



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:57 PM GMT

PDB ID : 1YJN  
Title : Crystal Structure Of Clindamycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui  
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2005-01-14  
Resolution : 3.00 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](mailto: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.

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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

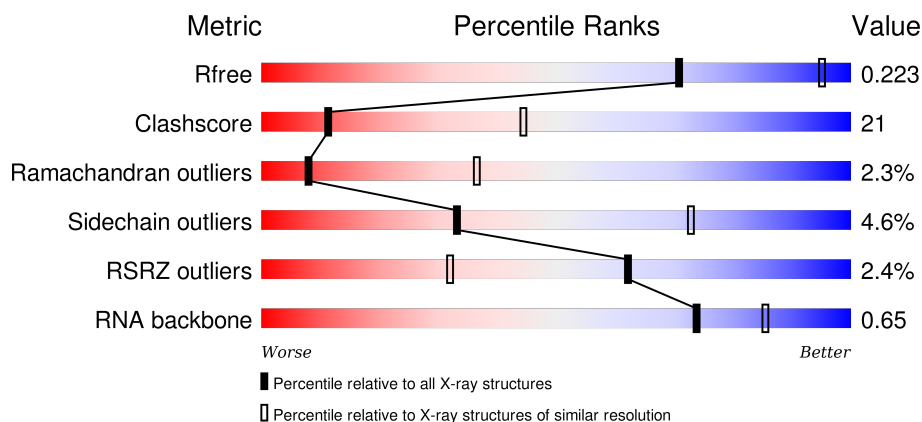
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




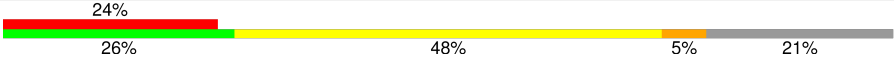

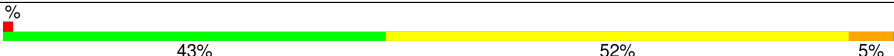

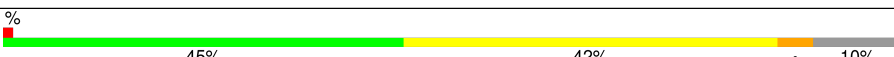
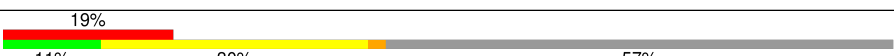



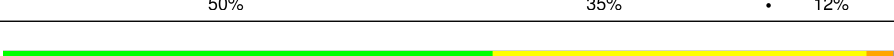
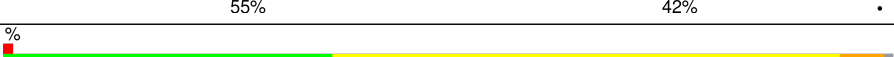

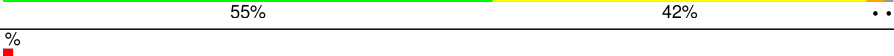
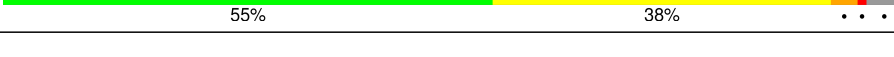





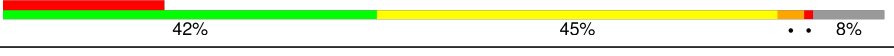




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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  $\geq 3$ , 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	0	2922	<div> <div>52%</div> <div>37%</div> <div>6%</div> <div>6%</div> </div>
2	9	122	<div> <div>39%</div> <div>52%</div> <div>9%</div> <div>.</div> </div>
3	A	240	<div> <div>52%</div> <div>40%</div> <div>7%</div> <div>.</div> </div>
4	B	338	<div> <div>47%</div> <div>46%</div> <div>6%</div> </div>

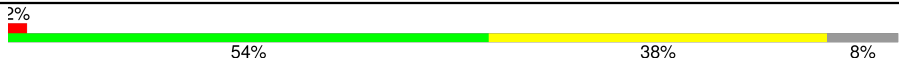

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	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	CLY	0	9000	-	-	-	X
33	MG	0	8053	-	-	-	X
34	K	0	8401	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8505	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8510	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8531	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8578	-	-	-	X
35	NA	0	8579	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	B	8561	-	-	-	X
35	NA	L	8580	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	R	8586	-	-	-	X
36	CL	O	8815	-	-	-	X
36	CL	B	8819	-	-	-	X
36	CL	J	8802	-	-	X	-

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99060 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	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

- 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
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- 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	S	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
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	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	S	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			

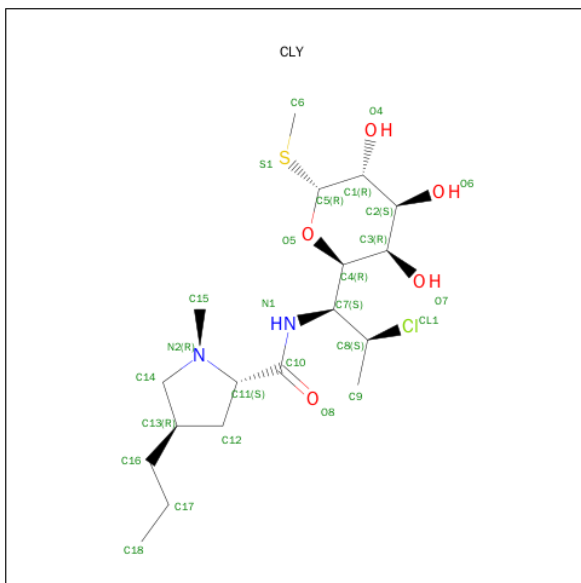
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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 CLINDAMYCIN (three-letter code: CLY) (formula:  $C_{18}H_{33}ClN_2O_5S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	S	0	0
			27	18	1	2	5	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	110	Total	Mg	0	0
			110	110		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	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		
33	3	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 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	72	Total Na 72 72	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	T	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5892	Total 5892	O 5892	0	0
38	9	139	Total 139	O 139	0	0
38	A	120	Total 120	O 120	0	0
38	B	146	Total 146	O 146	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	169	Total 169	O 169	0	0
38	D	49	Total 49	O 49	0	0
38	E	41	Total 41	O 41	0	0
38	F	25	Total 25	O 25	0	0
38	G	19	Total 19	O 19	0	0
38	H	68	Total 68	O 68	0	0
38	I	10	Total 10	O 10	0	0
38	J	56	Total 56	O 56	0	0
38	K	60	Total 60	O 60	0	0
38	L	82	Total 82	O 82	0	0
38	M	128	Total 128	O 128	0	0
38	N	64	Total 64	O 64	0	0
38	O	44	Total 44	O 44	0	0
38	P	64	Total 64	O 64	0	0
38	Q	49	Total 49	O 49	0	0
38	R	79	Total 79	O 79	0	0
38	S	31	Total 31	O 31	0	0
38	T	36	Total 36	O 36	0	0
38	U	27	Total 27	O 27	0	0
38	V	14	Total 14	O 14	0	0
38	W	68	Total 68	O 68	0	0

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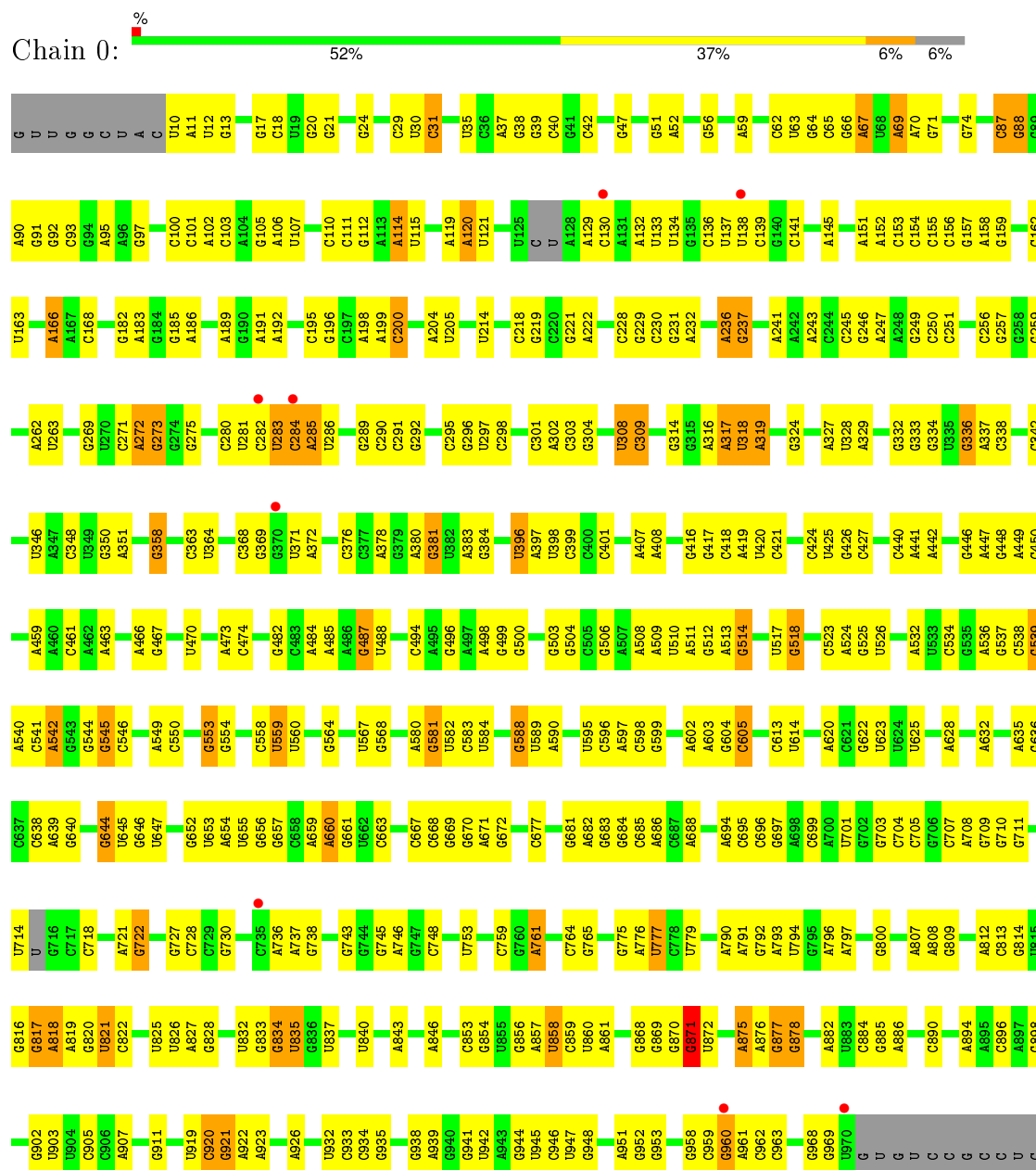
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	24	Total 24	O 24	0	0
38	Y	101	Total 101	O 101	0	0
38	Z	31	Total 31	O 31	0	0
38	1	57	Total 57	O 57	0	0
38	2	39	Total 39	O 39	0	0
38	3	74	Total 74	O 74	0	0

