



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 07:58 PM EDT

PDB ID : 3CCS  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A  
Authors : Blaha, G.; Gurel, G.  
Deposited on : unknown  
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

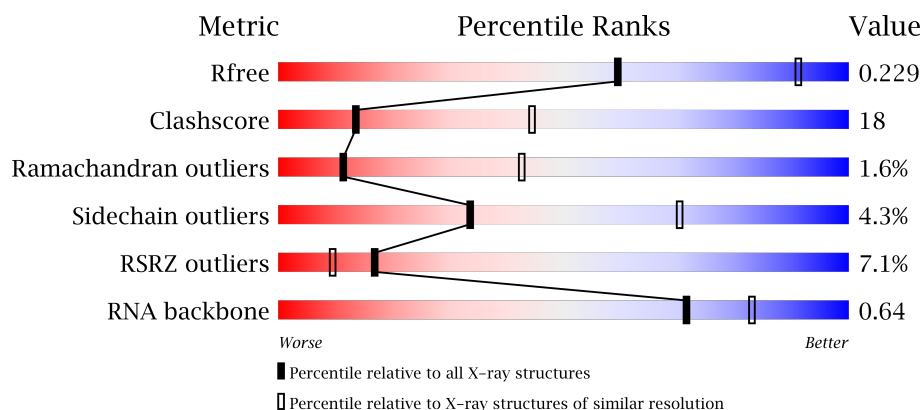
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)
RNA backbone	2435	1008 (3.30-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>3%</div> <div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>62%</div> <div>33%</div> <div>•</div> </div>
3	C	246	<div> <div>73%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>30%</div> <div>51%</div> <div>25%</div> <div>•</div> <div>21%</div> </div>



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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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	8009	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8079	-	-	-	X
32	MG	0	8080	-	-	-	X
32	MG	0	8085	-	-	-	X
33	CL	0	8812	-	-	X	-
33	CL	0	8816	-	-	-	X
33	CL	B	8819	-	-	-	X
33	CL	Y	8820	-	-	X	-
34	SR	0	8903	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8926	-	-	-	X
34	SR	0	8943	-	-	-	X
34	SR	0	8975	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8992	-	-	-	X
34	SR	B	8987	-	-	-	X
34	SR	L	8969	-	-	-	X
34	SR	R	8912	-	-	-	X
35	NA	0	8507	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8569	-	-	-	X
35	NA	0	8575	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	B	8552	-	-	-	X
36	K	0	8401	-	-	-	X
37	CD	3	8704	-	-	-	X
37	CD	U	8701	-	-	-	X
37	CD	Z	8703	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99121 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.



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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	86	Total	Mg	0	0
			86	86		
32	9	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	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	10	Total Cl 10 10	0	0
33	J	3	Total Cl 3 3	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	92	Total Sr 92 92	0	0
34	1	2	Total Sr 2 2	0	0
34	H	1	Total Sr 1 1	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	2	Total Sr 2 2	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	L	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	S	1	Total 1	Sr 1	0	0
34	F	1	Total 1	Sr 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total 65	Na 65	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	1	Total 1	K 1	0	0
36	M	1	Total 1	K 1	0	0

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	119	Total 119	O 119	0	0
38	B	152	Total 152	O 152	0	0
38	C	185	Total 185	O 185	0	0
38	D	42	Total 42	O 42	0	0
38	E	43	Total 43	O 43	0	0
38	F	26	Total 26	O 26	0	0
38	G	19	Total 19	O 19	0	0
38	H	65	Total 65	O 65	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	58	Total 58	O 58	0	0
38	L	85	Total 85	O 85	0	0
38	M	127	Total 127	O 127	0	0
38	N	59	Total 59	O 59	0	0
38	O	39	Total 39	O 39	0	0

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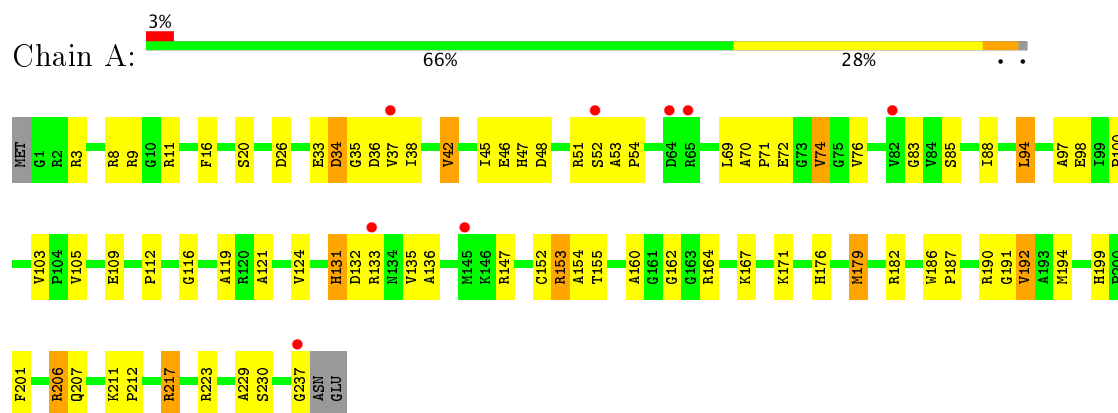
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	67	Total 67	O 67	0	0
38	Q	48	Total 48	O 48	0	0
38	R	77	Total 77	O 77	0	0
38	S	30	Total 30	O 30	0	0
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	31	Total 31	O 31	0	0
38	1	59	Total 59	O 59	0	0
38	2	43	Total 43	O 43	0	0
38	3	70	Total 70	O 70	0	0
38	0	5904	Total 5904	O 5904	0	0
38	9	149	Total 149	O 149	0	0

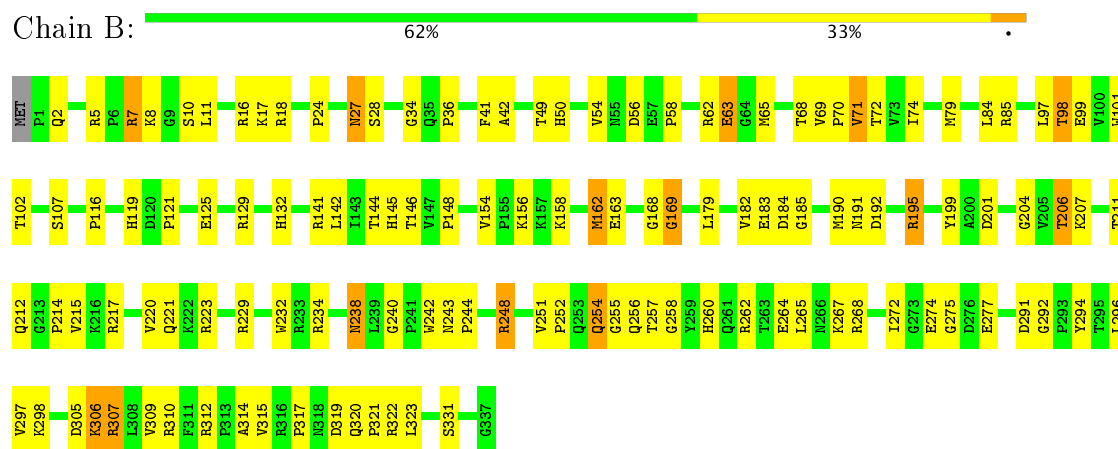
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

