



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2017 – 04:39 PM EDT

PDB ID : 2OTL
Title : Girodazole bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : unknown
Resolution : 2.70 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

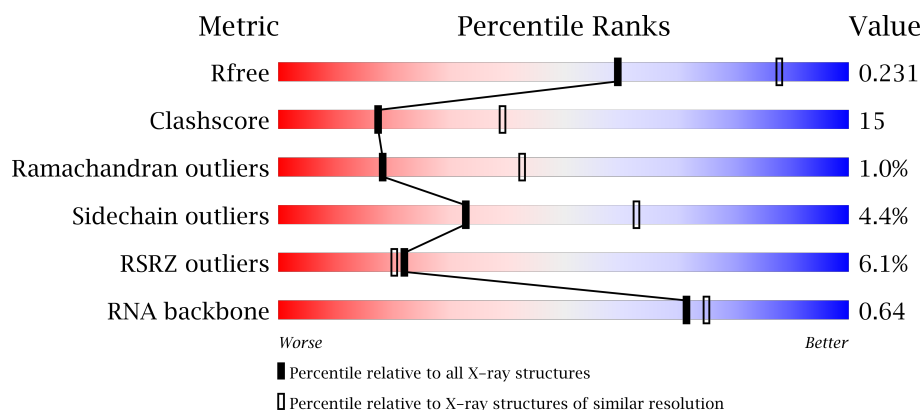
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)
RNA backbone	2435	1011 (3.06-2.34)

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	0	2922	
2	9	122	
3	A	239	
4	B	337	

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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	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	162	

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
33	MG	0	8060	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8503	-	-	-	X
35	NA	0	8514	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8529	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	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	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8537	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8705	-	-	-	X
36	CL	0	8713	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CL	0	8715	-	-	-	X
36	CL	J	8701	-	-	X	-
36	CL	M	8718	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99016 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
			59021	26350	10878	19048	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779
0	628	1MA	A	MODIFIED RESIDUE	GB 3377779
0	2587	OMU	U	MODIFIED RESIDUE	GB 3377779
0	2588	OMG	G	MODIFIED RESIDUE	GB 3377779
0	2619	UR3	U	MODIFIED RESIDUE	GB 3377779
0	2621	PSU	U	MODIFIED RESIDUE	GB 3377779

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

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

- Molecule 3 is a 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 L4P.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	CONFLICT	UNP P12735

- 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 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	CONFLICT	UNP P15825

- 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
			1266	785	237	238	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	-	INSERTION	UNP P60617
H	166	SER	-	INSERTION	UNP P60617
H	167	PRO	-	INSERTION	UNP P60617
H	168	ALA	-	INSERTION	UNP P60617
H	169	GLY	-	INSERTION	UNP P60617
H	170	ASN	-	INSERTION	UNP P60617
H	171	ALA	-	INSERTION	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	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 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	UNP P60618
M	194	ALA	-	INSERTION	UNP P60618

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

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

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

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

- Molecule 20 is a protein called 50S ribosomal protein L23P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

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

- Molecule 23 is a protein called 50S ribosomal protein L29P.

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

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

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

- Molecule 26 is a protein called 50S ribosomal protein L32e.

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

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			579	346	116	112	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	INSERTION	UNP P60619

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

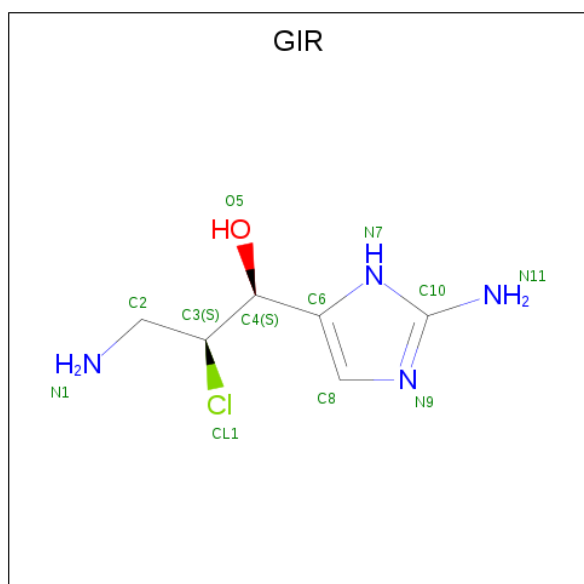
- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a protein called 50S ribosomal protein L11P.

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

- Molecule 32 is GIRODAZOLE (three-letter code: GIR) (formula: C₆H₁₁ClN₄O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	Cl	N	O	0	0
			12	6	1	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
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	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	C	1	Total	Na	0	0
			1	1		

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

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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5893	Total O 5893 5893	0	0
38	9	145	Total O 145 145	0	0
38	A	118	Total O 118 118	0	0
38	B	147	Total O 147 147	0	0
38	C	163	Total O 163 163	0	0
38	D	48	Total O 48 48	0	0
38	E	46	Total O 46 46	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	69	Total O 69 69	0	0
38	J	58	Total O 58 58	0	0
38	K	58	Total O 58 58	0	0
38	L	81	Total O 81 81	0	0
38	M	115	Total O 115 115	0	0
38	N	58	Total O 58 58	0	0

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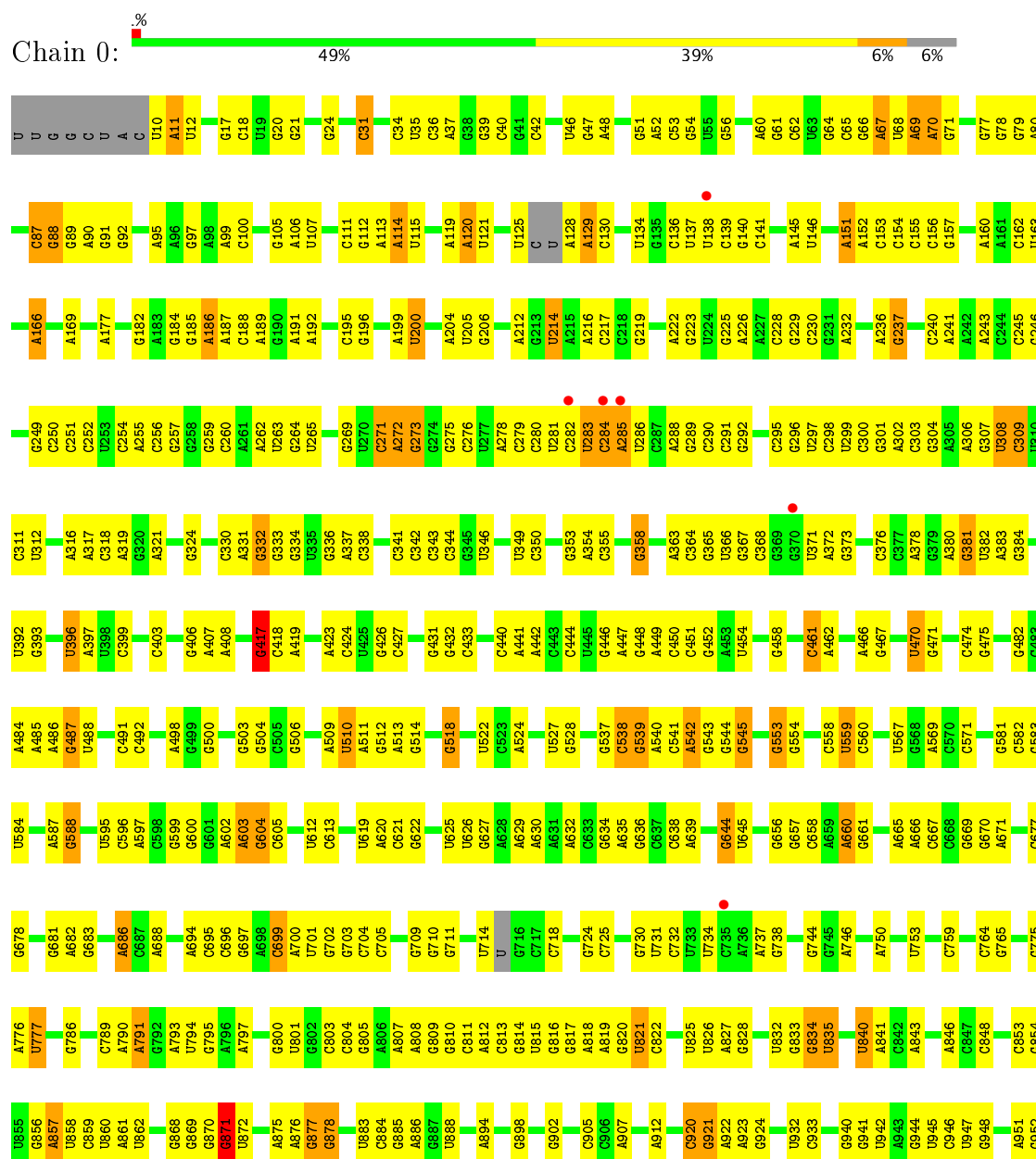
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	61	Total 61	O 61	0	0
38	Q	55	Total 55	O 55	0	0
38	R	81	Total 81	O 81	0	0
38	S	37	Total 37	O 37	0	0
38	T	39	Total 39	O 39	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	70	Total 70	O 70	0	0
38	X	26	Total 26	O 26	0	0
38	Y	99	Total 99	O 99	0	0
38	Z	32	Total 32	O 32	0	0
38	1	56	Total 56	O 56	0	0
38	2	40	Total 40	O 40	0	0
38	3	66	Total 66	O 66	0	0
38	I	4	Total 4	O 4	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 the various outlier classes 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.