### 3 Residue-property plots

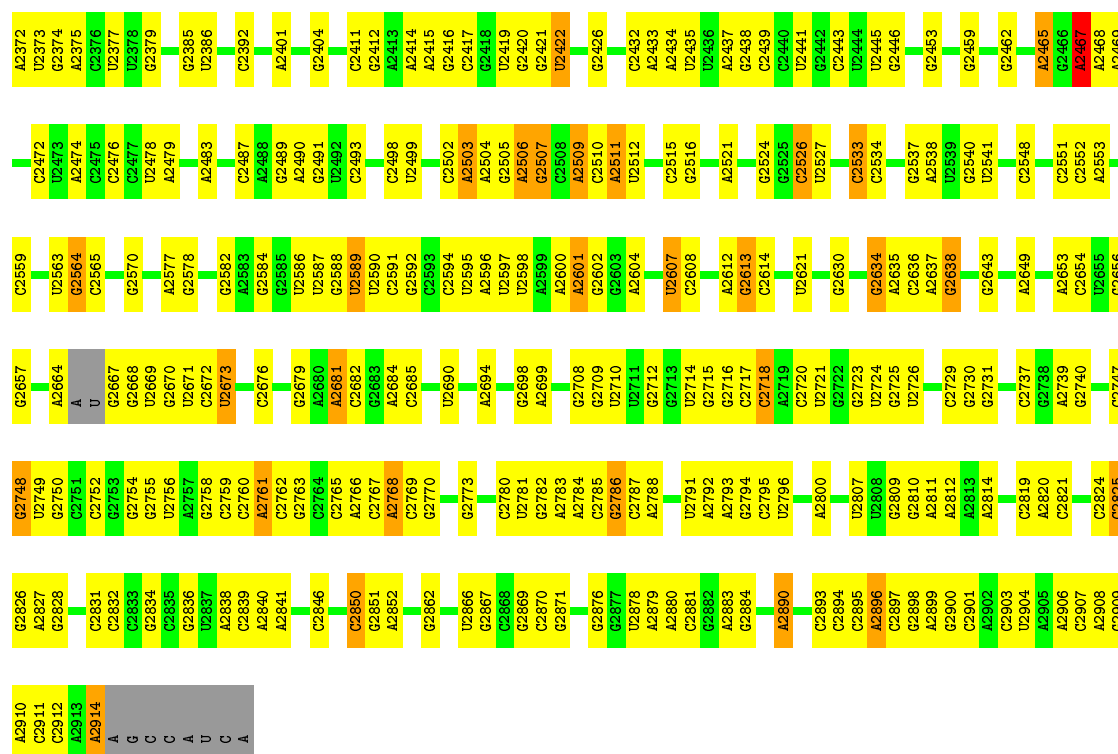
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

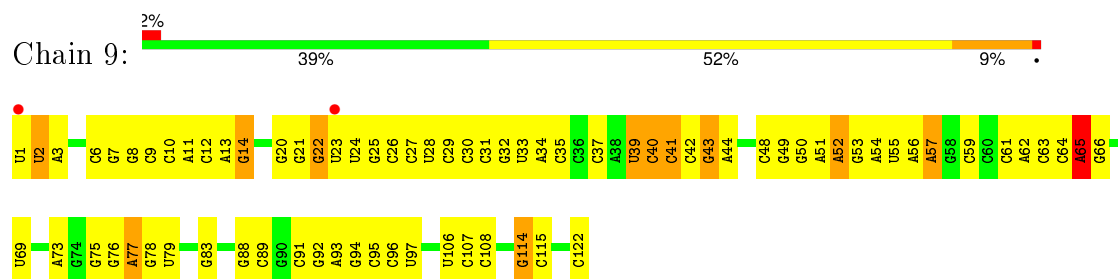




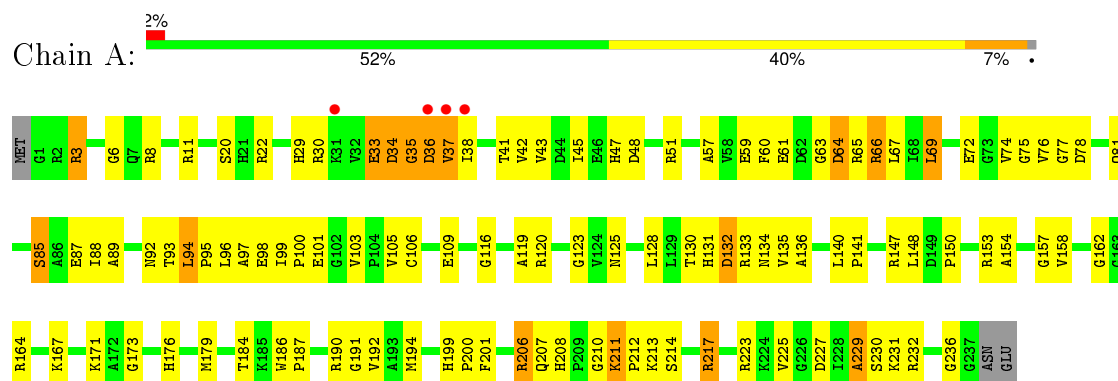
C2281	A	G	G2044	C	U1771	C1679	A1580	C1483	U1388	G1269	A1181	A1078	C
U2282	C	C	G2047	U	C1772	C1680	U1587	G1484	G1389	C1273	C1182	A1079	G
A2291	A	C	G2050	U	G1774	G1681	G1588	A1485	A1393	A1278	C1183	A1081	A
G2299	G	A	A2054	A	A1778	A1682	G1589	U1488	C1394	U1279	U1185	A1086	G
A2300	U	U	A2055	C	A1779	A1684	A1590	G1489	G1398	C1289	U1187	C1087	G
A2301	G	U	G2064	C	A1783	A1685	A1591	A1494	A1399	A1297	A1188	A1088	A
A2302	A	C	A2064	C	U1784	C1686	C1592	A1495	C1400	U1293	G1190	A1097	G
C2309	A	A	G2070	U	G1787	G1692	G1595	A1496	A1406	U1296	A1192	G1099	U
C2313	U	G	C2071	U	A1788	A1701	G1596	G1497	A1408	U1297	A1193	U1109	G
C2316	C	A	G2072	A	G1789	U1702	A1597	U1498	U1407	U1298	U1198	G1110	C
C2317	U	U	G2073	U	U1791	A1710	A1598	U1499	G1409	G1299	U1199	U1109	A
U2320	C	G	A2074	U	C1798	G1713	G1601	U1503	A1414	U1304	U1116	U1116	C
A2321	C	A	G2081	U	A1801	G1717	A1603	A1504	G1415	U1305	A1117	U1117	A
G2324	G	U	A2083	C	G1802	A1717	G1605	U1505	G1416	C1201	A1118	U1119	U
U2325	U	G	C2088	U	A1803	G1719	G1613	U1506	G1417	A1202	G1119	U1120	C
C2326	G	A	A2089	U	G1804	G1722	G1614	C1507	U1418	A1307	G1121	U1121	A
U2329	U	U	G2090	C	A1805	G1723	G1616	U1511	U1419	A1308	G1127	U1128	U
U2330	G	C	G2092	U	G1806	G1725	C1617	G1512	C1420	A1309	G1129	U1130	C
G2336	U	U	A2096	U	G1809	U1724	C1617	G1513	U1422	G1311	U1131	U1131	G
C2337	C	A	U2097	U	C1810	G1725	G1622	G1514	A1427	G1319	U1132	U1132	A
C2338	U	U	A1909	U	A1811	G1730	C1623	G1515	G1430	G1325	U1133	U1133	C
A	C	A	A1910	C	G1812	G1731	A1624	U1524	C1431	A1328	U1135	U1135	U
C2344	G	C	A1919	G	G1813	A1732	U1625	G1525	U1432	G1329	U1136	U1136	C
A2345	A	G	A1920	U	A1815	A1733	A1626	A1527	G1433	A1330	G1137	U1137	A
C2346	U	U	C1921	U	C1816	C1734	A1632	U1529	C1436	G1331	U1138	U1138	C
G2350	U	U	A1922	U	G1819	G1735	C1633	G1529	U1440	C1332	G1151	C1023	G
C2351	C	A	G1926	U	G1820	U1741	G1634	G1535	U1441	C1334	A1154	G1024	A
G2352	G	C	A1927	C	U1825	A1742	U1635	C1536	A1442	C1335	G1155	U1029	U
A2353	G	C	C1928	U	G1826	A1746	G1636	G1543	G1443	C1342	G1156	C1044	C
A2354	U	U	G1929	U	G1827	A1747	A1637	U1544	U1444	C1343	G1157	G1045	G
G2355	C	C	A1930	U	G1828	G1752	A1641	C1545	G1445	G1344	G1158	U1044	C
G2356	A	G	G1931	U	A1829	C1753	A1642	C1546	U1446	G1345	G1159	G1051	G
G2357	U	U	G1932	U	C1830	A1754	C1643	A1547	C1450	U1346	G1160	G1052	C
A2358	C	C	G1933	U	G1834	A1755	U1645	U1548	C1451	A1242	G1162	G1053	C
G2359	U	U	A1934	U	U1835	G1756	U1645	C1549	U1461	C1352	G1163	G1054	G
A2360	C	A	U1939	U	A1839	U1757	U1654	A1559	U1462	C1353	U1164	G1055	C
G2361	G	G	C1940	U	A1840	U1758	G1655	U	U1463	C1360	A1166	A1058	A
A2362	C	C	A1941	U	A1845	U1761	A1656	U1561	U1464	A1246	G1167	G1059	C
G2363	U	U	C1942	U	G1848	C1762	A1657	C1562	A1372	U1249	C1168	C1060	G
A2364	C	C	C1943	U	G1849	C1763	A1658	C1563	G1373	U1250	U1169	G1063	C
G2365	A	A	G1947	U	U1850	G1764	A1664	C1564	A1471	C1251	U1170	U1066	C
A2366	U	U	G1948	U	G1851	U1765	G1665	C1565	C1472	G1375	A1171	A1171	C
G2367	C	C	U1951	U	A1852	U1766	G1666	C1566	U1473	A1376	G1172	U1067	C
A2368	C	C	U1951	U	G1853	A1767	A1667	G1567	C1474	C1377	A1173	A1067	C
U2370	U	U	U	U	A1854	C1768	U1668	U1569	C1477	U1383	A1174	G1071	C
U2371	C	C	A	C	C1853	C1769	G1669	U1569	U1478	C1384	G1175	G1072	C
G2371	G	G	A	C		U1770	A1670	A1572	A1480				



