



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:10 PM UTC

PDB ID : 3I55 / pdb_00003i55
Title : Co-crystal structure of Mycalamide A Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 3.11 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:

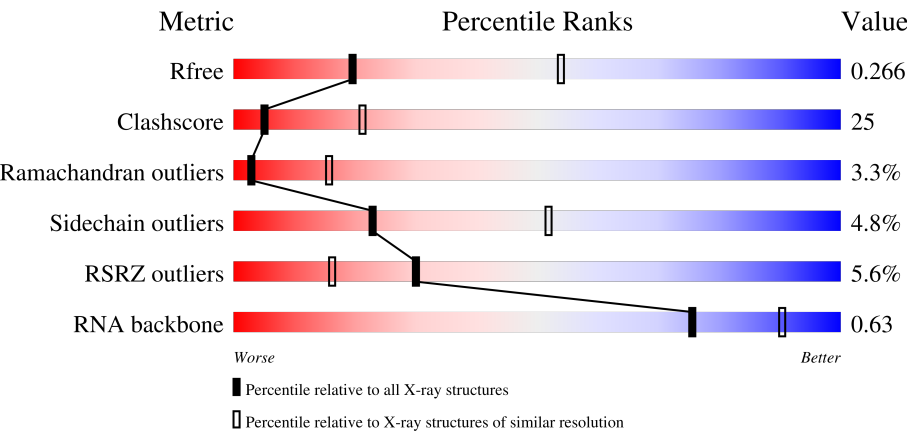
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 3.11 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	2923	42%46%6%6%
2	A	240	8%48%42%10%
3	B	338	4%42%51%7%
4	C	246	5%48%44%7%

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	178	
7	F	120	
8	G	348	
9	H	174	
10	I	162	
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	116	
28	1	57	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	
32	4	8	

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	5AA	4	76	-	-	X	-
34	K	0	8401	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	H	8518	-	-	-	X
38	MYL	0	2924	-	-	X	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99287 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	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

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

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

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

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

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

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 8 is a protein called 50S ribosomal protein L10E.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	160	Total	C	N	O	S	0	0	0
			1283	798	240	239	6			

- Molecule 10 is a protein called 50S ribosomal protein L11P.

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

- 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
			994	609	189	192	4			

- 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	333	282	1			

- 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	0	0	0
			950	568	180	202			

- 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	0	0	0
			410	244	75	86	5			

- 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	0	0	0
			499	304	94	100	1			

- 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	0	0	0
			1196	737	209	244	6			

- 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	0	0	0
			654	402	129	122	1			

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

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

- 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	0	0	0
			573	343	113	112	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	1	MET	-	expression tag	UNP P60619
Z	2	SER	-	expression tag	UNP P60619
Z	3	PRO	-	expression tag	UNP P60619
Z	4	ARG	-	expression tag	UNP P60619
Z	5	ALA	-	expression tag	UNP P60619
Z	6	ARG	-	expression tag	UNP P60619
Z	7	ARG	-	expression tag	UNP P60619
Z	8	GLU	-	expression tag	UNP P60619
Z	9	PRO	-	expression tag	UNP P60619
Z	10	ASN	-	expression tag	UNP P60619
Z	11	LEU	-	expression tag	UNP P60619
Z	12	GLU	-	expression tag	UNP P60619
Z	13	GLY	-	expression tag	UNP P60619
Z	14	LEU	-	expression tag	UNP P60619
Z	15	MET	-	expression tag	UNP P60619
Z	16	TRP	-	expression tag	UNP P60619
Z	17	PRO	-	expression tag	UNP P60619
Z	18	LEU	-	expression tag	UNP P60619
Z	19	GLY	-	expression tag	UNP P60619
Z	20	GLY	-	expression tag	UNP P60619
Z	21	GLN	-	expression tag	UNP P60619
Z	22	GLN	-	expression tag	UNP P60619
Z	23	THR	-	expression tag	UNP P60619
Z	24	THR	-	expression tag	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 RNA chain called 5S ribosomal RNA.

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

- Molecule 32 is DNA/RNA hybrid called DNA/RNA (5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	4	8	Total	C	N	O	P	0	0	0
			127	61	23	38	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	83	Total	Mg	0	0
			83	83		
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	2	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		
33	9	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	63	Total Na 63 63	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	S	1	Total Na 1 1	0	0
35	9	2	Total Na 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0

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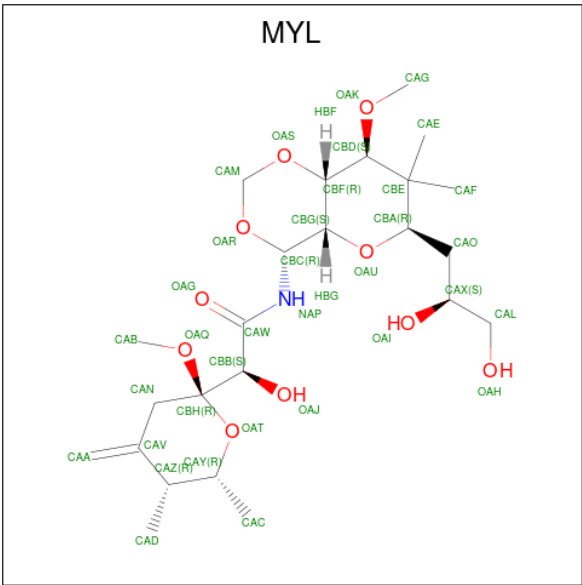
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	93	Total 93	Sr 93	0	0
37	A	2	Total 2	Sr 2	0	0
37	B	2	Total 2	Sr 2	0	0
37	F	1	Total 1	Sr 1	0	0
37	H	1	Total 1	Sr 1	0	0
37	L	1	Total 1	Sr 1	0	0
37	R	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	1	1	Total 1	Sr 1	0	0
37	3	2	Total 2	Sr 2	0	0
37	9	3	Total 3	Sr 3	0	0

- Molecule 38 is Mycalamide A (CCD ID: MYL) (formula: C₂₄H₄₁NO₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	0	1	Total	C	N	O	0	0
			35	24	1	10		

- Molecule 39 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total	Cd	0	0
			1	1		
39	U	1	Total	Cd	0	0
			1	1		
39	Z	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	3	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5841	Total	O	0	0
			5841	5841		
40	A	117	Total	O	0	0
			117	117		
40	B	151	Total	O	0	0
			151	151		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	175	Total 175	O 175	0	0
40	D	49	Total 49	O 49	0	0
40	E	40	Total 40	O 40	0	0
40	F	29	Total 29	O 29	0	0
40	G	18	Total 18	O 18	0	0
40	H	76	Total 76	O 76	0	0
40	I	10	Total 10	O 10	0	0
40	J	57	Total 57	O 57	0	0
40	K	62	Total 62	O 62	0	0
40	L	91	Total 91	O 91	0	0
40	M	148	Total 148	O 148	0	0
40	N	61	Total 61	O 61	0	0
40	O	41	Total 41	O 41	0	0
40	P	61	Total 61	O 61	0	0
40	Q	49	Total 49	O 49	0	0
40	R	83	Total 83	O 83	0	0
40	S	37	Total 37	O 37	0	0
40	T	36	Total 36	O 36	0	0
40	U	29	Total 29	O 29	0	0
40	V	13	Total 13	O 13	0	0
40	W	67	Total 67	O 67	0	0

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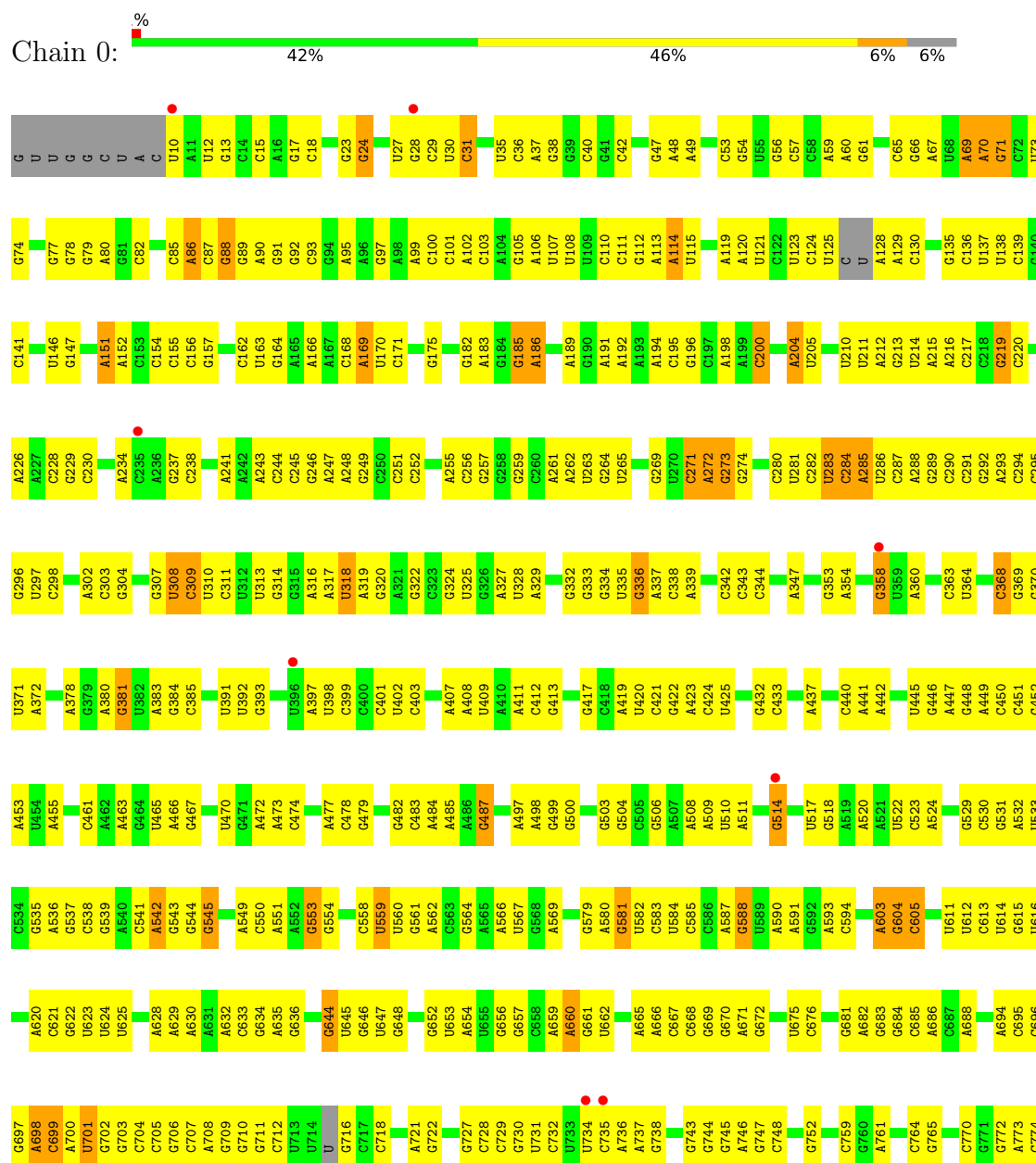
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	24	Total 24	O 24	0	0
40	Y	98	Total 98	O 98	0	0
40	Z	30	Total 30	O 30	0	0
40	1	58	Total 58	O 58	0	0
40	2	45	Total 45	O 45	0	0
40	3	70	Total 70	O 70	0	0
40	9	144	Total 144	O 144	0	0
40	4	13	Total 13	O 13	0	0

