



wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:42 am BST

PDB ID : 2QEX
Title : Negamycin Binds to the Wall of the Nascent Chain Exit Tunnel of the 50S Ribosomal Subunit
Authors : Schroeder, S.J.; Blaha, G.
Deposited on : 2007-06-26
Resolution : 2.90 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:

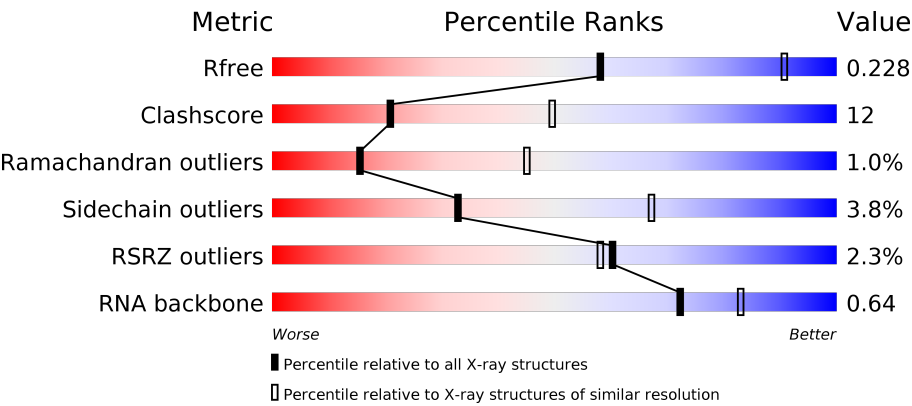
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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	2772	<div><div>0%</div><div><div>61%</div><div>32%</div><div>6%</div></div><div></div></div>
2	9	122	<div><div>2%</div><div><div>38%</div><div>50%</div><div>11%</div></div><div></div></div>
3	A	240	<div><div>0%</div><div><div>71%</div><div>25%</div><div></div></div><div></div></div>
4	B	338	<div><div></div><div><div>66%</div><div>31%</div><div></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	174	
11	J	145	
12	K	132	
13	L	165	
14	M	196	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	67	
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	 72% 27%
31	I	162	 36% 26% 17% 57%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8024	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8574	-	-	-	X
34	NA	0	8577	-	-	-	X
37	CD	O	8705	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99020 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			

- 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			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	3073	G	A	CONFLICT	GB 6468293
9	3106	C	U	CONFLICT	GB 6468293

- 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 Acidic ribosomal protein P0 homolog.

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

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 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	INSERTION	UNP P60617
H	165	SER	LYS	CONFLICT	UNP P60617
H	166	SER	VAL	CONFLICT	UNP P60617
H	167	PRO	GLU	CONFLICT	UNP P60617
H	168	ALA	ARG	CONFLICT	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	GLU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	?	-	LEU	DELETION	UNP P60617
H	170	ASN	ILE	CONFLICT	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
			1559	943	332	283	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	GLY	CONFLICT	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	SER	CONFLICT	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
			431	258	86	83	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	Y	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	72	Total	Na	0	0
			72	72		
34	J	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	A	1	Total	Na	0	0
			1	1		
34	R	3	Total	Na	0	0
			3	3		
34	9	3	Total	Na	0	0
			3	3		
34	L	1	Total	Na	0	0
			1	1		
34	S	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		

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

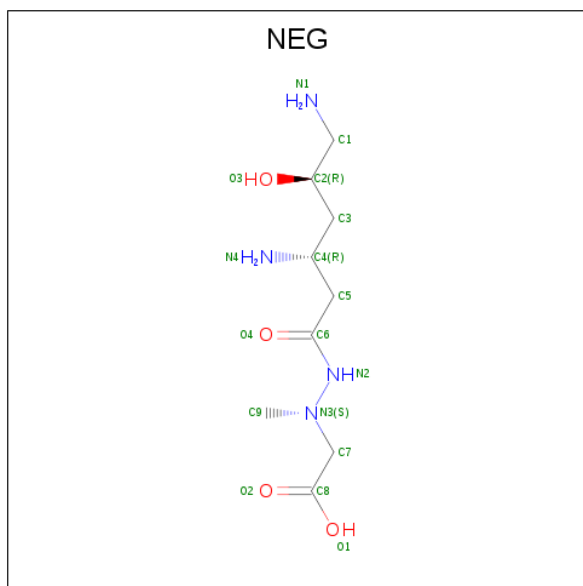
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	10	Total	Cl	0	0
			10	10		
35	J	3	Total	Cl	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Q	1	Total	Cl	0	0
			1	1		
35	B	1	Total	Cl	0	0
			1	1		
35	A	1	Total	Cl	0	0
			1	1		
35	N	1	Total	Cl	0	0
			1	1		
35	O	1	Total	Cl	0	0
			1	1		
35	R	1	Total	Cl	0	0
			1	1		
35	L	1	Total	Cl	0	0
			1	1		
35	3	1	Total	Cl	0	0
			1	1		
35	M	1	Total	Cl	0	0
			1	1		

- Molecule 36 is NEGAMYCIN (three-letter code: NEG) (formula: $C_9H_{20}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	0	1	Total	C	N	O	0	0
			17	9	4	4		

- 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	5923	Total O 5923 5923	0	0
38	9	142	Total O 142 142	0	0
38	A	112	Total O 112 112	0	0
38	B	137	Total O 137 137	0	0
38	C	167	Total O 167 167	0	0
38	D	44	Total O 44 44	0	0
38	E	45	Total O 45 45	0	0
38	F	27	Total O 27 27	0	0
38	G	16	Total O 16 16	0	0
38	H	70	Total O 70 70	0	0
38	J	51	Total O 51 51	0	0
38	K	57	Total O 57 57	0	0
38	L	85	Total O 85 85	0	0
38	M	122	Total O 122 122	0	0
38	N	61	Total O 61 61	0	0

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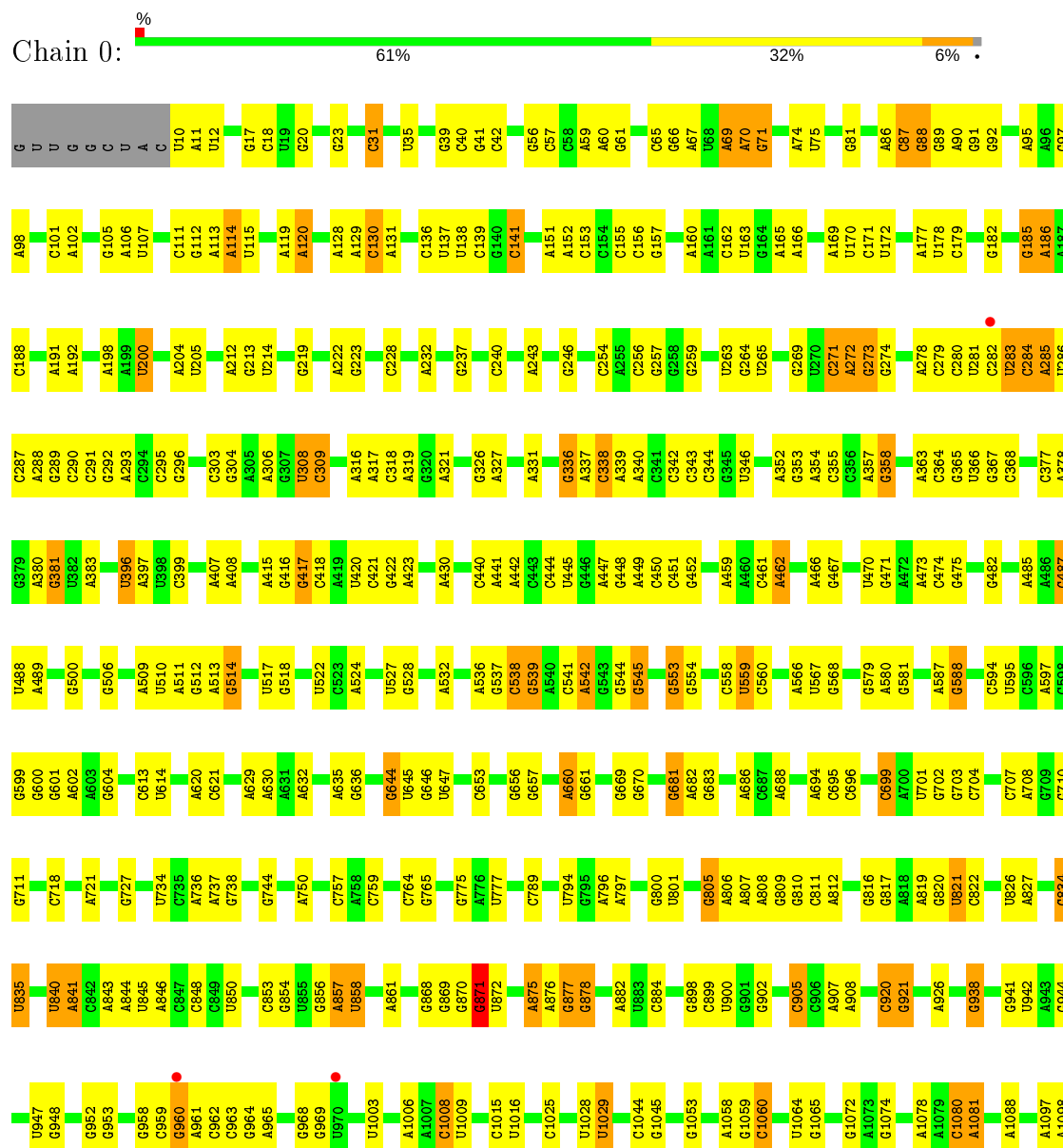
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	38	Total 38	O 38	0	0
38	P	63	Total 63	O 63	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	39	Total 39	O 39	0	0
38	T	30	Total 30	O 30	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0	0
38	W	69	Total 69	O 69	0	0
38	X	24	Total 24	O 24	0	0
38	Y	87	Total 87	O 87	0	0
38	Z	30	Total 30	O 30	0	0
38	1	60	Total 60	O 60	0	0
38	2	36	Total 36	O 36	0	0
38	3	74	Total 74	O 74	0	0
38	I	5	Total 5	O 5	0	0