### • Molecule 2: 5S Ribosomal RNA

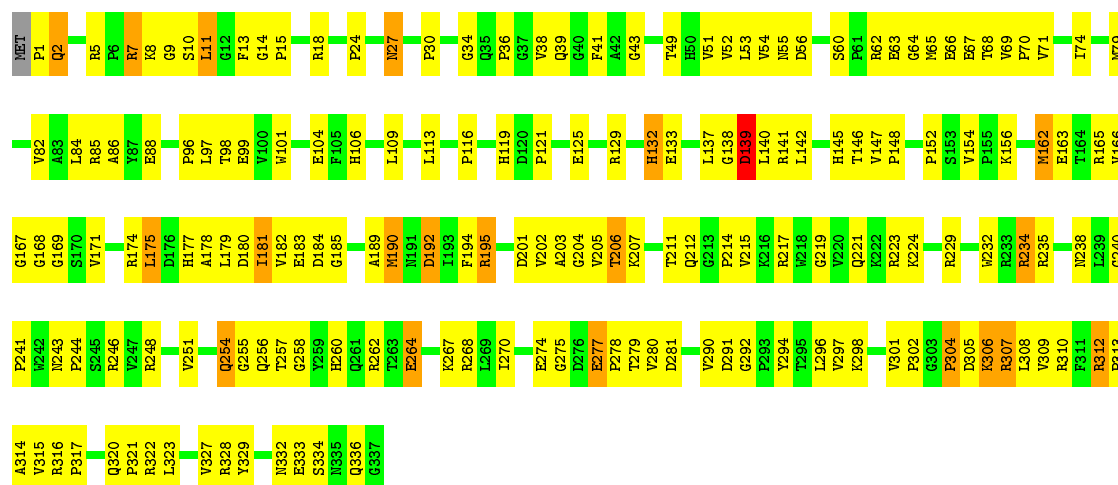


### • Molecule 3: 50S ribosomal protein L2P



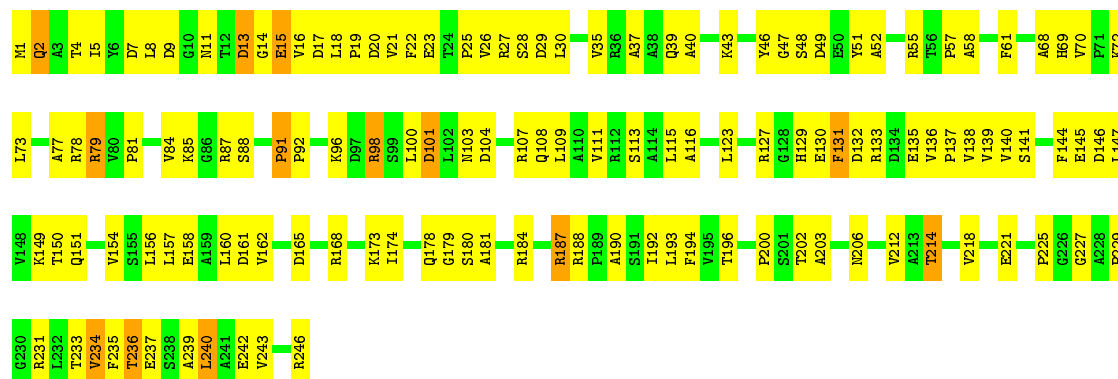
### • Molecule 4: 50S ribosomal protein L3P





