



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 04:51 am BST

PDB ID : 3OW2
Title : Crystal Structure of Enhanced Macrolide Bound to 50S Ribosomal Subunit
Authors : Kanyo, Z.F.
Deposited on : 2010-09-17
Resolution : 2.70 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

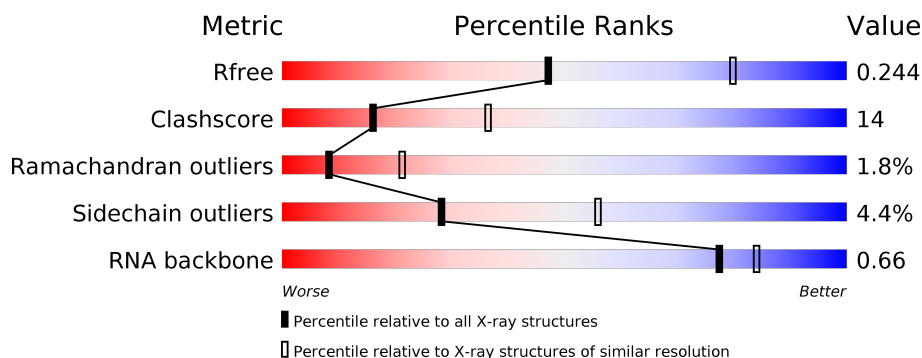
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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.






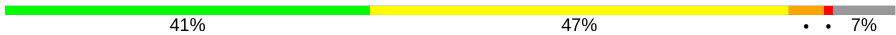




















Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	0	2902	55% 35% 5% 5%
2	9	122	51% 39% 9% .
3	A	237	67% 28% 5%
4	B	337	62% 34% .
5	C	246	63% 33% .
6	D	165	40% 37% 8% 15%

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Mol	Chain	Length	Quality of chain
7	E	172	
8	F	119	
9	G	62	
10	H	167	
11	I	142	
12	J	132	
13	K	150	
14	L	194	
15	M	186	
16	N	115	
17	O	143	
18	P	95	
19	Q	150	
20	R	81	
21	S	119	
22	T	53	
23	U	65	
24	V	154	
25	W	82	
26	X	142	
27	Y	73	
28	Z	56	
29	1	48	
30	2	92	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	EMK	0	8163	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90725 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
			59016	26346	10878	19047	2745			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	?	-	U	DELETION	GB 3377779
0	?	-	C	DELETION	GB 3377779
0	560	C	U	CONFLICT	GB 3377779
0	2099	A	G	CONFLICT	GB 3377779

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1755	1072	352	326	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1095	685	195	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			241	149	39	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	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	J	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	K	145	Total	C	N	O		0	0	0
			1119	670	222	227				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	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	N	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	O	143	Total	C	N	O		0	0	0
			1134	680	230	224				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	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	Q	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	U	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	142	Total	C	N	O		0	0	0
			1131	686	228	217				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	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	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	0	55	Total	Mg	0	0
			55	55		
31	J	1	Total	Mg	0	0
			1	1		
31	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total 1	Mg 1	0	0
31	X	1	Total 1	Mg 1	0	0
31	9	1	Total 1	Mg 1	0	0
31	S	1	Total 1	Mg 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	1	Total 1	K 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	19	Total 19	Na 19	0	0
33	P	1	Total 1	Na 1	0	0
33	Q	2	Total 2	Na 2	0	0
33	I	1	Total 1	Na 1	0	0
33	C	1	Total 1	Na 1	0	0
33	9	1	Total 1	Na 1	0	0
33	L	1	Total 1	Na 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	5	Total 5	Cl 5	0	0
34	Q	1	Total 1	Cl 1	0	0
34	D	1	Total 1	Cl 1	0	0

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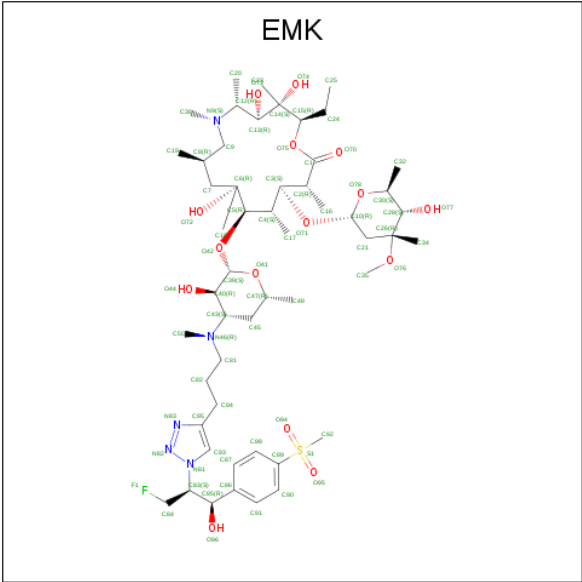
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	I	2	Total 2	Cl 2	0	0
34	A	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0

- Molecule 35 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total 82	Sr 82	0	0
35	Q	1	Total 1	Sr 1	0	0
35	B	2	Total 2	Sr 2	0	0
35	Z	2	Total 2	Sr 2	0	0
35	A	4	Total 4	Sr 4	0	0
35	R	1	Total 1	Sr 1	0	0
35	9	3	Total 3	Sr 3	0	0
35	2	2	Total 2	Sr 2	0	0
35	F	1	Total 1	Sr 1	0	0

- Molecule 36 is (2R,3S,4R,5R,8R,10R,11R,12S,13S,14R)-2-ethyl-3,4,10-trihydroxy-3,5,6,8,10,12,14-heptamethyl-15-oxo-11-[(3,4,6-trideoxy-3-{[3-(1-{(1S,2R)-1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl}-1H-1,2,3-triazol-4-yl)propyl](methyl)amino}-beta-D-xylo-hexopyranosyl)oxy]-1-oxa-6-azacyclopentadecan-13-yl 2,6-dideoxy-3-C-methyl-3-O-methyl-alpha-L-ribo-hexopyranoside (three-letter code: EMK) (formula: C₅₂H₈₈FN₅O₁₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	0	1	Total	C	F	N	O	S	0	0
			74	52	1	5	15	1		

