



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 04:43 pm BST

PDB ID : 2OTL
Title : Girodazole bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
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

<https://www.wwpdb.org/validation/2017/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:

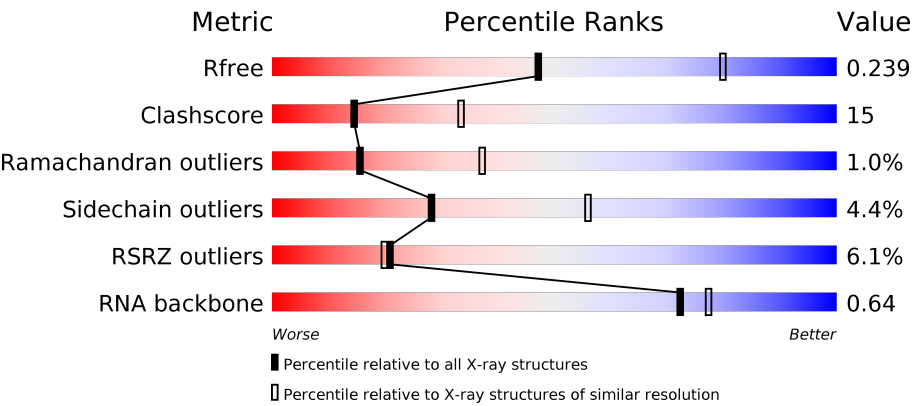
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 respectively. 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>%</div><div><div></div><div>49%</div><div>39%</div><div>6%</div><div>6%</div></div></div>
2	9	122	<div><div>3%</div><div><div></div><div>43%</div><div>44%</div><div>12%</div></div></div>
3	A	239	<div><div>12%</div><div><div></div><div>70%</div><div>26%</div><div>••</div></div></div>
4	B	337	<div><div>%</div><div><div></div><div>61%</div><div>35%</div><div>•</div></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	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	8090	-	-	-	X
35	NA	0	8529	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8713	-	-	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			

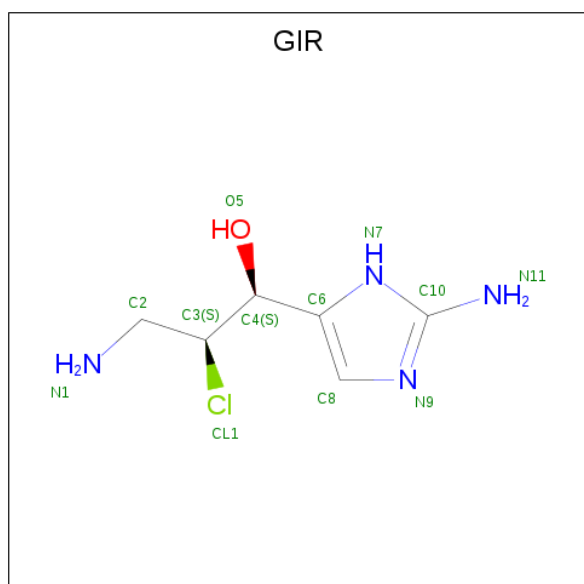
- Molecule 30 is a protein called 50S ribosomal protein L44E.

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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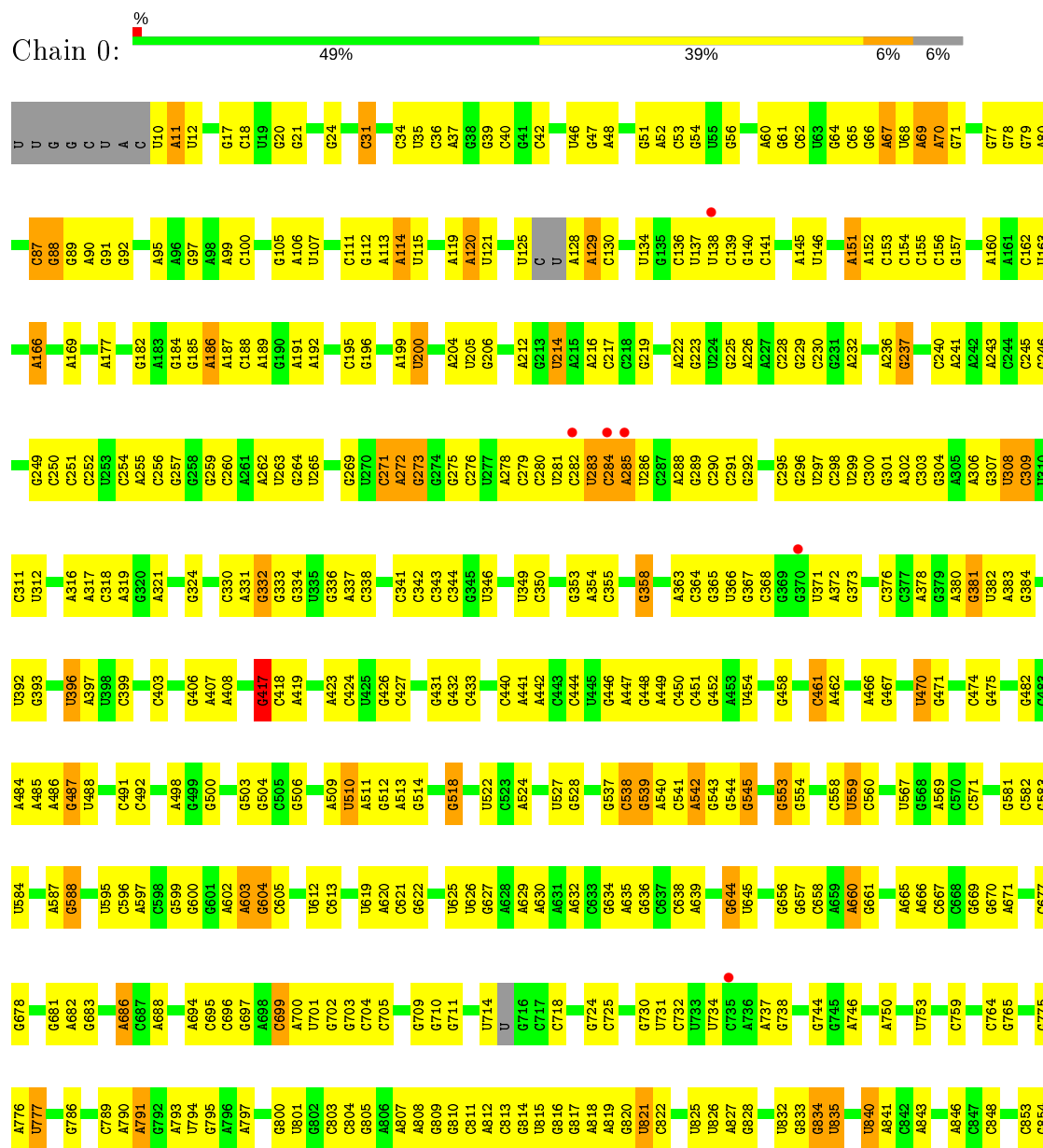
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	61	Total 61	O 61	0	0
38	Q	55	Total 55	O 55	0	0
38	R	81	Total 81	O 81	0	0
38	S	37	Total 37	O 37	0	0
38	T	39	Total 39	O 39	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	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

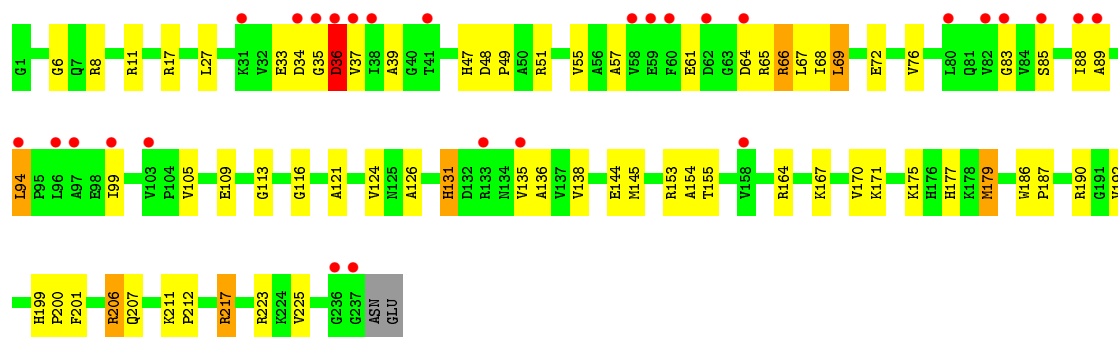
3 Residue-property plots

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.

