



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 07:59 PM UTC

PDB ID : 1YI2 / pdb_00001yi2
Title : Crystal Structure Of Erythromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-11
Resolution : 2.65 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)
Xtrriage (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

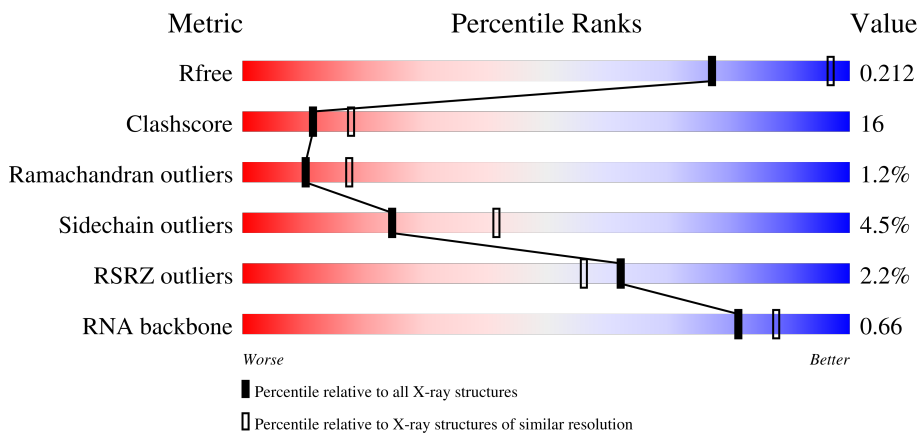
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.




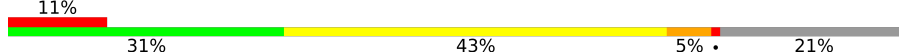

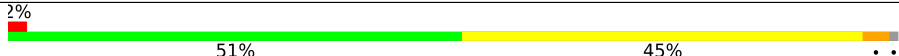
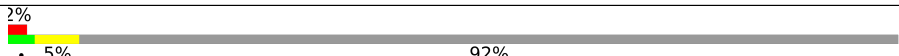
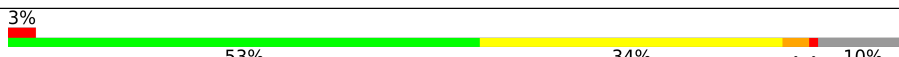
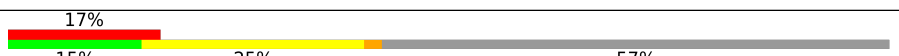
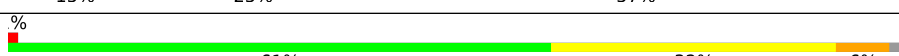
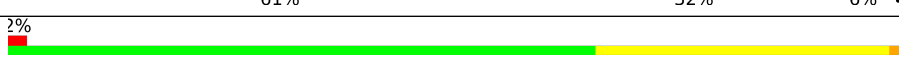

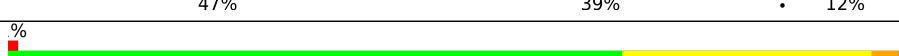
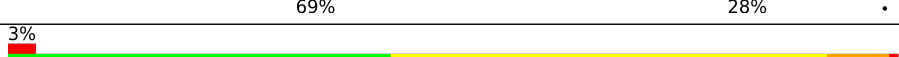

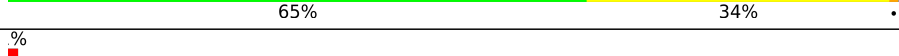
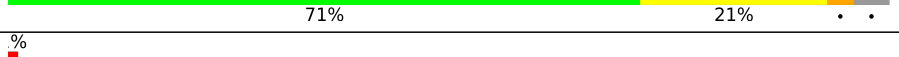





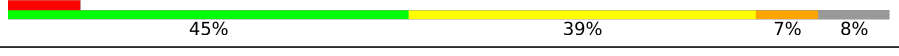


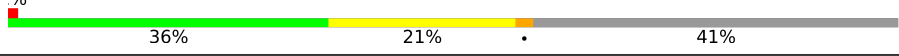

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)
RNA backbone	3983	1090 (2.90-2.42)

