



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 06:56 PM EDT

PDB ID : 3I56 / pdb_00003i56
Title : Co-crystal structure of Triacetyloleandomycin Bound to the Large Ribosomal Subunit
Authors : Gurel, G.; Blaha, G.; Steitz, T.A.; Moore, P.B.
Deposited on : 2009-07-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

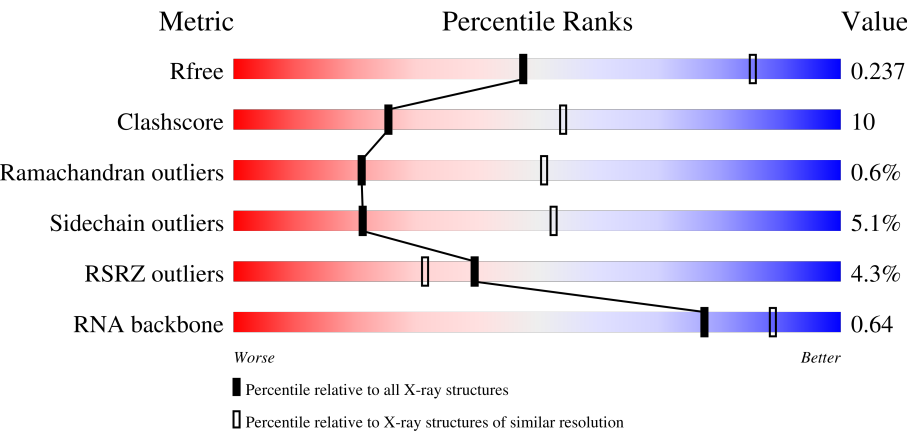
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	240	4% 80% 18% ..
2	B	338	% 79% 17% .
3	C	246	% 81% 18% .
4	D	177	28% 60% 16% .. 21%

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	174	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	194	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	66	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8071	-	-	-	X
33	CL	K	8812	-	-	X	-
34	SR	0	8928	-	-	-	X
34	SR	0	8967	-	-	-	X
34	SR	1	8952	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8557	-	-	-	X
35	NA	0	8564	-	-	-	X
38	TAO	0	2924	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99181 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

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

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59020	26349	10873	19053	2745			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	A	2	Total	Mg	0	0
			2	2		
32	B	2	Total	Mg	0	0
			2	2		
32	C	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	0	82	Total	Mg	0	0
			82	82		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	1	Total	Cl	0	0
			1	1		
33	B	1	Total	Cl	0	0
			1	1		
33	J	3	Total	Cl	0	0
			3	3		
33	K	1	Total	Cl	0	0
			1	1		
33	L	2	Total	Cl	0	0
			2	2		
33	M	1	Total	Cl	0	0
			1	1		
33	N	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total 1	Cl 1	0	0
33	Q	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	0	7	Total 7	Cl 7	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	3	Total 3	Sr 3	0	0
34	B	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	R	1	Total 1	Sr 1	0	0
34	S	1	Total 1	Sr 1	0	0
34	T	1	Total 1	Sr 1	0	0
34	Y	1	Total 1	Sr 1	0	0
34	1	2	Total 2	Sr 2	0	0
34	3	3	Total 3	Sr 3	0	0
34	0	91	Total 91	Sr 91	0	0
34	9	2	Total 2	Sr 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total Na 1 1	0	0
35	C	3	Total Na 3 3	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	2	1	Total Na 1 1	0	0
35	0	60	Total Na 60 60	0	0
35	9	2	Total Na 2 2	0	0

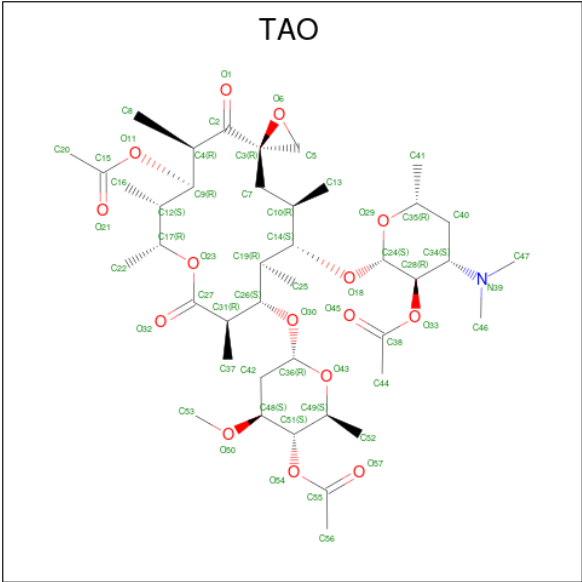
- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

- Molecule 37 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is TROLEANDOMYCIN (CCD ID: TAO) (formula: C₄₁H₆₇NO₁₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	0	1	Total	C	N	O	0	0
			57	41	1	15		

• Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	A	106	Total	O	0	0
			106	106		
39	B	135	Total	O	0	0
			135	135		
39	C	168	Total	O	0	0
			168	168		
39	D	45	Total	O	0	0
			45	45		
39	E	40	Total	O	0	0
			40	40		
39	F	23	Total	O	0	0
			23	23		
39	G	18	Total	O	0	0
			18	18		
39	H	71	Total	O	0	0
			71	71		
39	I	7	Total	O	0	0
			7	7		
39	J	46	Total	O	0	0
			46	46		
39	K	52	Total	O	0	0
			52	52		

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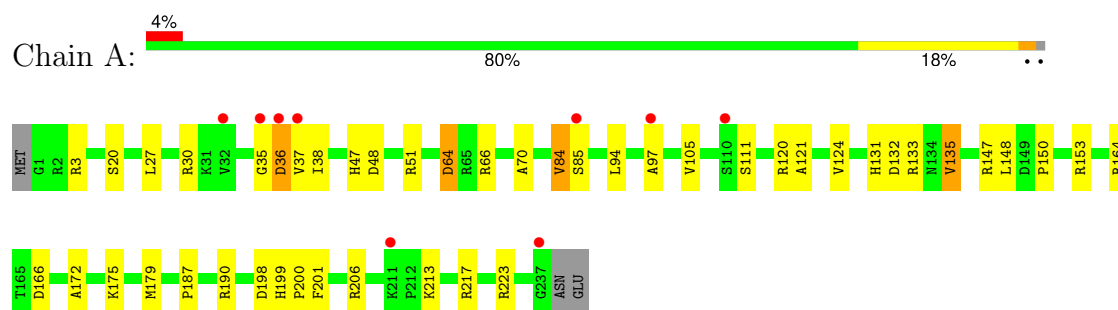
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	L	87	Total 87	O 87	0	0
39	M	123	Total 123	O 123	0	0
39	N	66	Total 66	O 66	0	0
39	O	44	Total 44	O 44	0	0
39	P	55	Total 55	O 55	0	0
39	Q	42	Total 42	O 42	0	0
39	R	78	Total 78	O 78	0	0
39	S	28	Total 28	O 28	0	0
39	T	35	Total 35	O 35	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	66	Total 66	O 66	0	0
39	X	22	Total 22	O 22	0	0
39	Y	94	Total 94	O 94	0	0
39	Z	27	Total 27	O 27	0	0
39	1	49	Total 49	O 49	0	0
39	2	34	Total 34	O 34	0	0
39	3	62	Total 62	O 62	0	0
39	0	6021	Total 6021	O 6021	0	0
39	9	142	Total 142	O 142	0	0

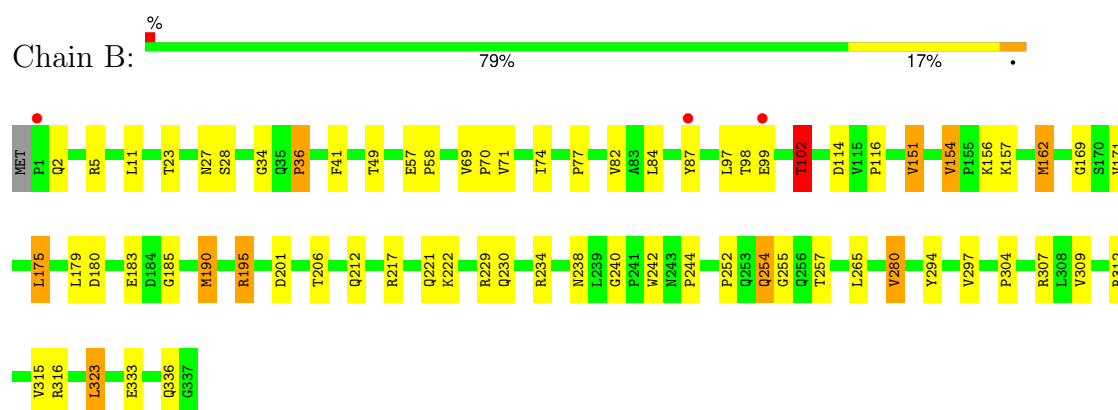
3 Residue-property plots [i](#)

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.