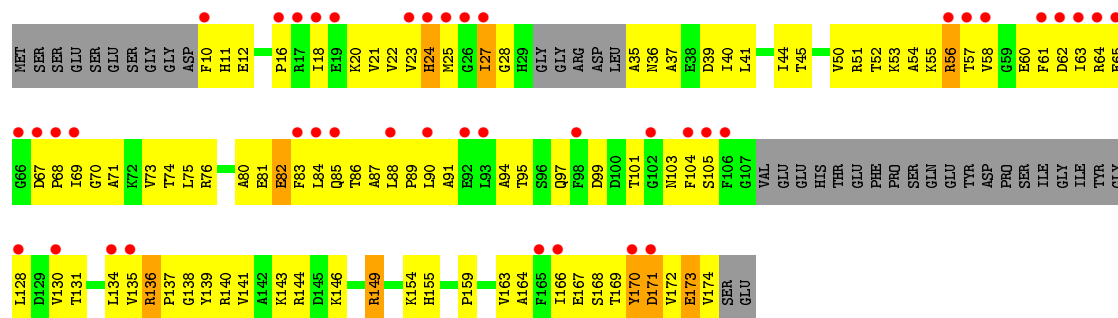
• Molecule 5: 50S ribosomal protein L4E

Chain C: 46% 49% 5%



• Molecule 6: 50S ribosomal protein L5P

Chain D: 24% 26% 48% 5% 21%



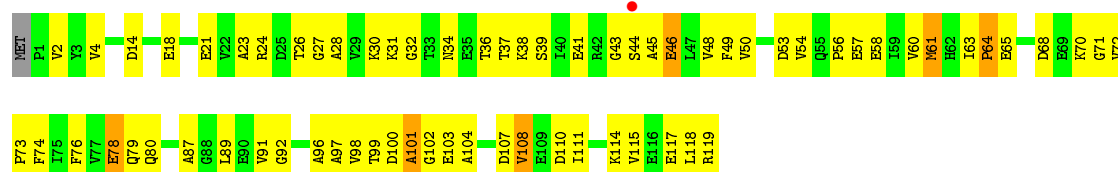
• Molecule 7: 50S ribosomal protein L6P

Chain E: 52% 42%

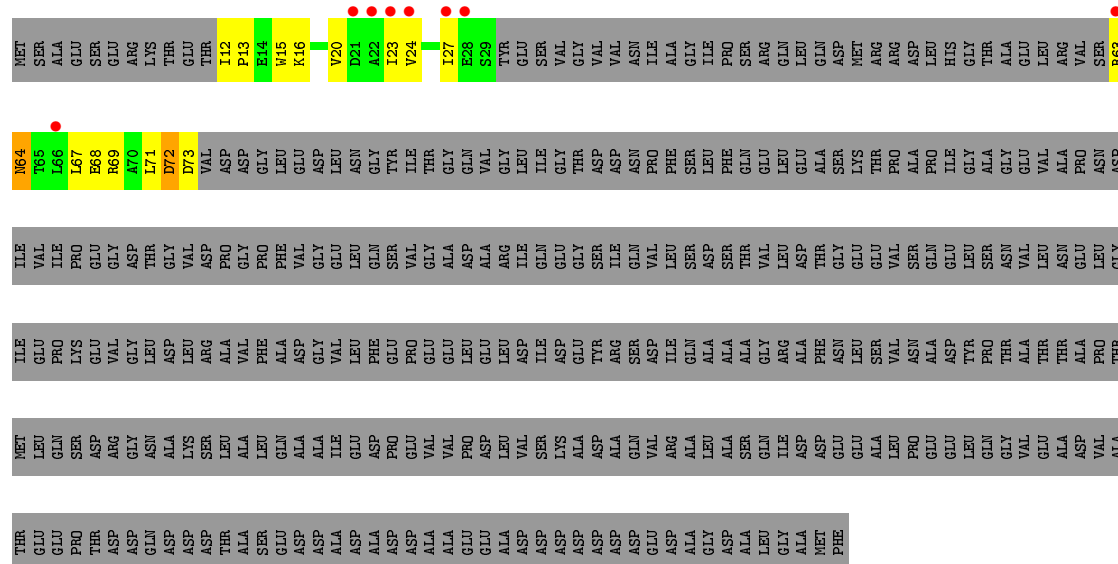




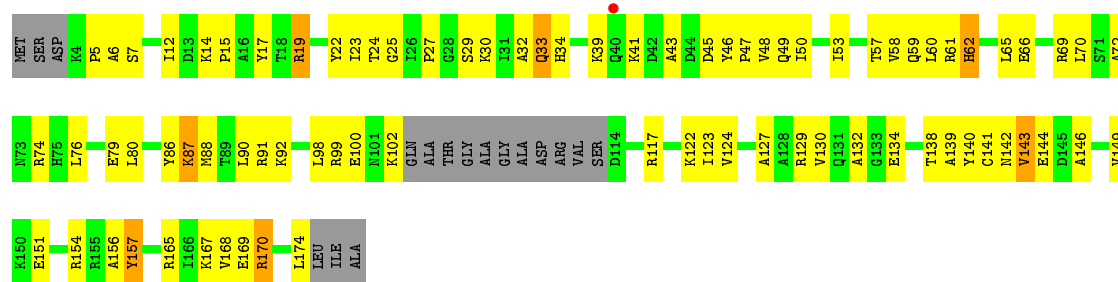
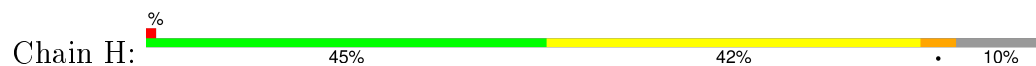
• Molecule 8: 50S ribosomal protein L7AE



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



• Molecule 10: 50S RIBOSOMAL PROTEIN L10E

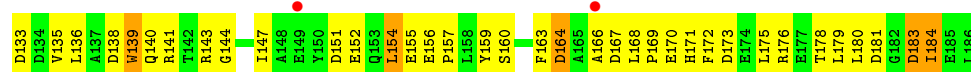
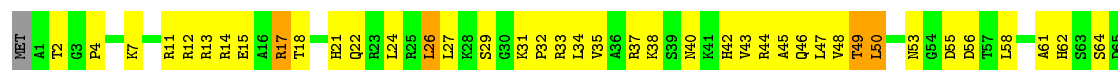


• Molecule 11: 50S RIBOSOMAL PROTEIN L11P

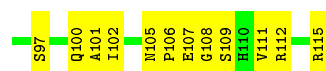




• Molecule 16: 50S ribosomal protein L18P



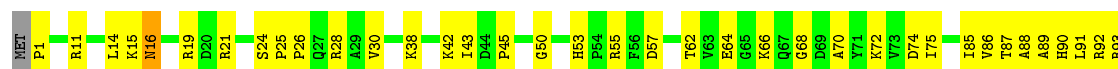
• Molecule 17: 50S ribosomal protein L18e



• Molecule 18: 50S ribosomal protein L19E

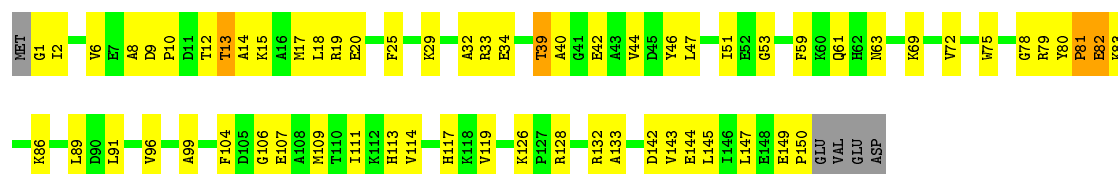


• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P

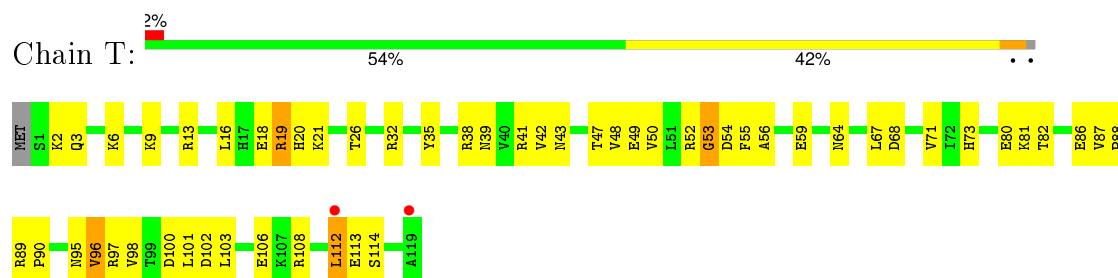




- Molecule 21: 50S ribosomal protein L23P



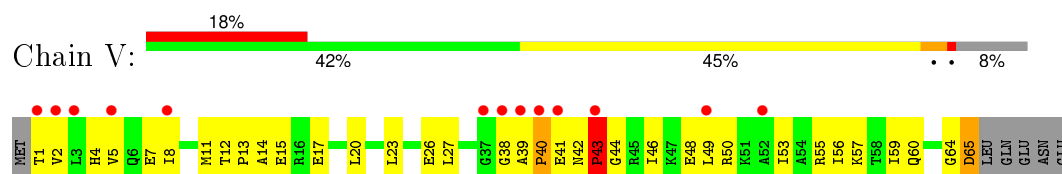
- Molecule 22: 50S ribosomal protein L24P



- Molecule 23: 50S ribosomal protein L24E



- Molecule 24: 50S ribosomal protein L29P



- Molecule 25: 50S ribosomal protein L30P

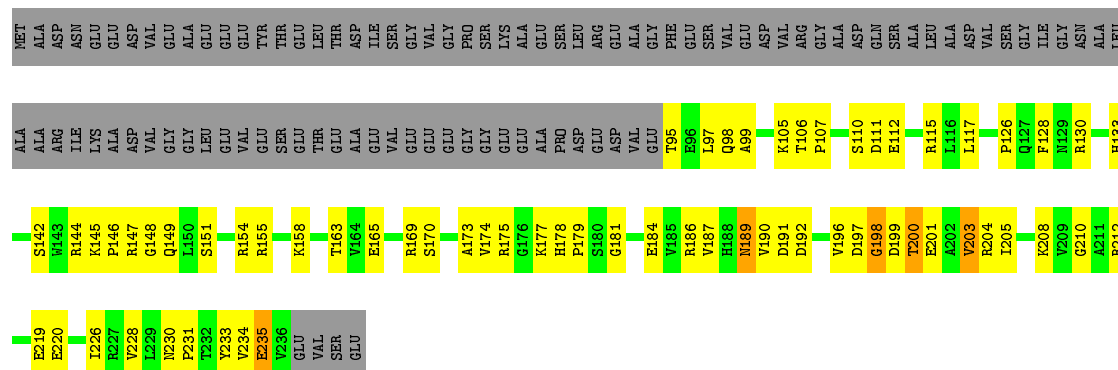
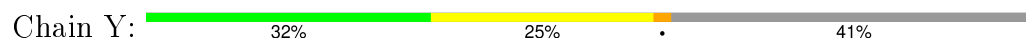


