



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:54 PM UTC

PDB ID : 2OTJ / pdb_00002otj
Title : 13-deoxytedanolide bound to the large subunit of Haloarcula marismortui
Authors : Blaha, G.; Schroeder, S.J.; Tirado-Rives, J.
Deposited on : 2007-02-08
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

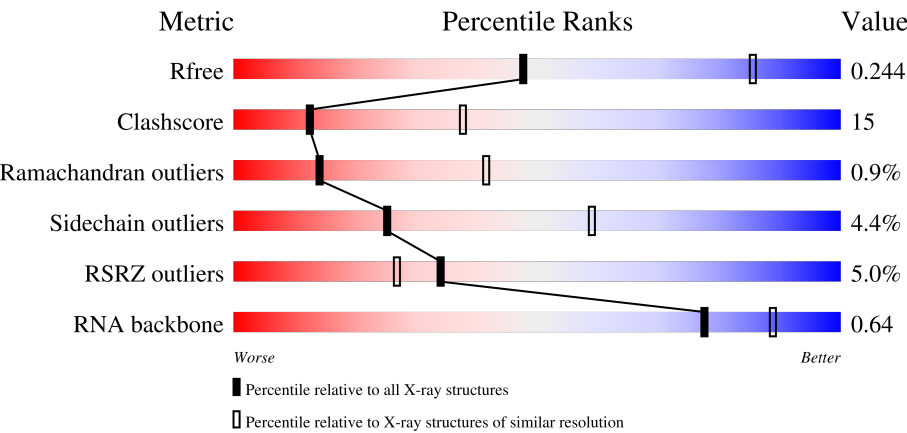
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	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	2922	1% 49% 39% 6% 6%
2	9	122	2% 38% 48% 12%
3	A	240	5% 63% 31% 5%
4	B	338	7% 58% 37% 5%

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	J	145	
12	K	132	
13	L	165	
14	M	194	
15	N	187	
16	O	116	
17	P	149	
18	Q	96	
19	R	155	
20	S	85	
21	T	120	
22	U	66	
23	V	71	
24	W	154	
25	X	92	
26	Y	241	
27	Z	73	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	I	161	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	13T	0	9000	-	-	X	-
33	MG	0	8024	-	-	-	X
35	NA	0	8542	-	-	X	-
35	NA	H	8522	-	-	-	X
36	CL	J	8801	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	GB 3377779

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

- Molecule 9 is a protein called 50S ribosomal protein L10E.

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	-	insertion	UNP P60617
H	166	SER	-	insertion	UNP P60617
H	167	PRO	-	insertion	UNP P60617
H	168	ALA	-	insertion	UNP P60617
H	169	GLY	-	insertion	UNP P60617
H	170	ASN	-	insertion	UNP P60617
H	171	ALA	-	insertion	UNP P60617

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	-	insertion	UNP P60619

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			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			

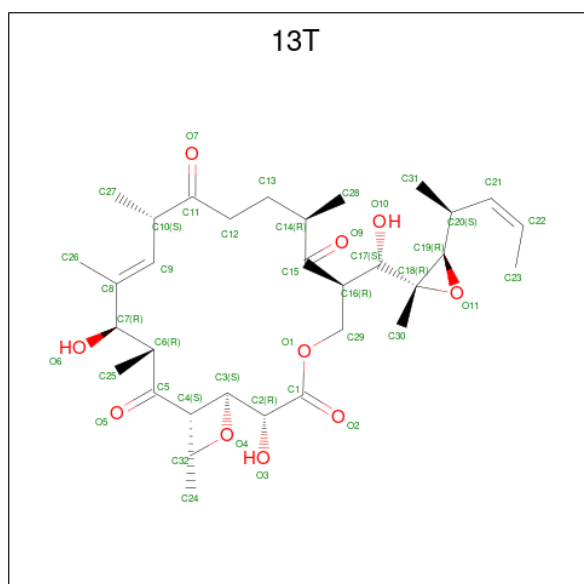
- Molecule 30 is a protein called 50S ribosomal protein L44E.

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 13-DEOXYTEDANOLIDE (CCD ID: 13T) (formula: C₃₂H₅₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	0	1	Total	C	O	0	0
			42	32	10		

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	9	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	2	Total	Mg	0	0
			2	2		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	74	Total	Na	0	0
			74	74		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	9	Total 9	Cl 9	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	2	Total 2	Cl 2	0	0
36	3	1	Total 1	Cl 1	0	0

- 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	5905	Total O 5905 5905	0	0
38	9	140	Total O 140 140	0	0
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	170	Total O 170 170	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	19	Total O 19 19	0	0
38	H	70	Total O 70 70	0	0
38	J	58	Total O 58 58	0	0
38	K	59	Total O 59 59	0	0
38	L	83	Total O 83 83	0	0
38	M	123	Total O 123 123	0	0
38	N	63	Total O 63 63	0	0

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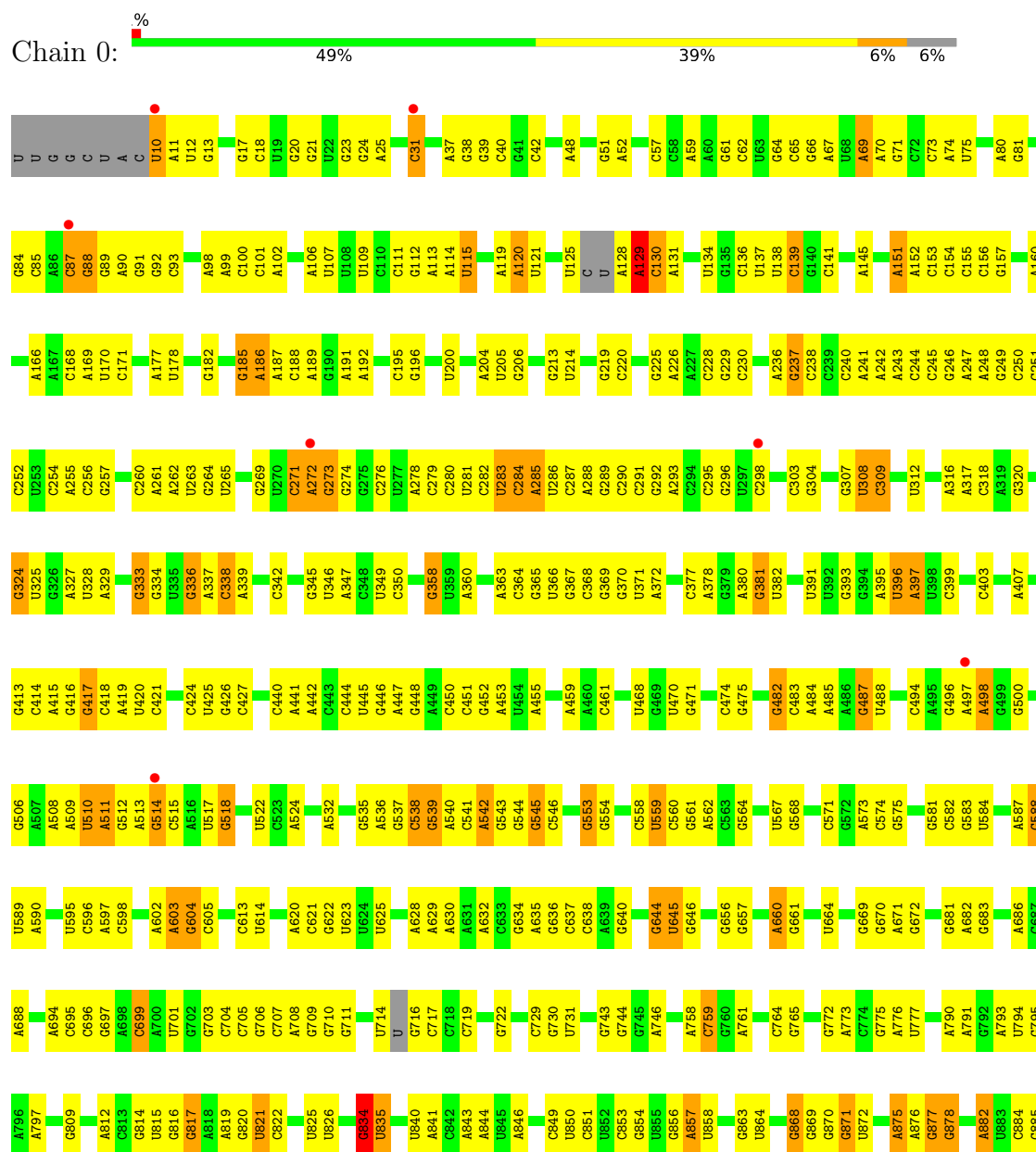
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	44	Total 44	O 44	0	0
38	P	56	Total 56	O 56	0	0
38	Q	51	Total 51	O 51	0	0
38	R	80	Total 80	O 80	0	0
38	S	36	Total 36	O 36	0	0
38	T	33	Total 33	O 33	0	0
38	U	26	Total 26	O 26	0	0
38	V	11	Total 11	O 11	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	31	Total 31	O 31	0	0
38	1	56	Total 56	O 56	0	0
38	2	45	Total 45	O 45	0	0
38	3	66	Total 66	O 66	0	0
38	I	8	Total 8	O 8	0	0

