



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 04:10 am GMT

PDB ID : 3CCR
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488C. Density for anisomycin is visible but not included in the model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

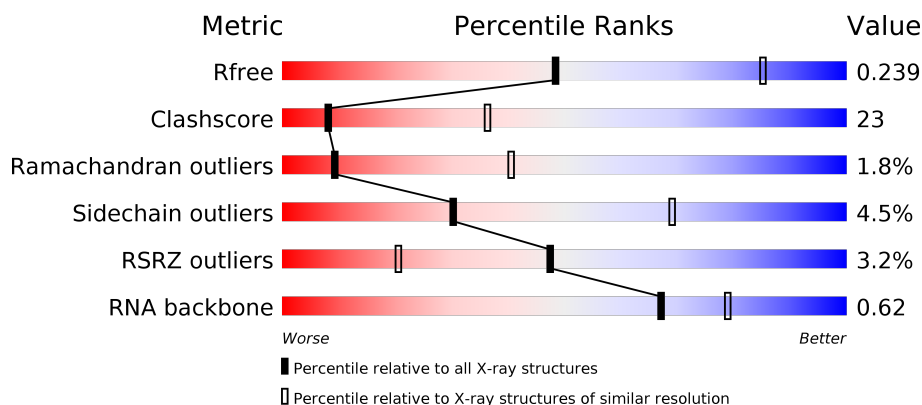
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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






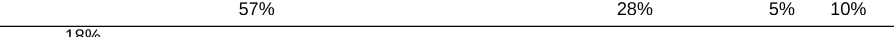

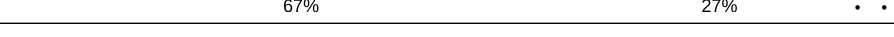
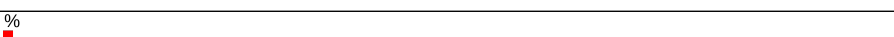

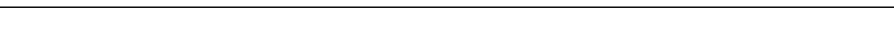




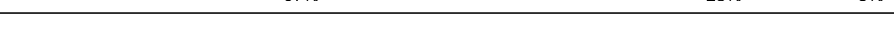




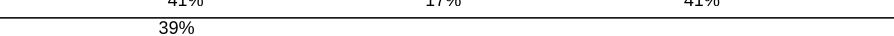






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	111664	1851 (3.00-3.00)
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)
RNA backbone	2636	1017 (3.30-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>8%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
2	B	338	<div> <div>58%</div> <div>37%</div> <div>.</div> </div>
3	C	246	<div> <div>68%</div> <div>27%</div> <div>5%</div> </div>
4	D	177	<div> <div>8%</div> <div>42%</div> <div>35%</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
33	CL	3	8804	-	-	X	-
33	CL	B	8819	-	-	X	-
33	CL	M	8818	-	-	X	-
34	SR	0	8957	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8563	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99120 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
			59018	26348	10871	19054	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	84	Total	Mg	0	0
			84	84		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	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	9	Total 9	Cl 9	0	0
33	J	3	Total 3	Cl 3	0	0
33	K	1	Total 1	Cl 1	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	93	Total 93	Sr 93	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	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	66	Total 66	Na 66	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	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
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	121	Total 121	O 121	0	0
38	B	145	Total 145	O 145	0	0
38	C	166	Total 166	O 166	0	0
38	D	46	Total 46	O 46	0	0
38	E	43	Total 43	O 43	0	0
38	F	31	Total 31	O 31	0	0
38	G	17	Total 17	O 17	0	0
38	H	72	Total 72	O 72	0	0
38	I	5	Total 5	O 5	0	0
38	J	52	Total 52	O 52	0	0
38	K	52	Total 52	O 52	0	0
38	L	81	Total 81	O 81	0	0
38	M	133	Total 133	O 133	0	0
38	N	56	Total 56	O 56	0	0
38	O	41	Total 41	O 41	0	0
38	P	63	Total 63	O 63	0	0
38	Q	52	Total 52	O 52	0	0

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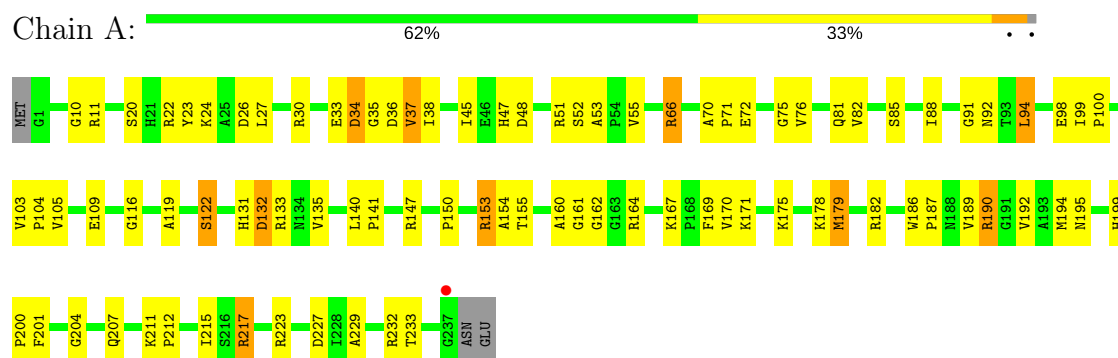
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	R	75	Total 75	O 75	0	0
38	S	37	Total 37	O 37	0	0
38	T	40	Total 40	O 40	0	0
38	U	28	Total 28	O 28	0	0
38	V	15	Total 15	O 15	0	0
38	W	69	Total 69	O 69	0	0
38	X	22	Total 22	O 22	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	28	Total 28	O 28	0	0
38	1	61	Total 61	O 61	0	0
38	2	45	Total 45	O 45	0	0
38	3	76	Total 76	O 76	0	0
38	0	5897	Total 5897	O 5897	0	0
38	9	154	Total 154	O 154	0	0

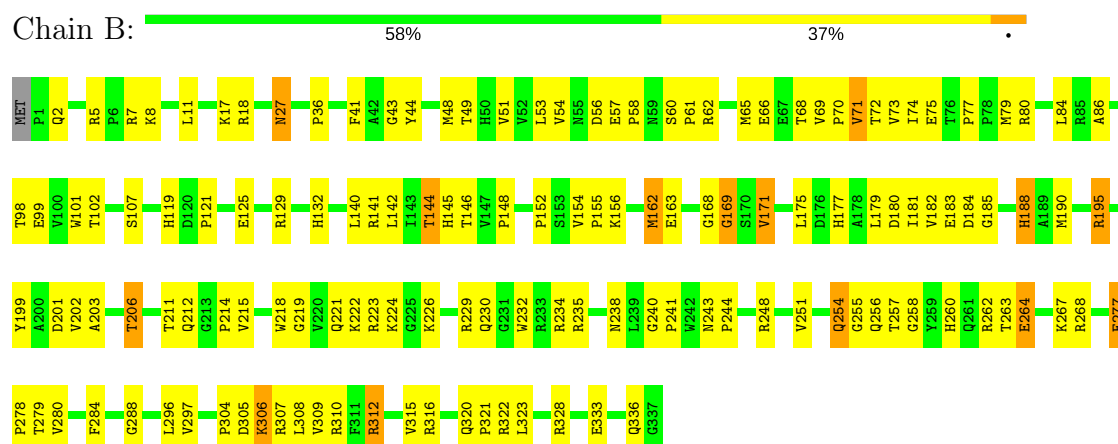
3 Residue-property plots

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.

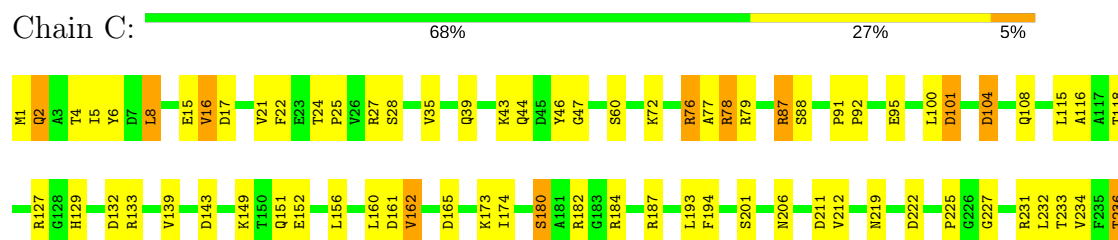
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P