- Molecule 26: 50S ribosomal protein L31e

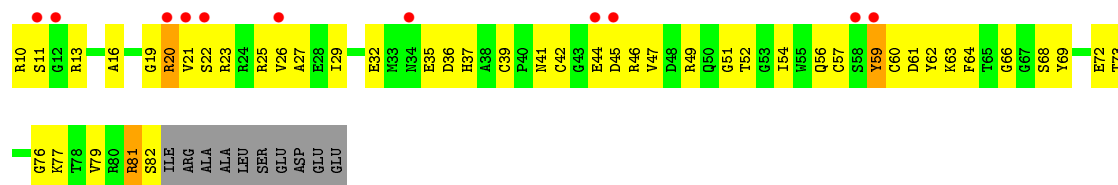




- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae



- Molecule 29: 50S ribosomal protein L37e



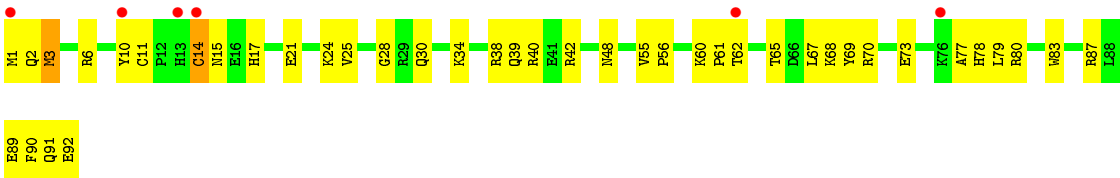
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E







E89  
F90  
Q91  
E92

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.51Å 300.12Å 573.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.00 49.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (29.97-3.00) 92.0 (49.96-3.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.170 , 0.228 0.170 , 0.223	Depositor DCC
$R_{free}$ test set	3274 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 78.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 333181 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, OMG, CL, NA, K, CD, CLY, 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	0.40	0/65957	0.69	11/102867 (0.0%)
2	9	0.36	0/2904	0.70	1/4526 (0.0%)
3	A	0.33	0/1786	0.64	0/2408
4	B	0.35	0/2690	0.64	0/3652
5	C	0.39	0/1884	0.65	0/2551
6	D	0.32	0/1111	0.57	0/1498
7	E	0.34	0/1382	0.60	0/1880
8	F	0.32	0/901	0.59	0/1224
9	G	0.32	0/241	0.49	0/324
10	H	0.35	0/1302	0.65	0/1743
11	I	0.32	0/526	0.57	0/716
12	J	0.38	0/1136	0.62	0/1530
13	K	0.37	0/1001	0.68	0/1347
14	L	0.33	0/1130	0.63	0/1509
15	M	0.37	0/1582	0.61	0/2117
16	N	0.31	0/1474	0.63	0/1999
17	O	0.36	0/874	0.59	0/1181
18	P	0.36	0/1147	0.55	0/1528
19	Q	0.36	0/749	0.69	0/1005
20	R	0.37	0/1172	0.64	0/1578
21	S	0.35	0/648	0.59	0/875
22	T	0.34	0/958	0.64	0/1289
23	U	0.34	0/417	0.58	0/562
24	V	0.31	0/502	0.60	0/675
25	W	0.37	0/1219	0.65	0/1655
26	X	0.36	0/664	0.61	0/895
27	Y	0.38	0/1146	0.65	0/1536
28	Z	0.35	0/589	0.59	0/787
29	1	0.40	0/438	0.60	0/578
30	2	0.34	0/401	0.54	0/529
31	3	0.34	0/771	0.55	0/1024
All	All	0.38	0/98702	0.67	12/147588 (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	0	30
2	9	0	1
All	All	0	31

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.13	129.59	109.50
1	0	1504	A	C1'-O4'-C4'	-6.53	104.68	109.90
1	0	871	G	C5'-C4'-O4'	-6.40	101.42	109.10
1	0	1942	A	C5'-C4'-C3'	6.35	126.17	116.00
2	9	39	U	N1-C1'-C2'	6.34	122.24	114.00

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	324	G	Sidechain
1	0	396	U	Sidechain
1	0	518	G	Sidechain
1	0	722	G	Sidechain
1	0	761	A	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	0	59020	0	29807	1145	0
2	9	2599	0	1325	94	0
3	A	1753	0	1766	153	0
4	B	2625	0	2533	198	0
5	C	1859	0	1816	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1094	0	1085	123	0
7	E	1357	0	1266	74	0
8	F	890	0	843	73	0
9	G	240	0	231	20	0
10	H	1282	0	1292	98	0
11	I	519	0	500	67	0
12	J	1120	0	1098	83	0
13	K	992	0	1031	85	0
14	L	1118	0	1076	57	0
15	M	1558	0	1566	81	0
16	N	1445	0	1401	138	0
17	O	865	0	873	50	0
18	P	1136	0	1123	74	0
19	Q	735	0	729	36	0
20	R	1149	0	1122	70	0
21	S	641	0	605	36	0
22	T	950	0	923	62	0
23	U	410	0	364	33	0
24	V	499	0	511	39	0
25	W	1196	0	1137	106	0
26	X	654	0	653	55	0
27	Y	1130	0	1133	64	0
28	Z	578	0	540	50	0
29	1	431	0	426	34	0
30	2	396	0	413	26	0
31	3	755	0	729	35	0
32	0	27	0	32	5	0
33	0	110	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	B	1	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
34	0	2	0	0	0	0
35	0	72	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	L	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	10	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	3	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	1	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5892	0	0	235	0
38	1	57	0	0	2	0
38	2	39	0	0	4	0
38	3	74	0	0	8	0
38	9	139	0	0	12	0
38	A	120	0	0	16	0
38	B	146	0	0	27	0
38	C	169	0	0	34	0
38	D	49	0	0	26	0
38	E	41	0	0	11	0
38	F	25	0	0	8	0
38	G	19	0	0	2	0
38	H	68	0	0	14	0
38	I	10	0	0	5	0
38	J	56	0	0	4	0
38	K	60	0	0	9	0
38	L	82	0	0	14	0
38	M	128	0	0	6	0
38	N	64	0	0	11	0
38	O	44	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	P	64	0	0	9	0
38	Q	49	0	0	6	0
38	R	79	0	0	8	0
38	S	31	0	0	4	0
38	T	36	0	0	9	0
38	U	27	0	0	2	0
38	V	14	0	0	4	0
38	W	68	0	0	14	0
38	X	24	0	0	8	0
38	Y	101	0	0	7	0
38	Z	31	0	0	7	0
All	All	99060	0	59949	3113	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 3113 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)
1:0:871:G:H8	1:0:871:G:H5'	1.15	1.12
2:9:6:C:H5''	16:N:37:ARG:HH12	1.16	1.10
13:K:10:GLN:H	13:K:10:GLN:NE2	1.49	1.09
13:K:10:GLN:N	13:K:10:GLN:HE21	1.52	1.07
1:0:156:C:H5''	15:M:171:ARG:HD3	1.31	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	235/240 (98%)	192 (82%)	34 (14%)	9 (4%)	<b>4</b> <b>22</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	B	335/338 (99%)	289 (86%)	38 (11%)	8 (2%)	7	35
5	C	244/246 (99%)	213 (87%)	24 (10%)	7 (3%)	6	29
6	D	134/177 (76%)	89 (66%)	35 (26%)	10 (8%)	1	6
7	E	170/178 (96%)	157 (92%)	13 (8%)	0	100	100
8	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	2	11
9	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	4	21
10	H	156/177 (88%)	140 (90%)	14 (9%)	2 (1%)	15	53
11	I	68/162 (42%)	45 (66%)	22 (32%)	1 (2%)	13	50
12	J	140/145 (97%)	124 (89%)	11 (8%)	5 (4%)	4	24
13	K	130/132 (98%)	114 (88%)	15 (12%)	1 (1%)	24	66
14	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	14	51
15	M	192/195 (98%)	172 (90%)	18 (9%)	2 (1%)	19	61
16	N	184/187 (98%)	151 (82%)	26 (14%)	7 (4%)	4	22
17	O	113/116 (97%)	100 (88%)	11 (10%)	2 (2%)	11	45
18	P	141/149 (95%)	128 (91%)	11 (8%)	2 (1%)	14	51
19	Q	93/96 (97%)	81 (87%)	11 (12%)	1 (1%)	17	58
20	R	148/155 (96%)	133 (90%)	13 (9%)	2 (1%)	14	51
21	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
22	T	117/120 (98%)	102 (87%)	14 (12%)	1 (1%)	21	64
23	U	51/66 (77%)	44 (86%)	5 (10%)	2 (4%)	4	21
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	5	27
25	W	152/154 (99%)	141 (93%)	9 (6%)	2 (1%)	15	53
26	X	80/92 (87%)	67 (84%)	9 (11%)	4 (5%)	3	15
27	Y	140/241 (58%)	125 (89%)	13 (9%)	2 (1%)	14	51
28	Z	71/83 (86%)	57 (80%)	11 (16%)	3 (4%)	3	20
29	1	54/57 (95%)	50 (93%)	4 (7%)	0	100	100
30	2	42/50 (84%)	39 (93%)	3 (7%)	0	100	100
31	3	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
All	All	3705/4437 (84%)	3196 (86%)	424 (11%)	85 (2%)	8	36

5 of 85 Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	A	34	ASP
3	A	36	ASP
3	A	132	ASP
4	B	139	ASP
5	C	234	VAL