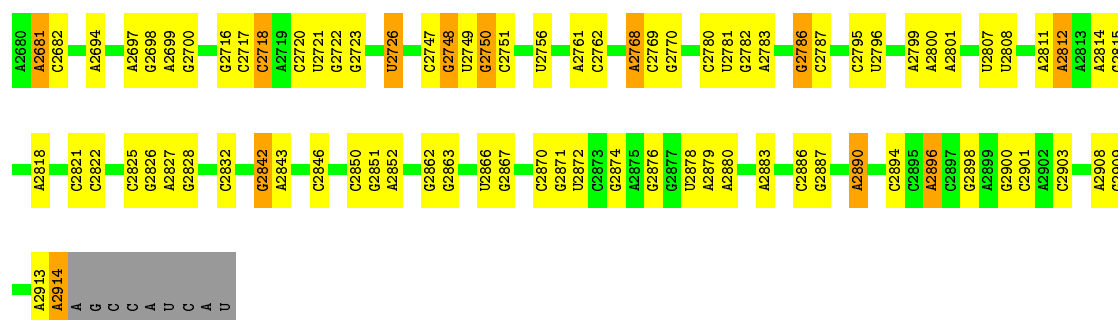
3 Residue-property plots

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.

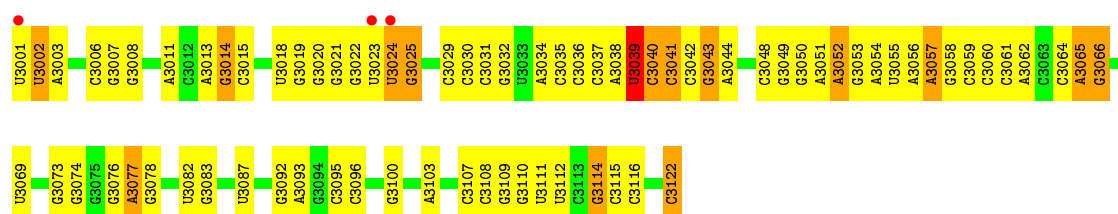
• Molecule 1: 23S ribosomal RNA



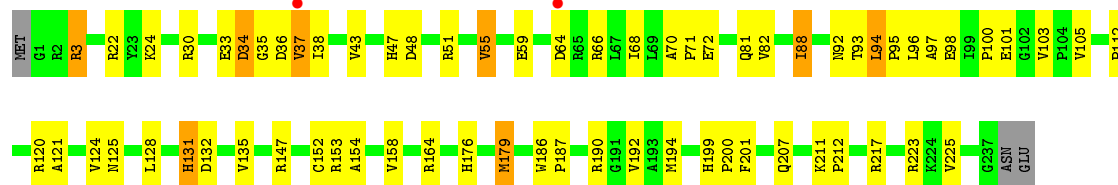
G2543	G2544	G2545	G2546	G2552	A2553	G2559	G2563	G2564	G2565	G2570	G2577	G2578	U2586	U2587	G2588	U2589	U2590	C2591	G2592	U2598	A2599	A2600	A2601	G2602	U2607	G2608	G2613	G2614	G2634	A2635	G2636	U2645	U2648	A2649	U2650	G2651	U2652	U2663	A2664	G2667	G2672	G2676	G2679							
G2350	C2351	A2354	A2361	A2362	G2363	A2364	A2369	A2372	U2373	A2374	G2375	A2382	G2385	U2386	U2387	C2388	A2401	A2402	C2403	G2404	G2412	A2413	A2414	A2415	G2416	U2419	G2420	G2421	U2422	A2423	U2424	A2425	G2426	A2429	A2430	A2433	A2434	U2435	G2438	C2439	G2446	A2447	G2453	G2542						
A2244	C2247	C2248	G2251	A2252	G2253	G2254	G2256	G2257	A2258	G2263	A2264	U2265	A2266	C2269	G2270	G2271	G2272	C2273	A2274	G2275	G2285	C2286	G2287	G2288	G2289	U2290	A2291	A2300	A2301	C2309	C2313	G2316	G2317	U2320	A2321	U2322	G2323	U2326	A2327	U2328	G2329	U2330	C2331	G2338	C2346					
A2010	A2011	U2012	G2013	U2016	U2017	A2018	A2019	G2033	U2034	C2047	C2048	G2049	G2050	A2054	U2063	U2064	G2072	G2073	A2074	A2081	G2090	G2091	G2092	G2093	A2096	A2100	A2101	G2102	U2107	A2108	U2109	G2110	C2114	U2115	U2133	G2134	A2135	G2136	G2237	C2243										
U1887	C1888	C1889	U1890	G1902	U1903	C1914	A1919	C1920	A1921	A1922	G1925	G1926	A1927	A1931	G1932	U1933	G1940	A1941	A1942	G1947	G1950	U1951	U1964	U1965	U1966	G1971	U1972	A1973	G1974	G1975	G1976	U1977	A1978	G1979	U1980	U1992	C1993	A1994	G1995	U1996	G2001	C2002	U2003	U2004	G2005	C2006	U2008			
G1774	G1777	A1778	A1779	C1787	U1788	G1789	U1791	G1795	A1796	A1797	C1798	G1803	A1804	G1805	G1806	U1807	A1808	G1809	G1818	G1819	G1820	A1821	G1823	C1826	G1827	G1828	A1829	C1834	U1835	A1839	A1840	G1867	G1868	U1871	C1872	G1873	G1874	U1874	G1877	G1878	U1879	U1883								
A1682	C1683	A1684	A1685	C1686	C1687	C1692	G1697	U1698	C1699	C1700	A1701	U1702	G1706	G1707	C1714	C1715	A1716	A1717	U1722	G1723	U1724	C1725	G1730	C1731	U1735	G1736	G1739	U1740	U1741	A1742	G1751	G1752	A1755	G1756	A1759	U1760	U1761	C1762	C1763	G1764	G1765	A1767	C1768	C1769	G1773					
C1584	C1585	G1586	U1587	G1588	G1589	C1592	C1593	C1594	G1595	U1596	U1597	A1603	G1604	G1605	A1606	A1607	A1624	U1625	A1626	G1627	C1633	G1634	U1635	U1636	A1637	A1641	A1642	U1654	G1655	A1656	A1657	A1658	A1659	G1660	A1661	G1662	A1667	U1668	A1669	G1670	U1677	A1678	C1679							
U1500	U1503	A1504	U1505	U1506	C1507	C1508	G1512	C1513	A1514	A1515	C1516	U1517	U1518	U1519	G1520	C1521	A1522	U1523	U1524	G1525	A1526	A1527	A1528	G1529	C1537	C1545	A1546	U1547	U1548	C1549	A1550	C1551	G1552	C1553	G1555	G1556	G1557	C1558	A1559	U1561	C1562	G1563	G1568	U1569	A1573	C1574	G1575	A1576	U1577	A1580
G1269	G1273	U1279	C1289	G1290	A1291	G1299	U1304	C1305	U1306	A1307	A1308	U1309	A1310	A1313	G1319	C1320	A1321	G1322	A1326	G1216	G1217	G1218	U1219	G1226	C1229	A1230	G1339	G1340	A1341	C1342	C1343	G1344	A1352	A1353	U1359	C1360	A1364	G1365	U1366	A1367	C1368	A1369	G1370	U1371	A1372	G1376	C1377	G1378		
A1379	A1393	C1394	C1395	C1396	C1397	G1398	A1399	A1407	U1408	G1409	G1410	U1419	C1420	C1423	A1424	G1430	G1431	G1441	A1442	U1446	U1447	C1450	G1451	G1452	U1453	U1454	C1455	C1456	U1457	C1462	A1463	C1472	U1473	C1474	C1477	G1481	A1482	C1483	G1484	U1488	A1492	C1495	G1496	G1497						
A1191	A1192	A1193	A1194	G1195	C1196	G1197	U1198	A1199	A1200	C1201	G1202	G1203	C1204	U1205	U1206	A1207	C1208	C1209	G1210	G1211	G1212	C1213	G1214	A1215	G1226	C1229	A1230	G1339	G1340	A1341	C1342	C1343	G1344	A1352	A1353	U1359	C1360	A1364	G1365	U1366	A1367	C1368	A1369	G1370	U1371	A1372	G1376	C1377	G1378	
G1099	U1109	G1110	U1116	A1117	A1118	G1119	U1119	A1120	G1121	U1122	A1123	C1126	C1127	U1128	U1206	A1207	C1208	C1209	G1210	G1211	G1212	C1213	G1214	A1215	G1226	C1229	A1230	G1339	G1340	A1341	C1342	C1343	G1344	A1352	A1353	U1359	C1360	A1364	G1365	U1366	A1367	C1368	A1369	G1370	U1371	A1372	G1376	C1377	G1378	



