



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 10:17 AM UTC

PDB ID : 2QEX / pdb_00002qex
Title : Negamycin Binds to the Wall of the Nascent Chain Exit Tunnel of the 50S Ribosomal Subunit
Authors : Schroeder, S.J.; Blaha, G.
Deposited on : 2007-06-26
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

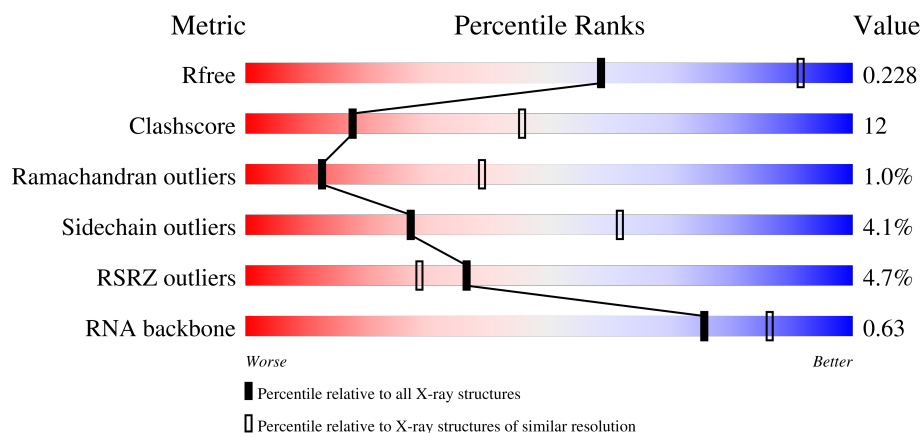
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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

Mol	Chain	Length	Quality of chain
1	0	2772	2% 61% 33% 6% .
2	9	122	3% 39% 49% 11% .
3	A	240	5% 67% 26% 6% .
4	B	338	2% 62% 34% .

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	174	
11	J	145	
12	K	132	
13	L	165	
14	M	196	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	67	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	0	8575	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99020 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4P.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 9 is a protein called Acidic ribosomal protein P0 homolog.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	LYS	conflict	UNP P60617
H	166	SER	VAL	conflict	UNP P60617
H	167	PRO	GLU	conflict	UNP P60617
H	168	ALA	ARG	conflict	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	170	ASN	ILE	conflict	UNP P60617

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	332	283	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	GLY	conflict	UNP P60618

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	UNP P60619

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

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

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

- Molecule 30 is a protein called 50S ribosomal protein L44e.

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

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

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

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

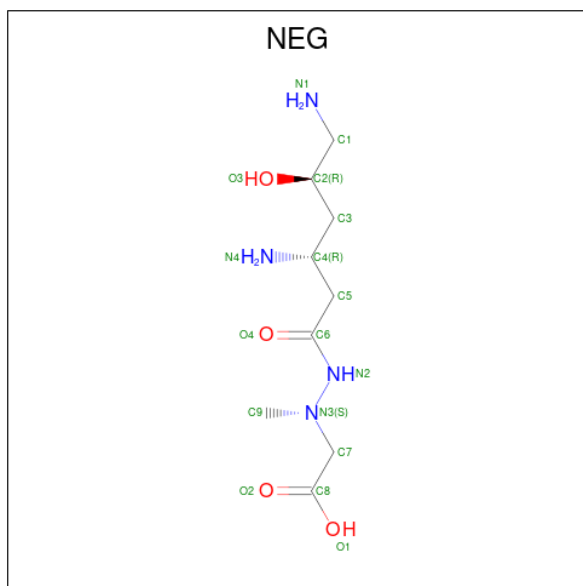
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	10	Total	Cl	0	0
			10	10		
35	A	1	Total	Cl	0	0
			1	1		

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

- Molecule 36 is NEGAMYCIN (CCD ID: NEG) (formula: $C_9H_{20}N_4O_4$).



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

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 38 is water.

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

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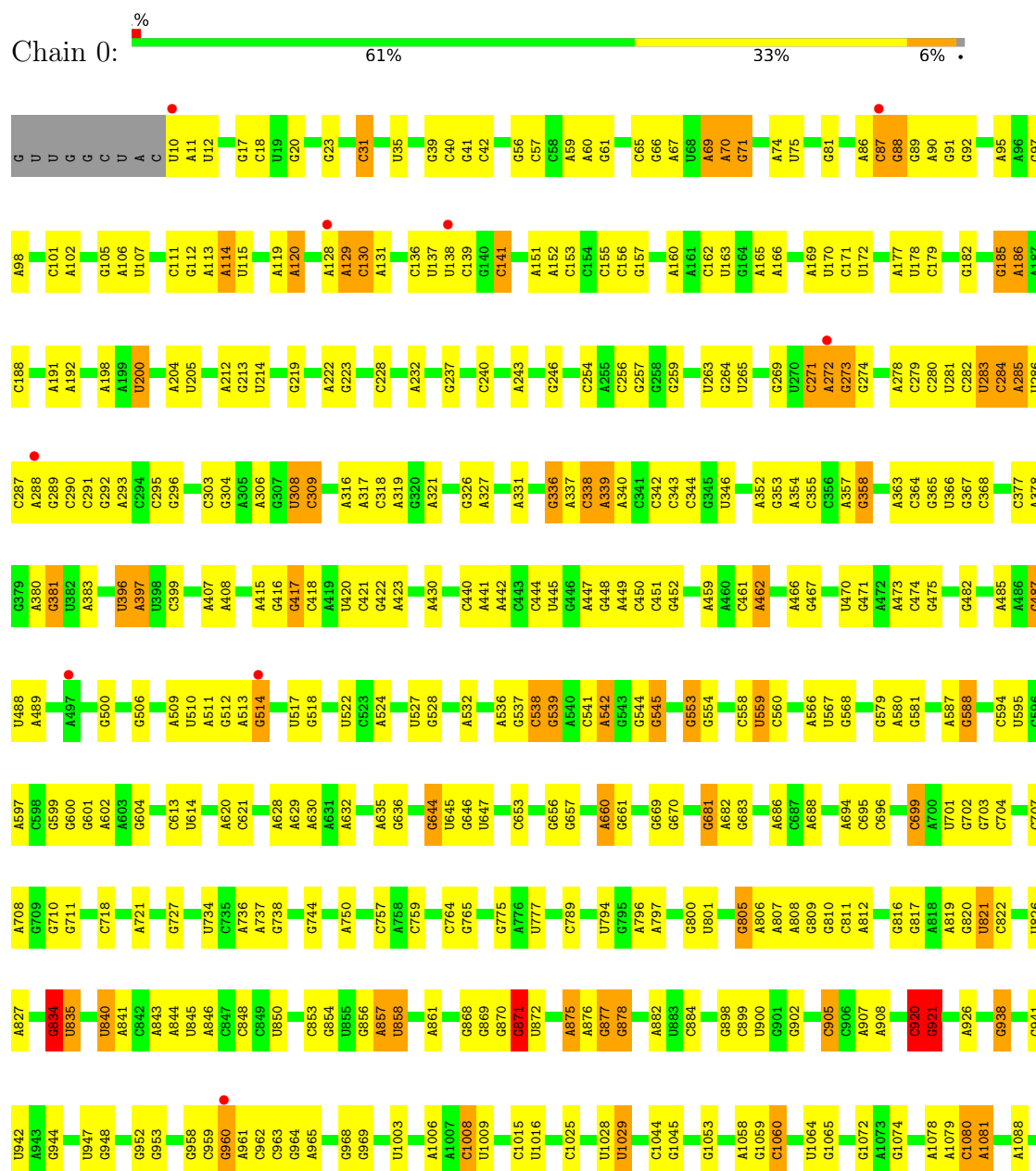
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	38	Total 38	O 38	0	0
38	P	63	Total 63	O 63	0	0
38	Q	50	Total 50	O 50	0	0
38	R	85	Total 85	O 85	0	0
38	S	39	Total 39	O 39	0	0
38	T	30	Total 30	O 30	0	0
38	U	28	Total 28	O 28	0	0
38	V	11	Total 11	O 11	0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