### 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	
3	A	179/182 (98%)	168 (94%)	11 (6%)	23	61
4	B	282/283 (100%)	263 (93%)	19 (7%)	20	57
5	C	193/193 (100%)	184 (95%)	9 (5%)	32	72
6	D	117/148 (79%)	112 (96%)	5 (4%)	35	75
7	E	152/156 (97%)	146 (96%)	6 (4%)	39	77
8	F	93/94 (99%)	90 (97%)	3 (3%)	46	82
9	G	27/283 (10%)	25 (93%)	2 (7%)	17	52
10	H	134/145 (92%)	129 (96%)	5 (4%)	41	79
11	I	58/130 (45%)	55 (95%)	3 (5%)	29	68
12	J	118/121 (98%)	111 (94%)	7 (6%)	24	63
13	K	106/106 (100%)	103 (97%)	3 (3%)	51	84
14	L	113/127 (89%)	106 (94%)	7 (6%)	23	60
15	M	158/159 (99%)	151 (96%)	7 (4%)	35	74
16	N	149/150 (99%)	142 (95%)	7 (5%)	32	72
17	O	93/94 (99%)	90 (97%)	3 (3%)	46	82
18	P	113/117 (97%)	106 (94%)	7 (6%)	23	60
19	Q	79/80 (99%)	76 (96%)	3 (4%)	40	78
20	R	117/122 (96%)	114 (97%)	3 (3%)	54	85
21	S	71/74 (96%)	70 (99%)	1 (1%)	74	93
22	T	105/106 (99%)	99 (94%)	6 (6%)	25	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	39	77
25	W	130/130 (100%)	125 (96%)	5 (4%)	40	78
26	X	66/74 (89%)	60 (91%)	6 (9%)	12	41
27	Y	120/196 (61%)	114 (95%)	6 (5%)	30	70
28	Z	60/68 (88%)	59 (98%)	1 (2%)	68	91
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	40 (95%)	2 (5%)	31	71
31	3	79/79 (100%)	76 (96%)	3 (4%)	40	78
All	All	3095/3619 (86%)	2953 (95%)	142 (5%)	33	73

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	52	GLN
14	L	140	VAL
27	Y	189	ASN
12	J	79	PHE
13	K	49	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	137	ASN
19	Q	16	ASN
29	1	28	HIS
15	M	190	ASN
16	N	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	243 (8%)	28 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	259 (9%)	29 (1%)

5 of 259 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 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1246	A
1	0	1450	C
1	0	2761	A
1	0	1352	A
1	0	1563	G

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

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	12,22,23	1.04	1 (8%)	19,31,34	3.16	2 (10%)
1	OMG	0	2588	1	17,26,27	1.02	1 (5%)	21,38,41	2.54	3 (14%)
1	UR3	0	2619	1	12,22,23	0.79	0	16,32,35	0.76	0
1	PSU	0	2621	1	13,21,22	1.56	2 (15%)	18,30,33	6.15	3 (16%)
1	1MA	0	628	1	14,25,26	0.96	1 (7%)	15,37,40	1.14	1 (6%)

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	-	0/5/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.60	1.48	1.52
1	0	2621	PSU	C4-N3	2.49	1.37	1.33
1	0	628	1MA	C6-N6	2.59	1.33	1.29
1	0	2587	OMU	C4-N3	2.68	1.38	1.33
1	0	2588	OMG	C6-N1	3.18	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.43	114.66	128.33
1	0	2588	OMG	C5-C6-N1	-8.73	111.66	123.59
1	0	628	1MA	C2-N3-C4	-3.68	110.70	116.40
1	0	2587	OMU	C5-C4-N3	-3.34	114.55	123.12
1	0	2588	OMG	N3-C2-N1	-2.34	123.89	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0
1	0	2621	PSU	1	0
1	0	628	1MA	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 232 ligands modelled in this entry, 231 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	$\# Z  > 2$
32	CLY	0	9000	-	26,28,28	1.90	7 (26%)	30,40,40	1.33	4 (13%)

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
32	CLY	0	9000	-	-	0/19/53/53	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	CLY	C3-C2	2.25	1.58	1.52
32	0	9000	CLY	C6-S1	2.32	1.84	1.79
32	0	9000	CLY	C10-N1	2.70	1.40	1.34
32	0	9000	CLY	C5-S1	3.07	1.86	1.81
32	0	9000	CLY	O5-C4	3.33	1.49	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	CLY	C11-C10-N1	-3.86	107.96	116.64
32	0	9000	CLY	C12-C13-C16	-2.32	111.86	114.72
32	0	9000	CLY	O8-C10-N1	2.61	128.03	122.93
32	0	9000	CLY	C7-C8-CL1	2.91	113.90	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	CLY	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.21	25 (0%) 85 64	23, 50, 94, 155	0
2	9	122/122 (100%)	-0.08	2 (1%) 74 47	37, 69, 94, 157	0
3	A	237/240 (98%)	-0.17	4 (1%) 73 45	31, 58, 94, 112	0
4	B	337/338 (99%)	-0.33	0 100 100	30, 59, 85, 94	0
5	C	246/246 (100%)	-0.40	0 100 100	26, 48, 72, 82	0
6	D	140/177 (79%)	1.30	42 (30%) 1 0	63, 104, 125, 135	0
7	E	172/178 (96%)	0.27	1 (0%) 90 73	50, 72, 95, 99	0
8	F	119/120 (99%)	0.18	1 (0%) 87 67	51, 75, 98, 116	0
9	G	29/348 (8%)	1.47	8 (27%) 1 0	77, 93, 105, 107	0
10	H	160/177 (90%)	-0.12	1 (0%) 90 73	43, 63, 96, 110	0
11	I	70/162 (43%)	2.23	31 (44%) 0 0	109, 125, 143, 145	0
12	J	142/145 (97%)	-0.25	0 100 100	38, 54, 76, 92	0
13	K	132/132 (100%)	-0.29	0 100 100	37, 56, 77, 87	0
14	L	145/165 (87%)	0.23	4 (2%) 56 27	28, 70, 109, 122	0
15	M	194/195 (99%)	-0.49	0 100 100	33, 47, 63, 70	0
16	N	186/187 (99%)	-0.13	2 (1%) 82 58	45, 69, 114, 121	0
17	O	115/116 (99%)	-0.38	0 100 100	43, 58, 74, 78	0
18	P	143/149 (95%)	-0.08	1 (0%) 89 70	41, 60, 75, 81	0
19	Q	95/96 (98%)	-0.47	0 100 100	36, 49, 65, 81	0
20	R	150/155 (96%)	-0.40	0 100 100	32, 47, 67, 79	0
21	S	81/85 (95%)	-0.37	0 100 100	45, 64, 82, 88	0
22	T	119/120 (99%)	-0.15	2 (1%) 73 45	40, 59, 86, 102	0
23	U	53/66 (80%)	0.22	0 100 100	49, 62, 78, 88	0
24	V	65/71 (91%)	1.27	13 (20%) 1 1	59, 78, 115, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.48	0 100 100	32, 49, 68, 82	0
26	X	82/92 (89%)	0.04	3 (3%) 45 19	48, 62, 86, 100	0
27	Y	142/241 (58%)	-0.25	0 100 100	31, 48, 69, 90	0
28	Z	73/83 (87%)	0.72	11 (15%) 3 1	72, 83, 98, 107	0
29	1	56/57 (98%)	-0.53	0 100 100	28, 35, 41, 49	0
30	2	46/50 (92%)	-0.14	1 (2%) 65 35	35, 66, 94, 108	0
31	3	92/92 (100%)	0.51	6 (6%) 22 8	53, 72, 82, 90	0
All	All	6646/7481 (88%)	-0.11	158 (2%) 62 32	23, 56, 102, 157	0

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	8.2
2	9	1	U	5.6
28	Z	11	SER	5.5
6	D	18	ILE	5.2
11	I	108	HIS	5.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.99	0.15	-	29,32,34,35	0
1	OMU	0	2587	21/22	0.98	0.17	-	37,39,41,44	0
1	OMG	0	2588	24/25	0.98	0.15	-	37,40,41,44	0
1	UR3	0	2619	21/22	0.98	0.15	-	39,43,46,50	0
1	PSU	0	2621	20/21	0.99	0.14	-	28,31,37,37	0