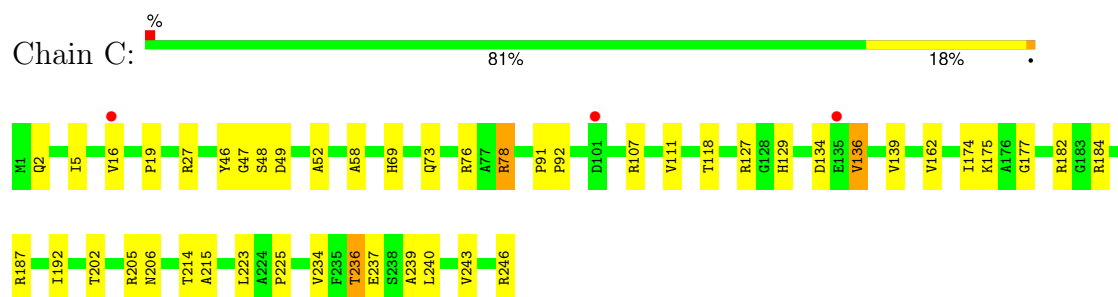
- Molecule 1: 50S ribosomal protein L2P



- Molecule 2: 50S ribosomal protein L3P

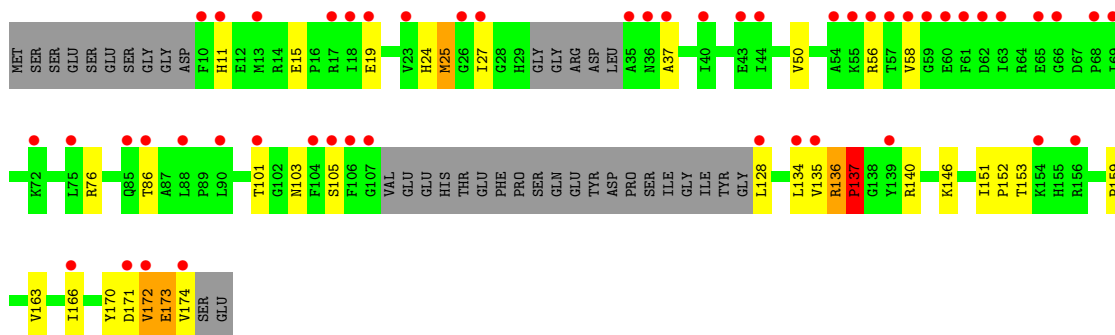


- Molecule 3: 50S ribosomal protein L4P

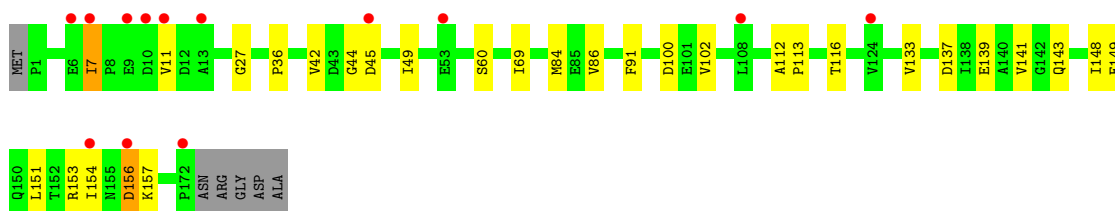
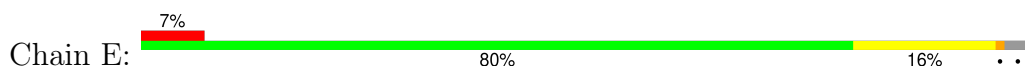


- Molecule 4: 50S ribosomal protein L5P

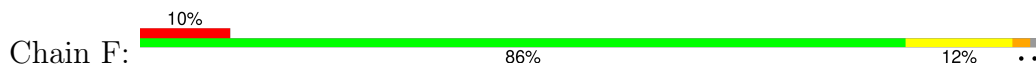




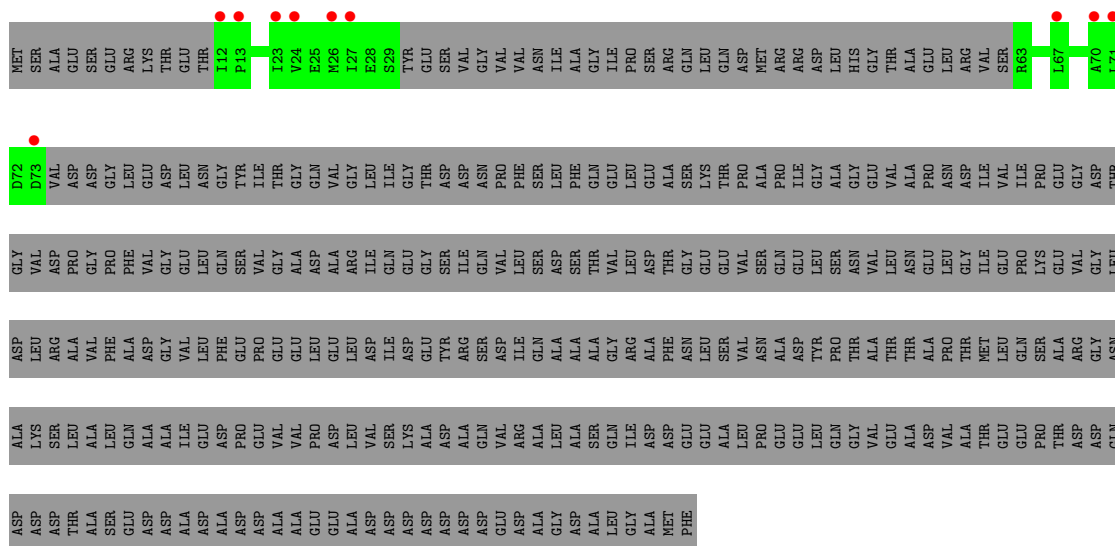
- Molecule 5: 50S ribosomal protein L6P



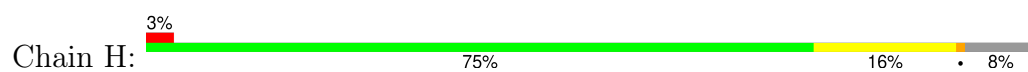
- Molecule 6: 50S ribosomal protein L7Ae



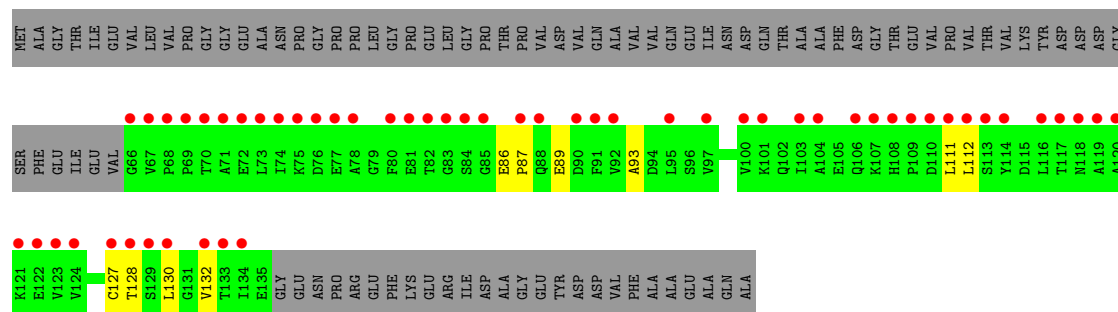
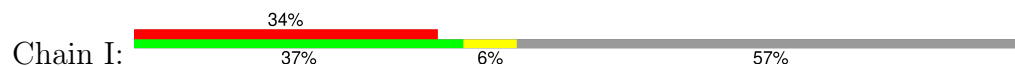
- Molecule 7: 50S ribosomal protein L10E



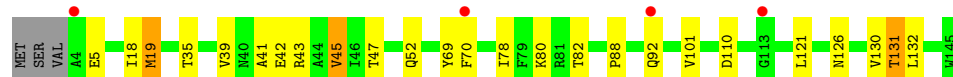
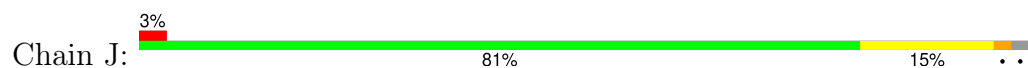
- Molecule 8: 50S ribosomal protein L10e



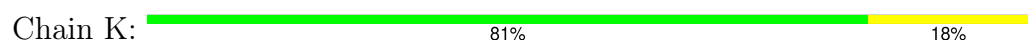
- Molecule 9: 50S ribosomal protein L11P



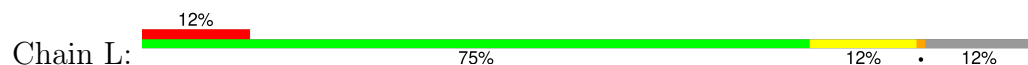
- Molecule 10: 50S ribosomal protein L13P



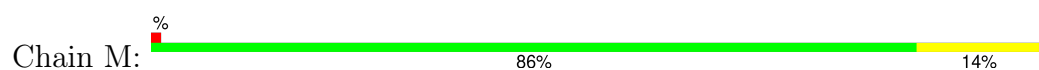
- Molecule 11: 50S ribosomal protein L14P



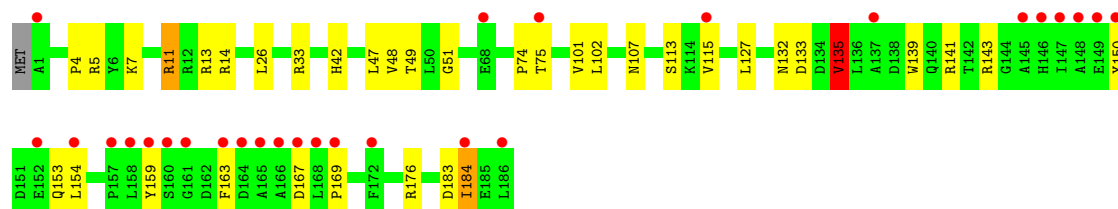
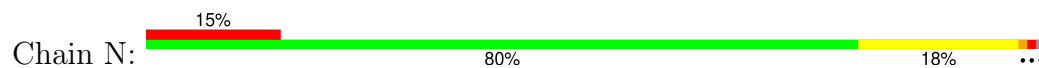
- Molecule 12: 50S ribosomal protein L15P



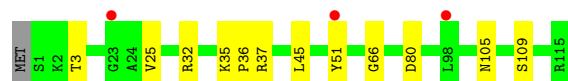
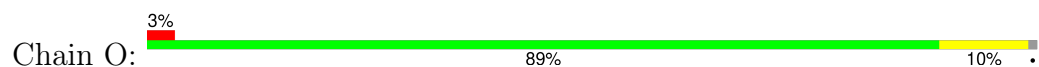
- Molecule 13: 50S ribosomal protein L15e



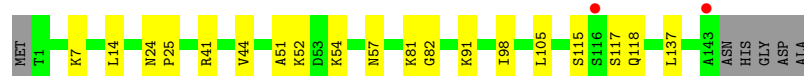
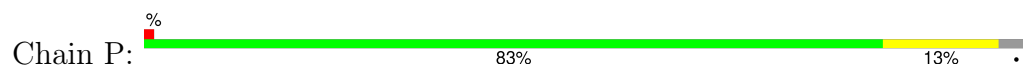
- Molecule 14: 50S ribosomal protein L18P



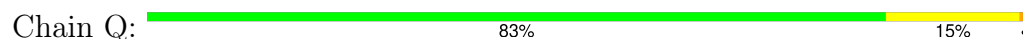
- Molecule 15: 50S ribosomal protein L18e