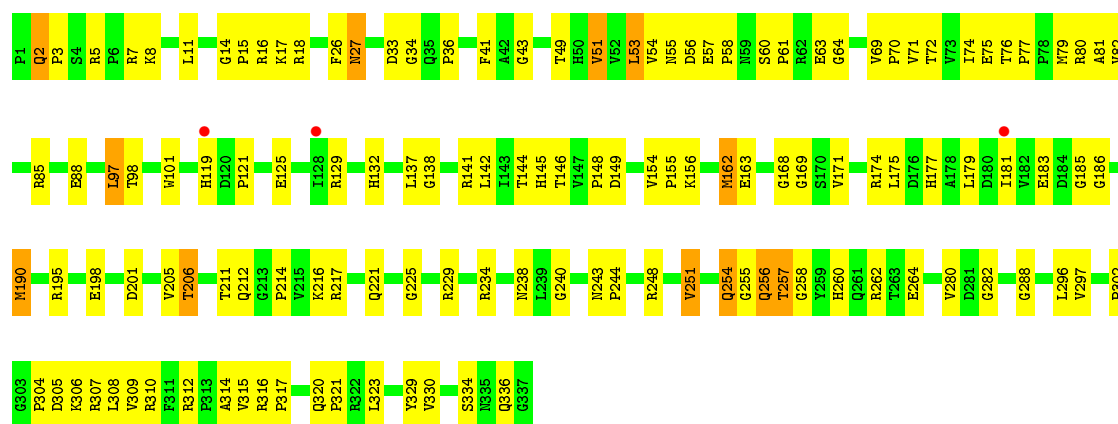
- Molecule 1: 23S ribosomal RNA



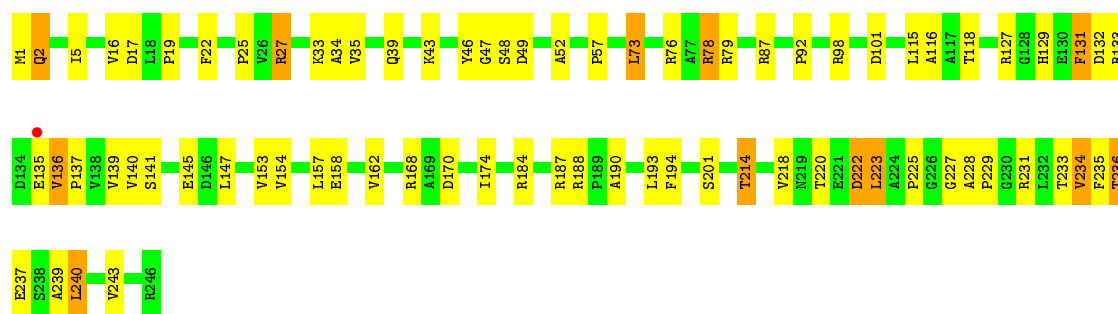
G2001	C1920	U1835	G1752	A1856	U1569	G1497	G1415	G1325	G1160	G1026	G953	U855
G2002	A1921	A1836	C1783	A1857	A1569	U1500	G1416	A1328	A1161	G1027	G954	G856
U2003	A1922			A1858	A1573	A1501	G1417	A1329	G1162	U1028	A955	U857
U2004		A1840	A1759	A1859	C1574	A1502	U1418	A1330	U1163	U1029		U858
G2005	G1925	A1841	G1765	A1661	U1577	A1503	G1419	A1331	U1164	A1032	G958	C959
U2008	A1927	A1842	U1766	C1862	C1578	A1504	G1421	C1832	U1165		G960	U860
G2009	C1928	A1845	A1767	G1863	C1579	U1505	G1422	U1333	A1166	C1044	A961	U861
A2011	G1929	U1846	C1768	A1664	U1506	C1507	G1423	U1334	G1167	G1045	C962	U862
A2012	A1930	A1847	U1769	G1665	C1508	U1508	A1424	G1340	U1169	G1052	G968	G868
U2012	U1931	G1848	U1770	C1666	C1509	G1509	G1426	A1341	A1171	G1053	G969	G870
G2013		G1849	U1771	A1667			A1427	C1342	G1172	G1054	U970	G871
U2016	C1936	U1850	C1772	U1668	G1586	G1512		C1343	A1173	G1055	U872	U872
U1937	U1937	G1851	G1773	A1669	U1587	C1513	U1432	C1344	A1174	U1056	U	A875
U1938	G1938	A1852	G1774	G1588	G1589	C1514	G1433	U1358	A1175	A1057	G	A876
C2028	U1939	C1853		U1671		A1515	G1434	U1359	C1176	A1058	U	A877
C2029	C1940	G1854	G1777	G1672	G1592	A1516	U1435	U1360	A1177	G1059	C	G877
G2033	A1941	G1855	A1778		G1593	U1517	C1436	A1352	G1178	C1060	C	G878
U2034	A1942	C1856	U1779	G1679	C1594			C1353	C1179	U1066	G	U883
U2039	G1943	A1857	G1780	C1880	C1595	G1520	U1440	A1358	A1180	A1067	C	C884
G2044	G1945	C1862	G1781	G1681	U1596	C1521	G1441	U1359	A1181		C	C885
G2045	C1946	G1863	A1782	A1682	U1597	A1522	A1442	A1358	C1182		U	G886
G2046	G1947	U1864	U1783	G1883	A1598	G1523	G1443	C1361	C1183	G1072	C	U887
	G1948	G1785	U1784	A1684		U1524	G1444	U1362	U1185	A1078	G	U888
	G1949	C1786	C1786	A1685	A1603	G1525	G1445	U1362	C1184			
G1950	G1873	C1787	C1787	C1886	G1604	A1526	U1446	U1362	U1266	A1079		
G1951	U1874	U1788	U1788	C1887	G1605	A1527	U1447	C1366	C1267	A1080	A	A894
A2054	U1874	C1789	C1789	C1692	A1606	A1528	U1447	U1366	G1268	A1081	A	
U2063	G1877	G1790	U1791	A1701	A1607	G1529	G1450	A1372	A1189		G	G898
U2064	A1878			U1702			G1451	G1373	A1190	A1086	A	
C2065	U1879		G1795	U1702	G1613	A1533	G1452	C1374	A1191	G1087	G	G902
C2066	C1880		A1796	A1710	G1614	C1534	G1453	A1375	A1192	A1088	G	C905
C2071	A1881		A1797	A1711	G1619	C1535	U1454	C1376	A1193		U	C906
G2072	C1882		C1798	A1712	C1620	C1536	U1454	C1377	A1194	C1102	C	A907
G2073	U1883			G1713		C1537	G1460	U1380	G1195	U1109	G	
A2074	G1884				U1635	U1538	U1461	U1380	C1196	G1110	C	A912
	A1885		C1803	A1717	A1635	U1539	C1462	U1383	U1196	U1116	C	C920
A2081	A1886		G1804	A1717	A1636	G1543	A1463	U1383	A1199	U1117	C	G921
G2082	A1887		G1805	G1627	G1627	U1544	A1471	U1388	A1200	A1118	A	A922
A2083	C1889		G1806	G1723	A1630	C1545	C1472	G1389	C1201	G1119	G	A923
C2088	U1890			U1724	A1633	G1546	U1473	A1390	A1202	U1120	U1001	G924
A2089	C1894		G1809	C1725	C1633	C1553	C1474	G1391	C1203			
G2090	A1895		A1811	C1725	G1634	C1554		A1392	C1204	U1130	C1004	U932
G2091	G1896		G1812	G1730	U1635	U1554	C1477	A1393	U1205	G1131	C1005	C933
G2092	U1897			C1731	G1636	G1555	U1478	C1394	A1206	G1132	A1006	C934
	C1975		C1818	A1732	A1637	G1556	U1479	C1395	A1207	A1132	U1007	G940
G1976	G1819		G1820	A1733	A1641	G1557	G1484	C1396	C1208	G1135	U1008	G941
U1977	G1820		A1821	C1734	A1642	C1558	A1485	C1397	C1209	U1136	U1009	U942
A1978	A1903		A1822	C1735	C1643	U1559		G1398	G1210	G1137	C1010	A943
	A1904			U1741	C1644	U	G1489	A1399	G1211	U1138		G944
A2101	U1909		G1823	A1742	U1645	U1561	G1490	C1400	C1212	G1139		U945
G2102	A1910		C1824	G1743	G1649	C1562	G1491	G1401	C1213	C1140	A1013	U946
C2104			U1825	G1744	C1650	C1563	A1492	A1406	G1214		A1014	C946
C2105	U1915		C1826	G1745	C1655	G1564	A1493	A1407	A1215	C1156	C1015	U947
C2106	C1916			G1746	C1566	C1565	A1494	U1408	G1216		U1016	G948
	G1917		A3329	A1747	U1567	U1567	A1495	A1407	G1217	C1157	G1024	A951
G2110	U1918			U1654	U1567		A1495	U1408	U1218	G1158		
G2111	A1919		C1834	G1655	G1568		G1496	A1414	U1219	G1159		G952