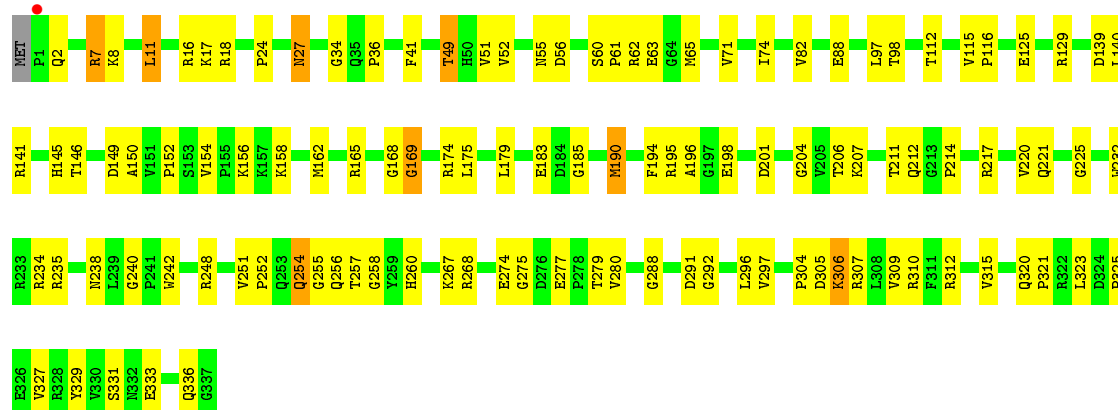
- Molecule 2: 5S ribosomal RNA




- Molecule 3: 50S ribosomal protein L2P

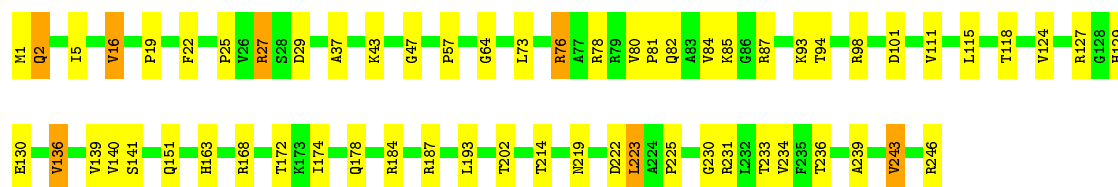


- Molecule 4: 50S ribosomal protein L3P



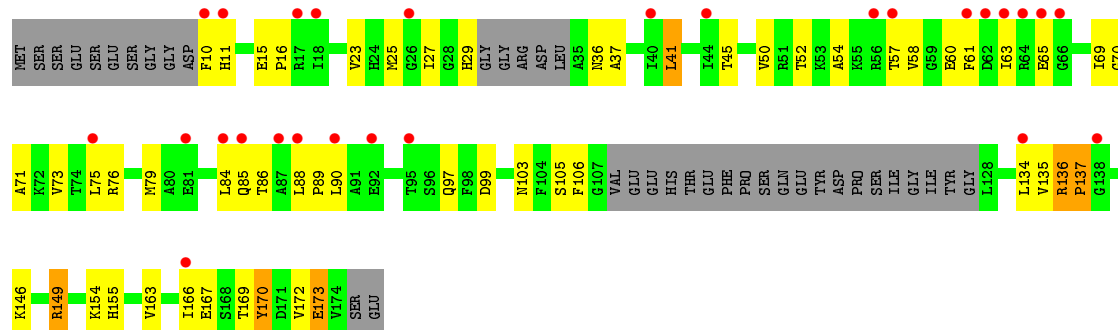
- Molecule 5: 50S ribosomal protein L4P

Chain C:  75% 22%



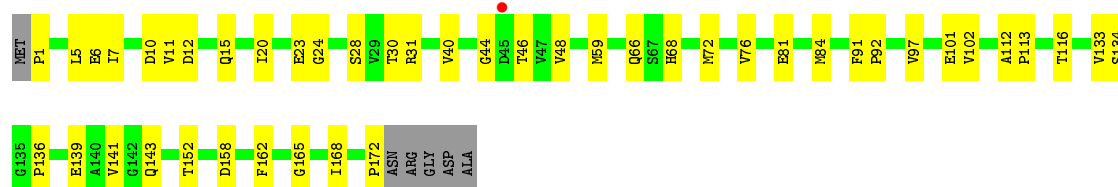
• Molecule 6: 50S ribosomal protein L5P

Chain D:  15% 49% 27% 21%



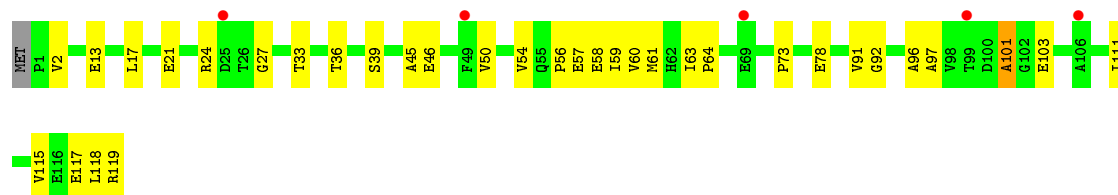
• Molecule 7: 50S ribosomal protein L6P

Chain E:  71% 25%



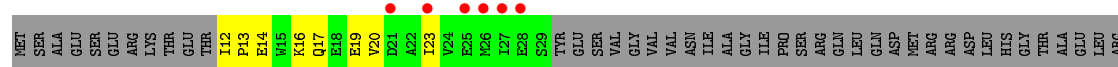
• Molecule 8: 50S ribosomal protein L7Ae

Chain F:  4% 71% 28%



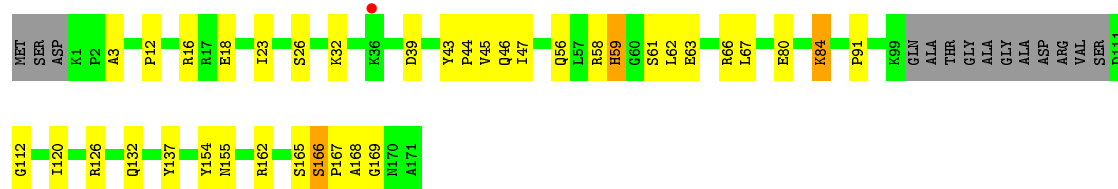
• Molecule 9: Acidic ribosomal protein P0 homolog