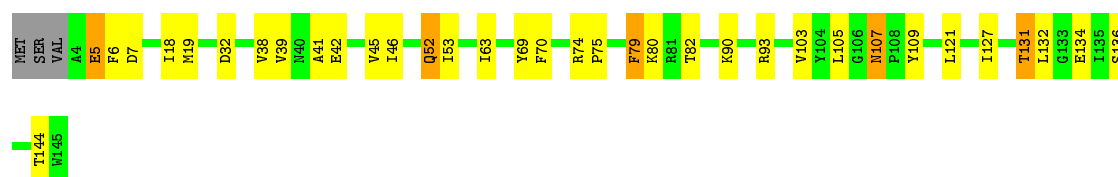
• Molecule 1: 23S ribosomal RNA



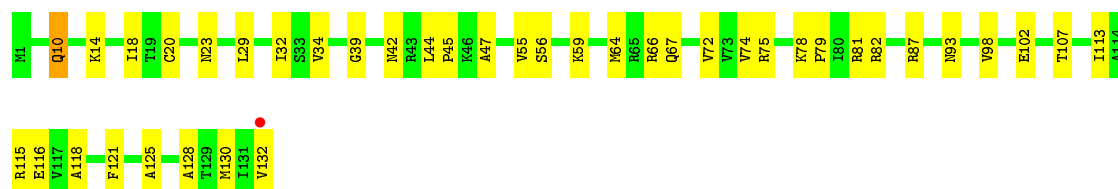
U	A2112	G2001	C1920	U1835	G1752	A1856	U1569	G1497	G1415	G1325	C1229	A1160	C1025	G953
A	G2113	C2002	A1921	A1836	C1753	A1857	A1572	U1500	G1416	A1328	A1230	A1161	G1027	U954
C	U2114	U2003	A1922	A1858	A1759	A1859	A1573	A1501	G1417	U1418	A1231	G1162	U1028	A955
C	U2115	U2004	G1925	A1840	G1765	G1860	C1574	A1502	U1419	A1329	A1232	G1163	U1029	G958
G	U2116	G2005	G1926	A1841	U1766	A1861	U1577	A1503	C1420	A1330	A1233	G1164	A1032	C959
C	C2119	U2008	A1927	A1842	G1767	C1862	U1578	A1504	C1421	A1331	U1234	G1165	C1044	G960
G	U2120	C2009	G1928	A1845	A1768	G1863	C1576	U1505	U1422	U1332	U1235	G1166	G1045	A961
C	C2128	A2010	G1929	U1846	C1769	A1864	U1581	U1506	C1423	U1333	A1236	G1167	C1044	C962
U	G2128	A2011	A1930	G1847	U1770	G1865	A1582	C1507	G1424	G1340	U1237	U1170	G1052	G968
A	U2012	U2012	A1931	G1848	U1771	C1866	C1582	U1508	G1425	C1342	C1238	A1171	G1053	G969
G	C2132	G2013	G1936	U1849	G1772	A1867	G1586	C1509	C1426	A1341	G1239	G1172	G1054	U970
C	U2133	U2013	U1937	U1850	G1773	A1868	U1587	G1512	A1427	C1343	A1242	A1173	G1055	G
G	G2134	U2016	U1938	G1851	G1774	A1869	U1588	C1513	U1432	G1344	C1243	A1174	G1056	U
G	A2135	U2028	U1939	A1852	G1774	G1870	G1589	C1514	G1433	U1350	U1244	A1175	U1057	U
C	G2136	C2029	C1940	G1853	G1777	U1871	U1592	A1515	A1434	A1351	A1245	G1176	A1058	U
C	A	G2033	A1941	C1854	A1778	G1872	G1593	C1516	U1435	A1352	A1246	G1177	G1059	C
G	U	U2034	C1855	G1855	A1779	C1873	C1594	U1517	C1436	C1353	A1252	G1178	C1060	C
A	C	A	C1856	C1856	A1780	G1879	C1594	U1517	U1440	U1358	A1253	U1180	U1066	C
C	U	U2039	A1857	G1859	G1781	G1880	C1594	G1520	G1441	A1358	C1253	U1181	A1067	C
C	G	G	G1944	G1944	G1782	G1881	G1594	C1521	A1442	U1359	C1254	C1182	U	U
G	U	A	C1945	C1945	A1783	G1882	A1597	A1522	G1443	G1360	C1262	C1183	C	C
G	C	G	G1946	G1946	U1784	A1884	A1598	G1523	G1444	C1361	U1266	C1184	C	C
G	U	G	G1947	G1947	G1785	A1885	A1603	U1524	G1445	U1362	U1267	U1185	G	G
C	C	C	G1948	G1948	G1786	G1886	A1604	G1525	U1446	U1362	C1267	U1186	A1078	A
C	C	G2046	G1949	G1949	C1787	C1887	G1605	A1526	U1447	C1366	C1268	U1187	A1079	G
A	A	A2054	G1950	U1874	U1788	G1888	A1606	A1527	U1447	U1366	G1269	U1188	A1080	A
C	C	C	G1951	C1951	G1789	C1889	A1607	A1528	U1447	U1366	G1269	U1188	A1081	A
C	A	U	U	U	C1790	C1892	A1607	G1529	U1447	U1366	G1269	U1188	A1081	A
C	U	U2063	U	U	U1791	A1701	A1607	G1529	U1447	U1366	G1269	U1188	A1081	A
C	U	U2064	A	A	U1791	U1702	A1607	G1529	U1447	U1366	G1269	U1188	A1081	A
U	U	U2065	C	C	G1795	U1702	A1607	G1529	U1447	U1366	G1269	U1188	A1081	A
U	U	C2066	U	U	A1796	A1710	A1614	C1533	G1452	G1374	C1273	U1190	A1086	G
G	G	C	C	C	A1797	A1711	A1614	C1533	G1452	G1374	C1273	U1190	A1086	G
A	A	A	U	U	C1798	A1712	C1620	C1536	U1454	C1375	A1278	A1191	A1087	A
U	U	G2071	U	U	C1798	G1713	C1620	C1536	U1454	C1375	A1278	A1191	A1087	A
U	U	G2072	U	U	C1798	G1713	C1620	C1536	U1454	C1375	A1278	A1191	A1087	A
U	U	G2073	U	U	C1798	G1713	C1620	C1536	U1454	C1375	A1278	A1191	A1087	A
A	A	A2074	U	U	C1798	G1713	C1620	C1536	U1454	C1375	A1278	A1191	A1087	A
C	C	C	C	C	C1803	A1804	U1625	U1539	G1460	U1380	U1285	G1195	C1102	C
C	U	A2081	C	C	A1804	A1805	A1626	U1539	G1460	U1380	U1285	G1195	C1102	C
U	U	G2082	C	C	G1806	G1806	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	A2083	U	U	G1809	G1809	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	U	C2088	G1970	U1890	G1810	G1810	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
A	A	A2089	G1971	C1894	A1811	A1811	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
G	G	U1972	U1972	A1895	G1812	G1812	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
U	U	A1973	A1973	G1896	G1812	G1812	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	G2091	G1974	U1897	G1812	G1812	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
G	G	G2092	C1975	C1975	C1818	C1818	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
G	G	A2096	G1976	G1976	G1819	G1819	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
U	U	C	U1977	U1977	G1820	G1820	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
U	U	C	U1978	U1978	A1821	A1821	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
G	A	A2101	G1979	G1979	A1822	A1822	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
A	C	G2102	U1980	U1980	G1823	G1823	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	U	A2103	A1910	A1910	A1741	A1741	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
G	G	C2104	U1992	U1992	A1742	A1742	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	A	C2105	U1993	U1993	G1743	G1743	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2106	U1994	U1994	G1744	G1744	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2107	U1995	U1995	G1745	G1745	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2108	U1996	U1996	G1746	G1746	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2109	U1997	U1997	A1747	A1747	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2110	U1998	U1998	A1748	A1748	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2111	G2000	G2000	A1749	A1749	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2112	G2001	G2001	A1750	A1750	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2113	G2002	G2002	A1751	A1751	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2114	G2003	G2003	A1752	A1752	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
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C	C	C2116	G2005	G2005	A1754	A1754	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2117	G2006	G2006	A1755	A1755	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2118	G2007	G2007	A1756	A1756	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2119	G2008	G2008	A1757	A1757	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2120	G2009	G2009	A1758	A1758	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2121	G2010	G2010	A1759	A1759	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2122	G2011	G2011	A1760	A1760	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2123	G2012	G2012	A1761	A1761	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2124	G2013	G2013	A1762	A1762	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2125	G2014	G2014	A1763	A1763	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2126	G2015	G2015	A1764	A1764	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2127	G2016	G2016	A1765	A1765	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2128	G2017	G2017	A1766	A1766	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2129	G2018	G2018	A1767	A1767	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2130	G2019	G2019	A1768	A1768	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2131	G2020	G2020	A1769	A1769	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2132	G2021	G2021	A1770	A1770	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2133	G2022	G2022	A1771	A1771	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2134	G2023	G2023	A1772	A1772	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2135	G2024	G2024	A1773	A1773	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2136	G2025	G2025	A1774	A1774	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2137	G2026	G2026	A1775	A1775	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2138	G2027	G2027	A1776	A1776	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2139	G2028	G2028	A1777	A1777	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2140	G2029	G2029	A1778	A1778	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2141	G2030	G2030	A1779	A1779	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2142	G2031	G2031	A1780	A1780	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2143	G2032	G2032	A1781	A1781	A1627	U1539	G1460	U1380	U1285	G1195	C1102	C
C	C	C2144	G2033	G2033	A1782	A1782	A							