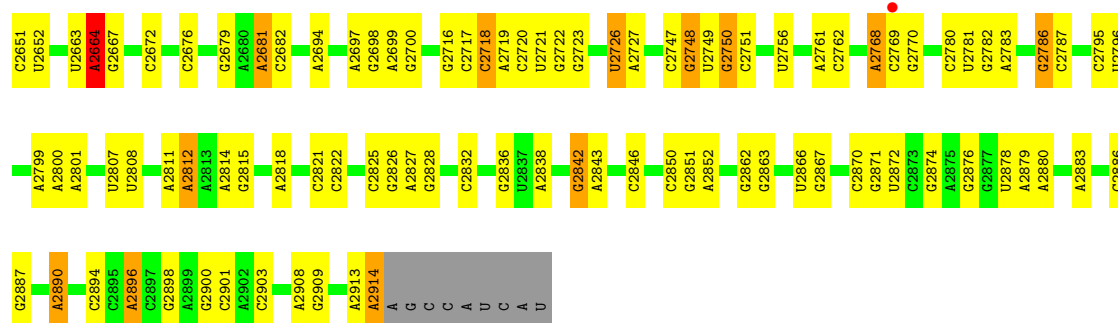
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

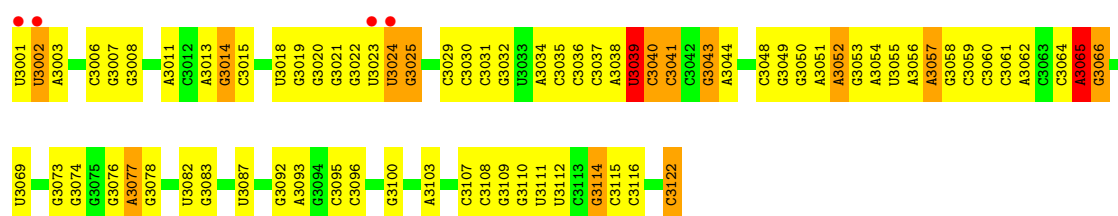
• Molecule 1: 23S ribosomal RNA



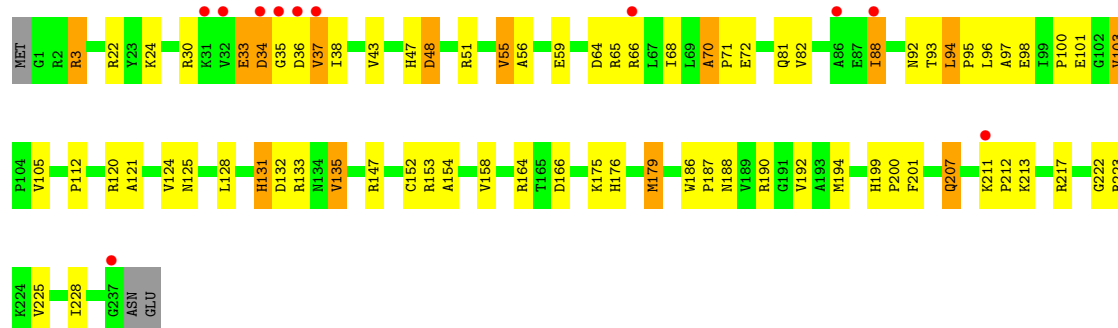
U2535	C2439	U2330	U2115	C2002	G1877	A1767	G1670	G1576	C1495	U1266	U1187	A1097
C2536	G2446	C2331	U2133	U2003	U1878	C1768	U1677	U1577	C1496	C1376	A1188	G1099
A2537	A2447	G2338	G2134	G2005	U1879	C1769	A1678	A1580	G1497	G1378	A1189	
G2453	G2453	A2345	A2135	C2006	U1883	G1773	C1679	C1584	U1500	C1273	U1191	U1109
C2542	A2456	C2346	G2237	A2007	U1887	G1774	A1682	C1585			A1192	G1110
G2543	U2457	G2350	C2247	G2008	C1888	G1777	G1683	C1586	U1503	U1279	A1193	
U2544	G2351	C2351	C2248	A2010	U1889	A1778	A1684	U1587	A1504	A1394	A1194	U1116
U2545	U2461	G2363	A2255	A2011	U1890	A1779	A1685	U1588	U1505	C1395	G1117	A1118
U2546	G2462	A2364	G2256	U2012	C1686		C1686	G1589	C1506	C1289	C1196	
C2552			G2257	G2013	C1687	C1787	C1687		U1507	G1398	U1198	U1120
A2553	A2465	A2361	A2252	U2016	U1903	U1788	C1692	G1592	C1508	A1399	U1199	G1121
C2559	G2466	A2362	G2254	U2017	G1789	C1789	C1692	C1593		G1299	A1200	U1122
U2563	A2467	G2363	A2255	A2018	C1790	U1791	G1697	C1594	G1512	A1407	C1201	A1123
G2564	A2468	A2364	G2257	A2019	G1795	U1795	U1698	U1596	C1513	U1408	A1202	C1126
C2472			G2257	G2033	A1796	A1796	C1699	A1597	C1514	G1409	G1203	C1127
C2476			A2258	U2034	A1921	A1921	C1700	A1598	A1515	A1307	U1205	U1128
C2477			G2263	G2047	A1922	A1922	U1702	A1598	U1517	U1418	U1206	U1128
U2478			U2265	C2048	G1925	G1925	G1706	A1603	U1519	U1419	A1207	G1131
A2479			A2266	C2049	G1926	G1926	G1707	G1604	G1520	C1420	C1208	G1132
A2483			C2269	G2050	A1927	A1927	U1707	A1606	C1521	G1423	C1209	
U2586			G2270	A2054	G1929	G1929	C1714	A1607	A1522	A1424	G1210	
U2587			G2271	G2058	U1930	U1930	C1715	C1613	G1523	G1319	G1211	G1137
G2588			G2272	U2059	A1931	A1931	A1716	G1614	U1524	U1320	C1212	
U2589			C2273	A2060	G1932	G1932	A1717	A1615	G1525	A1321	C1213	
U2590			A2274	A2060	C1940	C1940	U1722		A1527	G1441	G1214	A1154
C2591			G2275	U2063	A1941	A1941	G1723	U1625	A1528	A1328	G1216	G1155
G2592			G2275	U2064	A1942	A1942	U1724	A1626	G1529	A1329	G1217	C1156
U2598			G2285	G2068	G1947	G1947	C1725	G1627	C1537	A1330	U1219	
A2599			C2286				G1730	C1633	U1545	U1333	G1226	
A2600			G2287				C1731	G1634	G1546	C1334		
A2601			G2288				U1950	U1635	C1452	G1339	C1229	
G2602			U2290				C1826	G1636	G1453	U1230	A1165	
A2604			A2291				G1827	A1637	U1454	G1340	U1164	
U2607			A2415				G1828		C1455	A1341	A1166	
C2608			G2416				U1966		A1550	C1342	U1236	
			A2300				A1829		C1551	G1567	A1167	
			A2301						G1552	C1343	C1238	
			C2309				G1739		C1462	G1344	G1239	
			C2313				U1740		U1170		U1169	
			G2316				U1741		C1462	A1242	U1171	
			C2317				A1742		A1463	C1243	G1172	
			U2320				G1751		C1353	U1244	A1173	
			A2321				C1752		U1473	G1245	A1174	
			G2323				A1840		C1474	A1246	G1175	
			U2326				A1845		A1358	U1359	A1176	
			C2327				U1977		C1360	A1247	A1177	
			U2328				C1856		C1477	U1248	G1178	
			A2429				G1756		G1364	U1249	C1179	
			A2430				U1980		C1562	C1250	U1180	
			U2433				G1867		G1481			
			C2433				U1982		A1482	C1253	A1181	
			U2434				G1868		C1366		C1182	
			A2435				U1993		A1367	G1260	A1183	
			C2437				C1993		C1483	A1261	C1184	
			U2438				A1994		G1494	G1370	U1185	
			C2439				C1995		U1488	C1262	A1186	
			U2439				U1996		A1092			
			C2440				G2001		C1574			