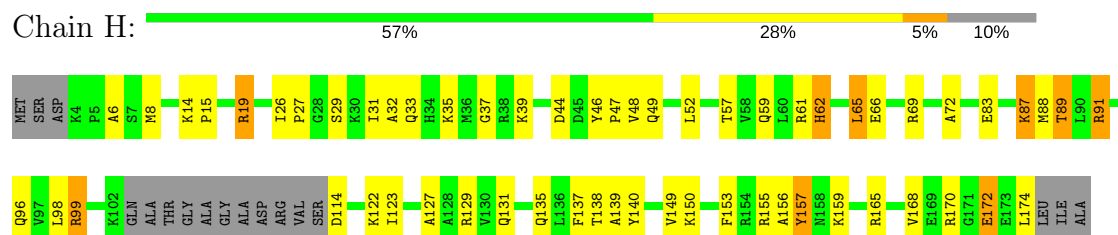


• Molecule 3: 50S ribosomal protein L4P

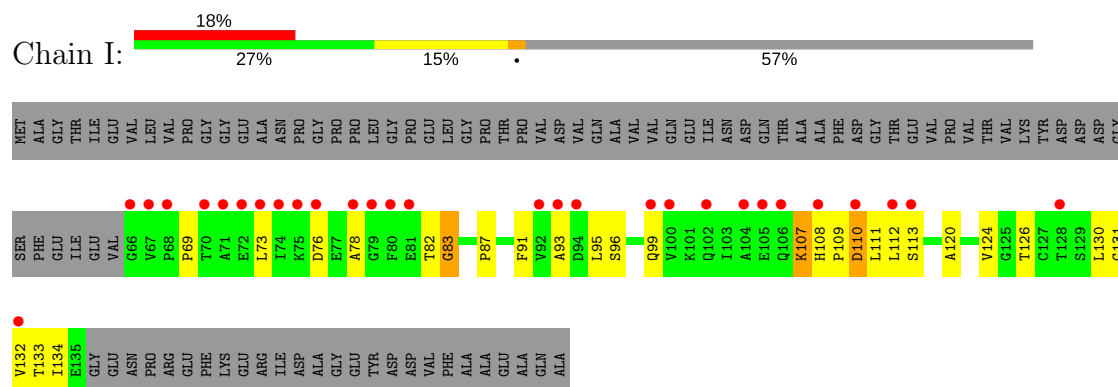


ASP	ASP	GLN	ASP	ASP	ASP	THR	ALA	ALA	SER	GLU	ASP	ASP	ALA	ASP	ASP	ALA	ALA	GLU	GLU	ALA	ASP	ASP	ASP	ASP	ASP	ASP	GLU	ASP	ALA	GLY	ASP	ALA	LEU	GLY	ALA	MET	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

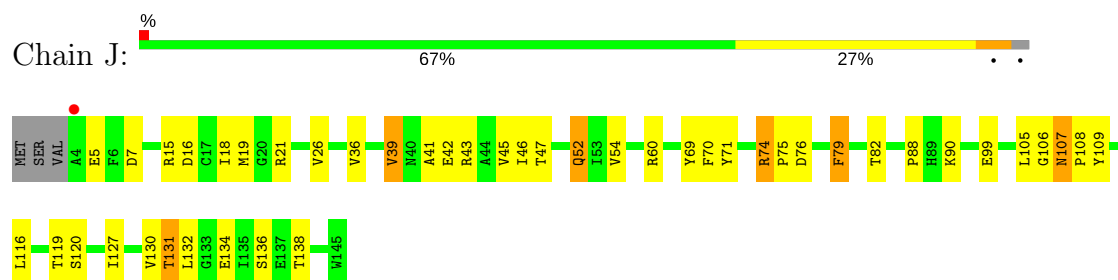
- Molecule 8: 50S ribosomal protein L10e



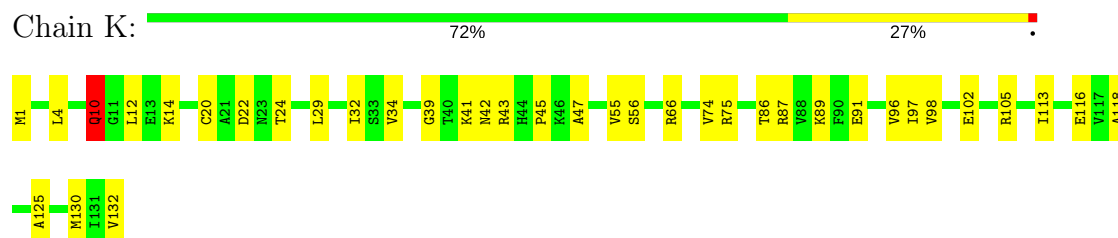
- Molecule 9: 50S ribosomal protein L11P



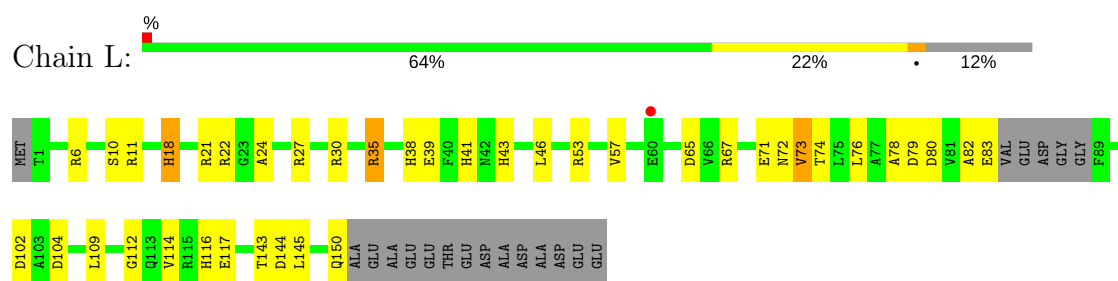
- Molecule 10: 50S ribosomal protein L13P



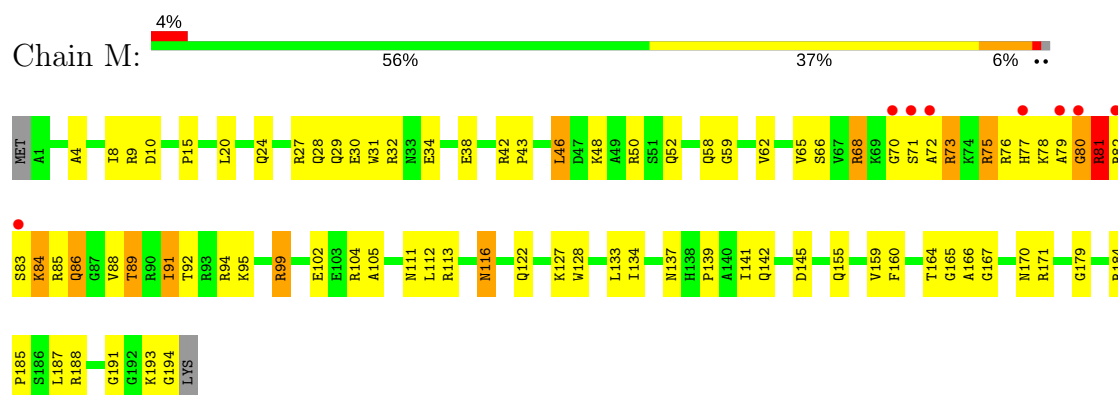
- Molecule 11: 50S ribosomal protein L14P



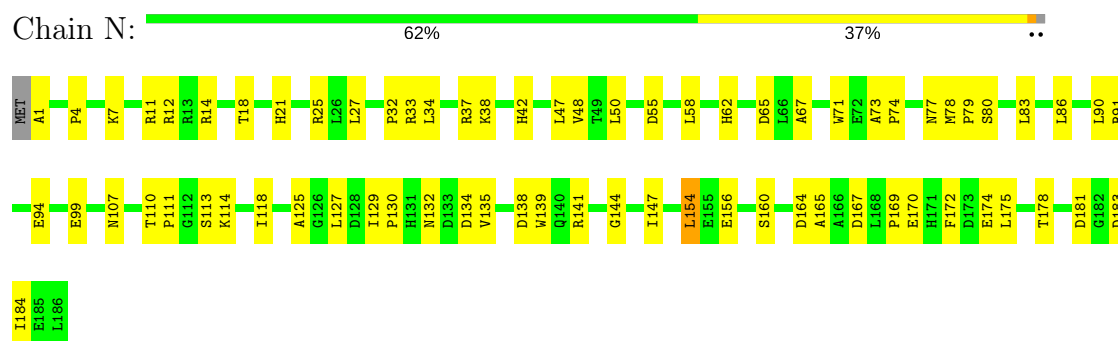
- Molecule 12: 50S ribosomal protein L15P



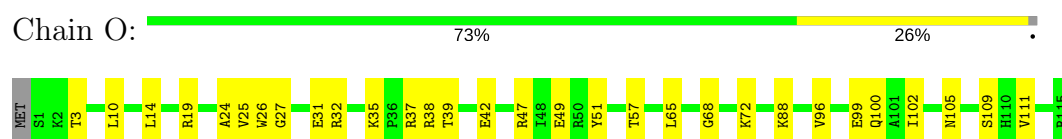
- Molecule 13: 50S ribosomal protein L15e



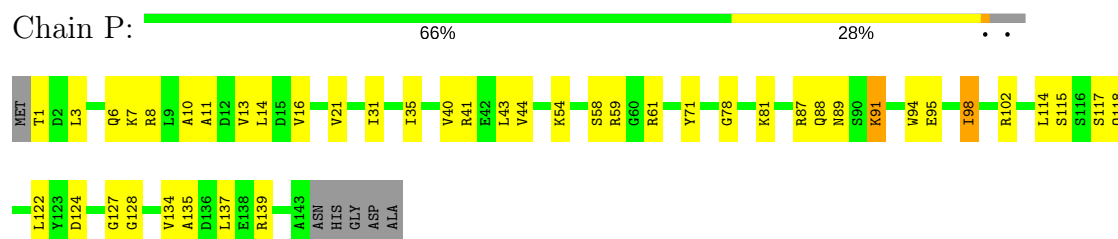
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e

Chain Q:  69% 27% ..



- Molecule 18: 50S ribosomal protein L22P

Chain R:  68% 26% . .