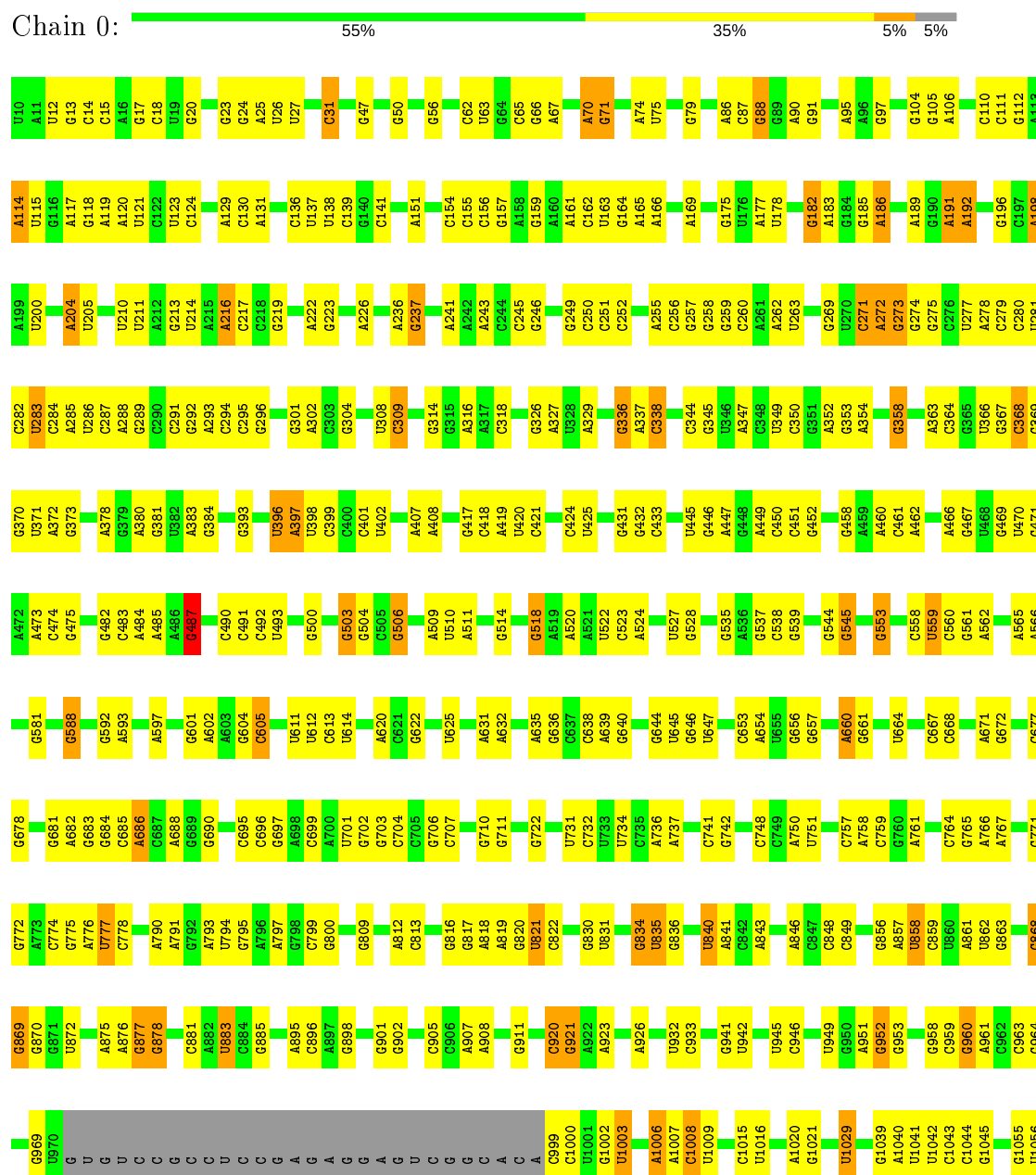
- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	Z	1	Total	Cd	0	0
			1	1		
37	Y	1	Total	Cd	0	0
			1	1		
37	T	1	Total	Cd	0	0
			1	1		
37	2	1	Total	Cd	0	0
			1	1		

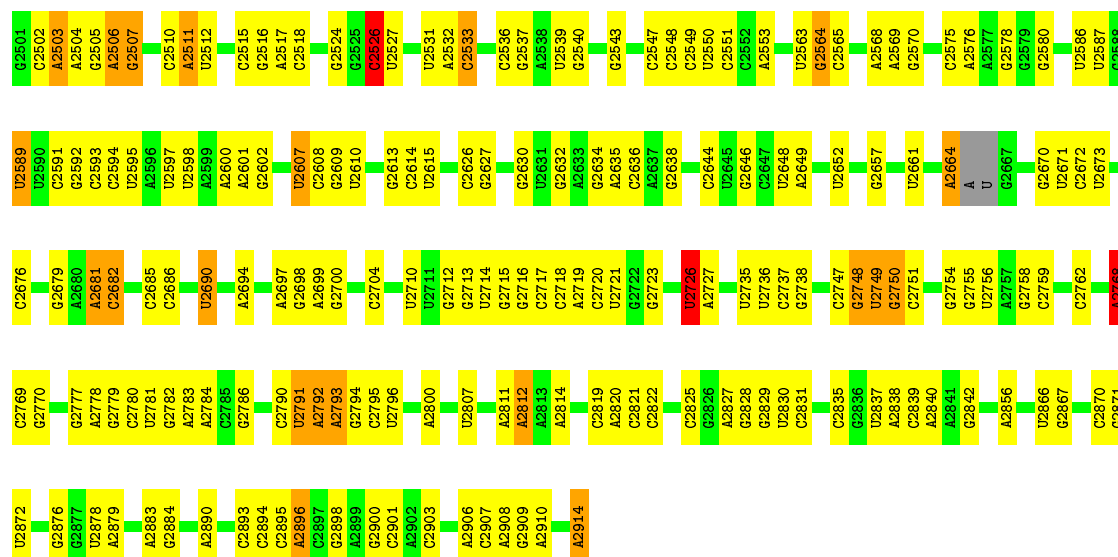
3 Residue-property plots

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. 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. 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