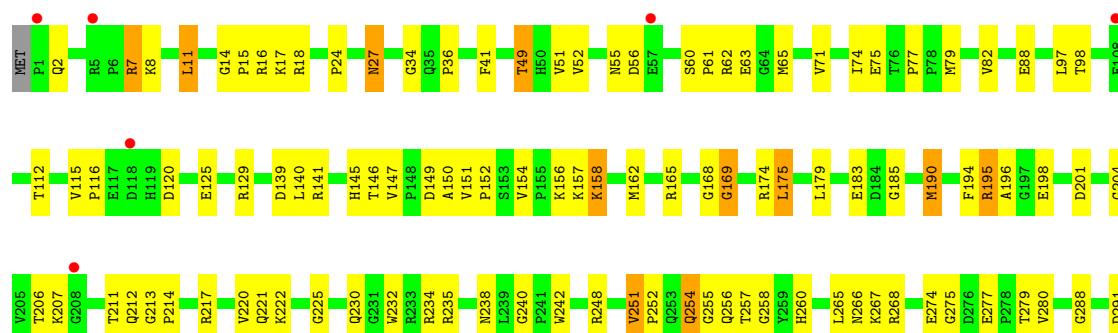
• Molecule 2: 5S ribosomal RNA

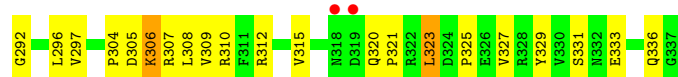


• Molecule 3: 50S ribosomal protein L2P

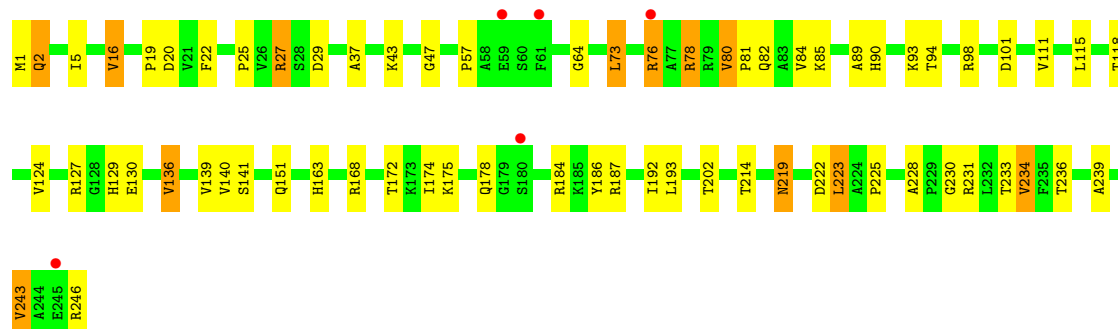
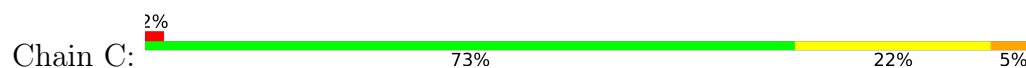


• Molecule 4: 50S ribosomal protein L3P

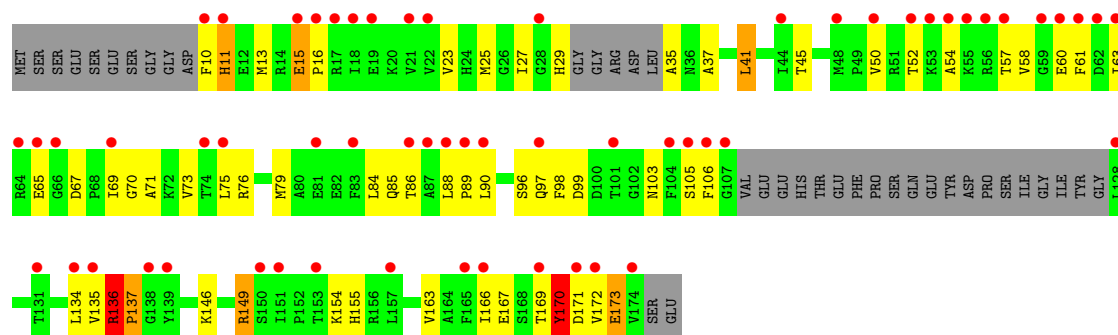




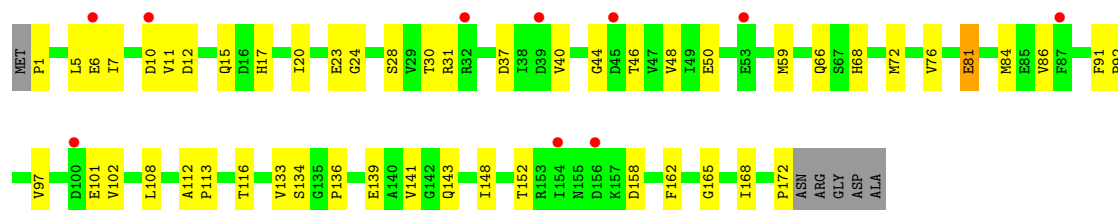
• Molecule 5: 50S ribosomal protein L4P



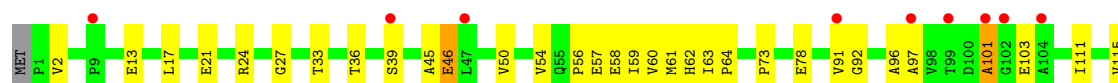
• Molecule 6: 50S ribosomal protein L5P

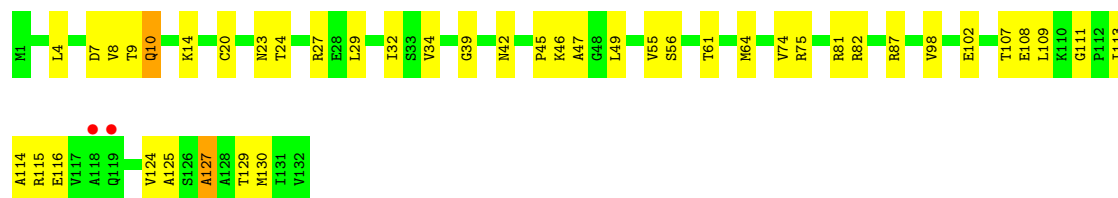


• Molecule 7: 50S ribosomal protein L6P

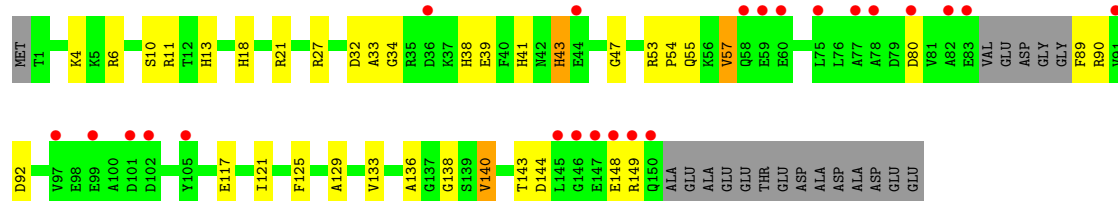


• Molecule 8: 50S ribosomal protein L7Ae

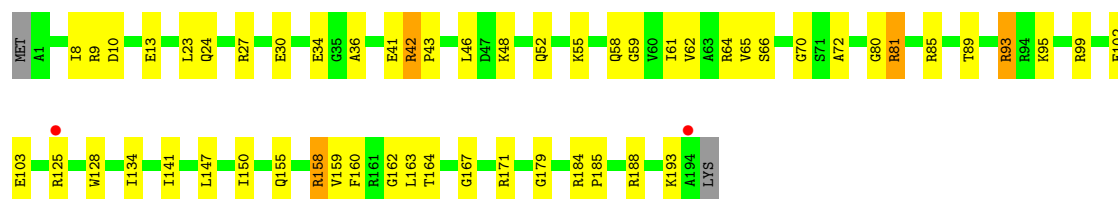




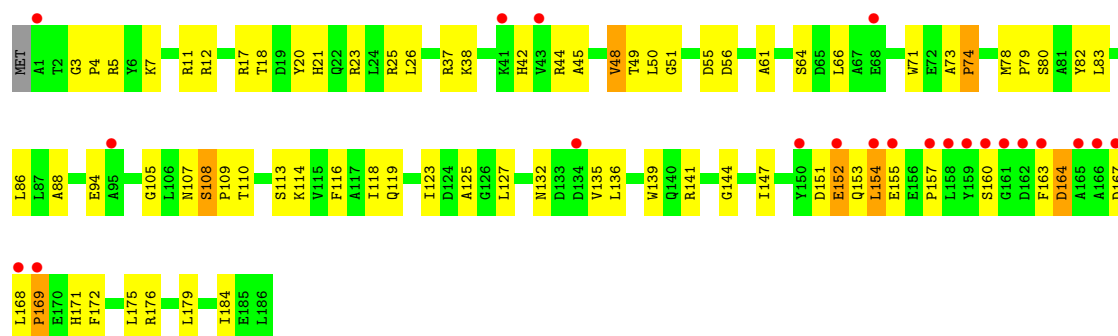
• Molecule 13: 50S ribosomal protein L15P