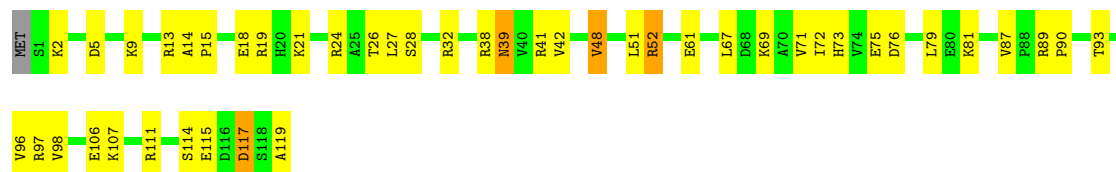
- Molecule 19: 50S ribosomal protein L23P

Chain S:  % 67% 28% 5%



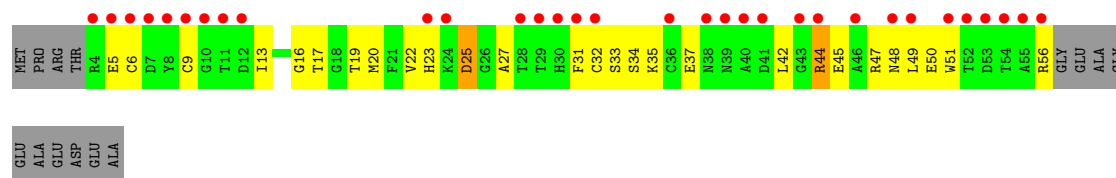
- Molecule 20: 50S ribosomal protein L24P

Chain T:  62% 34% ..



- Molecule 21: 50S ribosomal protein L24e

Chain U:  48% 39% 37% 21%

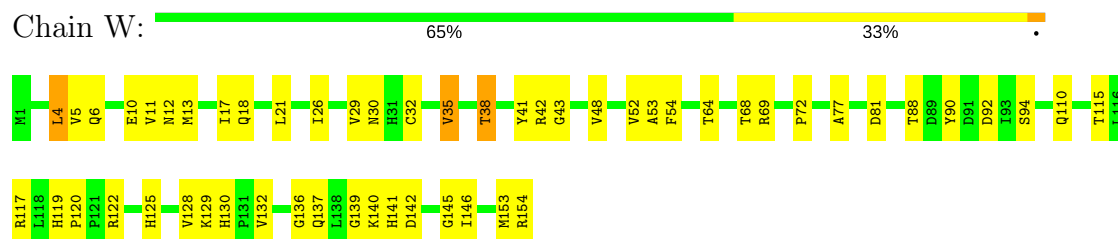


- Molecule 22: 50S ribosomal protein L29P

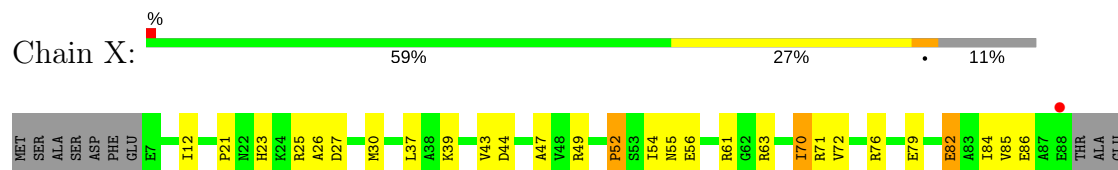
Chain V:  6% 62% 28% 8%



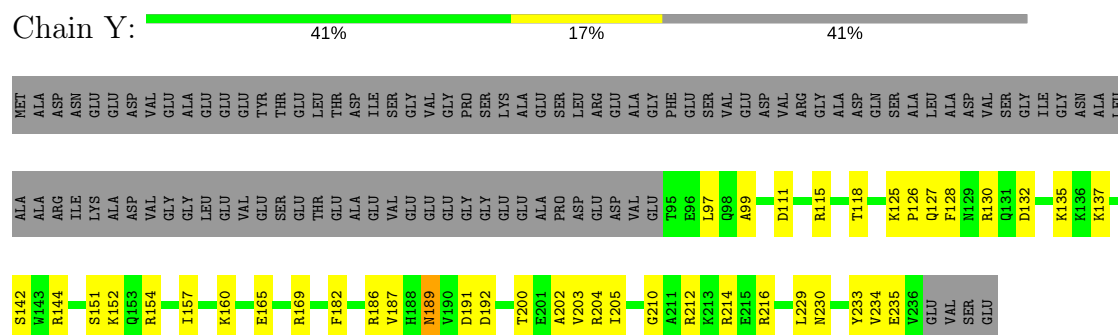
- Molecule 23: 50S ribosomal protein L30P



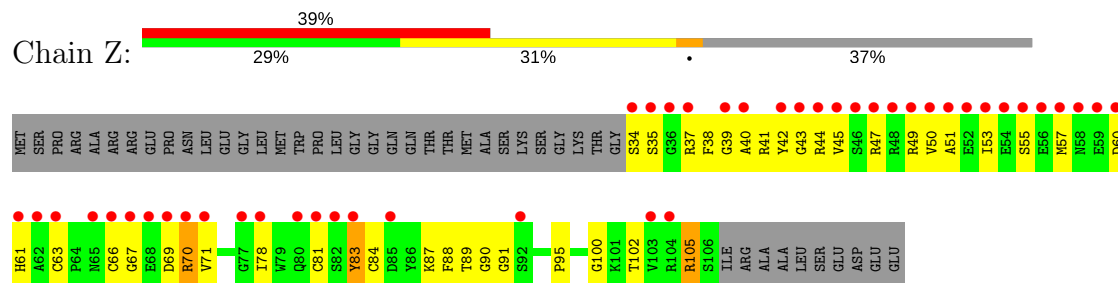
- Molecule 24: 50S ribosomal protein L31e



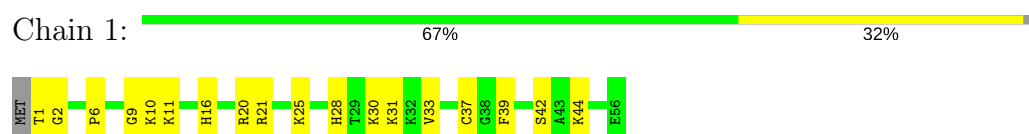
- Molecule 25: 50S ribosomal protein L32e