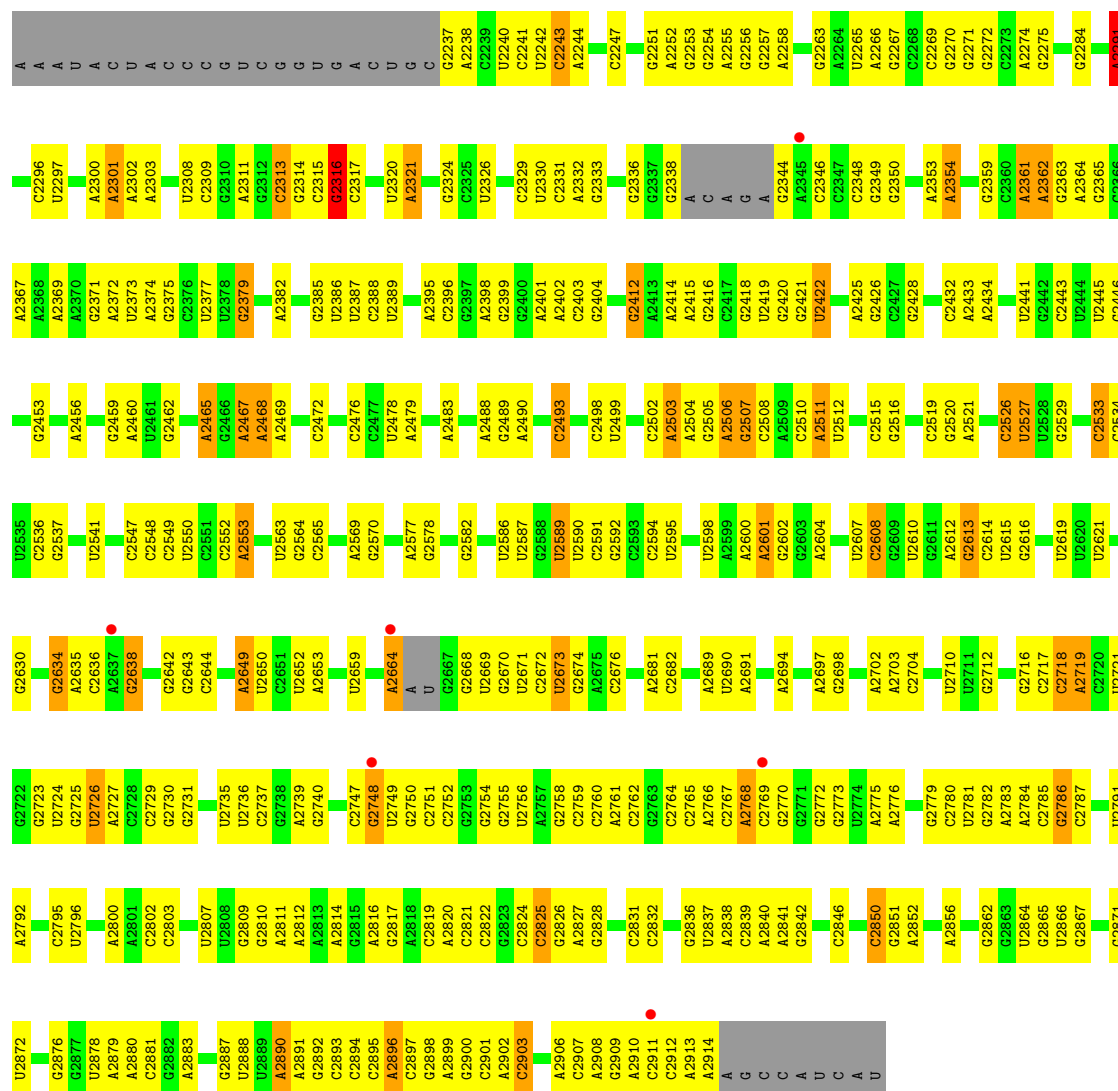
3 Residue-property plots

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.

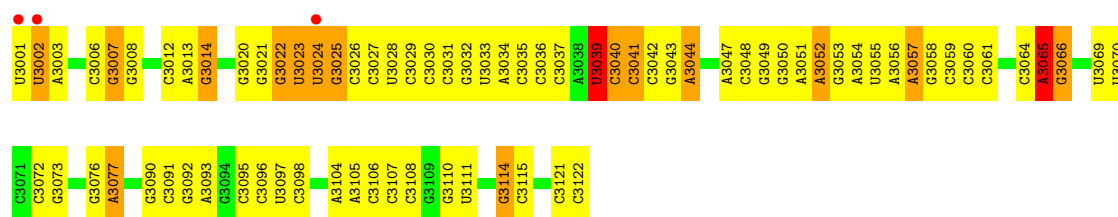
- Molecule 1: 23S ribosomal RNA



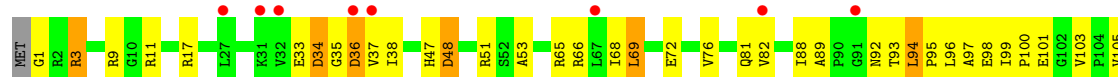
C	U2076	G1879	G1877	A1778	G1681	A1597	U1504	A1413	U1320	A1230	G1163	G1059	A886
A	C2077	U1985	G1878	A1779	A1682	A1598	U1505	A1414	A1321	A1231	U1164	CI060	A894
G	U2078	G1683	U1879	G1783	G1684	U1600	G1506	G1415	G1322	A1232	G1165	CI069	A894
C	G2079	A1684	G1685	A1784	A1685	G1601	G1524	A1419	G1323	A1233	A1166	CI070	G898
U	A2081	G1785	CI082	G1786	CI083	A1603	G1525	CI020	A1328	G1234	G1167	G1071	G899
A	G2082	CI082	U1906	CI087	CI088	G1604	A1526	CI021	A1329	G1235	CI072	G1072	G902
G	A2083	G2000	G1902	CI088	CI089	G1605	A1527	CI022	A1330	U1236	U1169	G1076	G905
G	C2087	G2001	U1903	CI089	CI090	G1609	A1528	CI023	A1331	U1237	U1170	CI077	G905
U	C2088	G2002	U1905	CI090	CI091	G1610	A1529	CI024	A1332	U1238	G1171	CI078	G911
A	G2089	U2003	U1906	CI091	CI092	G1611	G1535	CI025	A1333	U1239	G1172	CI079	G911
G	G2090	U2004	A1909	CI092	CI093	G1612	CI056	CI026	U1334	U1240	CI081	CI082	A912
A	G2091	G2005	U1909	CI093	CI094	G1613	CI057	CI027	U1335	U1241	CI082	CI083	G920
G	G2092	G2006	CI094	CI094	CI095	A1615	CI058	CI028	U1336	U1242	CI083	CI084	A922
A	A2096	A2007	CI095	CI095	CI096	A1616	CI059	CI029	U1337	U1243	CI084	CI085	A926
C	A2097	U2008	G1805	G1806	CI097	A1617	G1543	CI030	U1338	U1244	CI085	CI086	A929
A	U2009	G1806	G1807	G1808	CI098	A1618	G1544	CI031	U1339	U1245	CI086	CI087	A932
A	A2100	CI098	G1809	G1810	CI099	G1619	U1544	CI032	U1340	U1246	CI087	CI088	A936
U	A2101	A1919	G1811	CI099	CI100	G1620	G1545	CI033	U1341	U1247	CI088	CI089	A939
U	A2102	A1920	CI100	CI101	CI102	G1621	G1546	CI034	U1342	U1248	CI089	CI090	G940
A	G2103	G1923	CI101	CI102	CI103	G1622	G1552	CI035	U1343	U1249	CI090	CI091	G941
C	A2104	A1924	CI102	CI103	CI104	G1623	CI053	CI036	U1344	U1250	CI091	CI092	U942
A	C2105	G1925	CI103	CI104	CI105	G1624	CI054	CI037	U1345	U1251	CI092	CI093	U946
C	C2106	A1926	CI104	CI105	CI106	G1625	CI055	CI038	U1346	U1252	CI093	CI094	U947
A	U2016	G1927	CI105	CI106	CI107	U1626	CI056	CI039	U1347	U1253	CI094	CI095	U948
G	U2017	CI106	CI106	CI107	CI108	G1627	CI057	CI040	U1348	U1254	CI095	CI096	U949
G	U2018	CI107	CI107	CI108	CI109	G1628	CI058	CI041	U1349	U1255	CI096	CI097	U951
G	U2019	CI108	CI108	CI109	CI110	G1629	CI059	CI042	U1350	U1256	CI097	CI098	U952
G	U2020	CI109	CI109	CI110	CI111	G1630	CI060	CI043	U1351	U1257	CI098	CI099	U953
G	U2021	CI110	CI110	CI111	CI112	G1631	CI061	CI044	U1352	U1258	CI099	CI100	U954
G	U2022	CI111	CI111	CI112	CI113	G1632	CI062	CI045	U1353	U1259	CI100	CI101	U955
G	U2023	CI112	CI112	CI113	CI114	G1633	CI063	CI046	U1354	U1260	CI101	CI102	U956
G	U2024	CI113	CI113	CI114	CI115	G1634	CI064	CI047	U1355	U1261	CI102	CI103	U957
G	U2025	CI114	CI114	CI115	CI116	G1635	CI065	CI048	U1356	U1262	CI103	CI104	U958
G	U2026	CI115	CI115	CI116	CI117	G1636	CI066	CI049	U1357	U1263	CI104	CI105	U959
G	U2027	CI116	CI116	CI117	CI118	G1637	CI067	CI050	U1358	U1264	CI105	CI106	U960
G	U2028	CI117	CI117	CI118	CI119	G1638	CI068	CI051	U1359	U1265	CI106	CI107	U961
G	U2029	CI118	CI118	CI119	CI120	G1639	CI069	CI052	U1360	U1266	CI107	CI108	U962
G	U2030	CI119	CI119	CI120	CI121	G1640	CI070	CI053	U1361	U1267	CI108	CI109	U963
G	U2031	CI120	CI120	CI121	CI122	G1641	CI071	CI054	U1362	U1268	CI109	CI110	U966
G	U2032	CI121	CI121	CI122	CI123	G1642	CI072	CI055	U1363	U1269	CI110	CI111	U970
G	U2033	CI122	CI122	CI123	CI124	G1643	CI073	CI056	U1364	U1270	CI111	CI112	U
G	U2034	CI123	CI123	CI124	CI125	G1644	CI074	CI057	U1365	U1271	CI112	CI113	U
G	U2035	CI124	CI124	CI125	CI126	G1645	CI075	CI058	U1366	U1272	CI113	CI114	U
G	U2036	CI125	CI125	CI126	CI127	G1646	CI076	CI059	U1367	U1273	CI114	CI115	U
G	U2037	CI126	CI126	CI127	CI128	G1647	CI077	CI060	U1368	U1274	CI115	CI116	U
G	U2038	CI127	CI127	CI128	CI129	G1648	CI078	CI061	U1369	U1275	CI116	CI117	U
G	U2039	CI128	CI128	CI129	CI130	G1649	CI079	CI062	U1370	U1276	CI117	CI118	U
G	U2040	CI129	CI129	CI130	CI131	G1650	CI080	CI063	U1371	U1277	CI118	CI119	U
G	U2041	CI130	CI130	CI131	CI132	G1651	CI081	CI064	U1372	U1278	CI119	CI120	U
G	U2042	CI131	CI131	CI132	CI133	G1652	CI082	CI065	U1373	U1279	CI120	CI121	U
G	U2043	CI132	CI132	CI133	CI134	G1653	CI083	CI066	U1374	U1280	CI121	CI122	U
G	U2044	CI133	CI133	CI134	CI135	G1654	CI084	CI067	U1375	U1281	CI122	CI123	U
G	U2045	CI134	CI134	CI135	CI136	G1655	CI085	CI068	U1376	U1282	CI123	CI124	U
G	U2046	CI135	CI135	CI136	CI137	G1656	CI086	CI069	U1377	U1283	CI124	CI125	U
G	U2047	CI136	CI136	CI137	CI138	G1657	CI087	CI070	U1378	U1284	CI125	CI126	U
G	U2048	CI137	CI137	CI138	CI139	G1658	CI088	CI071	U1379	U1285	CI126	CI127	U
G	U2049	CI138	CI138	CI139	CI140	G1659	CI089	CI072	U1380	U1286	CI127	CI128	U
G	U2050	CI139	CI139	CI140	CI141	G1660	CI090	CI073	U1381	U1287	CI128	CI129	U
G	U2051	CI140	CI140	CI141	CI142	G1661	CI091	CI074	U1382	U1288	CI129	CI130	U
G	U2052	CI141	CI141	CI142	CI143	G1662	CI092	CI075	U1383	U1289	CI130	CI131	U
G	U2053	CI142	CI142	CI143	CI144	G1663	CI093	CI076	U1384	U1290	CI131	CI132	U
G	U2054	CI143	CI143	CI144	CI145	G1664	CI094	CI077	U1385	U1291	CI132	CI133	U
G	U2055	CI144	CI144	CI145	CI146	G1665	CI095	CI078	U1386	U1292	CI133	CI134	U
G	U2056	CI145	CI145	CI146	CI147	G1666	CI096	CI079	U1387	U1293	CI134	CI135	U
G	U2057	CI146	CI146	CI147	CI148	G1667	CI097	CI080	U1388	U1294	CI135	CI136	U
G	U2058	CI147	CI147	CI148	CI149	G1668	CI098	CI081	U1389	U1295	CI136	CI137	U
G	U2059	CI148	CI148	CI149	CI150	G1669	CI099	CI082	U1390	U1296	CI137	CI138	U
G	U2060	CI149	CI149	CI150	CI151	G1670	CI100	CI083	U1391	U1297	CI138	CI139	U
G	U2061	CI150	CI150	CI151	CI152	G1671	CI101	CI084	U1392	U1298	CI139	CI140	U
G	U2062	CI151	CI151	CI152	CI153	G1672	CI102	CI085	U1393	U1299	CI140	CI141	U
G	U2063	CI152	CI152	CI153	CI154	G1673	CI103	CI086	U1394	U1300	CI141	CI142	U
G	U2064	CI153	CI153	CI154	CI155	G1674	CI104	CI087	U1395	U1301	CI142	CI143	U
G	U2065	CI154	CI154	CI155	CI156	G1675	CI105	CI088	U1396	U1302	CI143	CI144	U
G	U2066	CI155	CI155	CI156	CI157	G1676	CI106	CI089	U1397	U1303	CI144	CI145	U
G	U2067	CI156	CI156	CI157	CI158	G1677	CI107	CI090	U1398	U1304	CI145	CI146	U
G	U2068	CI157	CI157	CI158	CI159	G1678	CI108	CI091	U1399	U1305	CI146	CI147	U
G	U2069	CI158	CI158	CI159	CI160	G1679	CI109	CI092	U1400	U1306	CI147	CI148	U
G	U2070	CI159	CI159	CI160	CI161	G1680	CI110	CI093	U1401	U1307	CI148	CI149	U
G	U2071	CI160	CI160	CI161	CI162	G1681	CI111	CI094	U1402	U1308	CI149	CI150	U
G	U2072	CI161	CI161	CI162	CI163	G1682	CI112	CI095	U1403	U1309	CI150	CI151	U
G	U2073	CI162	CI162	CI163	CI164	G1683	CI113	CI096	U1404	U1310	CI151	CI152	U
G	U2074	CI163	CI163	CI164	CI165	G1684	CI114	CI097	U1405	U1311	CI152	CI153	U
G	U2075	CI164	CI164	CI165	CI166	G1685	CI115	CI098	U1406	U1312	CI153	CI154	U
G	U2076	CI165	CI165	CI166	CI167	G1686	CI116	CI099	U1407	U1313	CI154	CI155	U
G	U2077	CI166	CI166	CI167	CI168	G1687	CI117	CI100	U1408	U1314	CI155	CI156	U
G	U2078	CI167	CI167	CI168	CI169	G1688	CI118	CI101	U1409	U1315	CI156	CI157	U
G	U2079	CI168	CI168	CI169	CI170	G1689	CI119	CI102	U1410	U1316	CI157	CI158	U
G	U2080	CI169	CI169	CI170	CI171	G1690	CI120	CI103	U1411	U1317	CI158	CI159	U
G	U2081	CI170	CI170	CI171	CI172	G1691	CI121	CI104	U1412	U1318	CI159	CI160	U
G	U2082	CI171	CI171	CI172	CI173	G1692	CI122	CI105	U1413	U1319	CI160	CI161	U
G	U2083	CI172	CI172	CI173	CI174	G1693	CI123	CI106	U1414	U1320	CI161	CI162	U
G	U2084	CI173	CI173	CI174	CI175	G1694	CI124	CI107	U1415	U1321	CI162	CI163	U
G	U2085	CI174	CI174	CI175	CI176	G1695	CI125	CI108	U1416	U1322	CI163	CI164	U
G	U2086	CI175	CI175	CI176	CI177	G1696	CI126	CI109	U1417	U1323	CI164	CI165	U
G	U2087	CI176	CI176	CI177	CI178	G1697	CI127	CI110	U1418	U1324	CI165	CI166	U