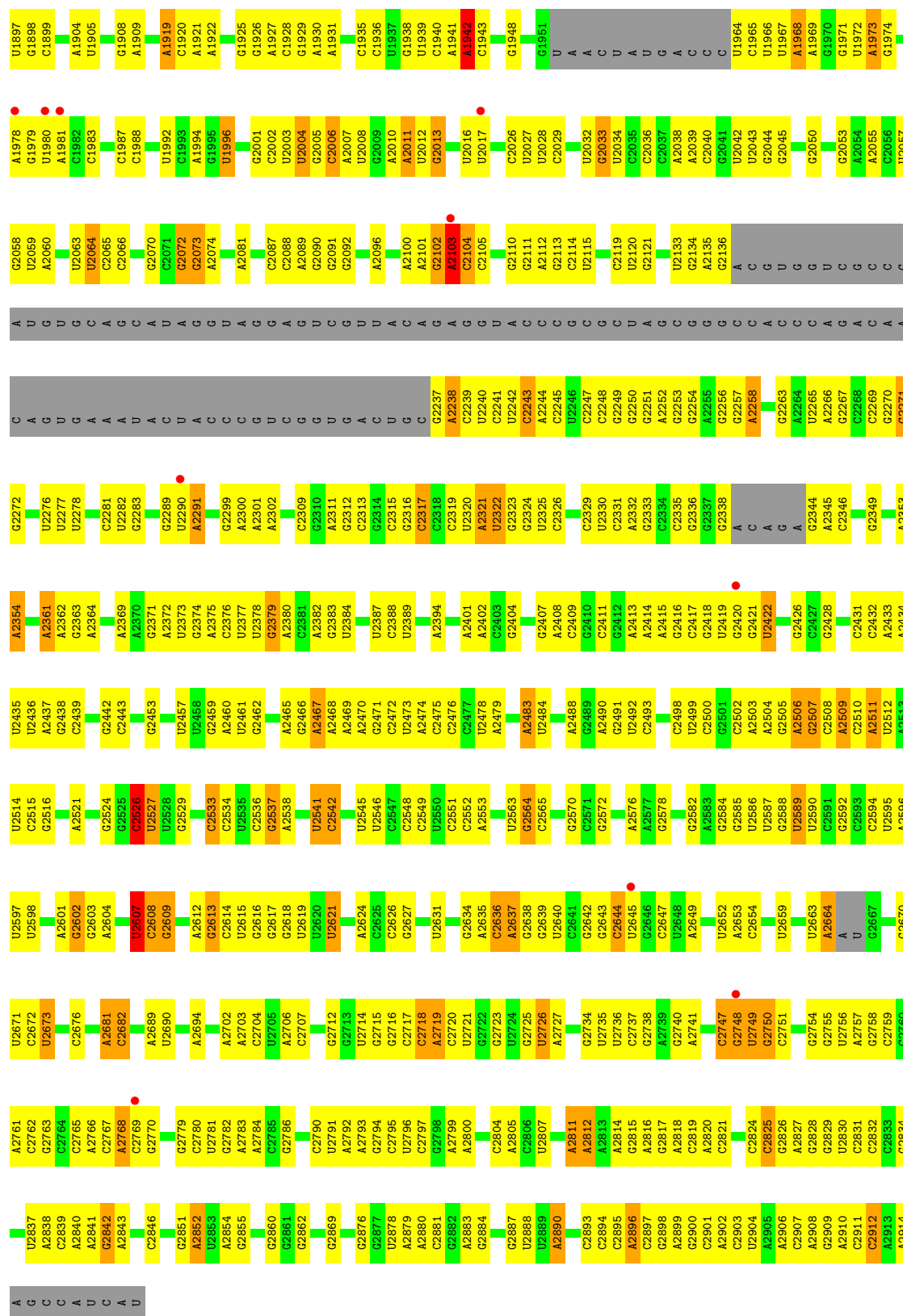
3 Residue-property plots

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

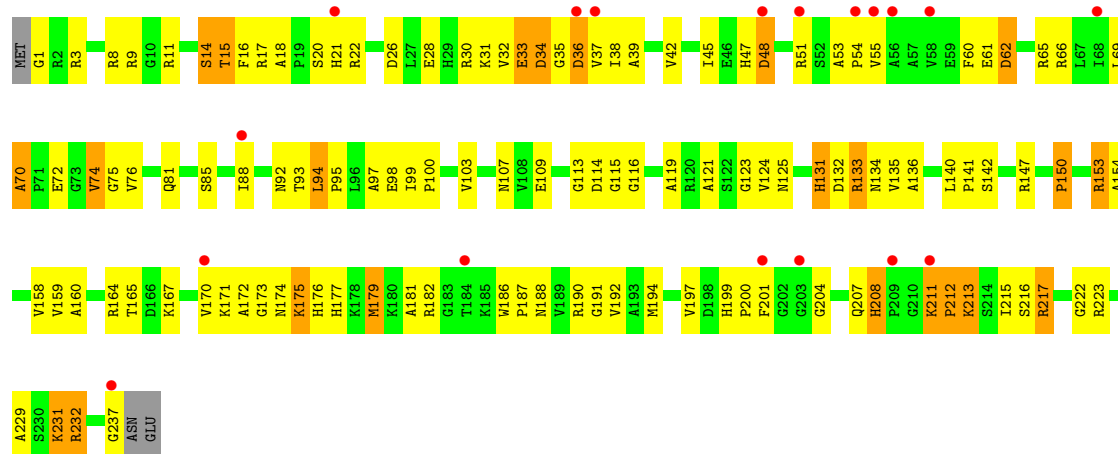


C1816	C1750	C1674	C1593	G1512	C1342	C1262	A1188	G1110	A1020	U954	C868	G775
U1817	G1751	C1675	C1594	C1513	C1343	C1263	A1189	A1114	A1021	A955	C869	A776
G1818	G1752	C1676	C1595	C1514	G1344	U1264	G1190	A1115	G1021	G956	G870	U777
G1820	C1753	U1596	U1597	A1515	U1350	C1268	A1191	U1116	C1025	G958	G871	U779
U1825	U1757	C1679	A1598	C1517	U1351	C1269	A1192	A1117	U1028	C959	U872	A788
C1826	U1758	G1681	U1599	U1434	A1352	C1273	A1194	A1118	U1029	G960	G873	C789
A1829	A1759	A1682	G1600	U1435	C1353	U1276	G1195	G1119	A874	A961	A875	A790
C1830	C1762	A1683	G1603	C1436	C1354	C1277	G1197	U1120	U1030	C962	A876	A791
C1833	C1763	A1684	G1604	U1524	A1355	U1278	G1199	G1121	G1031	G963	G877	G792
C1834	G1764	C1686	G1605	G1437	C1356	A1280	A1200	U1130	G1038	G964	G878	A793
U1835	U1766	A1687	A1606	C1439	U1359	U1279	C1201	G1131	G1039	A965	G879	U794
C1836	A1767	G1688	A1607	U1440	C1360	A1281	A1202	A1132	U1044	G969	A882	G795
U1838	C1692	C1613	C1613	A1441	G1363	A1286	G1203	G1135	G1045	U970	C885	G798
A1839	A1693	G1614	G1614	A1442	C1364	A1287	C1204	U1136	G1046	G	C890	C799
U1840	G1694	A1615	A1615	U1446	C1365	U1288	U1205	G1137	U1047	U	G891	G800
A1845	U1696	A1616	A1616	U1447	C1366	C1289	A1207	U1138	G1048	C	G892	U801
U1846	G1697	C1617	C1617	C1451	G1370	C1290	C1208	U1139	C1051	C	C896	A807
A1847	G1697	A1624	A1624	C1456	U1371	A1291	C1209	U1149	G1052	C	C897	G809
U1850	C1700	U1625	U1625	U1457	A1372	A1294	G1210	U1150	G1053	C	G898	A812
G1851	A1701	A1626	A1626	A1458	A1375	C1295	G1211	G1151	G1054	U	G901	C813
A1852	U1702	G1627	G1627	U1459	G1376	C1296	C1212	A1152	U1055	C	G902	C814
C1853	G1706	C1628	C1628	C1461	C1377	U1297	G1213	C1153	A1057	C	U815	U815
C1854	U1710	A1630	A1630	U1462	C1378	U1298	G1214	C1154	U1058	G	G905	G816
C1855	A1711	A1631	A1631	C1462	A1379	C1299	G1215	C1155	G1059	A	G911	G817
C1856	G1712	C1633	C1633	U1473	U1390	G1300	U1219	C1156	G1060	C	A912	A818
A1857	U1713	G1634	G1634	C1474	A1393	C1303	U1220	G1157	C1061	A	G820	A819
A1858	C1714	U1635	U1635	C1477	C1384	C1304	G1221	G1158	U1066	G	U821	G820
C1864	G1715	G1636	G1636	U1478	G1385	C1305	G1224	G1159	A1067	A	G918	G821
A1865	U1722	A1637	A1637	C1478	C1386	U1306	C1225	G1160	C1068	G	U919	U822
U1868	G1723	G1640	G1640	A1482	G1387	A1307	C1226	G1161	C1069	U	C920	U823
G1868	U1724	A1641	A1641	G1484	U1388	U1308	C1228	G1163	A1070	C	G921	A827
U1871	C1725	A1642	A1642	A1485	G1389	U1310	C1229	U1164	G1071	G	A922	G828
C1872	G1726	C1643	C1643	A1486	A1393	G1311	A1230	G1165	G1072	G	A923	G829
A1873	U1730	U1644	U1644	U1487	C1397	U1312	U1234	A1166	G1073	C	G925	G834
U1877	G1731	G1645	G1645	U1488	A1399	G1313	G1235	G1167	G1074	A	A926	U835
G1877	A1732	C1646	C1646	C1492	G1402	G1316	U1236	U1169	A1081	A	U932	G836
G1878	U1733	C1652	C1652	A1493	U1405	G1319	C1238	U1170	G1087	C999	U933	U840
U1879	C1734	A1653	A1653	A1494	U1406	G1325	G1239	A1171	A1088	C1000	G938	A843
C1882	C1735	G1654	G1654	C1495	A1407	U1328	G1240	A1172	G1089	U1001	G941	A844
U1883	A1736	A1655	A1655	A1496	U1408	G1329	G1241	A1174	A1090	U1003	U942	U845
G1884	C1737	A1656	A1656	G1497	U1409	U1330	C1242	G1175	U1091	C1004	A943	A846
A1885	G1738	A1657	A1657	U1498	G1410	G1331	U1243	U1178	U1095	A1005	G944	C853
C1888	C1739	C1662	C1662	U1499	G1411	U1332	C1244	U1179	U1096	A1007	U945	C854
U1889	U1740	G1663	G1663	U1500	A1411	G1333	U1245	U1180	A1097	C1008	U946	U855
C1890	A1741	A1664	A1664	A1504	U1412	U1334	A1246	A1181	A1098	U1009	U947	G856
U1891	G1743	G1665	G1665	U1505	U1416	C1334	U1247	C1182	G1099	C1010	G948	A857
C1894	A1746	U1667	U1667	U1506	G1417	G1339	C1250	C1184	C1102	A1013	U951	U858
A1895	U1747	C1668	C1668	C1507	U1418	G1340	G1260	U1185	C1103	C1014	G952	U862
G1896	U1748	U1669	U1669	U1508	U1419	A1341	A1261	C1186	U1109	U1016	G953	G863
	U1749			U1511	C1420			U1187				