- Molecule 26: 50S ribosomal protein L37Ae

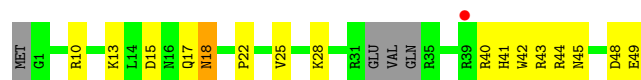


- Molecule 27: 50S ribosomal protein L37e

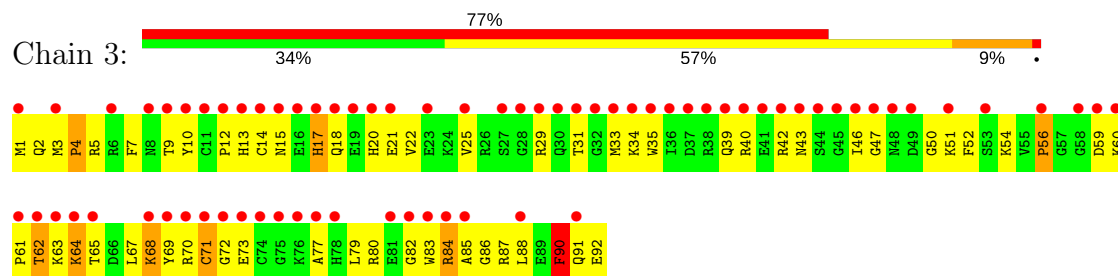


- Molecule 28: 50S ribosomal protein L39e

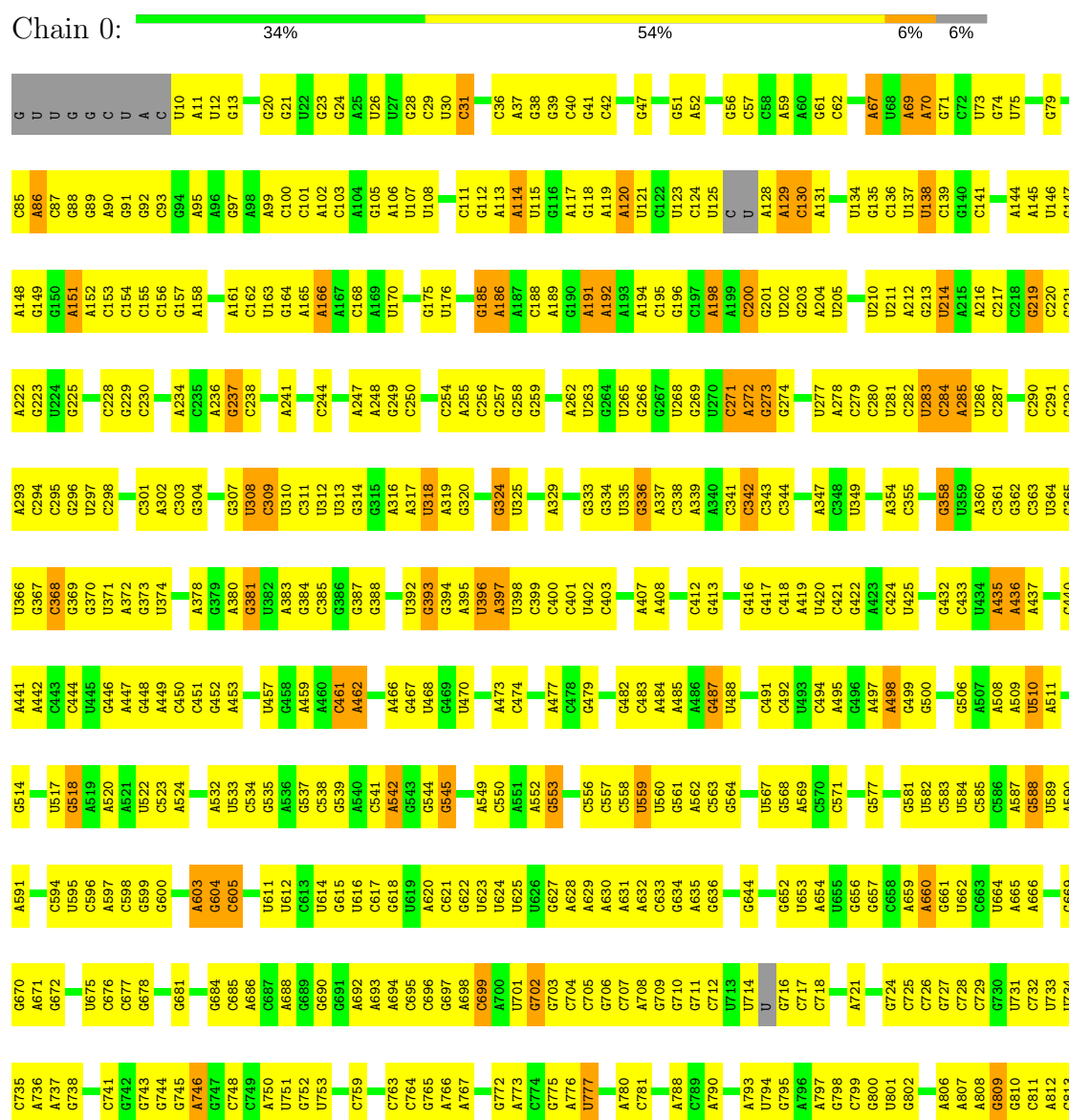




- Molecule 29: 50S ribosomal protein L44E



- Molecule 30: 23S RIBOSOMAL RNA



A1924	C1856	A1778	C1705	G1823	G1555	G1475	U1405	U1333	C1251	C1186	G1112	C1025	G964	G887	G814
G1925	A1857	A1778	G1706	A1624	G1556	A1476	A1406	U1334	C1255	U1187	U1115	U1026	A965	U888	U815
G1926	A1858	C1787	G1707	U1625	C1557	C1477	A1407	C1334	C1256	A1188	U1116	U1028	U967	C899	G816
A1927	A1859	C1787	G1708	A1626	C1558	U1478	A1408	U1337	C1260	A1189	A1117	U1029	G968	C890	G817
G1928	U1860	G1789	G1709	G1627	U1559	U1484	G1410	U1338	U1264	G1190	A1118	U1030	G969	A894	A818
G1929	C1861	G1789	A1710	U1630	U1561	A1485	A1413	G1339	U1265	A1191	G1119	U1031	U970	A895	A819
A1930	C1862	C1790	A1711	A1631	C1562	U1490	A1414	G1340	U1266	A1192	U1120	U1032	U970	C896	G820
A1931	C1863	U1791	G1712	A1632	G1563	G1495	A1415	A1341	U1267	A1193	G1121	U1041	U970	C897	G821
G1932	A1864	A1796	A1713	A1633	C1564	U1496	G1416	C1342	C1268	A1194	C1127	U1042	U970	A897	C822
G1933	A1865	A1797	A1716	C1634	C1566	C1495	G1416	C1343	C1269	A1195	C1127	U1043	U970	C898	G823
A1934	A1866	C1798	A1717	U1635	G1567	A1496	G1417	C1344	U1270	C1196	C1128	C1043	U970	C899	U824
G1935	G1867	G1799	G1718	U1636	G1568	G1497	U1418	G1344	U1271	G1197	U1128	C1044	U970	G902	U825
C1936	G1868	G1800	G1719	A1641	U1569	U1500	U1419	U1350	U1272	U1198	C1129	C1045	U970	U903	U826
U1937	U1871	A1801	G1720	A1642	U1570	U1500	U1420	U1351	U1273	A1199	U1130	U1046	U970	U904	A827
G1938	C1872	A1802	U1722	A1643	A1572	U1503	C1421	G1352	U1274	A1200	G1131	U1047	U970	C905	G828
U1939	G1873	C1803	G1723	U1644	A1573	A1504	C1422	C1353	C1275	A1201	A1132	U1048	U970	C906	A829
C1940	G1874	A1804	U1724	U1645	C1574	A1505	C1423	G1354	C1276	A1202	A1133	U1049	U970	C907	G830
A1941	A1875	G1805	C1725	G1649	C1575	U1506	A1424	A1355	C1277	C1203	G1134	U1050	U970	C908	U831
C1942	C1876	G1806	G1725	G1650	G1576	C1507	G1425	A1356	U1278	U1205	G1137	G1052	U970	C909	G834
C1943	G1877	U1807	G1730	A1653	U1577	C1507	C1426	A1357	U1279	U1206	G1138	G1053	U970	C910	G835
G1947	U1878	C1808	C1731	A1654	C1578	U1511	C1427	U1358	U1280	U1207	U1139	U1056	U970	A916	C838
G1948	U1879	G1809	A1732	U1654	C1579	G1512	C1428	C1360	U1281	C1208	C1140	U1057	U970	U917	C839
G1949	C1880	C1810	A1733	G1655	U1583	G1513	U1429	U1361	G1284	C1209	U1149	U1058	U970	C920	U840
G1950	A1881	A1811	C1734	U1656	C1584	G1514	G1430	U1362	U1285	G1210	A1150	C1060	U970	C921	A841
G1951	C1882	G1812	C1735	C1662	C1585	U1515	A1434	G1363	U1286	G1211	G1151	C1061	U970	A922	C842
U1952	U1883	U1813	A1736	G1663	U1586	A1516	U1435	G1364	A1287	C1212	A1152	U1062	U970	A923	A844
A1953	A1884	G1814	A1737	U1664	U1587	U1517	U1436	C1365	U1288	C1213	G1153	U1063	U970	C924	
A1954	A1885	A1815	U1741	A1665	U1588	C1517	C1437	C1366	U1289	G1214	A1154	U1064	U970	C925	
A1955	C1886	C1816	A1742	G1666	G1589	A1518	A1438	C1367	G1290	A1215	G1155	U1065	U970	C926	
U1956	A1887	U1817	G1743	U1667	U1590	U1519	G1439	A1368	U1291	G1216	G1156	U1066	U970	C927	
A1957	C1888	C1818	G1744	A1668	A1591	G1520	C1440	U1369	A1292	G1217	C1157	U1067	U970	C928	
U1958	U1889	G1819	G1745	U1669	G1592	C1521	U1441	A1370	G1293	U1218	G1158	U1068	U970	A927	C853
U1959	C1890	G1820	U1746	C1670	C1593	A1522	G1442	U1371	U1293	U1219	G1159	U1069	U970	A928	C854
C1960	C1891	U1825	U1747	U1671	U1594	G1523	A1443	A1372	A1294	U1220	G1160	A1070	U970	A929	U855
C1961	C1892	U1826	G1752	C1672	U1595	U1524	G1444	C1377	U1298	G1224	A1161	G1071	U970	G938	C856
C1962	C1893	G1827	C1753	G1673	U1596	G1525	G1445	G1378	G1299	C1225	G1162	A1073	U970	A939	A857
C1963	C1894	U1828	C1754	G1674	U1597	A1526	G1446	G1379	G1300	G1226	G1163	G1074	U970	G940	U858
C1964	C1895	A1829	A1755	U1677	U1598	A1527	U1447	U1380	C1303	G1227	U1164	G1075	U970	G941	C859
C1965	C1896	C1830	A1756	A1678	U1599	G1528	U1448	U1381	C1304	C1228	G1165	G1076	U970	U942	U862
C1966	C1897	U1831	G1757	C1679	G1600	G1529	G1449	G1382	U1305	C1229	G1166	C1080	U970	U943	U863
C1967	C1898	U1832	U1757	C1680	G1601	U1530	G1450	G1383	C1306	U1234	G1167	A1081	U970	U944	
C1968	C1899	U1833	U1758	G1681	A1602	A1533	C1451	U1384	U1309	U1235	U1169	G1087	U970	C945	C868
C1969	C1900	C1834	A1759	G1682	G1603	C1537	G1452	G1385	U1310	G1236	U1170	G1088	U970	U947	G869
C1970	C1901	U1835	G1760	G1683	G1604	U1538	G1453	G1386	G1311	A1237	A1171	A1089	U970	G948	G870
C1971	C1902	U1836	A1761	A1684	A1605	U1539	U1454	A1389	G1312	U1237	G1172	G1089	U970	U949	C871
C1972	C1903	A1840	C1762	A1685	A1606	G1540	G1461	A1390	G1313	C1238	G1173	U1095	U970	A951	U872
C1973	C1904	U1841	C1763	C1686	A1607	G1541	U1462	G1391	U1314	G1239	A1174	U1096	U970	A952	C873
C1974	C1905	C1841	C1764	C1687	G1608	G1542	C1463	A1392	U1315	G1240	G1175	U1097	U970	G953	A874
C1975	C1906	C1842	G1765	C1688	C1613	G1543	U1464	A1393	G1316	G1241	C1176	A1098	U970	G954	A875
C1976	C1907	C1843	G1766	A1691	G1614	U1544	U1465	C1394	G1317	G1242	G1177	A1099	U970	G955	A876
C1977	C1908	A1844	G1767	C1692	A1615	U1545	C1466	C1395	G1318	G1243	G1178	U1107	U970	G956	A877
C1978	C1909	G1848	C1769	G1697	A1616	G1546	C1467	C1396	G1319	U1244	G1179	C1102	U970	G957	C878
C1979	C1910	G1849	U1770	G1698	C1617	U1547	C1468	C1397	G1320	C1245	U1180	C1103	U970	G958	
C1980	C1911	U1850	U1771	G1699	C1618	U1548	A1470	G1398	G1321	A1246	A1181	C1104	U970	C959	A882
C1981	C1912	C1851	G1772	A1701	G1619	U1549	A1471	A1399	G1322	A1247	C1182	U1109	U970	G960	U883
C1982	C1913	U1852	G1773	U1702	G1620	C1552	C1472	A1400	G1323	A1248	C1183	G1110	U970	A961	C884
C1983	C1914	C1853	G1774	U1703	C1621	C1553	U1473	C1401	G1324	G1329	C1184	C1185	U970	C962	C885
C1984	C1915	C1854	A1775	G1704	C1622	C1554	C1474		A1330	C1250	U1185	U1111	U970	C963	A886



