



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 08:14 am BST

PDB ID : 3I55
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

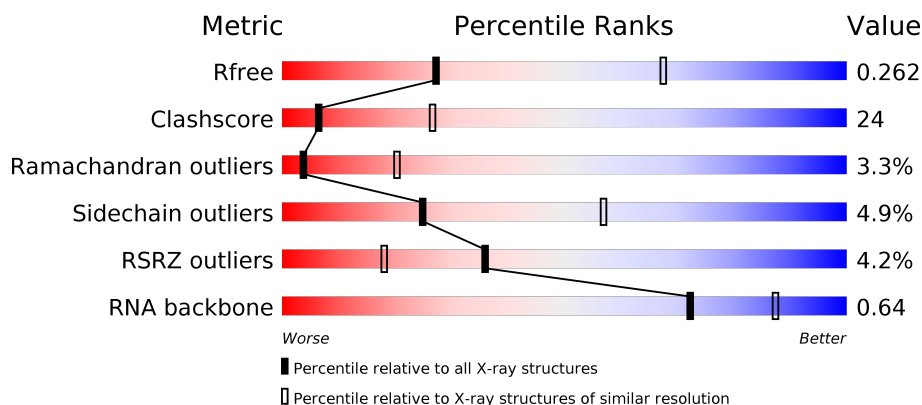
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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.



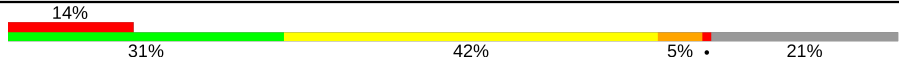



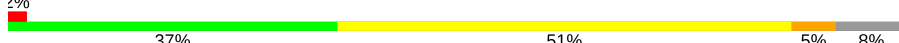


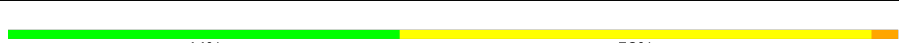
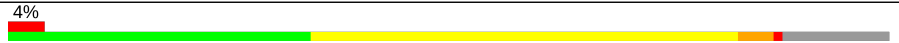
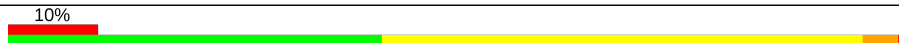
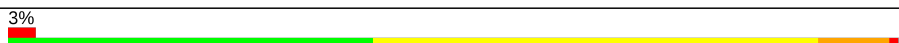


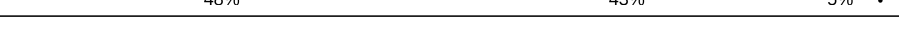
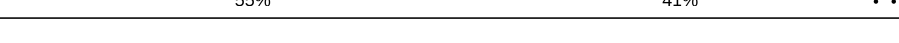

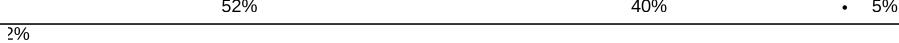



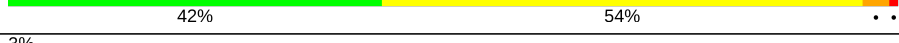

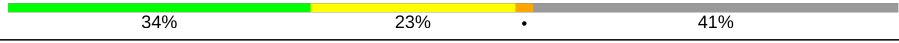

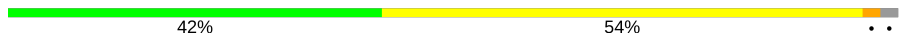
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	
2	A	240	
3	B	338	
4	C	246	

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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	-
33	MG	0	8055	-	-	-	X
33	MG	0	8069	-	-	-	X
33	MG	0	8081	-	-	-	X
33	MG	0	8092	-	-	-	X
33	MG	3	8090	-	-	-	X
34	K	0	8402	-	-	-	X
35	NA	0	8506	-	-	-	X
35	NA	0	8508	-	-	-	X
35	NA	0	8509	-	-	-	X
35	NA	0	8513	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8544	-	-	-	X
35	NA	0	8551	-	-	-	X
35	NA	0	8554	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8558	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	H	8518	-	-	-	X
36	CL	3	8804	-	-	-	X
37	SR	0	8922	-	-	-	X
37	SR	0	8949	-	-	-	X
37	SR	0	8953	-	-	-	X
37	SR	0	8962	-	-	-	X
37	SR	0	8986	-	-	-	X
37	SR	0	8997	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
37	SR	0	9000	-	-	-	X
37	SR	3	8999	-	-	-	X
37	SR	B	8987	-	-	-	X
37	SR	L	8969	-	-	-	X
38	MYL	0	2924	-	-	X	-
39	CD	3	8704	-	-	-	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			
			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			
			573	343	113	112	5	0	0	0

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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	83	Total	Mg	0	0
			83	83		
33	9	2	Total	Mg	0	0
			2	2		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		
33	3	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	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
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

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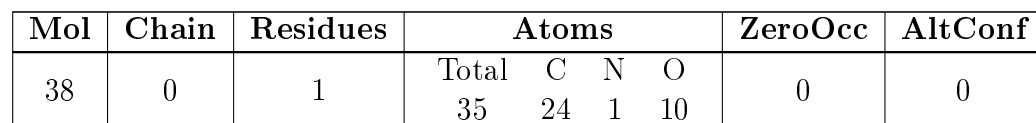
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Cl	0	0
			1	1		

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

- Molecule 38 is Mycalamide A (three-letter code: MYL) (formula: C₂₄H₄₁NO₁₀).



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

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



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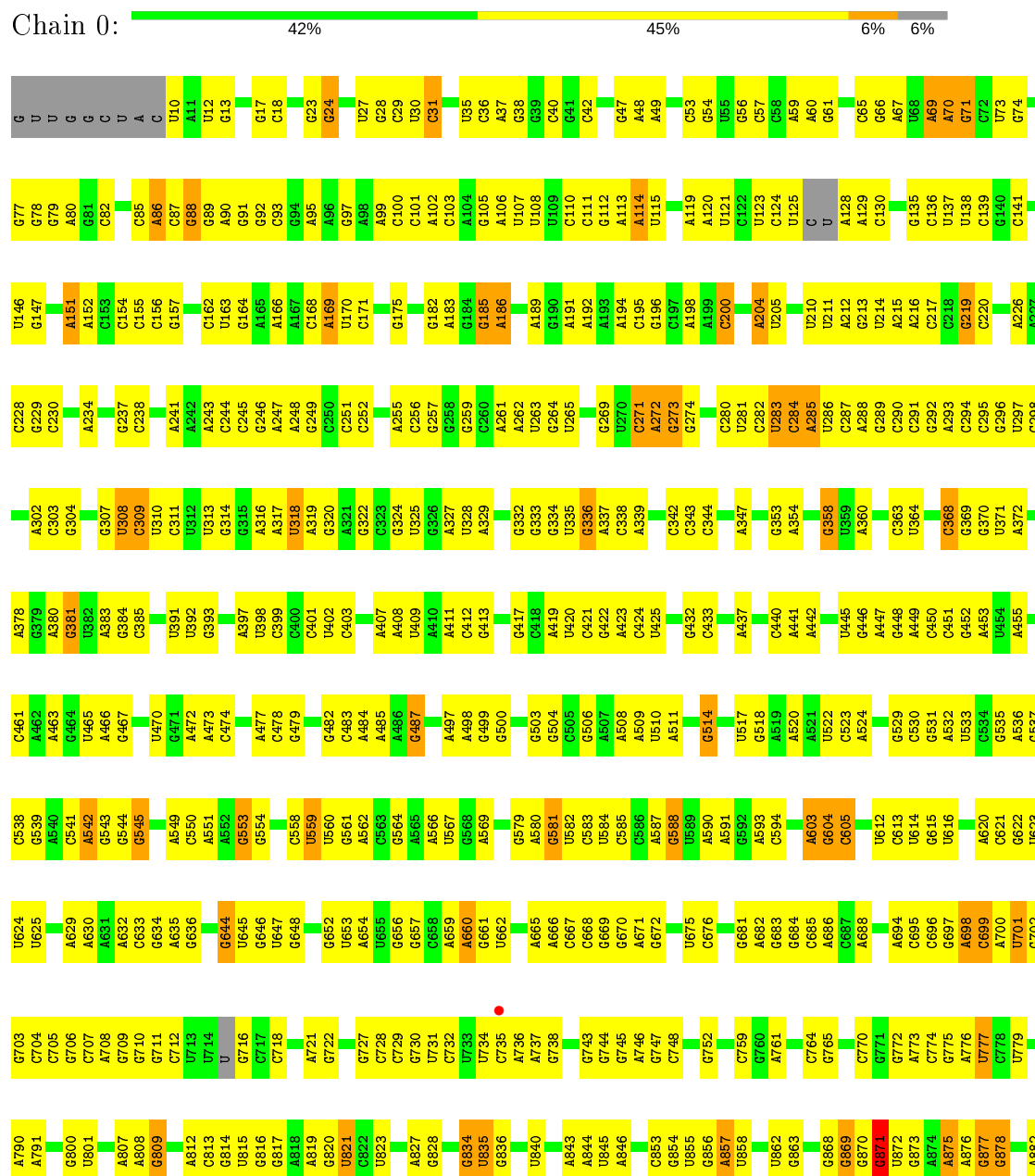
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	24	Total 24	O 24	0	0
40	Y	98	Total 98	O 98	0	0
40	Z	30	Total 30	O 30	0	0
40	1	58	Total 58	O 58	0	0
40	2	45	Total 45	O 45	0	0
40	3	70	Total 70	O 70	0	0
40	9	144	Total 144	O 144	0	0
40	4	13	Total 13	O 13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