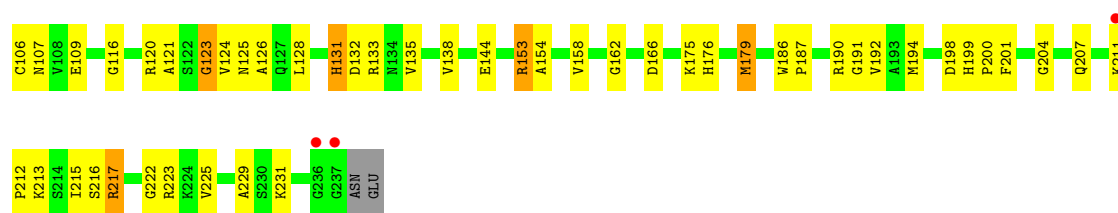


• Molecule 2: 5S ribosomal RNA

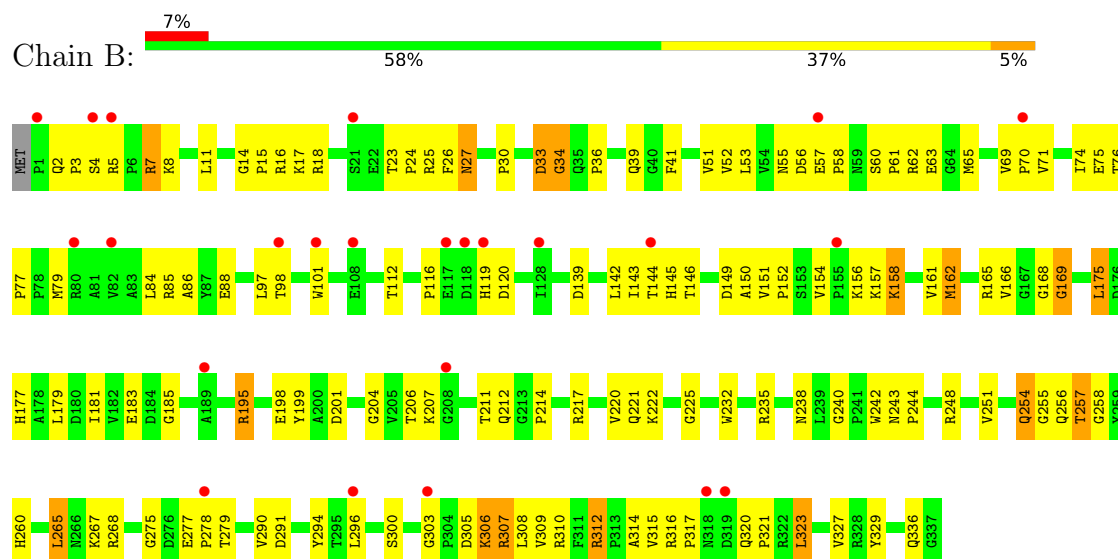


• Molecule 3: 50S ribosomal protein L2P

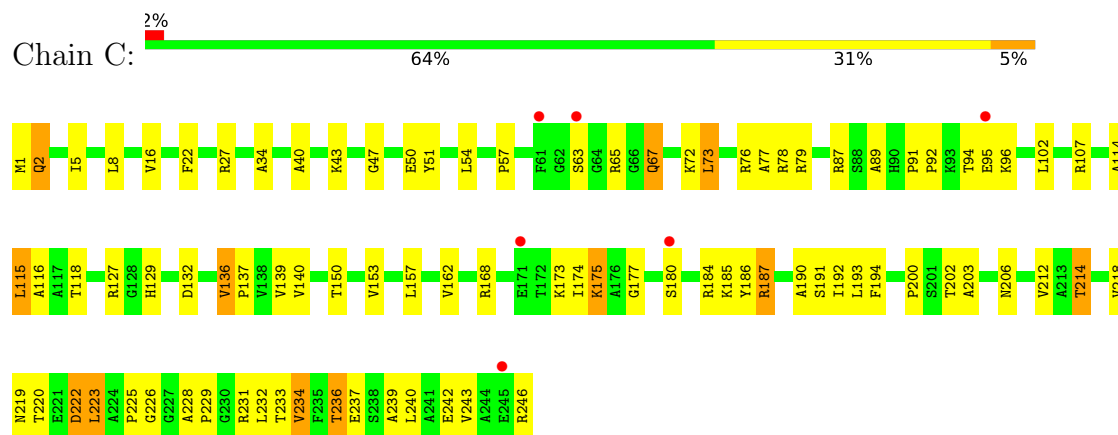




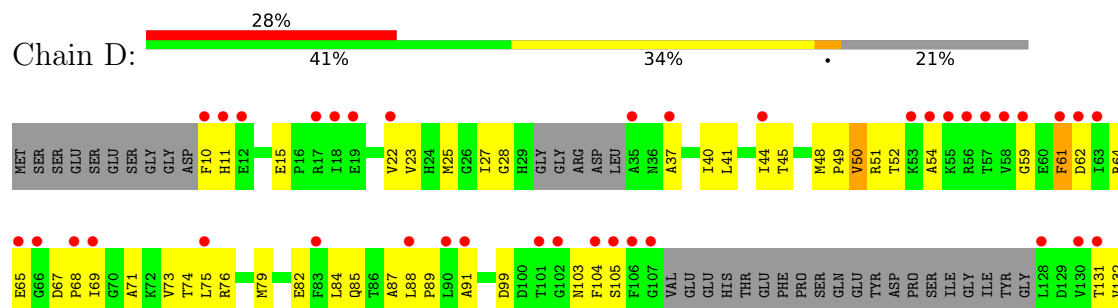
• Molecule 4: 50S ribosomal protein L3P

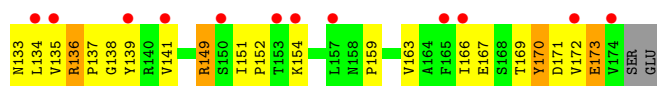


• Molecule 5: 50S ribosomal protein L4P

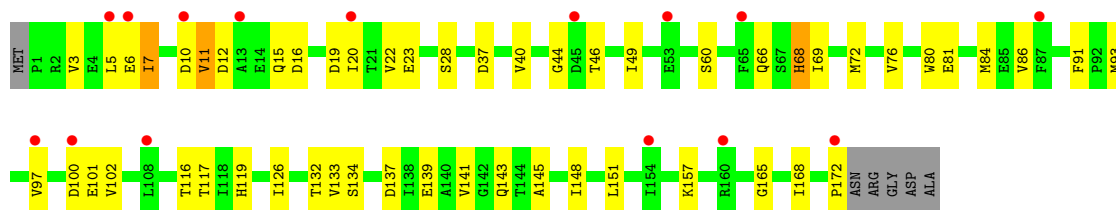


• Molecule 6: 50S ribosomal protein L5P

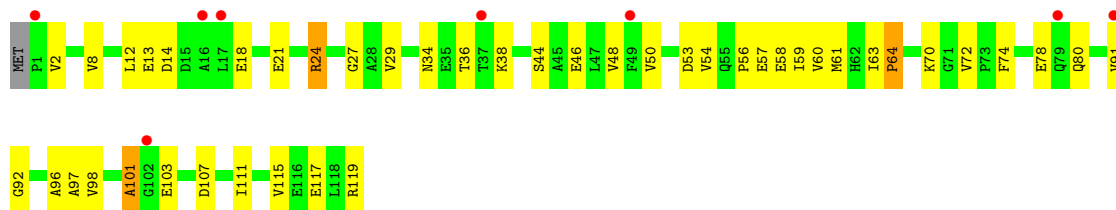




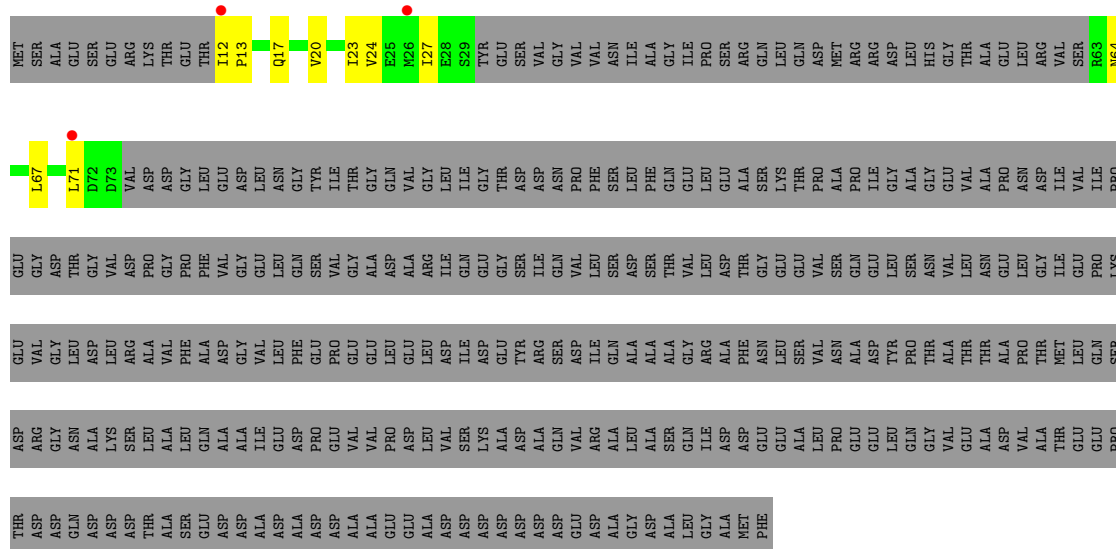
• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7Ae

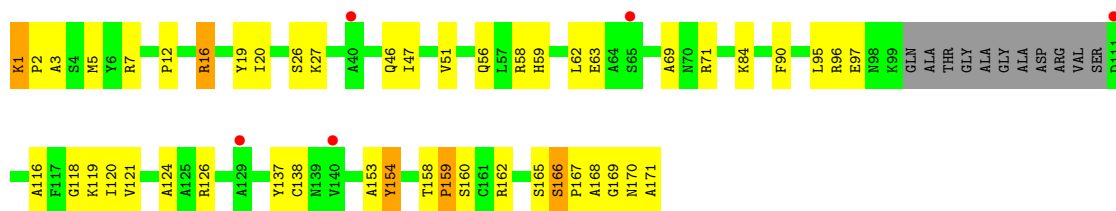


• Molecule 9: 50S ribosomal protein L10E

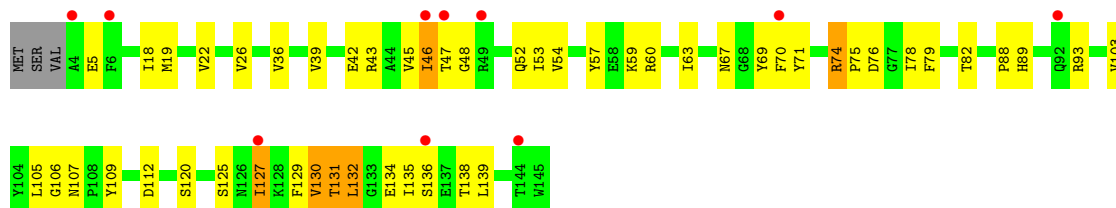


• Molecule 10: 50S ribosomal protein L10e

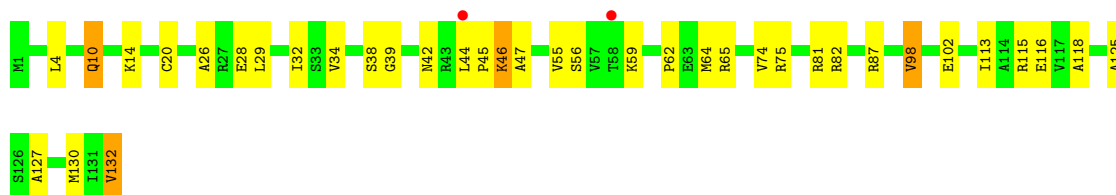
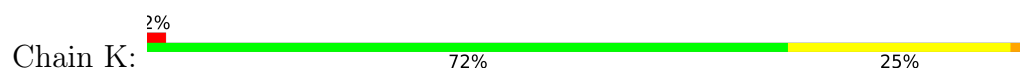




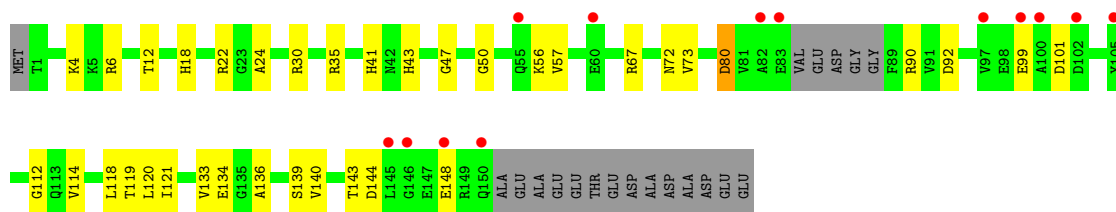
• Molecule 11: 50S ribosomal protein L13P



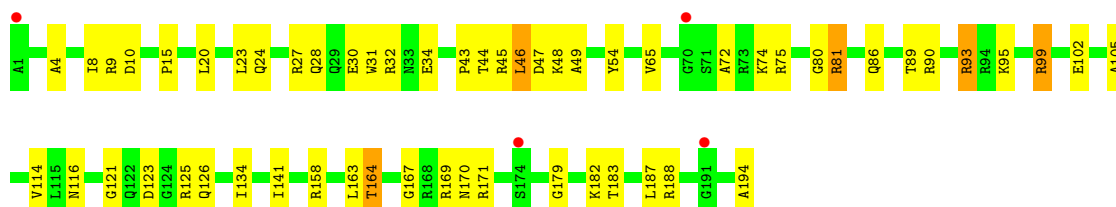
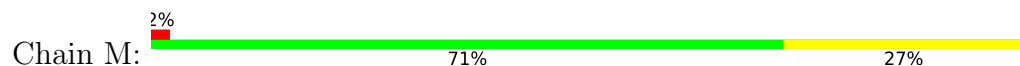
• Molecule 12: 50S ribosomal protein L14P



• Molecule 13: 50S ribosomal protein L15P

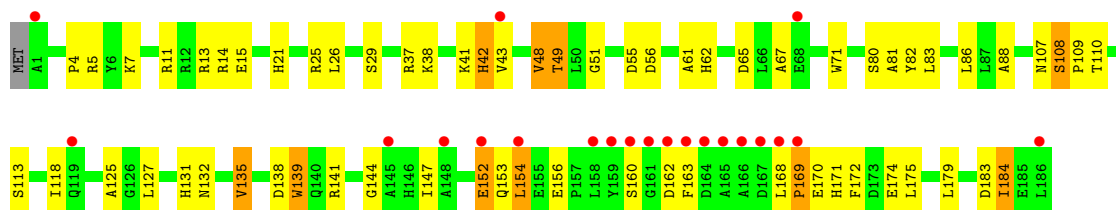


• Molecule 14: 50S ribosomal protein L15e



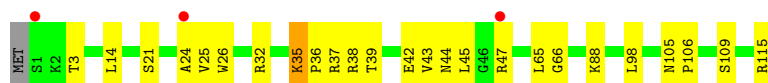
- Molecule 15: 50S ribosomal protein L18P

Chain N: 



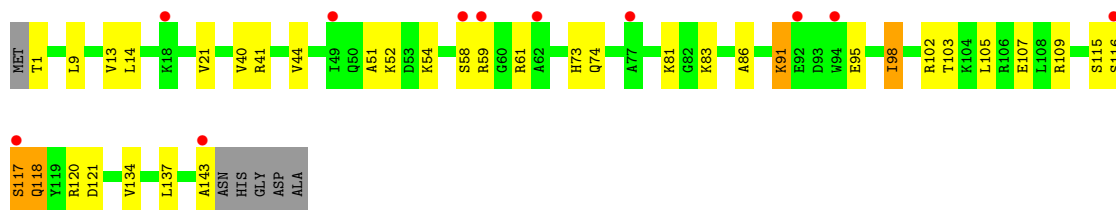
- Molecule 16: 50S ribosomal protein L18e

Chain O: 



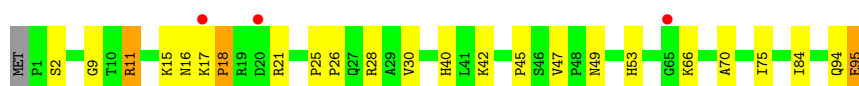
- Molecule 17: 50S ribosomal protein L19e

Chain P: 



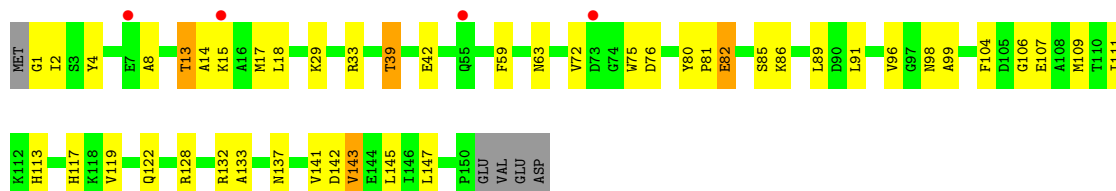
- Molecule 18: 50S ribosomal protein L21e

Chain Q: 