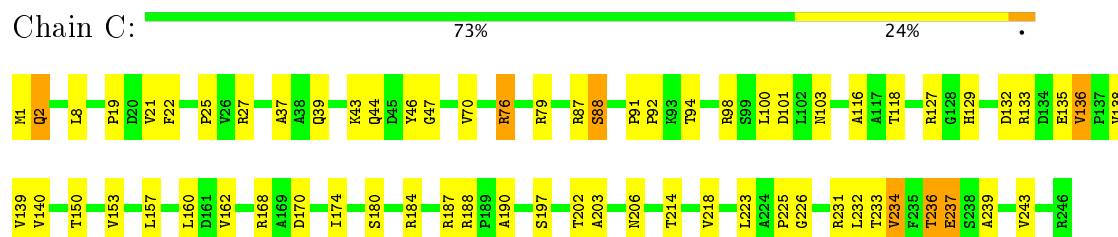
- Molecule 1: 50S ribosomal protein L2P



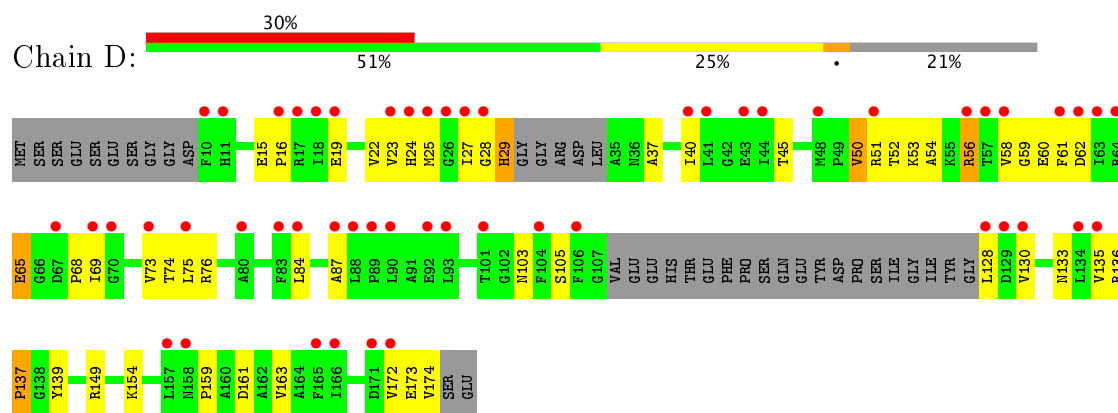
- Molecule 2: 50S ribosomal protein L3P



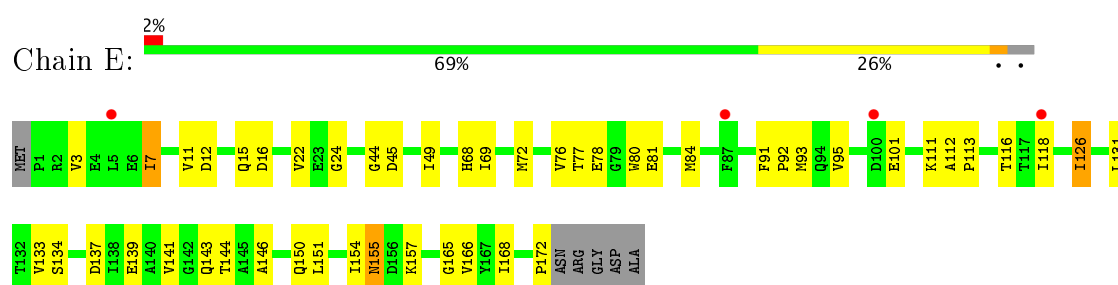
- Molecule 3: 50S ribosomal protein L4P



- Molecule 4: 50S ribosomal protein L5P



- Molecule 5: 50S ribosomal protein L6P

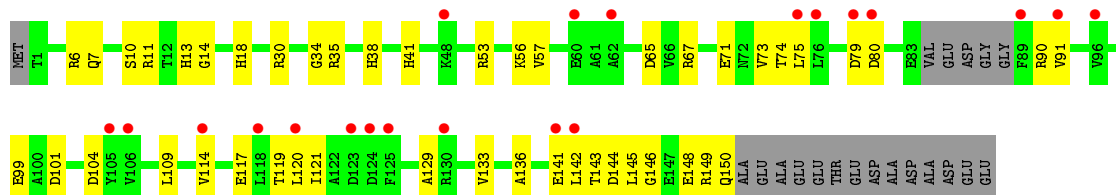




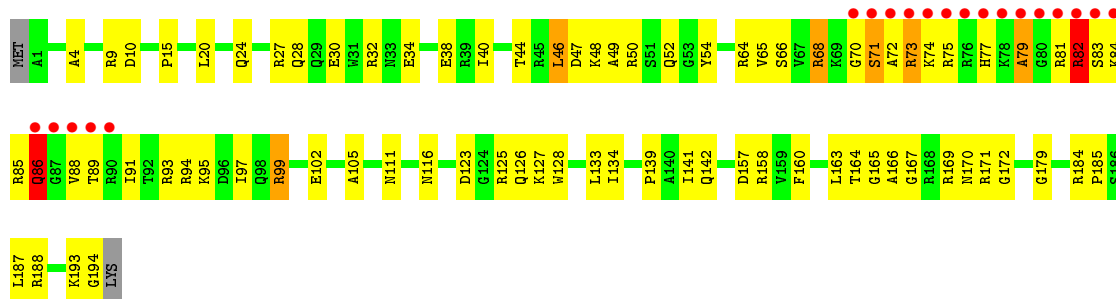




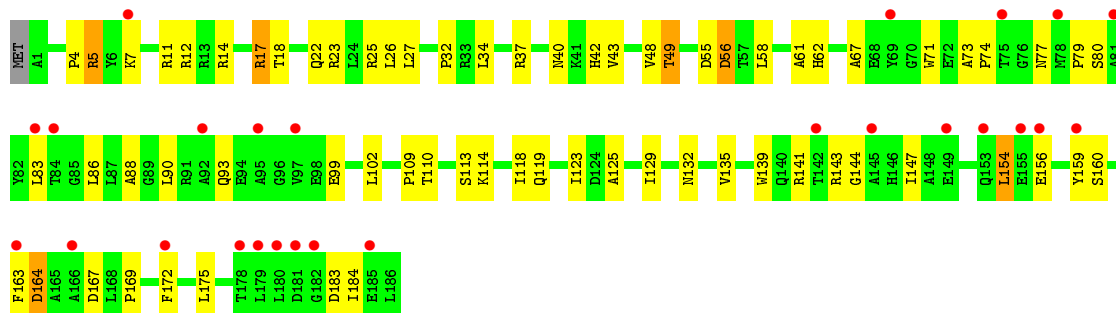
- Molecule 12: 50S ribosomal protein L15P



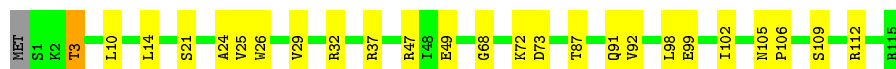
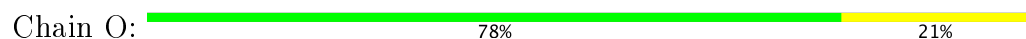
- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

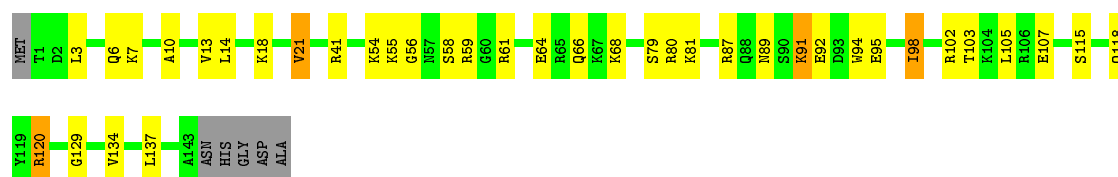


- Molecule 15: 50S ribosomal protein L18e

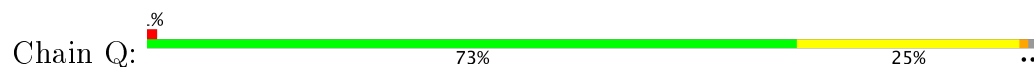


- Molecule 16: 50S ribosomal protein L19e

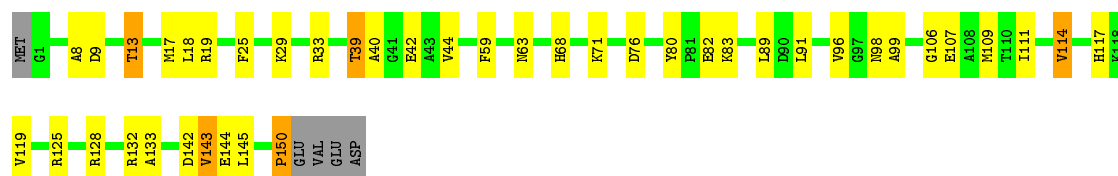




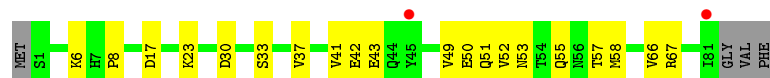
- Molecule 17: 50S ribosomal protein L21e