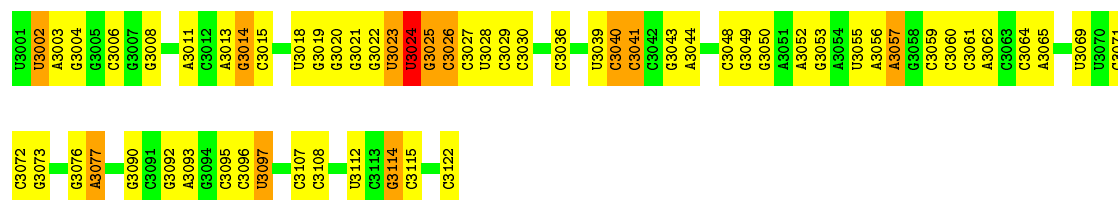






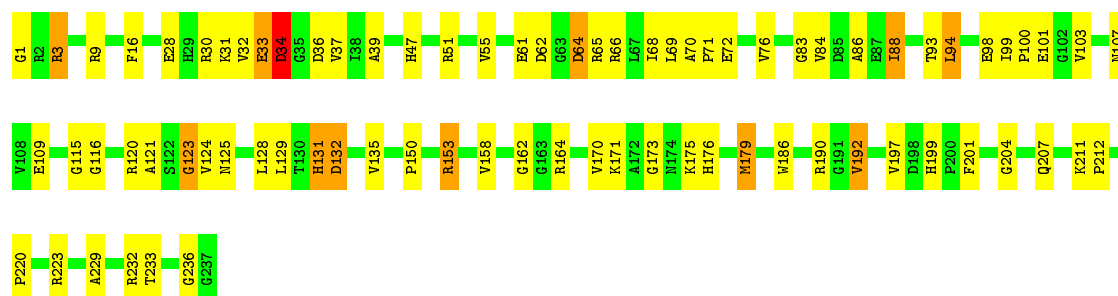
• Molecule 2: 5S RIBOSOMAL RNA

Chain 9: 51% 39% 9%



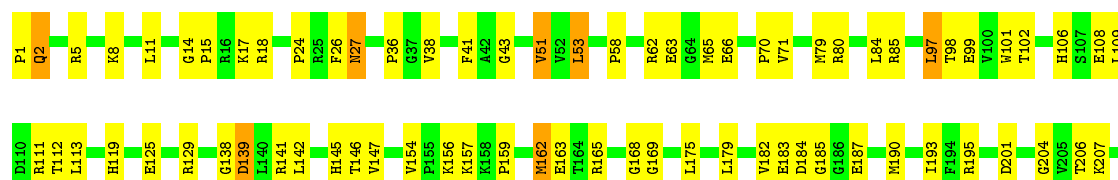
• Molecule 3: 50S ribosomal protein L2P

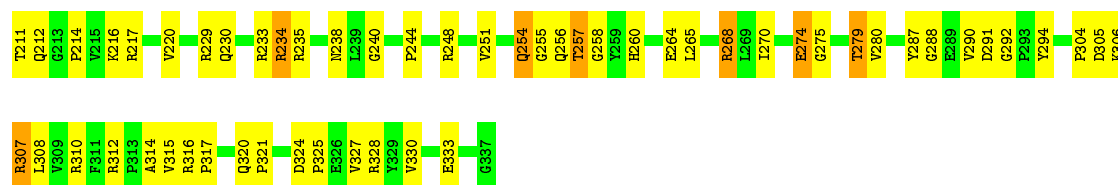
Chain A: 67% 28% 5%



• Molecule 4: 50S ribosomal protein L3P

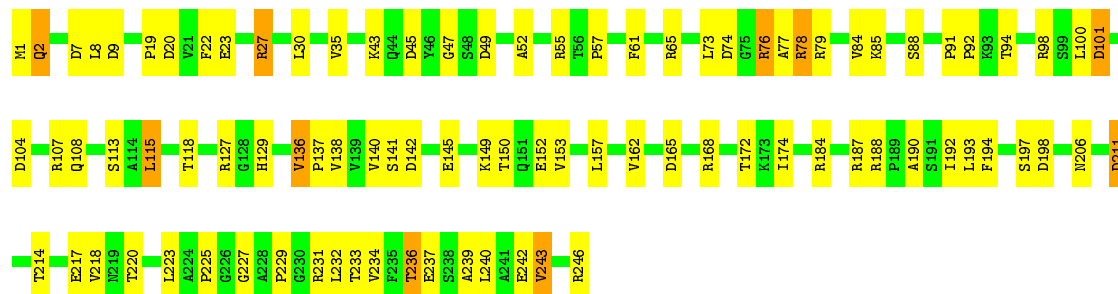
Chain B: 62% 34% 4%





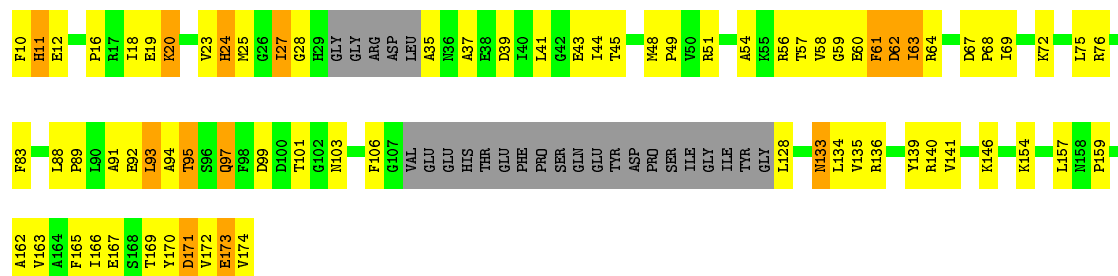
• Molecule 5: 50S ribosomal protein L4P

Chain C: 63% 33%



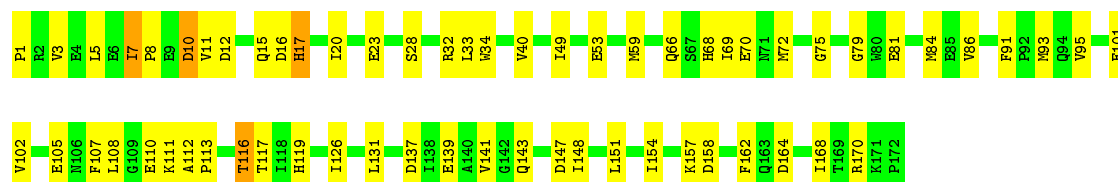
• Molecule 6: 50S ribosomal protein L5P

Chain D: 40% 37% 8% 15%



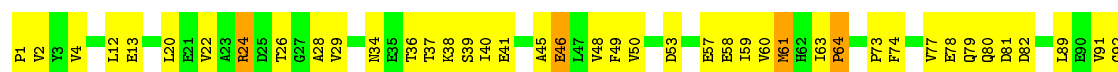
• Molecule 7: 50S ribosomal protein L6P