## 6.3 Carbohydrates [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
35	NA	0	8525	1/1	0.94	0.34	29.22	54,54,54,54	0
34	K	0	8401	1/1	0.96	0.62	26.19	99,99,99,99	0
35	NA	0	8562	1/1	0.89	0.44	25.50	66,66,66,66	0
35	NA	0	8574	1/1	0.98	0.60	24.54	62,62,62,62	0
35	NA	0	8573	1/1	0.94	0.47	24.13	61,61,61,61	0
35	NA	0	8556	1/1	0.95	0.61	23.22	49,49,49,49	0
35	NA	0	8559	1/1	0.94	0.56	21.58	61,61,61,61	0
35	NA	0	8577	1/1	0.59	0.50	19.54	65,65,65,65	0
35	NA	0	8578	1/1	0.96	0.53	18.79	52,52,52,52	0
35	NA	0	8572	1/1	0.70	0.56	17.55	66,66,66,66	0
35	NA	0	8555	1/1	0.87	0.65	16.43	81,81,81,81	0
35	NA	0	8571	1/1	0.77	0.30	15.19	52,52,52,52	0
36	CL	0	8815	1/1	0.90	0.31	13.14	92,92,92,92	0
35	NA	0	8532	1/1	0.96	0.30	13.09	53,53,53,53	0
35	NA	L	8580	1/1	0.87	0.55	13.00	63,63,63,63	0
35	NA	0	8579	1/1	0.96	0.31	11.90	39,39,39,39	0
35	NA	0	8531	1/1	0.93	0.30	11.72	77,77,77,77	0
35	NA	R	8586	1/1	0.74	0.42	9.58	63,63,63,63	0
35	NA	9	8583	1/1	0.92	0.34	9.16	70,70,70,70	0
35	NA	B	8561	1/1	0.91	0.29	8.95	70,70,70,70	0
35	NA	0	8526	1/1	0.69	0.73	8.47	57,57,57,57	0
34	K	0	8402	1/1	0.96	0.24	7.50	73,73,73,73	0
35	NA	0	8576	1/1	0.93	0.31	6.80	48,48,48,48	0
35	NA	0	8582	1/1	0.88	0.26	6.54	66,66,66,66	0
35	NA	0	8566	1/1	0.91	0.32	5.17	48,48,48,48	0
35	NA	0	8510	1/1	0.89	0.25	4.65	41,41,41,41	0
35	NA	0	8505	1/1	0.97	0.19	4.63	35,35,35,35	0
35	NA	0	8564	1/1	0.93	0.20	4.24	48,48,48,48	0
35	NA	0	8508	1/1	0.84	0.18	4.12	59,59,59,59	0
33	MG	0	8053	1/1	0.90	0.20	4.08	37,37,37,37	0
36	CL	B	8819	1/1	0.97	0.21	3.92	62,62,62,62	0
35	NA	0	8503	1/1	0.94	0.20	3.57	68,68,68,68	0
35	NA	0	8550	1/1	0.98	0.17	2.66	52,52,52,52	0
35	NA	0	8553	1/1	0.98	0.19	2.56	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	CLY	0	9000	27/27	0.86	0.26	2.43	50,56,61,61	0
35	NA	0	8565	1/1	0.94	0.31	2.18	50,50,50,50	0
35	NA	0	8502	1/1	0.95	0.16	1.93	45,45,45,45	0
35	NA	0	8569	1/1	0.79	0.27	1.77	86,86,86,86	0
36	CL	O	8808	1/1	0.96	0.31	1.70	90,90,90,90	0
33	MG	0	8013	1/1	0.98	0.18	1.65	45,45,45,45	0
35	NA	R	8537	1/1	0.95	0.20	1.55	50,50,50,50	0
35	NA	0	8521	1/1	0.99	0.17	1.47	53,53,53,53	0
35	NA	0	8523	1/1	0.94	0.19	1.40	42,42,42,42	0
35	NA	0	8567	1/1	0.96	0.15	1.04	54,54,54,54	0
33	MG	Y	8108	1/1	0.97	0.19	1.00	40,40,40,40	0
35	NA	Q	8548	1/1	0.94	0.21	0.63	49,49,49,49	0
35	NA	0	8535	1/1	0.96	0.16	0.04	42,42,42,42	0
35	NA	0	8527	1/1	0.96	0.15	-0.20	41,41,41,41	0
35	NA	0	8524	1/1	0.95	0.18	-0.27	44,44,44,44	0
36	CL	0	8812	1/1	0.98	0.16	-0.28	51,51,51,51	0
35	NA	T	8543	1/1	0.97	0.14	-0.57	31,31,31,31	0
35	NA	H	8509	1/1	0.98	0.15	-0.58	40,40,40,40	0
33	MG	0	8064	1/1	0.96	0.14	-0.59	33,33,33,33	0
36	CL	3	8804	1/1	0.94	0.22	-0.62	76,76,76,76	0
36	CL	M	8818	1/1	0.98	0.15	-0.94	50,50,50,50	0
33	MG	0	8018	1/1	0.99	0.14	-0.96	55,55,55,55	0
33	MG	0	8057	1/1	0.98	0.16	-0.98	50,50,50,50	0
36	CL	0	8805	1/1	0.98	0.13	-1.13	61,61,61,61	0
35	NA	C	8504	1/1	0.93	0.13	-1.22	29,29,29,29	0
35	NA	0	8517	1/1	0.97	0.14	-1.23	48,48,48,48	0
33	MG	0	8066	1/1	0.98	0.10	-1.25	87,87,87,87	0
35	NA	0	8544	1/1	0.97	0.15	-1.26	24,24,24,24	0
33	MG	0	8111	1/1	0.96	0.13	-1.31	38,38,38,38	0
36	CL	J	8821	1/1	0.95	0.14	-1.56	61,61,61,61	0
35	NA	M	8547	1/1	0.98	0.14	-1.64	33,33,33,33	0
36	CL	0	8813	1/1	0.99	0.12	-1.65	54,54,54,54	0
33	MG	0	8065	1/1	0.98	0.13	-1.85	41,41,41,41	0
33	MG	T	8073	1/1	0.78	0.15	-2.05	59,59,59,59	0
35	NA	J	8546	1/1	0.88	0.13	-2.18	52,52,52,52	0
33	MG	0	8107	1/1	0.95	0.12	-2.21	80,80,80,80	0
37	CD	Z	8703	1/1	0.99	0.04	-2.21	97,97,97,97	0
35	NA	0	8533	1/1	0.85	0.10	-2.24	44,44,44,44	0
33	MG	0	8060	1/1	0.97	0.13	-2.37	50,50,50,50	0
37	CD	1	8702	1/1	0.99	0.08	-2.45	64,64,64,64	0
33	MG	B	8055	1/1	0.95	0.10	-2.56	45,45,45,45	0
37	CD	U	8701	1/1	0.99	0.07	-2.57	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8062	1/1	0.99	0.11	-2.58	62,62,62,62	0
33	MG	0	8056	1/1	0.99	0.10	-2.65	55,55,55,55	0
33	MG	0	8067	1/1	0.99	0.13	-2.74	60,60,60,60	0
33	MG	0	8101	1/1	0.96	0.12	-2.89	56,56,56,56	0
37	CD	3	8704	1/1	0.99	0.03	-3.02	88,88,88,88	0
35	NA	0	8538	1/1	0.94	0.06	-3.22	54,54,54,54	0
33	MG	0	8044	1/1	0.95	0.09	-3.52	35,35,35,35	0
33	MG	0	8058	1/1	0.98	0.09	-3.65	40,40,40,40	0
33	MG	0	8038	1/1	0.99	0.11	-3.65	31,31,31,31	0
33	MG	0	8004	1/1	0.96	0.07	-3.65	43,43,43,43	0
35	NA	A	8545	1/1	0.99	0.11	-3.91	41,41,41,41	0
33	MG	0	8017	1/1	0.98	0.03	-3.98	26,26,26,26	0
33	MG	0	8003	1/1	0.99	0.14	-4.25	33,33,33,33	0
33	MG	0	8012	1/1	0.99	0.09	-4.30	43,43,43,43	0
35	NA	0	8539	1/1	0.96	0.11	-4.58	21,21,21,21	0
33	MG	0	8091	1/1	0.96	0.09	-4.65	53,53,53,53	0
33	MG	0	8019	1/1	0.99	0.07	-4.82	27,27,27,27	0
33	MG	0	8015	1/1	0.97	0.05	-5.14	43,43,43,43	0
33	MG	0	8035	1/1	0.97	0.07	-5.32	48,48,48,48	0
33	MG	0	8077	1/1	0.97	0.07	-5.42	39,39,39,39	0
33	MG	0	8010	1/1	0.99	0.08	-5.77	41,41,41,41	0
33	MG	0	8014	1/1	0.99	0.03	-5.92	36,36,36,36	0
33	MG	0	8033	1/1	0.98	0.06	-5.96	34,34,34,34	0
33	MG	0	8032	1/1	0.98	0.07	-5.97	41,41,41,41	0
33	MG	0	8109	1/1	0.99	0.07	-6.11	30,30,30,30	0
33	MG	0	8054	1/1	0.98	0.09	-6.31	43,43,43,43	0
33	MG	3	8078	1/1	0.98	0.07	-6.36	55,55,55,55	0
33	MG	0	8006	1/1	0.98	0.04	-6.43	37,37,37,37	0
33	MG	0	8071	1/1	0.96	0.08	-6.93	80,80,80,80	0
33	MG	0	8074	1/1	0.98	0.04	-6.96	29,29,29,29	0
33	MG	0	8008	1/1	0.98	0.06	-7.10	41,41,41,41	0
33	MG	0	8007	1/1	0.98	0.08	-7.80	34,34,34,34	0
33	MG	0	8052	1/1	0.93	0.06	-8.09	51,51,51,51	0
33	MG	0	8002	1/1	0.98	0.05	-8.67	41,41,41,41	0
33	MG	0	8020	1/1	0.99	0.06	-9.13	31,31,31,31	0