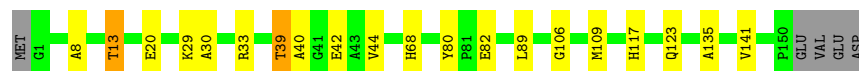
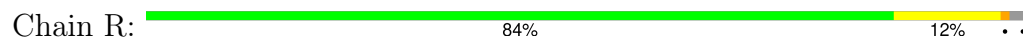
- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e



- Molecule 18: 50S ribosomal protein L22P

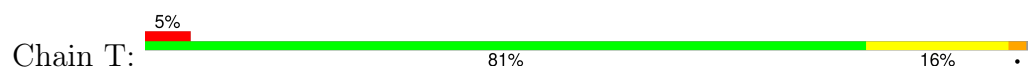


- Molecule 19: 50S ribosomal protein L23P





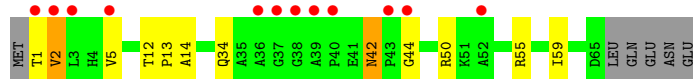
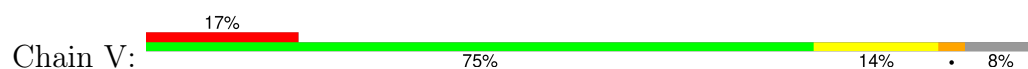
- Molecule 20: 50S ribosomal protein L24P



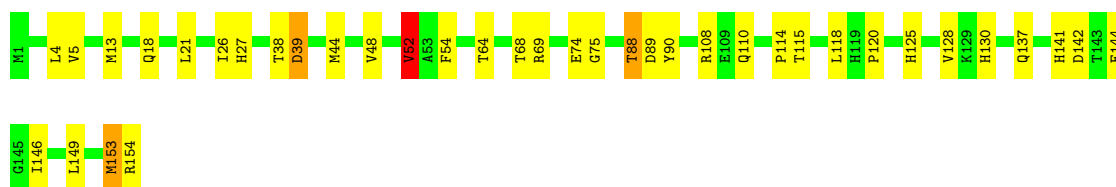
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P



- Molecule 23: 50S ribosomal protein L30P

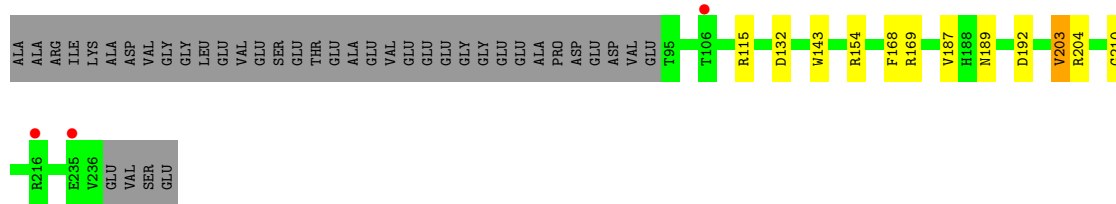


- Molecule 24: 50S ribosomal protein L31e

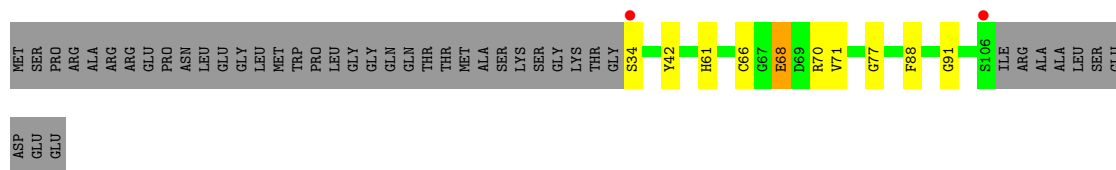


- Molecule 25: 50S ribosomal protein L32e





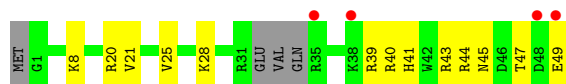
- Molecule 26: 50S ribosomal protein L37Ae



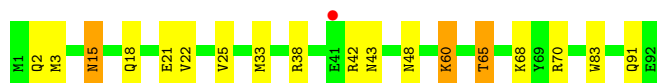
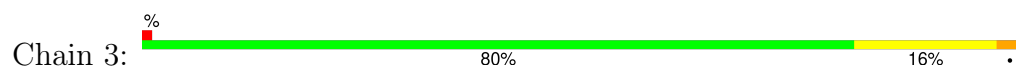
- Molecule 27: 50S ribosomal protein L37e



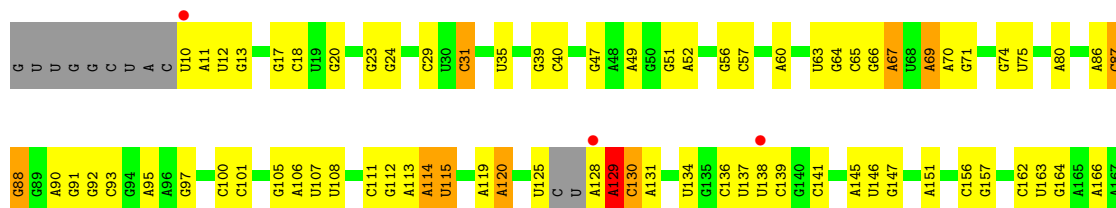
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E