Chain E: 64% 34%



• Molecule 8: 50S ribosomal protein L7Ae

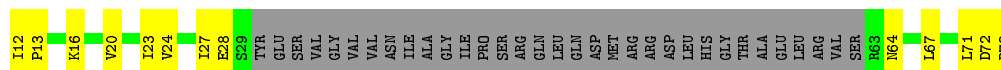
Chain F: 56% 39%





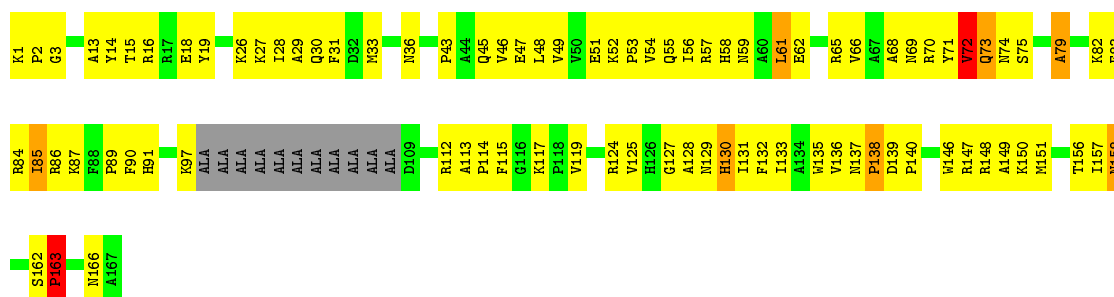
- Molecule 9: 50S ribosomal protein L10E

Chain G: 26% 21% 53%



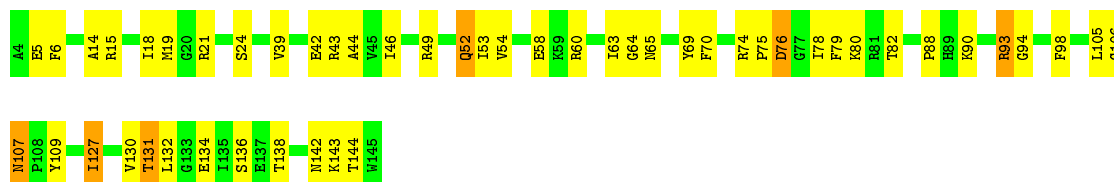
- Molecule 10: 50S ribosomal protein L10e

Chain H: 41% 47% 7%



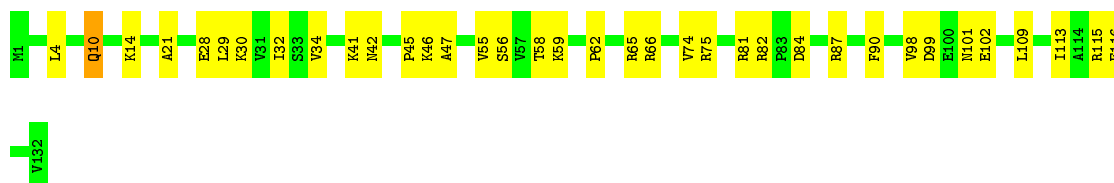
- Molecule 11: 50S ribosomal protein L13P

Chain I: 65% 31% 4%



- Molecule 12: 50S ribosomal protein L14P

Chain J: 73% 27% 0%



- Molecule 13: 50S ribosomal protein L15P

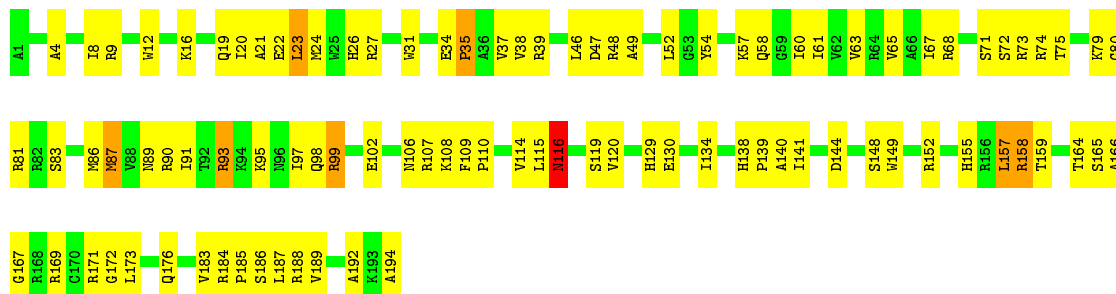
Chain K: 55% 39% 6%





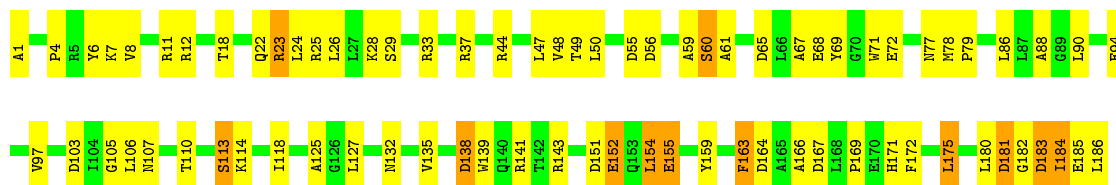
• Molecule 14: 50S ribosomal protein L15e