3 Residue-property plots

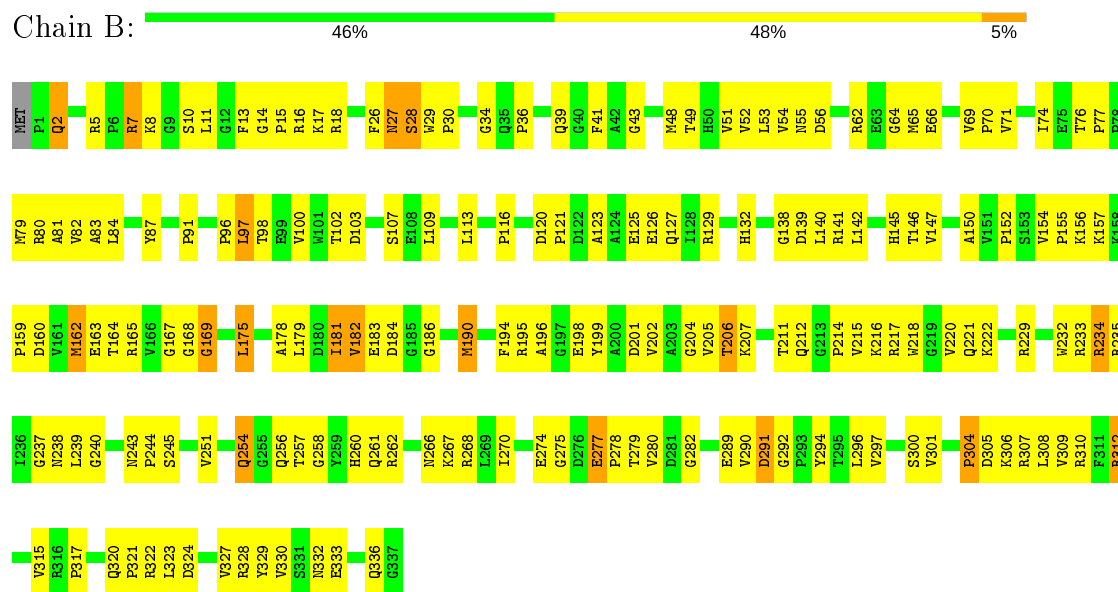
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 23S ribosomal RNA

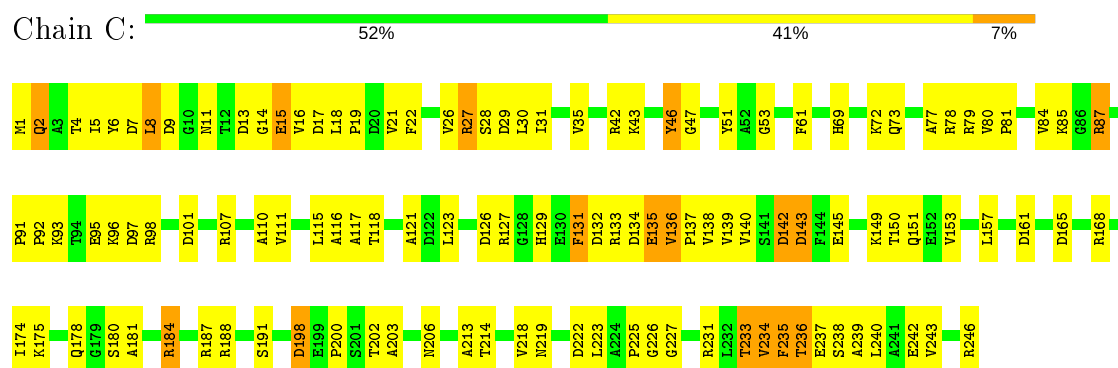


C2006	A1931	G1846	G1774	G1895	C1617	G1535	A1442	C1360	A1280	A1202	G1135	C1044	G885
A2007	C1935	A1847	A1775	A1701	A1624	C1536	U1446	G1363	A1286	G1203	U1136	G1045	C890
G2008	C1936	U1850	G1777	U1702	U1625	C1537	U1447	G1364	A1287	C1204	U1137	G1046	G891
A2010	U1937	G1851	A1778	G1706	A1626	G1541	G1451	C1365	U1288	U1206	U1138	G1048	G892
A2011	G1938	A1852	A1779	G1706	G1627	G1542	G1451	C1366	G1290	A1207	U1139		
U2012	U1939	C1853			G1628	G1543			G1290	C1208	C1140		
G2013	C1940	C1854	A1783	A1710	G1629	U1544	C1456	G1370	A1291	C1209	U1149	C1051	C896
U2016	A1941	G1855	U1784	A1711	A1630	C1545	U1457	U1371	A1294	G1210	U1150	G1052	A897
A1942	A1942	C1856	G1785	A1712	A1631	G1546	A1458	A1372	A1295	G1211	G1151	G1054	G898
U2017	C1943	A1857	G1786	G1713	A1632	A1547			G1296	C1212	U1151	G1055	
		A1858	C1787	G1714	C1633	U1548	U1461	A1375	A1296	C1213	A1152	U1056	G901
				C1715	G1634	C1549	C1462	G1376	U1297	G1214	A1153	A1057	G902
C2026	G1948				U1635	A1550		C1377	U1288	A1215	A1154	A1058	
U2027	C1864	C1636	C1790	U1722	U1636	C1551	U1473	C1378	G1299	G1216	C1155	G1059	C905
U2028	A1865	G1723	U1791	U1722	A1637	G1552	C1474	A1379	G1300		C1156	C1060	
C2029		G1723	G1792	G1723	A1637	G1553	C1474	A1379	G1300		C1156	C1061	
U2032	A	G1868	C1793	U1724	C1640	C1554	C1477	U1380	C1303	U1219	C1157	G1066	A912
G2033	A	U1871	G1794	U1724	A1641	C1554	U1478	C1384	U1304	U1220	G1158	U1066	
U2034	C	C1872	G1795	G1726	A1642	G1555		G1385	C1305	G1221	G1159	U1067	G918
C2035	U	G1873	A1796		C1643	G1556		G1386	C1306	G1224	A1161	C1068	U919
C2036	A	C1874	A1797	G1730	C1644	C1557	A1482	G1387	U1307	C1225	G1162	C1069	C920
C2037	U	G1875	G1798	A1731	U1645	C1558	C1483	G1388	A1308	A1070	G1163	A1071	G921
A2038	G	G1877	G1799	A1732	U1645	U	G1484	U1388	A1308		U1164	G1071	A922
C2039	A	G1878	G1800	A1733		U1561	A1485	G1389	U1309	C1228	U1165	G1072	A923
A2040	A	U1879	A1801	G1734	C1652	U1561	A1486		U1310	C1229	G1166	A1073	G924
G2041	C		G1802	C1735	A1653			A1393	G1311	A1230	A1167	G1074	A925
U2042	U1964	C1882	C1803	C1735	U1654	C1564	A1492		G1312		C1168	A1081	A926
C2043	C1883	U1883	A1804	A1737	G1655	C1565	A1493	C1397	U1234	U1234	U1170	G1087	U932
U2044	C1965	G1884	G1805	A1738	A1656	C1566	G1495	G1398	G1235	G1235	U1169	A1088	C933
G2045	U1966	A1885	G1806	G1739	A1657	G1567	C1496	A1399	A1236	G1239	A1173	G1089	G938
	U1967		U1807	U1740			A1497	U1405	U1237	C1238	G1172	A1090	G941
A1968	C1888	C1888	C1808	U1741	C1682	G1571	G1497	U1406	G1319	C1239	A1173	A1091	U942
A1969	C1889	U1889	A1809	A1742	G1683	A1572	G1498	A1406	G1320	G1240	A1173	U1095	A943
G1970	U1890	G1891	C1810	G1743	G1665	C1574	U1500	U1408	G1325	G1241	G1175	U1096	A944
U1972			G1812		C1666	C1575		G1409	G1326	A1242	U1178	A1097	U945
A1973	A1746	C1894	U1813	A1747	A1667	G1586	A1504	G1410	G1329	C1243	C1179	A1098	G946
G1974	U1748	A1895	G1814	U1748	U1688	U1587	U1505	A1411	G1330	U1244	U1180	A1099	U947
	G1896	U1897	A1815	U1749	G1689	U1588	C1507	U1412	G1331	G1245	A1181	G1099	G948
A1978	U1897	U1898	C1816	C1750	A1670	G1588	C1507		C1332	A1247	C1182		
U2059	G1898	U1898	U1817	G1751	G1675	G1589	C1508	G1416	U1333	A1248	C1183		
U1980	C1899	C1899	C1818	G1752	C1674			G1417	C1334	U1249	C1184		
A1981			G1819	C1753	C1675	G1592	U1511	U1418	U1185	C1250	U1185	A1013	A951
C1982			G1820		G1676	C1593	G1512	U1419	C1186	G1260	C1187	A1014	G952
C1983				U1757	U1677	C1594	C1514	C1420	G1340	A1261	A1187	C1015	G953
	G1908	G1908	U1825	U1758	A1678	G1595	A1515	C1426	A1341	C1262	A1188	U1016	U954
C2066	C1988	A1909	C1826	A1759	C1679	U1596	C1516	A1427	C1342	C1263	G1190	A1020	A955
					C1680	A1597	U1516	C1428	C1343	U1264	G1191	G1021	G956
G2070			A1823	C1762	G1681	A1598	C1517	U1429	G1344		A1192		A957
C2071	C1830		C1830	C1763	A1682			G1430			A1193	C1025	G958
G2072				C1764	G1683	A1603	C1521		U1350	C1268	A1194		C959
A2074	U1833	G1765	A1684	G1765	A1685	G1604	A1522		G1351	G1269	A1194	U1028	G960
	U1835	U1766	A1685	G1605	C1686	G1605	U1524	U1435	A1352	G1119	G1195	U1029	A961
A2081		A1767	C1686	A1606	C1687	A1607	U1525	C1436	C1353	C1273	C1196	U1030	C962
		C1768	G1687	C1688	G1688		A1526	A1437	G1354		G1197	G1031	C963
		C1769	G1688			C1613	A1527	G1438	A1355	U1276	U1198		G964
C2087		U1770				G1614	A1528	C1439	A1358	C1277	A1199	G1038	A965
C2088		U1771				A1615	G1529	U1440	A1358	U1279	A1200	G1039	
A2089		C1772				A1616		G1441	U1359		C1201	A1132	G969
G2090		G1773											