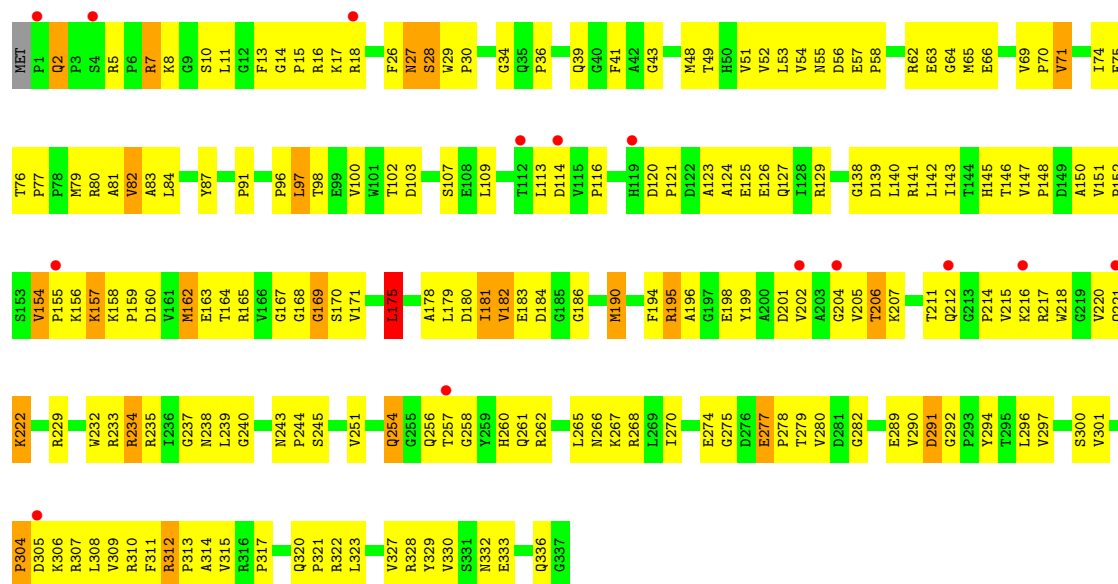


• Molecule 2: 50S ribosomal protein L2P

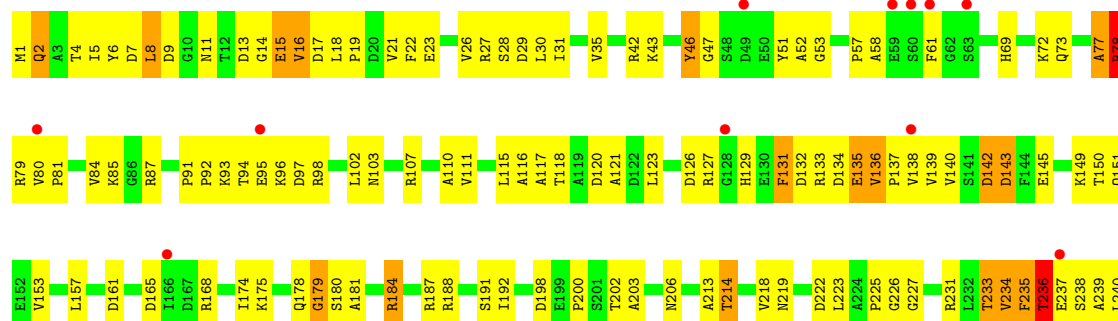
Chain A: 8% 48% 42% 10%

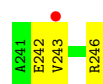


• Molecule 3: 50S ribosomal protein L3P

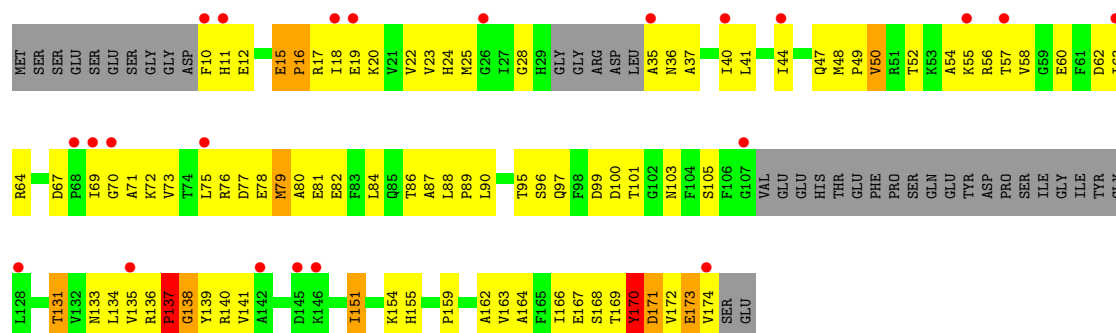


• Molecule 4: 50S ribosomal protein L4P

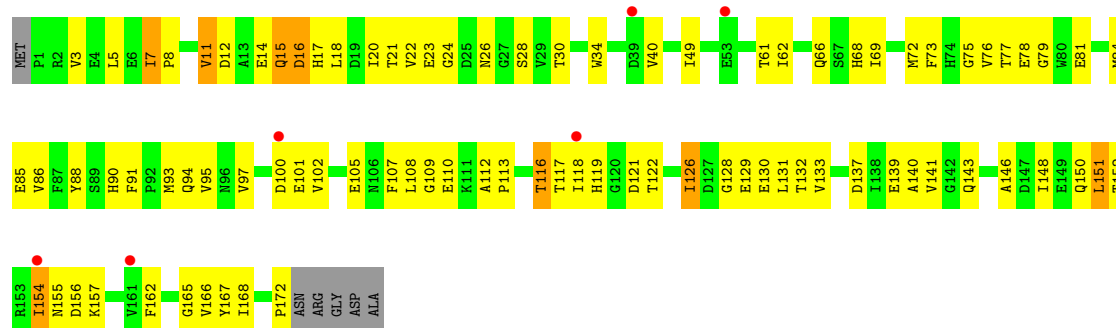




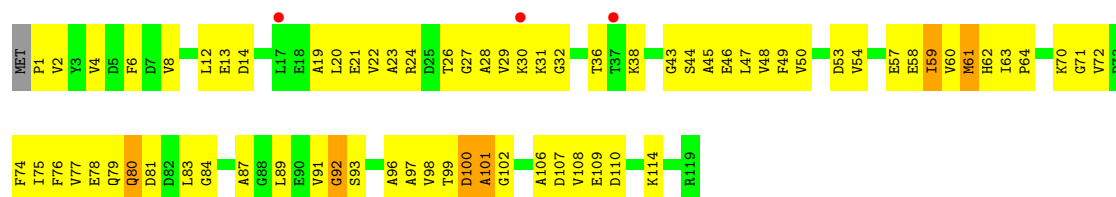
• Molecule 5: 50S ribosomal protein L5P



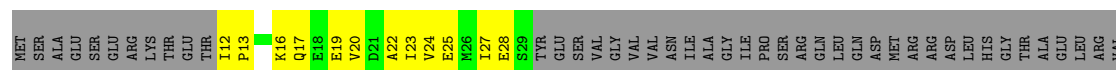
• Molecule 6: 50S ribosomal protein L6P



• Molecule 7: 50S ribosomal protein L7Ae

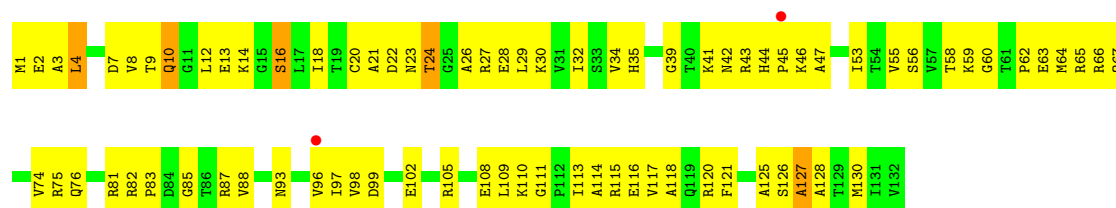


• Molecule 8: 50S ribosomal protein L10E

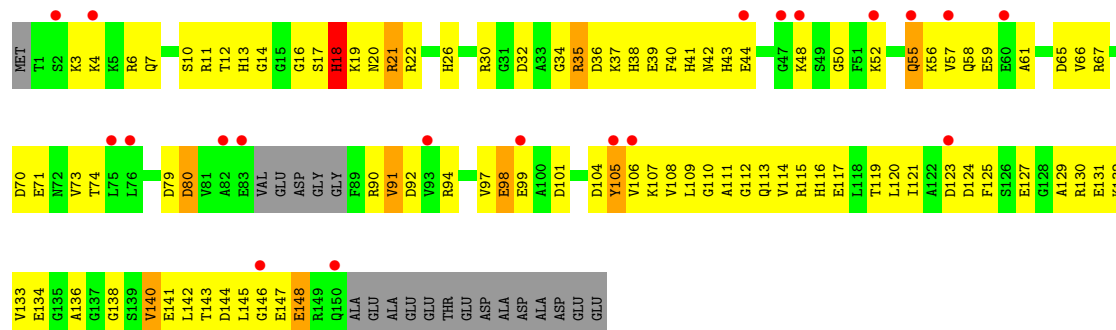




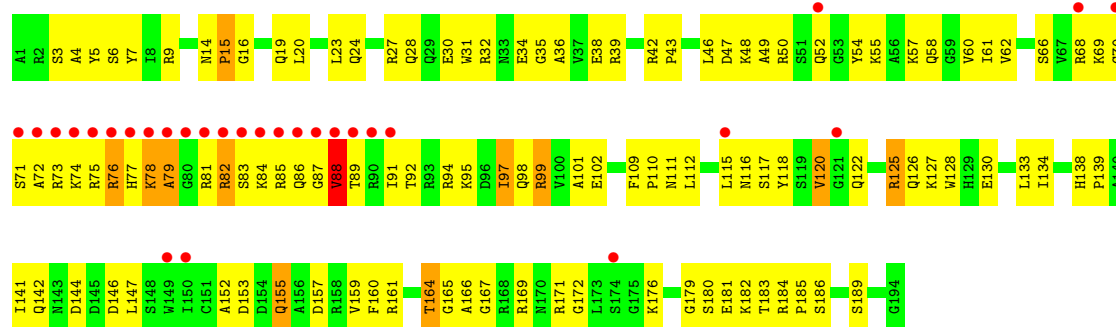
• Molecule 12: 50S ribosomal protein L14P



• Molecule 13: 50S ribosomal protein L15P



• Molecule 14: 50S ribosomal protein L15e

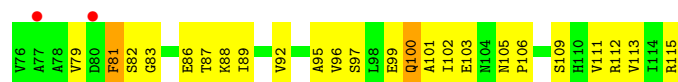
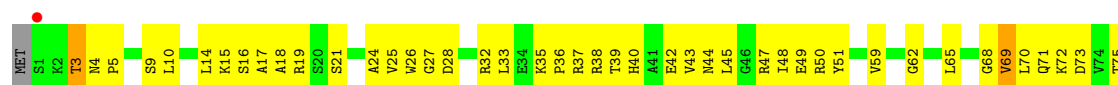


• Molecule 15: 50S ribosomal protein L18P

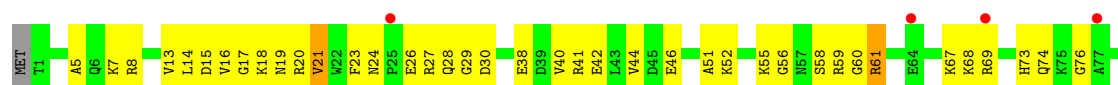
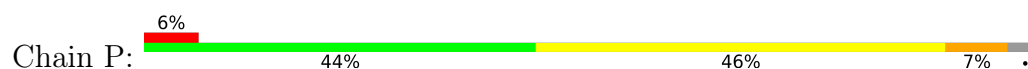




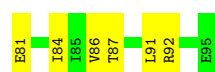
• Molecule 16: 50S ribosomal protein L18e