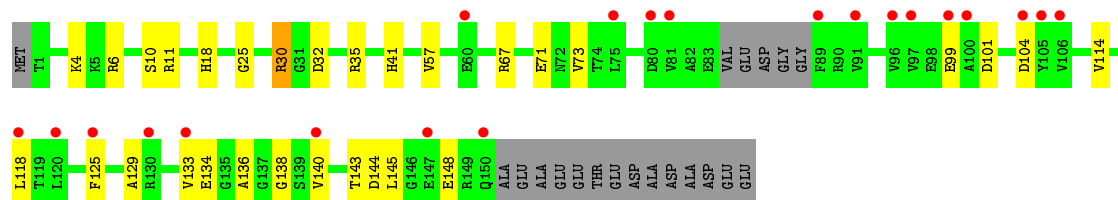
- Chain E:**
-
- | Category | Value (%) |
|----------|-----------|
| MET | - |
| P1 | - |
| R2 | - |
| V3 | - |
| E4 | - |
| L5 | - |
| E6 | - |
| I7 | - |
| P8 | - |
| E9 | - |
| D10 | - |
| V11 | - |
| D12 | - |
| Q15 | - |
| D16 | - |
| I20 | - |
| G24 | - |
| V40 | - |
| S41 | - |
| V42 | - |
| D45 | - |
| T46 | - |
| V47 | - |
| V48 | - |
| I49 | - |
| Q66 | - |
| S67 | - |
| H68 | - |
| I69 | - |
| M72 | - |
| V76 | - |
| H80 | - |
| E81 | - |
| M84 | - |
| E85 | - |
| V86 | - |
| F87 | - |
| F91 | - |
| V97 | - |
| D100 | - |
| E101 | - |
| L108 | - |
| K111 | - |
| A112 | - |
| D112 | - |



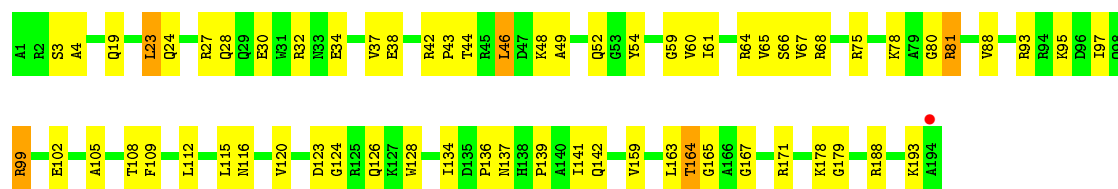
- Molecule 12: 50S ribosomal protein L14P



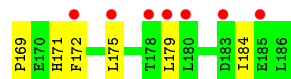
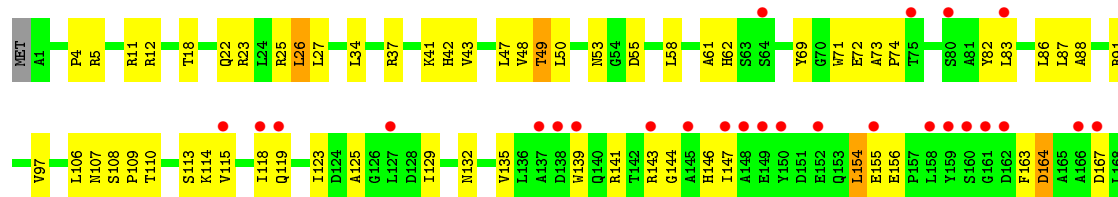
- Molecule 13: 50S ribosomal protein L15P



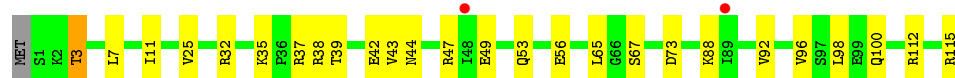
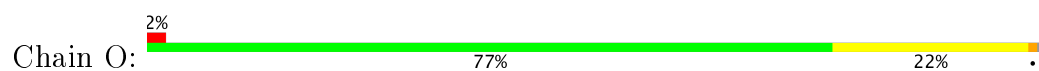
- Molecule 14: 50S ribosomal protein L15e



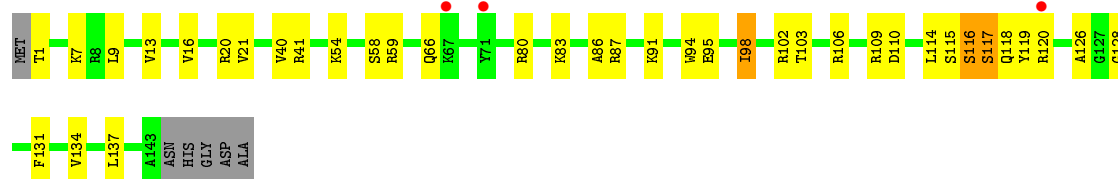
- Molecule 15: 50S ribosomal protein L18P



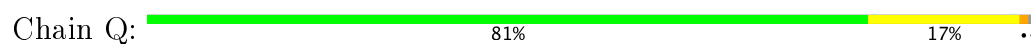
- Molecule 16: 50S ribosomal protein L18e



- Molecule 17: 50S ribosomal protein L19e



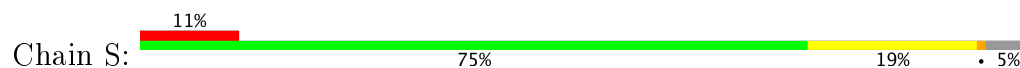
- Molecule 18: 50S ribosomal protein L21e