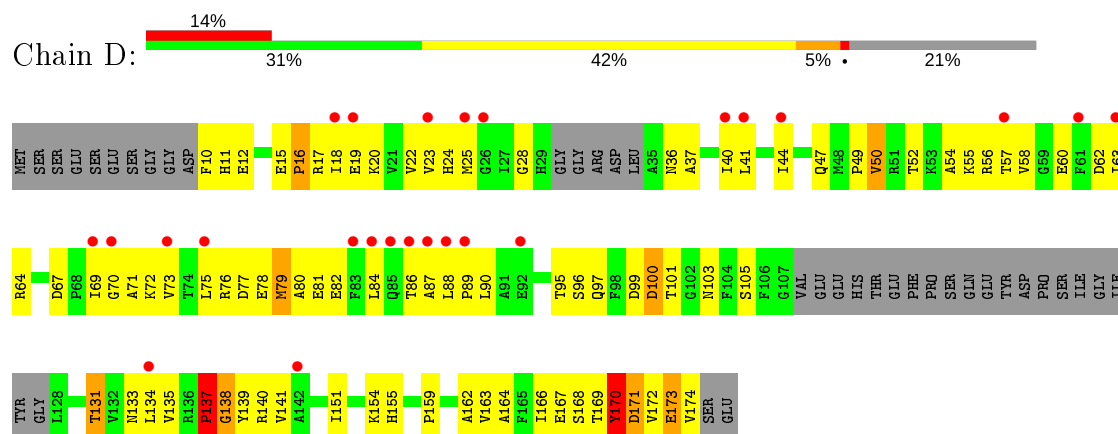
• Molecule 3: 50S ribosomal protein L3P



• Molecule 4: 50S ribosomal protein L4P

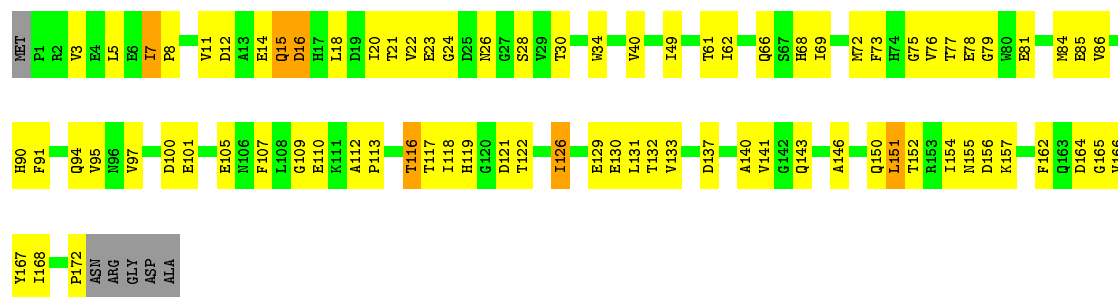


• Molecule 5: 50S ribosomal protein L5P



• Molecule 6: 50S ribosomal protein L6P





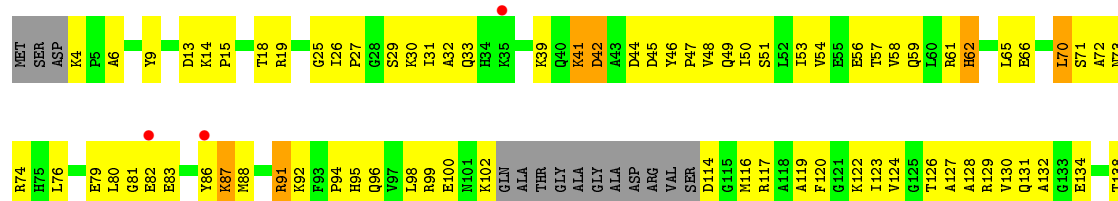
- Molecule 7: 50S ribosomal protein L7Ae

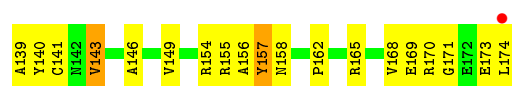


- Molecule 8: 50S ribosomal protein L10E

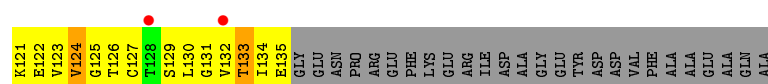
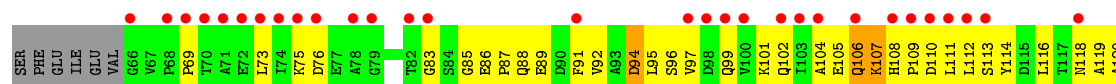
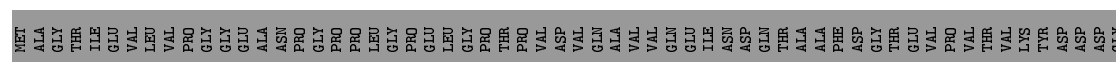


- Molecule 9: 50S ribosomal protein L10e





• Molecule 10: 50S ribosomal protein L11P



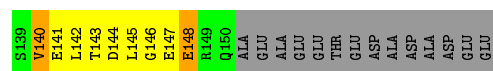
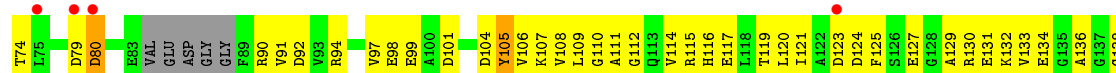
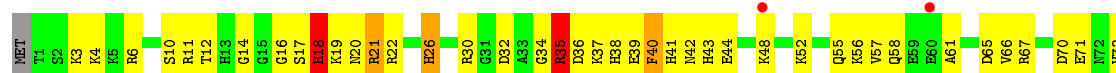
• Molecule 11: 50S ribosomal protein L13P



• Molecule 12: 50S ribosomal protein L14P



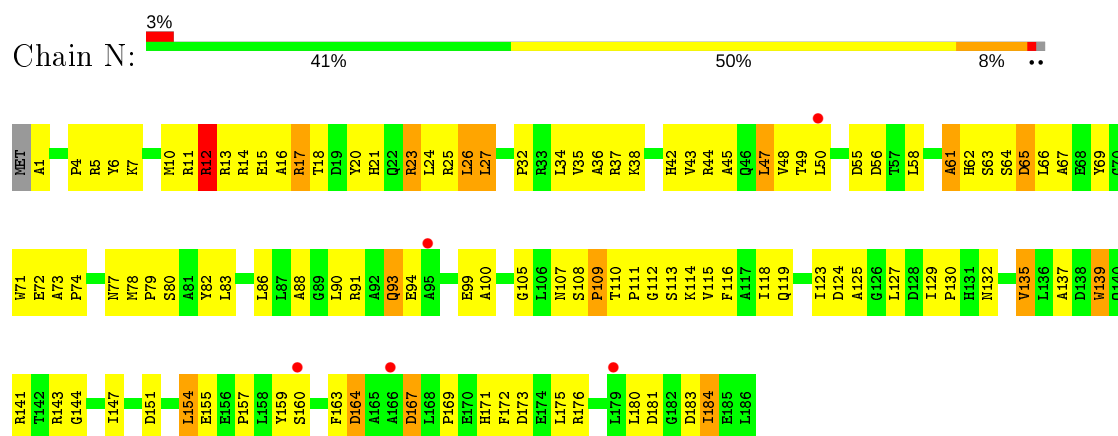
• Molecule 13: 50S ribosomal protein L15P



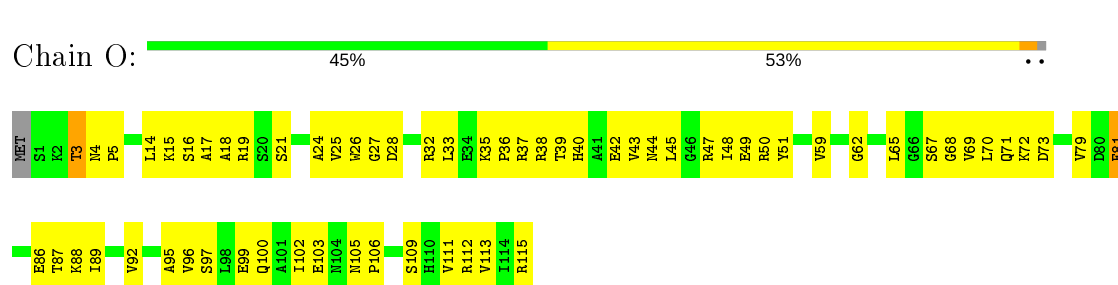
- Molecule 14: 50S ribosomal protein L15e

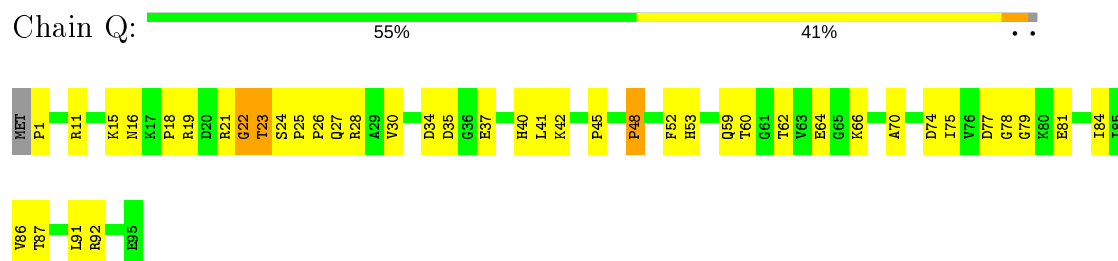


- Molecule 15: 50S ribosomal protein L18P

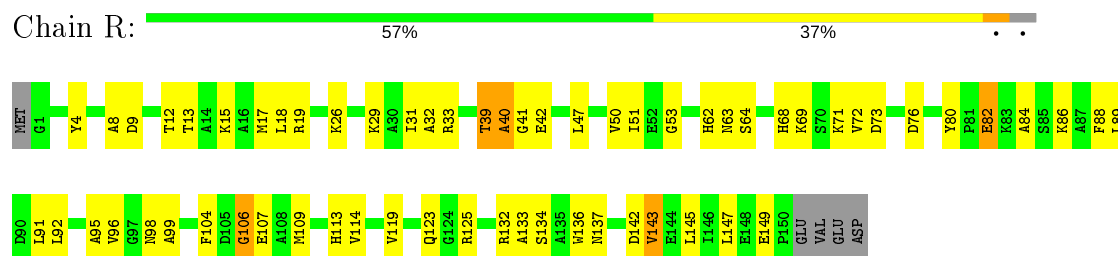


- Molecule 16: 50S ribosomal protein L18e

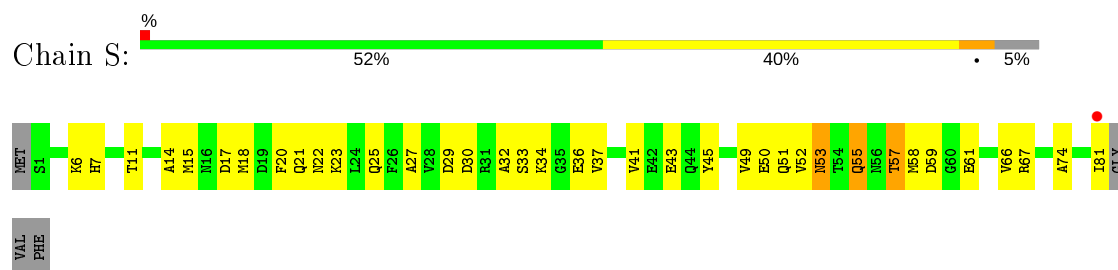




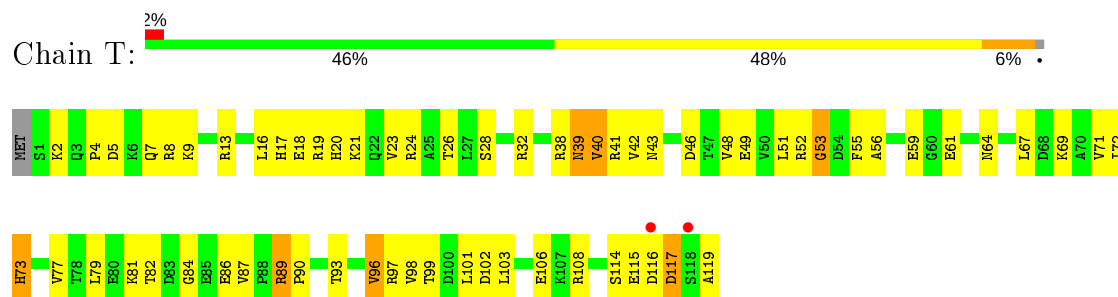
- Molecule 19: 50S ribosomal protein L22P