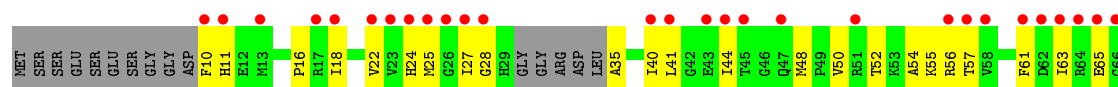
- Molecule 4: 50S ribosomal protein L3P

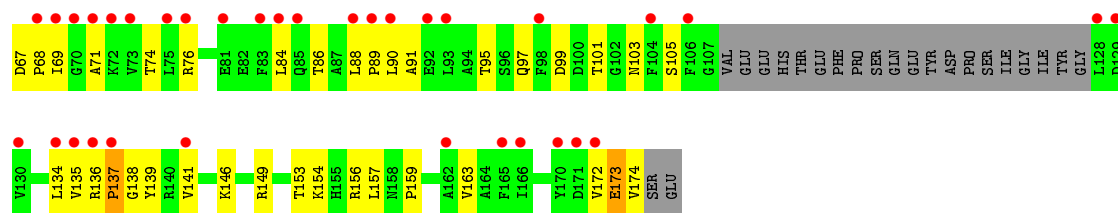


- Molecule 5: 50S ribosomal protein L4P

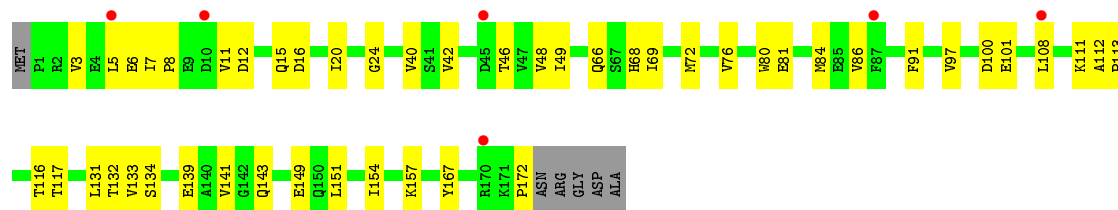


- Molecule 6: 50S ribosomal protein L5P

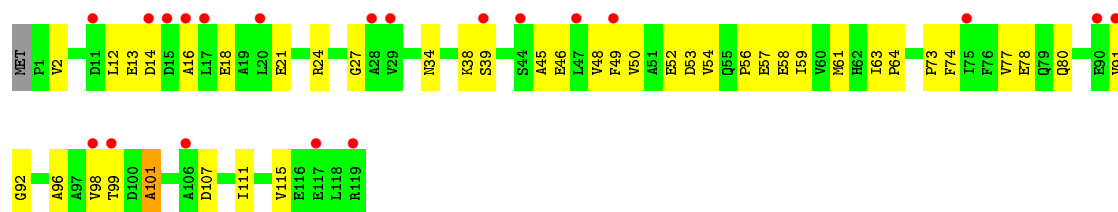




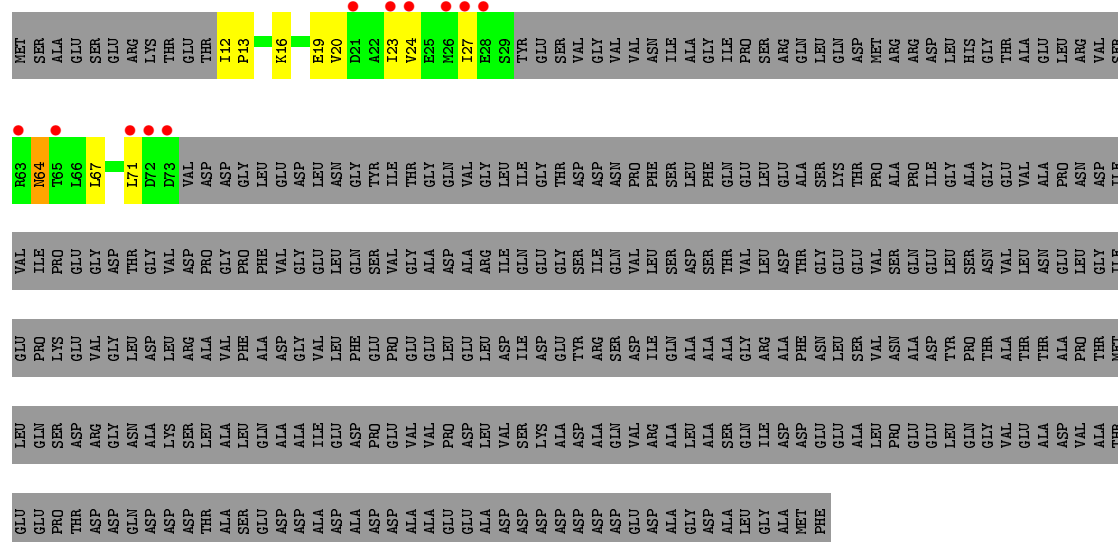
• Molecule 7: 50S ribosomal protein L6P



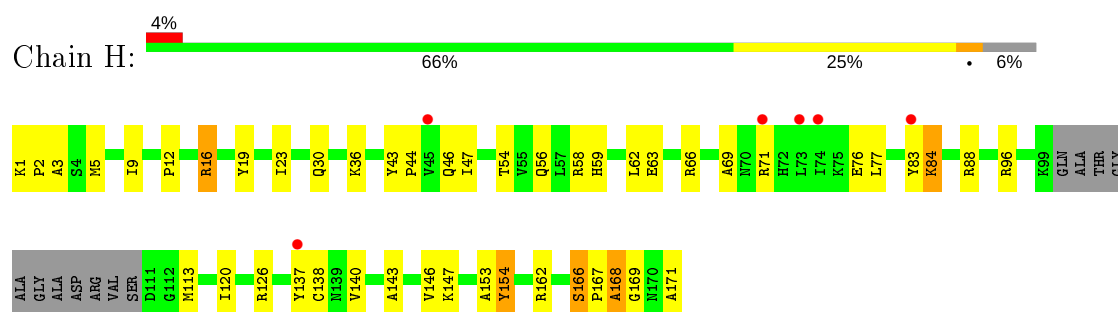
• Molecule 8: 50S ribosomal protein L7Ae