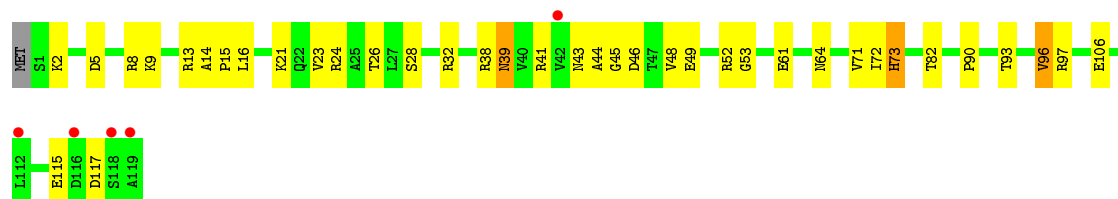
- Molecule 18: 50S ribosomal protein L22P



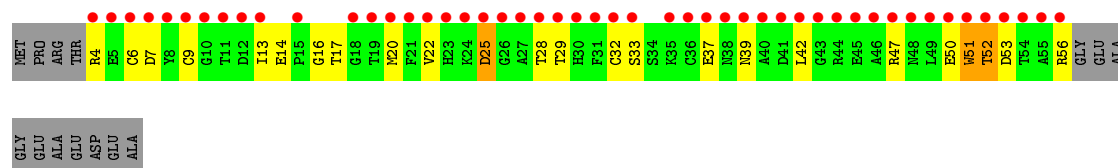
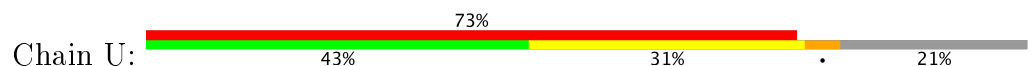
- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P



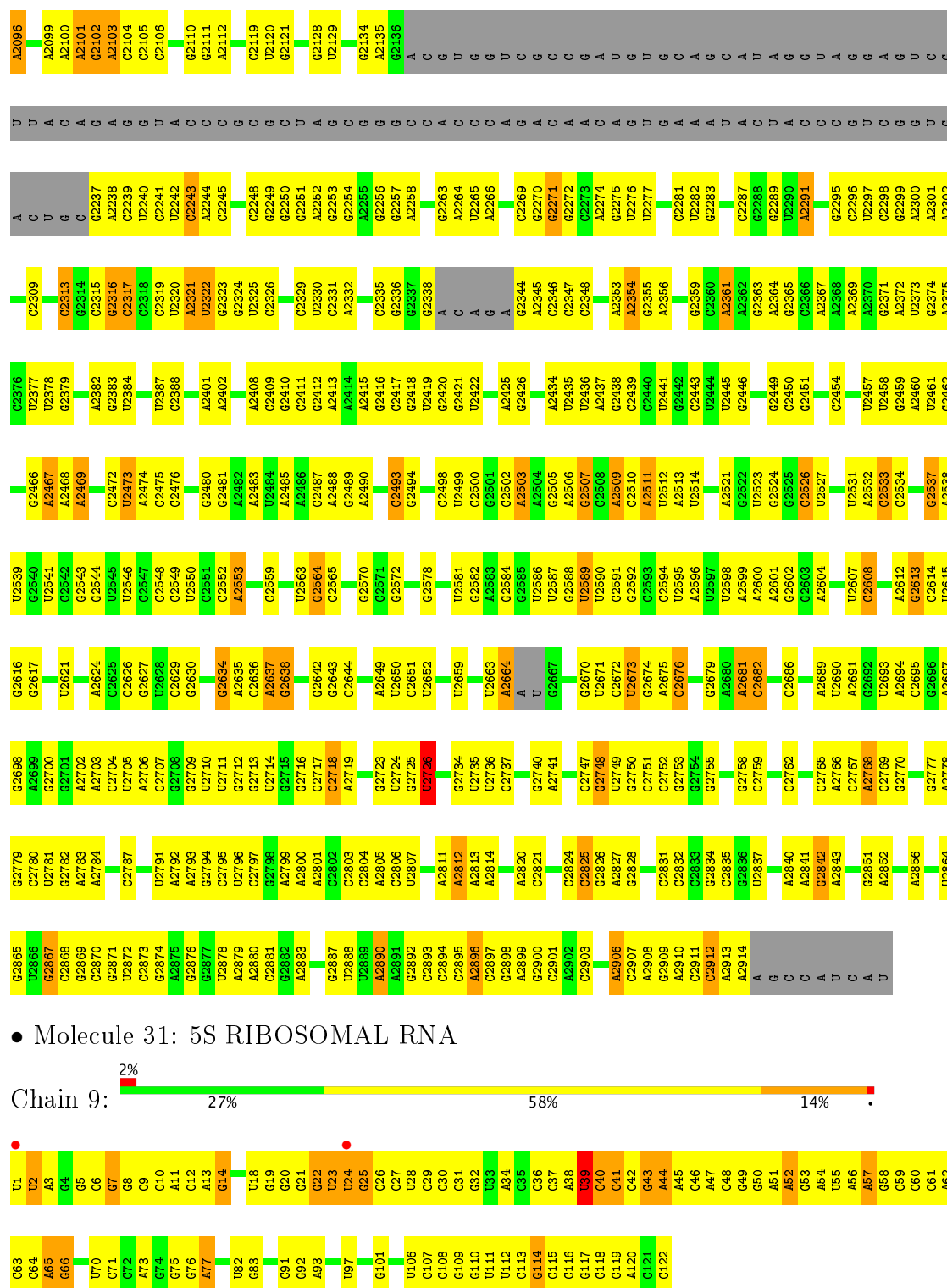
- Molecule 21: 50S ribosomal protein L24e



- Chain 1:  68% 30% .