A62	C63	C64	A65	G66	C67	G68	U69	C72	A73	G74	G75	G76	A77	C81	U82	G83	U87	G88	C89	G90	C91	G92	A93	A105	U106	C107	C108	G109	G110	U111	U112	C113	G114	C115	C116	C122
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.41Å 299.52Å 574.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 3.00 85.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.81-3.00) 77.4 (85.66-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.247 0.177 , 0.239	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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, 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	0.65	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.38	0/1885	0.65	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.34	0/1382	0.59	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.33	0/241	0.48	0/324
8	H	0.34	0/1302	0.65	0/1743
9	I	0.31	0/526	0.51	0/716
10	J	0.38	0/1136	0.62	0/1530
11	K	0.36	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.62	0/1509
13	M	0.38	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.63	0/1999
15	O	0.37	0/874	0.60	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.69	0/1005
18	R	0.37	0/1172	0.63	0/1578
19	S	0.38	0/648	0.60	0/875
20	T	0.34	0/958	0.66	1/1289 (0.1%)
21	U	0.45	0/417	0.67	0/562
22	V	0.32	0/502	0.55	0/675
23	W	0.36	0/1219	0.64	0/1655
24	X	0.35	0/664	0.61	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.45	0/584	0.63	0/781
27	1	0.43	0/438	0.57	0/578
28	2	0.35	0/401	0.60	0/529
29	3	0.48	0/771	0.66	0/1024
30	0	0.41	0/65954	0.68	4/102862 (0.0%)
31	9	0.35	0/2904	0.68	0/4526
All	All	0.39	0/98698	0.67	5/147581 (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
23	W	0	1
30	0	0	18
31	9	0	1
All	All	0	20

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C5'-C4'-C3'	5.99	125.59	116.00
30	0	871	G	C5'-C4'-O4'	-5.85	102.08	109.10
30	0	1504	A	C1'-O4'-C4'	-5.36	105.62	109.90
20	T	52	ARG	N-CA-C	5.08	124.73	111.00
30	0	2726	U	N1-C1'-C2'	5.01	120.52	114.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	214	U	Sidechain
30	0	324	G	Sidechain
30	0	393	G	Sidechain
30	0	435	A	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	97	0
2	B	2625	0	2532	127	0
3	C	1860	0	1813	70	0
4	D	1094	0	1085	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	55	0
6	F	890	0	843	27	0
7	G	240	0	231	11	0
8	H	1282	0	1292	55	0
9	I	519	0	500	26	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	98	0
14	N	1445	0	1401	59	0
15	O	865	0	873	32	0
16	P	1136	0	1123	44	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	16	0
20	T	950	0	924	33	0
21	U	410	0	368	38	0
22	V	499	0	511	19	0
23	W	1196	0	1137	52	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	44	0
26	Z	573	0	535	64	0
27	1	431	0	426	20	0
28	2	396	0	413	21	0
29	3	755	0	732	90	0
30	0	59018	0	29810	2239	0
31	9	2599	0	1325	161	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	2	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	9	0	0	2	0
33	3	1	0	0	3	0
33	A	1	0	0	1	0
33	B	1	0	0	2	0
33	J	3	0	0	2	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	1	0	0	1	0
33	M	1	0	0	2	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	0	0
34	0	93	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	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	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	2	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	5897	0	0	323	0
38	1	61	0	0	3	0
38	2	45	0	0	1	0
38	3	76	0	0	7	0
38	9	154	0	0	11	0
38	A	121	0	0	3	0
38	B	145	0	0	20	0
38	C	166	0	0	13	0
38	D	46	0	0	7	0
38	E	43	0	0	4	0
38	F	31	0	0	1	0
38	G	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	72	0	0	10	0
38	I	5	0	0	2	0
38	J	52	0	0	4	0
38	K	52	0	0	3	0
38	L	81	0	0	4	0
38	M	133	0	0	12	0
38	N	56	0	0	6	0
38	O	41	0	0	2	0
38	P	63	0	0	5	0
38	Q	52	0	0	1	0
38	R	75	0	0	2	0
38	S	37	0	0	0	0
38	T	40	0	0	3	0
38	U	28	0	0	5	0
38	V	15	0	0	1	0
38	W	69	0	0	7	0
38	X	22	0	0	4	0
38	Y	100	0	0	5	0
38	Z	28	0	0	5	0
All	All	99120	0	59922	3377	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 23.

The worst 5 of 3377 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)
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
30:0:1160:G:H5'	30:0:1161:A:C5'	1.70	1.20
30:0:1160:G:C5'	30:0:1161:A:H5'	1.73	1.18
30:0:1278:A:H4'	30:0:1279:U:C4	1.81	1.16
13:M:171:ARG:HD3	30:0:156:C:H5''	1.15	1.13

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	200 (85%)	30 (13%)	5 (2%)	8	36
2	B	335/338 (99%)	305 (91%)	23 (7%)	7 (2%)	8	36
3	C	244/246 (99%)	216 (88%)	26 (11%)	2 (1%)	21	61
4	D	134/177 (76%)	105 (78%)	23 (17%)	6 (4%)	3	16
5	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	27	67
6	F	117/120 (98%)	97 (83%)	16 (14%)	4 (3%)	4	22
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	156/177 (88%)	139 (89%)	16 (10%)	1 (1%)	27	67
9	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	3	16
10	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	12	47
11	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	21	61
12	L	141/165 (86%)	116 (82%)	22 (16%)	3 (2%)	8	36
13	M	192/196 (98%)	171 (89%)	17 (9%)	4 (2%)	8	36
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	7	34
15	O	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	7	34
18	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	24	64
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
21	U	51/67 (76%)	44 (86%)	6 (12%)	1 (2%)	8	37
22	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	11	43
23	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	24	64
24	X	80/92 (87%)	72 (90%)	6 (8%)	2 (2%)	6	31
25	Y	140/241 (58%)	132 (94%)	7 (5%)	1 (1%)	24	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	55 (78%)	12 (17%)	4 (6%)	2	11
27	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	64 (71%)	17 (19%)	9 (10%)	0	3
All	All	3705/4472 (83%)	3292 (89%)	348 (9%)	65 (2%)	9	40

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
2	B	306	LYS
4	D	137	PRO
6	F	61	MET
6	F	101	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	
1	A	179/182 (98%)	170 (95%)	9 (5%)	27	65
2	B	282/283 (100%)	263 (93%)	19 (7%)	18	52
3	C	193/193 (100%)	180 (93%)	13 (7%)	18	52
4	D	117/148 (79%)	110 (94%)	7 (6%)	21	57
5	E	152/156 (97%)	146 (96%)	6 (4%)	35	73
6	F	93/94 (99%)	92 (99%)	1 (1%)	76	92
7	G	27/282 (10%)	25 (93%)	2 (7%)	15	47
8	H	134/145 (92%)	124 (92%)	10 (8%)	15	47
9	I	58/130 (45%)	57 (98%)	1 (2%)	63	88
10	J	118/121 (98%)	109 (92%)	9 (8%)	14	46
11	K	106/106 (100%)	103 (97%)	3 (3%)	47	80
12	L	113/127 (89%)	106 (94%)	7 (6%)	20	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	147 (93%)	11 (7%)	16	50
14	N	149/150 (99%)	146 (98%)	3 (2%)	58	86
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	62	87
17	Q	79/80 (99%)	74 (94%)	5 (6%)	20	55
18	R	117/122 (96%)	113 (97%)	4 (3%)	40	76
19	S	71/74 (96%)	70 (99%)	1 (1%)	69	90
20	T	105/106 (99%)	98 (93%)	7 (7%)	18	52
21	U	44/53 (83%)	43 (98%)	1 (2%)	53	84
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	130/130 (100%)	126 (97%)	4 (3%)	43	78
24	X	66/74 (89%)	61 (92%)	5 (8%)	14	46
25	Y	120/196 (61%)	117 (98%)	3 (2%)	50	82
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	83
29	3	79/79 (100%)	73 (92%)	6 (8%)	14	46
All	All	3095/3646 (85%)	2955 (96%)	140 (4%)	30	69

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	99	ARG
11	K	24	THR
24	X	82	GLU
8	H	157	TYR
10	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	116	HIS
16	P	50	GLN
28	2	45	ASN
13	M	24	GLN

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Mol	Chain	Res	Type
13	M	137	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	243 (8%)	22 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	262 (9%)	24 (0%)

5 of 262 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 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	871	G
30	0	1237	U
31	9	43	G
30	0	877	G
30	0	1080	C