Chain G:  3% 5% 92%

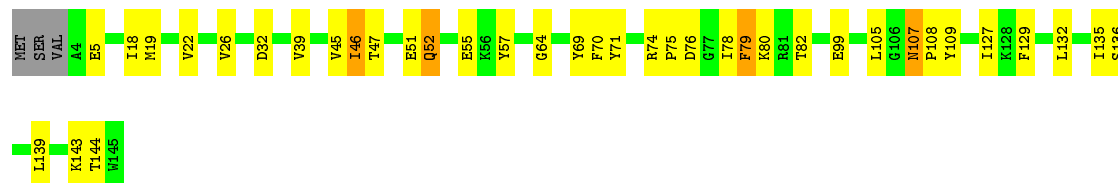




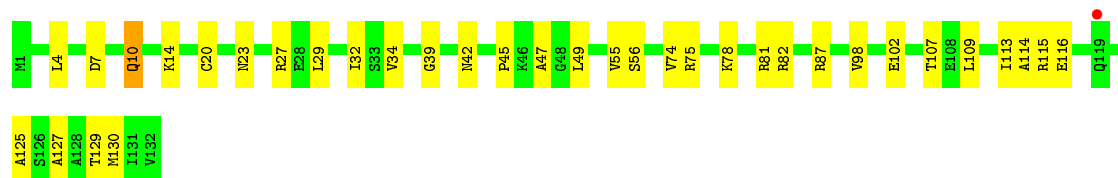
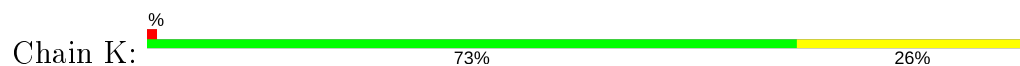
- Molecule 10: 50S ribosomal protein L10e



- Molecule 11: 50S ribosomal protein L13P

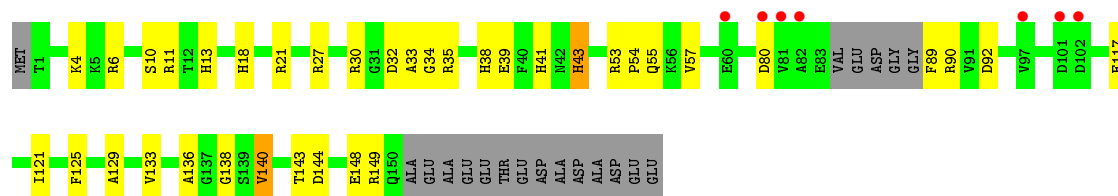


- Molecule 12: 50S ribosomal protein L14P

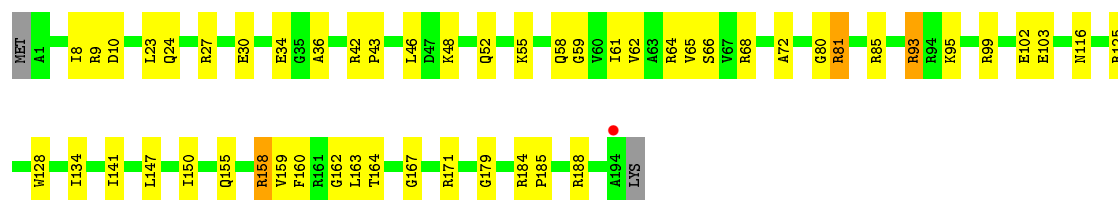


- Molecule 13: 50S ribosomal protein L15P

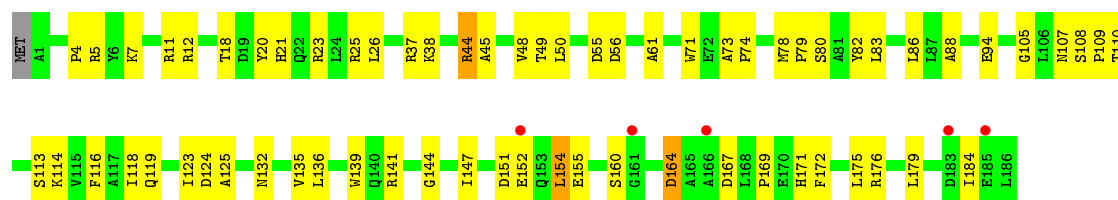




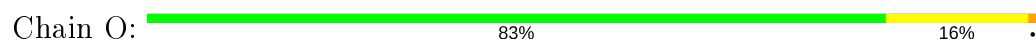
- Molecule 14: 50S ribosomal protein L15e



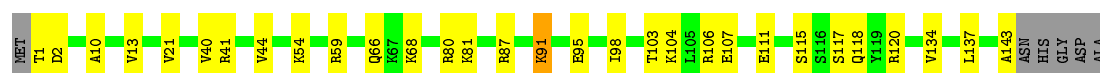
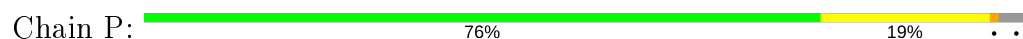
- Molecule 15: 50S ribosomal protein L18P



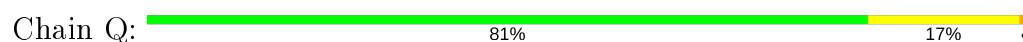
- Molecule 16: 50S ribosomal protein L18e




- Molecule 17: 50S ribosomal protein L19e

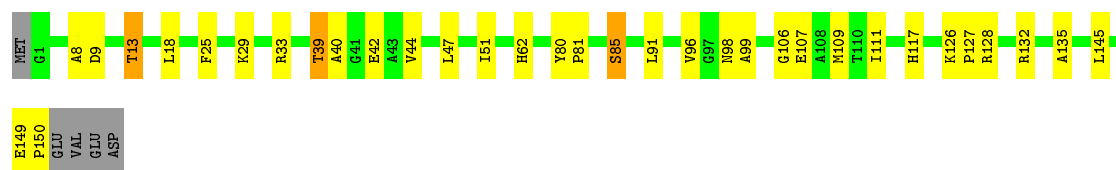


- Molecule 18: 50S ribosomal protein L21e




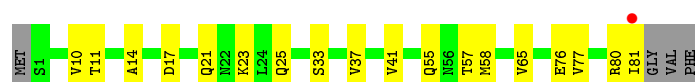
- Molecule 19: 50S ribosomal protein L22P

Chain R:  75% 20%



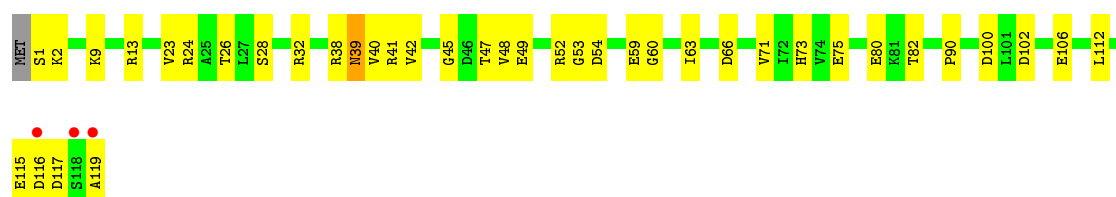
- Molecule 20: 50S ribosomal protein L23P

Chain S:  74% 21% 5%



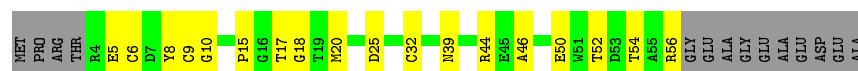
- Molecule 21: 50S ribosomal protein L24P

Chain T:  67% 32% 3%



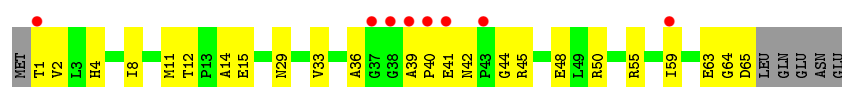
- Molecule 22: 50S ribosomal protein L24e

Chain U:  52% 27% 21%



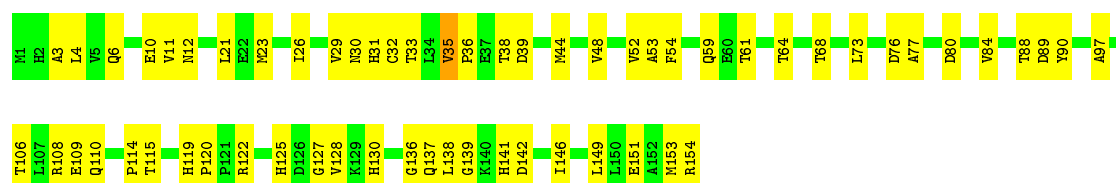
- Molecule 23: 50S ribosomal protein L29P