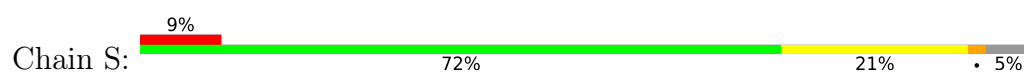


- Molecule 19: 50S ribosomal protein L22P

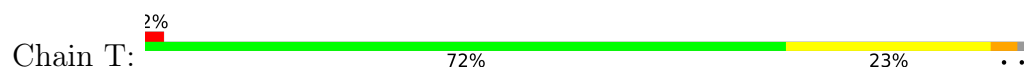
Chain R: 



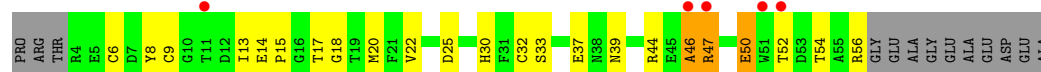
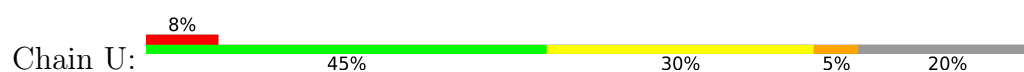
- Molecule 20: 50S ribosomal protein L23P



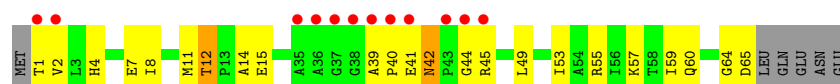
- Molecule 21: 50S ribosomal protein L24P



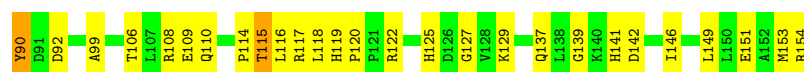
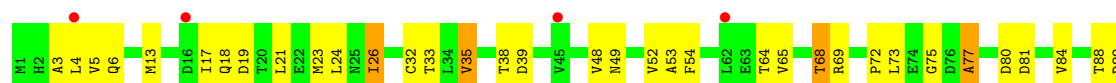
- Molecule 22: 50S ribosomal protein L24e



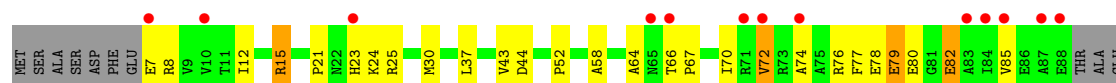
- Molecule 23: 50S ribosomal protein L29P



- Molecule 24: 50S ribosomal protein L30P

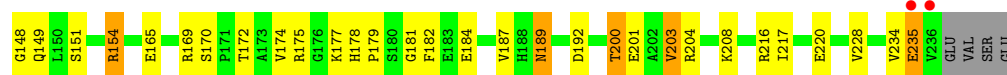


- Molecule 25: 50S ribosomal protein L31e

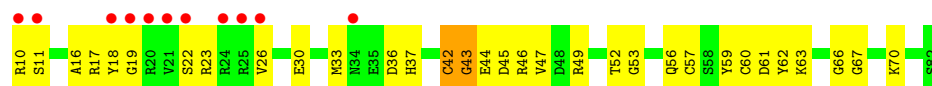


- Molecule 26: 50S ribosomal protein L32e





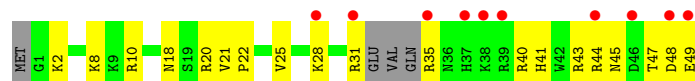
Chain Z: 15% 56% 41%



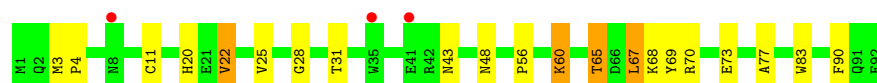
Chain 1: 63% 33% •



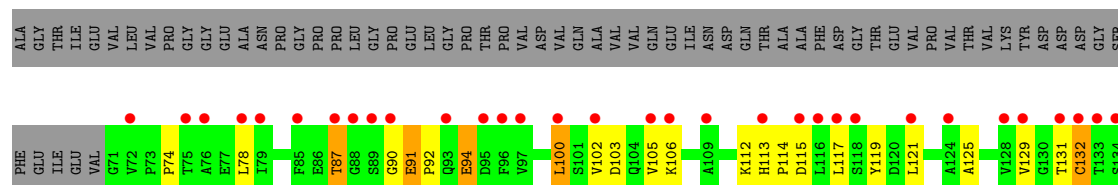
Chain 2:



Chain 3: 3% 77% 18%



Chain I:



L135	GLN	V137	I138	I139	E140	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	GLU	ALA	GLN	ALA
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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	211.74Å 299.52Å 573.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.90 49.70 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.90) 93.3 (49.70-2.90)	Depositor EDS
R_{merge}	0.16	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}	0.193 , 0.238 0.211 , 0.244	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.1	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	0.92	EDS
Total number of atoms	99043	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 13T, 1MA, PSU, OMG, MG, K, OMU, NA, CL, UR3, CD

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	0.39	0/65959	0.61	18/102870 (0.0%)
2	9	0.38	0/2905	0.60	2/4528 (0.0%)
3	A	0.46	0/1786	1.02	9/2408 (0.4%)
4	B	0.44	0/2690	1.03	18/3652 (0.5%)
5	C	0.48	0/1884	1.01	6/2551 (0.2%)
6	D	0.41	0/1111	0.96	5/1498 (0.3%)
7	E	0.41	0/1382	0.88	4/1880 (0.2%)
8	F	0.44	0/901	0.93	2/1224 (0.2%)
9	G	0.38	0/241	0.84	0/324
10	H	0.43	0/1287	0.99	10/1725 (0.6%)
11	J	0.43	0/1136	0.98	5/1530 (0.3%)
12	K	0.43	0/1001	0.99	1/1347 (0.1%)
13	L	0.41	0/1130	0.98	4/1509 (0.3%)
14	M	0.45	0/1584	0.93	5/2119 (0.2%)
15	N	0.38	0/1474	1.10	15/1999 (0.8%)
16	O	0.44	0/874	0.92	3/1181 (0.3%)
17	P	0.41	0/1147	0.89	1/1528 (0.1%)
18	Q	0.45	0/749	1.01	4/1005 (0.4%)
19	R	0.46	0/1172	0.95	3/1578 (0.2%)
20	S	0.39	0/648	0.89	2/875 (0.2%)
21	T	0.40	0/958	1.01	7/1289 (0.5%)
22	U	0.41	0/417	0.89	2/562 (0.4%)
23	V	0.44	0/502	1.05	2/675 (0.3%)
24	W	0.49	0/1219	1.00	5/1655 (0.3%)
25	X	0.44	0/664	0.97	3/895 (0.3%)
26	Y	0.45	0/1146	0.96	1/1536 (0.1%)
27	Z	0.41	0/590	0.98	1/787 (0.1%)
28	1	0.46	0/438	0.93	3/578 (0.5%)
29	2	0.46	0/401	0.82	0/529
30	3	0.41	0/771	0.82	3/1024 (0.3%)
31	I	0.47	0/526	1.08	4/716 (0.6%)
All	All	0.40	0/98693	0.73	148/147577 (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	42
2	9	0	2
24	W	0	1
All	All	1	45

There are no bond length outliers.

The worst 5 of 148 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	13.74	130.11	109.50
17	P	118	GLN	N-CA-C	-8.86	101.70	111.36
1	0	1563	G	C4'-C3'-O3'	8.66	122.39	109.40
18	Q	17	LYS	N-CA-C	-8.39	99.52	109.93
21	T	52	ARG	N-CA-C	8.37	124.31	113.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	131	A	Sidechain
1	0	220	C	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	48	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1341	0
2	9	2600	0	1326	95	0
3	A	1753	0	1766	81	0
4	B	2625	0	2533	110	0
5	C	1859	0	1816	76	0
6	D	1094	0	1085	57	0
7	E	1357	0	1266	41	0
8	F	890	0	843	33	0
9	G	240	0	231	9	0
10	H	1266	0	1268	40	0
11	J	1120	0	1098	49	0
12	K	992	0	1031	41	0
13	L	1118	0	1076	29	0
14	M	1560	0	1568	46	0
15	N	1445	0	1401	47	0
16	O	865	0	873	21	0
17	P	1136	0	1123	33	0
18	Q	735	0	728	22	0
19	R	1149	0	1122	45	0
20	S	641	0	605	15	0
21	T	950	0	923	25	0
22	U	410	0	364	23	0
23	V	499	0	511	19	0
24	W	1196	0	1137	57	0
25	X	654	0	653	23	0
26	Y	1130	0	1133	46	0
27	Z	579	0	539	25	0
28	1	431	0	426	20	0
29	2	396	0	413	18	0
30	3	755	0	728	18	0
31	I	519	0	500	23	0
32	0	42	0	50	24	0
33	0	108	0	0	0	0
33	3	2	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	74	0	0	2	0
35	9	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	1	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	9	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	2	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	5905	0	0	199	0
38	1	56	0	0	1	0
38	2	45	0	0	4	0
38	3	66	0	0	2	0
38	9	140	0	0	10	0
38	A	112	0	0	8	0
38	B	142	0	0	20	0
38	C	170	0	0	17	0
38	D	45	0	0	8	0
38	E	42	0	0	5	0
38	F	26	0	0	2	0
38	G	19	0	0	0	0
38	H	70	0	0	6	0
38	I	8	0	0	1	0
38	J	58	0	0	3	0
38	K	59	0	0	1	0
38	L	83	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	M	123	0	0	4	0
38	N	63	0	0	6	0
38	O	44	0	0	3	0
38	P	56	0	0	2	0
38	Q	51	0	0	5	0
38	R	80	0	0	2	0
38	S	36	0	0	2	0
38	T	33	0	0	1	0
38	U	26	0	0	2	0
38	V	11	0	0	1	0
38	W	67	0	0	6	0
38	X	21	0	0	2	0
38	Y	96	0	0	6	0
38	Z	31	0	0	2	0
All	All	99043	0	59948	2297	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2297 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)
1:0:871:G:C8	1:0:871:G:H5'	1.77	1.19
1:0:1160:G:C5'	1:0:1161:A:H5'	1.73	1.18
1:0:1160:G:H5'	1:0:1161:A:C5'	1.79	1.12
1:0:871:G:H5'	1:0:871:G:H8	1.01	1.09
1:0:1002:G:H2'	1:0:1003:U:H5''	1.37	1.07