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	30,35	14,22,23	0.98	1 (7%)	18,31,34	3.68	2 (11%)
30	OMG	0	2588	30	19,26,27	1.10	2 (10%)	22,38,41	2.45	4 (18%)
30	UR3	0	2619	30	13,22,23	0.74	0	15,32,35	0.66	0
30	PSU	0	2621	30	16,21,22	1.66	3 (18%)	20,30,33	5.36	4 (20%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	12,37,40	1.25	1 (8%)

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	30,35	-	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'	-5.10	1.47	1.52
30	0	2588	OMG	C8-N7	-2.09	1.30	1.34
30	0	2621	PSU	C4-N3	2.59	1.37	1.33
30	0	2621	PSU	C2-N1	2.59	1.43	1.38
30	0	2587	OMU	C4-N3	2.63	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.02	114.73	128.41
30	0	2588	OMG	C5-C6-N1	-8.28	111.69	123.47
30	0	2621	PSU	C5-C4-N3	-8.09	114.94	125.36
30	0	628	1MA	C2-N3-C4	-3.80	110.71	116.51
30	0	2587	OMU	C5-C4-N3	-3.72	114.53	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	2	0
30	0	2621	PSU	2	0
30	0	628	1MA	2	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 [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	A	237/240 (98%)	-0.60	1 (0%) 92 78	29, 65, 98, 115	0
2	B	337/338 (99%)	-0.73	0 100 100	31, 59, 87, 97	0
3	C	246/246 (100%)	-0.82	0 100 100	23, 47, 69, 80	0
4	D	140/177 (79%)	0.45	15 (10%) 6 2	74, 109, 132, 140	0
5	E	172/178 (96%)	-0.64	0 100 100	50, 74, 97, 103	0
6	F	119/120 (99%)	-0.30	1 (0%) 86 64	50, 73, 106, 113	0
7	G	29/348 (8%)	0.08	0 100 100	75, 96, 105, 109	0
8	H	160/177 (90%)	-0.49	0 100 100	48, 67, 99, 109	0
9	I	70/162 (43%)	1.80	29 (41%) 0 0	134, 152, 167, 169	0
10	J	142/145 (97%)	-0.79	1 (0%) 87 68	40, 58, 75, 97	0
11	K	132/132 (100%)	-0.87	0 100 100	39, 55, 81, 86	0
12	L	145/165 (87%)	-0.24	1 (0%) 87 68	35, 72, 113, 129	0
13	M	194/196 (98%)	-0.51	8 (4%) 37 15	31, 46, 99, 106	0
14	N	186/187 (99%)	-0.33	0 100 100	60, 80, 126, 132	0
15	O	115/116 (99%)	-0.86	0 100 100	43, 56, 74, 80	0
16	P	143/149 (95%)	-0.75	0 100 100	40, 59, 79, 85	0
17	Q	95/96 (98%)	-0.71	0 100 100	44, 56, 72, 88	0
18	R	150/155 (96%)	-0.83	0 100 100	33, 49, 70, 83	0
19	S	81/85 (95%)	-0.67	1 (1%) 79 53	40, 62, 82, 92	0
20	T	119/120 (99%)	-0.55	0 100 100	40, 59, 87, 116	0
21	U	53/67 (79%)	2.66	32 (60%) 0 0	107, 117, 125, 126	0
22	V	65/71 (91%)	-0.02	4 (6%) 20 7	47, 74, 118, 123	0
23	W	154/154 (100%)	-0.69	0 100 100	39, 54, 73, 87	0
24	X	82/92 (89%)	-0.45	1 (1%) 79 53	46, 65, 94, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.88	0 100 100	30, 49, 71, 92	0
26	Z	73/116 (62%)	3.62	45 (61%) 0 0	98, 116, 126, 130	0
27	1	56/57 (98%)	-0.78	0 100 100	28, 36, 43, 48	0
28	2	46/50 (92%)	-0.57	1 (2%) 62 33	31, 66, 97, 104	0
29	3	92/92 (100%)	4.21	71 (77%) 0 0	104, 119, 130, 134	0
30	0	2749/2923 (94%)	-0.83	2 (0%) 95 89	23, 51, 96, 175	0
31	9	122/122 (100%)	-0.97	1 (0%) 86 64	45, 75, 103, 154	0
All	All	6646/7517 (88%)	-0.53	214 (3%) 47 20	23, 57, 116, 175	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	46	SER	17.2
26	Z	58	ASN	13.1
29	3	39	GLN	12.1
26	Z	36	GLY	11.6
29	3	34	LYS	11.4