Chain V:  58% 34% 8%

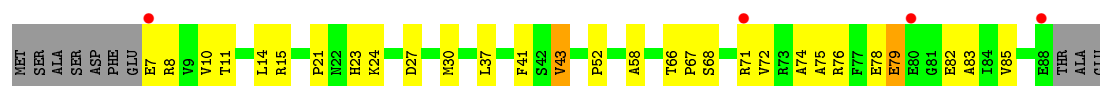


- Molecule 24: 50S ribosomal protein L30P

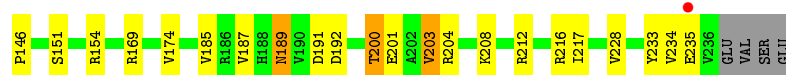
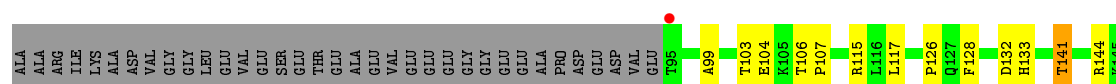
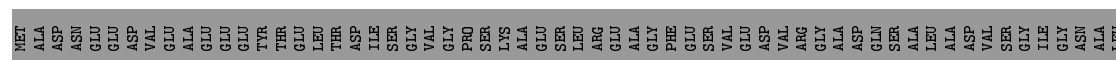
Chain W:  61% 38%



- Molecule 25: 50S ribosomal protein L31e



- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae



- Molecule 28: 50S ribosomal protein L37e



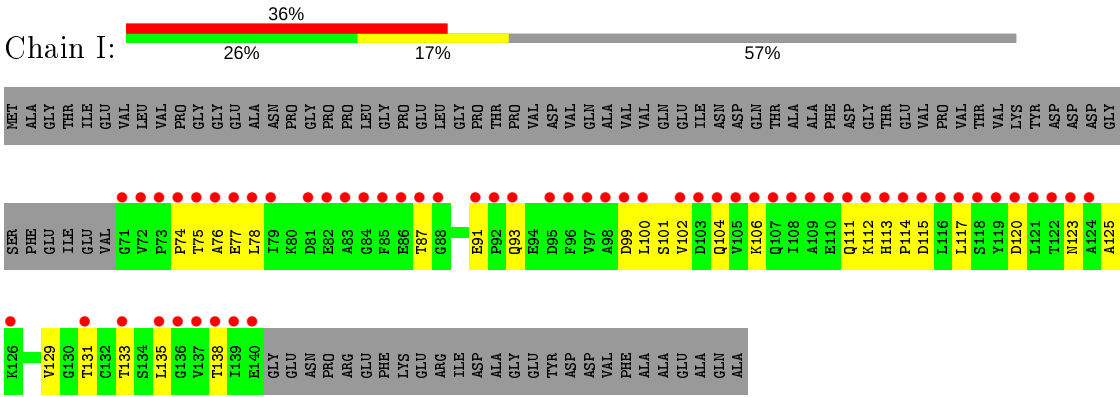
- Molecule 29: 50S ribosomal protein L39e



- 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	214.62Å 304.05Å 578.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 86.68 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.90) 90.6 (86.68-2.43)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.241 0.195 , 0.228	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.9	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	0.93	EDS
Total number of atoms	99020	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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, CL, NEG, K, UR3, CD, OMU, NA, 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	0.38	0/65959	0.69	10/102870 (0.0%)
2	9	0.35	0/2905	0.71	1/4528 (0.0%)
3	A	0.34	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.36	0/1884	0.63	0/2551
6	D	0.33	0/1111	0.57	0/1498
7	E	0.33	0/1382	0.57	0/1880
8	F	0.35	0/901	0.58	0/1224
9	G	0.35	0/241	0.52	0/324
10	H	0.34	0/1287	0.65	1/1725 (0.1%)
11	J	0.35	0/1136	0.60	0/1530
12	K	0.35	0/1001	0.65	0/1347
13	L	0.33	0/1130	0.65	0/1509
14	M	0.35	0/1583	0.61	0/2119
15	N	0.30	0/1474	0.65	0/1999
16	O	0.34	0/874	0.62	1/1181 (0.1%)
17	P	0.35	0/1147	0.53	0/1528
18	Q	0.37	0/749	0.67	0/1005
19	R	0.40	0/1172	0.65	0/1578
20	S	0.34	0/648	0.57	0/875
21	T	0.32	0/958	0.62	0/1289
22	U	0.36	0/417	0.53	0/562
23	V	0.31	0/502	0.55	0/675
24	W	0.34	0/1219	0.63	0/1655
25	X	0.35	0/664	0.60	0/895
26	Y	0.35	0/1146	0.62	0/1536
27	Z	0.35	0/590	0.63	0/787
28	1	0.41	0/438	0.66	0/578
29	2	0.36	0/401	0.57	0/529
30	3	0.37	0/771	0.57	0/1024
31	I	0.34	0/526	0.53	0/716
All	All	0.37	0/98692	0.67	13/147577 (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	1	37
2	9	0	2
All	All	1	39

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	805	G	C2'-C3'-O3'	7.33	125.62	109.50
1	0	1942	A	C5'-C4'-C3'	6.85	126.95	116.00
1	0	871	G	C5'-C4'-O4'	-5.95	101.95	109.10
2	9	3039	U	N1-C1'-C2'	5.83	121.57	114.00
1	0	1942	A	C5'-C4'-O4'	5.80	116.06	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	805	G	C3'

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	23	G	Sidechain
1	0	246	G	Sidechain
1	0	396	U	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain

5.2 Too-close contacts [i](#)

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	1019	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	2600	0	1326	87	0
3	A	1753	0	1766	61	0
4	B	2625	0	2533	85	0
5	C	1859	0	1816	53	0
6	D	1094	0	1085	39	0
7	E	1357	0	1266	32	0
8	F	890	0	843	24	0
9	G	240	0	231	12	0
10	H	1266	0	1268	31	0
11	J	1120	0	1098	36	0
12	K	992	0	1031	36	0
13	L	1118	0	1076	33	0
14	M	1559	0	1568	38	0
15	N	1445	0	1401	63	0
16	O	865	0	873	21	0
17	P	1136	0	1123	24	0
18	Q	735	0	729	12	0
19	R	1149	0	1122	29	0
20	S	641	0	605	15	0
21	T	950	0	923	27	0
22	U	410	0	364	19	0
23	V	499	0	511	17	0
24	W	1196	0	1137	54	0
25	X	654	0	653	22	0
26	Y	1130	0	1133	35	0
27	Z	579	0	539	19	0
28	1	431	0	426	19	0
29	2	396	0	413	18	0
30	3	755	0	730	19	0
31	I	519	0	500	30	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	1	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
36	0	17	0	19	5	0
37	1	1	0	0	0	0
37	3	1	0	0	1	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5923	0	0	177	0
38	1	60	0	0	2	0
38	2	36	0	0	3	0
38	3	74	0	0	6	0
38	9	142	0	0	14	0
38	A	112	0	0	7	0
38	B	137	0	0	14	0
38	C	167	0	0	10	0
38	D	44	0	0	5	0
38	E	45	0	0	3	0
38	F	27	0	0	2	0
38	G	16	0	0	1	0
38	H	70	0	0	5	0
38	I	5	0	0	2	0
38	J	51	0	0	3	0
38	K	57	0	0	6	0
38	L	85	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	122	0	0	2	0
38	N	61	0	0	7	0
38	O	38	0	0	5	0
38	P	63	0	0	1	0
38	Q	50	0	0	1	0
38	R	85	0	0	5	0
38	S	39	0	0	4	0
38	T	30	0	0	1	0
38	U	28	0	0	1	0
38	V	11	0	0	1	0
38	W	69	0	0	3	0
38	X	24	0	0	2	0
38	Y	87	0	0	7	0
38	Z	30	0	0	2	0
All	All	99020	0	59918	1837	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 12.