U1996	U1997	G1998	C2002	U2003	U2004	G2005	C2006	U2007	U2008	A2010	A2011	G2012	G2013	U2017	A2018	A2022	U2032	U2033	G2034	C2035	A2039	C2040	U2043	G2044	G2050	A2054	A2055	G2056	U2057	G2058	A2059	A2060	C2061	A2062	U2063	U2064	G2070	C2071	G2072	G2073	U2074	G2075	A2081	C2088	G2092																																																																																																																																																																																																																																																				
U1831	G1832	U1833	G1834	U1835	U1836	U1837	U1838	U1839	U1840	U1845	U1846	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883	U1884	U1885	U1886	U1887	U1888	U1889	U1890	U1891	U1892	U1893	U1894	U1895	U1896	U1897	U1898	U1899	U1900	U1901	U1902	U1903	U1904	U1905	U1906	U1907	U1908	U1909	U1910	U1911	U1912	U1913	U1914	U1915	U1916	U1917	U1918	U1919	U1920	U1921	U1922	U1923	U1924																																																																																																																																																																																																											
G1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830																																																																																																																																																																																																																			
U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751																																																																																																																																																																																																
A1486	A1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1503	A1504	U1505	U1506	U1511	U1512	U1515	U1516	U1594	U1595	U1596	U1597	U1598	U1599	U1603	U1604	U1605	U1606	U1607	U1608	U1610	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751																																																																																																																																					
G1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751																																																																																																									
U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751				
A1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.24Å 299.19Å 575.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 85.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 91.7 (85.59-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.179 , 0.238 0.177 , 0.229	Depositor DCC
$R_{free}$ test set	3430 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 79.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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, SR, 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	A	0.34	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.39	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.57	0/1498
5	E	0.34	0/1382	0.56	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.32	0/241	0.47	0/324
8	H	0.33	0/1302	0.62	0/1743
9	I	0.32	0/526	0.54	0/716
10	J	0.39	0/1136	0.61	0/1530
11	K	0.37	0/1004	0.66	0/1351
12	L	0.34	0/1130	0.61	0/1509
13	M	0.40	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.61	0/1999
15	O	0.37	0/874	0.62	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.64	0/1005
18	R	1.27	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.36	0/648	0.59	0/875
20	T	0.34	0/958	0.66	0/1289
21	U	0.45	0/417	0.60	0/562
22	V	0.34	0/502	0.53	0/675
23	W	0.38	0/1219	0.65	0/1655
24	X	0.36	0/664	0.61	0/895
25	Y	0.38	0/1146	0.62	0/1536
26	Z	0.43	0/584	0.63	0/781
27	1	0.47	0/438	0.64	0/578
28	2	0.36	0/401	0.61	0/529
29	3	0.46	0/771	0.60	0/1024
30	0	0.42	0/65956	0.68	7/102865 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.42	7/98700 (0.0%)	0.67	14/147584 (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
18	R	1	0
23	W	0	1
30	0	0	34
All	All	1	35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.15	2.85	1.50
18	R	150	PRO	CA-C	-18.51	1.15	1.52
18	R	150	PRO	CG-CD	13.84	1.96	1.50
18	R	150	PRO	C-O	11.87	1.47	1.23
18	R	150	PRO	N-CA	11.57	1.67	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.43	55.92	112.00
18	R	150	PRO	N-CA-C	-19.45	61.53	112.10
18	R	150	PRO	CA-N-CD	12.27	128.88	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.27	100.34	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	196	G	Sidechain
30	0	221	G	Sidechain
30	0	324	G	Sidechain
30	0	333	G	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	85	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	63	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	39	0
6	F	890	0	843	19	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	14	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	34	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	95	0
14	N	1445	0	1401	73	0
15	O	865	0	873	22	0
16	P	1136	0	1123	34	0
17	Q	735	0	729	28	0
18	R	1149	0	1122	41	0
19	S	641	0	605	15	0
20	T	950	0	924	36	0
21	U	410	0	368	26	0
22	V	499	0	511	21	0
23	W	1196	0	1137	58	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	39	0
26	Z	573	0	535	50	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	732	57	0
30	0	59019	0	29809	1661	0
31	9	2599	0	1325	127	0
32	0	86	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	3	0
33	3	1	0	0	1	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	2	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	L	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	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	5904	0	0	251	0
38	1	59	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	43	0	0	2	0
38	3	70	0	0	3	0
38	9	149	0	0	10	0
38	A	119	0	0	7	0
38	B	152	0	0	16	0
38	C	185	0	0	18	0
38	D	42	0	0	4	0
38	E	43	0	0	1	0
38	F	26	0	0	1	0
38	G	19	0	0	1	0
38	H	65	0	0	4	0
38	I	8	0	0	1	0
38	J	53	0	0	1	0
38	K	58	0	0	3	0
38	L	85	0	0	9	0
38	M	127	0	0	13	0
38	N	59	0	0	2	0
38	O	39	0	0	2	0
38	P	67	0	0	3	0
38	Q	48	0	0	1	0
38	R	77	0	0	2	0
38	S	30	0	0	2	0
38	T	36	0	0	3	0
38	U	28	0	0	4	0
38	V	13	0	0	2	0
38	W	67	0	0	3	0
38	X	21	0	0	2	0
38	Y	100	0	0	5	0
38	Z	31	0	0	7	0
All	All	99121	0	59922	2675	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 18.

The worst 5 of 2675 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.41
30:0:871:G:C8	30:0:871:G:H5'	1.77	1.19
10:J:82:THR:HG23	30:0:1242:A:H5'	1.23	1.16
30:0:1165:G:H1'	30:0:1174:A:H1'	1.17	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.19	1.13

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	
1	A	235/240 (98%)	202 (86%)	27 (12%)	6 (3%)	6	28
2	B	335/338 (99%)	309 (92%)	17 (5%)	9 (3%)	6	27
3	C	244/246 (99%)	222 (91%)	20 (8%)	2 (1%)	22	61
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	5	24
5	E	170/178 (96%)	157 (92%)	12 (7%)	1 (1%)	28	67
6	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	4	21
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	14	48
9	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	2	9
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	25	64
11	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	22	61
12	L	141/165 (86%)	120 (85%)	21 (15%)	0	100	100
13	M	192/196 (98%)	179 (93%)	9 (5%)	4 (2%)	8	35
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	8	33
15	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	17	53
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	25	64
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	11	41
21	U	51/67 (76%)	42 (82%)	8 (16%)	1 (2%)	9	36
22	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
23	W	152/154 (99%)	140 (92%)	10 (7%)	2 (1%)	14	48
24	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	6	29
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	58 (82%)	8 (11%)	5 (7%)	1	5
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	7	31
29	3	90/92 (98%)	74 (82%)	13 (14%)	3 (3%)	4	21
All	All	3705/4472 (83%)	3359 (91%)	286 (8%)	60 (2%)	11	42

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	37	VAL
1	A	74	VAL
4	D	65	GLU
4	D	137	PRO

### 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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	69
2	B	282/283 (100%)	264 (94%)	18 (6%)	20	54
3	C	193/193 (100%)	182 (94%)	11 (6%)	24	59
4	D	117/148 (79%)	110 (94%)	7 (6%)	22	57
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	82
6	F	93/94 (99%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	74
8	H	134/145 (92%)	126 (94%)	8 (6%)	22	57
9	I	58/130 (45%)	56 (97%)	2 (3%)	42	76
10	J	118/121 (98%)	113 (96%)	5 (4%)	34	71
11	K	106/106 (100%)	104 (98%)	2 (2%)	62	87
12	L	113/127 (89%)	108 (96%)	5 (4%)	33	69
13	M	158/160 (99%)	148 (94%)	10 (6%)	21	55
14	N	149/150 (99%)	144 (97%)	5 (3%)	42	76
15	O	93/94 (99%)	92 (99%)	1 (1%)	78	92
16	P	113/117 (97%)	107 (95%)	6 (5%)	26	62
17	Q	79/80 (99%)	78 (99%)	1 (1%)	73	91
18	R	117/122 (96%)	114 (97%)	3 (3%)	51	82
19	S	71/74 (96%)	70 (99%)	1 (1%)	71	90
20	T	105/106 (99%)	99 (94%)	6 (6%)	24	59
21	U	44/53 (83%)	41 (93%)	3 (7%)	18	51
22	V	51/57 (90%)	49 (96%)	2 (4%)	37	73
23	W	130/130 (100%)	124 (95%)	6 (5%)	31	68
24	X	66/74 (89%)	61 (92%)	5 (8%)	15	46
25	Y	120/196 (61%)	115 (96%)	5 (4%)	34	71
26	Z	60/94 (64%)	57 (95%)	3 (5%)	28	65
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	83
29	3	79/79 (100%)	76 (96%)	3 (4%)	38	73
All	All	3095/3646 (85%)	2963 (96%)	132 (4%)	33	70

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ILE
13	M	68	ARG
25	Y	189	ASN
10	J	74	ARG
12	L	99	GLU