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. 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
30	OMG	0	2588	24/25	0.98	0.13	39,41,42,45	0
30	UR3	0	2619	21/22	0.98	0.14	39,43,45,48	0
30	1MA	0	628	23/24	0.98	0.14	31,36,38,38	0
30	PSU	0	2621	20/21	0.98	0.18	40,43,44,44	0
30	OMU	0	2587	21/22	0.98	0.12	41,44,50,50	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. 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	SR	0	9006	1/1	0.31	0.83	180,180,180,180	0
35	NA	0	8557	1/1	0.41	0.08	59,59,59,59	0
34	SR	0	9004	1/1	0.44	1.01	200,200,200,200	0
34	SR	0	8985	1/1	0.45	0.12	182,182,182,182	0
35	NA	0	8567	1/1	0.50	0.30	68,68,68,68	0
35	NA	0	8563	1/1	0.53	0.68	65,65,65,65	0
34	SR	0	8971	1/1	0.54	0.11	170,170,170,170	0
34	SR	0	8997	1/1	0.54	0.83	194,194,194,194	0
33	CL	J	8802	1/1	0.54	0.08	76,76,76,76	0
34	SR	0	9001	1/1	0.55	0.08	166,166,166,166	0
34	SR	0	8959	1/1	0.56	0.28	200,200,200,200	0
34	SR	0	8974	1/1	0.57	0.14	164,164,164,164	0
34	SR	0	8957	1/1	0.57	0.73	200,200,200,200	0
34	SR	0	8979	1/1	0.61	0.18	198,198,198,198	0
35	NA	0	8553	1/1	0.62	0.33	70,70,70,70	0
35	NA	0	8528	1/1	0.63	0.91	83,83,83,83	0
34	SR	0	8986	1/1	0.63	0.45	200,200,200,200	0
34	SR	0	8975	1/1	0.64	0.11	171,171,171,171	0
34	SR	0	8962	1/1	0.67	0.08	179,179,179,179	0
34	SR	0	8977	1/1	0.72	0.11	181,181,181,181	0
32	MG	0	8091	1/1	0.73	0.07	58,58,58,58	0
37	CD	U	8701	1/1	0.74	0.35	200,200,200,200	0
34	SR	0	8998	1/1	0.75	0.30	184,184,184,184	0
34	SR	0	8922	1/1	0.75	0.29	169,169,169,169	0
34	SR	9	8980	1/1	0.75	0.14	182,182,182,182	0
36	K	0	8401	1/1	0.75	0.15	156,156,156,156	0
34	SR	0	8919	1/1	0.76	0.32	200,200,200,200	0
34	SR	0	8960	1/1	0.76	0.05	152,152,152,152	0
34	SR	0	8982	1/1	0.78	1.88	200,200,200,200	0
33	CL	0	8814	1/1	0.78	0.18	72,72,72,72	0
34	SR	0	8969	1/1	0.78	0.31	192,192,192,192	0
32	MG	0	8063	1/1	0.78	0.22	86,86,86,86	0
35	NA	0	8518	1/1	0.79	0.26	75,75,75,75	0
35	NA	0	8559	1/1	0.79	0.46	122,122,122,122	0
34	SR	0	8973	1/1	0.80	0.14	112,112,112,112	0
34	SR	0	8944	1/1	0.80	0.08	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8967	1/1	0.81	0.05	133,133,133,133	0
35	NA	0	8566	1/1	0.81	0.32	62,62,62,62	0
34	SR	0	8988	1/1	0.81	0.13	170,170,170,170	0
35	NA	0	8571	1/1	0.82	0.17	46,46,46,46	0
34	SR	0	9007	1/1	0.82	0.24	179,179,179,179	0
35	NA	0	8556	1/1	0.82	0.44	63,63,63,63	0
34	SR	0	8968	1/1	0.82	0.15	177,177,177,177	0
34	SR	3	8932	1/1	0.82	0.09	158,158,158,158	0
35	NA	9	8572	1/1	0.82	0.17	71,71,71,71	0
35	NA	0	8573	1/1	0.82	0.28	55,55,55,55	0
34	SR	0	8947	1/1	0.83	0.30	194,194,194,194	0
35	NA	0	8535	1/1	0.83	0.20	64,64,64,64	0
32	MG	A	8051	1/1	0.83	0.22	101,101,101,101	0
34	SR	0	8931	1/1	0.83	0.07	110,110,110,110	0
33	CL	0	8815	1/1	0.83	0.09	87,87,87,87	0
35	NA	0	8541	1/1	0.83	0.24	54,54,54,54	0
34	SR	0	9002	1/1	0.83	0.06	157,157,157,157	0
34	SR	0	8946	1/1	0.85	0.12	123,123,123,123	0
34	SR	0	8955	1/1	0.85	0.17	200,200,200,200	0
35	NA	0	8548	1/1	0.85	0.12	68,68,68,68	0
35	NA	0	8515	1/1	0.86	0.15	44,44,44,44	0
32	MG	0	8081	1/1	0.86	0.32	80,80,80,80	0
35	NA	0	8564	1/1	0.86	0.34	57,57,57,57	0
35	NA	0	8546	1/1	0.86	0.47	80,80,80,80	0
34	SR	A	8993	1/1	0.86	0.08	159,159,159,159	0
37	CD	Z	8703	1/1	0.86	0.28	200,200,200,200	0
35	NA	0	8507	1/1	0.86	0.16	32,32,32,32	0
34	SR	0	8989	1/1	0.86	0.18	200,200,200,200	0
32	MG	2	8060	1/1	0.86	0.10	35,35,35,35	0
35	NA	0	8525	1/1	0.87	0.25	85,85,85,85	0
32	MG	0	8093	1/1	0.87	0.05	28,28,28,28	0
34	SR	B	8987	1/1	0.87	0.39	200,200,200,200	0
34	SR	0	8953	1/1	0.88	0.07	200,200,200,200	0
35	NA	0	8562	1/1	0.88	0.53	89,89,89,89	0
35	NA	0	8530	1/1	0.88	0.37	49,49,49,49	0
34	SR	0	8942	1/1	0.88	0.07	130,130,130,130	0
34	SR	0	8915	1/1	0.88	0.07	118,118,118,118	0
34	SR	0	8964	1/1	0.88	0.08	129,129,129,129	0
34	SR	0	8939	1/1	0.88	0.08	152,152,152,152	0
35	NA	0	8545	1/1	0.88	0.24	33,33,33,33	0
34	SR	0	8991	1/1	0.88	0.35	193,193,193,193	0
33	CL	3	8804	1/1	0.89	0.19	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8071	1/1	0.89	0.13	31,31,31,31	0
37	CD	3	8704	1/1	0.89	0.71	200,200,200,200	0
35	NA	0	8570	1/1	0.89	0.07	25,25,25,25	0
34	SR	0	8928	1/1	0.89	0.09	146,146,146,146	0
35	NA	0	8549	1/1	0.90	0.17	77,77,77,77	0
32	MG	0	8047	1/1	0.90	0.15	67,67,67,67	0
34	SR	0	8976	1/1	0.90	0.23	197,197,197,197	0
35	NA	0	8522	1/1	0.90	0.21	45,45,45,45	0
32	MG	B	8042	1/1	0.90	0.08	56,56,56,56	0
32	MG	0	8036	1/1	0.90	0.05	37,37,37,37	0
32	MG	0	8069	1/1	0.90	0.19	55,55,55,55	0
35	NA	0	8552	1/1	0.90	0.26	58,58,58,58	0
34	SR	0	8981	1/1	0.91	0.13	157,157,157,157	0
32	MG	0	8052	1/1	0.91	0.04	51,51,51,51	0
35	NA	0	8505	1/1	0.91	1.13	53,53,53,53	0
34	SR	0	8965	1/1	0.91	0.07	127,127,127,127	0
34	SR	9	9003	1/1	0.91	0.09	177,177,177,177	0
34	SR	0	8956	1/1	0.91	0.05	151,151,151,151	0
32	MG	0	8032	1/1	0.91	0.05	27,27,27,27	0
32	MG	0	8050	1/1	0.91	0.08	52,52,52,52	0
34	SR	3	8999	1/1	0.91	0.28	172,172,172,172	0
32	MG	0	8075	1/1	0.92	0.09	83,83,83,83	0
34	SR	F	9005	1/1	0.92	0.09	131,131,131,131	0
32	MG	0	8049	1/1	0.92	0.38	74,74,74,74	0
35	NA	0	8565	1/1	0.92	0.94	70,70,70,70	0
34	SR	0	8984	1/1	0.92	0.07	105,105,105,105	0
35	NA	0	8509	1/1	0.92	0.14	54,54,54,54	0
34	SR	0	9000	1/1	0.92	0.31	200,200,200,200	0
32	MG	0	8068	1/1	0.92	0.11	49,49,49,49	0
32	MG	K	8054	1/1	0.92	0.15	40,40,40,40	0
32	MG	0	8046	1/1	0.92	0.13	26,26,26,26	0
35	NA	0	8519	1/1	0.92	0.27	51,51,51,51	0
34	SR	0	8937	1/1	0.93	0.17	100,100,100,100	0
32	MG	0	8016	1/1	0.93	0.22	48,48,48,48	0
32	MG	0	8010	1/1	0.93	0.17	24,24,24,24	0
34	SR	0	8994	1/1	0.93	0.24	200,200,200,200	0
35	NA	0	8511	1/1	0.93	0.09	48,48,48,48	0
33	CL	L	8810	1/1	0.93	0.10	64,64,64,64	0
35	NA	0	8521	1/1	0.93	0.20	53,53,53,53	0
32	MG	0	8039	1/1	0.94	0.18	71,71,71,71	0
35	NA	0	8547	1/1	0.94	0.67	47,47,47,47	0
33	CL	J	8821	1/1	0.94	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8560	1/1	0.94	0.76	74,74,74,74	0
34	SR	0	8970	1/1	0.94	0.04	131,131,131,131	0
35	NA	J	8538	1/1	0.94	0.08	49,49,49,49	0
34	SR	0	8910	1/1	0.94	0.08	99,99,99,99	0
32	MG	0	8037	1/1	0.94	0.17	76,76,76,76	0
32	MG	0	8088	1/1	0.94	0.16	35,35,35,35	0
32	MG	0	8033	1/1	0.94	0.13	40,40,40,40	0
35	NA	0	8544	1/1	0.94	0.11	41,41,41,41	0
33	CL	N	8807	1/1	0.94	0.35	99,99,99,99	0
35	NA	R	8532	1/1	0.94	0.14	37,37,37,37	0
34	SR	0	8916	1/1	0.94	0.10	114,114,114,114	0
33	CL	Y	8820	1/1	0.94	0.11	47,47,47,47	0
34	SR	0	8927	1/1	0.94	0.20	196,196,196,196	0
35	NA	0	8506	1/1	0.95	0.51	58,58,58,58	0
35	NA	0	8526	1/1	0.95	0.13	33,33,33,33	0
34	SR	0	8983	1/1	0.95	0.27	191,191,191,191	0
33	CL	K	8812	1/1	0.95	0.07	48,48,48,48	0
34	SR	0	8914	1/1	0.95	0.20	105,105,105,105	0
35	NA	0	8508	1/1	0.95	0.56	61,61,61,61	0
32	MG	0	8082	1/1	0.95	0.12	66,66,66,66	0
32	MG	0	8065	1/1	0.95	0.12	50,50,50,50	0
33	CL	0	8803	1/1	0.95	0.14	69,69,69,69	0
33	CL	R	8806	1/1	0.95	0.11	47,47,47,47	0
32	MG	0	8062	1/1	0.95	0.20	57,57,57,57	0
35	NA	0	8504	1/1	0.95	0.09	27,27,27,27	0
34	SR	0	8945	1/1	0.95	0.06	107,107,107,107	0