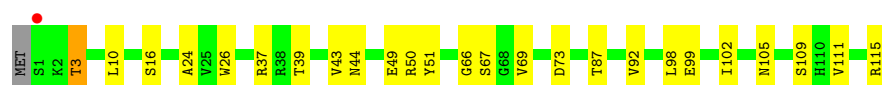
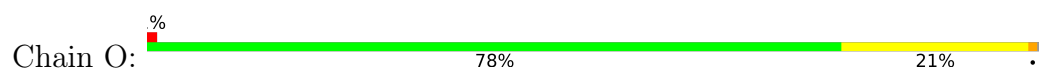
• Molecule 14: 50S ribosomal protein L15e



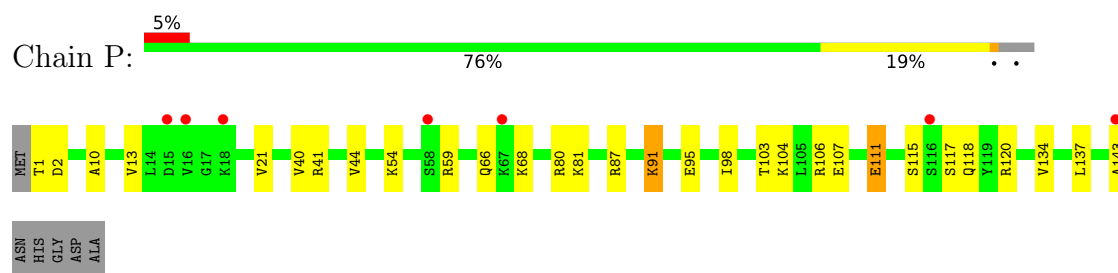
• Molecule 15: 50S ribosomal protein L18P



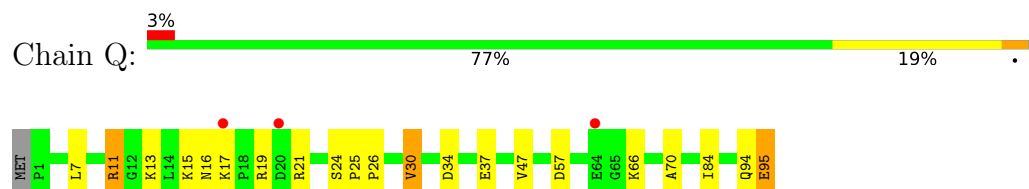
• Molecule 16: 50S ribosomal protein L18e



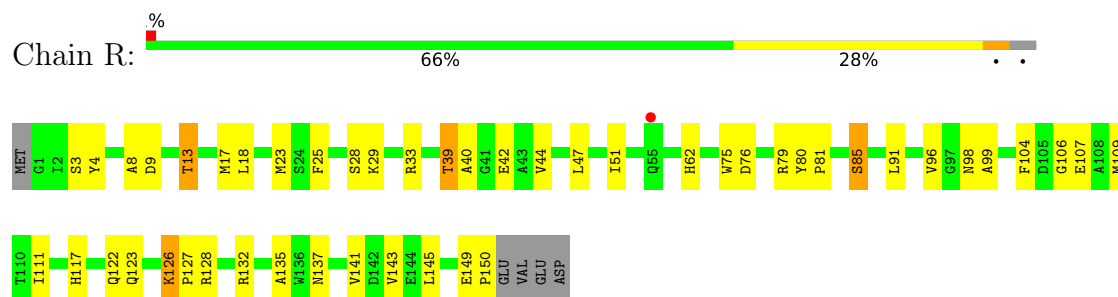
- Molecule 17: 50S ribosomal protein L19e



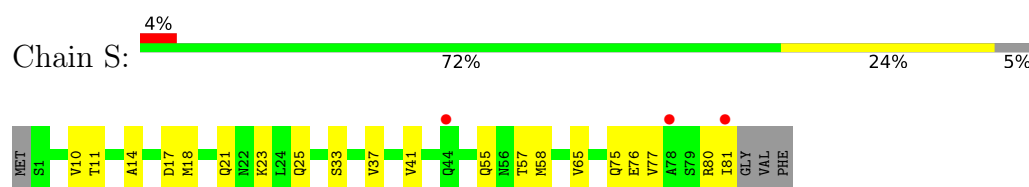
- Molecule 18: 50S ribosomal protein L21e



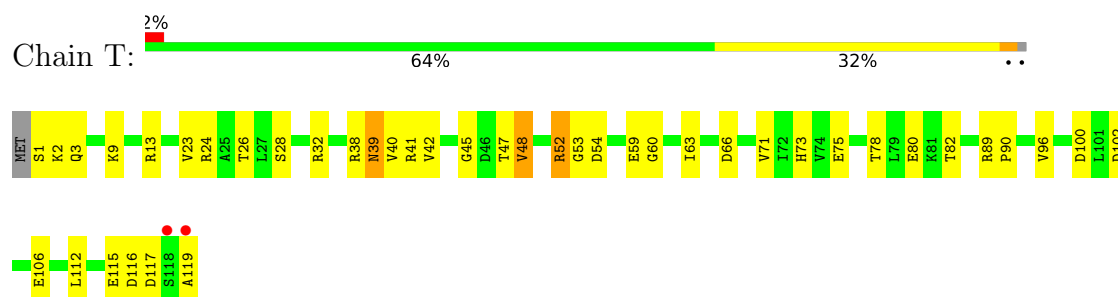
- Molecule 19: 50S ribosomal protein L22P



- Molecule 20: 50S ribosomal protein L23P

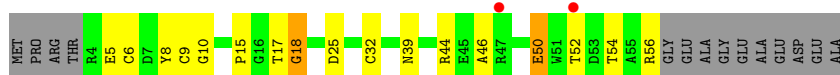


- Molecule 21: 50S ribosomal protein L24P

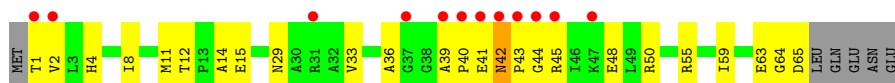


- Molecule 22: 50S ribosomal protein L24e

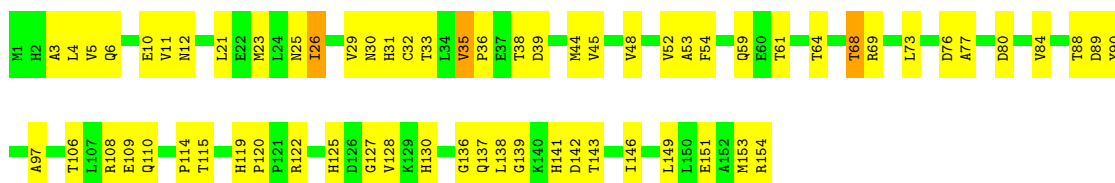




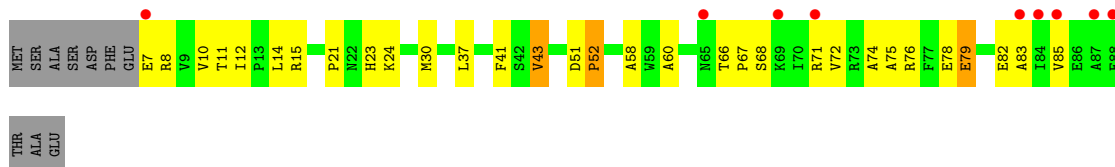
• Molecule 23: 50S ribosomal protein L29P



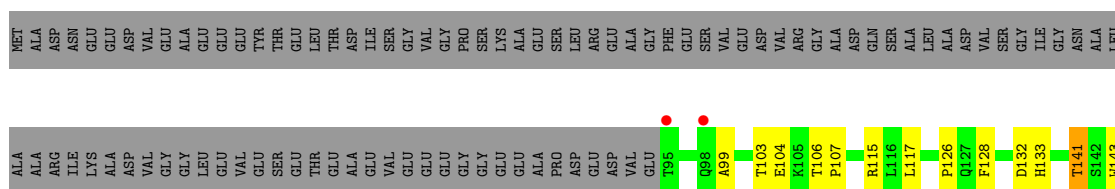
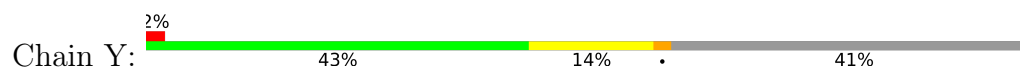
• Molecule 24: 50S ribosomal protein L30P