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	93	GLN
17	Q	16	ASN
27	1	28	HIS
14	N	107	ASN
16	P	66	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	250 (9%)	21 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	269 (9%)	23 (0%)

5 of 269 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1474	C
31	9	43	G
30	0	1377	C
30	0	1506	U

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

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
30	OMU	0	2587	30	14,22,23	0.96	1 (7%)	18,31,34	3.67	2 (11%)
30	OMG	0	2588	30	18,26,27	0.99	2 (11%)	22,38,41	2.49	4 (18%)
30	UR3	0	2619	30	14,22,23	0.75	0	16,32,35	0.65	0
30	PSU	0	2621	30	16,21,22	1.67	3 (18%)	20,30,33	6.12	5 (25%)
30	1MA	0	628	30,35	16,25,26	1.07	1 (6%)	13,37,40	1.25	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.22	1.47	1.52
30	0	2588	OMG	C8-N7	-2.07	1.30	1.34
30	0	2621	PSU	C2-N1	2.35	1.42	1.38
30	0	2587	OMU	C4-N3	2.35	1.37	1.33
30	0	2621	PSU	C4-N3	2.59	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.08	114.68	128.40
30	0	2621	PSU	C5-C4-N3	-12.95	114.81	125.43
30	0	2588	OMG	C5-C6-N1	-8.35	111.59	123.48
30	0	628	1MA	C2-N3-C4	-3.68	110.76	116.41
30	0	2587	OMU	C5-C4-N3	-3.51	114.75	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0
30	0	2588	OMG	1	0
30	0	2621	PSU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.14	8 (3%) 46 29	36, 71, 108, 128	0
2	B	337/338 (99%)	-0.45	0 100 100	38, 67, 98, 112	0
3	C	246/246 (100%)	-0.38	0 100 100	32, 56, 80, 91	0
4	D	140/177 (79%)	1.53	53 (37%) 0 0	89, 121, 144, 151	0
5	E	172/178 (96%)	-0.06	4 (2%) 61 41	57, 83, 104, 113	0
6	F	119/120 (99%)	0.51	15 (12%) 4 2	64, 88, 121, 131	0
7	G	29/348 (8%)	1.10	4 (13%) 3 2	92, 107, 116, 118	0
8	H	160/177 (90%)	0.89	30 (18%) 1 1	65, 89, 118, 127	0
9	I	70/162 (43%)	3.64	50 (71%) 0 0	145, 162, 177, 179	0
10	J	142/145 (97%)	-0.38	1 (0%) 87 74	47, 63, 86, 105	0
11	K	132/132 (100%)	-0.38	0 100 100	45, 63, 91, 100	0
12	L	145/165 (87%)	0.55	21 (14%) 3 1	41, 88, 131, 140	0
13	M	194/196 (98%)	0.25	20 (10%) 7 4	37, 53, 115, 122	0
14	N	186/187 (99%)	0.65	26 (13%) 3 1	70, 90, 134, 139	0
15	O	115/116 (99%)	-0.37	0 100 100	46, 64, 81, 87	0
16	P	143/149 (95%)	-0.30	0 100 100	48, 67, 85, 96	0
17	Q	95/96 (98%)	-0.17	1 (1%) 80 63	57, 69, 89, 97	0
18	R	150/155 (96%)	-0.50	0 100 100	39, 56, 79, 95	0
19	S	81/85 (95%)	-0.28	2 (2%) 58 39	52, 70, 89, 104	0
20	T	119/120 (99%)	-0.04	5 (4%) 37 23	48, 67, 95, 125	0
21	U	53/67 (79%)	4.50	49 (92%) 0 0	112, 125, 131, 134	0
22	V	65/71 (91%)	0.91	12 (18%) 1 1	51, 83, 131, 135	0
23	W	154/154 (100%)	-0.34	1 (0%) 89 77	45, 62, 79, 92	0
24	X	82/92 (89%)	0.03	4 (4%) 30 18	54, 72, 95, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.60	0 100 100	30, 53, 78, 97	0
26	Z	73/116 (62%)	7.40	59 (80%) 0 0	111, 130, 139, 142	0
27	1	56/57 (98%)	-0.51	0 100 100	30, 39, 47, 65	0
28	2	46/50 (92%)	-0.22	3 (6%) 20 11	39, 72, 104, 110	0
29	3	92/92 (100%)	8.52	91 (98%) 0 0	123, 135, 142, 148	0
30	0	2749/2923 (94%)	-0.63	10 (0%) 92 82	25, 58, 106, 183	0
31	9	122/122 (100%)	-0.81	2 (1%) 72 53	51, 90, 111, 159	0
All	All	6646/7517 (88%)	-0.00	471 (7%) 17 9	25, 66, 129, 183	0

The worst 5 of 471 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	58	ASN	25.8
29	3	39	GLN	21.9
29	3	41	GLU	19.9
29	3	47	GLY	19.1
29	3	35	TRP	18.9