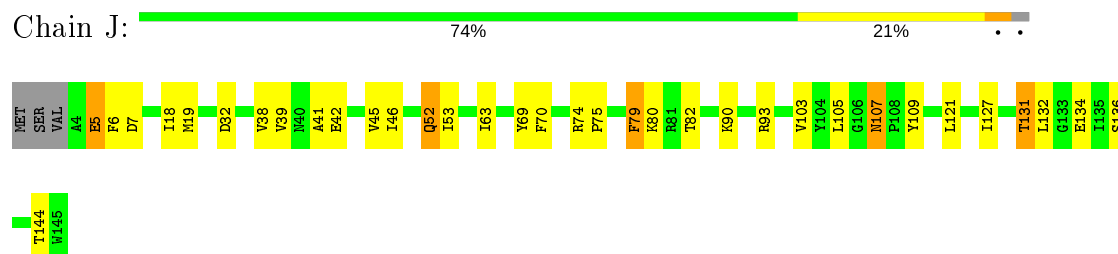
• Molecule 9: 50S ribosomal protein L10E



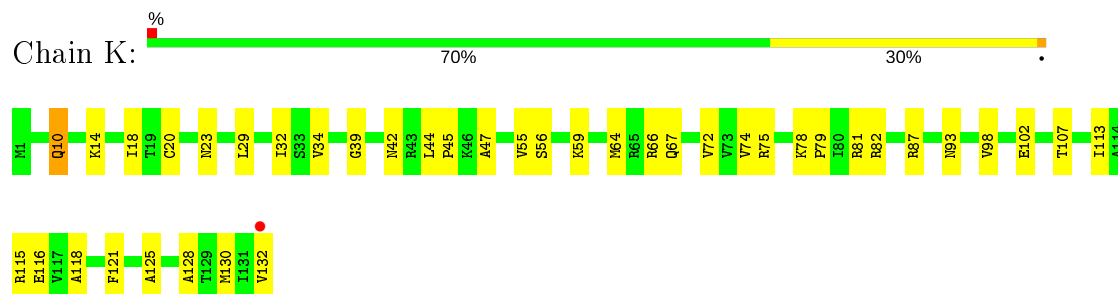
• Molecule 10: 50S ribosomal protein L10e



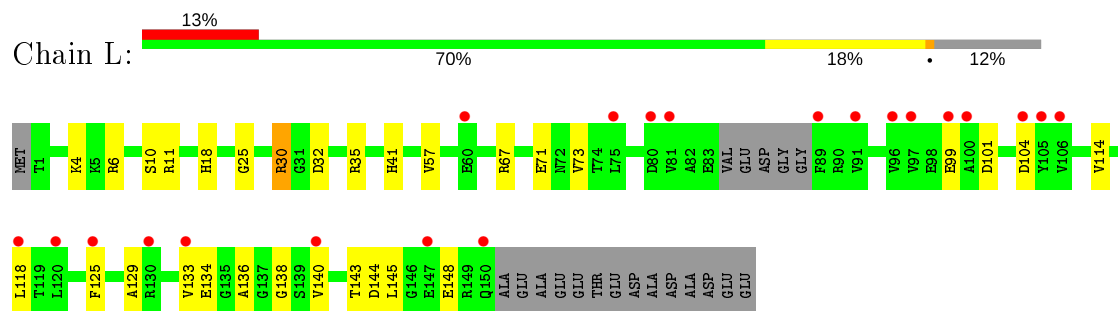
- Molecule 11: 50S ribosomal protein L13P



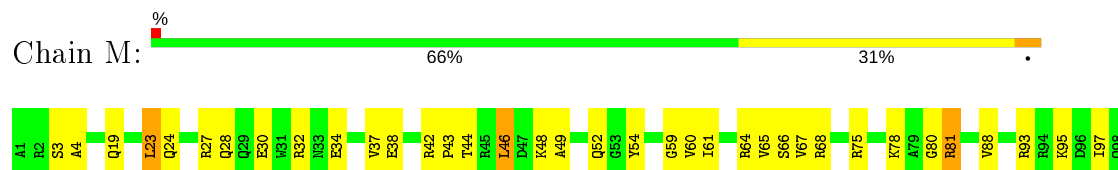
- Molecule 12: 50S ribosomal protein L14P



- Molecule 13: 50S ribosomal protein L15P

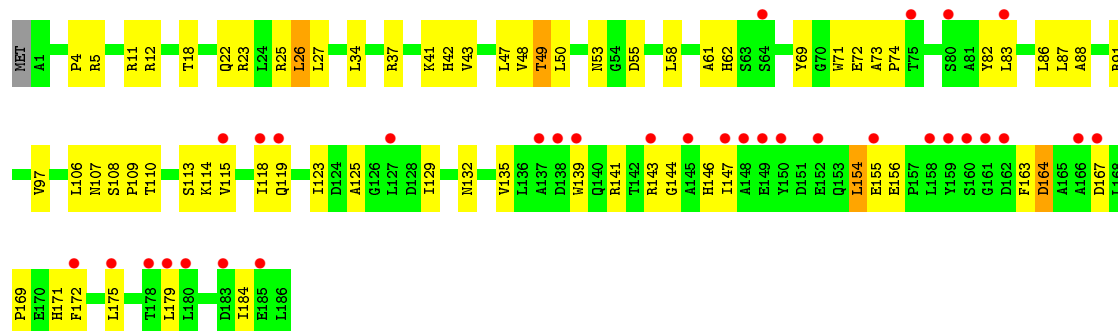


- Molecule 14: 50S ribosomal protein L15e

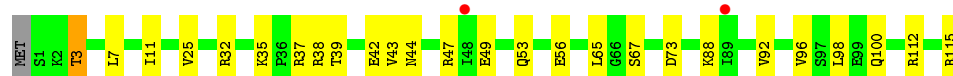
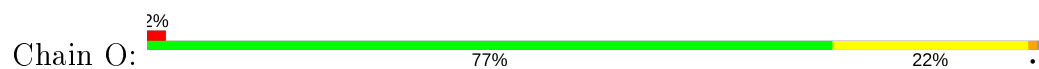




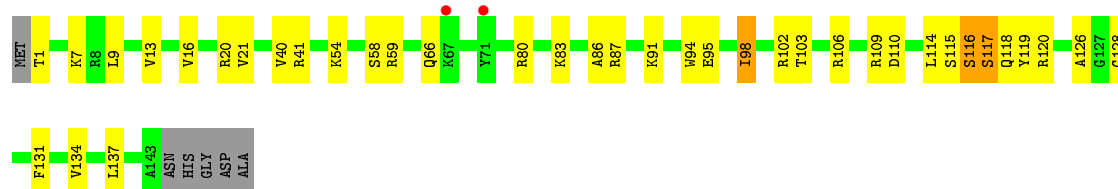
- Molecule 15: 50S ribosomal protein L18P