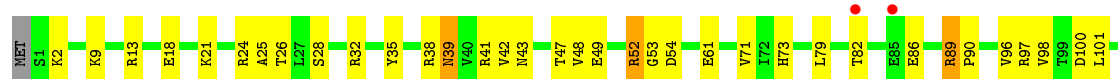
- Molecule 19: 50S ribosomal protein L22P

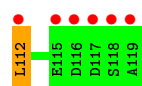


- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

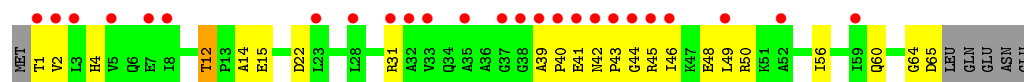




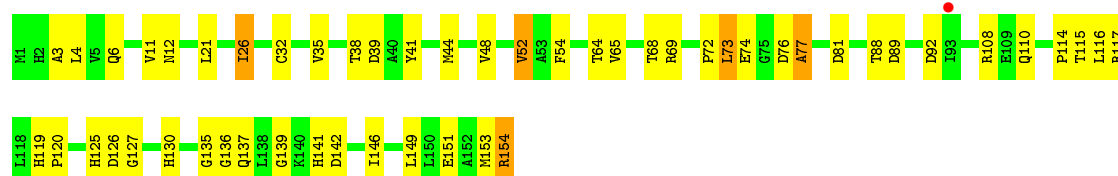
- Molecule 22: 50S ribosomal protein L24e



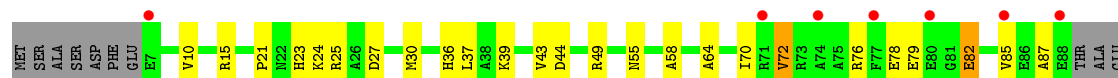
- Molecule 23: 50S ribosomal protein L29P



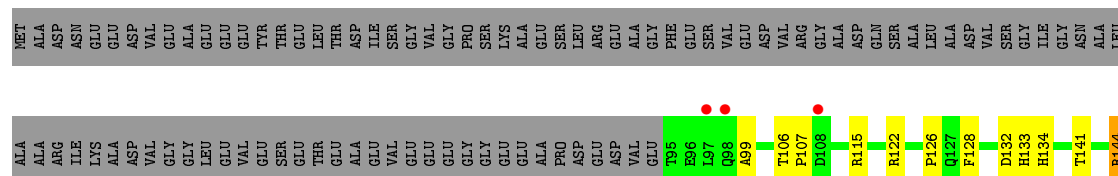
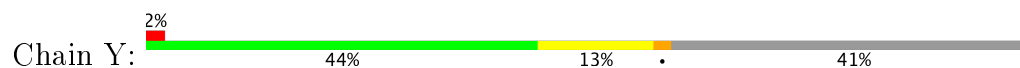
- Molecule 24: 50S ribosomal protein L30P



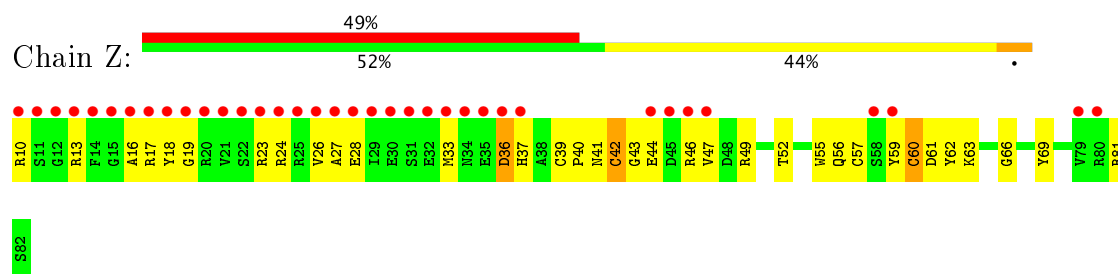
- Molecule 25: 50S ribosomal protein L31e



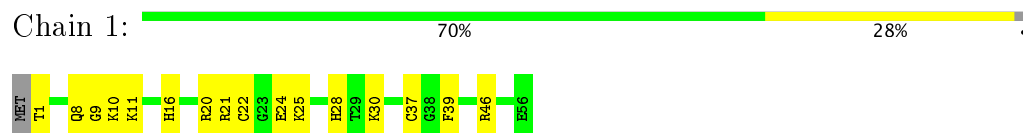
- Molecule 26: 50S ribosomal protein L32e



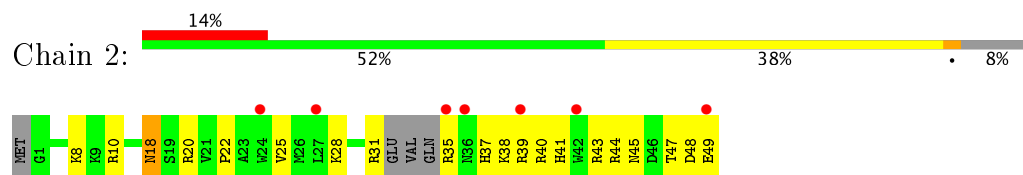
- Molecule 27: 50S ribosomal protein L37Ae



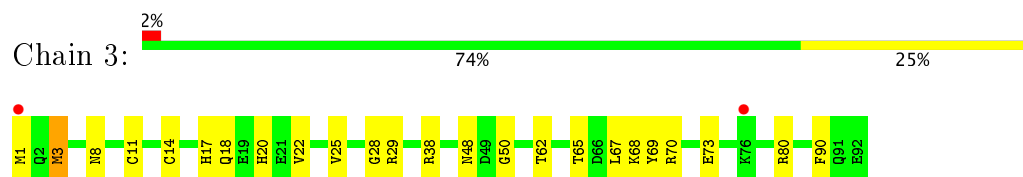
- Molecule 28: 50S ribosomal protein L37e



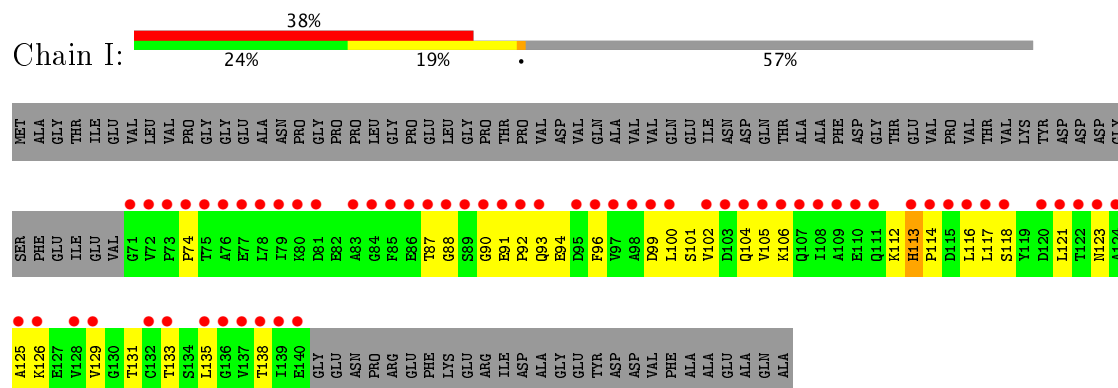
- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 50S ribosomal protein L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.08Å 300.60Å 575.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.70 85.94 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.36-2.70) 90.7 (85.94-2.41)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.248 0.192 , 0.231	Depositor DCC
R_{free} test set	4912 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99016	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.40	0/65959	0.69	14/102870 (0.0%)
2	9	0.34	0/2905	0.68	0/4528
3	A	0.36	0/1786	0.66	0/2408
4	B	0.33	0/2690	0.65	0/3652
5	C	0.39	0/1884	0.69	1/2551 (0.0%)
6	D	0.33	0/1111	0.55	0/1498
7	E	0.33	0/1382	0.57	0/1880
8	F	0.38	0/901	0.58	0/1224
9	G	0.30	0/241	0.47	0/324
10	H	0.35	0/1287	0.66	0/1725
11	J	0.36	0/1136	0.61	0/1530
12	K	0.36	0/1001	0.68	0/1347
13	L	0.38	0/1130	0.67	0/1509
14	M	0.38	0/1584	0.64	0/2119
15	N	0.33	0/1474	0.64	0/1999
16	O	0.35	0/874	0.59	0/1181
17	P	0.36	0/1147	0.55	0/1528
18	Q	0.36	0/749	0.70	0/1005
19	R	0.38	0/1172	0.65	0/1578
20	S	0.34	0/648	0.59	0/875
21	T	0.35	0/958	0.64	1/1289 (0.1%)
22	U	0.37	0/417	0.55	0/562
23	V	0.35	0/502	0.57	0/675
24	W	0.38	0/1219	0.64	0/1655
25	X	0.35	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.54	0/590	0.66	0/787
28	1	0.39	0/437	0.63	0/578
29	2	0.39	0/401	0.54	0/529
30	3	0.39	0/771	0.59	0/1024
31	I	0.33	0/526	0.55	0/716
All	All	0.39	0/98692	0.67	16/147577 (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	52