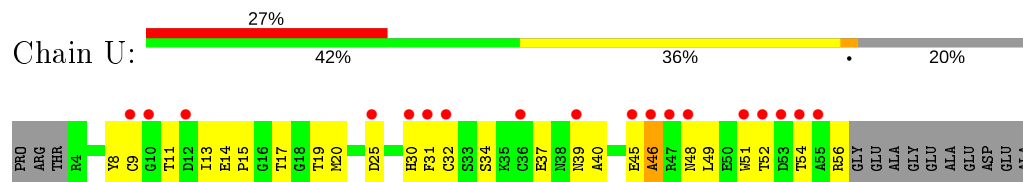
- Molecule 20: 50S ribosomal protein L23P



- Molecule 21: 50S ribosomal protein L24P

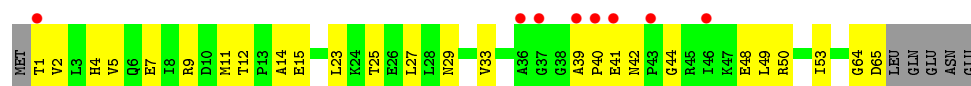


- Molecule 22: 50S ribosomal protein L24e

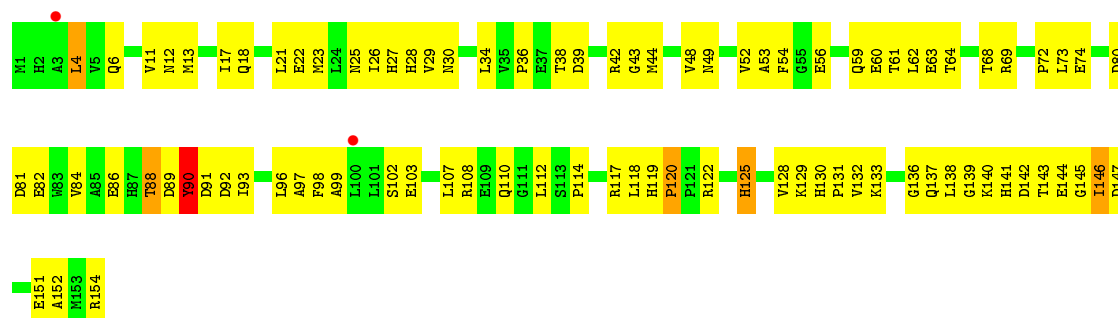
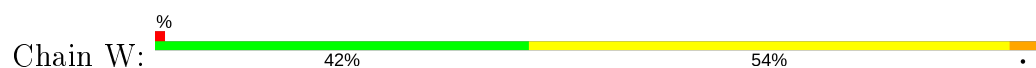


- Molecule 23: 50S ribosomal protein L29P

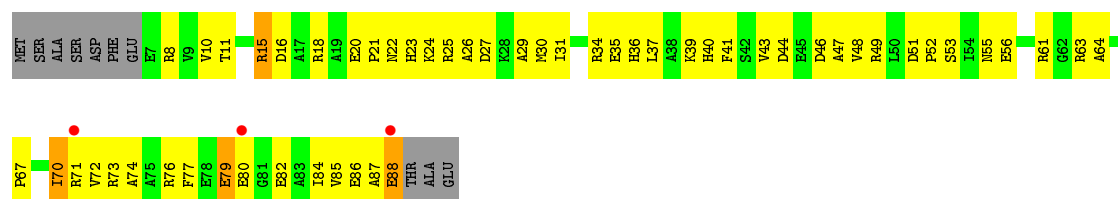




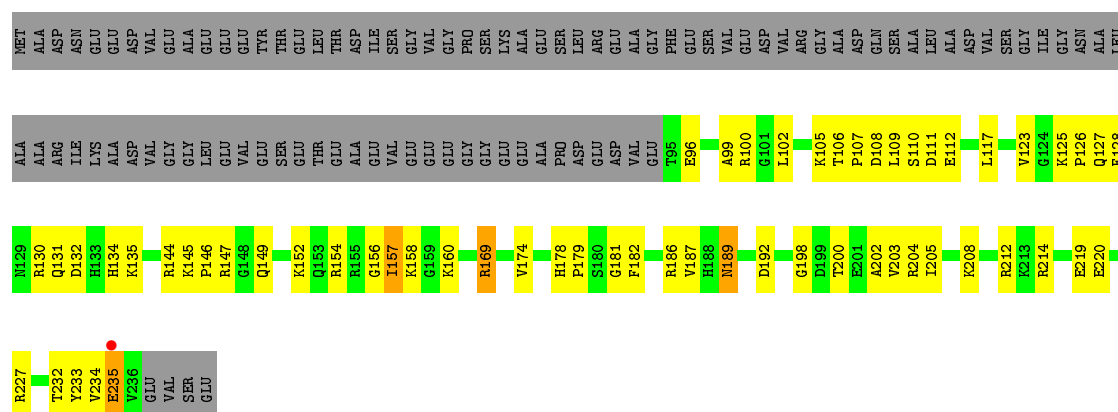
• Molecule 24: 50S ribosomal protein L30P



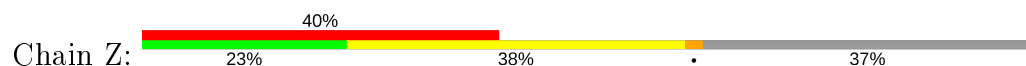
• Molecule 25: 50S ribosomal protein L31e

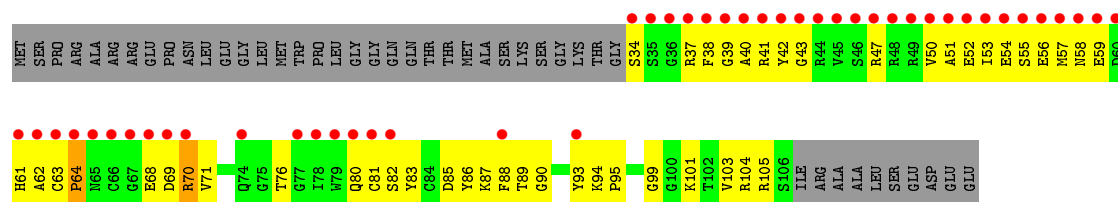


• Molecule 26: 50S ribosomal protein L32e



• Molecule 27: 50S ribosomal protein L37Ae





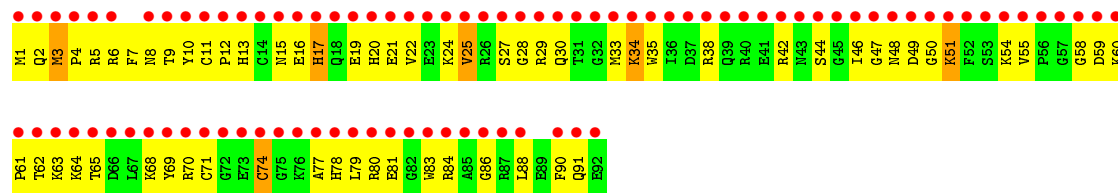
• Molecule 28: 50S ribosomal protein L37e



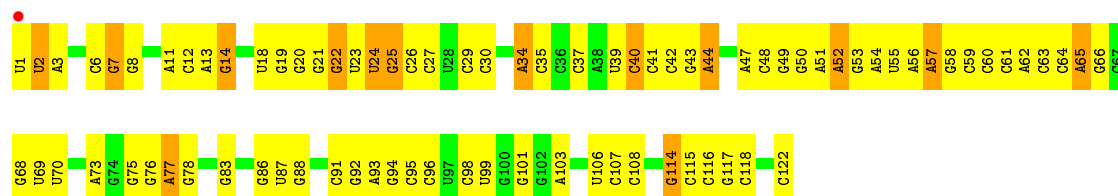
• Molecule 29: 50S ribosomal protein L39e



• 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 85.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.98-3.11) 93.9 (85.39-2.40)	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 0.230 , 0.262	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 , 92.2	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, PO2, CD, 5AA, MYL, OMU, UR3, 2OP, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.42	0/65958	0.68	6/102869 (0.0%)
2	A	0.33	0/1786	0.64	0/2408
3	B	0.36	0/2690	0.64	0/3652
4	C	0.38	0/1885	0.63	0/2552
5	D	0.31	0/1111	0.56	0/1498
6	E	0.35	0/1382	0.59	0/1880
7	F	0.32	0/901	0.59	0/1224
8	G	0.31	0/241	0.49	0/324
9	H	0.31	0/1303	0.63	0/1743
10	I	0.28	0/526	0.54	0/716
11	J	0.38	0/1136	0.62	0/1530
12	K	0.36	0/1004	0.65	0/1351
13	L	0.33	0/1130	0.62	0/1509
14	M	0.36	0/1583	0.59	0/2116
15	N	0.29	0/1474	0.62	0/1999
16	O	0.33	0/874	0.61	0/1181
17	P	0.36	0/1147	0.57	0/1528
18	Q	0.35	0/749	0.65	0/1005
19	R	0.40	0/1172	0.62	0/1578
20	S	0.35	0/648	0.58	0/875
21	T	0.33	0/958	0.63	0/1289
22	U	0.31	0/417	0.55	0/562
23	V	0.30	0/502	0.57	0/675
24	W	0.37	0/1219	0.66	0/1655
25	X	0.37	0/664	0.60	0/895
26	Y	0.38	0/1146	0.65	0/1536
27	Z	0.30	0/584	0.54	0/781
28	1	0.40	0/438	0.58	0/578
29	2	0.33	0/401	0.53	0/529
30	3	0.29	0/771	0.51	0/1024
31	9	0.35	0/2904	0.69	0/4526
32	4	0.46	0/102	0.73	0/149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.39	0/98806	0.66	6/147737 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.22	122.09	114.00
1	0	1819	G	C5'-C4'-C3'	5.93	125.50	116.00
1	0	2726	U	N1-C1'-C2'	5.42	121.04	114.00
1	0	871	G	C5'-C4'-O4'	-5.40	102.62	109.10
1	0	1942	A	C5'-C4'-C3'	5.19	124.30	116.00

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	1595	1
2	A	1753	0	1766	134	0
3	B	2625	0	2533	203	0
4	C	1860	0	1813	134	0
5	D	1094	0	1085	96	0
6	E	1357	0	1266	75	0
7	F	890	0	843	63	0
8	G	240	0	231	26	0
9	H	1283	0	1292	91	0
10	I	519	0	500	56	0
11	J	1120	0	1098	81	0
12	K	994	0	1027	84	0
13	L	1118	0	1076	94	0
14	M	1559	0	1573	155	0
15	N	1445	0	1401	122	0
16	O	865	0	873	59	0
17	P	1136	0	1123	84	0
18	Q	735	0	729	42	0
19	R	1149	0	1122	73	0
20	S	641	0	605	36	0
21	T	950	0	924	73	0
22	U	410	0	368	29	0
23	V	499	0	511	32	0
24	W	1196	0	1137	102	0
25	X	654	0	653	50	0
26	Y	1130	0	1133	62	0
27	Z	573	0	535	61	0
28	1	431	0	426	41	0
29	2	396	0	413	35	0
30	3	755	0	732	117	0
31	9	2599	0	1325	91	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	7	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	7	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	3609	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 24.