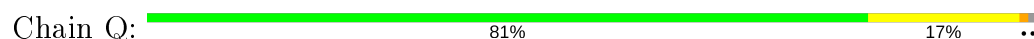
- Molecule 16: 50S ribosomal protein L18e



- Molecule 17: 50S ribosomal protein L19e



- Molecule 18: 50S ribosomal protein L21e

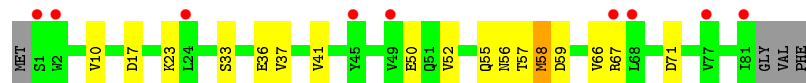
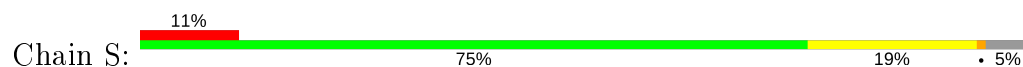


- Molecule 19: 50S ribosomal protein L22P

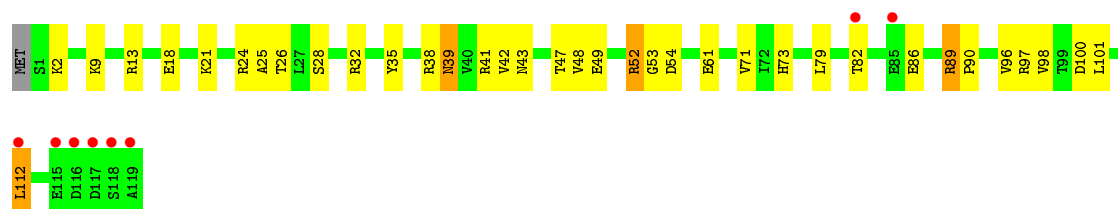




- Molecule 20: 50S ribosomal protein L23P



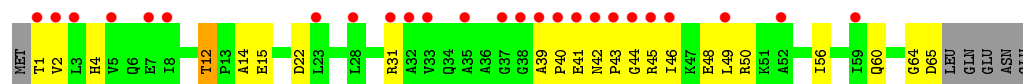
- Molecule 21: 50S ribosomal protein L24P



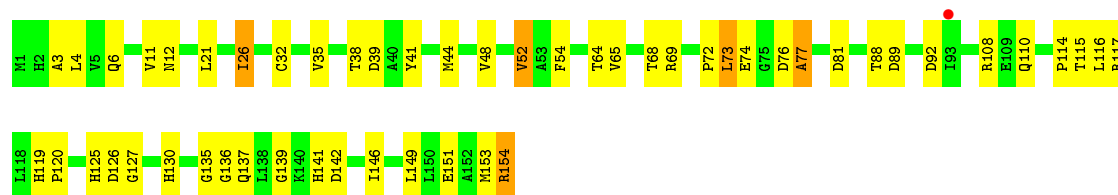
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P

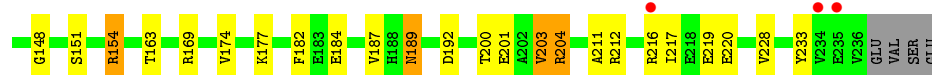
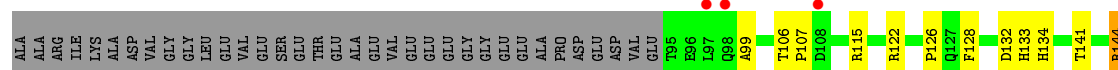


- Molecule 25: 50S ribosomal protein L31e

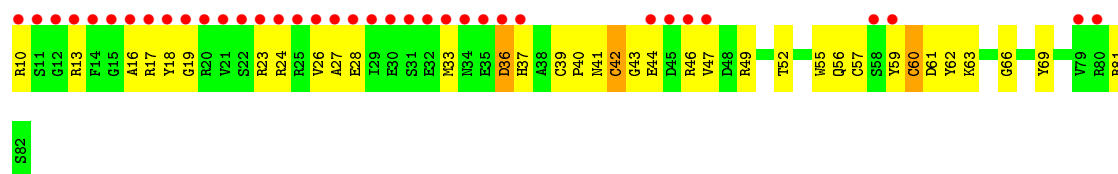




- Molecule 26: 50S ribosomal protein L32e



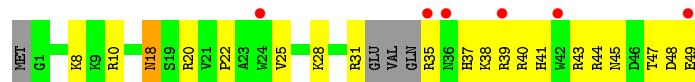
- Molecule 27: 50S ribosomal protein L37Ae



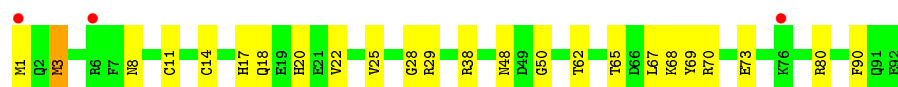
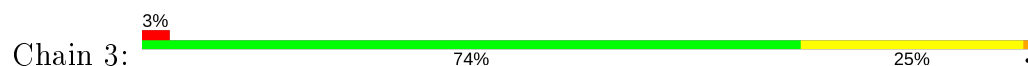
- Molecule 28: 50S ribosomal protein L37e



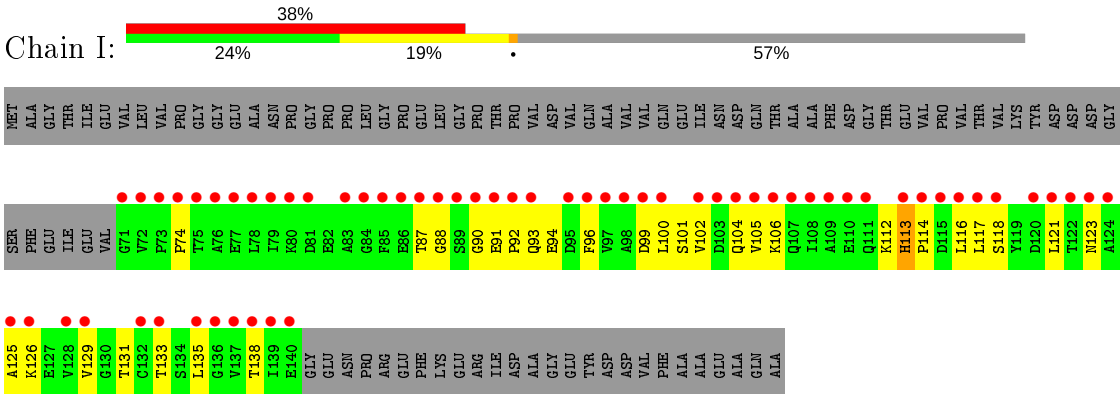
- Molecule 29: 50S ribosomal protein L39e



- 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	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.248 0.195 , 0.239	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	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	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 1.50% 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 ⓘ

5.1 Standard geometry ⓘ

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%)	12	30
4	B	335/337 (99%)	305 (91%)	24 (7%)	6 (2%)	8	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	C	244/246 (99%)	228 (93%)	15 (6%)	1 (0%)	34	60
6	D	134/177 (76%)	107 (80%)	23 (17%)	4 (3%)	4	10
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	106 (91%)	10 (8%)	1 (1%)	17	40
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	143 (92%)	9 (6%)	4 (3%)	5	13
11	J	140/145 (97%)	128 (91%)	11 (8%)	1 (1%)	22	46
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%)	29	54
15	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	9	24
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	136 (96%)	3 (2%)	2 (1%)	11	28
18	Q	93/96 (97%)	87 (94%)	5 (5%)	1 (1%)	14	34
19	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	22	46
20	S	79/85 (93%)	76 (96%)	2 (2%)	1 (1%)	12	30
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%)	9	24
24	W	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	12	30
25	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	5	14
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%)	15	37