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1878	G	N9-C1'-C2'	-6.83	104.49	112.00
1	0	1979	G	C2'-C3'-O3'	6.63	124.31	113.70
1	0	1504	A	C1'-O4'-C4'	-6.20	104.94	109.90
1	0	1559	A	C2'-C3'-O3'	5.63	122.71	113.70
1	0	2313	C	C5'-C4'-O4'	5.55	115.76	109.10

There are no chirality outliers.

5 of 52 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	214	U	Sidechain
1	0	332	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	48	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	59021	0	29810	1361	0
2	9	2600	0	1326	97	0
3	A	1753	0	1766	74	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	70	0
6	D	1094	0	1085	45	0
7	E	1357	0	1266	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	890	0	843	36	0
9	G	240	0	231	10	0
10	H	1266	0	1268	41	0
11	J	1120	0	1098	41	0
12	K	992	0	1031	38	0
13	L	1118	0	1076	24	0
14	M	1560	0	1568	55	0
15	N	1445	0	1401	64	0
16	O	865	0	873	21	0
17	P	1136	0	1123	35	0
18	Q	735	0	729	13	0
19	R	1149	0	1122	40	0
20	S	641	0	605	12	0
21	T	950	0	923	38	0
22	U	410	0	364	17	0
23	V	499	0	511	20	0
24	W	1196	0	1137	54	0
25	X	654	0	653	23	0
26	Y	1130	0	1133	37	0
27	Z	579	0	540	46	0
28	1	430	0	426	20	0
29	2	396	0	413	25	0
30	3	755	0	729	27	0
31	I	519	0	500	27	0
32	0	12	0	10	0	0
33	0	107	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	9	0	0	4	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	4	0
36	L	1	0	0	0	0
36	M	1	0	0	2	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	Q	1	0	0	0	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	5893	0	0	185	0
38	1	56	0	0	1	0
38	2	40	0	0	3	0
38	3	66	0	0	5	0
38	9	145	0	0	9	0
38	A	118	0	0	10	0
38	B	147	0	0	15	0
38	C	163	0	0	14	0
38	D	48	0	0	8	0
38	E	46	0	0	4	0
38	F	23	0	0	3	0
38	G	19	0	0	0	0
38	H	69	0	0	6	0
38	I	4	0	0	1	0
38	J	58	0	0	4	0
38	K	58	0	0	4	0
38	L	81	0	0	8	0
38	M	115	0	0	5	0
38	N	58	0	0	5	0
38	O	44	0	0	6	0
38	P	61	0	0	1	0
38	Q	55	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	R	81	0	0	4	0
38	S	37	0	0	0	0
38	T	39	0	0	3	0
38	U	28	0	0	2	0
38	V	11	0	0	3	0
38	W	70	0	0	5	0
38	X	26	0	0	2	0
38	Y	99	0	0	10	0
38	Z	32	0	0	5	0
All	All	99016	0	59909	2306	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 15.

The worst 5 of 2306 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)
10:H:46:GLN:HB3	10:H:167:PRO:HD2	1.29	1.15
1:0:871:G:H8	1:0:871:G:H5'	1.06	1.12
1:0:656:G:H5'	16:O:3:THR:HG22	1.16	1.12
2:9:3056:A:H2'	2:9:3057:A:H5''	1.31	1.10
5:C:236:THR:HG22	5:C:239:ALA:H	1.16	1.09

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	235/239 (98%)	209 (89%)	23 (10%)	3 (1%)	14	35
4	B	335/337 (99%)	305 (91%)	24 (7%)	6 (2%)	10	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	38	66
6	D	134/177 (76%)	107 (80%)	23 (17%)	4 (3%)	5	12
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	20	46
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	143 (92%)	9 (6%)	4 (3%)	6	15
11	J	140/145 (97%)	128 (91%)	11 (8%)	1 (1%)	25	53
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	127 (90%)	14 (10%)	0	100	100
14	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	32	60
15	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	11	28
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	13	33
18	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	17	40
19	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	25	53
20	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	14	35
21	T	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
22	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
23	V	63/71 (89%)	59 (94%)	3 (5%)	1 (2%)	11	28
24	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	14	35
25	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	6	17
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	58 (82%)	9 (13%)	4 (6%)	2	3
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
31	I	68/162 (42%)	65 (96%)	3 (4%)	0	100	100
All	All	3705/4418 (84%)	3435 (93%)	232 (6%)	38 (1%)	18	43

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	137	PRO

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Mol	Chain	Res	Type
6	D	173	GLU
8	F	101	ALA
10	H	166	SER
10	H	168	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	169 (94%)	10 (6%)	25	51
4	B	282/282 (100%)	264 (94%)	18 (6%)	20	45
5	C	193/193 (100%)	177 (92%)	16 (8%)	13	30
6	D	117/148 (79%)	113 (97%)	4 (3%)	42	73
7	E	152/156 (97%)	149 (98%)	3 (2%)	60	86
8	F	93/94 (99%)	92 (99%)	1 (1%)	78	93
9	G	27/283 (10%)	26 (96%)	1 (4%)	39	70
10	H	132/138 (96%)	125 (95%)	7 (5%)	26	54
11	J	118/121 (98%)	110 (93%)	8 (7%)	18	41
12	K	106/106 (100%)	105 (99%)	1 (1%)	82	94
13	L	113/127 (89%)	107 (95%)	6 (5%)	26	54
14	M	158/158 (100%)	150 (95%)	8 (5%)	28	56
15	N	149/150 (99%)	145 (97%)	4 (3%)	50	80
16	O	93/94 (99%)	89 (96%)	4 (4%)	33	64
17	P	113/117 (97%)	108 (96%)	5 (4%)	33	63
18	Q	79/80 (99%)	77 (98%)	2 (2%)	53	82
19	R	117/122 (96%)	112 (96%)	5 (4%)	33	64
20	S	71/74 (96%)	69 (97%)	2 (3%)	49	79
21	T	105/106 (99%)	100 (95%)	5 (5%)	30	59
22	U	44/52 (85%)	43 (98%)	1 (2%)	56	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	51/57 (90%)	49 (96%)	2 (4%)	37	68
24	W	130/130 (100%)	124 (95%)	6 (5%)	31	61
25	X	66/74 (89%)	62 (94%)	4 (6%)	22	47
26	Y	120/196 (61%)	114 (95%)	6 (5%)	28	57
27	Z	60/60 (100%)	58 (97%)	2 (3%)	43	73
28	1	46/47 (98%)	46 (100%)	0	100	100
29	2	42/46 (91%)	40 (95%)	2 (5%)	30	59
30	3	79/79 (100%)	77 (98%)	2 (2%)	53	82
31	I	58/130 (45%)	57 (98%)	1 (2%)	66	88
All	All	3093/3601 (86%)	2957 (96%)	136 (4%)	33	63

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

Mol	Chain	Res	Type
11	J	32	ASP
14	M	46	LEU
26	Y	163	THR
11	J	46	ILE
13	L	30	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	170	ASN
17	P	118	GLN
29	2	41	HIS
15	N	53	ASN
15	N	119	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	235 (8%)	35 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	253 (8%)	36 (1%)

5 of 253 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1667	A
1	0	2791	U
1	0	1450	C
1	0	1685	A