• Molecule 25: 50S ribosomal protein L31e

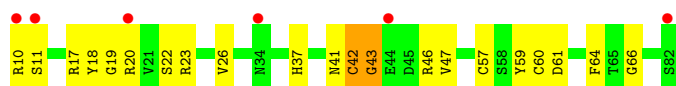


• Molecule 26: 50S ribosomal protein L32e



• Molecule 27: 50S ribosomal protein L37Ae





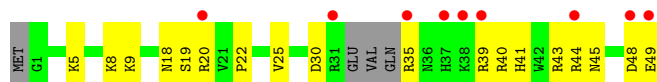
- Molecule 28: 50S ribosomal protein L37e

Chain 1: 74% 25%



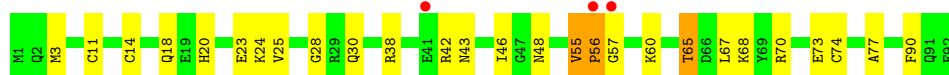
- Molecule 29: 50S ribosomal protein L39e

Chain 2: 18% 56% 36% 8%



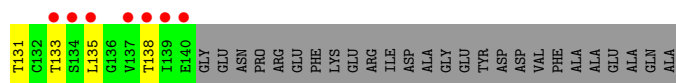
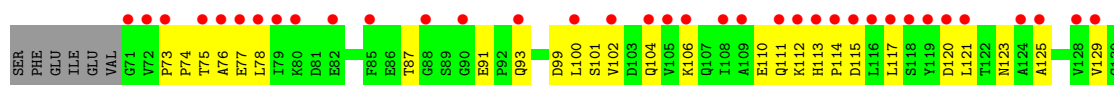
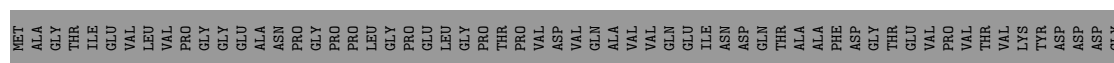
- Molecule 30: 50S ribosomal protein L44e

Chain 3: 3% 71% 26%



- Molecule 31: 50S ribosomal protein L11P

Chain I: 27% 24% 19% 57%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.62Å 304.05Å 578.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 49.92 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.90) 93.9 (49.92-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.241 0.195 , 0.228	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	99020	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.40	0/65959	0.60	16/102870 (0.0%)
2	9	0.39	0/2905	0.61	2/4528 (0.0%)
3	A	0.45	0/1786	1.03	14/2408 (0.6%)
4	B	0.41	0/2690	1.02	19/3652 (0.5%)
5	C	0.47	0/1884	1.02	12/2551 (0.5%)
6	D	0.42	0/1111	1.03	9/1498 (0.6%)
7	E	0.41	0/1382	0.90	4/1880 (0.2%)
8	F	0.44	0/901	0.95	1/1224 (0.1%)
9	G	0.40	0/241	0.95	0/324
10	H	0.43	0/1287	1.01	13/1725 (0.8%)
11	J	0.44	0/1136	0.98	4/1530 (0.3%)
12	K	0.44	0/1001	1.02	9/1347 (0.7%)
13	L	0.41	0/1130	0.97	2/1509 (0.1%)
14	M	0.46	0/1583	0.97	7/2119 (0.3%)
15	N	0.39	0/1474	1.07	13/1999 (0.7%)
16	O	0.45	0/874	0.96	3/1181 (0.3%)
17	P	0.43	0/1147	0.90	1/1528 (0.1%)
18	Q	0.45	0/749	1.03	6/1005 (0.6%)
19	R	0.50	0/1172	1.03	8/1578 (0.5%)
20	S	0.39	0/648	0.88	0/875
21	T	0.40	0/958	0.98	6/1289 (0.5%)
22	U	0.43	0/417	0.86	2/562 (0.4%)
23	V	0.41	0/502	1.00	2/675 (0.3%)
24	W	0.50	0/1219	0.98	4/1655 (0.2%)
25	X	0.47	0/664	1.04	5/895 (0.6%)
26	Y	0.47	0/1146	0.95	3/1536 (0.2%)
27	Z	0.42	0/590	0.95	3/787 (0.4%)
28	1	0.48	0/438	0.88	0/578
29	2	0.46	0/401	0.85	0/529
30	3	0.40	0/771	0.91	4/1024 (0.4%)
31	I	0.46	0/526	1.01	4/716 (0.6%)
All	All	0.41	0/98692	0.73	176/147577 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	37
2	9	0	2
All	All	1	39

There are no bond length outliers.

The worst 5 of 176 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	15	GLU	CA-C-N	9.32	129.40	119.89
6	D	15	GLU	C-N-CA	9.32	129.40	119.89
14	M	89	THR	N-CA-C	9.05	121.15	111.28
3	A	222	GLY	N-CA-C	-9.00	103.95	113.58
1	0	805	G	C2'-C3'-O3'	7.95	125.62	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	805	G	C3'

5 of 39 planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29810	1022	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	2600	0	1326	87	0
3	A	1753	0	1766	62	0
4	B	2625	0	2533	91	0
5	C	1859	0	1816	53	0
6	D	1094	0	1085	41	0
7	E	1357	0	1266	34	0
8	F	890	0	843	25	0
9	G	240	0	231	12	0
10	H	1266	0	1268	31	0
11	J	1120	0	1098	35	0
12	K	992	0	1031	37	0
13	L	1118	0	1076	33	0
14	M	1559	0	1568	39	0
15	N	1445	0	1401	65	0
16	O	865	0	873	22	0
17	P	1136	0	1123	24	0
18	Q	735	0	729	12	0
19	R	1149	0	1122	34	0
20	S	641	0	605	17	0
21	T	950	0	923	26	0
22	U	410	0	364	18	0
23	V	499	0	511	18	0
24	W	1196	0	1137	57	0
25	X	654	0	653	22	0
26	Y	1130	0	1133	35	0
27	Z	579	0	539	18	0
28	1	431	0	426	19	0
29	2	396	0	413	18	0
30	3	755	0	730	19	0
31	I	519	0	500	31	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	72	0	0	1	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	3	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	2	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
36	0	17	0	19	5	0
37	1	1	0	0	0	0
37	3	1	0	0	1	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5923	0	0	177	0
38	1	60	0	0	2	0
38	2	36	0	0	3	0
38	3	74	0	0	6	0
38	9	142	0	0	14	0
38	A	112	0	0	7	0
38	B	137	0	0	14	0
38	C	167	0	0	10	0
38	D	44	0	0	5	0
38	E	45	0	0	3	0
38	F	27	0	0	2	0
38	G	16	0	0	1	0
38	H	70	0	0	5	0
38	I	5	0	0	2	0
38	J	51	0	0	3	0
38	K	57	0	0	4	0
38	L	85	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	122	0	0	2	0
38	N	61	0	0	7	0
38	O	38	0	0	5	0
38	P	63	0	0	1	0
38	Q	50	0	0	1	0
38	R	85	0	0	5	0
38	S	39	0	0	4	0
38	T	30	0	0	1	0
38	U	28	0	0	1	0
38	V	11	0	0	1	0
38	W	69	0	0	3	0
38	X	24	0	0	2	0
38	Y	87	0	0	7	0
38	Z	30	0	0	2	0
All	All	99020	0	59918	1861	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 1861 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	215 (92%)	16 (7%)	4 (2%)	7	26
4	B	335/338 (99%)	307 (92%)	23 (7%)	5 (2%)	8	28
5	C	244/246 (99%)	220 (90%)	22 (9%)	2 (1%)	16	44
6	D	134/177 (76%)	108 (81%)	22 (16%)	4 (3%)	3	14
7	E	170/178 (96%)	161 (95%)	7 (4%)	2 (1%)	10	34
8	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	14	41
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/174 (90%)	144 (92%)	11 (7%)	1 (1%)	21	51
11	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	9	30
12	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
13	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	9	30
14	M	192/196 (98%)	184 (96%)	8 (4%)	0	100	100
15	N	184/187 (98%)	163 (89%)	18 (10%)	3 (2%)	7	27
16	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
17	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
18	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
19	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
20	S	79/85 (93%)	71 (90%)	8 (10%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	41
22	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	32
25	X	80/92 (87%)	71 (89%)	7 (9%)	2 (2%)	4	17
26	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
27	Z	71/73 (97%)	61 (86%)	7 (10%)	3 (4%)	2	9
28	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	36
31	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	8	28
All	All	3705/4426 (84%)	3419 (92%)	250 (7%)	36 (1%)	12	39