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%)	21	45
4	B	282/282 (100%)	264 (94%)	18 (6%)	17	39
5	C	193/193 (100%)	177 (92%)	16 (8%)	11	25
6	D	117/148 (79%)	113 (97%)	4 (3%)	37	66
7	E	152/156 (97%)	149 (98%)	3 (2%)	55	81
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	90
9	G	27/283 (10%)	26 (96%)	1 (4%)	34	63
10	H	132/138 (96%)	125 (95%)	7 (5%)	22	48
11	J	118/121 (98%)	110 (93%)	8 (7%)	16	36
12	K	106/106 (100%)	105 (99%)	1 (1%)	78	92
13	L	113/127 (89%)	107 (95%)	6 (5%)	22	48
14	M	158/158 (100%)	150 (95%)	8 (5%)	24	50
15	N	149/150 (99%)	145 (97%)	4 (3%)	44	74
16	O	93/94 (99%)	89 (96%)	4 (4%)	29	57
17	P	113/117 (97%)	108 (96%)	5 (4%)	28	56
18	Q	79/80 (99%)	77 (98%)	2 (2%)	47	76
19	R	117/122 (96%)	112 (96%)	5 (4%)	29	57
20	S	71/74 (96%)	69 (97%)	2 (3%)	43	73
21	T	105/106 (99%)	100 (95%)	5 (5%)	25	53
22	U	44/52 (85%)	43 (98%)	1 (2%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	51/57 (90%)	49 (96%)	2 (4%)	32	61
24	W	130/130 (100%)	124 (95%)	6 (5%)	27	54
25	X	66/74 (89%)	62 (94%)	4 (6%)	18	41
26	Y	120/196 (61%)	114 (95%)	6 (5%)	24	51
27	Z	60/60 (100%)	58 (97%)	2 (3%)	38	67
28	1	46/47 (98%)	46 (100%)	0	100	100
29	2	42/46 (91%)	40 (95%)	2 (5%)	25	53
30	3	79/79 (100%)	77 (98%)	2 (2%)	47	76
31	I	58/130 (45%)	57 (98%)	1 (2%)	60	84
All	All	3093/3601 (86%)	2957 (96%)	136 (4%)	28	56

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	1MA	0	628	1,35	15,25,26	0.75	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1	14,22,23	0.91	1 (7%)	14,31,34	1.18	1 (7%)
1	UR3	0	2619	1	14,22,23	0.67	0	15,32,35	0.61	0
1	PSU	0	2621	1	17,21,22	1.71	3 (17%)	20,30,33	5.46	5 (25%)
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.59	4 (20%)

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	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.25	1.47	1.52
1	0	2588	OMG	C6-N1	3.65	1.39	1.33
1	0	2621	PSU	C2-N1	2.74	1.43	1.38
1	0	2621	PSU	C4-N3	2.74	1.37	1.33
1	0	2587	OMU	C4-N3	2.27	1.37	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.62	114.42	128.43
1	0	2621	PSU	C4-N3-C2	14.08	127.03	115.14
1	0	2588	OMG	C5-C6-N1	-8.60	111.67	123.43
1	0	2621	PSU	C5-C4-N3	-7.92	115.15	125.36
1	0	2588	OMG	C6-N1-C2	5.75	125.06	115.93

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	-	7,12,12	0.75	0	4,16,16	0.76	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	39 (1%) 75 77	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.33	4 (3%) 46 46	38, 64, 91, 149	0
3	A	237/239 (99%)	0.62	28 (11%) 4 3	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%) 1 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%) 40 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 87	36, 54, 77, 87	0
13	L	145/165 (87%)	0.87	21 (14%) 2 1	29, 71, 118, 130	0
14	M	194/194 (100%)	0.01	1 (0%) 91 92	35, 47, 63, 73	0
15	N	186/187 (99%)	0.97	33 (17%) 1 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	2 (1%) 75 77	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%) 5 4	47, 67, 87, 94	0
21	T	119/120 (99%)	0.54	8 (6%) 17 16	41, 61, 88, 108	0
22	U	53/66 (80%)	0.41	1 (1%) 66 69	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 91	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%) 10 9	45, 61, 87, 102	0
26	Y	142/241 (58%)	0.17	6 (4%) 36 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	6 (13%) 3 2	39, 68, 101, 114	0
30	3	92/92 (100%)	0.48	3 (3%) 46 46	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	403 (6%) 21 20	24, 55, 105, 153	0