The worst 5 of 3609 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)
40:0:4863:HOH:O	32:4:77:2OP:HB3	1.31	1.30
1:0:656:G:H5'	16:O:3:THR:HG22	1.20	1.15
1:0:871:G:C8	1:0:871:G:H5'	1.84	1.12
19:R:8:ALA:HB1	19:R:13:THR:HG21	1.28	1.11
1:0:1160:G:H5'	1:0:1161: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	15
3	B	335/338 (99%)	285 (85%)	38 (11%)	12 (4%)	3	19
4	C	244/246 (99%)	204 (84%)	35 (14%)	5 (2%)	7	30
5	D	134/177 (76%)	91 (68%)	33 (25%)	10 (8%)	1	5
6	E	170/178 (96%)	149 (88%)	20 (12%)	1 (1%)	25	59
7	F	117/120 (98%)	95 (81%)	15 (13%)	7 (6%)	1	9
8	G	25/348 (7%)	18 (72%)	6 (24%)	1 (4%)	3	16
9	H	156/174 (90%)	134 (86%)	15 (10%)	7 (4%)	2	14
10	I	68/162 (42%)	43 (63%)	20 (29%)	5 (7%)	1	6
11	J	140/145 (97%)	120 (86%)	15 (11%)	5 (4%)	3	19
12	K	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	10	38
13	L	141/165 (86%)	105 (74%)	31 (22%)	5 (4%)	3	19
14	M	192/194 (99%)	153 (80%)	29 (15%)	10 (5%)	2	12
15	N	184/187 (98%)	147 (80%)	27 (15%)	10 (5%)	2	11
16	O	113/116 (97%)	89 (79%)	23 (20%)	1 (1%)	17	51
17	P	141/149 (95%)	118 (84%)	20 (14%)	3 (2%)	7	29
18	Q	93/96 (97%)	78 (84%)	10 (11%)	5 (5%)	2	11
19	R	148/155 (96%)	130 (88%)	16 (11%)	2 (1%)	11	39
20	S	79/85 (93%)	66 (84%)	12 (15%)	1 (1%)	12	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	117/120 (98%)	99 (85%)	15 (13%)	3 (3%)	5	25
22	U	51/66 (77%)	43 (84%)	6 (12%)	2 (4%)	3	17
23	V	63/71 (89%)	52 (82%)	11 (18%)	0	100	100
24	W	152/154 (99%)	121 (80%)	27 (18%)	4 (3%)	5	25
25	X	80/92 (87%)	65 (81%)	13 (16%)	2 (2%)	5	26
26	Y	140/241 (58%)	126 (90%)	13 (9%)	1 (1%)	22	56
27	Z	71/116 (61%)	58 (82%)	10 (14%)	3 (4%)	3	15
28	1	54/57 (95%)	46 (85%)	8 (15%)	0	100	100
29	2	42/50 (84%)	34 (81%)	7 (17%)	1 (2%)	6	26
30	3	90/92 (98%)	64 (71%)	23 (26%)	3 (3%)	4	20
All	All	3705/4466 (83%)	3039 (82%)	545 (15%)	121 (3%)	4	20

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%)	170 (95%)	9 (5%)	24	56
3	B	282/283 (100%)	264 (94%)	18 (6%)	17	47
4	C	193/193 (100%)	174 (90%)	19 (10%)	8	29
5	D	117/148 (79%)	111 (95%)	6 (5%)	24	55
6	E	152/156 (97%)	145 (95%)	7 (5%)	27	59
7	F	93/94 (99%)	92 (99%)	1 (1%)	73	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	G	27/282 (10%)	26 (96%)	1 (4%)	34	66
9	H	134/143 (94%)	128 (96%)	6 (4%)	27	59
10	I	58/130 (45%)	56 (97%)	2 (3%)	37	68
11	J	118/121 (98%)	114 (97%)	4 (3%)	37	68
12	K	106/106 (100%)	101 (95%)	5 (5%)	26	58
13	L	113/127 (89%)	103 (91%)	10 (9%)	10	35
14	M	158/158 (100%)	153 (97%)	5 (3%)	39	69
15	N	149/150 (99%)	139 (93%)	10 (7%)	16	45
16	O	93/94 (99%)	90 (97%)	3 (3%)	39	69
17	P	113/117 (97%)	106 (94%)	7 (6%)	18	48
18	Q	79/80 (99%)	78 (99%)	1 (1%)	69	86
19	R	117/122 (96%)	112 (96%)	5 (4%)	29	61
20	S	71/74 (96%)	68 (96%)	3 (4%)	30	62
21	T	105/106 (99%)	98 (93%)	7 (7%)	16	45
22	U	44/52 (85%)	44 (100%)	0	100	100
23	V	51/57 (90%)	51 (100%)	0	100	100
24	W	130/130 (100%)	123 (95%)	7 (5%)	22	53
25	X	66/74 (89%)	60 (91%)	6 (9%)	9	33
26	Y	120/196 (61%)	116 (97%)	4 (3%)	38	68
27	Z	60/94 (64%)	59 (98%)	1 (2%)	60	83
28	1	46/47 (98%)	45 (98%)	1 (2%)	52	77
29	2	42/46 (91%)	40 (95%)	2 (5%)	25	57
30	3	79/79 (100%)	76 (96%)	3 (4%)	33	65
All	All	3095/3641 (85%)	2942 (95%)	153 (5%)	25	57

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	39	VAL
13	L	127	GLU
25	X	88	GLU
11	J	74	ARG
12	K	83	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 107 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	58	GLN
17	P	28	GLN
29	2	41	HIS
14	M	24	GLN
14	M	98	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	248 (9%)	18 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
32	4	1/8 (12%)	0	0
All	All	2867/3053 (93%)	266 (9%)	19 (0%)

5 of 266 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	871	G
1	0	2011	A
1	0	2718	C
1	0	857	A
1	0	2726	U

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	UR3	0	2619	1	14,22,23	0.73	0	15,32,35	0.56	0
1	OMG	0	2588	1,32	18,26,27	0.98	2 (11%)	20,38,41	2.58	4 (20%)
1	PSU	0	2621	1	17,21,22	1.69	3 (17%)	20,30,33	5.43	4 (20%)
1	1MA	0	628	1	15,25,26	0.78	0	15,37,40	1.39	1 (6%)
1	OMU	0	2587	1,35	14,22,23	1.05	1 (7%)	14,31,34	1.17	1 (7%)
32	5AA	4	76	1,32	18,26,27	0.76	0	15,38,41	0.80	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1,32	-	0/5/27/28	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1,35	-	0/7/27/28	0/2/2/2
32	5AA	4	76	1,32	-	0/7/29/30	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.12	1.47	1.52
1	0	2588	OMG	C6-N1	3.06	1.38	1.33
1	0	2621	PSU	C4-N3	2.93	1.38	1.33
1	0	2621	PSU	C2-N1	2.89	1.43	1.38
1	0	2587	OMU	C4-N3	2.81	1.37	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.29	114.69	128.43
1	0	2621	PSU	C4-N3-C2	14.17	127.10	115.14
1	0	2588	OMG	C5-C6-N1	-8.51	111.78	123.43
1	0	2621	PSU	C5-C4-N3	-8.14	114.87	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-N1-C2	5.80	125.14	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2619	UR3	1	0
1	0	2588	OMG	5	0
1	0	2621	PSU	1	0
1	0	2587	OMU	2	0
32	4	76	5AA	10	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	1.19	4 (11%)	38,56,56	1.64	10 (26%)

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	4.80	1.49	1.43
38	0	2924	MYL	CAA-CAV	2.97	1.39	1.32
38	0	2924	MYL	OAR-CAM	2.14	1.44	1.41
38	0	2924	MYL	OAS-CAM	2.14	1.44	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	MYL	OAT-CAY-CAC	4.10	110.94	105.85
38	0	2924	MYL	CAN-CAV-CAZ	3.78	116.96	112.10
38	0	2924	MYL	CBC-NAP-CAW	3.04	126.58	122.69
38	0	2924	MYL	OAR-CBC-NAP	2.71	110.89	107.15
38	0	2924	MYL	OAR-CBC-CBG	-2.68	104.64	109.35

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:

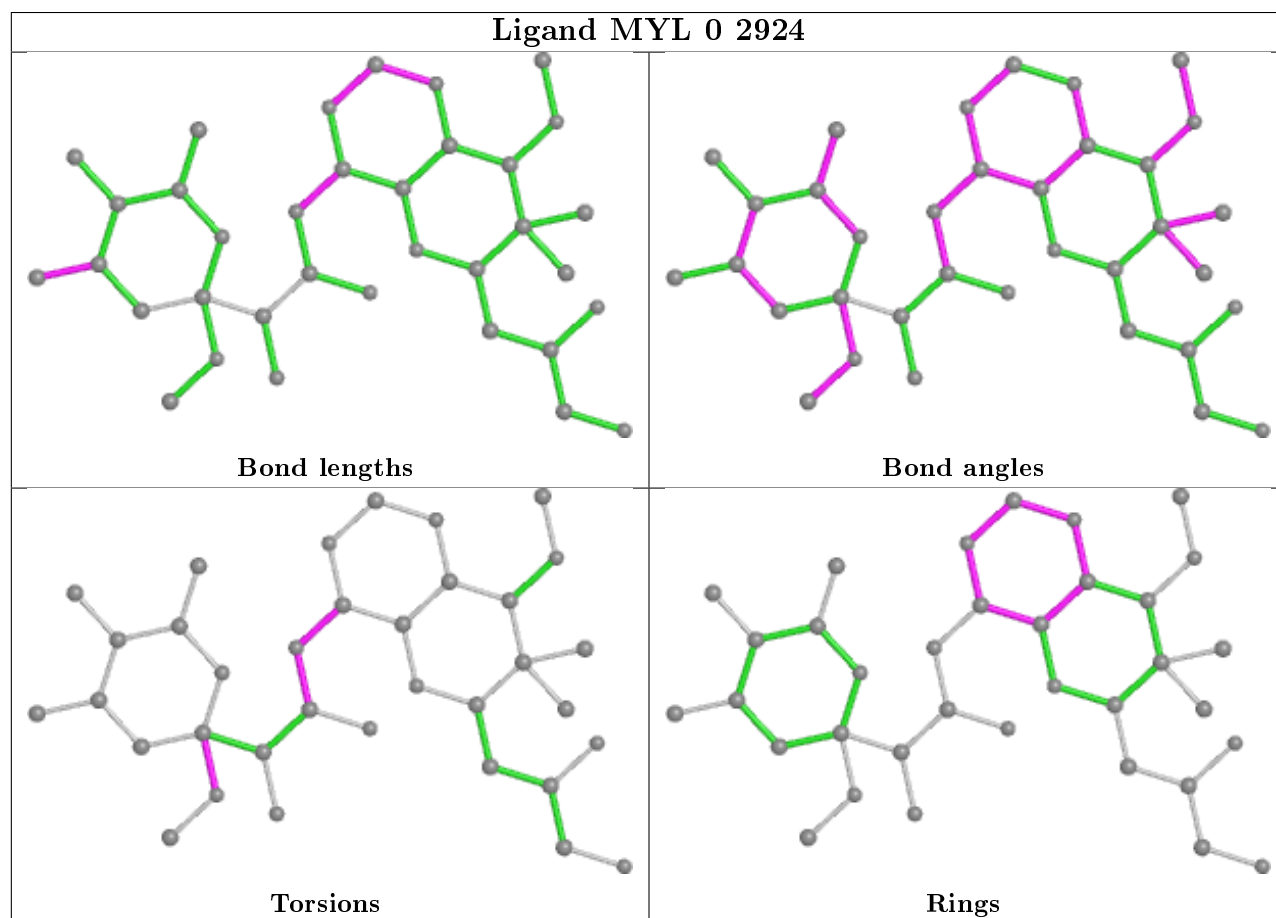
Mol	Chain	Res	Type	Atoms
38	0	2924	MYL	CAM-CBC-CBF-CBG-OAR-OAS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2923 (94%)	-0.36	3 (0%) 95 92	31, 61, 109, 181	0
2	A	237/240 (98%)	-0.02	5 (2%) 63 43	37, 75, 110, 131	0
3	B	337/338 (99%)	-0.41	0 100 100	37, 65, 93, 103	0
4	C	246/246 (100%)	-0.31	0 100 100	34, 60, 84, 96	0
5	D	140/177 (79%)	0.97	25 (17%) 1 0	80, 118, 140, 148	0
6	E	172/178 (96%)	-0.25	0 100 100	54, 81, 102, 112	0
7	F	119/120 (99%)	0.14	2 (1%) 70 50	65, 93, 121, 135	0
8	G	29/348 (8%)	0.36	1 (3%) 45 24	86, 102, 109, 114	0
9	H	160/174 (91%)	0.10	4 (2%) 57 35	58, 79, 111, 121	0
10	I	70/162 (43%)	1.92	32 (45%) 0 0	137, 154, 180, 181	0
11	J	142/145 (97%)	-0.45	0 100 100	48, 63, 82, 98	0
12	K	132/132 (100%)	-0.30	0 100 100	46, 63, 88, 95	0
13	L	145/165 (87%)	0.18	6 (4%) 37 18	38, 86, 124, 133	0
14	M	194/194 (100%)	0.21	19 (9%) 7 2	38, 60, 136, 151	0
15	N	186/187 (99%)	0.21	5 (2%) 54 31	65, 89, 138, 146	0
16	O	115/116 (99%)	-0.35	0 100 100	51, 70, 84, 91	0
17	P	143/149 (95%)	-0.15	1 (0%) 87 77	52, 69, 87, 93	0
18	Q	95/96 (98%)	-0.17	0 100 100	51, 62, 77, 85	0
19	R	150/155 (96%)	-0.41	0 100 100	42, 56, 77, 89	0
20	S	81/85 (95%)	-0.12	1 (1%) 79 63	57, 76, 99, 111	0
21	T	119/120 (99%)	-0.03	2 (1%) 70 50	55, 73, 106, 125	0
22	U	53/66 (80%)	1.58	18 (33%) 0 0	95, 117, 133, 135	0
23	V	65/71 (91%)	0.79	8 (12%) 4 1	65, 90, 140, 144	0
24	W	154/154 (100%)	-0.25	2 (1%) 77 60	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%)	-0.03	3 (3%) 41 21	52, 70, 88, 105	0
26	Y	142/241 (58%)	-0.43	1 (0%) 87 77	39, 58, 80, 99	0
27	Z	73/116 (62%)	4.94	46 (63%) 0 0	107, 143, 170, 176	0
28	1	56/57 (98%)	-0.23	0 100 100	34, 47, 58, 62	0
29	2	46/50 (92%)	0.14	3 (6%) 18 7	47, 80, 113, 121	0
30	3	92/92 (100%)	7.53	90 (97%) 0 0	164, 175, 184, 189	0
31	9	122/122 (100%)	-0.57	1 (0%) 86 74	52, 86, 113, 166	0
32	4	5/8 (62%)	1.30	0 100 100	41, 43, 47, 47	0
All	All	6651/7519 (88%)	-0.01	278 (4%) 36 18	31, 67, 132, 189	0

The worst 5 of 278 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	24.2
30	3	82	GLY	23.8
27	Z	35	SER	22.6
27	Z	58	ASN	21.8
27	Z	46	SER	20.6