Chain L: 51% 45%



• Molecule 15: 50S ribosomal protein L18P

Chain M: 59% 35% 6%



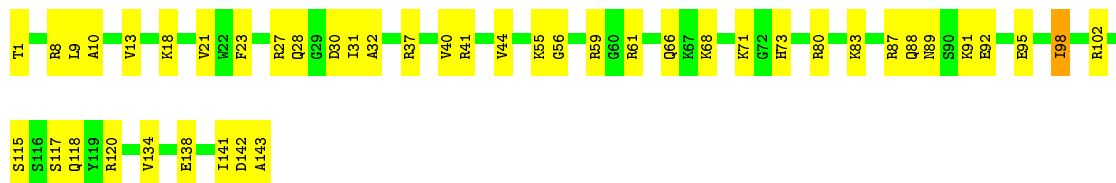
• Molecule 16: 50S ribosomal protein L18e

Chain N: 73% 24%



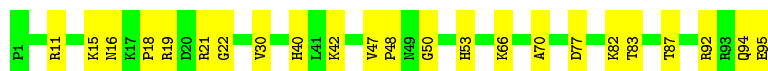
• Molecule 17: 50S ribosomal protein L19e

Chain O: 69% 30%

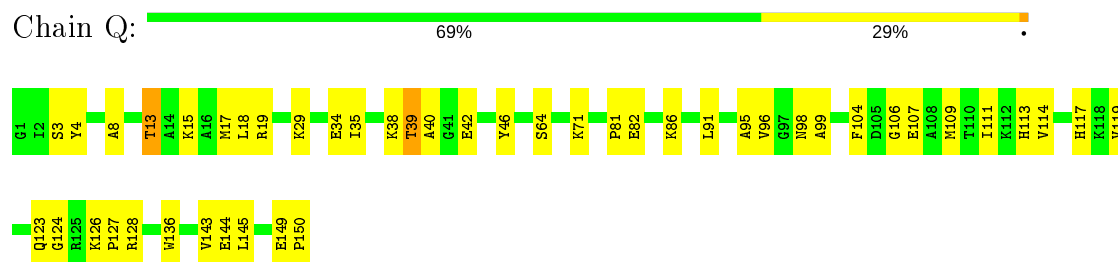


• Molecule 18: 50S ribosomal protein L21e

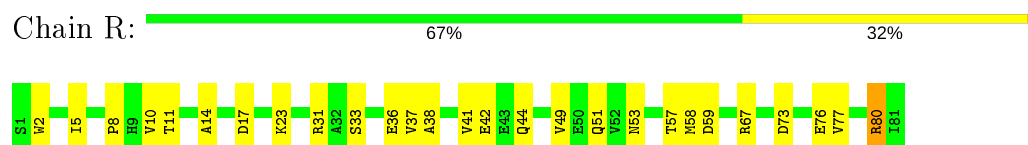
Chain P: 76% 24%



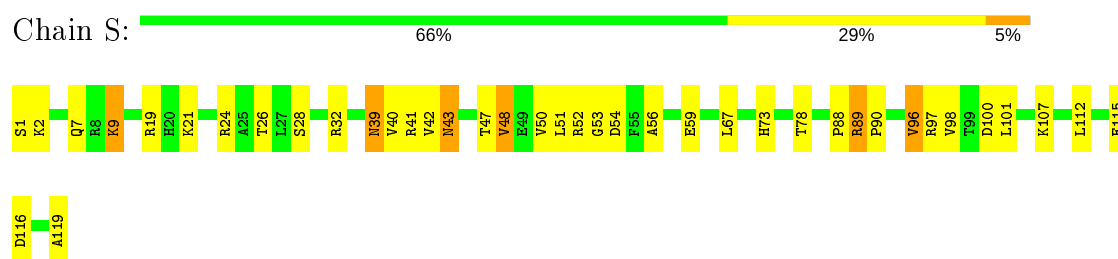
- Molecule 19: 50S ribosomal protein L22P



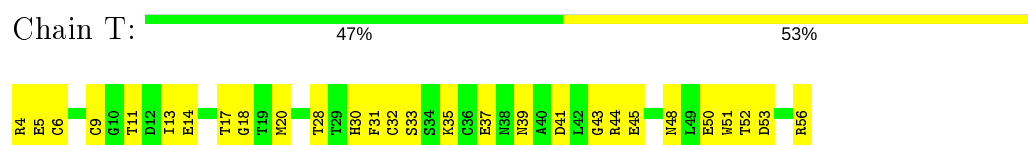
- Molecule 20: 50S ribosomal protein L23P



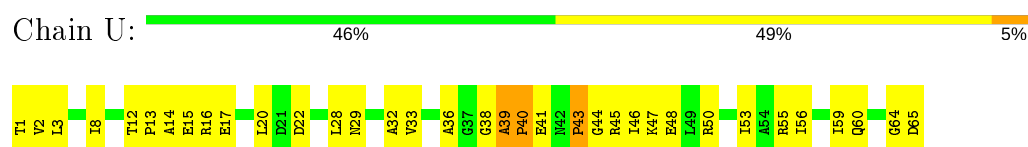
- Molecule 21: 50S ribosomal protein L24P



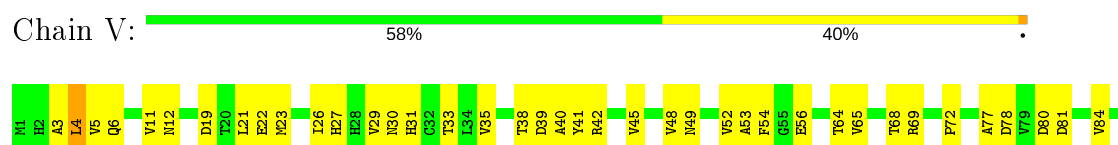
- Molecule 22: 50S ribosomal protein L24e