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	37	VAL
8	F	101	ALA
15	N	154	LEU
15	N	184	ILE
24	W	77	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	169 (94%)	10 (6%)	19	50
4	B	282/283 (100%)	270 (96%)	12 (4%)	26	60
5	C	193/193 (100%)	178 (92%)	15 (8%)	11	35
6	D	117/148 (79%)	110 (94%)	7 (6%)	17	47
7	E	152/156 (97%)	148 (97%)	4 (3%)	40	73
8	F	93/94 (99%)	91 (98%)	2 (2%)	45	77
9	G	27/283 (10%)	26 (96%)	1 (4%)	30	64
10	H	132/141 (94%)	128 (97%)	4 (3%)	36	70
11	J	118/121 (98%)	112 (95%)	6 (5%)	21	53
12	K	106/106 (100%)	102 (96%)	4 (4%)	29	64
13	L	113/127 (89%)	110 (97%)	3 (3%)	39	73
14	M	158/160 (99%)	151 (96%)	7 (4%)	25	59
15	N	149/150 (99%)	140 (94%)	9 (6%)	17	47
16	O	93/94 (99%)	90 (97%)	3 (3%)	34	68
17	P	113/117 (97%)	110 (97%)	3 (3%)	39	73
18	Q	79/80 (99%)	74 (94%)	5 (6%)	16	45
19	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
20	S	71/74 (96%)	71 (100%)	0	100	100
21	T	105/106 (99%)	97 (92%)	8 (8%)	12	36
22	U	44/53 (83%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	51/57 (90%)	49 (96%)	2 (4%)	28	63
24	W	130/130 (100%)	123 (95%)	7 (5%)	20	51
25	X	66/74 (89%)	62 (94%)	4 (6%)	17	46
26	Y	120/196 (61%)	116 (97%)	4 (3%)	33	67
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/47 (98%)	46 (100%)	0	100	100
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	75
30	3	79/79 (100%)	77 (98%)	2 (2%)	42	74
31	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3609 (86%)	2966 (96%)	127 (4%)	27	61

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	46	ILE
24	W	26	ILE
14	M	81	ARG
24	W	10	GLU
25	X	52	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	67	GLN
21	T	95	ASN
30	3	48	ASN
19	R	61	GLN
20	S	51	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2772 (99%)	242 (8%)	28 (1%)
2	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/2894 (99%)	259 (9%)	29 (1%)

5 of 259 RNA backbone outliers are listed below:

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

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	2761	A
1	0	1684	A
1	0	2649	A
1	0	1506	U

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UR3	0	2619	1	19,22,23	0.39	0	26,32,35	0.78	1 (3%)
1	OMG	0	2588	1	23,26,27	0.32	0	32,38,41	0.43	0
1	OMU	0	2587	1	19,22,23	0.24	0	25,31,34	0.44	0
1	PSU	0	2621	1	18,21,22	1.52	2 (11%)	21,30,33	1.34	3 (14%)
1	1MA	0	628	1	21,25,26	0.74	1 (4%)	30,37,40	0.66	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.94	1.43	1.36
1	0	2621	PSU	C6-C5	2.98	1.38	1.35
1	0	628	1MA	C6-N6	2.48	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.22	120.34	118.17
1	0	2621	PSU	C6-N1-C2	-3.19	119.73	122.69
1	0	2621	PSU	O2-C2-N1	2.99	125.87	122.79
1	0	2619	UR3	C4-N3-C2	2.91	126.92	124.58
1	0	628	1MA	N1-C2-N3	2.76	129.27	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	NEG	0	8823	32	14,16,16	1.49	1 (7%)	12,20,20	0.75	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEG	0	8823	32	-	5/18/18/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8823	NEG	N2-N3	-4.77	1.36	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	0	8823	NEG	N3-C7-C8-O1
36	0	8823	NEG	N3-C7-C8-O2
36	0	8823	NEG	C6-N2-N3-C7
36	0	8823	NEG	C2-C3-C4-N4
36	0	8823	NEG	C8-C7-N3-N2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2772 (99%)	-0.32	36 (1%) 75 67	19, 42, 86, 144	0
2	9	122/122 (100%)	0.16	4 (3%) 49 40	35, 59, 83, 147	0
3	A	237/240 (98%)	0.33	11 (4%) 37 29	25, 46, 78, 99	0
4	B	337/338 (99%)	0.34	8 (2%) 59 50	26, 50, 75, 85	0
5	C	246/246 (100%)	0.27	5 (2%) 65 56	22, 44, 66, 75	0
6	D	140/177 (79%)	1.91	59 (42%) 0 0	54, 94, 118, 126	0
7	E	172/178 (96%)	0.66	10 (5%) 29 22	40, 63, 83, 88	0
8	F	119/120 (99%)	0.80	9 (7%) 20 16	42, 67, 89, 100	0
9	G	29/348 (8%)	1.47	5 (17%) 4 3	73, 89, 96, 98	0
10	H	160/174 (91%)	0.54	6 (3%) 44 36	36, 56, 86, 95	0
11	J	142/145 (97%)	0.30	6 (4%) 40 32	32, 47, 68, 89	0
12	K	132/132 (100%)	0.13	2 (1%) 72 64	29, 45, 67, 78	0
13	L	145/165 (87%)	0.89	23 (15%) 5 4	23, 62, 102, 114	0
14	M	194/196 (98%)	0.13	2 (1%) 79 73	30, 40, 55, 63	0
15	N	186/187 (99%)	0.88	22 (11%) 9 7	37, 59, 103, 114	0
16	O	115/116 (99%)	0.43	1 (0%) 81 75	35, 51, 67, 76	0
17	P	143/149 (95%)	0.48	7 (4%) 35 27	36, 51, 63, 72	0
18	Q	95/96 (98%)	0.24	3 (3%) 50 41	33, 44, 56, 70	0
19	R	150/155 (96%)	0.14	1 (0%) 84 79	30, 43, 64, 79	0
20	S	81/85 (95%)	0.47	3 (3%) 45 37	43, 58, 78, 80	0
21	T	119/120 (99%)	0.47	2 (1%) 69 61	41, 54, 77, 95	0
22	U	53/67 (79%)	0.26	2 (3%) 44 36	37, 50, 70, 77	0
23	V	65/71 (91%)	1.13	12 (18%) 3 3	51, 72, 106, 114	0
24	W	154/154 (100%)	0.27	0 100 100	33, 47, 63, 73	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.76	9 (10%) 10 9	43, 56, 81, 96	0
26	Y	142/241 (58%)	0.25	6 (4%) 40 32	25, 42, 64, 84	0
27	Z	73/73 (100%)	0.62	6 (8%) 17 14	45, 57, 74, 93	0
28	1	56/57 (98%)	-0.22	0 100 100	28, 32, 39, 48	0
29	2	46/50 (92%)	1.07	9 (19%) 3 2	34, 60, 93, 102	0
30	3	92/92 (100%)	0.39	3 (3%) 49 40	32, 51, 64, 75	0
31	I	70/162 (43%)	2.53	43 (61%) 0 0	101, 115, 127, 129	0
All	All	6646/7320 (90%)	0.17	315 (4%) 36 28	19, 48, 93, 147	0

The worst 5 of 315 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	7.5
15	N	161	GLY	6.6
14	M	194	ALA	5.9
6	D	57	THR	5.9
6	D	10	PHE	5.9