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	0.77	0.29	38,44,48,48	0
1	PSU	0	2621	20/21	0.93	0.19	37,39,44,44	0
1	OMU	0	2587	21/22	0.95	0.14	43,46,50,50	0
1	UR3	0	2619	21/22	0.95	0.17	41,44,49,50	0
1	OMG	0	2588	24/25	0.96	0.16	37,42,44,45	0
1	1MA	0	628	23/24	0.96	0.17	38,41,42,43	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	8971	1/1	-0.30	0.33	200,200,200,200	0
37	SR	3	8932	1/1	-0.02	0.28	184,184,184,184	0
33	MG	3	8090	1/1	0.04	2.21	86,86,86,86	0
35	NA	0	8544	1/1	0.07	0.45	75,75,75,75	0
37	SR	0	8962	1/1	0.08	0.43	200,200,200,200	0
36	CL	3	8804	1/1	0.10	0.57	121,121,121,121	0
37	SR	0	8983	1/1	0.16	0.28	199,199,199,199	0
37	SR	0	8965	1/1	0.16	0.19	158,158,158,158	0
37	SR	0	8977	1/1	0.23	0.11	200,200,200,200	0
37	SR	0	8974	1/1	0.28	0.20	163,163,163,163	0
33	MG	0	8075	1/1	0.30	0.14	64,64,64,64	0
37	SR	0	8993	1/1	0.36	0.23	186,186,186,186	0
37	SR	0	8941	1/1	0.38	0.30	152,152,152,152	0
35	NA	0	8568	1/1	0.39	0.61	35,35,35,35	0
37	SR	9	8980	1/1	0.39	0.37	192,192,192,192	0
35	NA	0	8548	1/1	0.40	0.33	67,67,67,67	0
37	SR	0	8959	1/1	0.40	0.36	194,194,194,194	0
37	SR	0	9002	1/1	0.42	0.12	169,169,169,169	0
37	SR	0	8949	1/1	0.44	0.43	157,157,157,157	0
35	NA	0	8506	1/1	0.46	0.78	65,65,65,65	0
35	NA	0	8551	1/1	0.48	0.79	86,86,86,86	0
37	SR	A	8930	1/1	0.49	0.15	168,168,168,168	0
39	CD	Z	8703	1/1	0.51	0.38	200,200,200,200	0
33	MG	0	8088	1/1	0.53	0.18	37,37,37,37	0
37	SR	0	8986	1/1	0.53	0.84	200,200,200,200	0
37	SR	0	9000	1/1	0.53	1.07	200,200,200,200	0
37	SR	L	8969	1/1	0.55	1.29	200,200,200,200	0
35	NA	0	8574	1/1	0.56	0.62	72,72,72,72	0
39	CD	3	8704	1/1	0.56	0.62	200,200,200,200	0
35	NA	0	8528	1/1	0.57	0.68	91,91,91,91	0
33	MG	0	8066	1/1	0.57	0.25	75,75,75,75	0
33	MG	0	8010	1/1	0.57	0.14	25,25,25,25	0
37	SR	0	8908	1/1	0.57	0.22	116,116,116,116	0
37	SR	0	8938	1/1	0.57	0.32	200,200,200,200	0
35	NA	0	8557	1/1	0.57	0.15	72,72,72,72	0
35	NA	0	8522	1/1	0.57	0.27	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8536	1/1	0.58	0.20	72,72,72,72	0
33	MG	0	8093	1/1	0.59	0.11	29,29,29,29	0
33	MG	0	8044	1/1	0.60	0.16	51,51,51,51	0
35	NA	0	8521	1/1	0.60	0.47	59,59,59,59	0
37	SR	0	8968	1/1	0.61	0.15	180,180,180,180	0
37	SR	F	9005	1/1	0.61	0.07	153,153,153,153	0
35	NA	0	8509	1/1	0.62	0.58	90,90,90,90	0
33	MG	0	8081	1/1	0.63	0.58	80,80,80,80	0
33	MG	0	8055	1/1	0.63	0.53	87,87,87,87	0
36	CL	0	8803	1/1	0.63	0.12	68,68,68,68	0
33	MG	0	8069	1/1	0.64	0.43	63,63,63,63	0
37	SR	9	9003	1/1	0.64	0.06	195,195,195,195	0
35	NA	H	8518	1/1	0.65	0.77	92,92,92,92	0
37	SR	3	8999	1/1	0.66	0.69	200,200,200,200	0
37	SR	0	8944	1/1	0.66	0.17	169,169,169,169	0
37	SR	0	8991	1/1	0.67	0.14	197,197,197,197	0
36	CL	O	8808	1/1	0.67	0.14	109,109,109,109	0
33	MG	0	8038	1/1	0.68	0.20	92,92,92,92	0
37	SR	0	8989	1/1	0.68	0.16	129,129,129,129	0
35	NA	J	8538	1/1	0.69	0.14	56,56,56,56	0
35	NA	0	8571	1/1	0.69	0.36	101,101,101,101	0
35	NA	0	8559	1/1	0.69	0.32	99,99,99,99	0
33	MG	0	8092	1/1	0.69	0.47	133,133,133,133	0
35	NA	0	8502	1/1	0.70	0.39	53,53,53,53	0
35	NA	0	8570	1/1	0.70	0.26	61,61,61,61	0
35	NA	0	8561	1/1	0.71	0.26	66,66,66,66	0
35	NA	0	8554	1/1	0.71	0.46	106,106,106,106	0
35	NA	0	8558	1/1	0.71	0.58	60,60,60,60	0
34	K	0	8402	1/1	0.71	0.48	88,88,88,88	0
35	NA	0	8508	1/1	0.71	0.42	68,68,68,68	0
35	NA	0	8563	1/1	0.72	1.01	85,85,85,85	0
33	MG	K	8054	1/1	0.72	0.19	29,29,29,29	0
35	NA	0	8556	1/1	0.72	0.46	49,49,49,49	0
33	MG	2	8060	1/1	0.72	0.11	62,62,62,62	0
37	SR	0	8915	1/1	0.73	0.14	131,131,131,131	0
33	MG	0	8073	1/1	0.73	0.09	70,70,70,70	0
37	SR	0	8992	1/1	0.73	0.29	164,164,164,164	0
35	NA	0	8531	1/1	0.74	0.18	45,45,45,45	0
37	SR	0	8922	1/1	0.74	0.65	182,182,182,182	0
33	MG	0	8071	1/1	0.74	0.30	67,67,67,67	0
35	NA	9	8543	1/1	0.74	0.18	68,68,68,68	0
37	SR	0	8916	1/1	0.74	0.17	126,126,126,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8065	1/1	0.74	0.12	33,33,33,33	0
37	SR	0	8979	1/1	0.74	0.24	111,111,111,111	0
37	SR	0	8960	1/1	0.75	0.09	175,175,175,175	0
37	SR	0	8975	1/1	0.75	0.08	158,158,158,158	0
37	SR	0	8911	1/1	0.75	0.10	99,99,99,99	0
35	NA	Q	8540	1/1	0.75	0.30	84,84,84,84	0
37	SR	0	8966	1/1	0.76	0.13	117,117,117,117	0
35	NA	0	8513	1/1	0.76	0.67	62,62,62,62	0
35	NA	0	8549	1/1	0.76	0.34	124,124,124,124	0
37	SR	0	8957	1/1	0.76	0.29	200,200,200,200	0
37	SR	0	8953	1/1	0.76	1.09	200,200,200,200	0
33	MG	0	8053	1/1	0.76	0.10	61,61,61,61	0
37	SR	0	8976	1/1	0.77	0.38	200,200,200,200	0
37	SR	0	8927	1/1	0.77	0.16	176,176,176,176	0
37	SR	0	8945	1/1	0.77	0.13	131,131,131,131	0
37	SR	0	9007	1/1	0.78	0.37	200,200,200,200	0
33	MG	0	8029	1/1	0.78	0.18	79,79,79,79	0
35	NA	0	8567	1/1	0.78	0.82	57,57,57,57	0
37	SR	B	8987	1/1	0.78	0.99	200,200,200,200	0
35	NA	0	8560	1/1	0.78	0.78	61,61,61,61	0
33	MG	0	8091	1/1	0.78	0.10	111,111,111,111	0
37	SR	0	8988	1/1	0.78	0.17	183,183,183,183	0
37	SR	0	8926	1/1	0.79	0.16	127,127,127,127	0
33	MG	0	8036	1/1	0.79	0.16	59,59,59,59	0
33	MG	0	8024	1/1	0.79	0.24	55,55,55,55	0
35	NA	0	8530	1/1	0.79	0.68	68,68,68,68	0
36	CL	L	8810	1/1	0.79	0.16	76,76,76,76	0
37	SR	0	9001	1/1	0.79	0.18	200,200,200,200	0
33	MG	T	8057	1/1	0.80	0.07	68,68,68,68	0
37	SR	0	8997	1/1	0.80	0.73	200,200,200,200	0
33	MG	0	8064	1/1	0.80	0.29	53,53,53,53	0
37	SR	0	9006	1/1	0.80	0.12	190,190,190,190	0
37	SR	0	8964	1/1	0.80	0.08	160,160,160,160	0
35	NA	0	8534	1/1	0.81	0.38	53,53,53,53	0
35	NA	0	8569	1/1	0.81	0.36	63,63,63,63	0
35	NA	0	8517	1/1	0.81	0.35	62,62,62,62	0
33	MG	0	8031	1/1	0.81	0.63	77,77,77,77	0
33	MG	0	8076	1/1	0.81	0.24	52,52,52,52	0
39	CD	U	8701	1/1	0.81	0.40	200,200,200,200	0
35	NA	0	8507	1/1	0.81	0.17	27,27,27,27	0
37	SR	0	8924	1/1	0.82	0.20	140,140,140,140	0
36	CL	A	8809	1/1	0.82	0.76	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8541	1/1	0.82	0.38	65,65,65,65	0
33	MG	0	8004	1/1	0.82	0.18	25,25,25,25	0
33	MG	0	8017	1/1	0.82	0.17	26,26,26,26	0
37	SR	A	8929	1/1	0.82	0.07	124,124,124,124	0
36	CL	0	8813	1/1	0.82	0.10	77,77,77,77	0
37	SR	0	8943	1/1	0.82	0.14	105,105,105,105	0
33	MG	0	8056	1/1	0.82	0.13	44,44,44,44	0
34	K	0	8401	1/1	0.83	0.36	132,132,132,132	0
33	MG	9	8074	1/1	0.83	0.11	87,87,87,87	0
33	MG	0	8039	1/1	0.83	0.19	55,55,55,55	0
37	SR	0	8933	1/1	0.83	0.06	122,122,122,122	0
37	SR	0	8917	1/1	0.83	0.23	157,157,157,157	0
33	MG	0	8020	1/1	0.83	0.15	56,56,56,56	0
35	NA	M	8539	1/1	0.84	0.26	51,51,51,51	0
35	NA	0	8529	1/1	0.84	0.09	45,45,45,45	0
33	MG	0	8083	1/1	0.84	0.18	50,50,50,50	0
37	SR	0	8947	1/1	0.84	0.76	200,200,200,200	0
35	NA	0	8537	1/1	0.84	0.09	40,40,40,40	0
35	NA	S	8510	1/1	0.84	0.12	56,56,56,56	0
37	SR	0	8984	1/1	0.84	0.07	118,118,118,118	0
37	SR	0	8951	1/1	0.84	0.06	144,144,144,144	0
38	MYL	0	2924	35/35	0.84	0.26	80,83,86,87	0
35	NA	R	8533	1/1	0.84	0.20	62,62,62,62	0
35	NA	0	8523	1/1	0.84	0.20	52,52,52,52	0
35	NA	0	8564	1/1	0.84	0.21	94,94,94,94	0
37	SR	0	8995	1/1	0.85	0.45	191,191,191,191	0
35	NA	0	8546	1/1	0.85	0.62	65,65,65,65	0
33	MG	0	8046	1/1	0.85	0.13	46,46,46,46	0
35	NA	0	8525	1/1	0.85	0.25	67,67,67,67	0
37	SR	0	8918	1/1	0.85	0.14	92,92,92,92	0
37	SR	0	8973	1/1	0.85	0.12	162,162,162,162	0
37	SR	0	8942	1/1	0.85	0.21	139,139,139,139	0
33	MG	0	8047	1/1	0.85	0.55	68,68,68,68	0
33	MG	0	8026	1/1	0.87	0.20	39,39,39,39	0
37	SR	0	8982	1/1	0.87	1.35	200,200,200,200	0
33	MG	0	8019	1/1	0.87	0.16	11,11,11,11	0
33	MG	0	8045	1/1	0.87	0.10	64,64,64,64	0
35	NA	0	8520	1/1	0.87	0.18	63,63,63,63	0
36	CL	Y	8820	1/1	0.87	0.21	58,58,58,58	0
33	MG	0	8079	1/1	0.87	0.41	76,76,76,76	0
33	MG	Y	8086	1/1	0.87	0.25	53,53,53,53	0
35	NA	0	8550	1/1	0.87	0.27	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	8914	1/1	0.88	0.15	109,109,109,109	0
36	CL	B	8819	1/1	0.88	0.23	80,80,80,80	0
37	SR	0	8919	1/1	0.88	0.09	81,81,81,81	0
36	CL	J	8802	1/1	0.88	0.25	84,84,84,84	0
33	MG	0	8082	1/1	0.88	0.23	61,61,61,61	0
37	SR	0	8956	1/1	0.88	0.09	154,154,154,154	0
33	MG	0	8089	1/1	0.88	0.21	42,42,42,42	0
36	CL	N	8807	1/1	0.88	0.29	98,98,98,98	0
35	NA	0	8505	1/1	0.88	0.49	58,58,58,58	0
36	CL	0	8822	1/1	0.88	0.88	123,123,123,123	0
33	MG	0	8070	1/1	0.88	0.09	58,58,58,58	0
33	MG	0	8018	1/1	0.88	0.15	32,32,32,32	0
35	NA	C	8503	1/1	0.88	0.17	32,32,32,32	0
36	CL	0	8805	1/1	0.88	0.24	101,101,101,101	0
35	NA	0	8501	1/1	0.89	0.24	41,41,41,41	0
37	SR	0	8910	1/1	0.89	0.13	107,107,107,107	0
37	SR	0	8931	1/1	0.89	0.09	147,147,147,147	0
37	SR	0	8913	1/1	0.89	0.78	181,181,181,181	0
33	MG	0	8063	1/1	0.89	0.16	62,62,62,62	0
35	NA	0	8565	1/1	0.89	1.65	80,80,80,80	0
35	NA	0	8516	1/1	0.89	0.20	39,39,39,39	0
37	SR	0	8955	1/1	0.89	0.13	200,200,200,200	0
37	SR	0	8934	1/1	0.89	0.31	168,168,168,168	0
33	MG	0	8077	1/1	0.89	0.63	60,60,60,60	0
35	NA	0	8553	1/1	0.90	0.36	98,98,98,98	0
37	SR	0	8939	1/1	0.90	0.15	166,166,166,166	0
37	SR	0	8985	1/1	0.90	0.12	150,150,150,150	0
33	MG	0	8011	1/1	0.90	0.16	14,14,14,14	0
36	CL	J	8801	1/1	0.90	0.33	88,88,88,88	0
35	NA	0	8555	1/1	0.90	0.76	61,61,61,61	0
37	SR	B	8950	1/1	0.90	0.15	125,125,125,125	0
35	NA	0	8512	1/1	0.90	0.44	54,54,54,54	0
33	MG	0	8013	1/1	0.90	0.08	24,24,24,24	0
35	NA	0	8545	1/1	0.90	0.26	25,25,25,25	0
33	MG	0	8005	1/1	0.90	0.31	46,46,46,46	0
33	MG	0	8059	1/1	0.90	0.15	56,56,56,56	0
37	SR	0	8921	1/1	0.91	0.16	98,98,98,98	0
33	MG	0	8080	1/1	0.91	2.93	126,126,126,126	0
37	SR	0	8901	1/1	0.91	0.15	78,78,78,78	0
33	MG	A	8050	1/1	0.91	0.18	68,68,68,68	0
35	NA	0	8511	1/1	0.91	0.26	54,54,54,54	0
35	NA	0	8566	1/1	0.91	0.37	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8025	1/1	0.91	0.14	30,30,30,30	0
37	SR	S	8961	1/1	0.91	0.12	150,150,150,150	0
33	MG	0	8048	1/1	0.91	0.29	41,41,41,41	0
37	SR	0	8923	1/1	0.91	0.17	108,108,108,108	0
33	MG	0	8028	1/1	0.92	0.15	13,13,13,13	0
37	SR	0	8967	1/1	0.92	0.07	164,164,164,164	0
37	SR	0	8963	1/1	0.92	0.12	146,146,146,146	0
36	CL	0	8811	1/1	0.92	0.21	87,87,87,87	0
37	SR	0	8946	1/1	0.92	0.14	127,127,127,127	0
33	MG	0	8052	1/1	0.92	0.13	60,60,60,60	0
37	SR	0	8928	1/1	0.92	0.11	148,148,148,148	0
33	MG	0	8043	1/1	0.92	0.21	48,48,48,48	0
35	NA	0	8562	1/1	0.92	0.21	49,49,49,49	0
33	MG	0	8032	1/1	0.92	0.15	66,66,66,66	0
33	MG	B	8042	1/1	0.92	0.47	121,121,121,121	0
35	NA	0	8573	1/1	0.92	0.15	78,78,78,78	0
35	NA	0	8535	1/1	0.92	0.76	72,72,72,72	0
33	MG	0	8058	1/1	0.92	0.12	22,22,22,22	0
35	NA	0	8519	1/1	0.92	0.35	69,69,69,69	0
33	MG	0	8085	1/1	0.93	0.13	73,73,73,73	0
35	NA	B	8552	1/1	0.93	0.23	111,111,111,111	0
37	SR	0	8937	1/1	0.93	0.10	116,116,116,116	0
37	SR	0	9004	1/1	0.93	0.25	172,172,172,172	0
37	SR	0	8948	1/1	0.93	0.12	113,113,113,113	0
35	NA	R	8532	1/1	0.93	0.08	52,52,52,52	0
33	MG	9	8040	1/1	0.93	0.23	89,89,89,89	0
33	MG	0	8008	1/1	0.93	0.15	23,23,23,23	0
33	MG	0	8003	1/1	0.93	0.17	32,32,32,32	0
35	NA	9	8572	1/1	0.93	0.04	78,78,78,78	0
33	MG	0	8061	1/1	0.93	0.41	48,48,48,48	0
33	MG	0	8034	1/1	0.93	0.19	57,57,57,57	0
36	CL	J	8821	1/1	0.93	0.19	90,90,90,90	0
35	NA	0	8515	1/1	0.93	0.17	39,39,39,39	0
37	SR	0	9008	1/1	0.93	0.16	107,107,107,107	0
37	SR	0	8935	1/1	0.93	0.09	91,91,91,91	0
37	SR	0	8954	1/1	0.93	0.15	108,108,108,108	0
33	MG	0	8023	1/1	0.94	0.18	41,41,41,41	0
35	NA	0	8526	1/1	0.94	0.12	40,40,40,40	0
33	MG	0	8014	1/1	0.94	0.20	24,24,24,24	0
37	SR	0	8981	1/1	0.94	0.28	198,198,198,198	0
36	CL	M	8818	1/1	0.94	0.18	62,62,62,62	0
37	SR	1	8952	1/1	0.94	0.16	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8049	1/1	0.94	0.35	82,82,82,82	0
33	MG	0	8030	1/1	0.94	0.39	88,88,88,88	0
39	CD	1	8702	1/1	0.94	0.11	78,78,78,78	0
35	NA	0	8547	1/1	0.94	0.60	82,82,82,82	0
33	MG	0	8035	1/1	0.94	0.25	52,52,52,52	0
35	NA	0	8542	1/1	0.94	0.34	51,51,51,51	0
36	CL	0	8816	1/1	0.94	0.80	89,89,89,89	0
37	SR	0	8970	1/1	0.94	0.13	148,148,148,148	0
33	MG	0	8022	1/1	0.94	0.07	56,56,56,56	0
33	MG	0	8041	1/1	0.94	0.21	29,29,29,29	0
36	CL	0	8815	1/1	0.94	0.21	83,83,83,83	0
39	CD	O	8705	1/1	0.95	0.07	117,117,117,117	0
37	SR	0	8998	1/1	0.95	0.20	196,196,196,196	0
37	SR	9	8978	1/1	0.95	0.10	154,154,154,154	0
35	NA	0	8514	1/1	0.95	0.56	38,38,38,38	0
37	SR	0	8920	1/1	0.95	0.14	130,130,130,130	0
36	CL	0	8817	1/1	0.95	0.34	80,80,80,80	0
37	SR	0	8906	1/1	0.95	0.21	64,64,64,64	0
33	MG	0	8087	1/1	0.95	0.11	29,29,29,29	0
33	MG	0	8072	1/1	0.95	0.40	60,60,60,60	0
36	CL	0	8812	1/1	0.95	0.12	66,66,66,66	0
33	MG	0	8078	1/1	0.95	0.84	91,91,91,91	0
36	CL	R	8806	1/1	0.95	0.08	56,56,56,56	0
37	SR	0	8903	1/1	0.96	0.15	62,62,62,62	0
37	SR	0	8996	1/1	0.96	0.22	200,200,200,200	0
37	SR	0	8907	1/1	0.96	0.14	59,59,59,59	0
33	MG	0	8007	1/1	0.96	0.12	27,27,27,27	0
37	SR	0	8905	1/1	0.96	0.27	78,78,78,78	0
37	SR	0	8936	1/1	0.96	0.13	125,125,125,125	0
35	NA	0	8524	1/1	0.96	0.12	67,67,67,67	0
37	SR	0	8940	1/1	0.96	0.16	110,110,110,110	0
33	MG	0	8033	1/1	0.96	0.20	79,79,79,79	0
37	SR	0	8958	1/1	0.96	0.16	120,120,120,120	0
33	MG	0	8012	1/1	0.96	0.17	23,23,23,23	0
33	MG	0	8067	1/1	0.97	0.17	33,33,33,33	0
33	MG	0	8015	1/1	0.97	0.17	26,26,26,26	0
33	MG	0	8016	1/1	0.97	0.19	34,34,34,34	0
35	NA	0	8527	1/1	0.97	0.34	75,75,75,75	0
37	SR	0	8909	1/1	0.97	0.18	105,105,105,105	0
36	CL	0	8814	1/1	0.97	0.17	55,55,55,55	0
33	MG	0	8021	1/1	0.97	0.10	53,53,53,53	0
37	SR	H	8972	1/1	0.97	0.11	139,139,139,139	0