The worst 5 of 1837 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1160:G:C5'	1:0:1161:A:H5'	1.70	1.22
1:0:871:G:C8	1:0:871:G:H5'	1.81	1.14
2:9:3006:C:H5''	15:N:37:ARG:NH1	1.63	1.12
1:0:871:G:H8	1:0:871:G:H5'	1.10	1.11
1:0:656:G:H5'	16:O:3:THR:HG22	1.18	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	215 (92%)	16 (7%)	4 (2%)	9	31
4	B	335/338 (99%)	307 (92%)	23 (7%)	5 (2%)	10	34
5	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	19	51
6	D	134/177 (76%)	108 (81%)	22 (16%)	4 (3%)	4	17
7	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	13	40
8	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	17	48
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/174 (90%)	144 (92%)	11 (7%)	1 (1%)	25	58
11	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	11	36
12	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
13	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	11	36
14	M	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
15	N	184/187 (98%)	163 (89%)	18 (10%)	3 (2%)	9	32
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	17	48
22	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	12	37
25	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	5	21
26	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	3	10
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%)	85 (94%)	4 (4%)	1 (1%)	14	42
31	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	10	34
All	All	3705/4426 (84%)	3419 (92%)	250 (7%)	36 (1%)	15	45

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	37	VAL
8	F	101	ALA
15	N	154	LEU
15	N	184	ILE
24	W	77	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	179/182 (98%)	171 (96%)	8 (4%)	27	61
4	B	282/283 (100%)	271 (96%)	11 (4%)	32	66
5	C	193/193 (100%)	179 (93%)	14 (7%)	14	38
6	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
7	E	152/156 (97%)	150 (99%)	2 (1%)	69	90
8	F	93/94 (99%)	92 (99%)	1 (1%)	73	92
9	G	27/283 (10%)	26 (96%)	1 (4%)	34	68
10	H	132/141 (94%)	125 (95%)	7 (5%)	22	54
11	J	118/121 (98%)	112 (95%)	6 (5%)	24	56
12	K	106/106 (100%)	102 (96%)	4 (4%)	33	67
13	L	113/127 (89%)	108 (96%)	5 (4%)	28	61
14	M	158/160 (99%)	149 (94%)	9 (6%)	20	51
15	N	149/150 (99%)	142 (95%)	7 (5%)	26	59
16	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
17	P	113/117 (97%)	110 (97%)	3 (3%)	44	77
18	Q	79/80 (99%)	76 (96%)	3 (4%)	33	67
19	R	117/122 (96%)	114 (97%)	3 (3%)	46	77
20	S	71/74 (96%)	71 (100%)	0	100	100
21	T	105/106 (99%)	99 (94%)	6 (6%)	20	51
22	U	44/53 (83%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	V	51/57 (90%)	50 (98%)	1 (2%)	55 82
24	W	130/130 (100%)	125 (96%)	5 (4%)	33 67
25	X	66/74 (89%)	61 (92%)	5 (8%)	13 36
26	Y	120/196 (61%)	116 (97%)	4 (3%)	38 72
27	Z	60/60 (100%)	59 (98%)	1 (2%)	60 86
28	1	46/47 (98%)	46 (100%)	0	100 100
29	2	42/46 (91%)	41 (98%)	1 (2%)	49 79
30	3	79/79 (100%)	77 (98%)	2 (2%)	47 78
31	I	58/130 (45%)	58 (100%)	0	100 100
All	All	3093/3609 (86%)	2975 (96%)	118 (4%)	33 67

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	39	VAL
13	L	140	VAL
25	X	79	GLU
11	J	46	ILE
12	K	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	58	GLN
19	R	98	ASN
29	2	45	ASN
14	M	137	ASN
17	P	118	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2772 (99%)	234 (8%)	28 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/2894 (99%)	251 (8%)	29 (1%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1506	U
1	0	2726	U
1	0	1450	C
1	0	1684	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	1.05	1 (7%)	14,31,34	1.18	1 (7%)
1	UR3	0	2619	1	14,22,23	0.81	1 (7%)	15,32,35	0.70	0
1	1MA	0	628	1	15,25,26	0.80	0	15,37,40	1.38	1 (6%)
1	OMG	0	2588	1	18,26,27	1.12	1 (5%)	20,38,41	2.59	5 (25%)
1	PSU	0	2621	1	17,21,22	1.54	3 (17%)	20,30,33	5.42	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	OMU	0	2587	1	-	0/7/27/28	0/2/2/2

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

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'	-4.67	1.48	1.52
1	0	2588	OMG	C6-N1	3.47	1.39	1.33
1	0	2587	OMU	C4-N3	2.85	1.38	1.33
1	0	2621	PSU	C4-N3	2.72	1.37	1.33
1	0	2621	PSU	C2-N1	2.49	1.43	1.38

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	-17.27	114.70	128.43
1	0	2621	PSU	C4-N3-C2	14.32	127.23	115.14
1	0	2588	OMG	C5-C6-N1	-8.67	111.57	123.43
1	0	2621	PSU	C5-C4-N3	-8.12	114.89	125.36
1	0	2588	OMG	C6-N1-C2	5.73	125.04	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
36	NEG	0	8823	32	9,16,16	0.53	0	10,20,20	0.72	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
36	NEG	0	8823	32	-	3/15/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	0	8823	NEG	C6-N2-N3-C7
36	0	8823	NEG	C2-C3-C4-N4
36	0	8823	NEG	C6-N2-N3-C9

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8823	NEG	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	2749/2772 (99%)	-0.77	14 (0%) 91 91	19, 42, 86, 144	0
2	9	122/122 (100%)	-0.80	3 (2%) 57 55	35, 59, 83, 147	0
3	A	237/240 (98%)	-0.49	2 (0%) 86 86	25, 46, 78, 99	0
4	B	337/338 (99%)	-0.70	1 (0%) 94 94	26, 50, 75, 85	0
5	C	246/246 (100%)	-0.63	0 100 100	23, 44, 66, 75	0
6	D	140/177 (79%)	1.00	27 (19%) 1 0	54, 94, 118, 126	0
7	E	172/178 (96%)	-0.53	1 (0%) 89 89	40, 63, 83, 88	0
8	F	119/120 (99%)	0.15	5 (4%) 36 32	42, 67, 89, 100	0
9	G	29/348 (8%)	1.07	9 (31%) 0 0	73, 89, 96, 98	0
10	H	160/174 (91%)	-0.18	1 (0%) 89 89	36, 56, 86, 95	0
11	J	142/145 (97%)	-0.70	0 100 100	32, 47, 68, 89	0
12	K	132/132 (100%)	-0.80	1 (0%) 86 86	29, 45, 67, 78	0
13	L	145/165 (87%)	-0.08	7 (4%) 30 27	23, 62, 102, 114	0
14	M	194/196 (98%)	-0.77	1 (0%) 91 91	30, 40, 55, 63	0
15	N	186/187 (99%)	-0.21	5 (2%) 54 50	37, 59, 103, 114	0
16	O	115/116 (99%)	-0.65	0 100 100	35, 51, 67, 76	0
17	P	143/149 (95%)	-0.62	0 100 100	36, 51, 63, 72	0
18	Q	95/96 (98%)	-0.65	0 100 100	33, 44, 56, 70	0
19	R	150/155 (96%)	-0.70	0 100 100	30, 43, 64, 79	0
20	S	81/85 (95%)	-0.12	1 (1%) 79 79	43, 58, 78, 80	0
21	T	119/120 (99%)	-0.35	3 (2%) 57 55	41, 54, 77, 95	0
22	U	53/67 (79%)	-0.60	0 100 100	37, 50, 70, 77	0
23	V	65/71 (91%)	0.74	8 (12%) 4 3	51, 72, 106, 114	0
24	W	154/154 (100%)	-0.58	0 100 100	33, 47, 63, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	-0.27	4 (4%) 29 26	43, 56, 81, 96	0
26	Y	142/241 (58%)	-0.72	2 (1%) 75 75	25, 42, 64, 84	0
27	Z	73/73 (100%)	-0.45	0 100 100	45, 57, 74, 93	0
28	1	56/57 (98%)	-0.80	0 100 100	28, 32, 39, 48	0
29	2	46/50 (92%)	-0.25	3 (6%) 18 14	34, 60, 93, 102	0
30	3	92/92 (100%)	-0.63	0 100 100	32, 51, 64, 75	0
31	I	70/162 (43%)	3.73	58 (82%) 0 0	101, 115, 127, 129	0
All	All	6646/7320 (90%)	-0.53	156 (2%) 60 58	19, 48, 93, 147	0

The worst 5 of 156 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	11.8
31	I	79	ILE	9.5
31	I	71	GLY	9.4
6	D	63	ILE	8.7
31	I	75	THR	7.5