• Molecule 17: 50S ribosomal protein L19e



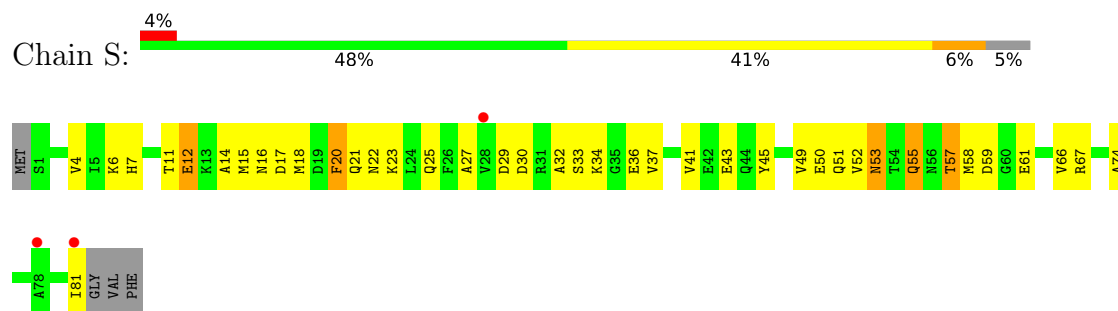
• Molecule 18: 50S ribosomal protein L21e



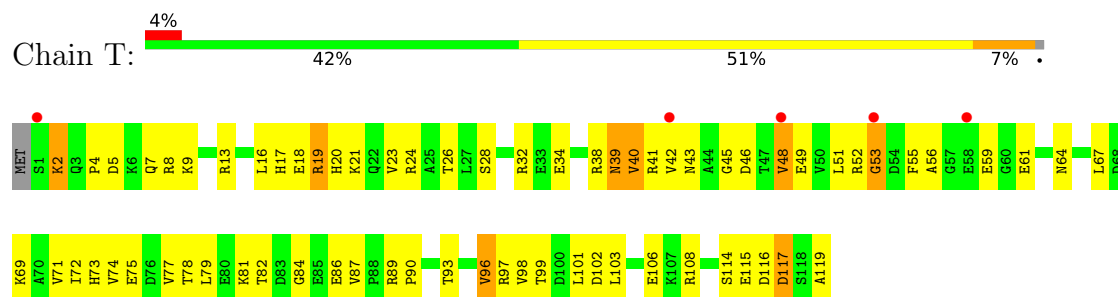
• Molecule 19: 50S ribosomal protein L22P



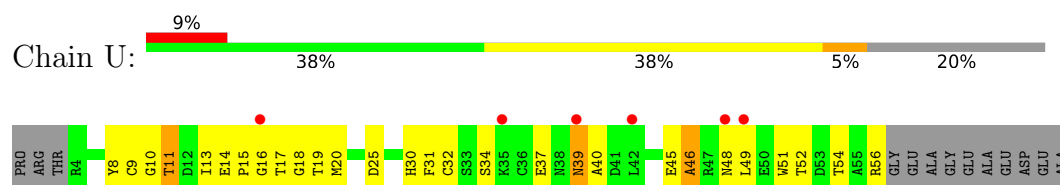
• Molecule 20: 50S ribosomal protein L23P



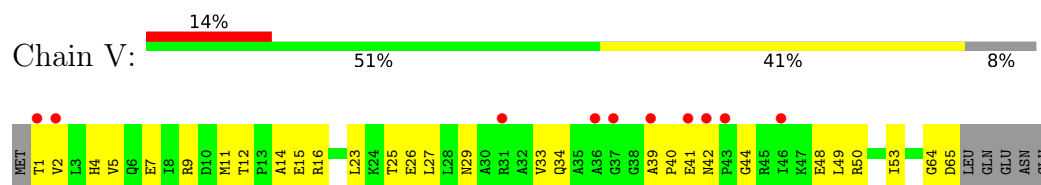
• Molecule 21: 50S ribosomal protein L24P



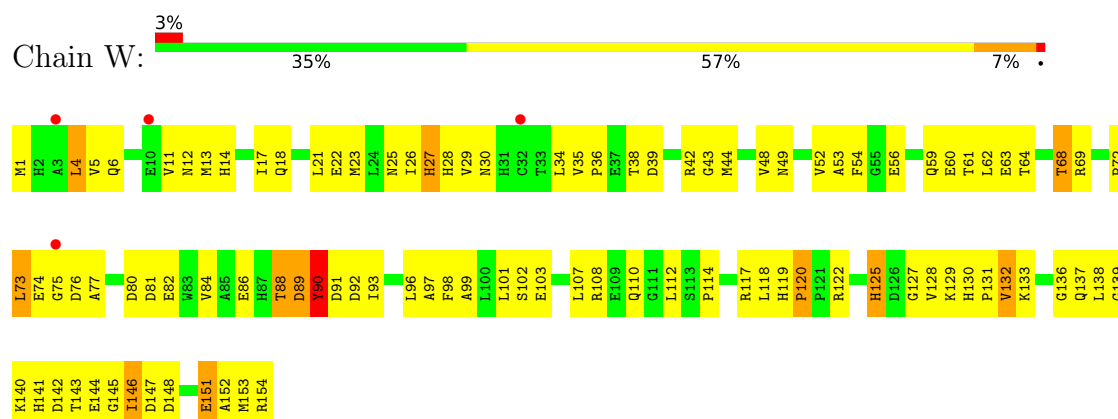
• Molecule 22: 50S ribosomal protein L24e



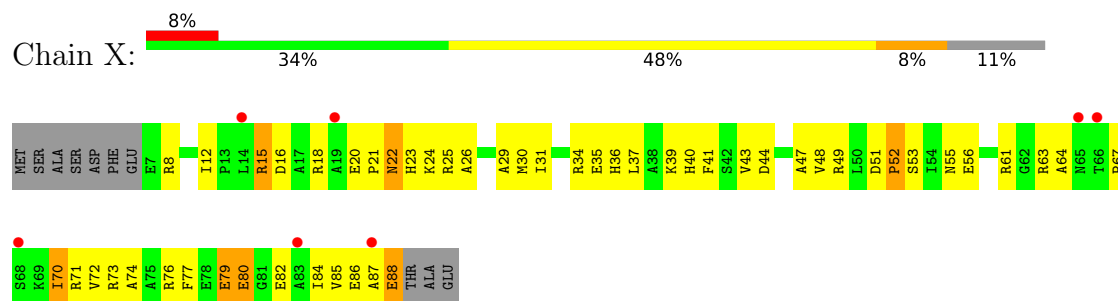
• Molecule 23: 50S ribosomal protein L29P



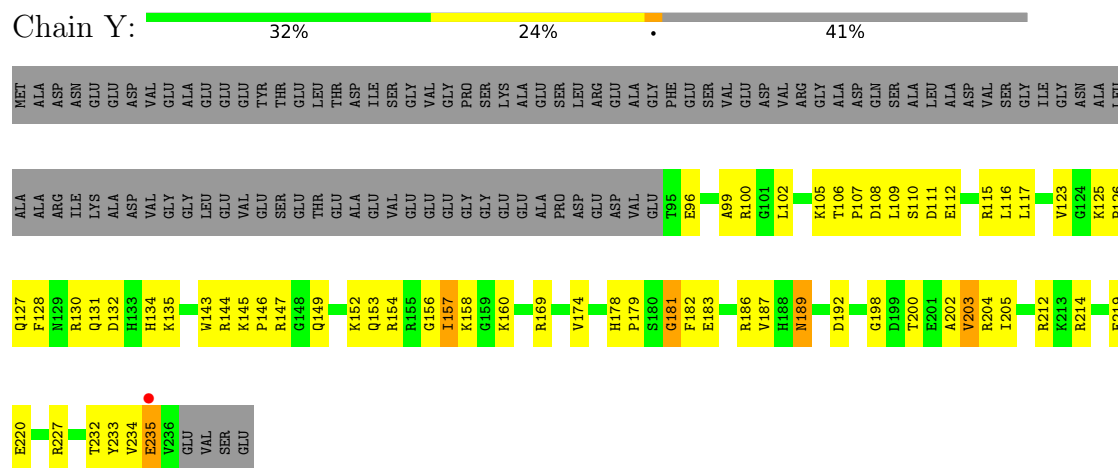
• Molecule 24: 50S ribosomal protein L30P



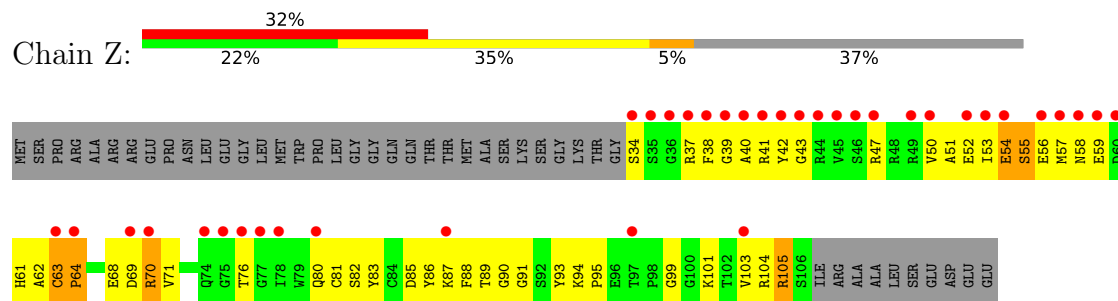
- Molecule 25: 50S ribosomal protein L31e



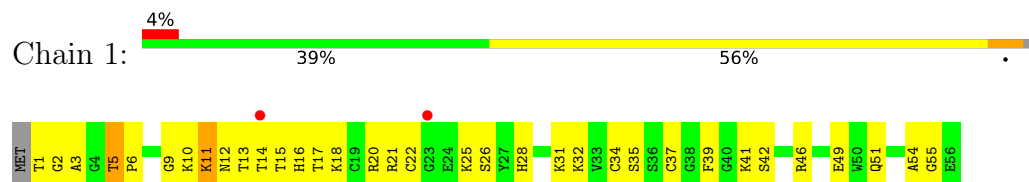
- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae

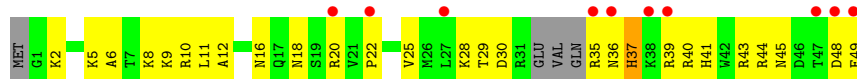


- Molecule 28: 50S ribosomal protein L37e

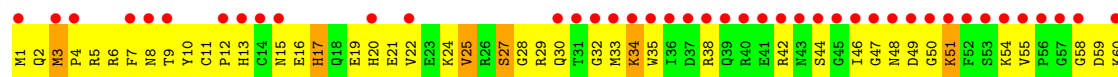


- Molecule 29: 50S ribosomal protein L39e

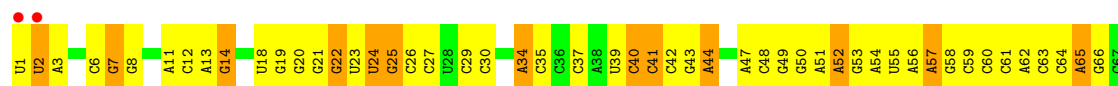




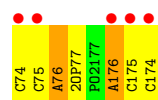
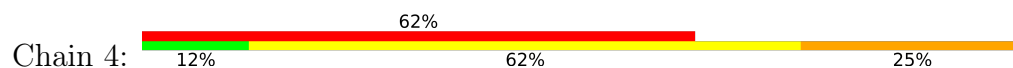
- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



- Molecule 32: DNA/RNA (5'-R(*CP*CP*(5AA)P*(2OP)P*(PO2)P*AP*CP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.32Å 299.65Å 574.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.98 – 3.11 49.98 – 3.11	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.98-3.11) 93.9 (49.98-3.11)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.260 0.232 , 0.266	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	99287	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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: UR3, NA, OMU, MG, PSU, K, 5AA, SR, CD, PO2, OMG, CL, 1MA, 2OP, MYL