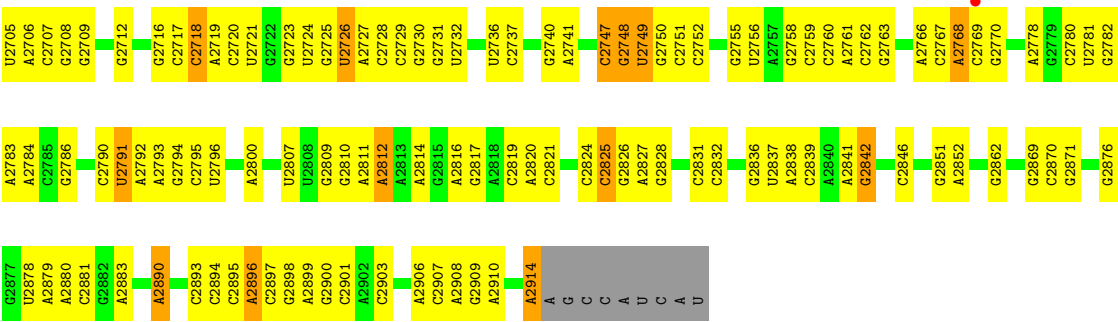


- Molecule 30: 23S ribosomal RNA

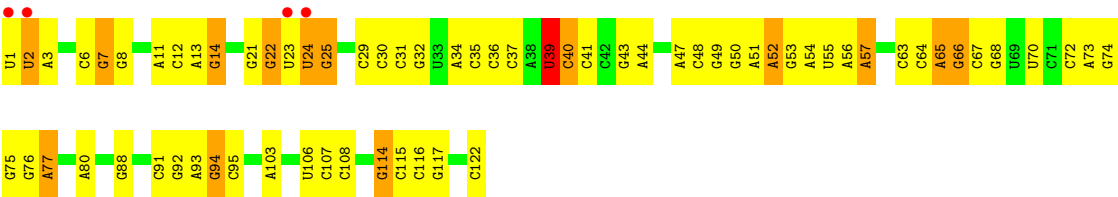


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G1398	A1308	G1217	A1152	G1063	G	G	G	C881	U794	C696	U612	C515	A419	G334	C250	A169
A1399	U1310	U1218	C1153	G1063	C	U	C	A882	G795	G697	U613	A516	A429	U335	U170	C171
C1400	G1311	G1221	U1066	U1066	U	C	C	G885	A797	C699	U614	G518	A430	G336	C256	G175
A1407	G1312	G1221	G1155	C1068	C	C	C	A886	G798	A700	A620	A519	C440	C337	G257	U176
U1408	A1313	G1224	C1157	G1068	G	C	C	G887	C799	U701	G621	U522	A441	C338	G258	U177
G1409	G1319	C1225	G1158	C1069	A	A	A	U888	G800	G702	U625	G523	A442	A339	G259	U178
G1410	G1320	C1228	G1159	G1072	G	G	G	U888	A806	G703	U625	G524	U445	C342	C260	G182
A1413	A1328	C1229	G1160	A1073	A	A	A	C896	A807	C704	U626	G525	U446	C343	A261	G183
G1414	G1329	A1230	G1162	G1074	G	G	G	A897	A808	G705	U627	G526	U447	C344	A262	G184
G1415	G1330	U1234	G1163	A1078	A	A	A	G898	G809	C707	A628	U527	U448	C345	U265	G185
G1416	A1331	G1235	G1165	A1079	G	G	G	G902	A812	G709	A632	A532	A449	C346	C271	A186
G1417	G1332	U1236	G1166	C1080	U	U	U	U903	C813	G710	C633	G537	A450	C347	A272	A187
U1418	C1332	C1237	G1167	A1081	C	C	C	U904	C814	G711	A635	U538	A451	C348	G273	C188
U1419	U1333	C1238	G1168	A1082	G	G	G	C905	U815	G712	C636	G539	C452	C349	G274	A189
U1422	C1334	G1239	C	C	C	C	C	C906	C816	U713	C637	A540	A453	C350	G275	G190
C1423	G1335	G1240	A1171	G1087	C	C	C	C907	C817	U714	C638	A541	U454	G358	A191	A192
A1424	G1339	G1241	G1172	A1088	A	A	A	C920	A818	U	A639	C542	A455	U359	C280	C195
G1425	C1342	C1242	A1173	G1089	C	C	C	G921	A819	G716	G644	G544	C458	A360	U281	G196
A1426	G1343	U1244	A1174	A1090	A	A	A	A922	G820	C729	U645	G545	A459	C363	C282	C199
A1427	G1344	C1245	G1175	A1091	C	C	C	A923	C822	U731	G646	G546	A460	C364	U283	G205
G1433	U1345	A1246	G1177	G1092	A1006	A1006	A1006	G924	U823	G732	U647	C546	C461	C365	A285	A199
A1434	U1346	C1250	G1178	G1099	C1008	C1008	C1008	G925	U824	U733	A654	C553	A466	U366	C286	C200
C1439	A1352	C1251	U1180	G1100	U1007	U1007	U1007	G940	G828	U734	U655	U555	U468	C368	U287	A204
U1440	C1353	C1253	C1104	C1104	C1010	C1010	C1010	G941	G834	A737	G656	C556	U469	C371	G289	A205
A1441	A1357	G1260	A1107	A1107	A1014	A1014	A1014	U942	U835	G738	G657	C557	U470	A372	C290	C291
G1443	U1358	A1261	G1108	G1108	C1015	C1015	C1015	A943	G836	G743	C658	U559	U471	C376	C292	A212
G1444	U1359	C1262	G1109	G1109	U1016	U1016	U1016	U944	U840	G744	A659	U560	A472	C377	G213	G214
U1445	C1360	U1266	G1110	G1110	G1023	G1023	G1023	C946	A841	G745	A660	G561	A473	C378	U214	U215
U1446	G1361	G1267	U1116	U1116	G1024	G1024	G1024	U947	C842	A746	G661	A562	A474	A378	C217	C218
U1447	U1362	C1268	A1117	A1117	G1027	G1027	G1027	G948	A843	G747	A666	C583	C483	G381	G219	G220
C1450	G1363	G1269	U1118	U1118	U1028	U1028	U1028	A951	A844	C748	C667	G564	A484	U392	G301	G302
C1456	C1365	A1278	G1119	G1119	U1029	U1029	U1029	G952	U845	A761	C668	A565	A485	U393	A303	G303
U1457	C1366	U1279	U1120	U1120	U1039	U1039	U1039	G953	A846	G764	C669	A566	A486	G394	G304	G221
U1461	U1370	G1283	G1121	G1121	G1040	G1040	G1040	U954	C848	C765	A671	U567	C487	C395	U308	A222
C1462	U1371	U1284	C1127	C1127	U1041	U1041	U1041	A955	C853	A766	G672	G579	C489	U396	C309	G225
A1471	A1375	U1285	U1128	U1128	U1042	U1042	U1042	G958	G854	A767	C677	A580	U493	A397	A226	A227
C1472	G1376	A1286	C1129	C1129	G1043	G1043	G1043	C959	U855	C678	G678	U582	A487	U398	U312	C228
U1473	U1377	U1287	G1131	G1131	C1044	C1044	C1044	G960	G856	C772	C583	U584	A488	C400	G229	G229
C1474	G1378	U1288	A1132	A1132	G1045	G1045	G1045	A961	A857	A773	G681	G503	C401	C401	A316	A317
C1477	U1379	C1289	G1133	G1133	G1046	G1046	G1046	C962	U858	G776	A682	G504	U402	U402	U318	U318
G1481	G1384	G1290	U1135	U1135	C1051	C1051	C1051	G963	G868	A777	G683	G588	C505	A407	A319	A236
A1482	U1380	U1295	G1136	G1136	G1052	G1052	G1052	G968	C869	U778	G684	C589	G506	A408	A320	G237
C1483	G1391	G300	U1137	U1137	G1053	G1053	G1053	G969	G870	U779	A686	C598	A507	U409	A321	G237
G1484	A1392	U1304	G1138	G1138	G1054	G1054	G1054	U970	G871	G782	C687	G600	A508	A410	G322	A241
A1485	A1393	U1306	U1139	U1139	G1055	G1055	G1055	G	U872	G782	A688	A602	A509	A411	G323	A241
			C1140	C1140	U1056	U1056	U1056	U	U875	A790	G691	A603	U510	A415	G324	C244
			G1145	G1145	A1057	A1057	A1057	U	A876	A791	G691	A604	A511	A416	U325	A247
					G1058	G1058	G1058	C	G877	G792	A694	C605	A513	G417	A248	A248

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U2607	A2511	C2427	A	C2242	A2103	U2012	A1931	A1822	G1745	A1657	A1573	A1494
C2608	U2512	G2428	C	U2243	C2104	G2013	G1932	C1823	U1749	A1658	G1586	C1495
G2613	A2517	A2434	G	A2244	C2106	U2016	G1933	C1825	G1752	A1660	G1587	A1496
U2614	A2521	U2435	A	C2247	G2110	U2017	A1934	C1826	C1753	G1662	G1588	G1497
U2615	G2524	G2436	C	C2250	G2112	C2020	C1936	G1828	G1756	G1663	G1589	U1498
G2616	U2525	C2439	C	G2251	A2111	C2021	U1937	A1829	U1757	C1666	G1592	U1500
U2619	C2526	U2440	G	A2252	G2113	A2030	G1938	C1830	U1758	C1667	C1593	U1503
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U2621	U2531	U2443	U	G2256	U2115	U2032	A1941	U1835	G1760	G1669	U1595	U1505
C2629	A2532	U2444	A	G2257	U2116	G2033	A1942	U1838	U1761	A1670	A1597	U1506
G2630	C2533	G2446	G	A2258	U2120	U2034	C1943	U1839	C1762	A1598	U1599	U1511
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C2644	U2541	A2465	C	C2269	G	C2047	U	U1850	C1772	A1682	A1606	C1521
U2645	C2542	C2466	C	G2270	C	G2050	A	G1851	G1773	G1683	A1607	U1521
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C2668	U2585	A2485	C	A2301	C	A2081	G1974	U1883	C1798	G1712	A1632	C1551
U2669	U2586	C2488	U	A2302	G	G2082	A1994	U1884	C1798	A1717	C1633	G1552
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U2671	U2590	A2490	C	U2307	U	G2087	G2000	C1894	A1804	G1723	U1635	C1554
C2672	C2591	G2491	C	C2309	C	A2088	G1995	U1903	G1805	U1724	G1636	G1555
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	G2602	C2508	G						G1820	G1743		
	G2603	A2509	G									



● Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.43Å 300.77Å 575.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 50.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	84.3 (50.00-2.90) 84.2 (50.00-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.243 0.189 , 0.237	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99181	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: SR, CL, OMU, NA, PSU, MG, CD, TAO, 1MA, K, OMG, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.63	0/1786	1.12	10/2408 (0.4%)
2	B	0.63	2/2690 (0.1%)	1.10	13/3652 (0.4%)
3	C	0.63	0/1885	1.13	9/2552 (0.4%)
4	D	0.73	1/1111 (0.1%)	1.17	9/1498 (0.6%)
5	E	0.66	0/1382	1.02	4/1880 (0.2%)
6	F	0.69	1/901 (0.1%)	1.12	3/1224 (0.2%)
7	G	0.61	0/241	1.00	0/324
8	H	0.61	0/1303	1.05	8/1743 (0.5%)
9	I	0.72	0/526	1.14	1/716 (0.1%)
10	J	0.62	1/1136 (0.1%)	1.08	4/1530 (0.3%)
11	K	0.61	0/1004	1.14	8/1351 (0.6%)
12	L	0.55	0/1130	1.09	8/1509 (0.5%)
13	M	0.55	0/1583	1.06	5/2116 (0.2%)
14	N	0.60	0/1474	1.20	17/1999 (0.9%)
15	O	0.59	0/874	1.08	4/1181 (0.3%)
16	P	0.54	0/1147	1.03	1/1528 (0.1%)
17	Q	0.58	0/749	1.11	6/1005 (0.6%)
18	R	0.66	1/1172 (0.1%)	1.10	4/1578 (0.3%)
19	S	0.57	0/648	0.97	0/875
20	T	0.57	0/958	1.12	5/1289 (0.4%)
21	U	0.56	0/417	1.05	1/562 (0.2%)
22	V	0.59	0/502	1.19	3/675 (0.4%)
23	W	0.67	1/1219 (0.1%)	1.16	7/1655 (0.4%)
24	X	0.69	0/664	1.22	7/895 (0.8%)
25	Y	0.58	0/1146	1.07	2/1536 (0.1%)
26	Z	0.60	0/584	1.14	3/781 (0.4%)
27	1	0.57	0/438	1.02	4/578 (0.7%)
28	2	0.50	0/401	1.00	1/529 (0.2%)
29	3	0.53	0/771	0.93	2/1024 (0.2%)
30	0	0.39	0/65957	0.61	18/102867 (0.0%)
31	9	0.38	0/2904	0.59	2/4526 (0.0%)
All	All	0.47	7/98703 (0.0%)	0.77	169/147586 (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
23	W	0	1
30	0	0	35
31	9	0	2
All	All	0	38

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	63	ILE	CA-CB	8.72	1.58	1.54
18	R	109	MET	SD-CE	-7.01	1.62	1.79
2	B	190	MET	SD-CE	-6.59	1.63	1.79
2	B	162	MET	SD-CE	-6.40	1.63	1.79
23	W	153	MET	SD-CE	-5.97	1.64	1.79

The worst 5 of 169 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	170	TYR	N-CA-C	9.59	124.51	112.24
23	W	75	GLY	N-CA-C	9.21	120.70	111.95
20	T	52	ARG	N-CA-C	9.15	124.95	113.43
4	D	136	ARG	CA-C-N	7.83	129.63	119.84
4	D	136	ARG	C-N-CA	7.83	129.63	119.84

There are no chirality outliers.