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	UR3	0	2619	21/22	0.97	0.12	32,34,35,37	0
1	OMG	0	2588	24/25	0.97	0.12	26,32,34,36	0
1	1MA	0	628	23/24	0.98	0.14	26,29,30,31	0
1	PSU	0	2621	20/21	0.98	0.11	23,27,32,33	0
1	OMU	0	2587	21/22	0.99	0.09	29,31,33,36	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
34	NA	0	8574	1/1	0.03	0.84	73,73,73,73	0
37	CD	O	8705	1/1	0.49	0.41	187,187,187,187	0
32	MG	0	8106	1/1	0.51	0.17	63,63,63,63	0
34	NA	R	8538	1/1	0.53	0.10	55,55,55,55	0
32	MG	0	8076	1/1	0.56	0.12	44,44,44,44	0
34	NA	0	8577	1/1	0.58	0.53	70,70,70,70	0
34	NA	0	8582	1/1	0.59	0.26	88,88,88,88	0
34	NA	0	8584	1/1	0.63	0.36	68,68,68,68	0
32	MG	0	8050	1/1	0.66	0.15	66,66,66,66	0
32	MG	0	8080	1/1	0.68	0.18	48,48,48,48	0
34	NA	0	8558	1/1	0.70	0.41	68,68,68,68	0
34	NA	9	8551	1/1	0.71	0.23	95,95,95,95	0
32	MG	0	8024	1/1	0.72	0.67	80,80,80,80	0
34	NA	0	8567	1/1	0.75	0.28	51,51,51,51	0
32	MG	0	8071	1/1	0.77	0.12	62,62,62,62	0
32	MG	0	8113	1/1	0.77	0.13	49,49,49,49	0
34	NA	Q	8548	1/1	0.78	0.19	43,43,43,43	0
34	NA	0	8508	1/1	0.78	0.22	36,36,36,36	0
32	MG	B	8055	1/1	0.79	0.08	43,43,43,43	0
32	MG	0	8085	1/1	0.80	0.14	48,48,48,48	0
34	NA	A	8545	1/1	0.80	0.11	57,57,57,57	0
32	MG	0	8094	1/1	0.80	0.10	66,66,66,66	0
32	MG	0	8086	1/1	0.81	0.04	46,46,46,46	0
34	NA	0	8507	1/1	0.81	0.12	54,54,54,54	0
34	NA	0	8568	1/1	0.81	0.12	61,61,61,61	0
34	NA	0	8585	1/1	0.82	0.31	59,59,59,59	0
32	MG	0	8092	1/1	0.82	0.11	66,66,66,66	0
34	NA	0	8571	1/1	0.82	0.28	46,46,46,46	0
32	MG	0	8083	1/1	0.83	0.06	40,40,40,40	0
35	CL	L	8810	1/1	0.83	0.09	54,54,54,54	0
34	NA	0	8569	1/1	0.84	0.31	63,63,63,63	0
35	CL	0	8805	1/1	0.84	0.07	58,58,58,58	0
32	MG	0	8043	1/1	0.84	0.19	61,61,61,61	0
32	MG	0	8102	1/1	0.85	0.14	70,70,70,70	0
34	NA	0	8506	1/1	0.85	0.35	52,52,52,52	0
34	NA	9	8552	1/1	0.85	0.15	47,47,47,47	0
32	MG	0	8032	1/1	0.85	0.06	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8544	1/1	0.85	0.05	14,14,14,14	0
32	MG	0	8059	1/1	0.85	0.09	38,38,38,38	0
34	NA	0	8564	1/1	0.85	0.22	50,50,50,50	0
34	NA	0	8535	1/1	0.85	0.19	39,39,39,39	0
34	NA	0	8513	1/1	0.85	0.09	46,46,46,46	0
32	MG	0	8040	1/1	0.86	0.12	46,46,46,46	0
32	MG	0	8087	1/1	0.86	0.10	61,61,61,61	0
32	MG	0	8082	1/1	0.86	0.22	65,65,65,65	0
34	NA	0	8555	1/1	0.86	0.90	81,81,81,81	0
32	MG	0	8015	1/1	0.86	0.12	34,34,34,34	0
32	MG	0	8045	1/1	0.86	0.09	51,51,51,51	0
34	NA	0	8549	1/1	0.87	0.19	45,45,45,45	0
32	MG	0	8041	1/1	0.87	0.07	54,54,54,54	0
34	NA	0	8559	1/1	0.87	0.28	48,48,48,48	0
32	MG	0	8060	1/1	0.87	0.21	43,43,43,43	0
32	MG	0	8070	1/1	0.88	0.10	34,34,34,34	0
35	CL	O	8808	1/1	0.88	0.09	66,66,66,66	0
34	NA	R	8537	1/1	0.88	0.06	35,35,35,35	0
32	MG	0	8088	1/1	0.88	0.08	22,22,22,22	0
32	MG	0	8046	1/1	0.88	0.06	45,45,45,45	0
34	NA	0	8562	1/1	0.88	0.33	65,65,65,65	0
32	MG	0	8099	1/1	0.89	0.15	42,42,42,42	0
34	NA	H	8522	1/1	0.89	0.34	71,71,71,71	0
34	NA	0	8539	1/1	0.89	0.12	30,30,30,30	0
32	MG	0	8063	1/1	0.89	0.30	89,89,89,89	0
35	CL	J	8821	1/1	0.89	0.11	60,60,60,60	0
35	CL	0	8815	1/1	0.89	0.13	61,61,61,61	0
32	MG	0	8096	1/1	0.89	0.12	52,52,52,52	0
34	NA	0	8578	1/1	0.89	0.36	49,49,49,49	0
32	MG	0	8114	1/1	0.89	0.23	41,41,41,41	0
33	K	0	8401	1/1	0.90	0.35	78,78,78,78	0
34	NA	9	8583	1/1	0.90	0.21	63,63,63,63	0
32	MG	0	8072	1/1	0.90	0.09	55,55,55,55	0
34	NA	0	8573	1/1	0.90	0.33	56,56,56,56	0
32	MG	0	8035	1/1	0.90	0.06	36,36,36,36	0
36	NEG	0	8823	17/17	0.90	0.18	68,72,82,83	0
32	MG	0	8028	1/1	0.90	0.06	39,39,39,39	0
34	NA	R	8586	1/1	0.91	0.28	29,29,29,29	0
34	NA	0	8505	1/1	0.91	0.13	36,36,36,36	0
32	MG	Y	8109	1/1	0.91	0.10	36,36,36,36	0
34	NA	0	8529	1/1	0.91	0.14	56,56,56,56	0
34	NA	S	8512	1/1	0.91	0.67	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8502	1/1	0.91	0.11	51,51,51,51	0
34	NA	0	8572	1/1	0.91	0.19	68,68,68,68	0
32	MG	T	8073	1/1	0.91	0.04	63,63,63,63	0
32	MG	0	8047	1/1	0.91	0.05	72,72,72,72	0
32	MG	0	8110	1/1	0.91	0.12	54,54,54,54	0
35	CL	J	8802	1/1	0.91	0.12	58,58,58,58	0
32	MG	9	8095	1/1	0.92	0.05	55,55,55,55	0
35	CL	R	8806	1/1	0.92	0.07	52,52,52,52	0
32	MG	0	8004	1/1	0.92	0.15	23,23,23,23	0
34	NA	0	8554	1/1	0.92	0.23	39,39,39,39	0
34	NA	0	8566	1/1	0.92	0.12	74,74,74,74	0
32	MG	0	8108	1/1	0.92	0.04	66,66,66,66	0
32	MG	0	8062	1/1	0.92	0.21	5,5,5,5	0
32	MG	0	8019	1/1	0.92	0.04	26,26,26,26	0
32	MG	0	8057	1/1	0.92	0.10	29,29,29,29	0
35	CL	N	8807	1/1	0.92	0.12	57,57,57,57	0
34	NA	0	8532	1/1	0.92	0.09	34,34,34,34	0
34	NA	0	8527	1/1	0.93	0.15	46,46,46,46	0
32	MG	0	8117	1/1	0.93	0.09	45,45,45,45	0
32	MG	0	8075	1/1	0.93	0.10	57,57,57,57	0
34	NA	0	8517	1/1	0.93	0.07	24,24,24,24	0
32	MG	0	8021	1/1	0.93	0.07	37,37,37,37	0
34	NA	0	8523	1/1	0.93	0.26	56,56,56,56	0
34	NA	0	8561	1/1	0.93	0.33	61,61,61,61	0
34	NA	0	8550	1/1	0.93	0.17	40,40,40,40	0
34	NA	0	8511	1/1	0.93	0.09	46,46,46,46	0
32	MG	0	8042	1/1	0.93	0.05	35,35,35,35	0
34	NA	0	8526	1/1	0.93	0.16	63,63,63,63	0
32	MG	0	8054	1/1	0.94	0.14	24,24,24,24	0
32	MG	0	8017	1/1	0.94	0.12	25,25,25,25	0
34	NA	0	8524	1/1	0.94	0.10	45,45,45,45	0
32	MG	0	8112	1/1	0.94	0.07	38,38,38,38	0
32	MG	0	8100	1/1	0.94	0.21	37,37,37,37	0
32	MG	0	8011	1/1	0.94	0.08	23,23,23,23	0