- Molecule 23: 50S ribosomal protein L29P

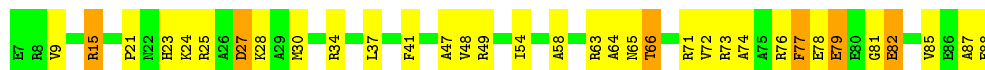


- Molecule 24: 50S ribosomal protein L30P

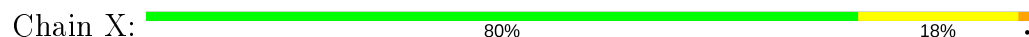




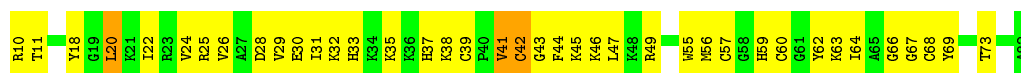
- Molecule 25: 50S ribosomal protein L31e



- 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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.85Å 298.00Å 574.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.90 – 2.72	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.70) 90.9 (49.90-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.73Å)	Xtriage
Refinement program	CNS, CNX	Depositor
R, R_{free}	0.222 , 0.253 0.210 , 0.244	Depositor DCC
R_{free} test set	4458 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	90725	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% 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, CL, NA, K, EMK, CD, SR

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	0.41	0/66075	0.69	18/103050 (0.0%)
2	9	0.37	0/2905	0.72	2/4528 (0.0%)
3	A	0.36	0/1788	0.66	0/2409
4	B	0.39	0/2690	0.67	0/3652
5	C	0.39	0/1884	0.65	0/2551
6	D	0.32	0/1112	0.58	0/1498
7	E	0.35	0/1383	0.59	0/1880
8	F	0.37	0/897	0.58	0/1219
9	G	0.30	0/242	0.45	0/324
10	H	0.40	0/1247	0.74	1/1686 (0.1%)
11	I	0.38	0/1136	0.63	0/1530
12	J	0.39	0/1004	0.70	0/1351
13	K	0.39	0/1131	0.68	0/1509
14	L	0.39	0/1634	0.69	1/2180 (0.0%)
15	M	0.32	0/1474	0.61	0/1999
16	N	0.33	0/874	0.62	0/1181
17	O	0.37	0/1144	0.57	0/1521
18	P	0.38	0/749	0.72	0/1005
19	Q	0.36	0/1173	0.63	0/1578
20	R	0.36	0/649	0.58	0/875
21	S	0.35	0/958	0.65	0/1289
22	T	0.39	0/418	0.59	0/562
23	U	0.31	0/503	0.52	0/675
24	V	0.36	0/1219	0.65	0/1655
25	W	0.36	0/665	0.60	0/895
26	X	0.38	0/1147	0.66	0/1536
27	Y	0.40	0/576	0.71	0/763
28	Z	0.49	0/438	0.70	0/578
29	1	0.37	0/399	0.60	0/527
30	2	0.41	0/771	0.60	0/1024
All	All	0.40	0/98285	0.68	22/147030 (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	75
2	9	1	2
24	V	0	1
All	All	1	78

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	9.36	130.09	109.50
1	0	1559	A	C2'-C3'-O3'	8.36	127.88	109.50
1	0	2338	G	C2'-C3'-O3'	7.19	125.32	109.50
1	0	1120	U	C5'-C4'-C3'	-6.74	105.22	116.00
1	0	777	U	O4'-C1'-N1	6.46	113.37	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	9	3024	U	C3'

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	216	A	Sidechain
1	0	314	G	Sidechain
1	0	396	U	Sidechain
1	0	50	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	59016	0	29808	892	0
2	9	2600	0	1326	67	0
3	A	1755	0	1763	77	0
4	B	2625	0	2533	124	0
5	C	1859	0	1816	85	0
6	D	1095	0	1085	84	0
7	E	1358	0	1266	53	0
8	F	886	0	854	50	0
9	G	241	0	231	8	0
10	H	1216	0	1215	132	0
11	I	1120	0	1098	57	0
12	J	994	0	1027	37	0
13	K	1119	0	1076	57	0
14	L	1606	0	1676	123	0
15	M	1445	0	1401	69	0
16	N	865	0	873	23	0
17	O	1134	0	1127	42	0
18	P	735	0	729	17	0
19	Q	1150	0	1122	53	0
20	R	642	0	605	25	0
21	S	950	0	924	31	0
22	T	411	0	364	22	0
23	U	500	0	511	32	0
24	V	1196	0	1137	69	0
25	W	655	0	653	35	0
26	X	1131	0	1133	26	0
27	Y	564	0	598	46	0
28	Z	431	0	426	24	0
29	1	394	0	406	24	0
30	2	755	0	729	22	0
31	0	55	0	0	0	0
31	9	1	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	S	1	0	0	0	0
31	X	1	0	0	0	0
32	0	1	0	0	0	0
33	0	19	0	0	0	0
33	9	1	0	0	0	0
33	C	1	0	0	0	0
33	I	1	0	0	0	0
33	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
34	0	5	0	0	0	0
34	A	1	0	0	0	0
34	D	1	0	0	0	0
34	I	2	0	0	0	0
34	L	1	0	0	1	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	0	82	0	0	0	0
35	2	2	0	0	0	0
35	9	3	0	0	0	0
35	A	4	0	0	0	0
35	B	2	0	0	0	0
35	F	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Z	2	0	0	0	0
36	0	74	0	88	30	0
37	2	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
All	All	90725	0	59600	2169	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 14.

The worst 5 of 2169 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)
36:0:8163:EMK:C15	36:0:8163:EMK:C14	1.75	1.63
36:0:8163:EMK:C20	36:0:8163:EMK:C12	1.76	1.58
36:0:8163:EMK:C13	36:0:8163:EMK:C14	1.78	1.58
36:0:8163:EMK:C8	36:0:8163:EMK:C9	1.75	1.57
36:0:8163:EMK:N9	36:0:8163:EMK:C12	1.71	1.49