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%)	212 (90%)	21 (9%)	2 (1%)	14	41
4	B	335/338 (99%)	310 (92%)	21 (6%)	4 (1%)	10	34
5	C	244/246 (99%)	224 (92%)	18 (7%)	2 (1%)	16	44
6	D	134/177 (76%)	113 (84%)	18 (13%)	3 (2%)	5	20
7	E	170/178 (96%)	163 (96%)	6 (4%)	1 (1%)	21	51
8	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	4	17
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	6	23
11	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	30
12	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	L	141/165 (86%)	121 (86%)	20 (14%)	0	100	100
14	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
15	N	184/187 (98%)	167 (91%)	13 (7%)	4 (2%)	5	20
16	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
17	P	141/149 (95%)	136 (96%)	4 (3%)	1 (1%)	18	48
18	Q	93/96 (97%)	86 (92%)	6 (6%)	1 (1%)	11	36
19	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
20	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
21	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	41
22	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
24	W	152/154 (99%)	150 (99%)	0	2 (1%)	9	32
25	X	80/92 (87%)	72 (90%)	7 (9%)	1 (1%)	9	32
26	Y	140/241 (58%)	140 (100%)	0	0	100	100
27	Z	71/73 (97%)	60 (84%)	9 (13%)	2 (3%)	4	15
28	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
30	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
31	I	68/161 (42%)	62 (91%)	6 (9%)	0	100	100
All	All	3705/4419 (84%)	3436 (93%)	237 (6%)	32 (1%)	14	41

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	F	101	ALA
10	H	166	SER
11	J	5	GLU
15	N	154	LEU
15	N	183	ASP

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%)	170 (95%)	9 (5%)	22	53
4	B	282/283 (100%)	266 (94%)	16 (6%)	18	49
5	C	193/193 (100%)	175 (91%)	18 (9%)	8	27
6	D	117/148 (79%)	114 (97%)	3 (3%)	40	73
7	E	152/156 (97%)	146 (96%)	6 (4%)	28	63
8	F	93/94 (99%)	89 (96%)	4 (4%)	26	60
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	132/138 (96%)	128 (97%)	4 (3%)	36	70
11	J	118/121 (98%)	110 (93%)	8 (7%)	14	42
12	K	106/106 (100%)	103 (97%)	3 (3%)	38	72
13	L	113/127 (89%)	108 (96%)	5 (4%)	25	59
14	M	158/158 (100%)	150 (95%)	8 (5%)	21	53
15	N	149/150 (99%)	144 (97%)	5 (3%)	32	66
16	O	93/94 (99%)	90 (97%)	3 (3%)	34	68
17	P	113/117 (97%)	109 (96%)	4 (4%)	32	66
18	Q	79/80 (99%)	76 (96%)	3 (4%)	29	64
19	R	117/122 (96%)	113 (97%)	4 (3%)	32	66
20	S	71/74 (96%)	68 (96%)	3 (4%)	26	60
21	T	105/106 (99%)	101 (96%)	4 (4%)	29	64
22	U	44/52 (85%)	43 (98%)	1 (2%)	44	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	V	51/57 (90%)	50 (98%)	1 (2%)	48 78
24	W	130/130 (100%)	124 (95%)	6 (5%)	24 57
25	X	66/74 (89%)	62 (94%)	4 (6%)	17 46
26	Y	120/196 (61%)	114 (95%)	6 (5%)	22 53
27	Z	60/60 (100%)	60 (100%)	0	100 100
28	1	46/47 (98%)	45 (98%)	1 (2%)	45 77
29	2	42/46 (91%)	40 (95%)	2 (5%)	23 55
30	3	79/79 (100%)	77 (98%)	2 (2%)	42 74
31	I	58/129 (45%)	56 (97%)	2 (3%)	32 66
All	All	3093/3602 (86%)	2958 (96%)	135 (4%)	25 59

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	W	142	ASP
25	X	52	PRO
29	2	31	ARG
7	E	68	HIS
7	E	16	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
20	S	53	ASN
25	X	23	HIS
21	T	39	ASN
24	W	27	HIS
26	Y	149	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	249 (9%)	33 (1%)
2	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2867/3044 (94%)	267 (9%)	34 (1%)

5 of 267 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2526	C
1	0	2536	C
1	0	2761	A
1	0	1165	G
1	0	1080	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	1	19,22,23	0.32	0	25,31,34	0.43	0
1	OMG	0	2588	1	23,26,27	0.33	0	32,38,41	0.42	0
1	UR3	0	2619	1	19,22,23	0.49	0	26,32,35	0.75	1 (3%)
1	1MA	0	628	1	21,25,26	0.70	1 (4%)	30,37,40	0.71	1 (3%)
1	PSU	0	2621	1	18,21,22	1.57	2 (11%)	21,30,33	1.42	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	1	-	0/9/27/28	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	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.21	1.43	1.36
1	0	2621	PSU	C6-C5	2.83	1.38	1.35
1	0	628	1MA	C6-N6	2.35	1.33	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	3.68	120.66	118.17
1	0	2621	PSU	C6-N1-C2	-3.16	119.75	122.69
1	0	2621	PSU	O2-C2-N1	2.98	125.86	122.79
1	0	2619	UR3	C4-N3-C2	2.83	126.86	124.58
1	0	628	1MA	N1-C2-N3	2.66	129.16	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	13T	0	9000	-	42,43,43	2.00	10 (23%)	51,63,63	1.83	9 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	13T	0	9000	-	-	16/73/81/81	0/1/2/2

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	13T	C18-C19	6.97	1.56	1.47
32	0	9000	13T	C10-C9	4.13	1.57	1.50
32	0	9000	13T	O5-C5	3.42	1.26	1.21
32	0	9000	13T	O2-C1	3.31	1.29	1.21
32	0	9000	13T	O7-C11	3.13	1.26	1.21

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	13T	C18-O11-C19	8.03	65.36	60.81
32	0	9000	13T	O11-C18-C19	-4.35	56.62	59.38
32	0	9000	13T	O4-C3-C4	4.13	115.61	105.83
32	0	9000	13T	O11-C19-C18	-2.66	58.01	59.82
32	0	9000	13T	C27-C10-C9	2.51	113.14	110.73

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

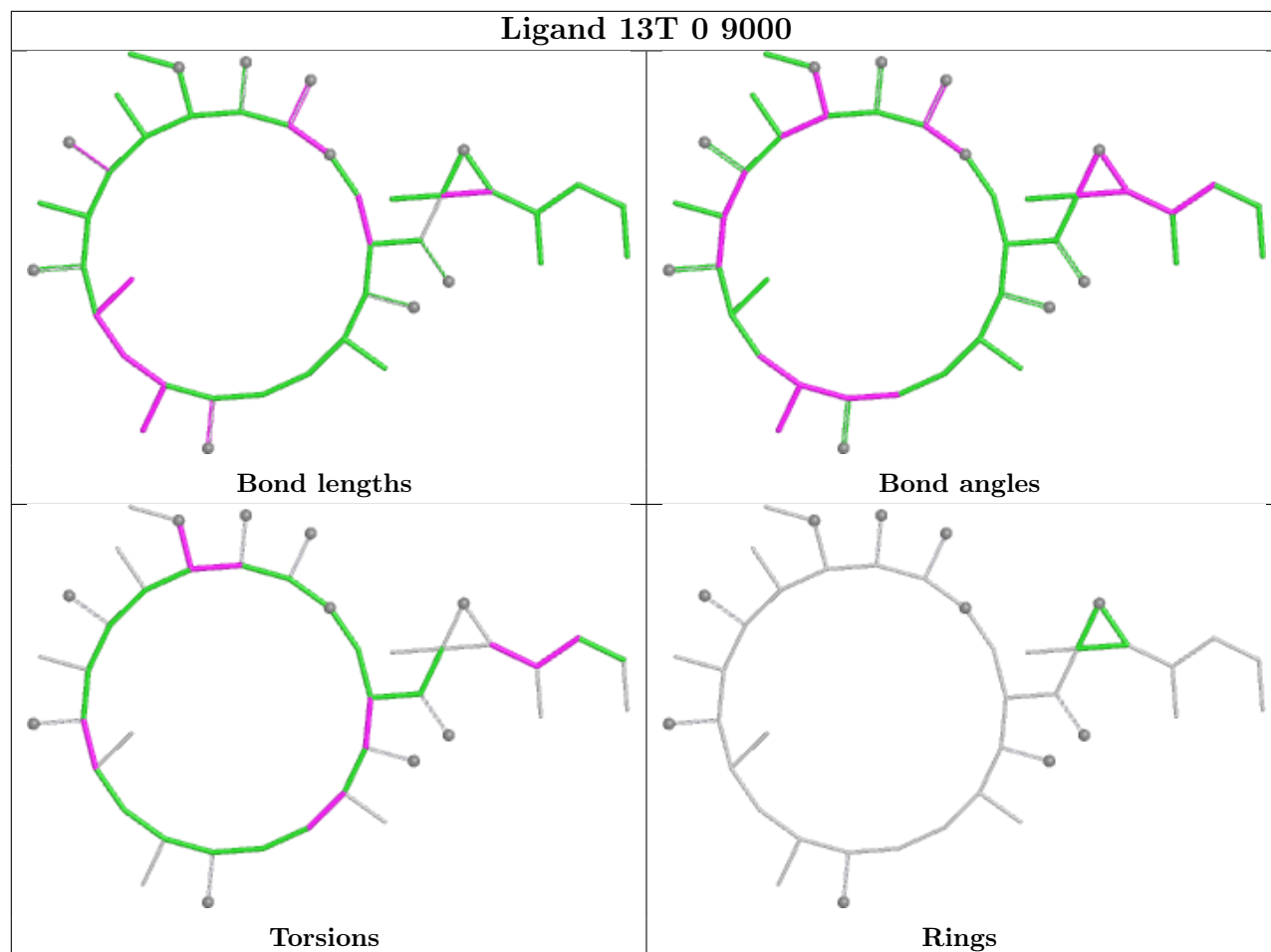
Mol	Chain	Res	Type	Atoms
32	0	9000	13T	C2-C3-O4-C32
32	0	9000	13T	C1-C2-C3-O4
32	0	9000	13T	O6-C7-C8-C9
32	0	9000	13T	O6-C7-C8-C26
32	0	9000	13T	C6-C7-C8-C9

There are no ring outliers.