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	0/65958	0.60	13/102869 (0.0%)
2	A	0.44	0/1786	1.03	10/2408 (0.4%)
3	B	0.46	0/2690	1.03	14/3652 (0.4%)
4	C	0.49	0/1885	0.97	5/2552 (0.2%)
5	D	0.36	0/1111	0.94	5/1498 (0.3%)
6	E	0.42	0/1382	0.90	2/1880 (0.1%)
7	F	0.38	0/901	0.97	4/1224 (0.3%)
8	G	0.39	0/241	0.75	0/324
9	H	0.39	0/1303	0.98	7/1743 (0.4%)
10	I	0.35	0/526	0.87	0/716
11	J	0.47	0/1136	0.96	6/1530 (0.4%)
12	K	0.45	0/1004	0.96	2/1351 (0.1%)
13	L	0.38	0/1130	0.94	5/1509 (0.3%)
14	M	0.46	0/1583	0.94	7/2116 (0.3%)
15	N	0.38	0/1474	1.09	14/1999 (0.7%)
16	O	0.43	0/874	0.94	2/1181 (0.2%)
17	P	0.46	0/1147	0.96	3/1528 (0.2%)
18	Q	0.45	0/749	1.00	7/1005 (0.7%)
19	R	0.52	0/1172	0.95	1/1578 (0.1%)
20	S	0.40	0/648	0.89	2/875 (0.2%)
21	T	0.41	0/958	0.98	4/1289 (0.3%)
22	U	0.35	0/417	0.93	2/562 (0.4%)
23	V	0.41	0/502	0.98	3/675 (0.4%)
24	W	0.50	0/1219	1.01	6/1655 (0.4%)
25	X	0.48	0/664	0.97	2/895 (0.2%)
26	Y	0.47	0/1146	1.02	5/1536 (0.3%)
27	Z	0.34	0/584	0.96	4/781 (0.5%)
28	1	0.45	0/438	0.86	3/578 (0.5%)
29	2	0.42	0/401	0.82	0/529
30	3	0.35	0/771	0.84	2/1024 (0.2%)
31	9	0.38	0/2904	0.58	0/4526
32	4	0.35	0/102	0.79	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	0/98806	0.72	140/147737 (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	0	12
24	W	0	1
31	9	0	1
32	4	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	N	163	PHE	N-CA-C	-12.07	98.03	113.12
15	N	14	ARG	N-CA-C	-9.10	101.05	110.97
15	N	51	GLY	CA-C-N	8.03	127.75	119.56
15	N	51	GLY	C-N-CA	8.03	127.75	119.56
22	U	18	GLY	N-CA-C	7.78	119.98	112.04

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1236	A	Sidechain
1	0	1430	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	24	G	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	1592	1
2	A	1753	0	1766	140	0
3	B	2625	0	2533	218	0
4	C	1860	0	1813	144	0
5	D	1094	0	1085	105	0
6	E	1357	0	1266	82	0
7	F	890	0	843	68	0
8	G	240	0	231	26	0
9	H	1283	0	1292	96	0
10	I	519	0	500	58	0
11	J	1120	0	1098	87	0
12	K	994	0	1027	89	0
13	L	1118	0	1076	100	0
14	M	1559	0	1573	160	0
15	N	1445	0	1401	129	0
16	O	865	0	873	67	0
17	P	1136	0	1123	89	0
18	Q	735	0	729	43	0
19	R	1149	0	1122	79	0
20	S	641	0	605	40	0
21	T	950	0	924	76	0
22	U	410	0	368	31	0
23	V	499	0	511	33	0
24	W	1196	0	1137	108	0
25	X	654	0	653	52	0
26	Y	1130	0	1133	63	0
27	Z	573	0	535	62	0
28	1	431	0	426	42	0
29	2	396	0	413	36	0
30	3	755	0	732	122	0
31	9	2599	0	1325	92	0
32	4	127	0	76	37	0
33	0	83	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	2	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	63	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	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	1	0	0	0	0
37	0	93	0	0	0	0
37	1	1	0	0	0	0
37	3	2	0	0	0	0
37	9	3	0	0	0	0
37	A	2	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	0	35	0	41	22	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5841	0	0	203	0
40	1	58	0	0	4	0
40	2	45	0	0	2	0
40	3	70	0	0	6	0
40	4	13	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	9	144	0	0	7	0
40	A	117	0	0	8	0
40	B	151	0	0	16	0
40	C	175	0	0	21	0
40	D	49	0	0	6	0
40	E	40	0	0	8	0
40	F	29	0	0	5	0
40	G	18	0	0	1	0
40	H	76	0	0	11	0
40	I	10	0	0	3	0
40	J	57	0	0	2	0
40	K	62	0	0	6	0
40	L	91	0	0	12	0
40	M	148	0	0	13	0
40	N	61	0	0	8	0
40	O	41	0	0	2	0
40	P	61	0	0	3	0
40	Q	49	0	0	3	0
40	R	83	0	0	3	0
40	S	37	0	0	1	0
40	T	36	0	0	4	0
40	U	29	0	0	2	0
40	V	13	0	0	3	0
40	W	67	0	0	6	0
40	X	24	0	0	1	0
40	Y	98	0	0	5	0
40	Z	30	0	0	6	0
All	All	99287	0	60042	3740	1

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 25.

The worst 5 of 3740 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)
40:O:4863:HOH:O	32:O:77:2OP:HB3	1.31	1.30
1:O:656:G:H5'	16:O:3:THR:HG22	1.20	1.15
1:O:871:G:C8	1:O:871:G:H5'	1.84	1.12
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.28	1.11
1:O:1160:G:H5'	1:O:1161:A:H5'	1.28	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	1.73	0.47

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	
2	A	235/240 (98%)	193 (82%)	32 (14%)	10 (4%)	2	11
3	B	335/338 (99%)	285 (85%)	38 (11%)	12 (4%)	2	14
4	C	244/246 (99%)	204 (84%)	35 (14%)	5 (2%)	6	24
5	D	134/177 (76%)	91 (68%)	33 (25%)	10 (8%)	1	4
6	E	170/178 (96%)	149 (88%)	20 (12%)	1 (1%)	21	50
7	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	1	7
8	G	25/348 (7%)	18 (72%)	6 (24%)	1 (4%)	2	12
9	H	156/174 (90%)	134 (86%)	15 (10%)	7 (4%)	2	11
10	I	68/162 (42%)	43 (63%)	20 (29%)	5 (7%)	1	4
11	J	140/145 (97%)	120 (86%)	15 (11%)	5 (4%)	2	14
12	K	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	8	30
13	L	141/165 (86%)	105 (74%)	31 (22%)	5 (4%)	3	15
14	M	192/194 (99%)	153 (80%)	29 (15%)	10 (5%)	1	9
15	N	184/187 (98%)	147 (80%)	27 (15%)	10 (5%)	1	8
16	O	113/116 (97%)	89 (79%)	23 (20%)	1 (1%)	14	42
17	P	141/149 (95%)	118 (84%)	20 (14%)	3 (2%)	5	23
18	Q	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	1	8
19	R	148/155 (96%)	130 (88%)	16 (11%)	2 (1%)	9	31
20	S	79/85 (93%)	66 (84%)	12 (15%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	117/120 (98%)	99 (85%)	15 (13%)	3 (3%)	4	19
22	U	51/66 (77%)	43 (84%)	6 (12%)	2 (4%)	2	13
23	V	63/71 (89%)	52 (82%)	11 (18%)	0	100	100
24	W	152/154 (99%)	121 (80%)	27 (18%)	4 (3%)	4	19
25	X	80/92 (87%)	65 (81%)	13 (16%)	2 (2%)	4	20
26	Y	140/241 (58%)	126 (90%)	13 (9%)	1 (1%)	18	47
27	Z	71/116 (61%)	58 (82%)	10 (14%)	3 (4%)	2	12
28	1	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
29	2	42/50 (84%)	34 (81%)	7 (17%)	1 (2%)	4	21
30	3	90/92 (98%)	64 (71%)	23 (26%)	3 (3%)	3	16
All	All	3705/4466 (83%)	3039 (82%)	545 (15%)	121 (3%)	3	16

5 of 121 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	36	ASP
2	A	37	VAL
3	B	184	ASP
3	B	206	THR
4	C	8	LEU

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	
2	A	179/182 (98%)	169 (94%)	10 (6%)	19	47
3	B	282/283 (100%)	263 (93%)	19 (7%)	15	41
4	C	193/193 (100%)	174 (90%)	19 (10%)	7	28
5	D	117/148 (79%)	112 (96%)	5 (4%)	26	55
6	E	152/156 (97%)	143 (94%)	9 (6%)	18	45
7	F	93/94 (99%)	92 (99%)	1 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/143 (94%)	128 (96%)	6 (4%)	24	54
10	I	58/130 (45%)	56 (97%)	2 (3%)	32	60
11	J	118/121 (98%)	113 (96%)	5 (4%)	26	56
12	K	106/106 (100%)	100 (94%)	6 (6%)	18	47
13	L	113/127 (89%)	107 (95%)	6 (5%)	20	49
14	M	158/158 (100%)	153 (97%)	5 (3%)	34	61
15	N	149/150 (99%)	143 (96%)	6 (4%)	28	57
16	O	93/94 (99%)	90 (97%)	3 (3%)	34	61
17	P	113/117 (97%)	106 (94%)	7 (6%)	16	44
18	Q	79/80 (99%)	79 (100%)	0	100	100
19	R	117/122 (96%)	112 (96%)	5 (4%)	26	55
20	S	71/74 (96%)	67 (94%)	4 (6%)	19	47
21	T	105/106 (99%)	99 (94%)	6 (6%)	18	47
22	U	44/52 (85%)	43 (98%)	1 (2%)	44	68
23	V	51/57 (90%)	51 (100%)	0	100	100
24	W	130/130 (100%)	121 (93%)	9 (7%)	14	40
25	X	66/74 (89%)	60 (91%)	6 (9%)	9	30
26	Y	120/196 (61%)	117 (98%)	3 (2%)	42	66
27	Z	60/94 (64%)	59 (98%)	1 (2%)	53	72
28	1	46/47 (98%)	45 (98%)	1 (2%)	45	68
29	2	42/46 (91%)	42 (100%)	0	100	100
30	3	79/79 (100%)	76 (96%)	3 (4%)	29	58
All	All	3095/3641 (85%)	2947 (95%)	148 (5%)	23	52

5 of 148 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S	30	ASP
27	Z	70	ARG
21	T	19	ARG
24	W	120	PRO
5	D	24	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	58	GLN
29	2	18	ASN
18	Q	16	ASN
29	2	16	ASN
30	3	78	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	253 (9%)	18 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/8 (12%)	0	0
All	All	2867/3053 (93%)	271 (9%)	19 (0%)

5 of 271 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2541	U
1	0	2791	U
31	9	65	A
1	0	2726	U
1	0	871	G

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

6 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	35,1	19,22,23	0.26	0	25,31,34	0.38	0
32	5AA	4	76	32,1	23,26,27	0.44	0	29,38,41	0.82	2 (6%)
1	UR3	0	2619	1	19,22,23	0.42	0	26,32,35	0.71	1 (3%)
1	PSU	0	2621	1	18,21,22	1.67	2 (11%)	21,30,33	1.43	3 (14%)
1	1MA	0	628	1	21,25,26	0.75	1 (4%)	30,37,40	0.88	2 (6%)
1	OMG	0	2588	32,1	23,26,27	0.33	0	32,38,41	0.40	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
1	OMU	0	2587	35,1	-	0/9/27/28	0/2/2/2
32	5AA	4	76	32,1	-	0/11/29/30	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	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
1	OMG	0	2588	32,1	-	0/9/27/28	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	5.55	1.43	1.36
1	0	2621	PSU	C6-C5	3.30	1.38	1.35
1	0	628	1MA	C6-N6	2.62	1.34	1.28