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	14,22,23	0.90	1 (7%)	18,31,34	3.70	2 (11%)
1	OMG	0	2588	1	18,26,27	1.05	2 (11%)	22,38,41	2.45	4 (18%)
1	UR3	0	2619	1	14,22,23	0.67	0	16,32,35	0.74	0
1	PSU	0	2621	1	16,21,22	1.71	3 (18%)	20,30,33	6.11	5 (25%)
1	1MA	0	628	1,35	16,25,26	1.05	1 (6%)	13,37,40	1.14	1 (7%)

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	1,35	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.16	1.47	1.52
1	0	2588	OMG	C8-N7	-2.02	1.30	1.34
1	0	2587	OMU	C4-N3	2.17	1.37	1.33
1	0	2621	PSU	C4-N3	2.63	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.44	114.42	128.40
1	0	2621	PSU	C5-C4-N3	-12.53	115.15	125.43
1	0	2588	OMG	C5-C6-N1	-8.30	111.67	123.48
1	0	628	1MA	C2-N3-C4	-3.63	110.84	116.41
1	0	2587	OMU	C5-C4-N3	-3.56	114.62	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2588	OMG	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 230 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	GIR	0	9000	-	9,12,12	0.76	0	5,16,16	0.71	0

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	GIR	0	9000	-	-	0/4/10/10	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.34	40 (1%) 74 75	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.33	4 (3%) 47 46	38, 64, 91, 149	0
3	A	237/239 (99%)	0.62	28 (11%) 5 4	30, 58, 99, 119	0
4	B	337/337 (100%)	0.15	3 (0%) 84 85	28, 56, 84, 95	0
5	C	246/246 (100%)	0.22	1 (0%) 92 93	25, 49, 74, 80	0
6	D	140/177 (79%)	2.12	62 (44%) 0 0	61, 105, 127, 136	0
7	E	172/178 (96%)	0.45	6 (3%) 44 44	46, 68, 87, 93	0
8	F	119/120 (99%)	0.95	20 (16%) 2 1	53, 78, 99, 117	0
9	G	29/348 (8%)	1.99	11 (37%) 0 0	77, 94, 105, 107	0
10	H	160/171 (93%)	0.41	6 (3%) 41 39	40, 58, 92, 100	0
11	J	142/145 (97%)	-0.02	0 100 100	35, 50, 74, 90	0
12	K	132/132 (100%)	0.09	1 (0%) 86 86	36, 54, 77, 87	0
13	L	145/165 (87%)	0.87	21 (14%) 3 2	29, 71, 118, 130	0
14	M	194/194 (100%)	0.01	1 (0%) 90 92	35, 47, 63, 73	0
15	N	186/187 (99%)	0.97	33 (17%) 2 1	41, 68, 115, 120	0
16	O	115/116 (99%)	0.26	2 (1%) 70 72	41, 57, 75, 80	0
17	P	143/149 (95%)	0.26	3 (2%) 64 65	43, 59, 78, 83	0
18	Q	95/96 (98%)	0.00	0 100 100	37, 48, 62, 78	0
19	R	150/155 (96%)	-0.03	0 100 100	33, 47, 66, 74	0
20	S	81/85 (95%)	0.84	9 (11%) 6 5	47, 67, 87, 94	0
21	T	119/120 (99%)	0.54	8 (6%) 19 16	41, 61, 88, 108	0
22	U	53/66 (80%)	0.41	1 (1%) 67 68	44, 61, 77, 83	0
23	V	65/71 (91%)	1.96	25 (38%) 0 0	60, 84, 118, 121	0
24	W	154/154 (100%)	0.05	1 (0%) 89 90	34, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.42	7 (8%) 11 9	45, 61, 87, 102	0
26	Y	142/241 (58%)	0.17	6 (4%) 37 35	28, 47, 71, 92	0
27	Z	73/73 (100%)	2.91	36 (49%) 0 0	61, 98, 111, 115	0
28	1	56/57 (98%)	-0.00	0 100 100	29, 37, 43, 50	0
29	2	46/50 (92%)	0.61	7 (15%) 2 2	39, 68, 101, 114	0
30	3	92/92 (100%)	0.48	2 (2%) 62 63	40, 62, 75, 83	0
31	I	70/162 (43%)	3.94	61 (87%) 0 0	105, 124, 141, 141	0
All	All	6646/7462 (89%)	0.18	405 (6%) 22 20	24, 55, 105, 153	0

The worst 5 of 405 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	12.9
27	Z	26	VAL	12.8
27	Z	20	ARG	11.1
27	Z	11	SER	9.8
27	Z	34	ASN	9.3