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/237 (99%)	209 (89%)	21 (9%)	5 (2%)	7	18
4	B	335/337 (99%)	309 (92%)	20 (6%)	6 (2%)	8	21
5	C	244/246 (99%)	229 (94%)	13 (5%)	2 (1%)	19	43
6	D	134/165 (81%)	103 (77%)	20 (15%)	11 (8%)	1	1
7	E	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	25	50
8	F	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	9	23
9	G	25/62 (40%)	23 (92%)	1 (4%)	1 (4%)	3	6
10	H	152/167 (91%)	134 (88%)	13 (9%)	5 (3%)	4	8
11	I	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	7	18
12	J	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	19	43
13	K	141/150 (94%)	117 (83%)	22 (16%)	2 (1%)	11	28
14	L	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	15	37
15	M	184/186 (99%)	159 (86%)	17 (9%)	8 (4%)	2	5
16	N	113/115 (98%)	107 (95%)	5 (4%)	1 (1%)	17	40
17	O	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
18	P	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	14	34
19	Q	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	22	46
20	R	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
21	S	117/119 (98%)	111 (95%)	4 (3%)	2 (2%)	9	23
22	T	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	U	63/65 (97%)	58 (92%)	1 (2%)	4 (6%)	1	2
24	V	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	46
25	W	80/82 (98%)	71 (89%)	5 (6%)	4 (5%)	2	4
26	X	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
27	Y	71/73 (97%)	63 (89%)	5 (7%)	3 (4%)	3	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
29	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
30	2	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	34
All	All	3633/3777 (96%)	3317 (91%)	249 (7%)	67 (2%)	8	21

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	63	ILE
6	D	93	LEU
6	D	95	THR
6	D	173	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/179 (100%)	168 (94%)	11 (6%)	18	41
4	B	282/282 (100%)	264 (94%)	18 (6%)	17	39
5	C	193/193 (100%)	179 (93%)	14 (7%)	14	33
6	D	117/138 (85%)	113 (97%)	4 (3%)	37	66
7	E	152/152 (100%)	148 (97%)	4 (3%)	46	75
8	F	92/92 (100%)	88 (96%)	4 (4%)	29	57
9	G	27/55 (49%)	27 (100%)	0	100	100
10	H	122/122 (100%)	113 (93%)	9 (7%)	13	32
11	I	118/118 (100%)	110 (93%)	8 (7%)	16	36
12	J	106/106 (100%)	104 (98%)	2 (2%)	57	82
13	K	113/116 (97%)	106 (94%)	7 (6%)	18	40
14	L	166/166 (100%)	158 (95%)	8 (5%)	25	53
15	M	149/149 (100%)	142 (95%)	7 (5%)	26	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	93/93 (100%)	89 (96%)	4 (4%)	29	57
17	O	113/113 (100%)	112 (99%)	1 (1%)	78	92
18	P	79/79 (100%)	77 (98%)	2 (2%)	47	76
19	Q	117/117 (100%)	114 (97%)	3 (3%)	46	75
20	R	71/71 (100%)	70 (99%)	1 (1%)	67	86
21	S	105/105 (100%)	98 (93%)	7 (7%)	16	37
22	T	44/44 (100%)	44 (100%)	0	100	100
23	U	51/51 (100%)	50 (98%)	1 (2%)	55	81
24	V	130/130 (100%)	126 (97%)	4 (3%)	40	69
25	W	66/66 (100%)	61 (92%)	5 (8%)	13	30
26	X	120/120 (100%)	115 (96%)	5 (4%)	30	58
27	Y	56/56 (100%)	55 (98%)	1 (2%)	59	83
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	49	77
30	2	79/79 (100%)	78 (99%)	1 (1%)	69	87
All	All	3028/3082 (98%)	2896 (96%)	132 (4%)	28	56

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	85	ILE
12	J	84	ASP
25	W	49	ARG
10	H	138	PRO
11	I	79	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
14	L	89	ASN
19	Q	61	GLN
28	Z	16	HIS
15	M	93	GLN
17	O	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2902 (94%)	233 (8%)	22 (0%)
2	9	121/122 (99%)	14 (11%)	2 (1%)
All	All	2866/3024 (94%)	247 (8%)	24 (0%)

5 of 247 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	70	A
1	0	71	G
1	0	86	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1237	U
1	0	1752	G
2	9	3024	U
1	0	1352	A
1	0	1684	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 204 ligands modelled in this entry, 203 are monoatomic - leaving 1 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	EMK	0	8163	-	76,78,78	5.99	58 (76%)	107,118,118	3.32	42 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	EMK	0	8163	-	-	29/93/133/133	0/5/5/5

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8163	EMK	C12-N9	14.11	1.71	1.49
36	0	8163	EMK	C20-C12	12.79	1.76	1.52
36	0	8163	EMK	O42-C5	-11.85	1.13	1.44
36	0	8163	EMK	C14-C15	10.87	1.75	1.54
36	0	8163	EMK	O74-C14	10.85	1.63	1.44

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	8163	EMK	C7-C8-C9	-14.28	91.72	112.06
36	0	8163	EMK	C39-O42-C5	13.13	139.06	116.25
36	0	8163	EMK	C92-S1-C89	8.67	114.82	104.58
36	0	8163	EMK	C81-N46-C43	-7.98	96.03	112.53
36	0	8163	EMK	C6-C7-C8	-6.07	100.28	117.06