1 monomer is involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9000	13T	24	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	0.13	26 (0%) 81 75	23, 50, 93, 150	0
2	9	122/122 (100%)	0.15	3 (2%) 58 48	43, 69, 91, 151	0
3	A	237/240 (98%)	0.67	11 (4%) 37 29	32, 55, 86, 105	0
4	B	337/338 (99%)	0.90	24 (7%) 22 17	33, 60, 82, 90	0
5	C	246/246 (100%)	0.53	6 (2%) 59 50	30, 50, 73, 82	0
6	D	140/177 (79%)	1.73	50 (35%) 1 0	63, 103, 124, 130	0
7	E	172/178 (96%)	0.94	15 (8%) 16 13	55, 73, 90, 96	0
8	F	119/120 (99%)	0.84	8 (6%) 24 19	57, 74, 96, 106	0
9	G	29/348 (8%)	1.11	3 (10%) 12 10	81, 94, 103, 103	0
10	H	160/171 (93%)	0.70	5 (3%) 51 42	52, 67, 93, 100	0
11	J	142/145 (97%)	0.77	10 (7%) 22 18	45, 56, 74, 94	0
12	K	132/132 (100%)	0.72	2 (1%) 72 64	41, 54, 75, 81	0
13	L	145/165 (87%)	0.90	13 (8%) 15 13	32, 71, 107, 118	0
14	M	194/194 (100%)	0.45	4 (2%) 63 54	36, 47, 60, 64	0
15	N	186/187 (99%)	0.94	21 (11%) 10 9	50, 67, 110, 119	0
16	O	115/116 (99%)	0.67	3 (2%) 57 48	44, 59, 71, 76	0
17	P	143/149 (95%)	0.97	11 (7%) 19 16	46, 60, 70, 75	0
18	Q	95/96 (98%)	0.49	3 (3%) 50 41	43, 52, 64, 72	0
19	R	150/155 (96%)	0.54	4 (2%) 56 47	38, 50, 68, 73	0
20	S	81/85 (95%)	0.79	8 (9%) 13 11	52, 65, 81, 85	0
21	T	119/120 (99%)	0.75	3 (2%) 58 48	47, 62, 83, 96	0
22	U	53/66 (80%)	0.88	5 (9%) 14 12	51, 61, 75, 81	0
23	V	65/71 (91%)	1.21	12 (18%) 3 3	59, 79, 109, 114	0
24	W	154/154 (100%)	0.55	4 (2%) 57 48	42, 56, 70, 77	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	1.25	13 (15%) 5 4	52, 64, 87, 97	0
26	Y	142/241 (58%)	0.54	3 (2%) 63 54	30, 51, 70, 86	0
27	Z	73/73 (100%)	1.01	11 (15%) 5 4	58, 69, 80, 94	0
28	1	56/57 (98%)	0.21	0 100 100	31, 37, 43, 51	0
29	2	46/50 (92%)	1.16	10 (21%) 2 2	41, 69, 90, 99	0
30	3	92/92 (100%)	0.50	3 (3%) 49 40	42, 60, 71, 82	0
31	I	70/161 (43%)	2.38	37 (52%) 0 0	109, 119, 135, 135	0
All	All	6646/7463 (89%)	0.52	331 (4%) 34 27	23, 57, 100, 151	0

The worst 5 of 331 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	6.5
25	X	88	GLU	6.4
6	D	10	PHE	6.2
15	N	166	ALA	6.2
4	B	1	PRO	6.0

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	OMU	0	2587	21/22	0.94	0.11	38,39,40,41	0
1	UR3	0	2619	21/22	0.94	0.10	36,38,39,40	0
1	1MA	0	628	23/24	0.95	0.10	33,35,36,37	0
1	PSU	0	2621	20/21	0.95	0.09	30,32,39,40	0
1	OMG	0	2588	24/25	0.96	0.10	37,38,39,40	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
35	NA	9	8551	1/1	0.55	0.22	92,92,92,92	0
35	NA	0	8584	1/1	0.56	0.23	90,90,90,90	0
35	NA	0	8560	1/1	0.60	0.30	60,60,60,60	0
35	NA	0	8571	1/1	0.60	0.27	59,59,59,59	0
33	MG	0	8050	1/1	0.70	0.15	74,74,74,74	0
33	MG	9	8095	1/1	0.70	0.18	77,77,77,77	0
35	NA	0	8510	1/1	0.72	0.16	45,45,45,45	0
35	NA	0	8569	1/1	0.73	0.32	64,64,64,64	0
35	NA	0	8577	1/1	0.74	0.31	81,81,81,81	0
35	NA	0	8557	1/1	0.75	0.14	45,45,45,45	0
33	MG	0	8024	1/1	0.76	0.73	65,65,65,65	0
35	NA	0	8582	1/1	0.76	0.20	85,85,85,85	0
35	NA	0	8502	1/1	0.76	0.17	57,57,57,57	0
35	NA	0	8559	1/1	0.76	0.25	53,53,53,53	0
35	NA	0	8538	1/1	0.78	0.10	55,55,55,55	0
33	MG	0	8082	1/1	0.79	0.23	84,84,84,84	0
35	NA	0	8585	1/1	0.79	0.32	65,65,65,65	0
35	NA	0	8511	1/1	0.79	0.14	56,56,56,56	0
35	NA	0	8534	1/1	0.80	0.15	40,40,40,40	0
35	NA	H	8522	1/1	0.80	0.42	77,77,77,77	0
35	NA	J	8546	1/1	0.80	0.14	39,39,39,39	0
35	NA	S	8512	1/1	0.80	0.29	57,57,57,57	0
35	NA	9	8583	1/1	0.81	0.23	73,73,73,73	0
33	MG	0	8104	1/1	0.81	0.20	78,78,78,78	0
36	CL	0	8816	1/1	0.81	0.23	69,69,69,69	0
33	MG	0	8046	1/1	0.82	0.09	56,56,56,56	0
35	NA	0	8508	1/1	0.82	0.18	58,58,58,58	0
35	NA	0	8540	1/1	0.82	0.19	50,50,50,50	0
35	NA	0	8524	1/1	0.82	0.17	48,48,48,48	0
35	NA	0	8528	1/1	0.82	0.18	54,54,54,54	0
35	NA	0	8532	1/1	0.82	0.17	44,44,44,44	0
35	NA	0	8507	1/1	0.83	0.16	69,69,69,69	0
35	NA	0	8563	1/1	0.83	0.23	68,68,68,68	0
35	NA	0	8564	1/1	0.83	0.16	49,49,49,49	0
35	NA	0	8516	1/1	0.83	0.17	49,49,49,49	0
35	NA	0	8529	1/1	0.83	0.14	68,68,68,68	0
33	MG	0	8051	1/1	0.84	0.10	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8102	1/1	0.84	0.09	50,50,50,50	0
35	NA	0	8566	1/1	0.84	0.08	48,48,48,48	0
32	13T	0	9000	42/42	0.85	0.20	58,67,73,74	0
35	NA	0	8565	1/1	0.85	0.30	47,47,47,47	0
33	MG	0	8070	1/1	0.85	0.08	43,43,43,43	0
35	NA	0	8562	1/1	0.85	0.27	70,70,70,70	0
36	CL	0	8815	1/1	0.85	0.22	89,89,89,89	0
33	MG	0	8072	1/1	0.85	0.08	57,57,57,57	0
36	CL	J	8802	1/1	0.85	0.13	76,76,76,76	0
35	NA	0	8579	1/1	0.86	0.23	65,65,65,65	0
33	MG	0	8096	1/1	0.86	0.11	48,48,48,48	0
33	MG	0	8093	1/1	0.86	0.08	61,61,61,61	0
35	NA	0	8520	1/1	0.86	0.12	36,36,36,36	0
33	MG	0	8113	1/1	0.87	0.08	44,44,44,44	0
33	MG	0	8103	1/1	0.87	0.22	78,78,78,78	0
36	CL	0	8822	1/1	0.87	0.41	90,90,90,90	0
35	NA	0	8568	1/1	0.87	0.40	87,87,87,87	0
35	NA	0	8544	1/1	0.88	0.09	29,29,29,29	0
35	NA	0	8552	1/1	0.88	0.36	68,68,68,68	0
35	NA	0	8509	1/1	0.88	0.09	48,48,48,48	0
35	NA	0	8573	1/1	0.88	0.07	56,56,56,56	0
33	MG	0	8041	1/1	0.88	0.11	68,68,68,68	0
36	CL	A	8809	1/1	0.88	0.23	82,82,82,82	0
35	NA	0	8541	1/1	0.88	0.06	46,46,46,46	0
33	MG	0	8108	1/1	0.89	0.12	77,77,77,77	0
35	NA	A	8545	1/1	0.89	0.12	61,61,61,61	0
34	K	0	8401	1/1	0.89	0.29	84,84,84,84	0
35	NA	0	8525	1/1	0.89	0.18	59,59,59,59	0
35	NA	0	8515	1/1	0.89	0.16	49,49,49,49	0
33	MG	0	8087	1/1	0.89	0.13	63,63,63,63	0
35	NA	0	8531	1/1	0.89	0.17	57,57,57,57	0
35	NA	0	8554	1/1	0.89	0.13	42,42,42,42	0
35	NA	0	8567	1/1	0.89	0.19	61,61,61,61	0
35	NA	0	8517	1/1	0.89	0.09	37,37,37,37	0
35	NA	0	8550	1/1	0.90	0.26	65,65,65,65	0
33	MG	0	8114	1/1	0.90	0.17	54,54,54,54	0
33	MG	0	8097	1/1	0.90	0.09	45,45,45,45	0
33	MG	0	8112	1/1	0.90	0.10	39,39,39,39	0
35	NA	0	8558	1/1	0.90	0.24	75,75,75,75	0