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, 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
1	1MA	0	628	23/24	0.99	0.18	-	28,32,33,35	0
1	OMU	0	2587	21/22	0.98	0.13	-	34,36,37,39	0
1	UR3	0	2619	21/22	0.98	0.16	-	36,39,42,48	0
1	PSU	0	2621	20/21	0.99	0.14	-	28,30,33,34	0
1	OMG	0	2588	24/25	0.98	0.15	-	33,36,38,39	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, 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
35	NA	0	8574	1/1	0.82	0.54	31.81	66,66,66,66	0
35	NA	0	8529	1/1	0.55	0.45	20.44	77,77,77,77	0
35	NA	R	8586	1/1	0.48	0.79	20.05	95,95,95,95	0
35	NA	0	8503	1/1	0.90	0.36	18.55	47,47,47,47	0
35	NA	0	8571	1/1	0.78	0.42	15.79	65,65,65,65	0
35	NA	9	8583	1/1	0.86	0.43	15.38	65,65,65,65	0
35	NA	0	8577	1/1	0.80	0.38	13.98	71,71,71,71	0
35	NA	0	8526	1/1	0.89	0.64	13.85	58,58,58,58	0
35	NA	0	8532	1/1	0.90	0.30	13.35	49,49,49,49	0
35	NA	0	8566	1/1	0.87	0.29	11.53	66,66,66,66	0
35	NA	0	8569	1/1	0.90	0.37	10.70	74,74,74,74	0
36	CL	0	8715	1/1	0.93	0.24	9.67	86,86,86,86	0
35	NA	0	8502	1/1	0.97	0.21	8.71	51,51,51,51	0
35	NA	0	8572	1/1	0.95	0.28	8.43	54,54,54,54	0
35	NA	0	8573	1/1	0.93	0.29	8.41	69,69,69,69	0
35	NA	0	8550	1/1	0.93	0.26	8.16	45,45,45,45	0
35	NA	0	8514	1/1	0.96	0.27	8.07	38,38,38,38	0
35	NA	0	8564	1/1	0.93	0.29	7.64	53,53,53,53	0
35	NA	0	8578	1/1	0.97	0.28	7.06	51,51,51,51	0
35	NA	0	8521	1/1	0.94	0.28	5.98	61,61,61,61	0
35	NA	0	8582	1/1	0.78	0.21	5.33	79,79,79,79	0
35	NA	0	8561	1/1	0.92	0.23	5.12	56,56,56,56	0
35	NA	L	8580	1/1	0.97	0.28	5.12	57,57,57,57	0
35	NA	0	8576	1/1	0.98	0.24	4.85	46,46,46,46	0
35	NA	0	8555	1/1	0.97	0.34	4.50	57,57,57,57	0
33	MG	0	8060	1/1	0.99	0.27	4.33	40,40,40,40	0
36	CL	0	8705	1/1	0.89	0.20	4.23	67,67,67,67	0
35	NA	0	8568	1/1	0.69	0.18	3.24	71,71,71,71	0
35	NA	R	8537	1/1	0.89	0.25	2.82	48,48,48,48	0
35	NA	0	8535	1/1	0.95	0.22	2.55	56,56,56,56	0
35	NA	0	8556	1/1	0.92	0.20	2.46	49,49,49,49	0
35	NA	0	8565	1/1	0.93	0.38	2.24	40,40,40,40	0
35	NA	0	8562	1/1	0.92	0.20	2.12	60,60,60,60	0
33	MG	0	8080	1/1	0.97	0.20	1.92	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8527	1/1	0.92	0.17	1.91	44,44,44,44	0
35	NA	C	8504	1/1	0.83	0.27	1.81	49,49,49,49	0
35	NA	0	8579	1/1	0.97	0.19	1.21	64,64,64,64	0
35	NA	0	8524	1/1	0.95	0.19	1.18	62,62,62,62	0
32	GIR	0	9000	12/12	0.91	0.21	1.17	23,40,50,53	0
34	K	0	8401	1/1	0.96	0.18	1.09	85,85,85,85	0
35	NA	M	8547	1/1	0.94	0.18	1.03	34,34,34,34	0
35	NA	0	8543	1/1	0.96	0.19	0.74	39,39,39,39	0
36	CL	O	8708	1/1	0.91	0.21	0.59	73,73,73,73	0
33	MG	0	8057	1/1	0.97	0.18	0.48	45,45,45,45	0
35	NA	0	8505	1/1	0.95	0.18	0.12	33,33,33,33	0
33	MG	0	8054	1/1	0.97	0.17	-0.57	37,37,37,37	0
35	NA	A	8545	1/1	0.96	0.16	-0.70	62,62,62,62	0
33	MG	0	8010	1/1	1.00	0.17	-0.91	33,33,33,33	0
37	CD	Z	8603	1/1	0.97	0.09	-1.02	98,98,98,98	0
36	CL	M	8718	1/1	0.99	0.13	-1.19	47,47,47,47	0
33	MG	0	8008	1/1	0.97	0.14	-1.24	37,37,37,37	0
35	NA	0	8533	1/1	0.85	0.14	-1.27	39,39,39,39	0
35	NA	0	8531	1/1	0.97	0.15	-1.28	50,50,50,50	0
35	NA	0	8523	1/1	0.95	0.17	-1.30	43,43,43,43	0
33	MG	0	8018	1/1	0.98	0.14	-1.38	50,50,50,50	0
33	MG	0	8076	1/1	0.98	0.12	-1.39	55,55,55,55	0
36	CL	3	8704	1/1	0.93	0.16	-1.43	71,71,71,71	0
35	NA	J	8546	1/1	0.93	0.13	-1.46	53,53,53,53	0
33	MG	0	8017	1/1	0.98	0.13	-1.53	26,26,26,26	0
35	NA	0	8544	1/1	0.97	0.10	-1.55	28,28,28,28	0
37	CD	3	8604	1/1	0.99	0.08	-1.59	68,68,68,68	0
33	MG	0	8053	1/1	0.94	0.16	-1.65	45,45,45,45	0
33	MG	0	8014	1/1	0.96	0.16	-1.68	32,32,32,32	0
33	MG	0	8038	1/1	0.99	0.13	-1.70	34,34,34,34	0
36	CL	0	8716	1/1	0.96	0.10	-1.81	56,56,56,56	0
35	NA	0	8510	1/1	0.92	0.12	-1.95	36,36,36,36	0
37	CD	U	8601	1/1	1.00	0.09	-1.99	62,62,62,62	0
33	MG	0	8012	1/1	0.97	0.10	-2.02	39,39,39,39	0
35	NA	0	8525	1/1	0.96	0.15	-2.05	56,56,56,56	0
36	CL	J	8721	1/1	0.98	0.10	-2.16	58,58,58,58	0
35	NA	0	8539	1/1	0.96	0.15	-2.25	30,30,30,30	0
33	MG	T	8073	1/1	0.85	0.12	-2.32	71,71,71,71	0
35	NA	H	8509	1/1	0.95	0.10	-2.36	39,39,39,39	0
36	CL	0	8712	1/1	0.98	0.08	-2.46	49,49,49,49	0
33	MG	0	8015	1/1	0.97	0.14	-2.50	35,35,35,35	0
34	K	0	8402	1/1	0.99	0.14	-2.50	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	R	8538	1/1	0.85	0.08	-2.58	60,60,60,60	0
35	NA	0	8517	1/1	0.93	0.06	-2.62	51,51,51,51	0
33	MG	0	8112	1/1	0.99	0.12	-2.63	42,42,42,42	0
33	MG	0	8021	1/1	0.98	0.12	-2.63	30,30,30,30	0
33	MG	0	8007	1/1	0.98	0.13	-2.68	22,22,22,22	0
33	MG	0	8058	1/1	0.97	0.06	-2.98	39,39,39,39	0
35	NA	Q	8548	1/1	0.95	0.06	-3.01	42,42,42,42	0
35	NA	0	8520	1/1	0.97	0.14	-3.02	34,34,34,34	0
33	MG	0	8074	1/1	0.98	0.05	-3.04	36,36,36,36	0
33	MG	0	8107	1/1	0.98	0.07	-3.05	36,36,36,36	0
33	MG	0	8004	1/1	0.98	0.09	-3.05	29,29,29,29	0
33	MG	0	8039	1/1	0.94	0.11	-3.06	52,52,52,52	0
33	MG	0	8067	1/1	0.97	0.12	-3.15	52,52,52,52	0
33	MG	0	8013	1/1	0.97	0.12	-3.23	38,38,38,38	0
33	MG	B	8055	1/1	0.94	0.05	-3.30	48,48,48,48	0
33	MG	0	8096	1/1	0.87	0.11	-3.41	52,52,52,52	0
33	MG	Y	8109	1/1	0.99	0.09	-3.42	37,37,37,37	0
33	MG	B	8056	1/1	0.98	0.05	-3.45	55,55,55,55	0
36	CL	0	8713	1/1	0.93	0.08	-3.49	65,65,65,65	0
36	CL	B	8719	1/1	0.98	0.12	-3.65	51,51,51,51	0
37	CD	1	8602	1/1	0.99	0.10	-3.66	63,63,63,63	0
33	MG	0	8001	1/1	0.99	0.14	-3.86	36,36,36,36	0
33	MG	0	8032	1/1	0.97	0.06	-4.41	28,28,28,28	0
33	MG	0	8091	1/1	0.96	0.07	-4.76	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.14	-5.13	33,33,33,33	0
33	MG	3	8078	1/1	0.98	0.05	-5.22	43,43,43,43	0
33	MG	0	8108	1/1	0.99	0.09	-5.55	70,70,70,70	0
33	MG	0	8044	1/1	0.91	0.10	-5.58	46,46,46,46	0
33	MG	0	8110	1/1	0.97	0.11	-5.65	27,27,27,27	0
35	NA	0	8553	1/1	0.97	0.11	-5.89	30,30,30,30	0
33	MG	0	8052	1/1	0.98	0.07	-7.12	54,54,54,54	0