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.96	0.08	32,34,35,37	0
1	OMG	0	2588	24/25	0.97	0.07	26,32,34,36	0
1	1MA	0	628	23/24	0.97	0.07	26,29,30,31	0
1	PSU	0	2621	20/21	0.97	0.07	23,27,32,33	0
1	OMU	0	2587	21/22	0.98	0.06	29,31,33,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	9	8551	1/1	0.52	0.25	95,95,95,95	0
34	NA	0	8571	1/1	0.59	0.19	46,46,46,46	0
32	MG	0	8050	1/1	0.67	0.10	66,66,66,66	0
32	MG	0	8063	1/1	0.67	0.20	89,89,89,89	0
34	NA	0	8584	1/1	0.72	0.15	68,68,68,68	0
34	NA	0	8569	1/1	0.72	0.33	63,63,63,63	0
34	NA	0	8574	1/1	0.74	0.35	73,73,73,73	0
34	NA	S	8512	1/1	0.76	0.18	62,62,62,62	0
32	MG	0	8106	1/1	0.77	0.18	63,63,63,63	0
34	NA	0	8575	1/1	0.78	0.41	52,52,52,52	0
34	NA	0	8566	1/1	0.79	0.25	74,74,74,74	0
34	NA	0	8577	1/1	0.79	0.32	70,70,70,70	0
34	NA	0	8582	1/1	0.79	0.20	88,88,88,88	0
32	MG	0	8082	1/1	0.81	0.18	65,65,65,65	0
34	NA	H	8522	1/1	0.81	0.32	71,71,71,71	0
32	MG	9	8095	1/1	0.81	0.14	55,55,55,55	0
34	NA	0	8562	1/1	0.82	0.28	65,65,65,65	0
32	MG	0	8108	1/1	0.82	0.11	66,66,66,66	0
32	MG	0	8024	1/1	0.82	0.36	80,80,80,80	0
34	NA	0	8507	1/1	0.82	0.15	54,54,54,54	0
34	NA	0	8557	1/1	0.82	0.20	49,49,49,49	0
34	NA	0	8558	1/1	0.82	0.29	68,68,68,68	0
34	NA	0	8585	1/1	0.83	0.32	59,59,59,59	0
34	NA	0	8563	1/1	0.83	0.21	52,52,52,52	0
32	MG	0	8092	1/1	0.83	0.12	66,66,66,66	0
32	MG	0	8087	1/1	0.83	0.14	61,61,61,61	0
32	MG	T	8073	1/1	0.84	0.17	63,63,63,63	0
32	MG	0	8094	1/1	0.84	0.27	66,66,66,66	0
34	NA	0	8539	1/1	0.84	0.11	30,30,30,30	0
34	NA	0	8555	1/1	0.84	0.27	81,81,81,81	0
32	MG	A	8066	1/1	0.84	0.18	47,47,47,47	0
33	K	0	8401	1/1	0.85	0.26	78,78,78,78	0
34	NA	9	8583	1/1	0.85	0.11	63,63,63,63	0
37	CD	O	8705	1/1	0.85	0.33	187,187,187,187	0
34	NA	0	8567	1/1	0.86	0.21	51,51,51,51	0
34	NA	0	8511	1/1	0.86	0.09	46,46,46,46	0
34	NA	0	8516	1/1	0.87	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8076	1/1	0.87	0.10	44,44,44,44	0
34	NA	9	8552	1/1	0.87	0.13	47,47,47,47	0
34	NA	0	8578	1/1	0.87	0.33	49,49,49,49	0
34	NA	0	8581	1/1	0.87	0.06	38,38,38,38	0
34	NA	R	8586	1/1	0.87	0.29	29,29,29,29	0
32	MG	0	8102	1/1	0.87	0.10	70,70,70,70	0
34	NA	0	8513	1/1	0.87	0.11	46,46,46,46	0
34	NA	0	8565	1/1	0.88	0.38	52,52,52,52	0
34	NA	Q	8548	1/1	0.88	0.11	43,43,43,43	0
34	NA	0	8559	1/1	0.88	0.31	48,48,48,48	0
34	NA	0	8554	1/1	0.88	0.15	39,39,39,39	0
34	NA	0	8535	1/1	0.88	0.15	39,39,39,39	0
34	NA	0	8520	1/1	0.89	0.17	35,35,35,35	0
34	NA	0	8530	1/1	0.89	0.07	33,33,33,33	0
32	MG	0	8110	1/1	0.89	0.12	54,54,54,54	0
32	MG	0	8114	1/1	0.89	0.10	41,41,41,41	0
34	NA	0	8573	1/1	0.89	0.08	56,56,56,56	0
32	MG	0	8043	1/1	0.89	0.19	61,61,61,61	0
35	CL	0	8805	1/1	0.89	0.11	58,58,58,58	0
35	CL	J	8802	1/1	0.89	0.08	58,58,58,58	0
36	NEG	0	8823	17/17	0.89	0.22	68,72,82,83	0
34	NA	0	8502	1/1	0.89	0.15	51,51,51,51	0
35	CL	A	8809	1/1	0.90	0.17	71,71,71,71	0
34	NA	A	8545	1/1	0.90	0.10	57,57,57,57	0
34	NA	0	8529	1/1	0.90	0.06	56,56,56,56	0
34	NA	0	8540	1/1	0.90	0.07	43,43,43,43	0
32	MG	0	8047	1/1	0.91	0.12	72,72,72,72	0
34	NA	0	8527	1/1	0.91	0.13	46,46,46,46	0
32	MG	0	8090	1/1	0.91	0.15	72,72,72,72	0
34	NA	0	8568	1/1	0.91	0.18	61,61,61,61	0
32	MG	0	8070	1/1	0.91	0.06	34,34,34,34	0
35	CL	L	8810	1/1	0.91	0.13	54,54,54,54	0
34	NA	0	8532	1/1	0.91	0.10	34,34,34,34	0
34	NA	0	8564	1/1	0.91	0.16	50,50,50,50	0
34	NA	0	8541	1/1	0.92	0.12	47,47,47,47	0
35	CL	0	8815	1/1	0.92	0.12	61,61,61,61	0
35	CL	0	8817	1/1	0.92	0.09	59,59,59,59	0
35	CL	0	8820	1/1	0.92	0.09	36,36,36,36	0
35	CL	0	8822	1/1	0.92	0.24	71,71,71,71	0
34	NA	0	8501	1/1	0.92	0.08	51,51,51,51	0
34	NA	0	8579	1/1	0.92	0.14	46,46,46,46	0
34	NA	R	8537	1/1	0.92	0.07	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8044	1/1	0.92	0.08	33,33,33,33	0
34	NA	0	8561	1/1	0.92	0.23	61,61,61,61	0
34	NA	C	8504	1/1	0.93	0.08	41,41,41,41	0
34	NA	0	8549	1/1	0.93	0.11	45,45,45,45	0
32	MG	0	8111	1/1	0.93	0.10	50,50,50,50	0
32	MG	0	8113	1/1	0.93	0.07	49,49,49,49	0
34	NA	0	8515	1/1	0.93	0.09	33,33,33,33	0
32	MG	0	8041	1/1	0.93	0.08	54,54,54,54	0
32	MG	0	8096	1/1	0.93	0.11	52,52,52,52	0
34	NA	0	8524	1/1	0.93	0.19	45,45,45,45	0
32	MG	0	8099	1/1	0.93	0.07	42,42,42,42	0
32	MG	0	8101	1/1	0.93	0.15	71,71,71,71	0
32	MG	0	8085	1/1	0.93	0.12	48,48,48,48	0
32	MG	0	8072	1/1	0.93	0.11	55,55,55,55	0
32	MG	0	8064	1/1	0.93	0.08	28,28,28,28	0
32	MG	0	8080	1/1	0.93	0.10	48,48,48,48	0
35	CL	R	8806	1/1	0.93	0.10	52,52,52,52	0
34	NA	0	8508	1/1	0.93	0.14	36,36,36,36	0
34	NA	0	8510	1/1	0.93	0.14	22,22,22,22	0
32	MG	0	8117	1/1	0.94	0.09	45,45,45,45	0
32	MG	0	8057	1/1	0.94	0.07	29,29,29,29	0
32	MG	0	8088	1/1	0.94	0.04	22,22,22,22	0
32	MG	0	8060	1/1	0.94	0.09	43,43,43,43	0
32	MG	0	8045	1/1	0.94	0.09	51,51,51,51	0
34	NA	0	8518	1/1	0.94	0.10	40,40,40,40	0
32	MG	0	8046	1/1	0.94	0.06	45,45,45,45	0
34	NA	0	8550	1/1	0.94	0.10	40,40,40,40	0
32	MG	0	8052	1/1	0.94	0.17	77,77,77,77	0
35	CL	B	8819	1/1	0.94	0.20	39,39,39,39	0
34	NA	0	8525	1/1	0.94	0.14	71,71,71,71	0
34	NA	0	8572	1/1	0.94	0.20	68,68,68,68	0
35	CL	N	8807	1/1	0.94	0.11	57,57,57,57	0
35	CL	O	8808	1/1	0.94	0.13	66,66,66,66	0
35	CL	Q	8811	1/1	0.94	0.13	58,58,58,58	0
32	MG	0	8098	1/1	0.94	0.16	31,31,31,31	0