35	NA	R	8586	1/1	0.90	0.26	23,23,23,23	0
35	NA	0	8536	1/1	0.90	0.09	54,54,54,54	0
35	NA	0	8526	1/1	0.90	0.17	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8052	1/1	0.90	0.13	68,68,68,68	0
35	NA	0	8518	1/1	0.90	0.21	58,58,58,58	0
35	NA	0	8530	1/1	0.90	0.12	45,45,45,45	0
35	NA	0	8549	1/1	0.90	0.15	53,53,53,53	0
36	CL	Y	8817	1/1	0.90	0.12	70,70,70,70	0
37	CD	O	8705	1/1	0.90	0.29	186,186,186,186	0
33	MG	0	8117	1/1	0.91	0.08	34,34,34,34	0
35	NA	0	8506	1/1	0.91	0.20	49,49,49,49	0
35	NA	0	8572	1/1	0.91	0.25	73,73,73,73	0
33	MG	0	8089	1/1	0.91	0.14	62,62,62,62	0
35	NA	0	8513	1/1	0.91	0.09	72,72,72,72	0
35	NA	C	8504	1/1	0.91	0.06	35,35,35,35	0
36	CL	J	8801	1/1	0.91	0.12	58,58,58,58	0
33	MG	0	8092	1/1	0.91	0.17	72,72,72,72	0
35	NA	0	8539	1/1	0.91	0.10	40,40,40,40	0
35	NA	R	8537	1/1	0.91	0.14	45,45,45,45	0
35	NA	0	8561	1/1	0.92	0.10	50,50,50,50	0
36	CL	0	8812	1/1	0.92	0.11	49,49,49,49	0
33	MG	0	8115	1/1	0.92	0.09	45,45,45,45	0
35	NA	0	8533	1/1	0.92	0.09	39,39,39,39	0
35	NA	0	8556	1/1	0.92	0.22	61,61,61,61	0
35	NA	0	8575	1/1	0.92	0.35	72,72,72,72	0
33	MG	0	8043	1/1	0.92	0.08	47,47,47,47	0
35	NA	0	8535	1/1	0.92	0.16	54,54,54,54	0
36	CL	J	8821	1/1	0.92	0.16	77,77,77,77	0
33	MG	0	8084	1/1	0.92	0.09	58,58,58,58	0
33	MG	0	8080	1/1	0.92	0.08	39,39,39,39	0
33	MG	Y	8109	1/1	0.93	0.09	44,44,44,44	0
33	MG	0	8063	1/1	0.93	0.09	63,63,63,63	0
33	MG	0	8090	1/1	0.93	0.12	73,73,73,73	0
33	MG	0	8076	1/1	0.93	0.06	49,49,49,49	0
33	MG	0	8085	1/1	0.93	0.07	48,48,48,48	0
33	MG	0	8116	1/1	0.93	0.06	56,56,56,56	0
33	MG	0	8045	1/1	0.93	0.15	67,67,67,67	0
33	MG	0	8111	1/1	0.93	0.07	46,46,46,46	0
33	MG	B	8055	1/1	0.93	0.12	64,64,64,64	0
35	NA	M	8547	1/1	0.93	0.12	41,41,41,41	0
36	CL	R	8806	1/1	0.93	0.09	49,49,49,49	0
35	NA	Q	8548	1/1	0.93	0.06	46,46,46,46	0
35	NA	0	8555	1/1	0.93	0.18	85,85,85,85	0
36	CL	0	8803	1/1	0.94	0.12	56,56,56,56	0
36	CL	0	8805	1/1	0.94	0.10	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8570	1/1	0.94	0.34	65,65,65,65	0
36	CL	0	8813	1/1	0.94	0.08	54,54,54,54	0
36	CL	0	8814	1/1	0.94	0.13	57,57,57,57	0
33	MG	0	8044	1/1	0.94	0.06	55,55,55,55	0
33	MG	0	8047	1/1	0.94	0.12	57,57,57,57	0
35	NA	0	8527	1/1	0.94	0.17	61,61,61,61	0
33	MG	0	8057	1/1	0.94	0.06	41,41,41,41	0
33	MG	0	8049	1/1	0.94	0.13	36,36,36,36	0
33	MG	0	8067	1/1	0.94	0.06	37,37,37,37	0
35	NA	0	8581	1/1	0.94	0.05	42,42,42,42	0
33	MG	0	8094	1/1	0.94	0.12	59,59,59,59	0
33	MG	0	8040	1/1	0.94	0.09	53,53,53,53	0
33	MG	T	8073	1/1	0.94	0.14	57,57,57,57	0
33	MG	A	8065	1/1	0.95	0.09	45,45,45,45	0
33	MG	0	8075	1/1	0.95	0.07	56,56,56,56	0
33	MG	K	8069	1/1	0.95	0.06	51,51,51,51	0
33	MG	0	8071	1/1	0.95	0.06	50,50,50,50	0
33	MG	0	8100	1/1	0.95	0.06	42,42,42,42	0
33	MG	0	8110	1/1	0.95	0.08	53,53,53,53	0
35	NA	0	8542	1/1	0.95	0.16	15,15,15,15	0
36	CL	B	8819	1/1	0.95	0.15	53,53,53,53	0
34	K	0	8402	1/1	0.95	0.12	61,61,61,61	0
33	MG	0	8101	1/1	0.95	0.06	45,45,45,45	0
35	NA	0	8503	1/1	0.95	0.15	1,1,1,1	0
36	CL	L	8810	1/1	0.95	0.10	59,59,59,59	0
36	CL	N	8807	1/1	0.95	0.10	71,71,71,71	0
36	CL	O	8808	1/1	0.95	0.09	67,67,67,67	0
35	NA	0	8505	1/1	0.95	0.06	37,37,37,37	0
35	NA	0	8553	1/1	0.95	0.08	44,44,44,44	0
33	MG	0	8035	1/1	0.95	0.08	46,46,46,46	0
33	MG	3	8118	1/1	0.96	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.96	0.04	33,33,33,33	0
35	NA	0	8514	1/1	0.96	0.07	38,38,38,38	0
33	MG	0	8061	1/1	0.96	0.05	44,44,44,44	0
35	NA	0	8501	1/1	0.96	0.06	50,50,50,50	0
33	MG	0	8037	1/1	0.96	0.06	42,42,42,42	0
33	MG	0	8028	1/1	0.96	0.05	33,33,33,33	0
33	MG	0	8068	1/1	0.96	0.06	56,56,56,56	0
35	NA	0	8521	1/1	0.96	0.16	77,77,77,77	0
33	MG	0	8048	1/1	0.96	0.05	49,49,49,49	0
35	NA	0	8574	1/1	0.96	0.13	67,67,67,67	0
33	MG	0	8053	1/1	0.96	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8025	1/1	0.96	0.05	43,43,43,43	0
35	NA	0	8578	1/1	0.96	0.13	57,57,57,57	0
33	MG	0	8098	1/1	0.96	0.12	42,42,42,42	0
33	MG	0	8099	1/1	0.96	0.12	70,70,70,70	0
36	CL	3	8804	1/1	0.96	0.07	56,56,56,56	0
36	CL	0	8811	1/1	0.96	0.08	58,58,58,58	0
33	MG	0	8106	1/1	0.97	0.10	71,71,71,71	0
33	MG	0	8042	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8523	1/1	0.97	0.19	38,38,38,38	0
33	MG	0	8022	1/1	0.97	0.05	37,37,37,37	0
33	MG	0	8029	1/1	0.97	0.05	42,42,42,42	0
35	NA	0	8543	1/1	0.97	0.13	35,35,35,35	0
33	MG	0	8039	1/1	0.97	0.06	64,64,64,64	0
36	CL	Y	8820	1/1	0.97	0.05	44,44,44,44	0
33	MG	0	8031	1/1	0.97	0.06	30,30,30,30	0
33	MG	0	8033	1/1	0.97	0.06	38,38,38,38	0
37	CD	Z	8703	1/1	0.97	0.04	71,71,71,71	0
33	MG	0	8059	1/1	0.98	0.04	39,39,39,39	0
33	MG	0	8060	1/1	0.98	0.06	45,45,45,45	0
33	MG	0	8036	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8011	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8064	1/1	0.98	0.06	41,41,41,41	0
33	MG	0	8012	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8091	1/1	0.98	0.04	65,65,65,65	0
33	MG	0	8027	1/1	0.98	0.03	40,40,40,40	0
33	MG	0	8016	1/1	0.98	0.04	18,18,18,18	0
33	MG	0	8018	1/1	0.98	0.06	39,39,39,39	0
33	MG	0	8021	1/1	0.98	0.05	37,37,37,37	0
36	CL	M	8818	1/1	0.98	0.05	44,44,44,44	0
33	MG	0	8008	1/1	0.98	0.05	29,29,29,29	0
33	MG	0	8056	1/1	0.98	0.05	56,56,56,56	0
33	MG	0	8023	1/1	0.98	0.12	61,61,61,61	0
33	MG	A	8066	1/1	0.98	0.05	73,73,73,73	0
35	NA	0	8576	1/1	0.98	0.04	33,33,33,33	0
33	MG	0	8081	1/1	0.98	0.07	43,43,43,43	0
33	MG	0	8058	1/1	0.98	0.06	42,42,42,42	0
37	CD	U	8701	1/1	0.98	0.03	67,67,67,67	0
33	MG	0	8083	1/1	0.98	0.04	41,41,41,41	0
33	MG	0	8032	1/1	0.99	0.04	35,35,35,35	0
33	MG	0	8077	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8079	1/1	0.99	0.03	27,27,27,27	0
33	MG	0	8005	1/1	0.99	0.04	32,32,32,32	0