35	CL	B	8819	1/1	0.94	0.06	39,39,39,39	0
34	NA	C	8504	1/1	0.94	0.18	41,41,41,41	0
34	NA	0	8501	1/1	0.94	0.04	51,51,51,51	0
34	NA	0	8557	1/1	0.94	0.05	49,49,49,49	0
35	CL	0	8820	1/1	0.94	0.06	36,36,36,36	0
34	NA	0	8528	1/1	0.94	0.18	39,39,39,39	0
35	CL	0	8803	1/1	0.94	0.07	52,52,52,52	0
32	MG	0	8116	1/1	0.94	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8111	1/1	0.94	0.13	50,50,50,50	0
34	NA	0	8543	1/1	0.94	0.09	32,32,32,32	0
32	MG	0	8009	1/1	0.94	0.15	31,31,31,31	0
35	CL	J	8801	1/1	0.94	0.08	54,54,54,54	0
32	MG	0	8044	1/1	0.95	0.06	33,33,33,33	0
32	MG	0	8098	1/1	0.95	0.17	31,31,31,31	0
32	MG	0	8052	1/1	0.95	0.14	77,77,77,77	0
34	NA	0	8581	1/1	0.95	0.05	38,38,38,38	0
32	MG	0	8104	1/1	0.95	0.16	67,67,67,67	0
32	MG	A	8065	1/1	0.95	0.12	37,37,37,37	0
34	NA	0	8536	1/1	0.95	0.06	38,38,38,38	0
33	K	0	8402	1/1	0.95	0.10	49,49,49,49	0
32	MG	0	8008	1/1	0.95	0.08	27,27,27,27	0
32	MG	0	8012	1/1	0.95	0.08	30,30,30,30	0
34	NA	0	8530	1/1	0.95	0.07	33,33,33,33	0
34	NA	J	8546	1/1	0.95	0.05	27,27,27,27	0
32	MG	0	8048	1/1	0.95	0.10	48,48,48,48	0
34	NA	0	8579	1/1	0.95	0.08	46,46,46,46	0
32	MG	0	8090	1/1	0.95	0.23	72,72,72,72	0
32	MG	0	8068	1/1	0.96	0.06	54,54,54,54	0
34	NA	0	8509	1/1	0.96	0.07	23,23,23,23	0
34	NA	0	8540	1/1	0.96	0.11	43,43,43,43	0
34	NA	0	8560	1/1	0.96	0.08	44,44,44,44	0
34	NA	L	8580	1/1	0.96	0.27	1,1,1,1	0
34	NA	0	8556	1/1	0.96	0.09	54,54,54,54	0
35	CL	0	8817	1/1	0.96	0.12	59,59,59,59	0
34	NA	0	8520	1/1	0.96	0.33	35,35,35,35	0
34	NA	0	8575	1/1	0.96	0.29	52,52,52,52	0
35	CL	0	8822	1/1	0.96	0.30	71,71,71,71	0
32	MG	A	8066	1/1	0.96	0.14	47,47,47,47	0
34	NA	0	8565	1/1	0.96	0.97	52,52,52,52	0
34	NA	0	8515	1/1	0.96	0.15	33,33,33,33	0
32	MG	0	8097	1/1	0.96	0.07	35,35,35,35	0
32	MG	0	8061	1/1	0.96	0.10	30,30,30,30	0
32	MG	0	8064	1/1	0.96	0.06	28,28,28,28	0
34	NA	0	8516	1/1	0.96	0.25	45,45,45,45	0
34	NA	0	8570	1/1	0.96	0.36	64,64,64,64	0
32	MG	0	8091	1/1	0.96	0.12	53,53,53,53	0
34	NA	0	8533	1/1	0.96	0.06	22,22,22,22	0
35	CL	0	8814	1/1	0.97	0.06	46,46,46,46	0
34	NA	0	8534	1/1	0.97	0.05	41,41,41,41	0
34	NA	0	8553	1/1	0.97	0.16	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8034	1/1	0.97	0.07	15,15,15,15	0
32	MG	0	8081	1/1	0.97	0.11	34,34,34,34	0
32	MG	0	8022	1/1	0.97	0.05	40,40,40,40	0
32	MG	0	8051	1/1	0.97	0.08	40,40,40,40	0
34	NA	0	8514	1/1	0.97	0.25	37,37,37,37	0
32	MG	0	8031	1/1	0.97	0.13	33,33,33,33	0
32	MG	0	8020	1/1	0.97	0.10	26,26,26,26	0
32	MG	0	8006	1/1	0.97	0.14	32,32,32,32	0
35	CL	0	8812	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8093	1/1	0.97	0.06	43,43,43,43	0
32	MG	0	8013	1/1	0.97	0.10	26,26,26,26	0
32	MG	0	8026	1/1	0.97	0.15	32,32,32,32	0
35	CL	A	8809	1/1	0.97	0.13	71,71,71,71	0
32	MG	0	8001	1/1	0.97	0.09	25,25,25,25	0
32	MG	0	8103	1/1	0.97	0.21	77,77,77,77	0
35	CL	Q	8811	1/1	0.97	0.07	58,58,58,58	0
34	NA	0	8525	1/1	0.98	0.14	71,71,71,71	0
32	MG	K	8069	1/1	0.98	0.07	54,54,54,54	0
32	MG	0	8003	1/1	0.98	0.08	29,29,29,29	0
32	MG	0	8107	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8037	1/1	0.98	0.09	38,38,38,38	0
34	NA	0	8541	1/1	0.98	0.11	47,47,47,47	0
32	MG	0	8018	1/1	0.98	0.17	26,26,26,26	0
32	MG	0	8038	1/1	0.98	0.14	21,21,21,21	0
32	MG	0	8115	1/1	0.98	0.03	41,41,41,41	0
32	MG	0	8101	1/1	0.98	0.21	71,71,71,71	0
32	MG	0	8067	1/1	0.98	0.11	52,52,52,52	0
32	MG	0	8058	1/1	0.98	0.07	32,32,32,32	0
34	NA	0	8503	1/1	0.98	0.26	1,1,1,1	0
34	NA	0	8518	1/1	0.98	0.12	40,40,40,40	0
34	NA	0	8576	1/1	0.98	0.20	24,24,24,24	0
34	NA	0	8531	1/1	0.98	0.12	35,35,35,35	0
35	CL	0	8813	1/1	0.98	0.06	55,55,55,55	0
32	MG	0	8023	1/1	0.98	0.15	39,39,39,39	0
34	NA	0	8563	1/1	0.98	0.19	52,52,52,52	0
32	MG	0	8056	1/1	0.98	0.06	42,42,42,42	0
32	MG	0	8029	1/1	0.98	0.06	36,36,36,36	0
32	MG	0	8030	1/1	0.99	0.06	20,20,20,20	0
37	CD	3	8704	1/1	0.99	0.05	53,53,53,53	0
32	MG	0	8027	1/1	0.99	0.06	39,39,39,39	0
32	MG	0	8039	1/1	0.99	0.11	43,43,43,43	0
32	MG	0	8084	1/1	0.99	0.03	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	CD	U	8701	1/1	0.99	0.06	63,63,63,63	0
35	CL	0	8816	1/1	0.99	0.12	57,57,57,57	0
32	MG	0	8079	1/1	0.99	0.14	27,27,27,27	0
35	CL	M	8818	1/1	0.99	0.09	36,36,36,36	0
32	MG	0	8074	1/1	0.99	0.04	28,28,28,28	0
32	MG	0	8077	1/1	0.99	0.13	30,30,30,30	0
34	NA	0	8521	1/1	0.99	0.21	43,43,43,43	0
32	MG	0	8016	1/1	0.99	0.13	19,19,19,19	0
34	NA	0	8519	1/1	0.99	0.12	21,21,21,21	0
32	MG	0	8036	1/1	0.99	0.04	29,29,29,29	0
34	NA	0	8510	1/1	0.99	0.13	22,22,22,22	0
32	MG	0	8025	1/1	0.99	0.10	32,32,32,32	0
37	CD	1	8702	1/1	0.99	0.09	55,55,55,55	0
34	NA	0	8542	1/1	0.99	0.28	1,1,1,1	0
32	MG	0	8010	1/1	0.99	0.16	13,13,13,13	0
32	MG	0	8049	1/1	0.99	0.12	30,30,30,30	0
32	MG	3	8078	1/1	0.99	0.15	11,11,11,11	0
32	MG	0	8053	1/1	0.99	0.03	50,50,50,50	0
32	MG	0	8089	1/1	0.99	0.12	32,32,32,32	0
32	MG	0	8002	1/1	0.99	0.14	27,27,27,27	0
34	NA	M	8547	1/1	0.99	0.04	35,35,35,35	0
32	MG	0	8005	1/1	1.00	0.14	32,32,32,32	0
32	MG	0	8007	1/1	1.00	0.15	9,9,9,9	0
35	CL	3	8804	1/1	1.00	0.04	42,42,42,42	0
37	CD	Z	8703	1/1	1.00	0.09	63,63,63,63	0
32	MG	0	8014	1/1	1.00	0.10	34,34,34,34	0
32	MG	0	8033	1/1	1.00	0.09	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.