61	0
32	MG	A	8098	1/1	0.98	0.17	-	33,33,33,33	0
32	MG	A	8113	1/1	0.76	0.32	-	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	MG	A	8005	1/1	0.99	0.07	-	38,38,38,38	0
32	MG	A	8088	1/1	0.85	0.15	-	65,65,65,65	0
34	NA	B	8351	1/1	0.56	0.39	-	75,75,75,75	0
32	MG	A	8068	1/1	0.95	0.11	-	46,46,46,46	0
35	CL	A	8513	1/1	0.96	0.12	-	56,56,56,56	0
32	MG	A	8085	1/1	0.85	0.16	-	95,95,95,95	0
34	NA	A	8318	1/1	0.97	0.27	-	43,43,43,43	0
32	MG	A	8115	1/1	0.85	0.09	-	59,59,59,59	0
32	MG	A	8046	1/1	0.83	0.10	-	53,53,53,53	0
32	MG	A	8083	1/1	0.97	0.08	-	37,37,37,37	0
34	NA	A	8313	1/1	0.94	0.10	-	74,74,74,74	0
32	MG	A	8036	1/1	0.98	0.06	-	38,38,38,38	0
32	MG	A	8049	1/1	0.33	0.69	-	95,95,95,95	0
32	MG	A	8050	1/1	0.95	0.10	-	52,52,52,52	0
34	NA	A	8302	1/1	0.90	0.20	-	31,31,31,31	0
32	MG	A	8079	1/1	0.94	0.07	-	48,48,48,48	0
34	NA	A	8301	1/1	0.82	0.14	-	31,31,31,31	0
35	CL	O	8507	1/1	0.87	0.23	-	65,65,65,65	0
34	NA	A	8340	1/1	0.52	0.59	-	58,58,58,58	0
32	MG	A	8081	1/1	0.95	0.08	-	39,39,39,39	0
32	MG	A	8066	1/1	0.94	0.16	-	65,65,65,65	0
32	MG	A	8029	1/1	0.95	0.10	-	38,38,38,38	0
34	NA	A	8384	1/1	0.12	0.76	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.