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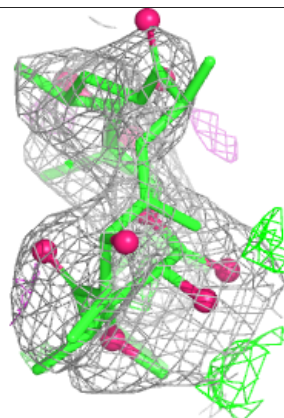
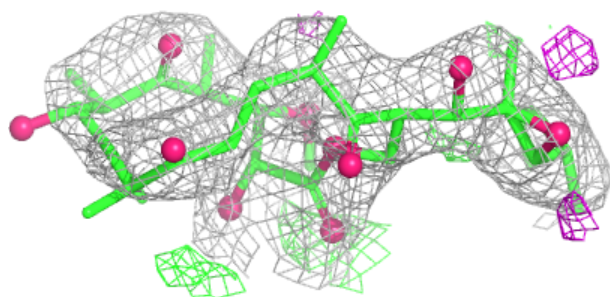
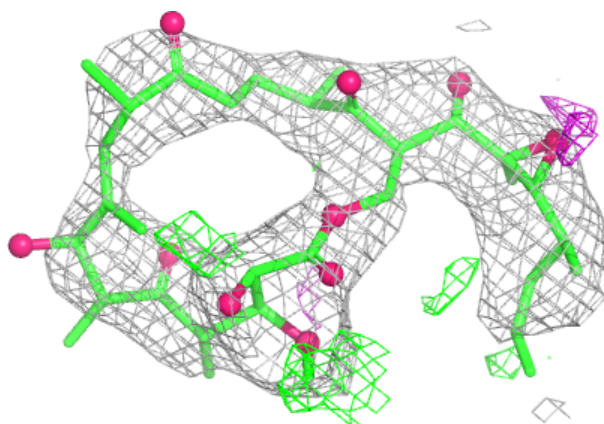
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8107	1/1	0.99	0.05	38,38,38,38	0
33	MG	0	8034	1/1	0.99	0.03	25,25,25,25	0
33	MG	0	8017	1/1	0.99	0.03	31,31,31,31	0
33	MG	0	8054	1/1	0.99	0.03	30,30,30,30	0
33	MG	0	8006	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8019	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8086	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8038	1/1	0.99	0.03	31,31,31,31	0
33	MG	0	8020	1/1	0.99	0.04	39,39,39,39	0
33	MG	0	8007	1/1	0.99	0.06	26,26,26,26	0
33	MG	0	8001	1/1	0.99	0.03	44,44,44,44	0
35	NA	0	8519	1/1	0.99	0.05	17,17,17,17	0
33	MG	0	8062	1/1	0.99	0.11	13,13,13,13	0
33	MG	0	8009	1/1	0.99	0.03	36,36,36,36	0
33	MG	0	8010	1/1	0.99	0.04	11,11,11,11	0
33	MG	0	8002	1/1	0.99	0.08	40,40,40,40	0
33	MG	0	8026	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	8004	1/1	0.99	0.04	37,37,37,37	0
33	MG	0	8013	1/1	0.99	0.07	38,38,38,38	0
33	MG	3	8078	1/1	0.99	0.02	16,16,16,16	0
33	MG	0	8014	1/1	0.99	0.05	41,41,41,41	0
35	NA	L	8580	1/1	0.99	0.10	1,1,1,1	0
33	MG	0	8074	1/1	0.99	0.02	30,30,30,30	0
33	MG	0	8015	1/1	0.99	0.03	35,35,35,35	0
37	CD	1	8702	1/1	0.99	0.05	65,65,65,65	0
37	CD	3	8704	1/1	0.99	0.03	65,65,65,65	0
33	MG	0	8003	1/1	1.00	0.02	36,36,36,36	0
33	MG	0	8030	1/1	1.00	0.04	35,35,35,35	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 13T 0 9000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.