32	MG	0	8080	1/1	0.95	0.28	68,68,68,68	0
33	CL	0	8822	1/1	0.95	0.60	97,97,97,97	0
35	NA	0	8501	1/1	0.96	0.14	43,43,43,43	0
35	NA	0	8561	1/1	0.96	0.36	57,57,57,57	0
35	NA	0	8554	1/1	0.96	0.55	65,65,65,65	0
35	NA	Q	8540	1/1	0.96	0.11	67,67,67,67	0
32	MG	0	8004	1/1	0.96	0.18	21,21,21,21	0
33	CL	0	8817	1/1	0.96	0.20	69,69,69,69	0
33	CL	0	8816	1/1	0.96	0.39	94,94,94,94	0
34	SR	0	8917	1/1	0.96	0.10	109,109,109,109	0
32	MG	B	8043	1/1	0.96	0.11	53,53,53,53	0
34	SR	0	8972	1/1	0.96	0.10	150,150,150,150	0
34	SR	0	8943	1/1	0.96	0.09	72,72,72,72	0
35	NA	S	8510	1/1	0.96	0.04	26,26,26,26	0
35	NA	0	8527	1/1	0.96	0.15	54,54,54,54	0
32	MG	0	8041	1/1	0.96	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8990	1/1	0.96	0.15	125,125,125,125	0
35	NA	0	8513	1/1	0.96	0.34	66,66,66,66	0
35	NA	0	8533	1/1	0.96	0.08	53,53,53,53	0
33	CL	J	8801	1/1	0.96	0.13	71,71,71,71	0
34	SR	0	8996	1/1	0.96	0.22	199,199,199,199	0
32	MG	3	8090	1/1	0.96	0.12	80,80,80,80	0
35	NA	M	8539	1/1	0.96	0.09	32,32,32,32	0
35	NA	0	8574	1/1	0.96	0.35	54,54,54,54	0
35	NA	0	8516	1/1	0.96	0.08	20,20,20,20	0
32	MG	0	8035	1/1	0.96	0.10	61,61,61,61	0
32	MG	0	8040	1/1	0.96	0.21	54,54,54,54	0
34	SR	A	8929	1/1	0.96	0.04	117,117,117,117	0
34	SR	0	8948	1/1	0.97	0.08	103,103,103,103	0
35	NA	0	8536	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8020	1/1	0.97	0.14	29,29,29,29	0
34	SR	0	8995	1/1	0.97	0.14	140,140,140,140	0
32	MG	0	8055	1/1	0.97	0.10	45,45,45,45	0
32	MG	0	8089	1/1	0.97	0.17	59,59,59,59	0
35	NA	0	8550	1/1	0.97	0.27	47,47,47,47	0
32	MG	0	8029	1/1	0.97	0.07	68,68,68,68	0
32	MG	0	8025	1/1	0.97	0.10	30,30,30,30	0
34	SR	0	8924	1/1	0.97	0.17	133,133,133,133	0
32	MG	0	8064	1/1	0.97	0.06	33,33,33,33	0
32	MG	Y	8086	1/1	0.97	0.06	37,37,37,37	0
33	CL	A	8809	1/1	0.97	0.35	100,100,100,100	0
32	MG	T	8057	1/1	0.97	0.04	63,63,63,63	0
34	SR	0	8920	1/1	0.97	0.05	106,106,106,106	0
35	NA	0	8529	1/1	0.97	0.18	41,41,41,41	0
35	NA	0	8534	1/1	0.97	0.18	37,37,37,37	0
32	MG	0	8083	1/1	0.97	0.12	71,71,71,71	0
32	MG	0	8027	1/1	0.97	0.12	26,26,26,26	0
32	MG	0	8067	1/1	0.98	0.13	32,32,32,32	0
32	MG	0	8021	1/1	0.98	0.11	25,25,25,25	0
34	SR	0	8940	1/1	0.98	0.11	77,77,77,77	0
34	SR	0	8963	1/1	0.98	0.05	123,123,123,123	0
32	MG	0	8078	1/1	0.98	0.23	51,51,51,51	0
34	SR	0	8926	1/1	0.98	0.09	109,109,109,109	0
34	SR	S	8961	1/1	0.98	0.05	126,126,126,126	0
32	MG	0	8002	1/1	0.98	0.08	29,29,29,29	0
35	NA	0	8555	1/1	0.98	0.34	50,50,50,50	0
32	MG	0	8018	1/1	0.98	0.14	34,34,34,34	0
32	MG	0	8092	1/1	0.98	0.02	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8005	1/1	0.98	0.22	34,34,34,34	0
35	NA	R	8575	1/1	0.98	0.34	89,89,89,89	0
32	MG	0	8024	1/1	0.98	0.12	96,96,96,96	0
35	NA	0	8551	1/1	0.98	0.15	55,55,55,55	0
34	SR	0	8908	1/1	0.98	0.13	77,77,77,77	0
32	MG	0	8053	1/1	0.98	0.05	45,45,45,45	0
32	MG	0	8014	1/1	0.98	0.19	21,21,21,21	0
32	MG	0	8009	1/1	0.98	0.21	24,24,24,24	0
32	MG	0	8087	1/1	0.98	0.09	26,26,26,26	0
34	SR	0	8936	1/1	0.98	0.08	87,87,87,87	0
32	MG	0	8034	1/1	0.98	0.13	53,53,53,53	0
34	SR	0	8901	1/1	0.98	0.14	63,63,63,63	0
32	MG	0	8006	1/1	0.98	0.13	20,20,20,20	0
34	SR	B	8950	1/1	0.98	0.16	113,113,113,113	0
34	SR	0	8958	1/1	0.98	0.07	114,114,114,114	0
34	SR	0	8921	1/1	0.98	0.09	75,75,75,75	0
37	CD	O	8705	1/1	0.98	0.08	93,93,93,93	0
34	SR	0	8923	1/1	0.98	0.12	85,85,85,85	0
36	K	M	8402	1/1	0.98	0.11	60,60,60,60	0
34	SR	0	8992	1/1	0.98	0.08	130,130,130,130	0
35	NA	0	8568	1/1	0.98	0.10	38,38,38,38	0
34	SR	0	8951	1/1	0.98	0.09	139,139,139,139	0
34	SR	0	8938	1/1	0.98	0.07	164,164,164,164	0
34	SR	0	8941	1/1	0.98	0.18	122,122,122,122	0
32	MG	0	8073	1/1	0.98	0.06	51,51,51,51	0
35	NA	0	8542	1/1	0.98	0.16	51,51,51,51	0
34	SR	0	8935	1/1	0.98	0.09	87,87,87,87	0
35	NA	0	8520	1/1	0.98	0.10	39,39,39,39	0
35	NA	0	8558	1/1	0.98	0.22	44,44,44,44	0
32	MG	0	8023	1/1	0.98	0.18	24,24,24,24	0
34	SR	0	8911	1/1	0.98	0.06	79,79,79,79	0
32	MG	0	8017	1/1	0.98	0.10	20,20,20,20	0
32	MG	0	8066	1/1	0.98	0.31	75,75,75,75	0
34	SR	0	8909	1/1	0.98	0.13	89,89,89,89	0
34	SR	0	8918	1/1	0.99	0.09	71,71,71,71	0
32	MG	0	8019	1/1	0.99	0.15	23,23,23,23	0
32	MG	0	8038	1/1	0.99	0.05	61,61,61,61	0
32	MG	0	8084	1/1	0.99	0.14	24,24,24,24	0
32	MG	0	8072	1/1	0.99	0.08	47,47,47,47	0
32	MG	0	8030	1/1	0.99	0.34	86,86,86,86	0
32	MG	0	8070	1/1	0.99	0.10	40,40,40,40	0
32	MG	0	8077	1/1	0.99	0.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8045	1/1	0.99	0.10	24,24,24,24	0
32	MG	0	8044	1/1	0.99	0.14	52,52,52,52	0
35	NA	0	8512	1/1	0.99	0.08	36,36,36,36	0
32	MG	0	8056	1/1	0.99	0.08	75,75,75,75	0
34	SR	0	8905	1/1	0.99	0.23	62,62,62,62	0
32	MG	0	8085	1/1	0.99	0.12	67,67,67,67	0
34	SR	0	9008	1/1	0.99	0.17	97,97,97,97	0
32	MG	0	8012	1/1	0.99	0.14	15,15,15,15	0
34	SR	0	8902	1/1	0.99	0.16	67,67,67,67	0
34	SR	0	8966	1/1	0.99	0.07	97,97,97,97	0
32	MG	0	8061	1/1	0.99	0.18	19,19,19,19	0
35	NA	0	8524	1/1	0.99	0.40	54,54,54,54	0
32	MG	0	8048	1/1	0.99	0.21	20,20,20,20	0
32	MG	0	8058	1/1	0.99	0.06	22,22,22,22	0
33	CL	B	8819	1/1	0.99	0.15	59,59,59,59	0
33	CL	M	8818	1/1	0.99	0.05	39,39,39,39	0
33	CL	0	8813	1/1	0.99	0.03	46,46,46,46	0
34	SR	A	8930	1/1	0.99	0.07	125,125,125,125	0
32	MG	0	8013	1/1	0.99	0.04	24,24,24,24	0
32	MG	0	8031	1/1	0.99	0.23	52,52,52,52	0
32	MG	0	8001	1/1	0.99	0.12	26,26,26,26	0
32	MG	0	8079	1/1	0.99	0.11	36,36,36,36	0
35	NA	0	8502	1/1	0.99	0.05	56,56,56,56	0
34	SR	0	8934	1/1	0.99	0.09	99,99,99,99	0
34	SR	1	8913	1/1	0.99	0.11	100,100,100,100	0
32	MG	0	8022	1/1	0.99	0.12	17,17,17,17	0
35	NA	0	8569	1/1	0.99	0.20	67,67,67,67	0
32	MG	0	8003	1/1	0.99	0.17	22,22,22,22	0
35	NA	0	8517	1/1	0.99	0.15	21,21,21,21	0
32	MG	0	8015	1/1	0.99	0.13	25,25,25,25	0
34	SR	0	8933	1/1	0.99	0.07	126,126,126,126	0
35	NA	0	8523	1/1	0.99	0.11	51,51,51,51	0
34	SR	0	8949	1/1	0.99	0.05	102,102,102,102	0
35	NA	0	8514	1/1	0.99	0.19	17,17,17,17	0
32	MG	9	8074	1/1	0.99	0.05	63,63,63,63	0
35	NA	9	8543	1/1	0.99	0.11	38,38,38,38	0
33	CL	0	8811	1/1	0.99	0.38	79,79,79,79	0
35	NA	C	8503	1/1	0.99	0.17	45,45,45,45	0
32	MG	0	8008	1/1	0.99	0.14	26,26,26,26	0
33	CL	O	8808	1/1	0.99	0.11	87,87,87,87	0
32	MG	0	8076	1/1	0.99	0.11	27,27,27,27	0
32	MG	0	8059	1/1	0.99	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8531	1/1	0.99	0.10	15,15,15,15	0
33	CL	0	8805	1/1	0.99	0.14	70,70,70,70	0
34	SR	0	8925	1/1	0.99	0.15	94,94,94,94	0
34	SR	0	8906	1/1	1.00	0.20	64,64,64,64	0
34	SR	0	8903	1/1	1.00	0.13	46,46,46,46	0
32	MG	0	8028	1/1	1.00	0.13	19,19,19,19	0
35	NA	0	8537	1/1	1.00	0.17	29,29,29,29	0
34	SR	1	8952	1/1	1.00	0.11	72,72,72,72	0
32	MG	0	8011	1/1	1.00	0.21	24,24,24,24	0
32	MG	0	8007	1/1	1.00	0.19	18,18,18,18	0
34	SR	0	8907	1/1	1.00	0.12	40,40,40,40	0
34	SR	0	8904	1/1	1.00	0.17	58,58,58,58	0
37	CD	1	8702	1/1	1.00	0.13	61,61,61,61	0
34	SR	0	8954	1/1	1.00	0.12	103,103,103,103	0
32	MG	0	8026	1/1	1.00	0.04	27,27,27,27	0
34	SR	R	8912	1/1	1.00	0.12	86,86,86,86	0
34	SR	9	8978	1/1	1.00	0.07	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.