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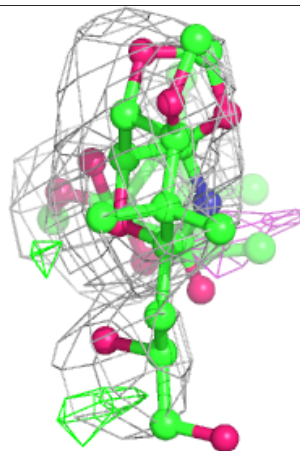
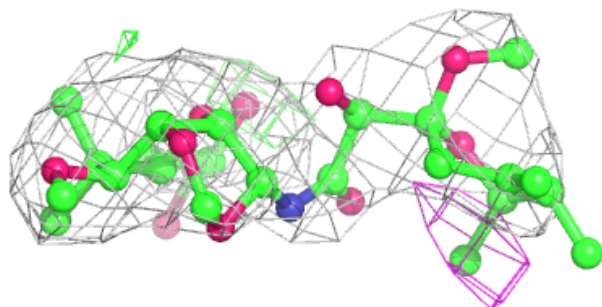
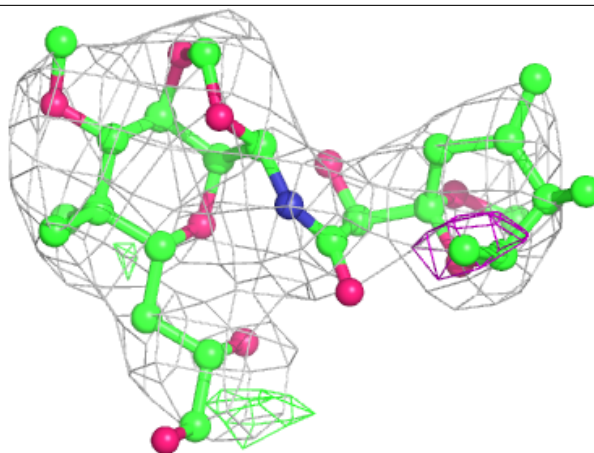
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	8994	1/1	0.97	0.61	200,200,200,200	0
35	NA	R	8575	1/1	0.97	0.18	92,92,92,92	0
37	SR	R	8912	1/1	0.97	0.16	93,93,93,93	0
37	SR	0	8925	1/1	0.97	0.10	99,99,99,99	0
33	MG	0	8002	1/1	0.97	0.17	40,40,40,40	0
33	MG	0	8084	1/1	0.97	0.11	31,31,31,31	0
33	MG	0	8009	1/1	0.98	0.13	22,22,22,22	0
33	MG	0	8006	1/1	0.98	0.16	44,44,44,44	0
33	MG	0	8027	1/1	0.98	0.08	47,47,47,47	0
33	MG	0	8062	1/1	0.98	0.20	53,53,53,53	0
37	SR	0	8990	1/1	0.98	0.19	108,108,108,108	0
33	MG	0	8001	1/1	0.98	0.17	24,24,24,24	0
33	MG	A	8051	1/1	0.99	0.20	81,81,81,81	0
37	SR	0	8904	1/1	0.99	0.23	65,65,65,65	0
35	NA	0	8504	1/1	0.99	0.13	32,32,32,32	0
33	MG	0	8068	1/1	0.99	0.12	64,64,64,64	0
33	MG	0	8037	1/1	0.99	0.10	67,67,67,67	0
37	SR	0	8902	1/1	0.99	0.20	44,44,44,44	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.