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	PSU	0	2621	20/21	0.98	0.18	-	39,41,53,53	0
30	OMG	0	2588	24/25	0.98	0.12	-	41,43,46,50	0
30	1MA	0	628	23/24	0.98	0.14	-	38,44,47,47	0
30	UR3	0	2619	21/22	0.98	0.13	-	47,49,51,54	0
30	OMU	0	2587	21/22	0.98	0.11	-	43,47,50,51	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8565	1/1	0.91	1.07	93.90	78,78,78,78	0
35	NA	0	8547	1/1	0.93	0.99	61.90	67,67,67,67	0
35	NA	0	8562	1/1	0.83	0.97	46.93	82,82,82,82	0
35	NA	0	8564	1/1	0.95	0.43	40.53	69,69,69,69	0
34	SR	L	8969	1/1	0.92	0.30	21.44	200,200,200,200	0
34	SR	0	8986	1/1	0.98	1.04	20.37	200,200,200,200	0
35	NA	0	8521	1/1	0.93	0.46	19.54	64,64,64,64	0
35	NA	0	8542	1/1	0.93	0.53	17.94	58,58,58,58	0
34	SR	B	8987	1/1	0.93	0.62	16.03	200,200,200,200	0
35	NA	0	8528	1/1	0.51	0.66	15.81	76,76,76,76	0
35	NA	0	8546	1/1	0.94	0.74	14.85	94,94,94,94	0
35	NA	0	8530	1/1	0.93	0.43	12.64	74,74,74,74	0
36	K	0	8401	1/1	0.92	0.64	11.84	139,139,139,139	0
35	NA	0	8556	1/1	0.98	0.81	10.04	71,71,71,71	0
35	NA	9	8572	1/1	0.95	0.27	9.29	88,88,88,88	0
35	NA	0	8507	1/1	0.99	0.24	8.58	43,43,43,43	0
35	NA	0	8535	1/1	0.83	0.29	8.43	67,67,67,67	0
35	NA	0	8513	1/1	0.96	0.41	8.23	68,68,68,68	0
35	NA	0	8555	1/1	0.87	0.42	8.12	52,52,52,52	0
35	NA	0	8527	1/1	0.94	0.28	6.49	72,72,72,72	0
34	SR	0	8903	1/1	1.00	0.19	6.37	57,57,57,57	0
35	NA	0	8559	1/1	0.98	0.17	5.92	77,77,77,77	0
32	MG	0	8085	1/1	0.96	0.17	5.59	76,76,76,76	0
35	NA	0	8568	1/1	0.94	0.34	5.51	54,54,54,54	0
32	MG	0	8047	1/1	0.97	0.30	5.30	66,66,66,66	0
35	NA	0	8575	1/1	0.99	0.23	5.23	103,103,103,103	0
33	CL	0	8816	1/1	0.96	0.43	5.10	85,85,85,85	0
35	NA	B	8552	1/1	0.78	0.28	4.99	89,89,89,89	0
34	SR	0	8926	1/1	0.98	0.14	4.63	122,122,122,122	0
35	NA	0	8553	1/1	0.93	0.28	4.46	89,89,89,89	0
34	SR	0	8992	1/1	0.84	0.22	3.96	159,159,159,159	0
32	MG	0	8009	1/1	0.99	0.24	3.93	34,34,34,34	0
32	MG	0	8079	1/1	0.97	0.20	3.76	66,66,66,66	0
33	CL	B	8819	1/1	0.93	0.21	3.45	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	R	8912	1/1	0.98	0.19	3.30	95,95,95,95	0
34	SR	0	8904	1/1	1.00	0.20	2.81	57,57,57,57	0
34	SR	0	8975	1/1	0.90	0.14	2.65	149,149,149,149	0
34	SR	0	8943	1/1	0.95	0.13	2.26	84,84,84,84	0
35	NA	0	8569	1/1	0.94	0.18	2.14	50,50,50,50	0
32	MG	0	8011	1/1	0.99	0.22	1.81	25,25,25,25	0
34	SR	0	8949	1/1	0.98	0.15	1.73	117,117,117,117	0
32	MG	0	8003	1/1	0.97	0.17	1.56	38,38,38,38	0
32	MG	0	8014	1/1	0.99	0.17	1.50	37,37,37,37	0
32	MG	0	8028	1/1	0.94	0.17	1.48	34,34,34,34	0
32	MG	0	8080	1/1	0.90	0.76	1.15	83,83,83,83	0
35	NA	0	8537	1/1	0.95	0.16	1.14	50,50,50,50	0
32	MG	0	8016	1/1	0.99	0.17	1.00	40,40,40,40	0
32	MG	A	8051	1/1	0.76	0.26	0.93	94,94,94,94	0
34	SR	0	8964	1/1	0.99	0.12	0.73	134,134,134,134	0
35	NA	M	8539	1/1	0.97	0.14	0.70	42,42,42,42	0
32	MG	0	8084	1/1	0.99	0.14	0.60	35,35,35,35	0
32	MG	0	8008	1/1	0.99	0.13	0.59	31,31,31,31	0
32	MG	0	8041	1/1	0.97	0.16	0.55	36,36,36,36	0
32	MG	0	8043	1/1	0.98	0.13	0.39	52,52,52,52	0
34	SR	0	8922	1/1	0.94	0.17	0.20	168,168,168,168	0
34	SR	0	8923	1/1	1.00	0.13	0.12	109,109,109,109	0
32	MG	0	8006	1/1	0.94	0.12	0.02	44,44,44,44	0
32	MG	0	8062	1/1	0.97	0.17	-0.04	56,56,56,56	0
34	SR	0	8918	1/1	0.99	0.12	-0.06	85,85,85,85	0
32	MG	0	8012	1/1	0.98	0.16	-0.07	25,25,25,25	0
34	SR	0	8935	1/1	0.99	0.11	-0.10	103,103,103,103	0
35	NA	C	8503	1/1	0.95	0.17	-0.15	46,46,46,46	0
34	SR	0	8902	1/1	0.99	0.15	-0.15	68,68,68,68	0
35	NA	0	8515	1/1	0.96	0.15	-0.22	32,32,32,32	0
35	NA	0	8523	1/1	0.98	0.13	-0.29	54,54,54,54	0
36	K	M	8402	1/1	0.92	0.19	-0.34	87,87,87,87	0
34	SR	A	8930	1/1	0.93	0.15	-0.46	142,142,142,142	0
35	NA	J	8538	1/1	0.58	0.15	-0.48	78,78,78,78	0
32	MG	0	8045	1/1	0.97	0.10	-0.53	31,31,31,31	0
35	NA	0	8520	1/1	0.97	0.10	-0.54	56,56,56,56	0
33	CL	O	8808	1/1	0.92	0.17	-0.57	86,86,86,86	0
34	SR	A	8929	1/1	0.95	0.11	-0.58	139,139,139,139	0
35	NA	R	8532	1/1	0.98	0.11	-0.59	50,50,50,50	0
35	NA	Q	8540	1/1	0.86	0.11	-0.67	79,79,79,79	0
34	SR	0	8936	1/1	0.99	0.11	-0.70	95,95,95,95	0
34	SR	H	8972	1/1	0.92	0.11	-0.78	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CD	Z	8703	1/1	0.78	0.46	-0.78	200,200,200,200	0
37	CD	U	8701	1/1	0.95	0.45	-0.87	200,200,200,200	0
35	NA	0	8504	1/1	1.00	0.12	-1.07	40,40,40,40	0
37	CD	3	8704	1/1	0.78	0.67	-1.14	200,200,200,200	0
32	MG	0	8058	1/1	0.97	0.06	-1.16	18,18,18,18	0
35	NA	0	8563	1/1	0.59	0.12	-1.21	117,117,117,117	0
33	CL	J	8821	1/1	0.96	0.10	-1.34	77,77,77,77	0
34	SR	F	9005	1/1	0.98	0.07	-1.35	147,147,147,147	0
35	NA	0	8534	1/1	0.98	0.12	-1.41	50,50,50,50	0
35	NA	0	8519	1/1	0.95	0.15	-1.50	52,52,52,52	0
35	NA	0	8533	1/1	0.95	0.09	-1.66	70,70,70,70	0
37	CD	1	8702	1/1	1.00	0.10	-1.69	61,61,61,61	0
34	SR	0	8985	1/1	0.86	0.06	-1.74	164,164,164,164	0
32	MG	0	8004	1/1	0.99	0.12	-1.75	29,29,29,29	0
34	SR	0	8910	1/1	0.98	0.09	-1.84	108,108,108,108	0
32	MG	0	8052	1/1	0.96	0.08	-2.05	44,44,44,44	0
32	MG	0	8025	1/1	0.98	0.10	-2.06	37,37,37,37	0
35	NA	0	8557	1/1	0.94	0.06	-2.47	65,65,65,65	0