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.72	120.68	118.17
1	0	2621	PSU	C6-N1-C2	-3.13	119.79	122.69
32	4	76	5AA	C2-N1-C6	2.95	119.04	111.83
1	0	2621	PSU	O2-C2-N1	2.87	125.74	122.79
1	0	628	1MA	N1-C2-N3	2.86	129.39	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.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
32	4	76	5AA	10	0
1	0	2621	PSU	1	0
1	0	2588	OMG	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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	$\# Z > 2$
38	MYL	0	2924	-	34,37,37	1.16	4 (11%)	42,56,56	1.77	12 (28%)

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
38	MYL	0	2924	-	-	7/23/77/77	1/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	MYL	CBC-NAP	4.32	1.49	1.43
38	0	2924	MYL	CAA-CAV	3.18	1.39	1.32
38	0	2924	MYL	OAR-CAM	2.16	1.44	1.41
38	0	2924	MYL	OAS-CAM	2.15	1.44	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	OAT-CAY-CAC	4.11	110.94	105.94
38	0	2924	MYL	CAN-CAV-CAZ	3.85	116.96	112.09
38	0	2924	MYL	OAQ-CBH-OAT	-3.52	107.76	111.16
38	0	2924	MYL	OAT-CAY-CAZ	3.13	114.42	110.16
38	0	2924	MYL	CBC-NAP-CAW	3.00	126.58	122.51

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	OAG-CAW-NAP-CBC
38	0	2924	MYL	CBB-CAW-NAP-CBC
38	0	2924	MYL	OAR-CBC-NAP-CAW
38	0	2924	MYL	CBG-CBC-NAP-CAW
38	0	2924	MYL	CAN-CBH-OAQ-CAB

All (1) ring outliers are listed below:

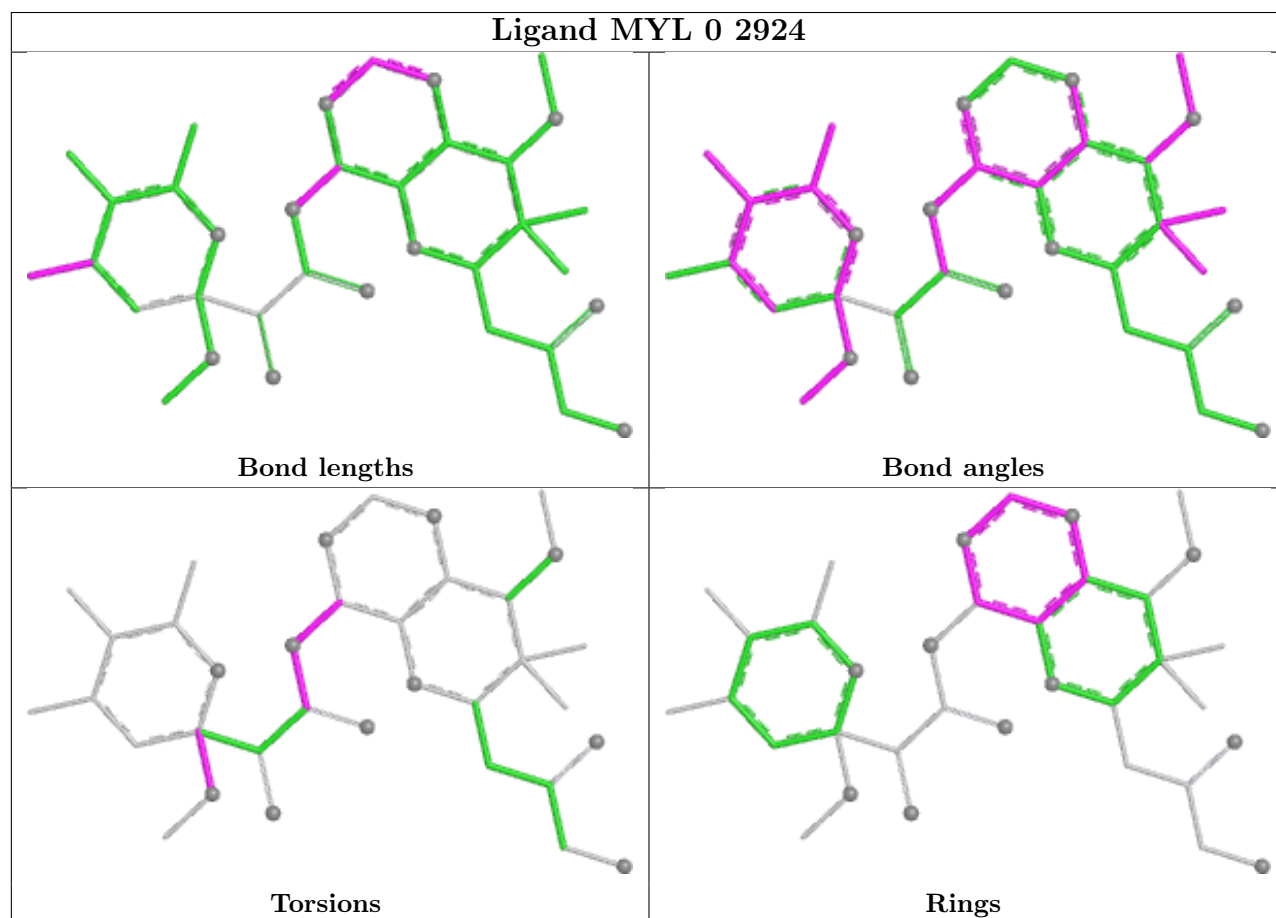
Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	CAM-CBC-CBF-CBG-OAR-OAS

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	MYL	22	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	2749/2923 (94%)	0.52	41 (1%) 72 52	31, 61, 109, 181	0
2	A	237/240 (98%)	1.01	18 (7%) 20 10	37, 75, 110, 131	0
3	B	337/338 (99%)	0.65	14 (4%) 40 22	37, 65, 93, 103	0
4	C	246/246 (100%)	0.71	12 (4%) 35 18	34, 60, 84, 96	0
5	D	140/177 (79%)	1.25	22 (15%) 5 2	80, 118, 140, 148	0
6	E	172/178 (96%)	0.47	6 (3%) 47 27	54, 81, 102, 112	0
7	F	119/120 (99%)	0.79	3 (2%) 58 37	65, 93, 121, 135	0
8	G	29/348 (8%)	0.57	0 100 100	86, 102, 109, 114	0
9	H	160/174 (91%)	0.60	3 (1%) 66 45	58, 79, 111, 121	0
10	I	70/162 (43%)	1.31	13 (18%) 3 2	137, 154, 180, 181	0
11	J	142/145 (97%)	0.44	2 (1%) 73 53	48, 63, 82, 98	0
12	K	132/132 (100%)	0.65	2 (1%) 72 52	46, 63, 88, 95	0
13	L	145/165 (87%)	1.02	20 (13%) 6 3	38, 86, 124, 133	0
14	M	194/194 (100%)	1.25	29 (14%) 5 3	38, 60, 136, 151	0
15	N	186/187 (99%)	1.10	20 (10%) 11 6	65, 89, 138, 146	0
16	O	115/116 (99%)	0.67	3 (2%) 57 36	51, 70, 84, 91	0
17	P	143/149 (95%)	1.00	9 (6%) 26 14	52, 69, 87, 93	0
18	Q	95/96 (98%)	0.82	3 (3%) 50 30	51, 62, 77, 85	0
19	R	150/155 (96%)	0.48	2 (1%) 75 56	42, 56, 77, 89	0
20	S	81/85 (95%)	0.83	3 (3%) 45 25	57, 76, 99, 111	0
21	T	119/120 (99%)	0.79	5 (4%) 40 22	55, 73, 106, 125	0
22	U	53/66 (80%)	1.21	6 (11%) 10 5	95, 117, 133, 135	0
23	V	65/71 (91%)	0.93	10 (15%) 5 2	65, 90, 140, 144	0
24	W	154/154 (100%)	0.50	4 (2%) 57 36	46, 62, 79, 95	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/92 (89%)	0.91	7 (8%) 16 9	52, 70, 88, 105	0
26	Y	142/241 (58%)	0.58	1 (0%) 84 68	39, 58, 80, 99	0
27	Z	73/116 (62%)	2.39	37 (50%) 0 0	107, 143, 170, 176	0
28	1	56/57 (98%)	0.78	2 (3%) 46 26	34, 47, 58, 62	0
29	2	46/50 (92%)	1.42	10 (21%) 2 1	47, 80, 113, 121	0
30	3	92/92 (100%)	2.93	57 (61%) 0 0	164, 175, 184, 189	0
31	9	122/122 (100%)	0.42	2 (1%) 70 49	52, 86, 113, 166	0
32	4	5/8 (62%)	3.28	5 (100%) 0 0	41, 43, 47, 47	0
All	All	6651/7519 (88%)	0.73	371 (5%) 30 16	31, 67, 132, 189	0

The worst 5 of 371 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
14	M	80	GLY	9.7
14	M	78	LYS	8.1
14	M	89	THR	8.0
27	Z	36	GLY	8.0
27	Z	42	TYR	7.7

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
32	5AA	4	76	24/25	0.74	0.19	38,44,48,48	0
1	UR3	0	2619	21/22	0.90	0.14	41,44,49,50	0
1	PSU	0	2621	20/21	0.91	0.13	37,39,44,44	0
1	1MA	0	628	23/24	0.94	0.11	38,41,42,43	0
1	OMU	0	2587	21/22	0.94	0.11	43,46,50,50	0
1	OMG	0	2588	24/25	0.94	0.11	37,42,44,45	0