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	482	G	Sidechain
30	0	49	A	Sidechain
23	W	90	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	22	0
2	B	2625	0	2533	36	0
3	C	1860	0	1813	28	0
4	D	1094	0	1085	16	0
5	E	1357	0	1266	15	0
6	F	890	0	843	5	0
7	G	240	0	231	0	0
8	H	1283	0	1292	17	0
9	I	519	0	500	6	0
10	J	1120	0	1098	17	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	10	0
13	M	1559	0	1573	19	0
14	N	1445	0	1401	15	0
15	O	865	0	873	6	0
16	P	1136	0	1123	12	0
17	Q	735	0	729	9	0
18	R	1149	0	1122	11	0
19	S	641	0	605	9	0
20	T	950	0	924	10	0
21	U	410	0	364	5	0
22	V	499	0	511	7	0
23	W	1196	0	1137	21	0
24	X	654	0	653	8	0
25	Y	1130	0	1133	10	0
26	Z	573	0	531	5	0
27	1	431	0	426	15	0
28	2	396	0	413	10	0
29	3	755	0	728	9	0
30	0	59020	0	29812	1177	0
31	9	2599	0	1325	71	0
32	0	82	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	0	0
33	K	1	0	0	2	0
33	L	2	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	91	0	0	0	0
34	1	2	0	0	0	0
34	3	3	0	0	0	0
34	9	2	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	60	0	0	0	0
35	2	1	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	3	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	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	57	0	67	14	0
39	0	6021	0	0	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	1	49	0	0	0	0
39	2	34	0	0	0	0
39	3	62	0	0	0	0
39	9	142	0	0	3	0
39	A	106	0	0	4	0
39	B	135	0	0	4	0
39	C	168	0	0	2	0
39	D	45	0	0	0	0
39	E	40	0	0	1	0
39	F	23	0	0	0	0
39	G	18	0	0	0	0
39	H	71	0	0	1	0
39	I	7	0	0	0	0
39	J	46	0	0	1	0
39	K	52	0	0	0	0
39	L	87	0	0	2	0
39	M	123	0	0	0	0
39	N	66	0	0	2	0
39	O	44	0	0	1	0
39	P	55	0	0	0	0
39	Q	42	0	0	0	0
39	R	78	0	0	2	0
39	S	28	0	0	0	0
39	T	35	0	0	1	0
39	U	26	0	0	0	0
39	V	11	0	0	0	0
39	W	66	0	0	1	0
39	X	22	0	0	0	0
39	Y	94	0	0	3	0
39	Z	27	0	0	0	0
All	All	99181	0	59980	1437	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

The worst 5 of 1437 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.25	1.16
30:0:871:G:H5'	30:0:871:G:H8	1.06	1.08
30:0:871:G:H5'	30:0:871:G:C8	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2717:C:H2'	30:0:2718:C:H5''	1.42	1.01
10:J:82:THR:HG23	30:0:1242:A:H5'	1.42	1.01

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	219 (93%)	14 (6%)	2 (1%)	14	41
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	14	41
3	C	244/246 (99%)	225 (92%)	19 (8%)	0	100	100
4	D	134/177 (76%)	121 (90%)	10 (8%)	3 (2%)	5	20
5	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
6	F	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	4	17
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/174 (90%)	146 (94%)	9 (6%)	1 (1%)	21	51
9	I	68/162 (42%)	62 (91%)	6 (9%)	0	100	100
10	J	140/145 (97%)	133 (95%)	6 (4%)	1 (1%)	18	48
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	131 (93%)	10 (7%)	0	100	100
13	M	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	4	16
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	4 (4%)	1 (1%)	11	36
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	18	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	111 (95%)	4 (3%)	2 (2%)	7	26
21	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	4	17
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	62 (87%)	9 (13%)	0	100	100
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	4 (4%)	0	100	100
All	All	3705/4466 (83%)	3492 (94%)	189 (5%)	24 (1%)	21	51

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
4	D	137	PRO
6	F	101	ALA
10	J	5	GLU
14	N	154	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	
1	A	179/182 (98%)	164 (92%)	15 (8%)	10	31
2	B	282/283 (100%)	264 (94%)	18 (6%)	16	44
3	C	193/193 (100%)	178 (92%)	15 (8%)	11	35
4	D	117/148 (79%)	106 (91%)	11 (9%)	8	26
5	E	152/156 (97%)	146 (96%)	6 (4%)	28	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	93/94 (99%)	89 (96%)	4 (4%)	26	60
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/143 (94%)	128 (96%)	6 (4%)	24	58
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	82
10	J	118/121 (98%)	113 (96%)	5 (4%)	26	60
11	K	106/106 (100%)	98 (92%)	8 (8%)	12	37
12	L	113/127 (89%)	109 (96%)	4 (4%)	32	66
13	M	158/158 (100%)	152 (96%)	6 (4%)	29	64
14	N	149/150 (99%)	141 (95%)	8 (5%)	20	51
15	O	93/94 (99%)	91 (98%)	2 (2%)	45	77
16	P	113/117 (97%)	110 (97%)	3 (3%)	39	73
17	Q	79/80 (99%)	74 (94%)	5 (6%)	16	45
18	R	117/122 (96%)	115 (98%)	2 (2%)	53	82
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	60
20	T	105/106 (99%)	98 (93%)	7 (7%)	15	43
21	U	44/52 (85%)	43 (98%)	1 (2%)	44	76
22	V	51/57 (90%)	48 (94%)	3 (6%)	18	48
23	W	130/130 (100%)	124 (95%)	6 (5%)	24	57
24	X	66/74 (89%)	59 (89%)	7 (11%)	6	22
25	Y	120/196 (61%)	117 (98%)	3 (2%)	42	74
26	Z	60/94 (64%)	59 (98%)	1 (2%)	53	82
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	77
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	72 (91%)	7 (9%)	9	28
All	All	3095/3641 (85%)	2937 (95%)	158 (5%)	21	53

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	Q	75	ILE
24	X	72	VAL
19	S	10	VAL
22	V	5	VAL
27	1	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
19	S	9	HIS
25	Y	134	HIS
19	S	53	ASN
22	V	60	GLN
27	1	8	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	22 (0%)
31	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3045 (94%)	255 (8%)	23 (0%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1730	G
30	0	2313	C
30	0	2103	A
30	0	2467	A
30	0	877	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	1MA	0	628	30	21,25,26	0.73	1 (4%)	30,37,40	0.78	1 (3%)
30	UR3	0	2619	30	19,22,23	0.44	0	26,32,35	0.71	1 (3%)
30	PSU	0	2621	30	18,21,22	1.58	2 (11%)	21,30,33	1.36	3 (14%)
30	OMU	0	2587	30,35	19,22,23	0.32	0	25,31,34	0.36	0
30	OMG	0	2588	30	23,26,27	0.28	0	32,38,41	0.42	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
30	1MA	0	628	30	-	2/7/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30,35	-	0/9/27/28	0/2/2/2
30	OMG	0	2588	30	-	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)
30	0	2621	PSU	C2-N1	5.12	1.43	1.36
30	0	2621	PSU	C6-C5	3.17	1.38	1.35
30	0	628	1MA	C6-N6	2.56	1.34	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.22	120.34	118.17
30	0	2621	PSU	C6-N1-C2	-3.11	119.81	122.69
30	0	2621	PSU	O2-C2-N1	3.04	125.92	122.79
30	0	2619	UR3	C4-N3-C2	2.82	126.84	124.58
30	0	628	1MA	N1-C2-N3	2.78	129.30	126.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	1	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	TAO	0	2924	-	59,60,60	0.69	1 (1%)	78,89,89	1.88	17 (21%)

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	TAO	0	2924	-	2/2/24/24	14/77/113/113	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	0	2924	TAO	C5-C3	2.34	1.52	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	TAO	O33-C38-C44	6.10	121.97	111.09
38	0	2924	TAO	C17-O23-C27	-4.82	110.42	117.55
38	0	2924	TAO	O54-C55-C56	4.80	119.65	111.09
38	0	2924	TAO	O11-C15-C20	4.51	119.13	111.09
38	0	2924	TAO	C51-O54-C55	-4.25	111.12	117.72

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
38	0	2924	TAO	C10
38	0	2924	TAO	C9

5 of 14 torsion outliers are listed below:

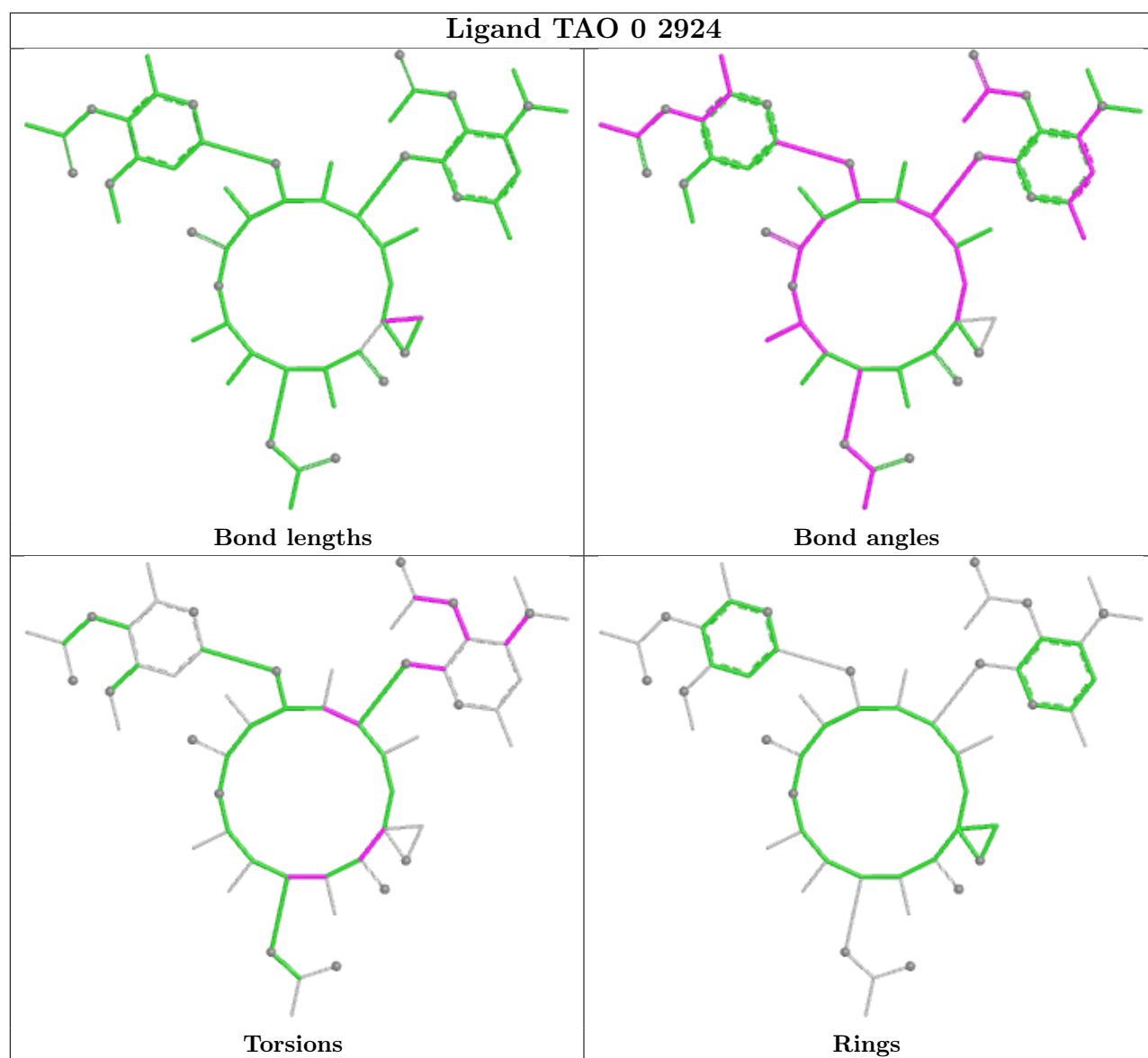
Mol	Chain	Res	Type	Atoms
38	0	2924	TAO	C44-C38-O33-C28
38	0	2924	TAO	O45-C38-O33-C28
38	0	2924	TAO	C10-C14-C19-C25
38	0	2924	TAO	C34-C28-O33-C38
38	0	2924	TAO	C40-C34-N39-C47