32	MG	T	8057	1/1	0.98	0.07	-2.48	65,65,65,65	0
32	MG	Y	8086	1/1	0.95	0.08	-2.50	50,50,50,50	0
32	MG	0	8021	1/1	0.95	0.09	-3.00	33,33,33,33	0
33	CL	0	8812	1/1	0.98	0.05	-3.02	61,61,61,61	0
32	MG	A	8050	1/1	0.94	0.06	-3.05	64,64,64,64	0
32	MG	0	8001	1/1	0.98	0.11	-3.33	36,36,36,36	0
32	MG	0	8088	1/1	0.99	0.10	-3.33	35,35,35,35	0
32	MG	0	8044	1/1	0.94	0.05	-3.35	58,58,58,58	0
32	MG	0	8059	1/1	0.93	0.09	-3.35	51,51,51,51	0
32	MG	0	8002	1/1	0.97	0.10	-3.61	40,40,40,40	0
32	MG	0	8076	1/1	0.98	0.06	-3.72	40,40,40,40	0
32	MG	0	8034	1/1	1.00	0.07	-3.82	50,50,50,50	0
33	CL	M	8818	1/1	0.99	0.05	-3.95	49,49,49,49	0
32	MG	0	8075	1/1	0.85	0.05	-4.42	55,55,55,55	0
35	NA	0	8517	1/1	0.96	0.09	-4.54	38,38,38,38	0
34	SR	9	8978	1/1	0.93	0.06	-4.55	157,157,157,157	0
32	MG	0	8013	1/1	0.99	0.06	-5.07	28,28,28,28	0
34	SR	0	8970	1/1	0.96	0.05	-5.52	125,125,125,125	0
32	MG	0	8065	1/1	0.97	0.05	-6.10	42,42,42,42	0
34	SR	1	8913	1/1	0.99	0.06	-10.48	95,95,95,95	0
34	SR	0	8945	1/1	0.98	0.09	-	105,105,105,105	0
35	NA	0	8529	1/1	0.95	0.12	-	48,48,48,48	0
34	SR	B	8950	1/1	0.96	0.16	-	130,130,130,130	0
32	MG	0	8068	1/1	0.96	0.10	-	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8046	1/1	1.00	0.10	-	45,45,45,45	0
34	SR	0	8995	1/1	0.98	0.19	-	150,150,150,150	0
32	MG	0	8030	1/1	0.90	0.48	-	90,90,90,90	0
33	CL	0	8811	1/1	0.99	0.20	-	81,81,81,81	0
32	MG	0	8070	1/1	0.99	0.17	-	66,66,66,66	0
35	NA	0	8531	1/1	0.99	0.06	-	39,39,39,39	0
34	SR	0	8957	1/1	0.86	0.34	-	200,200,200,200	0
32	MG	0	8038	1/1	0.98	0.08	-	74,74,74,74	0
34	SR	0	8959	1/1	0.81	0.28	-	200,200,200,200	0
34	SR	0	8947	1/1	0.95	0.26	-	200,200,200,200	0
34	SR	0	8967	1/1	0.97	0.04	-	131,131,131,131	0
37	CD	O	8705	1/1	0.99	0.08	-	100,100,100,100	0
34	SR	0	8934	1/1	0.99	0.13	-	133,133,133,133	0
33	CL	0	8813	1/1	0.99	0.07	-	60,60,60,60	0
35	NA	0	8522	1/1	0.91	0.14	-	82,82,82,82	0
34	SR	0	8998	1/1	0.99	0.18	-	178,178,178,178	0
35	NA	0	8536	1/1	0.90	0.17	-	64,64,64,64	0
32	MG	0	8039	1/1	0.96	0.20	-	84,84,84,84	0
34	SR	0	8982	1/1	0.67	1.93	-	200,200,200,200	0
34	SR	0	8979	1/1	0.54	0.19	-	196,196,196,196	0
34	SR	0	8973	1/1	0.99	0.16	-	146,146,146,146	0
32	MG	0	8072	1/1	0.98	0.06	-	59,59,59,59	0
34	SR	0	8901	1/1	0.99	0.18	-	66,66,66,66	0
35	NA	0	8549	1/1	0.98	0.84	-	56,56,56,56	0
35	NA	9	8543	1/1	0.91	0.21	-	61,61,61,61	0
32	MG	0	8061	1/1	0.94	0.17	-	36,36,36,36	0
32	MG	0	8060	1/1	0.94	0.06	-	53,53,53,53	0
32	MG	0	8081	1/1	0.85	0.16	-	88,88,88,88	0
32	MG	0	8024	1/1	0.99	0.17	-	62,62,62,62	0
34	SR	0	8951	1/1	0.85	0.10	-	155,155,155,155	0
35	NA	0	8514	1/1	0.96	0.29	-	55,55,55,55	0
33	CL	0	8803	1/1	0.98	0.09	-	60,60,60,60	0
34	SR	0	8981	1/1	0.99	0.13	-	161,161,161,161	0
32	MG	0	8031	1/1	0.92	0.40	-	83,83,83,83	0
35	NA	0	8509	1/1	0.83	0.13	-	69,69,69,69	0
32	MG	0	8010	1/1	0.96	0.13	-	72,72,72,72	0
32	MG	0	8048	1/1	0.99	0.24	-	29,29,29,29	0
33	CL	0	8817	1/1	0.98	0.14	-	72,72,72,72	0
34	SR	0	8920	1/1	0.95	0.05	-	127,127,127,127	0
32	MG	0	8090	1/1	0.95	0.17	-	97,97,97,97	0
32	MG	0	8055	1/1	0.94	0.07	-	62,62,62,62	0
32	MG	0	8017	1/1	0.99	0.17	-	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8940	1/1	0.99	0.09	-	93,93,93,93	0
33	CL	R	8806	1/1	0.99	0.14	-	58,58,58,58	0
32	MG	0	8067	1/1	0.89	0.11	-	35,35,35,35	0
34	SR	S	8961	1/1	0.95	0.09	-	128,128,128,128	0
34	SR	0	8962	1/1	0.84	0.09	-	172,172,172,172	0
32	MG	0	8063	1/1	0.93	0.30	-	116,116,116,116	0
34	SR	0	8991	1/1	0.66	0.08	-	180,180,180,180	0
34	SR	0	9006	1/1	0.56	0.98	-	200,200,200,200	0
33	CL	N	8807	1/1	0.94	0.22	-	87,87,87,87	0
35	NA	0	8558	1/1	0.93	0.20	-	58,58,58,58	0
35	NA	0	8566	1/1	0.92	0.30	-	63,63,63,63	0
35	NA	0	8525	1/1	0.77	0.16	-	75,75,75,75	0
32	MG	0	8027	1/1	0.98	0.12	-	47,47,47,47	0
32	MG	0	8023	1/1	0.99	0.17	-	28,28,28,28	0
34	SR	0	9000	1/1	0.95	0.08	-	183,183,183,183	0
35	NA	0	8505	1/1	0.98	0.66	-	53,53,53,53	0
34	SR	0	8906	1/1	1.00	0.21	-	67,67,67,67	0
35	NA	0	8573	1/1	0.94	0.12	-	73,73,73,73	0
34	SR	0	8905	1/1	0.99	0.25	-	72,72,72,72	0
34	SR	0	8939	1/1	0.94	0.04	-	144,144,144,144	0
35	NA	0	8550	1/1	0.94	0.26	-	71,71,71,71	0
32	MG	0	8069	1/1	0.98	0.09	-	102,102,102,102	0
34	SR	0	8911	1/1	0.98	0.12	-	88,88,88,88	0
34	SR	0	8927	1/1	0.96	0.06	-	181,181,181,181	0
35	NA	0	8567	1/1	0.93	0.24	-	78,78,78,78	0
34	SR	0	8993	1/1	0.89	0.08	-	167,167,167,167	0
35	NA	0	8544	1/1	0.90	0.20	-	79,79,79,79	0
34	SR	0	8971	1/1	0.92	0.06	-	192,192,192,192	0
34	SR	0	8944	1/1	0.90	0.07	-	172,172,172,172	0
35	NA	0	8541	1/1	0.98	0.22	-	64,64,64,64	0
32	MG	0	8071	1/1	0.84	0.12	-	60,60,60,60	0
34	SR	0	8996	1/1	0.92	0.51	-	200,200,200,200	0
34	SR	0	8924	1/1	0.99	0.20	-	124,124,124,124	0
32	MG	9	8074	1/1	0.89	0.07	-	87,87,87,87	0
35	NA	0	8554	1/1	0.97	0.85	-	69,69,69,69	0
32	MG	0	8018	1/1	0.99	0.24	-	33,33,33,33	0
34	SR	0	8997	1/1	0.93	0.15	-	189,189,189,189	0
35	NA	0	8545	1/1	0.88	0.81	-	58,58,58,58	0
32	MG	0	8053	1/1	0.93	0.05	-	63,63,63,63	0
34	SR	0	8965	1/1	0.95	0.06	-	134,134,134,134	0