33	MG	A	8065	1/1	0.99	0.06	-7.63	41,41,41,41	0
33	MG	0	8019	1/1	0.98	0.06	-8.09	35,35,35,35	0
33	MG	0	8020	1/1	0.98	0.09	-8.52	33,33,33,33	0
33	MG	0	8022	1/1	0.98	0.10	-8.67	38,38,38,38	0
33	MG	0	8006	1/1	0.99	0.06	-9.02	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.05	-9.19	47,47,47,47	0
33	MG	0	8035	1/1	0.97	0.05	-9.96	46,46,46,46	0
33	MG	0	8033	1/1	0.97	0.09	-10.68	31,31,31,31	0
33	MG	0	8003	1/1	0.99	0.09	-11.24	35,35,35,35	0
33	MG	0	8064	1/1	0.97	0.07	-11.92	30,30,30,30	0
33	MG	0	8002	1/1	0.98	0.09	-16.72	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8536	1/1	0.95	0.10	-	55,55,55,55	0
33	MG	0	8011	1/1	0.98	0.18	-	27,27,27,27	0
33	MG	0	8036	1/1	0.98	0.06	-	33,33,33,33	0
33	MG	0	8090	1/1	0.68	0.75	-	69,69,69,69	0
33	MG	0	8075	1/1	0.95	0.06	-	44,44,44,44	0
33	MG	0	8027	1/1	0.97	0.04	-	44,44,44,44	0
35	NA	0	8575	1/1	0.96	0.27	-	61,61,61,61	0
33	MG	0	8115	1/1	0.98	0.08	-	52,52,52,52	0
35	NA	0	8563	1/1	0.85	0.46	-	57,57,57,57	0
33	MG	0	8059	1/1	0.99	0.06	-	43,43,43,43	0
33	MG	0	8063	1/1	0.97	0.21	-	60,60,60,60	0
36	CL	R	8706	1/1	0.96	0.15	-	46,46,46,46	0
33	MG	0	8079	1/1	0.98	0.17	-	37,37,37,37	0
33	MG	0	8106	1/1	0.98	0.09	-	65,65,65,65	0
35	NA	0	8567	1/1	0.89	0.29	-	59,59,59,59	0
33	MG	0	8046	1/1	0.92	0.09	-	53,53,53,53	0
33	MG	0	8116	1/1	0.88	0.07	-	58,58,58,58	0
33	MG	0	8083	1/1	0.99	0.12	-	43,43,43,43	0
36	CL	0	8717	1/1	0.91	0.11	-	65,65,65,65	0
33	MG	0	8072	1/1	0.97	0.07	-	63,63,63,63	0
33	MG	0	8031	1/1	0.96	0.12	-	34,34,34,34	0
35	NA	0	8518	1/1	0.97	0.19	-	42,42,42,42	0
33	MG	0	8048	1/1	0.98	0.12	-	54,54,54,54	0
35	NA	S	8512	1/1	0.87	0.09	-	43,43,43,43	0
33	MG	0	8093	1/1	0.97	0.09	-	56,56,56,56	0
33	MG	0	8111	1/1	0.98	0.09	-	42,42,42,42	0
36	CL	A	8709	1/1	0.93	0.24	-	77,77,77,77	0
36	CL	0	8714	1/1	0.96	0.14	-	54,54,54,54	0
35	NA	0	8515	1/1	0.97	0.20	-	42,42,42,42	0
33	MG	0	8034	1/1	0.99	0.09	-	33,33,33,33	0
33	MG	A	8066	1/1	0.91	0.04	-	72,72,72,72	0
33	MG	0	8088	1/1	0.97	0.14	-	38,38,38,38	0
36	CL	0	8703	1/1	0.98	0.08	-	58,58,58,58	0
35	NA	0	8540	1/1	0.78	0.21	-	58,58,58,58	0
33	MG	0	8098	1/1	0.98	0.08	-	40,40,40,40	0
33	MG	0	8117	1/1	0.98	0.06	-	32,32,32,32	0
36	CL	J	8701	1/1	0.94	0.22	-	66,66,66,66	0
33	MG	0	8041	1/1	0.91	0.19	-	56,56,56,56	0
36	CL	0	8722	1/1	0.87	0.37	-	81,81,81,81	0
35	NA	0	8584	1/1	0.88	0.14	-	62,62,62,62	0
33	MG	0	8045	1/1	0.98	0.07	-	53,53,53,53	0
33	MG	0	8026	1/1	0.98	0.17	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8042	1/1	0.96	0.10	-	38,38,38,38	0
35	NA	0	8552	1/1	0.78	0.21	-	62,62,62,62	0
33	MG	0	8089	1/1	0.97	0.14	-	74,74,74,74	0
33	MG	0	8087	1/1	0.88	0.12	-	66,66,66,66	0
35	NA	0	8528	1/1	0.98	0.32	-	42,42,42,42	0
35	NA	0	8511	1/1	0.90	0.15	-	50,50,50,50	0
33	MG	0	8101	1/1	0.93	0.19	-	69,69,69,69	0
33	MG	0	8071	1/1	0.96	0.04	-	69,69,69,69	0
35	NA	0	8558	1/1	0.95	0.35	-	82,82,82,82	0
33	MG	0	8103	1/1	0.93	0.18	-	82,82,82,82	0
35	NA	0	8541	1/1	0.94	0.10	-	50,50,50,50	0
33	MG	0	8099	1/1	0.96	0.16	-	45,45,45,45	0
33	MG	0	8092	1/1	0.79	0.13	-	89,89,89,89	0
33	MG	0	8016	1/1	0.98	0.09	-	40,40,40,40	0
33	MG	0	8062	1/1	0.98	0.09	-	54,54,54,54	0
33	MG	0	8081	1/1	0.94	0.10	-	49,49,49,49	0
33	MG	K	8069	1/1	0.97	0.05	-	58,58,58,58	0
33	MG	0	8086	1/1	0.95	0.07	-	52,52,52,52	0
35	NA	0	8559	1/1	0.94	0.24	-	49,49,49,49	0
33	MG	0	8050	1/1	0.90	0.08	-	59,59,59,59	0
33	MG	0	8114	1/1	0.86	0.65	-	67,67,67,67	0
35	NA	0	8516	1/1	0.92	0.25	-	54,54,54,54	0
35	NA	0	8542	1/1	0.90	0.39	-	47,47,47,47	0
36	CL	Q	8711	1/1	0.98	0.08	-	55,55,55,55	0
33	MG	0	8068	1/1	0.96	0.04	-	61,61,61,61	0
33	MG	9	8095	1/1	0.89	0.12	-	76,76,76,76	0
33	MG	0	8040	1/1	0.97	0.13	-	60,60,60,60	0
35	NA	0	8506	1/1	0.90	0.37	-	48,48,48,48	0
33	MG	0	8030	1/1	0.99	0.10	-	25,25,25,25	0
35	NA	0	8501	1/1	0.95	0.21	-	32,32,32,32	0
33	MG	0	8049	1/1	0.75	0.19	-	92,92,92,92	0
35	NA	0	8554	1/1	0.98	0.16	-	40,40,40,40	0
33	MG	0	8082	1/1	0.88	0.14	-	63,63,63,63	0
36	CL	N	8707	1/1	0.95	0.11	-	66,66,66,66	0
35	NA	0	8581	1/1	0.95	0.08	-	48,48,48,48	0
35	NA	0	8534	1/1	0.95	0.07	-	45,45,45,45	0
33	MG	0	8061	1/1	0.97	0.17	-	41,41,41,41	0
33	MG	0	8113	1/1	0.91	0.12	-	53,53,53,53	0
36	CL	Y	8720	1/1	0.98	0.13	-	46,46,46,46	0
33	MG	0	8051	1/1	0.97	0.05	-	59,59,59,59	0
33	MG	0	8028	1/1	0.97	0.05	-	38,38,38,38	0
37	CD	O	8605	1/1	0.96	0.08	-	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8009	1/1	0.99	0.17	-	35,35,35,35	0
33	MG	0	8085	1/1	0.94	0.12	-	54,54,54,54	0
36	CL	J	8702	1/1	0.97	0.10	-	57,57,57,57	0
36	CL	L	8710	1/1	0.95	0.19	-	60,60,60,60	0
35	NA	0	8513	1/1	0.90	0.09	-	62,62,62,62	0
35	NA	0	8570	1/1	0.95	0.34	-	69,69,69,69	0
35	NA	9	8551	1/1	0.71	0.19	-	50,50,50,50	0
35	NA	0	8549	1/1	0.96	0.18	-	51,51,51,51	0
33	MG	0	8097	1/1	0.94	0.10	-	34,34,34,34	0
33	MG	0	8043	1/1	0.96	0.08	-	48,48,48,48	0
35	NA	0	8557	1/1	0.92	0.12	-	61,61,61,61	0
33	MG	0	8094	1/1	0.97	0.07	-	77,77,77,77	0
33	MG	0	8029	1/1	0.98	0.07	-	35,35,35,35	0
33	MG	0	8102	1/1	0.91	0.29	-	73,73,73,73	0
35	NA	0	8507	1/1	0.94	0.32	-	59,59,59,59	0
33	MG	0	8104	1/1	0.91	0.23	-	65,65,65,65	0
33	MG	0	8100	1/1	0.91	0.18	-	66,66,66,66	0
35	NA	0	8560	1/1	0.95	0.30	-	51,51,51,51	0
33	MG	0	8024	1/1	0.98	0.13	-	21,21,21,21	0
33	MG	0	8070	1/1	0.97	0.16	-	50,50,50,50	0
33	MG	0	8037	1/1	0.98	0.09	-	43,43,43,43	0
35	NA	H	8522	1/1	0.83	0.33	-	67,67,67,67	0
35	NA	0	8530	1/1	0.97	0.15	-	50,50,50,50	0
33	MG	0	8047	1/1	0.93	0.13	-	74,74,74,74	0
35	NA	0	8585	1/1	0.86	0.26	-	51,51,51,51	0
33	MG	0	8005	1/1	0.99	0.16	-	33,33,33,33	0
33	MG	0	8023	1/1	0.97	0.27	-	41,41,41,41	0
33	MG	0	8025	1/1	0.97	0.09	-	37,37,37,37	0
35	NA	0	8508	1/1	0.92	0.15	-	56,56,56,56	0

6.5 Other polymers

There are no such residues in this entry.