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	TAO	14	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	A	237/240 (98%)	0.20	9 (3%) 44 36	19, 43, 83, 105	0
2	B	337/338 (99%)	0.34	3 (0%) 81 75	17, 47, 75, 90	0
3	C	246/246 (100%)	0.25	3 (1%) 76 69	12, 41, 66, 78	0
4	D	140/177 (79%)	1.74	50 (35%) 1 0	51, 92, 120, 131	0
5	E	172/178 (96%)	0.70	13 (7%) 20 16	39, 62, 89, 96	0
6	F	119/120 (99%)	0.94	12 (10%) 12 10	43, 70, 104, 120	0
7	G	29/348 (8%)	1.69	10 (34%) 1 1	62, 88, 97, 98	0
8	H	160/174 (91%)	0.38	6 (3%) 44 36	24, 48, 85, 99	0
9	I	70/162 (43%)	2.90	55 (78%) 0 0	124, 138, 160, 161	0
10	J	142/145 (97%)	0.29	4 (2%) 55 46	25, 43, 65, 80	0
11	K	132/132 (100%)	0.22	0 100 100	25, 43, 68, 75	0
12	L	145/165 (87%)	0.73	19 (13%) 7 6	13, 60, 107, 118	0
13	M	194/194 (100%)	0.04	1 (0%) 87 83	22, 36, 55, 62	0
14	N	186/187 (99%)	0.93	28 (15%) 5 4	32, 58, 111, 119	0
15	O	115/116 (99%)	0.51	3 (2%) 57 48	30, 49, 66, 74	0
16	P	143/149 (95%)	0.48	2 (1%) 73 65	30, 49, 64, 67	0
17	Q	95/96 (98%)	0.01	0 100 100	25, 36, 51, 71	0
18	R	150/155 (96%)	-0.05	0 100 100	21, 37, 61, 73	0
19	S	81/85 (95%)	0.35	1 (1%) 76 69	35, 57, 74, 82	0
20	T	119/120 (99%)	0.56	6 (5%) 34 27	32, 53, 80, 100	0
21	U	53/66 (80%)	0.30	0 100 100	30, 49, 70, 74	0
22	V	65/71 (91%)	1.32	12 (18%) 3 3	49, 72, 108, 116	0
23	W	154/154 (100%)	0.10	0 100 100	26, 40, 59, 70	0
24	X	82/92 (89%)	0.47	4 (4%) 35 27	36, 49, 73, 84	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.15	3 (2%) 63 54	18, 39, 64, 81	0
26	Z	73/116 (62%)	0.61	2 (2%) 56 47	34, 54, 77, 93	0
27	1	56/57 (98%)	-0.41	0 100 100	16, 26, 35, 43	0
28	2	46/50 (92%)	0.65	4 (8%) 16 13	29, 56, 81, 98	0
29	3	92/92 (100%)	0.24	1 (1%) 78 71	27, 47, 62, 73	0
30	0	2749/2923 (94%)	-0.45	31 (1%) 78 71	11, 36, 81, 154	0
31	9	122/122 (100%)	-0.07	4 (3%) 49 40	22, 51, 78, 129	0
All	All	6646/7511 (88%)	0.09	286 (4%) 40 31	11, 44, 93, 161	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	128	THR	7.5
22	V	1	THR	7.3
9	I	97	VAL	6.1
9	I	112	LEU	6.1
4	D	10	PHE	5.8