34	SR	0	8955	1/1	0.96	0.07	-	200,200,200,200	0
34	SR	0	8954	1/1	0.91	0.12	-	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8524	1/1	0.97	0.69	-	73,73,73,73	0
34	SR	3	8932	1/1	0.90	0.24	-	178,178,178,178	0
32	MG	0	8019	1/1	0.94	0.19	-	29,29,29,29	0
35	NA	H	8518	1/1	0.86	0.42	-	91,91,91,91	0
33	CL	A	8809	1/1	0.99	0.15	-	104,104,104,104	0
32	MG	0	8020	1/1	0.95	0.16	-	41,41,41,41	0
33	CL	L	8810	1/1	0.96	0.05	-	64,64,64,64	0
34	SR	0	8988	1/1	0.62	0.08	-	173,173,173,173	0
35	NA	0	8571	1/1	0.94	0.12	-	79,79,79,79	0
35	NA	S	8510	1/1	0.93	0.03	-	44,44,44,44	0
34	SR	0	8919	1/1	0.87	0.09	-	168,168,168,168	0
34	SR	0	8974	1/1	0.97	0.07	-	166,166,166,166	0
32	MG	0	8078	1/1	0.98	0.25	-	65,65,65,65	0
34	SR	0	9007	1/1	0.79	1.78	-	200,200,200,200	0
34	SR	0	8908	1/1	0.96	0.11	-	85,85,85,85	0
33	CL	0	8815	1/1	0.93	0.22	-	89,89,89,89	0
34	SR	0	8968	1/1	0.94	0.06	-	177,177,177,177	0
34	SR	0	8953	1/1	0.86	0.54	-	200,200,200,200	0
33	CL	0	8814	1/1	0.97	0.16	-	79,79,79,79	0
34	SR	0	8914	1/1	0.98	0.27	-	133,133,133,133	0
32	MG	0	8007	1/1	0.99	0.18	-	36,36,36,36	0
32	MG	0	8033	1/1	0.96	0.06	-	63,63,63,63	0
34	SR	0	8983	1/1	0.91	0.34	-	197,197,197,197	0
32	MG	0	8089	1/1	0.81	0.24	-	65,65,65,65	0
32	MG	0	8066	1/1	0.94	0.17	-	69,69,69,69	0
32	MG	0	8073	1/1	0.96	0.08	-	72,72,72,72	0
32	MG	0	8056	1/1	0.89	0.06	-	57,57,57,57	0
35	NA	0	8548	1/1	0.88	0.12	-	56,56,56,56	0
34	SR	0	9004	1/1	0.71	0.84	-	200,200,200,200	0
33	CL	Y	8820	1/1	0.95	0.07	-	52,52,52,52	0
34	SR	0	8917	1/1	0.94	0.16	-	114,114,114,114	0
33	CL	0	8805	1/1	0.93	0.17	-	98,98,98,98	0
32	MG	K	8054	1/1	0.99	0.17	-	57,57,57,57	0
34	SR	0	8938	1/1	0.80	0.08	-	183,183,183,183	0
35	NA	0	8502	1/1	0.86	0.12	-	69,69,69,69	0
32	MG	0	8029	1/1	1.00	0.13	-	59,59,59,59	0
34	SR	9	9003	1/1	0.89	0.10	-	187,187,187,187	0
32	MG	0	8049	1/1	0.99	0.23	-	64,64,64,64	0
35	NA	0	8551	1/1	0.90	0.46	-	63,63,63,63	0
33	CL	J	8801	1/1	0.84	0.12	-	95,95,95,95	0
35	NA	0	8511	1/1	0.68	0.08	-	81,81,81,81	0
32	MG	0	8015	1/1	1.00	0.13	-	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8976	1/1	0.90	0.29	-	193,193,193,193	0
34	SR	0	8909	1/1	1.00	0.14	-	93,93,93,93	0
34	SR	0	9002	1/1	0.82	0.12	-	193,193,193,193	0
35	NA	0	8560	1/1	0.86	0.55	-	118,118,118,118	0
34	SR	0	8942	1/1	0.97	0.09	-	124,124,124,124	0
32	MG	0	8091	1/1	0.95	0.12	-	56,56,56,56	0
34	SR	0	8921	1/1	0.99	0.13	-	83,83,83,83	0
34	SR	0	8966	1/1	0.96	0.09	-	105,105,105,105	0
34	SR	0	8990	1/1	0.99	0.14	-	137,137,137,137	0
34	SR	3	8999	1/1	0.84	0.28	-	187,187,187,187	0
32	MG	0	8092	1/1	0.95	0.08	-	76,76,76,76	0
34	SR	0	8937	1/1	0.96	0.15	-	113,113,113,113	0
34	SR	0	8994	1/1	0.86	0.48	-	200,200,200,200	0
34	SR	0	8946	1/1	0.91	0.20	-	137,137,137,137	0
32	MG	0	8040	1/1	0.59	0.39	-	86,86,86,86	0
32	MG	0	8093	1/1	0.96	0.06	-	36,36,36,36	0
32	MG	0	8087	1/1	0.96	0.09	-	38,38,38,38	0
34	SR	0	8984	1/1	0.97	0.09	-	119,119,119,119	0
32	MG	0	8005	1/1	0.98	0.21	-	42,42,42,42	0
32	MG	0	8036	1/1	0.95	0.10	-	48,48,48,48	0
35	NA	0	8526	1/1	0.93	0.14	-	46,46,46,46	0
34	SR	0	8915	1/1	0.93	0.09	-	126,126,126,126	0
35	NA	0	8561	1/1	0.96	0.31	-	65,65,65,65	0
34	SR	0	9008	1/1	0.98	0.14	-	92,92,92,92	0
34	SR	0	8960	1/1	0.96	0.02	-	151,151,151,151	0
34	SR	0	9001	1/1	0.75	0.13	-	177,177,177,177	0
32	MG	0	8064	1/1	0.96	0.18	-	45,45,45,45	0
32	MG	0	8022	1/1	0.99	0.20	-	33,33,33,33	0
32	MG	0	8077	1/1	0.98	0.08	-	48,48,48,48	0
34	SR	0	8963	1/1	0.95	0.06	-	133,133,133,133	0
35	NA	0	8506	1/1	0.72	0.20	-	83,83,83,83	0
32	MG	B	8042	1/1	0.97	0.07	-	69,69,69,69	0
34	SR	0	8916	1/1	0.99	0.05	-	105,105,105,105	0
34	SR	1	8952	1/1	1.00	0.15	-	90,90,90,90	0
33	CL	3	8804	1/1	0.24	0.20	-	128,128,128,128	0
34	SR	0	8989	1/1	0.89	0.20	-	178,178,178,178	0
34	SR	0	8958	1/1	0.97	0.07	-	116,116,116,116	0
34	SR	0	8977	1/1	0.79	0.07	-	200,200,200,200	0
33	CL	0	8822	1/1	0.97	0.43	-	88,88,88,88	0
34	SR	0	8941	1/1	0.97	0.11	-	114,114,114,114	0
35	NA	0	8516	1/1	0.99	0.19	-	39,39,39,39	0
32	MG	0	8037	1/1	0.99	0.21	-	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8032	1/1	0.98	0.04	-	52,52,52,52	0
35	NA	0	8508	1/1	0.89	0.48	-	52,52,52,52	0
34	SR	9	8980	1/1	0.87	0.15	-	183,183,183,183	0
32	MG	0	8082	1/1	0.94	0.23	-	76,76,76,76	0
34	SR	0	8931	1/1	0.97	0.10	-	111,111,111,111	0
34	SR	0	8928	1/1	0.85	0.04	-	137,137,137,137	0
34	SR	0	8907	1/1	0.99	0.13	-	63,63,63,63	0
34	SR	0	8925	1/1	0.99	0.13	-	98,98,98,98	0
34	SR	0	8956	1/1	0.95	0.12	-	169,169,169,169	0
34	SR	0	8933	1/1	0.96	0.05	-	135,135,135,135	0
32	MG	0	8026	1/1	0.95	0.08	-	50,50,50,50	0
35	NA	0	8574	1/1	0.95	0.58	-	60,60,60,60	0
32	MG	0	8083	1/1	0.95	0.10	-	55,55,55,55	0
33	CL	J	8802	1/1	0.93	0.06	-	67,67,67,67	0
32	MG	0	8035	1/1	0.98	0.10	-	66,66,66,66	0
35	NA	0	8570	1/1	0.66	0.09	-	61,61,61,61	0
34	SR	0	8948	1/1	0.99	0.10	-	115,115,115,115	0
35	NA	0	8512	1/1	0.98	0.15	-	56,56,56,56	0
35	NA	0	8501	1/1	0.99	0.16	-	39,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.