33	MG	0	8080	1/1	0.99	0.05	-9.31	50,50,50,50	0
33	MG	0	8088	1/1	0.98	0.06	-9.72	36,36,36,36	0
33	MG	0	8084	1/1	0.99	0.04	-10.95	55,55,55,55	0
35	NA	0	8520	1/1	0.99	0.10	-13.08	29,29,29,29	0
33	MG	0	8001	1/1	0.99	0.06	-15.98	35,35,35,35	0
33	MG	0	8110	1/1	0.98	0.09	-	47,47,47,47	0
35	NA	0	8554	1/1	0.92	0.30	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8581	1/1	0.93	0.55	-	70,70,70,70	0
36	CL	0	8817	1/1	0.95	0.32	-	68,68,68,68	0
33	MG	0	8072	1/1	0.99	0.07	-	46,46,46,46	0
33	MG	0	8022	1/1	0.99	0.08	-	48,48,48,48	0
33	MG	0	8102	1/1	0.97	0.28	-	77,77,77,77	0
33	MG	0	8099	1/1	0.98	0.14	-	64,64,64,64	0
33	MG	0	8106	1/1	0.99	0.03	-	34,34,34,34	0
33	MG	0	8114	1/1	0.96	0.14	-	52,52,52,52	0
33	MG	0	8048	1/1	0.98	0.16	-	60,60,60,60	0
35	NA	0	8568	1/1	0.88	0.34	-	84,84,84,84	0
33	MG	0	8027	1/1	0.98	0.11	-	48,48,48,48	0
36	CL	A	8809	1/1	0.89	0.30	-	84,84,84,84	0
36	CL	L	8810	1/1	0.88	0.21	-	74,74,74,74	0
33	MG	0	8100	1/1	0.98	0.16	-	80,80,80,80	0
33	MG	K	8069	1/1	0.98	0.10	-	59,59,59,59	0
33	MG	0	8083	1/1	0.98	0.09	-	45,45,45,45	0
33	MG	0	8063	1/1	0.99	0.08	-	70,70,70,70	0
33	MG	9	8095	1/1	0.96	0.08	-	54,54,54,54	0
35	NA	0	8513	1/1	0.91	0.14	-	52,52,52,52	0
33	MG	0	8047	1/1	0.99	0.09	-	74,74,74,74	0
33	MG	0	8115	1/1	0.94	0.08	-	58,58,58,58	0
33	MG	0	8043	1/1	0.98	0.20	-	43,43,43,43	0
33	MG	0	8021	1/1	0.99	0.10	-	28,28,28,28	0
33	MG	0	8011	1/1	0.93	0.28	-	8,8,8,8	0
33	MG	0	8089	1/1	0.96	0.09	-	58,58,58,58	0
33	MG	0	8081	1/1	0.96	0.13	-	56,56,56,56	0
33	MG	0	8042	1/1	0.92	0.07	-	36,36,36,36	0
33	MG	0	8096	1/1	0.86	0.09	-	47,47,47,47	0
35	NA	0	8522	1/1	0.82	0.29	-	61,61,61,61	0
33	MG	0	8045	1/1	0.96	0.12	-	54,54,54,54	0
33	MG	0	8061	1/1	0.96	0.07	-	40,40,40,40	0
33	MG	0	8093	1/1	0.94	0.07	-	45,45,45,45	0
33	MG	0	8050	1/1	0.95	0.13	-	107,107,107,107	0
35	NA	0	8530	1/1	0.97	0.41	-	41,41,41,41	0
33	MG	0	8105	1/1	0.96	0.27	-	64,64,64,64	0
36	CL	0	8803	1/1	0.94	0.23	-	75,75,75,75	0
35	NA	0	8542	1/1	0.98	0.18	-	39,39,39,39	0
35	NA	0	8536	1/1	0.94	0.09	-	61,61,61,61	0
35	NA	0	8552	1/1	0.85	0.19	-	49,49,49,49	0
33	MG	0	8051	1/1	0.95	0.11	-	67,67,67,67	0
33	MG	0	8116	1/1	0.99	0.10	-	23,23,23,23	0
33	MG	0	8023	1/1	0.98	0.07	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8560	1/1	0.95	0.55	-	63,63,63,63	0
33	MG	0	8076	1/1	0.91	0.13	-	79,79,79,79	0
35	NA	0	8541	1/1	0.95	0.19	-	50,50,50,50	0
33	MG	0	8112	1/1	0.97	0.08	-	50,50,50,50	0
35	NA	0	8549	1/1	0.97	0.17	-	50,50,50,50	0
35	NA	9	8551	1/1	0.95	0.11	-	46,46,46,46	0
35	NA	0	8540	1/1	0.85	0.50	-	49,49,49,49	0
33	MG	0	8113	1/1	0.92	0.26	-	69,69,69,69	0
36	CL	0	8814	1/1	0.97	0.13	-	64,64,64,64	0
35	NA	0	8558	1/1	0.93	0.57	-	70,70,70,70	0
33	MG	0	8009	1/1	0.99	0.06	-	38,38,38,38	0
33	MG	0	8059	1/1	0.93	0.08	-	44,44,44,44	0
35	NA	S	8512	1/1	0.88	0.17	-	32,32,32,32	0
35	NA	0	8575	1/1	0.94	0.16	-	67,67,67,67	0
33	MG	0	8068	1/1	0.97	0.11	-	68,68,68,68	0
35	NA	0	8514	1/1	0.98	0.14	-	28,28,28,28	0
36	CL	R	8806	1/1	0.93	0.14	-	46,46,46,46	0
33	MG	0	8036	1/1	0.97	0.06	-	42,42,42,42	0
33	MG	0	8098	1/1	0.98	0.17	-	45,45,45,45	0
33	MG	0	8031	1/1	0.99	0.07	-	28,28,28,28	0
33	MG	0	8085	1/1	0.98	0.09	-	67,67,67,67	0
33	MG	0	8040	1/1	0.94	0.11	-	72,72,72,72	0
37	CD	O	8705	1/1	0.97	0.07	-	87,87,87,87	0
36	CL	Y	8820	1/1	0.95	0.14	-	42,42,42,42	0
35	NA	0	8534	1/1	0.95	0.15	-	49,49,49,49	0
35	NA	0	8563	1/1	0.84	0.29	-	46,46,46,46	0
33	MG	0	8087	1/1	0.94	0.10	-	51,51,51,51	0
35	NA	0	8570	1/1	0.98	0.21	-	55,55,55,55	0
33	MG	0	8082	1/1	0.87	0.16	-	70,70,70,70	0
36	CL	J	8801	1/1	0.94	0.15	-	80,80,80,80	0
33	MG	0	8029	1/1	0.98	0.11	-	38,38,38,38	0
33	MG	0	8049	1/1	0.81	0.41	-	79,79,79,79	0
35	NA	0	8511	1/1	0.90	0.30	-	58,58,58,58	0
33	MG	0	8037	1/1	0.99	0.07	-	46,46,46,46	0
33	MG	0	8034	1/1	0.97	0.11	-	36,36,36,36	0
33	MG	0	8075	1/1	0.94	0.12	-	73,73,73,73	0
33	MG	0	8070	1/1	0.95	0.10	-	52,52,52,52	0
35	NA	0	8528	1/1	0.89	0.33	-	56,56,56,56	0
35	NA	0	8515	1/1	0.96	0.48	-	46,46,46,46	0
33	MG	0	8005	1/1	0.99	0.07	-	35,35,35,35	0
36	CL	0	8816	1/1	0.89	0.25	-	74,74,74,74	0
33	MG	0	8104	1/1	0.92	0.20	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8519	1/1	0.98	0.07	-	33,33,33,33	0
33	MG	0	8086	1/1	1.00	0.09	-	46,46,46,46	0
33	MG	0	8041	1/1	0.90	0.24	-	56,56,56,56	0
36	CL	N	8807	1/1	0.95	0.18	-	58,58,58,58	0
36	CL	0	8811	1/1	0.95	0.14	-	63,63,63,63	0
36	CL	J	8802	1/1	0.82	0.17	-	83,83,83,83	0
33	MG	0	8097	1/1	0.94	0.09	-	39,39,39,39	0
33	MG	0	8079	1/1	0.96	0.05	-	33,33,33,33	0
33	MG	0	8090	1/1	0.91	0.24	-	74,74,74,74	0
35	NA	0	8585	1/1	0.87	0.42	-	52,52,52,52	0
33	MG	0	8016	1/1	0.99	0.12	-	33,33,33,33	0
35	NA	0	8501	1/1	0.95	0.29	-	31,31,31,31	0
35	NA	0	8507	1/1	0.91	0.41	-	65,65,65,65	0
35	NA	0	8516	1/1	0.97	0.18	-	39,39,39,39	0
33	MG	0	8046	1/1	0.86	0.13	-	43,43,43,43	0
33	MG	0	8103	1/1	0.95	0.14	-	68,68,68,68	0
35	NA	0	8518	1/1	0.90	0.12	-	28,28,28,28	0
33	MG	0	8039	1/1	0.99	0.07	-	49,49,49,49	0
35	NA	0	8506	1/1	0.87	0.58	-	40,40,40,40	0
33	MG	0	8092	1/1	0.90	0.28	-	89,89,89,89	0
33	MG	0	8030	1/1	0.98	0.08	-	31,31,31,31	0
33	MG	0	8024	1/1	0.95	0.12	-	33,33,33,33	0
36	CL	0	8822	1/1	0.97	0.21	-	92,92,92,92	0
35	NA	0	8529	1/1	0.46	0.53	-	79,79,79,79	0
35	NA	0	8584	1/1	0.71	0.43	-	63,63,63,63	0
33	MG	0	8028	1/1	0.95	0.12	-	44,44,44,44	0
33	MG	0	8026	1/1	0.97	0.12	-	27,27,27,27	0
33	MG	0	8094	1/1	0.95	0.14	-	66,66,66,66	0
35	NA	0	8557	1/1	0.96	0.14	-	45,45,45,45	0
33	MG	0	8025	1/1	0.97	0.05	-	45,45,45,45	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.