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	OMG	0	2588	24/25	0.97	0.07	20,23,24,28	0
30	UR3	0	2619	21/22	0.97	0.07	21,24,26,29	0
30	1MA	0	628	23/24	0.98	0.06	13,18,20,21	0
30	OMU	0	2587	21/22	0.98	0.07	22,25,29,32	0
30	PSU	0	2621	20/21	0.98	0.05	18,19,25,25	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
35	NA	0	8525	1/1	0.13	0.72	107,107,107,107	0
34	SR	0	8977	1/1	0.31	0.16	194,194,194,194	0
35	NA	0	8557	1/1	0.37	0.70	89,89,89,89	0
35	NA	0	8571	1/1	0.41	0.32	73,73,73,73	0
34	SR	0	8991	1/1	0.51	0.20	162,162,162,162	0
34	SR	A	8993	1/1	0.51	0.18	200,200,200,200	0
35	NA	0	8573	1/1	0.53	0.34	65,65,65,65	0
34	SR	0	8954	1/1	0.57	0.27	198,198,198,198	0
34	SR	0	8967	1/1	0.58	0.41	191,191,191,191	0
34	SR	9	9003	1/1	0.59	0.23	195,195,195,195	0
34	SR	0	8970	1/1	0.60	0.23	200,200,200,200	0
35	NA	0	8511	1/1	0.62	0.22	56,56,56,56	0
34	SR	0	8925	1/1	0.63	0.17	178,178,178,178	0
34	SR	A	8930	1/1	0.63	0.36	200,200,200,200	0
34	SR	0	9005	1/1	0.63	0.20	190,190,190,190	0
32	MG	0	8071	1/1	0.65	0.74	136,136,136,136	0
34	SR	0	8971	1/1	0.66	0.23	195,195,195,195	0
34	SR	0	8923	1/1	0.66	0.22	165,165,165,165	0
34	SR	0	8983	1/1	0.66	0.27	170,170,170,170	0
34	SR	0	8984	1/1	0.66	0.26	170,170,170,170	0
34	SR	B	8950	1/1	0.66	0.38	196,196,196,196	0
34	SR	0	8926	1/1	0.66	0.30	199,199,199,199	0
34	SR	T	8939	1/1	0.67	0.25	200,200,200,200	0
34	SR	0	8906	1/1	0.67	0.28	191,191,191,191	0
34	SR	Y	9002	1/1	0.68	0.23	200,200,200,200	0
34	SR	0	8973	1/1	0.68	0.18	178,178,178,178	0
35	NA	0	8548	1/1	0.68	0.33	59,59,59,59	0
34	SR	0	8907	1/1	0.68	0.24	180,180,180,180	0
34	SR	0	8911	1/1	0.68	0.19	200,200,200,200	0
35	NA	C	8558	1/1	0.68	0.21	33,33,33,33	0
34	SR	1	8952	1/1	0.69	0.41	200,200,200,200	0
34	SR	9	8980	1/1	0.69	0.23	200,200,200,200	0
34	SR	0	8988	1/1	0.70	0.14	177,177,177,177	0
34	SR	0	8959	1/1	0.70	0.18	195,195,195,195	0
34	SR	0	8966	1/1	0.70	0.13	178,178,178,178	0
34	SR	3	8999	1/1	0.70	0.23	200,200,200,200	0
35	NA	0	8574	1/1	0.70	0.35	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8535	1/1	0.71	0.34	68,68,68,68	0
35	NA	0	8522	1/1	0.71	0.40	73,73,73,73	0
34	SR	0	9001	1/1	0.71	0.21	187,187,187,187	0
34	SR	0	8920	1/1	0.72	0.33	200,200,200,200	0
34	SR	0	8960	1/1	0.72	0.23	200,200,200,200	0
34	SR	0	8964	1/1	0.72	0.23	188,188,188,188	0
32	MG	0	8034	1/1	0.73	0.22	60,60,60,60	0
34	SR	R	8912	1/1	0.73	0.20	157,157,157,157	0
35	NA	0	8570	1/1	0.73	0.37	81,81,81,81	0
34	SR	0	8942	1/1	0.74	0.23	162,162,162,162	0
34	SR	0	8944	1/1	0.74	0.33	200,200,200,200	0
34	SR	0	8938	1/1	0.74	0.25	200,200,200,200	0
35	NA	0	8564	1/1	0.74	0.42	91,91,91,91	0
34	SR	0	8941	1/1	0.75	0.32	180,180,180,180	0
34	SR	0	8937	1/1	0.76	0.19	155,155,155,155	0
35	NA	0	8520	1/1	0.76	0.24	44,44,44,44	0
34	SR	0	8931	1/1	0.76	0.26	193,193,193,193	0
35	NA	0	8502	1/1	0.76	0.23	54,54,54,54	0
34	SR	0	8986	1/1	0.77	0.32	200,200,200,200	0
34	SR	0	8958	1/1	0.77	0.19	147,147,147,147	0
34	SR	3	8932	1/1	0.77	0.16	133,133,133,133	0
34	SR	0	8922	1/1	0.77	0.21	155,155,155,155	0
34	SR	0	9004	1/1	0.77	0.28	200,200,200,200	0
35	NA	0	8507	1/1	0.77	0.32	68,68,68,68	0
34	SR	0	8956	1/1	0.78	0.11	147,147,147,147	0
34	SR	0	8943	1/1	0.78	0.24	179,179,179,179	0
34	SR	0	8976	1/1	0.78	0.25	195,195,195,195	0
34	SR	0	9000	1/1	0.78	0.34	200,200,200,200	0
35	NA	9	8572	1/1	0.78	0.32	103,103,103,103	0
34	SR	0	8928	1/1	0.79	0.43	200,200,200,200	0
35	NA	R	8532	1/1	0.80	0.20	39,39,39,39	0
35	NA	0	8501	1/1	0.80	0.19	29,29,29,29	0
34	SR	0	8968	1/1	0.80	0.20	170,170,170,170	0
35	NA	0	8559	1/1	0.80	0.60	94,94,94,94	0
33	CL	0	8822	1/1	0.80	0.17	59,59,59,59	0
35	NA	0	8567	1/1	0.80	0.38	63,63,63,63	0
34	SR	0	8933	1/1	0.80	0.22	137,137,137,137	0
34	SR	0	8965	1/1	0.80	0.15	143,143,143,143	0
34	SR	0	8927	1/1	0.80	0.19	184,184,184,184	0
35	NA	0	8523	1/1	0.80	0.15	46,46,46,46	0
34	SR	0	8919	1/1	0.80	0.18	188,188,188,188	0
34	SR	0	8917	1/1	0.81	0.35	199,199,199,199	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8995	1/1	0.81	0.28	164,164,164,164	0
32	MG	0	8091	1/1	0.81	0.18	79,79,79,79	0
34	SR	0	9006	1/1	0.81	0.24	192,192,192,192	0
35	NA	0	8560	1/1	0.81	0.40	104,104,104,104	0
35	NA	0	8531	1/1	0.81	0.24	47,47,47,47	0
37	K	0	8401	1/1	0.81	0.44	150,150,150,150	0
38	TAO	0	2924	57/57	0.81	0.28	83,95,107,109	0
35	NA	0	8509	1/1	0.82	0.27	53,53,53,53	0
34	SR	0	8997	1/1	0.82	0.45	200,200,200,200	0
35	NA	S	8510	1/1	0.82	0.14	35,35,35,35	0
32	MG	2	8060	1/1	0.82	0.20	67,67,67,67	0
34	SR	0	9008	1/1	0.82	0.14	135,135,135,135	0
35	NA	J	8538	1/1	0.82	0.13	49,49,49,49	0
35	NA	0	8561	1/1	0.82	0.32	52,52,52,52	0
35	NA	0	8526	1/1	0.82	0.12	51,51,51,51	0
35	NA	0	8556	1/1	0.83	0.21	41,41,41,41	0
35	NA	0	8505	1/1	0.83	0.32	31,31,31,31	0
35	NA	0	8528	1/1	0.83	0.17	49,49,49,49	0
35	NA	0	8529	1/1	0.83	0.20	33,33,33,33	0
32	MG	0	8059	1/1	0.83	0.10	33,33,33,33	0
34	SR	0	8963	1/1	0.83	0.14	182,182,182,182	0
33	CL	J	8802	1/1	0.83	0.16	66,66,66,66	0
34	SR	0	8955	1/1	0.84	0.26	184,184,184,184	0
34	SR	0	8946	1/1	0.84	0.33	190,190,190,190	0
34	SR	0	8951	1/1	0.84	0.14	164,164,164,164	0
34	SR	0	8924	1/1	0.84	0.17	184,184,184,184	0
34	SR	0	8989	1/1	0.84	0.27	200,200,200,200	0
35	NA	0	8546	1/1	0.84	0.38	106,106,106,106	0
34	SR	0	8978	1/1	0.84	0.18	200,200,200,200	0
34	SR	A	8929	1/1	0.85	0.26	174,174,174,174	0
32	MG	0	8039	1/1	0.85	0.24	56,56,56,56	0
34	SR	0	8903	1/1	0.85	0.16	168,168,168,168	0
34	SR	0	8914	1/1	0.85	0.23	198,198,198,198	0
35	NA	0	8519	1/1	0.85	0.34	76,76,76,76	0
34	SR	0	8915	1/1	0.85	0.25	200,200,200,200	0
32	MG	0	8036	1/1	0.86	0.11	46,46,46,46	0
34	SR	0	8905	1/1	0.86	0.14	161,161,161,161	0
34	SR	0	8918	1/1	0.86	0.18	122,122,122,122	0
32	MG	0	8066	1/1	0.86	0.37	87,87,87,87	0
32	MG	0	8035	1/1	0.86	0.24	65,65,65,65	0
34	SR	0	8994	1/1	0.86	0.26	192,192,192,192	0
35	NA	Q	8540	1/1	0.86	0.13	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	SR	0	8921	1/1	0.86	0.17	155,155,155,155	0
35	NA	R	8533	1/1	0.86	0.34	51,51,51,51	0
34	SR	0	8947	1/1	0.86	0.20	200,200,200,200	0
32	MG	0	8081	1/1	0.86	0.33	94,94,94,94	0
34	SR	0	8979	1/1	0.86	0.15	180,180,180,180	0
34	SR	0	8981	1/1	0.86	0.29	200,200,200,200	0
34	SR	S	8961	1/1	0.86	0.14	165,165,165,165	0
34	SR	3	8953	1/1	0.87	0.22	200,200,200,200	0
34	SR	0	8908	1/1	0.87	0.28	200,200,200,200	0
34	SR	0	8949	1/1	0.87	0.20	132,132,132,132	0
34	SR	0	8909	1/1	0.87	0.24	189,189,189,189	0
35	NA	C	8503	1/1	0.87	0.08	31,31,31,31	0
34	SR	0	8969	1/1	0.87	0.30	181,181,181,181	0
34	SR	0	8935	1/1	0.87	0.17	159,159,159,159	0
35	NA	0	8565	1/1	0.87	0.30	79,79,79,79	0
33	CL	0	8816	1/1	0.87	0.15	60,60,60,60	0
32	MG	K	8054	1/1	0.87	0.15	62,62,62,62	0
34	SR	0	8940	1/1	0.87	0.24	159,159,159,159	0
34	SR	0	8904	1/1	0.87	0.27	200,200,200,200	0
34	SR	0	8916	1/1	0.87	0.25	178,178,178,178	0
32	MG	A	8051	1/1	0.87	0.23	117,117,117,117	0
35	NA	0	8536	1/1	0.87	0.20	46,46,46,46	0
32	MG	0	8053	1/1	0.87	0.25	78,78,78,78	0
34	SR	0	8901	1/1	0.88	0.10	73,73,73,73	0
34	SR	0	8982	1/1	0.88	0.26	200,200,200,200	0
35	NA	0	8563	1/1	0.88	0.32	61,61,61,61	0
34	SR	B	8987	1/1	0.88	0.40	199,199,199,199	0
35	NA	0	8506	1/1	0.88	0.12	50,50,50,50	0
34	SR	0	8975	1/1	0.88	0.16	131,131,131,131	0
34	SR	0	8985	1/1	0.88	0.17	128,128,128,128	0
35	NA	M	8539	1/1	0.88	0.09	19,19,19,19	0
33	CL	A	8809	1/1	0.88	0.18	86,86,86,86	0
32	MG	0	8072	1/1	0.88	0.13	44,44,44,44	0
35	NA	0	8521	1/1	0.88	0.09	28,28,28,28	0
34	SR	0	8936	1/1	0.88	0.12	100,100,100,100	0
34	SR	0	8910	1/1	0.88	0.14	92,92,92,92	0
34	SR	0	8934	1/1	0.89	0.28	168,168,168,168	0
35	NA	R	8575	1/1	0.89	0.21	65,65,65,65	0
34	SR	0	8996	1/1	0.89	0.23	200,200,200,200	0
32	MG	Y	8086	1/1	0.89	0.10	69,69,69,69	0
35	NA	0	8541	1/1	0.89	0.38	86,86,86,86	0
34	SR	0	8948	1/1	0.89	0.14	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	C	8554	1/1	0.89	0.24	52,52,52,52	0
35	NA	0	8553	1/1	0.89	0.26	59,59,59,59	0
34	SR	0	8974	1/1	0.90	0.20	165,165,165,165	0
32	MG	0	8075	1/1	0.90	0.09	32,32,32,32	0
32	MG	0	8029	1/1	0.90	0.30	111,111,111,111	0
35	NA	0	8566	1/1	0.90	0.20	69,69,69,69	0
34	SR	0	8998	1/1	0.90	0.24	196,196,196,196	0
35	NA	0	8568	1/1	0.90	0.17	46,46,46,46	0
35	NA	0	8569	1/1	0.90	0.16	40,40,40,40	0
35	NA	0	8549	1/1	0.90	0.35	60,60,60,60	0
32	MG	0	8082	1/1	0.90	0.13	39,39,39,39	0
32	MG	0	8089	1/1	0.90	0.11	56,56,56,56	0
32	MG	0	8026	1/1	0.90	0.09	22,22,22,22	0
35	NA	9	8543	1/1	0.90	0.16	22,22,22,22	0
32	MG	0	8092	1/1	0.90	0.15	61,61,61,61	0
34	SR	0	8992	1/1	0.90	0.23	151,151,151,151	0
34	SR	0	8945	1/1	0.90	0.19	131,131,131,131	0
32	MG	0	8055	1/1	0.91	0.11	49,49,49,49	0
34	SR	0	8902	1/1	0.91	0.17	107,107,107,107	0
32	MG	9	8040	1/1	0.91	0.18	71,71,71,71	0
34	SR	0	9007	1/1	0.91	0.31	200,200,200,200	0
35	NA	0	8537	1/1	0.91	0.08	22,22,22,22	0
32	MG	0	8068	1/1	0.91	0.12	54,54,54,54	0
35	NA	0	8524	1/1	0.91	0.15	43,43,43,43	0
32	MG	0	8038	1/1	0.91	0.08	52,52,52,52	0
34	SR	0	8957	1/1	0.91	0.24	200,200,200,200	0
37	K	0	8402	1/1	0.91	0.17	78,78,78,78	0
33	CL	3	8804	1/1	0.91	0.11	59,59,59,59	0
33	CL	J	8801	1/1	0.92	0.10	58,58,58,58	0
35	NA	0	8547	1/1	0.92	0.18	49,49,49,49	0
34	SR	0	8962	1/1	0.92	0.23	197,197,197,197	0
32	MG	0	8064	1/1	0.92	0.10	29,29,29,29	0
33	CL	L	8810	1/1	0.92	0.16	69,69,69,69	0
32	MG	0	8073	1/1	0.92	0.19	47,47,47,47	0
33	CL	0	8805	1/1	0.92	0.12	62,62,62,62	0
34	SR	0	8990	1/1	0.92	0.09	91,91,91,91	0
32	MG	0	8037	1/1	0.92	0.24	88,88,88,88	0
32	MG	0	8033	1/1	0.92	0.23	78,78,78,78	0
32	MG	0	8031	1/1	0.92	0.14	69,69,69,69	0
34	SR	1	8913	1/1	0.92	0.24	179,179,179,179	0
35	NA	0	8545	1/1	0.92	0.14	41,41,41,41	0
35	NA	2	8515	1/1	0.93	0.06	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8555	1/1	0.93	0.18	38,38,38,38	0
35	NA	0	8508	1/1	0.93	0.12	41,41,41,41	0
32	MG	0	8017	1/1	0.93	0.06	31,31,31,31	0
32	MG	0	8063	1/1	0.93	0.16	47,47,47,47	0
32	MG	0	8088	1/1	0.93	0.08	33,33,33,33	0
32	MG	0	8052	1/1	0.93	0.15	59,59,59,59	0
35	NA	0	8562	1/1	0.93	0.30	45,45,45,45	0
33	CL	0	8815	1/1	0.94	0.13	72,72,72,72	0
32	MG	T	8057	1/1	0.94	0.14	60,60,60,60	0
35	NA	B	8552	1/1	0.94	0.35	56,56,56,56	0
33	CL	0	8817	1/1	0.94	0.07	57,57,57,57	0
32	MG	0	8079	1/1	0.94	0.11	51,51,51,51	0
33	CL	N	8807	1/1	0.94	0.08	45,45,45,45	0
33	CL	O	8808	1/1	0.94	0.16	68,68,68,68	0
32	MG	0	8080	1/1	0.94	0.07	39,39,39,39	0
32	MG	0	8032	1/1	0.94	0.09	47,47,47,47	0
33	CL	0	8813	1/1	0.94	0.07	43,43,43,43	0
34	SR	H	8972	1/1	0.94	0.16	131,131,131,131	0
33	CL	B	8819	1/1	0.95	0.11	42,42,42,42	0
35	NA	0	8512	1/1	0.95	0.20	32,32,32,32	0
35	NA	0	8527	1/1	0.95	0.19	44,44,44,44	0
32	MG	0	8020	1/1	0.95	0.10	36,36,36,36	0
32	MG	0	8090	1/1	0.95	0.11	50,50,50,50	0
35	NA	0	8530	1/1	0.95	0.17	46,46,46,46	0
32	MG	0	8056	1/1	0.95	0.13	37,37,37,37	0
36	CD	O	8705	1/1	0.95	0.05	91,91,91,91	0
32	MG	0	8018	1/1	0.95	0.15	53,53,53,53	0
32	MG	0	8087	1/1	0.95	0.04	14,14,14,14	0
32	MG	0	8027	1/1	0.95	0.10	37,37,37,37	0
32	MG	0	8005	1/1	0.96	0.11	26,26,26,26	0
32	MG	0	8069	1/1	0.96	0.11	38,38,38,38	0
32	MG	0	8024	1/1	0.96	0.13	43,43,43,43	0
35	NA	0	8534	1/1	0.96	0.06	15,15,15,15	0
35	NA	H	8518	1/1	0.96	0.20	48,48,48,48	0
32	MG	0	8044	1/1	0.96	0.07	38,38,38,38	0
33	CL	J	8821	1/1	0.96	0.08	61,61,61,61	0
35	NA	0	8516	1/1	0.96	0.10	18,18,18,18	0
32	MG	0	8049	1/1	0.96	0.16	43,43,43,43	0
33	CL	L	8814	1/1	0.96	0.11	51,51,51,51	0
32	MG	B	8042	1/1	0.96	0.12	41,41,41,41	0
32	MG	0	8077	1/1	0.96	0.07	36,36,36,36	0
32	MG	B	8043	1/1	0.96	0.12	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8550	1/1	0.96	0.10	25,25,25,25	0
35	NA	0	8551	1/1	0.96	0.10	36,36,36,36	0
33	CL	0	8803	1/1	0.96	0.07	50,50,50,50	0
32	MG	0	8093	1/1	0.96	0.04	13,13,13,13	0
32	MG	0	8067	1/1	0.96	0.21	51,51,51,51	0
35	NA	0	8504	1/1	0.96	0.10	18,18,18,18	0
32	MG	9	8074	1/1	0.96	0.11	45,45,45,45	0
32	MG	0	8047	1/1	0.97	0.14	34,34,34,34	0
33	CL	Q	8811	1/1	0.97	0.05	51,51,51,51	0
35	NA	0	8513	1/1	0.97	0.14	34,34,34,34	0
35	NA	0	8514	1/1	0.97	0.19	40,40,40,40	0
33	CL	Y	8820	1/1	0.97	0.08	33,33,33,33	0
35	NA	0	8517	1/1	0.97	0.07	14,14,14,14	0
32	MG	0	8022	1/1	0.97	0.09	20,20,20,20	0
32	MG	0	8083	1/1	0.97	0.06	41,41,41,41	0
32	MG	0	8085	1/1	0.97	0.20	51,51,51,51	0
33	CL	K	8812	1/1	0.97	0.13	39,39,39,39	0
32	MG	0	8014	1/1	0.97	0.09	15,15,15,15	0
35	NA	0	8542	1/1	0.97	0.13	36,36,36,36	0
35	NA	0	8544	1/1	0.97	0.24	49,49,49,49	0
32	MG	0	8002	1/1	0.97	0.05	14,14,14,14	0
32	MG	0	8046	1/1	0.97	0.08	25,25,25,25	0
32	MG	0	8008	1/1	0.98	0.06	8,8,8,8	0
32	MG	0	8021	1/1	0.98	0.07	16,16,16,16	0
32	MG	0	8084	1/1	0.98	0.13	37,37,37,37	0
32	MG	0	8004	1/1	0.98	0.06	23,23,23,23	0
32	MG	0	8070	1/1	0.98	0.06	31,31,31,31	0
32	MG	0	8041	1/1	0.98	0.14	28,28,28,28	0
32	MG	0	8028	1/1	0.98	0.08	16,16,16,16	0
33	CL	M	8818	1/1	0.98	0.07	36,36,36,36	0
32	MG	0	8045	1/1	0.98	0.06	13,13,13,13	0
32	MG	0	8062	1/1	0.98	0.20	64,64,64,64	0
32	MG	0	8023	1/1	0.98	0.07	14,14,14,14	0
33	CL	R	8806	1/1	0.98	0.07	32,32,32,32	0
32	MG	0	8078	1/1	0.98	0.07	28,28,28,28	0
36	CD	1	8702	1/1	0.98	0.03	58,58,58,58	0
32	MG	0	8030	1/1	0.98	0.13	45,45,45,45	0
32	MG	0	8065	1/1	0.98	0.07	16,16,16,16	0
32	MG	0	8048	1/1	0.98	0.19	44,44,44,44	0
32	MG	0	8010	1/1	0.99	0.12	3,3,3,3	0
32	MG	0	8013	1/1	0.99	0.05	11,11,11,11	0
32	MG	0	8025	1/1	0.99	0.04	10,10,10,10	0