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

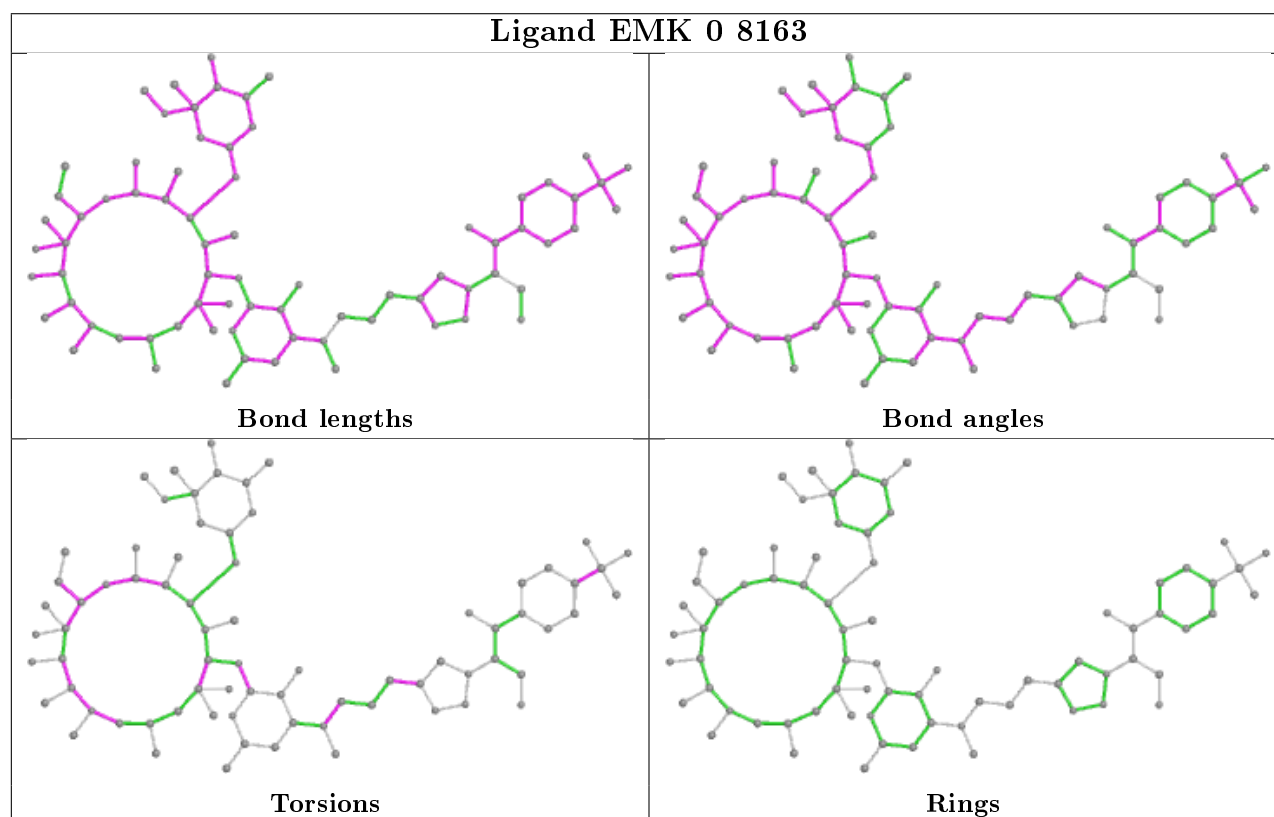
Mol	Chain	Res	Type	Atoms
36	0	8163	EMK	O70-C1-C2-C3
36	0	8163	EMK	O75-C1-C2-C3
36	0	8163	EMK	C8-C9-N9-C12
36	0	8163	EMK	C13-C12-N9-C9
36	0	8163	EMK	N9-C12-C13-C14

There are no ring outliers.

1 monomer is involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8163	EMK	30	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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

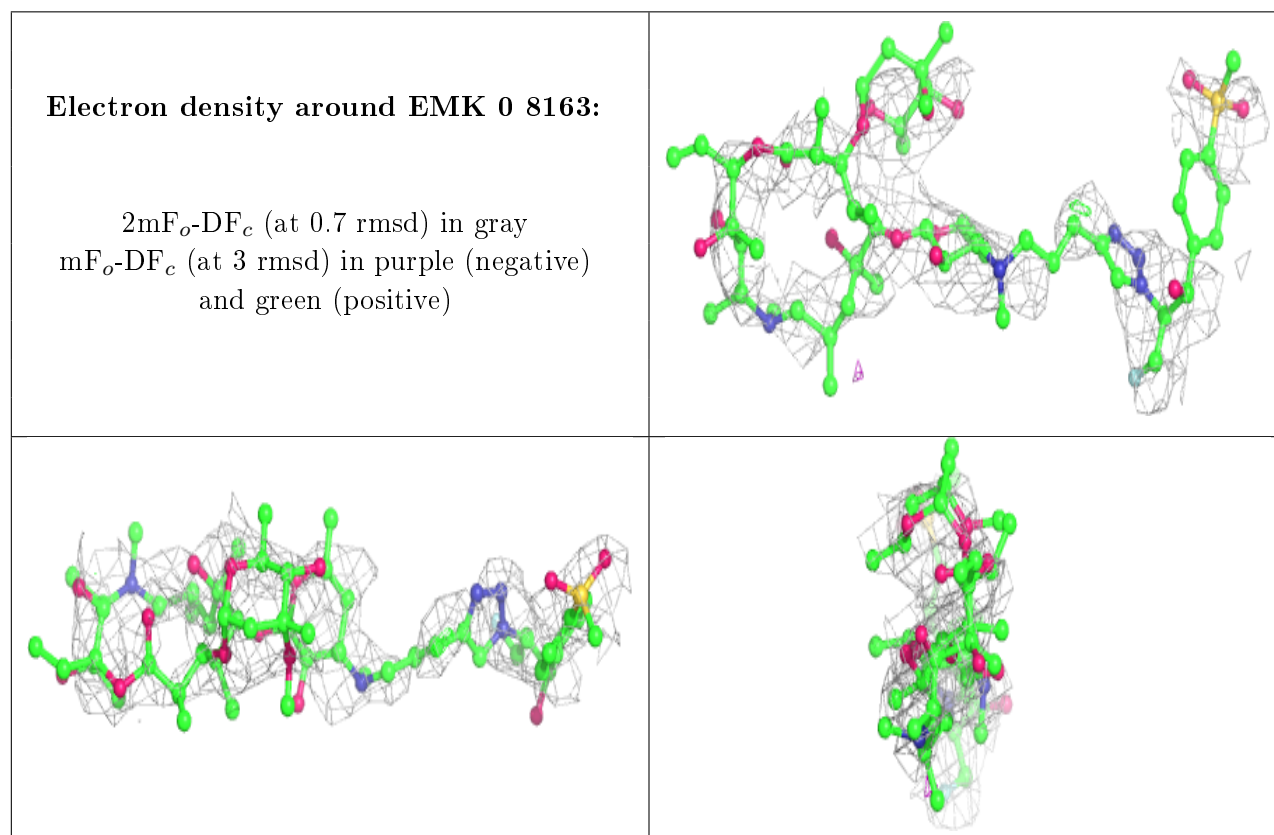
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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.



6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.