34	NA	0	8528	1/1	0.94	0.08	39,39,39,39	0
32	MG	0	8086	1/1	0.94	0.06	46,46,46,46	0
34	NA	0	8570	1/1	0.95	0.37	64,64,64,64	0
34	NA	0	8544	1/1	0.95	0.04	14,14,14,14	0
34	NA	R	8538	1/1	0.95	0.08	55,55,55,55	0
34	NA	0	8521	1/1	0.95	0.23	43,43,43,43	0
34	NA	0	8506	1/1	0.95	0.12	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8093	1/1	0.95	0.06	43,43,43,43	0
35	CL	0	8812	1/1	0.95	0.09	40,40,40,40	0
35	CL	0	8813	1/1	0.95	0.08	55,55,55,55	0
32	MG	0	8103	1/1	0.95	0.15	77,77,77,77	0
34	NA	0	8556	1/1	0.95	0.13	54,54,54,54	0
32	MG	0	8035	1/1	0.95	0.06	36,36,36,36	0
32	MG	0	8053	1/1	0.95	0.10	50,50,50,50	0
32	MG	0	8089	1/1	0.95	0.08	32,32,32,32	0
32	MG	Y	8109	1/1	0.95	0.08	36,36,36,36	0
34	NA	0	8533	1/1	0.95	0.12	22,22,22,22	0
35	CL	J	8821	1/1	0.95	0.10	60,60,60,60	0
34	NA	0	8534	1/1	0.95	0.13	41,41,41,41	0
32	MG	0	8075	1/1	0.95	0.06	57,57,57,57	0
34	NA	0	8536	1/1	0.95	0.07	38,38,38,38	0
34	NA	0	8517	1/1	0.95	0.06	24,24,24,24	0
32	MG	0	8112	1/1	0.95	0.06	38,38,38,38	0
32	MG	0	8051	1/1	0.95	0.08	40,40,40,40	0
34	NA	0	8543	1/1	0.95	0.07	32,32,32,32	0
32	MG	0	8083	1/1	0.96	0.07	40,40,40,40	0
35	CL	0	8803	1/1	0.96	0.08	52,52,52,52	0
32	MG	0	8091	1/1	0.96	0.06	53,53,53,53	0
33	K	0	8402	1/1	0.96	0.06	49,49,49,49	0
35	CL	M	8818	1/1	0.96	0.08	36,36,36,36	0
32	MG	0	8081	1/1	0.96	0.06	34,34,34,34	0
32	MG	K	8069	1/1	0.96	0.05	54,54,54,54	0
34	NA	0	8523	1/1	0.96	0.20	56,56,56,56	0
34	NA	0	8514	1/1	0.96	0.11	37,37,37,37	0
32	MG	0	8097	1/1	0.96	0.08	35,35,35,35	0
34	NA	0	8526	1/1	0.96	0.13	63,63,63,63	0
32	MG	0	8048	1/1	0.97	0.06	48,48,48,48	0
34	NA	0	8560	1/1	0.97	0.07	44,44,44,44	0
35	CL	J	8801	1/1	0.97	0.09	54,54,54,54	0
34	NA	0	8509	1/1	0.97	0.05	23,23,23,23	0
32	MG	0	8104	1/1	0.97	0.08	67,67,67,67	0
34	NA	0	8553	1/1	0.97	0.07	32,32,32,32	0
32	MG	B	8055	1/1	0.97	0.04	43,43,43,43	0
32	MG	0	8023	1/1	0.97	0.10	39,39,39,39	0
34	NA	0	8576	1/1	0.97	0.08	24,24,24,24	0
32	MG	0	8059	1/1	0.97	0.06	38,38,38,38	0
34	NA	0	8531	1/1	0.97	0.05	35,35,35,35	0
35	CL	3	8804	1/1	0.97	0.04	42,42,42,42	0
34	NA	M	8547	1/1	0.97	0.06	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8067	1/1	0.97	0.07	52,52,52,52	0
32	MG	0	8100	1/1	0.98	0.11	37,37,37,37	0
32	MG	0	8042	1/1	0.98	0.03	35,35,35,35	0
32	MG	0	8019	1/1	0.98	0.04	26,26,26,26	0
32	MG	0	8039	1/1	0.98	0.17	43,43,43,43	0
32	MG	0	8115	1/1	0.98	0.03	41,41,41,41	0
32	MG	0	8116	1/1	0.98	0.05	47,47,47,47	0
34	NA	0	8542	1/1	0.98	0.14	1,1,1,1	0
32	MG	0	8056	1/1	0.98	0.04	42,42,42,42	0
34	NA	0	8505	1/1	0.98	0.08	36,36,36,36	0
32	MG	0	8032	1/1	0.98	0.05	29,29,29,29	0
35	CL	0	8814	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8058	1/1	0.98	0.04	32,32,32,32	0
35	CL	0	8816	1/1	0.98	0.16	57,57,57,57	0
32	MG	0	8071	1/1	0.98	0.06	62,62,62,62	0
34	NA	J	8546	1/1	0.98	0.05	27,27,27,27	0
32	MG	0	8037	1/1	0.99	0.03	38,38,38,38	0
32	MG	0	8011	1/1	0.99	0.03	23,23,23,23	0
32	MG	0	8107	1/1	0.99	0.06	36,36,36,36	0
32	MG	0	8040	1/1	0.99	0.03	46,46,46,46	0
32	MG	0	8012	1/1	0.99	0.03	30,30,30,30	0
32	MG	0	8014	1/1	0.99	0.03	34,34,34,34	0
34	NA	0	8519	1/1	0.99	0.07	21,21,21,21	0
32	MG	0	8077	1/1	0.99	0.03	30,30,30,30	0
32	MG	0	8015	1/1	0.99	0.03	34,34,34,34	0
32	MG	0	8017	1/1	0.99	0.03	25,25,25,25	0
32	MG	0	8018	1/1	0.99	0.06	26,26,26,26	0
32	MG	0	8004	1/1	0.99	0.04	23,23,23,23	0
32	MG	0	8020	1/1	0.99	0.04	26,26,26,26	0
32	MG	0	8021	1/1	0.99	0.03	37,37,37,37	0
32	MG	A	8065	1/1	0.99	0.07	37,37,37,37	0
32	MG	0	8049	1/1	0.99	0.09	30,30,30,30	0
32	MG	0	8022	1/1	0.99	0.04	40,40,40,40	0
32	MG	0	8005	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8006	1/1	0.99	0.06	32,32,32,32	0
32	MG	0	8025	1/1	0.99	0.02	32,32,32,32	0
32	MG	3	8078	1/1	0.99	0.05	11,11,11,11	0
32	MG	0	8054	1/1	0.99	0.05	24,24,24,24	0
32	MG	0	8027	1/1	0.99	0.04	39,39,39,39	0
32	MG	0	8028	1/1	0.99	0.03	39,39,39,39	0
32	MG	0	8029	1/1	0.99	0.02	36,36,36,36	0
34	NA	0	8503	1/1	0.99	0.12	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8031	1/1	0.99	0.03	33,33,33,33	0
32	MG	0	8008	1/1	0.99	0.03	27,27,27,27	0
32	MG	0	8061	1/1	0.99	0.04	30,30,30,30	0
32	MG	0	8034	1/1	0.99	0.04	15,15,15,15	0
32	MG	0	8009	1/1	0.99	0.04	31,31,31,31	0
32	MG	0	8036	1/1	0.99	0.03	29,29,29,29	0
32	MG	0	8068	1/1	0.99	0.05	54,54,54,54	0
37	CD	Z	8703	1/1	0.99	0.03	63,63,63,63	0
37	CD	1	8702	1/1	0.99	0.04	55,55,55,55	0
32	MG	0	8084	1/1	1.00	0.06	42,42,42,42	0
32	MG	0	8030	1/1	1.00	0.03	20,20,20,20	0
32	MG	0	8002	1/1	1.00	0.02	27,27,27,27	0
32	MG	0	8016	1/1	1.00	0.06	19,19,19,19	0
32	MG	0	8033	1/1	1.00	0.02	21,21,21,21	0
32	MG	0	8010	1/1	1.00	0.04	13,13,13,13	0
32	MG	0	8074	1/1	1.00	0.02	28,28,28,28	0
32	MG	0	8003	1/1	1.00	0.02	29,29,29,29	0
32	MG	0	8026	1/1	1.00	0.05	32,32,32,32	0
32	MG	0	8007	1/1	1.00	0.05	9,9,9,9	0
32	MG	0	8079	1/1	1.00	0.02	27,27,27,27	0
32	MG	0	8038	1/1	1.00	0.03	21,21,21,21	0
32	MG	0	8062	1/1	1.00	0.12	5,5,5,5	0
32	MG	0	8013	1/1	1.00	0.02	26,26,26,26	0
37	CD	U	8701	1/1	1.00	0.02	63,63,63,63	0
32	MG	0	8001	1/1	1.00	0.02	25,25,25,25	0
34	NA	L	8580	1/1	1.00	0.12	1,1,1,1	0
37	CD	3	8704	1/1	1.00	0.03	53,53,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.