The worst 5 of 403 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	26	VAL	12.9
23	V	1	THR	12.9
27	Z	20	ARG	11.0
27	Z	11	SER	9.9
27	Z	34	ASN	9.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
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	OMG	0	2588	24/25	0.98	0.15	33,36,38,39	0
1	PSU	0	2621	20/21	0.99	0.14	28,30,33,34	0
1	1MA	0	628	23/24	0.99	0.18	28,32,33,35	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
35	NA	R	8586	1/1	0.48	0.80	95,95,95,95	0
35	NA	0	8529	1/1	0.55	0.45	77,77,77,77	0
33	MG	0	8090	1/1	0.68	0.75	69,69,69,69	0
35	NA	0	8568	1/1	0.69	0.18	71,71,71,71	0
35	NA	9	8551	1/1	0.71	0.19	50,50,50,50	0
33	MG	0	8049	1/1	0.75	0.19	92,92,92,92	0
35	NA	0	8540	1/1	0.78	0.21	58,58,58,58	0
35	NA	0	8552	1/1	0.78	0.21	62,62,62,62	0
35	NA	0	8571	1/1	0.78	0.42	65,65,65,65	0
35	NA	0	8582	1/1	0.78	0.21	79,79,79,79	0
35	NA	0	8577	1/1	0.80	0.38	71,71,71,71	0
33	MG	0	8092	1/1	0.80	0.13	89,89,89,89	0
35	NA	0	8574	1/1	0.82	0.54	66,66,66,66	0
35	NA	H	8522	1/1	0.83	0.34	67,67,67,67	0
35	NA	C	8504	1/1	0.84	0.27	49,49,49,49	0
35	NA	0	8533	1/1	0.85	0.14	39,39,39,39	0
35	NA	0	8563	1/1	0.85	0.46	57,57,57,57	0
33	MG	T	8073	1/1	0.85	0.12	71,71,71,71	0
35	NA	R	8538	1/1	0.85	0.08	60,60,60,60	0
33	MG	0	8114	1/1	0.85	0.66	67,67,67,67	0
35	NA	9	8583	1/1	0.86	0.43	65,65,65,65	0
35	NA	0	8585	1/1	0.86	0.26	51,51,51,51	0
35	NA	S	8512	1/1	0.87	0.09	43,43,43,43	0
33	MG	0	8096	1/1	0.87	0.11	52,52,52,52	0
35	NA	0	8566	1/1	0.87	0.30	66,66,66,66	0
36	CL	0	8722	1/1	0.87	0.36	81,81,81,81	0
33	MG	0	8087	1/1	0.88	0.12	66,66,66,66	0
35	NA	0	8584	1/1	0.88	0.14	62,62,62,62	0
33	MG	0	8116	1/1	0.88	0.07	58,58,58,58	0
33	MG	0	8082	1/1	0.88	0.14	63,63,63,63	0
35	NA	0	8526	1/1	0.89	0.64	58,58,58,58	0
36	CL	0	8705	1/1	0.89	0.20	67,67,67,67	0
35	NA	0	8567	1/1	0.89	0.29	59,59,59,59	0
35	NA	R	8537	1/1	0.89	0.25	48,48,48,48	0
33	MG	9	8095	1/1	0.90	0.12	76,76,76,76	0
33	MG	A	8066	1/1	0.90	0.04	72,72,72,72	0
35	NA	0	8506	1/1	0.90	0.37	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8569	1/1	0.90	0.37	74,74,74,74	0
35	NA	0	8511	1/1	0.90	0.15	50,50,50,50	0
35	NA	0	8532	1/1	0.90	0.30	49,49,49,49	0
35	NA	0	8513	1/1	0.90	0.09	62,62,62,62	0
35	NA	0	8542	1/1	0.90	0.39	47,47,47,47	0
33	MG	0	8050	1/1	0.90	0.08	59,59,59,59	0
35	NA	0	8503	1/1	0.90	0.36	47,47,47,47	0
36	CL	0	8717	1/1	0.91	0.11	65,65,65,65	0
33	MG	0	8102	1/1	0.91	0.29	73,73,73,73	0
33	MG	0	8113	1/1	0.91	0.12	53,53,53,53	0
33	MG	0	8041	1/1	0.91	0.20	56,56,56,56	0
32	GIR	0	9000	12/12	0.91	0.21	23,40,50,53	0
36	CL	O	8708	1/1	0.91	0.21	73,73,73,73	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
33	MG	0	8044	1/1	0.91	0.10	46,46,46,46	0
35	NA	0	8557	1/1	0.92	0.12	61,61,61,61	0
35	NA	0	8516	1/1	0.92	0.25	54,54,54,54	0
35	NA	0	8510	1/1	0.92	0.12	36,36,36,36	0
35	NA	0	8556	1/1	0.92	0.20	49,49,49,49	0
35	NA	0	8562	1/1	0.92	0.20	60,60,60,60	0
35	NA	0	8508	1/1	0.92	0.15	56,56,56,56	0
35	NA	0	8527	1/1	0.92	0.17	44,44,44,44	0
35	NA	0	8561	1/1	0.92	0.24	56,56,56,56	0
33	MG	0	8046	1/1	0.92	0.09	53,53,53,53	0
35	NA	0	8564	1/1	0.93	0.29	53,53,53,53	0
35	NA	0	8565	1/1	0.93	0.38	40,40,40,40	0
36	CL	0	8715	1/1	0.93	0.25	86,86,86,86	0
35	NA	J	8546	1/1	0.93	0.13	53,53,53,53	0
36	CL	3	8704	1/1	0.93	0.16	71,71,71,71	0
33	MG	0	8103	1/1	0.93	0.18	82,82,82,82	0
35	NA	0	8573	1/1	0.93	0.29	69,69,69,69	0
35	NA	0	8517	1/1	0.93	0.06	51,51,51,51	0
35	NA	0	8550	1/1	0.93	0.26	45,45,45,45	0
36	CL	A	8709	1/1	0.93	0.24	77,77,77,77	0
33	MG	0	8101	1/1	0.93	0.19	69,69,69,69	0
33	MG	0	8047	1/1	0.93	0.13	74,74,74,74	0
36	CL	0	8713	1/1	0.93	0.08	65,65,65,65	0
33	MG	0	8053	1/1	0.94	0.16	45,45,45,45	0
35	NA	0	8541	1/1	0.94	0.10	50,50,50,50	0
35	NA	0	8507	1/1	0.94	0.32	59,59,59,59	0
35	NA	0	8521	1/1	0.94	0.28	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	B	8055	1/1	0.94	0.05	48,48,48,48	0
36	CL	J	8701	1/1	0.94	0.22	66,66,66,66	0
35	NA	0	8581	1/1	0.94	0.07	48,48,48,48	0
33	MG	0	8039	1/1	0.94	0.11	52,52,52,52	0
33	MG	0	8081	1/1	0.94	0.10	49,49,49,49	0
33	MG	0	8097	1/1	0.94	0.10	34,34,34,34	0
35	NA	0	8559	1/1	0.94	0.24	49,49,49,49	0
35	NA	0	8536	1/1	0.95	0.10	55,55,55,55	0
33	MG	0	8084	1/1	0.95	0.05	47,47,47,47	0
35	NA	0	8534	1/1	0.95	0.07	45,45,45,45	0
35	NA	0	8560	1/1	0.95	0.30	51,51,51,51	0
35	NA	Q	8548	1/1	0.95	0.06	42,42,42,42	0
35	NA	0	8524	1/1	0.95	0.19	62,62,62,62	0
35	NA	0	8558	1/1	0.95	0.35	82,82,82,82	0
33	MG	0	8085	1/1	0.95	0.12	54,54,54,54	0
36	CL	L	8710	1/1	0.95	0.19	60,60,60,60	0
33	MG	0	8075	1/1	0.95	0.06	44,44,44,44	0
35	NA	0	8570	1/1	0.95	0.35	69,69,69,69	0
33	MG	0	8086	1/1	0.95	0.07	52,52,52,52	0
36	CL	N	8707	1/1	0.95	0.11	66,66,66,66	0
35	NA	0	8523	1/1	0.95	0.17	43,43,43,43	0
35	NA	0	8535	1/1	0.95	0.22	56,56,56,56	0
35	NA	0	8572	1/1	0.95	0.28	54,54,54,54	0
35	NA	H	8509	1/1	0.95	0.10	39,39,39,39	0
35	NA	0	8501	1/1	0.95	0.21	32,32,32,32	0
35	NA	M	8547	1/1	0.95	0.18	34,34,34,34	0
35	NA	0	8505	1/1	0.95	0.18	33,33,33,33	0
35	NA	A	8545	1/1	0.96	0.16	62,62,62,62	0
34	K	0	8401	1/1	0.96	0.18	85,85,85,85	0
33	MG	0	8099	1/1	0.96	0.16	45,45,45,45	0
33	MG	0	8071	1/1	0.96	0.04	69,69,69,69	0
35	NA	0	8515	1/1	0.96	0.20	42,42,42,42	0