6.3 Carbohydrates ⓘ

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	0	8570	1/1	0.19	0.14	61,61,61,61	0
35	NA	0	8528	1/1	0.34	0.46	91,91,91,91	0
37	SR	0	9001	1/1	0.41	0.19	200,200,200,200	0
35	NA	0	8502	1/1	0.47	0.27	53,53,53,53	0
35	NA	0	8573	1/1	0.48	0.20	78,78,78,78	0
35	NA	0	8568	1/1	0.48	0.24	35,35,35,35	0
35	NA	0	8536	1/1	0.50	0.23	72,72,72,72	0
35	NA	0	8564	1/1	0.53	0.26	94,94,94,94	0
37	SR	0	8971	1/1	0.54	0.21	200,200,200,200	0
33	MG	0	8066	1/1	0.54	0.21	75,75,75,75	0
35	NA	0	8525	1/1	0.55	0.17	67,67,67,67	0
37	SR	0	8959	1/1	0.56	0.09	194,194,194,194	0
37	SR	0	8938	1/1	0.57	0.21	200,200,200,200	0
33	MG	3	8090	1/1	0.58	0.36	86,86,86,86	0
37	SR	0	8977	1/1	0.58	0.11	200,200,200,200	0
37	SR	0	8983	1/1	0.58	0.19	199,199,199,199	0
35	NA	H	8518	1/1	0.58	0.44	92,92,92,92	0
35	NA	0	8559	1/1	0.59	0.40	99,99,99,99	0
37	SR	0	8997	1/1	0.59	0.39	200,200,200,200	0
35	NA	0	8571	1/1	0.59	0.28	101,101,101,101	0
35	NA	0	8560	1/1	0.60	0.30	61,61,61,61	0
37	SR	0	8995	1/1	0.60	0.19	191,191,191,191	0
35	NA	0	8557	1/1	0.61	0.27	72,72,72,72	0
35	NA	0	8558	1/1	0.61	0.28	60,60,60,60	0
35	NA	0	8554	1/1	0.63	0.39	106,106,106,106	0
36	CL	3	8804	1/1	0.63	0.10	121,121,121,121	0
37	SR	9	8980	1/1	0.65	0.21	192,192,192,192	0
36	CL	0	8815	1/1	0.67	0.20	83,83,83,83	0
37	SR	0	8953	1/1	0.68	0.22	200,200,200,200	0
37	SR	0	9000	1/1	0.68	0.31	200,200,200,200	0
35	NA	0	8561	1/1	0.68	0.28	66,66,66,66	0
35	NA	0	8506	1/1	0.68	0.20	65,65,65,65	0
37	SR	9	9003	1/1	0.68	0.14	195,195,195,195	0
33	MG	0	8092	1/1	0.69	0.34	133,133,133,133	0
37	SR	3	8932	1/1	0.69	0.17	184,184,184,184	0
37	SR	3	8999	1/1	0.69	0.24	200,200,200,200	0
33	MG	0	8044	1/1	0.69	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8574	1/1	0.69	0.36	72,72,72,72	0
35	NA	0	8541	1/1	0.70	0.30	65,65,65,65	0
35	NA	0	8520	1/1	0.71	0.26	63,63,63,63	0
35	NA	0	8522	1/1	0.72	0.32	71,71,71,71	0
35	NA	0	8569	1/1	0.72	0.21	63,63,63,63	0
37	SR	0	8965	1/1	0.72	0.20	158,158,158,158	0
37	SR	0	8993	1/1	0.72	0.14	186,186,186,186	0
37	SR	0	8989	1/1	0.73	0.18	129,129,129,129	0
37	SR	A	8930	1/1	0.73	0.16	168,168,168,168	0
35	NA	M	8539	1/1	0.73	0.18	51,51,51,51	0
37	SR	0	8941	1/1	0.73	0.20	152,152,152,152	0
35	NA	0	8508	1/1	0.73	0.29	68,68,68,68	0
35	NA	0	8544	1/1	0.73	0.26	75,75,75,75	0
39	CD	3	8704	1/1	0.73	0.25	200,200,200,200	0
33	MG	B	8042	1/1	0.74	0.22	121,121,121,121	0
35	NA	0	8530	1/1	0.74	0.31	68,68,68,68	0
37	SR	0	9002	1/1	0.75	0.15	169,169,169,169	0
37	SR	0	8964	1/1	0.75	0.15	160,160,160,160	0
37	SR	0	8949	1/1	0.75	0.23	157,157,157,157	0
35	NA	0	8563	1/1	0.75	0.43	85,85,85,85	0
37	SR	0	8955	1/1	0.75	0.27	200,200,200,200	0
37	SR	0	8947	1/1	0.75	0.19	200,200,200,200	0
37	SR	0	8988	1/1	0.75	0.10	183,183,183,183	0
37	SR	0	8937	1/1	0.76	0.16	116,116,116,116	0
35	NA	0	8535	1/1	0.76	0.33	72,72,72,72	0
39	CD	Z	8703	1/1	0.76	0.18	200,200,200,200	0
33	MG	0	8091	1/1	0.76	0.22	111,111,111,111	0
34	K	0	8401	1/1	0.77	0.41	132,132,132,132	0
37	SR	0	9006	1/1	0.77	0.23	190,190,190,190	0
35	NA	0	8548	1/1	0.77	0.29	67,67,67,67	0
37	SR	B	8987	1/1	0.77	0.37	200,200,200,200	0
37	SR	0	8991	1/1	0.77	0.17	197,197,197,197	0
33	MG	0	8048	1/1	0.77	0.14	41,41,41,41	0
35	NA	0	8556	1/1	0.77	0.23	49,49,49,49	0
35	NA	R	8533	1/1	0.77	0.28	62,62,62,62	0
33	MG	0	8071	1/1	0.77	0.36	67,67,67,67	0
36	CL	J	8802	1/1	0.77	0.16	84,84,84,84	0
33	MG	0	8043	1/1	0.78	0.15	48,48,48,48	0
33	MG	0	8064	1/1	0.78	0.17	53,53,53,53	0
33	MG	0	8029	1/1	0.78	0.20	79,79,79,79	0
36	CL	0	8813	1/1	0.78	0.16	77,77,77,77	0
37	SR	0	8982	1/1	0.78	0.25	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	K	0	8402	1/1	0.78	0.29	88,88,88,88	0
33	MG	Y	8086	1/1	0.79	0.12	53,53,53,53	0
35	NA	0	8551	1/1	0.79	0.28	86,86,86,86	0
33	MG	0	8069	1/1	0.79	0.38	63,63,63,63	0
37	SR	0	8960	1/1	0.79	0.12	175,175,175,175	0
33	MG	0	8073	1/1	0.79	0.23	70,70,70,70	0
35	NA	9	8543	1/1	0.79	0.30	68,68,68,68	0
35	NA	0	8562	1/1	0.79	0.14	49,49,49,49	0
37	SR	0	8974	1/1	0.79	0.21	163,163,163,163	0
37	SR	0	8976	1/1	0.79	0.23	200,200,200,200	0
33	MG	0	8076	1/1	0.79	0.16	52,52,52,52	0
37	SR	0	8975	1/1	0.80	0.16	158,158,158,158	0
37	SR	0	8986	1/1	0.80	0.17	200,200,200,200	0
35	NA	J	8538	1/1	0.80	0.15	56,56,56,56	0
33	MG	A	8051	1/1	0.80	0.11	81,81,81,81	0
35	NA	0	8524	1/1	0.80	0.18	67,67,67,67	0
35	NA	Q	8540	1/1	0.81	0.18	84,84,84,84	0
35	NA	R	8532	1/1	0.81	0.11	52,52,52,52	0
37	SR	0	8939	1/1	0.81	0.20	166,166,166,166	0
33	MG	0	8017	1/1	0.81	0.12	26,26,26,26	0
35	NA	0	8521	1/1	0.81	0.13	59,59,59,59	0
38	MYL	0	2924	35/35	0.81	0.19	80,83,86,87	0
39	CD	U	8701	1/1	0.81	0.25	200,200,200,200	0
37	SR	0	8992	1/1	0.81	0.28	164,164,164,164	0
37	SR	0	8916	1/1	0.81	0.14	126,126,126,126	0
33	MG	0	8080	1/1	0.82	0.23	126,126,126,126	0
37	SR	L	8969	1/1	0.82	0.27	200,200,200,200	0
36	CL	O	8808	1/1	0.82	0.23	109,109,109,109	0
37	SR	0	8917	1/1	0.82	0.18	157,157,157,157	0
37	SR	0	8924	1/1	0.82	0.17	140,140,140,140	0
33	MG	9	8040	1/1	0.83	0.30	89,89,89,89	0
35	NA	0	8534	1/1	0.83	0.15	53,53,53,53	0
35	NA	0	8567	1/1	0.83	0.23	57,57,57,57	0
37	SR	0	8942	1/1	0.83	0.16	139,139,139,139	0
35	NA	0	8526	1/1	0.83	0.08	40,40,40,40	0
37	SR	0	8931	1/1	0.83	0.17	147,147,147,147	0
37	SR	0	8973	1/1	0.83	0.14	162,162,162,162	0
37	SR	0	8951	1/1	0.83	0.07	144,144,144,144	0
33	MG	0	8081	1/1	0.83	0.20	80,80,80,80	0
35	NA	0	8512	1/1	0.84	0.20	54,54,54,54	0
33	MG	0	8055	1/1	0.84	0.35	87,87,87,87	0
35	NA	B	8552	1/1	0.84	0.40	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8038	1/1	0.84	0.11	92,92,92,92	0
35	NA	0	8550	1/1	0.84	0.21	76,76,76,76	0
37	SR	0	8923	1/1	0.84	0.15	108,108,108,108	0
33	MG	0	8036	1/1	0.84	0.20	59,59,59,59	0
37	SR	0	8927	1/1	0.84	0.17	176,176,176,176	0
36	CL	0	8822	1/1	0.84	0.38	123,123,123,123	0
37	SR	0	8944	1/1	0.85	0.19	169,169,169,169	0
37	SR	0	8945	1/1	0.85	0.15	131,131,131,131	0
36	CL	0	8816	1/1	0.85	0.29	89,89,89,89	0
35	NA	0	8566	1/1	0.85	0.24	64,64,64,64	0
37	SR	0	9004	1/1	0.85	0.19	172,172,172,172	0
35	NA	0	8555	1/1	0.85	0.23	61,61,61,61	0
37	SR	0	9007	1/1	0.85	0.37	200,200,200,200	0
37	SR	0	8928	1/1	0.85	0.13	148,148,148,148	0
36	CL	N	8807	1/1	0.85	0.25	98,98,98,98	0
37	SR	0	8984	1/1	0.85	0.11	118,118,118,118	0
33	MG	0	8072	1/1	0.85	0.25	60,60,60,60	0
35	NA	0	8511	1/1	0.85	0.13	54,54,54,54	0
37	SR	9	8978	1/1	0.85	0.13	154,154,154,154	0
37	SR	0	8963	1/1	0.85	0.14	146,146,146,146	0
37	SR	0	8908	1/1	0.85	0.17	116,116,116,116	0
33	MG	0	8047	1/1	0.85	0.29	68,68,68,68	0
37	SR	0	8967	1/1	0.85	0.12	164,164,164,164	0
37	SR	0	8994	1/1	0.85	0.33	200,200,200,200	0
33	MG	2	8060	1/1	0.85	0.11	62,62,62,62	0
35	NA	0	8565	1/1	0.86	0.43	80,80,80,80	0
35	NA	0	8501	1/1	0.86	0.16	41,41,41,41	0
37	SR	0	8956	1/1	0.86	0.12	154,154,154,154	0
37	SR	0	8943	1/1	0.86	0.17	105,105,105,105	0
33	MG	0	8030	1/1	0.86	0.28	88,88,88,88	0
37	SR	0	8934	1/1	0.86	0.17	168,168,168,168	0
35	NA	0	8519	1/1	0.86	0.21	69,69,69,69	0
33	MG	0	8082	1/1	0.86	0.16	61,61,61,61	0
33	MG	0	8037	1/1	0.86	0.22	67,67,67,67	0
35	NA	0	8529	1/1	0.87	0.16	45,45,45,45	0
35	NA	0	8547	1/1	0.87	0.57	82,82,82,82	0
37	SR	F	9005	1/1	0.87	0.09	153,153,153,153	0
33	MG	0	8093	1/1	0.87	0.10	29,29,29,29	0
33	MG	9	8074	1/1	0.87	0.20	87,87,87,87	0
37	SR	0	8981	1/1	0.87	0.20	198,198,198,198	0
35	NA	S	8510	1/1	0.87	0.12	56,56,56,56	0
37	SR	0	8946	1/1	0.87	0.11	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8079	1/1	0.87	0.22	76,76,76,76	0
37	SR	0	8985	1/1	0.87	0.16	150,150,150,150	0
35	NA	9	8572	1/1	0.87	0.14	78,78,78,78	0
35	NA	0	8507	1/1	0.87	0.10	27,27,27,27	0
33	MG	0	8065	1/1	0.87	0.11	33,33,33,33	0
35	NA	0	8509	1/1	0.88	0.30	90,90,90,90	0
37	SR	0	8919	1/1	0.88	0.10	81,81,81,81	0
37	SR	0	8922	1/1	0.88	0.20	182,182,182,182	0
36	CL	A	8809	1/1	0.88	0.34	128,128,128,128	0
33	MG	0	8083	1/1	0.88	0.11	50,50,50,50	0
33	MG	0	8075	1/1	0.88	0.13	64,64,64,64	0
35	NA	0	8513	1/1	0.88	0.21	62,62,62,62	0
36	CL	R	8806	1/1	0.88	0.12	56,56,56,56	0
37	SR	0	8968	1/1	0.88	0.13	180,180,180,180	0
35	NA	0	8523	1/1	0.88	0.16	52,52,52,52	0
35	NA	0	8514	1/1	0.88	0.27	38,38,38,38	0
35	NA	0	8549	1/1	0.88	0.37	124,124,124,124	0
35	NA	0	8517	1/1	0.89	0.24	62,62,62,62	0
37	SR	0	8901	1/1	0.89	0.12	78,78,78,78	0
33	MG	0	8005	1/1	0.89	0.18	46,46,46,46	0
37	SR	0	8933	1/1	0.89	0.11	122,122,122,122	0
37	SR	0	8913	1/1	0.89	0.27	181,181,181,181	0
33	MG	0	8089	1/1	0.89	0.11	42,42,42,42	0
35	NA	0	8546	1/1	0.89	0.19	65,65,65,65	0
33	MG	0	8035	1/1	0.89	0.14	52,52,52,52	0
37	SR	0	8920	1/1	0.89	0.12	130,130,130,130	0
37	SR	0	8979	1/1	0.89	0.14	111,111,111,111	0
37	SR	0	8998	1/1	0.89	0.22	196,196,196,196	0
33	MG	0	8056	1/1	0.89	0.09	44,44,44,44	0
37	SR	0	8962	1/1	0.89	0.23	200,200,200,200	0
33	MG	0	8067	1/1	0.89	0.10	33,33,33,33	0
33	MG	0	8068	1/1	0.89	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.90	0.13	64,64,64,64	0
37	SR	B	8950	1/1	0.90	0.10	125,125,125,125	0
35	NA	0	8527	1/1	0.90	0.30	75,75,75,75	0
33	MG	0	8039	1/1	0.90	0.17	55,55,55,55	0
35	NA	0	8545	1/1	0.90	0.17	25,25,25,25	0
37	SR	R	8912	1/1	0.90	0.09	93,93,93,93	0
37	SR	0	8996	1/1	0.90	0.21	200,200,200,200	0
33	MG	0	8031	1/1	0.90	0.12	77,77,77,77	0
35	NA	0	8516	1/1	0.90	0.17	39,39,39,39	0
37	SR	0	8935	1/1	0.90	0.08	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	J	8821	1/1	0.90	0.14	90,90,90,90	0
33	MG	0	8033	1/1	0.90	0.21	79,79,79,79	0
33	MG	0	8077	1/1	0.90	0.19	60,60,60,60	0
36	CL	0	8803	1/1	0.90	0.15	68,68,68,68	0
37	SR	0	8957	1/1	0.90	0.28	200,200,200,200	0
33	MG	0	8063	1/1	0.91	0.14	62,62,62,62	0
36	CL	Y	8820	1/1	0.91	0.15	58,58,58,58	0
33	MG	0	8085	1/1	0.91	0.21	73,73,73,73	0
33	MG	0	8078	1/1	0.91	0.27	91,91,91,91	0
37	SR	0	8926	1/1	0.91	0.11	127,127,127,127	0
33	MG	0	8024	1/1	0.91	0.11	55,55,55,55	0
37	SR	0	8910	1/1	0.91	0.12	107,107,107,107	0
35	NA	0	8505	1/1	0.91	0.18	58,58,58,58	0
36	CL	M	8818	1/1	0.91	0.14	62,62,62,62	0
33	MG	T	8057	1/1	0.91	0.16	68,68,68,68	0
37	SR	0	8918	1/1	0.91	0.09	92,92,92,92	0
37	SR	0	8970	1/1	0.91	0.10	148,148,148,148	0
35	NA	0	8537	1/1	0.91	0.10	40,40,40,40	0
37	SR	0	8954	1/1	0.91	0.08	108,108,108,108	0
33	MG	0	8052	1/1	0.92	0.10	60,60,60,60	0
37	SR	A	8929	1/1	0.92	0.13	124,124,124,124	0
36	CL	0	8817	1/1	0.92	0.09	80,80,80,80	0
35	NA	R	8575	1/1	0.92	0.26	92,92,92,92	0
37	SR	0	8903	1/1	0.92	0.10	62,62,62,62	0
35	NA	C	8503	1/1	0.92	0.08	32,32,32,32	0
37	SR	H	8972	1/1	0.92	0.11	139,139,139,139	0
36	CL	J	8801	1/1	0.92	0.23	88,88,88,88	0
33	MG	0	8013	1/1	0.92	0.08	24,24,24,24	0
37	SR	0	8914	1/1	0.92	0.10	109,109,109,109	0
35	NA	0	8531	1/1	0.92	0.17	45,45,45,45	0
37	SR	0	8936	1/1	0.92	0.13	125,125,125,125	0
36	CL	L	8810	1/1	0.92	0.13	76,76,76,76	0
33	MG	0	8046	1/1	0.92	0.12	46,46,46,46	0
36	CL	0	8805	1/1	0.92	0.15	101,101,101,101	0
39	CD	O	8705	1/1	0.92	0.09	117,117,117,117	0
33	MG	0	8010	1/1	0.92	0.08	25,25,25,25	0
37	SR	0	8921	1/1	0.92	0.08	98,98,98,98	0
33	MG	0	8020	1/1	0.92	0.19	56,56,56,56	0
35	NA	0	8553	1/1	0.93	0.27	98,98,98,98	0
33	MG	0	8088	1/1	0.93	0.09	37,37,37,37	0
35	NA	0	8515	1/1	0.93	0.09	39,39,39,39	0
33	MG	0	8032	1/1	0.93	0.10	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8003	1/1	0.93	0.10	32,32,32,32	0
33	MG	0	8026	1/1	0.93	0.10	39,39,39,39	0
36	CL	B	8819	1/1	0.93	0.16	80,80,80,80	0
37	SR	S	8961	1/1	0.93	0.10	150,150,150,150	0
33	MG	0	8028	1/1	0.93	0.09	13,13,13,13	0
37	SR	0	8911	1/1	0.94	0.07	99,99,99,99	0
36	CL	0	8814	1/1	0.94	0.15	55,55,55,55	0
37	SR	1	8952	1/1	0.94	0.07	81,81,81,81	0
33	MG	0	8070	1/1	0.94	0.11	58,58,58,58	0
33	MG	0	8059	1/1	0.94	0.11	56,56,56,56	0
37	SR	0	8925	1/1	0.94	0.07	99,99,99,99	0
37	SR	0	8948	1/1	0.94	0.09	113,113,113,113	0
33	MG	0	8053	1/1	0.94	0.09	61,61,61,61	0
33	MG	0	8049	1/1	0.94	0.19	82,82,82,82	0
37	SR	0	8966	1/1	0.94	0.10	117,117,117,117	0
37	SR	0	8940	1/1	0.94	0.09	110,110,110,110	0
36	CL	0	8811	1/1	0.94	0.12	87,87,87,87	0
33	MG	0	8009	1/1	0.94	0.07	22,22,22,22	0
33	MG	0	8002	1/1	0.95	0.07	40,40,40,40	0
33	MG	0	8061	1/1	0.95	0.17	48,48,48,48	0
33	MG	0	8022	1/1	0.95	0.07	56,56,56,56	0
33	MG	0	8014	1/1	0.95	0.11	24,24,24,24	0
33	MG	0	8016	1/1	0.95	0.06	34,34,34,34	0
33	MG	0	8034	1/1	0.95	0.10	57,57,57,57	0
37	SR	0	8906	1/1	0.95	0.07	64,64,64,64	0
33	MG	0	8008	1/1	0.95	0.10	23,23,23,23	0
33	MG	0	8018	1/1	0.95	0.06	32,32,32,32	0
35	NA	0	8542	1/1	0.96	0.14	51,51,51,51	0
37	SR	0	8909	1/1	0.96	0.10	105,105,105,105	0
33	MG	0	8041	1/1	0.96	0.08	29,29,29,29	0
33	MG	K	8054	1/1	0.96	0.09	29,29,29,29	0
33	MG	0	8012	1/1	0.96	0.07	23,23,23,23	0
33	MG	0	8025	1/1	0.96	0.07	30,30,30,30	0
37	SR	0	8915	1/1	0.96	0.11	131,131,131,131	0
36	CL	0	8812	1/1	0.96	0.10	66,66,66,66	0
37	SR	0	8990	1/1	0.96	0.14	108,108,108,108	0
37	SR	0	9008	1/1	0.96	0.07	107,107,107,107	0
37	SR	0	8958	1/1	0.96	0.10	120,120,120,120	0
33	MG	0	8087	1/1	0.96	0.08	29,29,29,29	0
33	MG	A	8050	1/1	0.96	0.16	68,68,68,68	0
37	SR	0	8905	1/1	0.96	0.16	78,78,78,78	0
33	MG	0	8007	1/1	0.96	0.06	27,27,27,27	0