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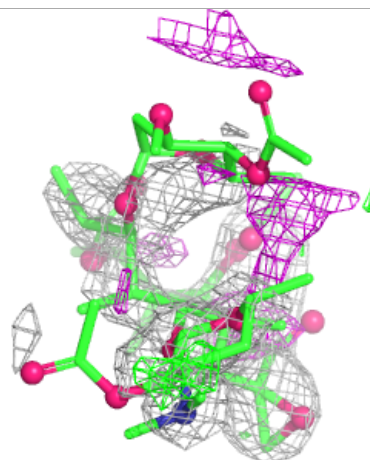
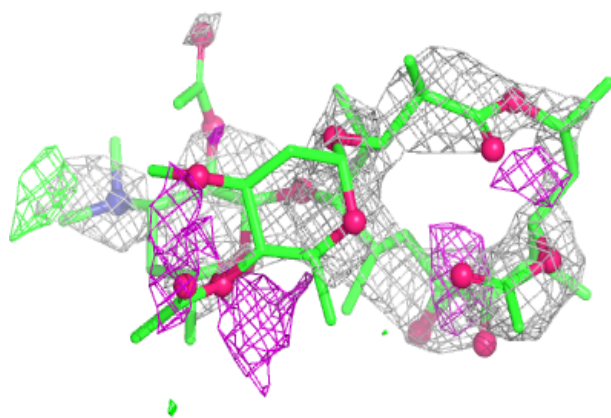
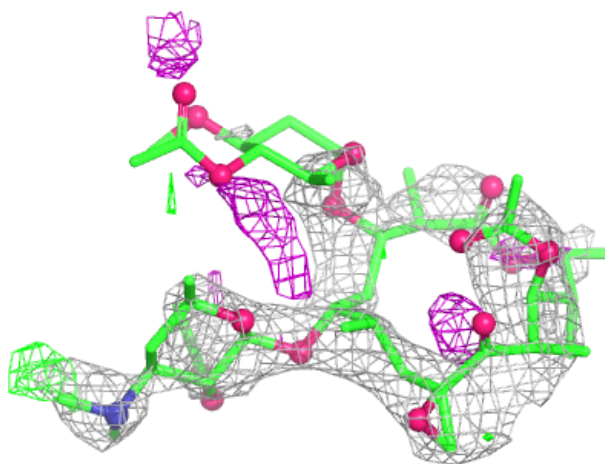
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8001	1/1	0.99	0.05	2,2,2,2	0
32	MG	0	8016	1/1	0.99	0.09	2,2,2,2	0
32	MG	A	8050	1/1	0.99	0.07	18,18,18,18	0
32	MG	0	8058	1/1	0.99	0.03	1,1,1,1	0
32	MG	0	8006	1/1	0.99	0.04	7,7,7,7	0
32	MG	0	8061	1/1	0.99	0.08	23,23,23,23	0
32	MG	0	8076	1/1	0.99	0.04	9,9,9,9	0
36	CD	U	8701	1/1	0.99	0.02	58,58,58,58	0
36	CD	Z	8703	1/1	0.99	0.04	55,55,55,55	0
32	MG	0	8019	1/1	0.99	0.10	1,1,1,1	0
32	MG	0	8007	1/1	0.99	0.05	3,3,3,3	0
32	MG	0	8003	1/1	0.99	0.05	16,16,16,16	0
32	MG	0	8009	1/1	0.99	0.10	15,15,15,15	0
36	CD	3	8704	1/1	1.00	0.02	56,56,56,56	0
32	MG	C	8012	1/1	1.00	0.04	10,10,10,10	0
32	MG	0	8011	1/1	1.00	0.07	1,1,1,1	0
32	MG	0	8015	1/1	1.00	0.07	5,5,5,5	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 TAO 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.