33	MG	0	8031	1/1	0.96	0.12	34,34,34,34	0
33	MG	0	8014	1/1	0.96	0.16	32,32,32,32	0
33	MG	0	8068	1/1	0.96	0.04	61,61,61,61	0
35	NA	0	8514	1/1	0.96	0.27	38,38,38,38	0
33	MG	0	8042	1/1	0.96	0.10	38,38,38,38	0
35	NA	0	8549	1/1	0.96	0.18	51,51,51,51	0
33	MG	0	8043	1/1	0.96	0.08	48,48,48,48	0
35	NA	0	8539	1/1	0.96	0.15	30,30,30,30	0
37	CD	O	8605	1/1	0.96	0.08	93,93,93,93	0
35	NA	0	8575	1/1	0.96	0.27	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	0	8714	1/1	0.96	0.14	54,54,54,54	0
35	NA	0	8543	1/1	0.96	0.19	39,39,39,39	0
36	CL	R	8706	1/1	0.96	0.15	46,46,46,46	0
35	NA	0	8525	1/1	0.96	0.15	56,56,56,56	0
36	CL	0	8716	1/1	0.96	0.09	56,56,56,56	0
33	MG	0	8091	1/1	0.96	0.07	51,51,51,51	0
33	MG	0	8035	1/1	0.97	0.05	46,46,46,46	0
35	NA	0	8520	1/1	0.97	0.14	34,34,34,34	0
33	MG	0	8027	1/1	0.97	0.04	44,44,44,44	0
33	MG	K	8069	1/1	0.97	0.05	58,58,58,58	0
35	NA	0	8579	1/1	0.97	0.19	64,64,64,64	0
35	NA	0	8531	1/1	0.97	0.15	50,50,50,50	0
33	MG	0	8058	1/1	0.97	0.06	39,39,39,39	0
33	MG	0	8051	1/1	0.97	0.05	59,59,59,59	0
33	MG	0	8012	1/1	0.97	0.10	39,39,39,39	0
33	MG	0	8094	1/1	0.97	0.07	77,77,77,77	0
35	NA	0	8530	1/1	0.97	0.15	50,50,50,50	0
33	MG	0	8032	1/1	0.97	0.06	28,28,28,28	0
33	MG	0	8033	1/1	0.97	0.09	31,31,31,31	0
33	MG	0	8072	1/1	0.97	0.07	63,63,63,63	0
33	MG	0	8054	1/1	0.97	0.17	37,37,37,37	0
35	NA	0	8555	1/1	0.97	0.34	57,57,57,57	0
33	MG	0	8040	1/1	0.97	0.13	60,60,60,60	0
33	MG	0	8063	1/1	0.97	0.21	60,60,60,60	0
33	MG	0	8080	1/1	0.97	0.19	45,45,45,45	0
33	MG	0	8057	1/1	0.97	0.18	45,45,45,45	0
33	MG	0	8028	1/1	0.97	0.05	38,38,38,38	0
35	NA	0	8518	1/1	0.97	0.19	42,42,42,42	0
35	NA	0	8502	1/1	0.97	0.21	51,51,51,51	0
33	MG	0	8061	1/1	0.97	0.17	41,41,41,41	0
36	CL	J	8702	1/1	0.97	0.10	57,57,57,57	0
33	MG	0	8013	1/1	0.97	0.12	38,38,38,38	0
33	MG	0	8093	1/1	0.97	0.09	56,56,56,56	0
35	NA	0	8553	1/1	0.97	0.11	30,30,30,30	0
35	NA	0	8544	1/1	0.97	0.10	28,28,28,28	0
33	MG	0	8088	1/1	0.97	0.14	38,38,38,38	0
33	MG	0	8015	1/1	0.97	0.14	35,35,35,35	0
33	MG	0	8064	1/1	0.97	0.07	30,30,30,30	0
36	CL	0	8703	1/1	0.97	0.08	58,58,58,58	0
35	NA	0	8578	1/1	0.97	0.28	51,51,51,51	0
33	MG	0	8023	1/1	0.97	0.26	41,41,41,41	0
33	MG	0	8110	1/1	0.97	0.11	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	CD	Z	8603	1/1	0.97	0.09	98,98,98,98	0
33	MG	0	8070	1/1	0.97	0.16	50,50,50,50	0
33	MG	0	8025	1/1	0.97	0.09	37,37,37,37	0
35	NA	L	8580	1/1	0.97	0.28	57,57,57,57	0
33	MG	0	8089	1/1	0.97	0.14	74,74,74,74	0
33	MG	0	8067	1/1	0.97	0.12	52,52,52,52	0
33	MG	0	8008	1/1	0.97	0.14	37,37,37,37	0
33	MG	0	8117	1/1	0.98	0.06	32,32,32,32	0
33	MG	0	8079	1/1	0.98	0.17	37,37,37,37	0
35	NA	0	8554	1/1	0.98	0.16	40,40,40,40	0
33	MG	0	8020	1/1	0.98	0.09	33,33,33,33	0
33	MG	0	8076	1/1	0.98	0.12	55,55,55,55	0
33	MG	0	8022	1/1	0.98	0.10	38,38,38,38	0
33	MG	0	8045	1/1	0.98	0.07	53,53,53,53	0
33	MG	0	8106	1/1	0.98	0.09	65,65,65,65	0
33	MG	0	8002	1/1	0.98	0.09	34,34,34,34	0
36	CL	B	8719	1/1	0.98	0.12	51,51,51,51	0
35	NA	0	8576	1/1	0.98	0.24	46,46,46,46	0
33	MG	0	8107	1/1	0.98	0.08	36,36,36,36	0
33	MG	3	8078	1/1	0.98	0.06	43,43,43,43	0
35	NA	0	8528	1/1	0.98	0.32	42,42,42,42	0
33	MG	0	8011	1/1	0.98	0.18	27,27,27,27	0
36	CL	Y	8720	1/1	0.98	0.13	46,46,46,46	0
33	MG	0	8029	1/1	0.98	0.07	35,35,35,35	0
33	MG	0	8074	1/1	0.98	0.05	36,36,36,36	0
33	MG	0	8036	1/1	0.98	0.06	33,33,33,33	0
36	CL	0	8712	1/1	0.98	0.08	49,49,49,49	0
33	MG	0	8048	1/1	0.98	0.12	54,54,54,54	0
33	MG	0	8004	1/1	0.98	0.09	29,29,29,29	0
33	MG	0	8007	1/1	0.98	0.13	22,22,22,22	0
36	CL	J	8721	1/1	0.98	0.10	58,58,58,58	0
33	MG	0	8077	1/1	0.98	0.14	33,33,33,33	0
33	MG	0	8111	1/1	0.98	0.09	42,42,42,42	0
33	MG	0	8115	1/1	0.98	0.08	52,52,52,52	0
33	MG	0	8016	1/1	0.98	0.09	40,40,40,40	0
33	MG	0	8017	1/1	0.98	0.13	26,26,26,26	0
33	MG	0	8062	1/1	0.98	0.09	54,54,54,54	0
33	MG	0	8024	1/1	0.98	0.13	21,21,21,21	0
33	MG	0	8026	1/1	0.98	0.17	26,26,26,26	0
33	MG	0	8037	1/1	0.98	0.09	43,43,43,43	0
33	MG	0	8019	1/1	0.98	0.06	35,35,35,35	0
33	MG	B	8056	1/1	0.98	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	Q	8711	1/1	0.98	0.09	55,55,55,55	0
33	MG	0	8052	1/1	0.98	0.07	54,54,54,54	0
33	MG	0	8098	1/1	0.98	0.08	40,40,40,40	0
33	MG	0	8018	1/1	0.98	0.14	50,50,50,50	0
33	MG	0	8021	1/1	0.98	0.12	30,30,30,30	0
33	MG	0	8059	1/1	0.99	0.06	43,43,43,43	0
36	CL	M	8718	1/1	0.99	0.13	47,47,47,47	0
33	MG	0	8006	1/1	0.99	0.06	33,33,33,33	0
33	MG	0	8009	1/1	0.99	0.17	35,35,35,35	0
33	MG	A	8065	1/1	0.99	0.06	41,41,41,41	0
33	MG	Y	8109	1/1	0.99	0.09	37,37,37,37	0
33	MG	0	8112	1/1	0.99	0.12	42,42,42,42	0
34	K	0	8402	1/1	0.99	0.14	57,57,57,57	0
37	CD	1	8602	1/1	0.99	0.10	63,63,63,63	0
33	MG	0	8038	1/1	0.99	0.13	34,34,34,34	0
33	MG	0	8001	1/1	0.99	0.14	36,36,36,36	0
33	MG	0	8030	1/1	0.99	0.10	25,25,25,25	0
33	MG	0	8108	1/1	0.99	0.09	70,70,70,70	0
37	CD	3	8604	1/1	0.99	0.08	68,68,68,68	0
33	MG	0	8083	1/1	0.99	0.12	43,43,43,43	0
33	MG	0	8005	1/1	0.99	0.16	33,33,33,33	0
33	MG	0	8003	1/1	0.99	0.09	35,35,35,35	0
33	MG	0	8034	1/1	0.99	0.09	33,33,33,33	0
33	MG	0	8060	1/1	0.99	0.27	40,40,40,40	0
37	CD	U	8601	1/1	1.00	0.09	62,62,62,62	0
33	MG	0	8010	1/1	1.00	0.17	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.