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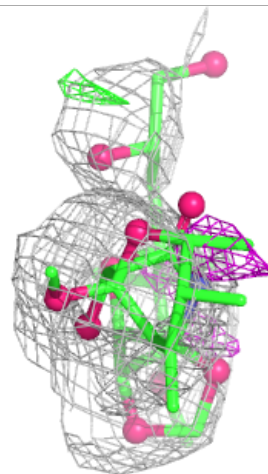
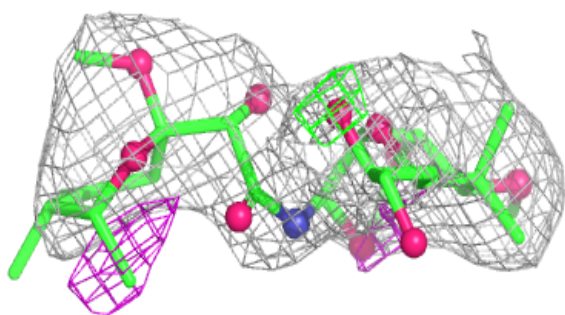
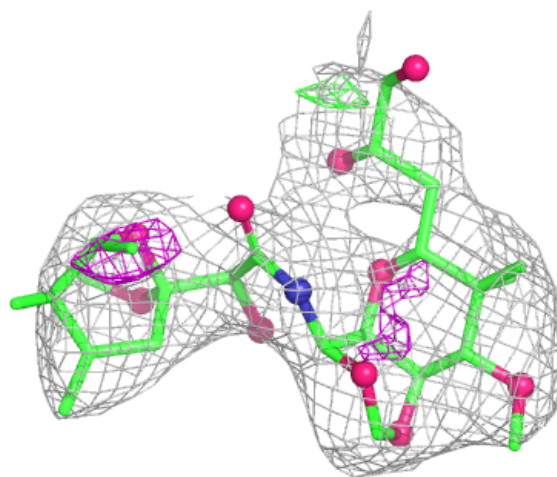
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8904	1/1	0.97	0.12	65,65,65,65	0
33	MG	0	8011	1/1	0.97	0.07	14,14,14,14	0
33	MG	0	8001	1/1	0.97	0.05	24,24,24,24	0
37	SR	0	8907	1/1	0.97	0.05	59,59,59,59	0
35	NA	0	8504	1/1	0.97	0.06	32,32,32,32	0
33	MG	0	8006	1/1	0.97	0.07	44,44,44,44	0
33	MG	0	8019	1/1	0.97	0.05	11,11,11,11	0
33	MG	0	8004	1/1	0.97	0.07	25,25,25,25	0
33	MG	0	8015	1/1	0.97	0.08	26,26,26,26	0
33	MG	0	8058	1/1	0.97	0.09	22,22,22,22	0
39	CD	1	8702	1/1	0.97	0.05	78,78,78,78	0
33	MG	0	8023	1/1	0.97	0.11	41,41,41,41	0
33	MG	0	8021	1/1	0.98	0.11	53,53,53,53	0
37	SR	0	8902	1/1	0.98	0.07	44,44,44,44	0
33	MG	0	8062	1/1	0.98	0.09	53,53,53,53	0
33	MG	0	8027	1/1	0.99	0.04	47,47,47,47	0
33	MG	0	8084	1/1	0.99	0.08	31,31,31,31	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 MYL 0 2924:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.