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

Mol	Chain	Length	Quality of chain
1	0	2922	 61% 27% 5% • 6%
2	9	122	 55% 35% 8% •
3	A	240	 61% 32% 6% •
4	B	338	 49% 46% 5%



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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	195	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	 2% 48% 44% 8%
31	3	92	 63% 34%

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
35	NA	R	8586	-	-	-	X

2 Entry composition i

There are 38 unique types of molecules in this entry. The entry contains 99086 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
			Total	C	N	O	P			
1	0	2754	59020	26349	10873	19053	2745	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2599	1160	471	847	121	0	0	0

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

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

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

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	160	1282	798	240	238	6	0	0	0

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	Z	73	578	346	116	111	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	1	56	431	258	86	83	4	0	0	0

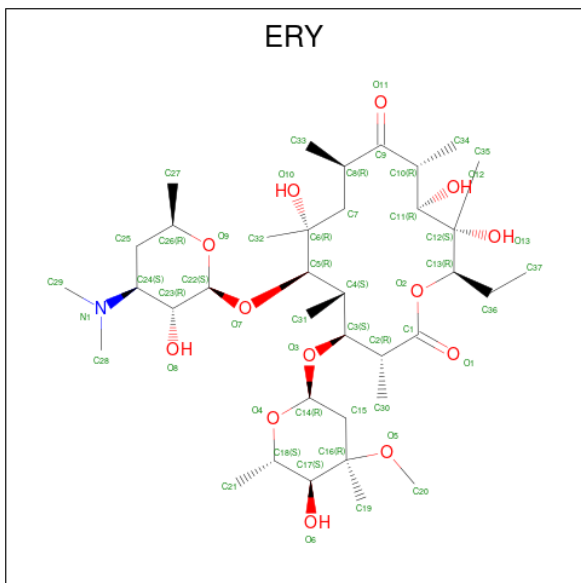
- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	2	46	396	239	89	67	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	3	92	755	458	153	137	7	0	0	0

- Molecule 32 is ERYTHROMYCIN A (CCD ID: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
32	0	1	51	37	1	13	0	0

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

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	3	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	71	Total	Na	0	0
			71	71		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	J	1	Total	Na	0	0
			1	1		
35	L	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	R	3	Total	Na	0	0
			3	3		
35	S	1	Total	Na	0	0
			1	1		
35	T	1	Total	Na	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total	Cl	0	0
			10	10		

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

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	O	1	Total Cd 1 1	0	0
37	U	1	Total Cd 1 1	0	0
37	Z	1	Total Cd 1 1	0	0
37	1	1	Total Cd 1 1	0	0
37	3	1	Total Cd 1 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	5869	Total O 5869 5869	0	0
38	9	138	Total O 138 138	0	0

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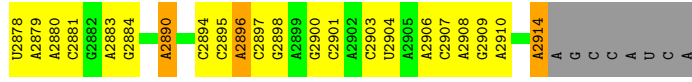
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total 121	O 121	0	0
38	B	151	Total 151	O 151	0	0
38	C	168	Total 168	O 168	0	0
38	D	50	Total 50	O 50	0	0
38	E	42	Total 42	O 42	0	0
38	F	28	Total 28	O 28	0	0
38	G	19	Total 19	O 19	0	0
38	H	71	Total 71	O 71	0	0
38	I	9	Total 9	O 9	0	0
38	J	55	Total 55	O 55	0	0
38	K	61	Total 61	O 61	0	0
38	L	81	Total 81	O 81	0	0
38	M	124	Total 124	O 124	0	0
38	N	67	Total 67	O 67	0	0
38	O	43	Total 43	O 43	0	0
38	P	66	Total 66	O 66	0	0
38	Q	49	Total 49	O 49	0	0
38	R	80	Total 80	O 80	0	0
38	S	37	Total 37	O 37	0	0
38	T	37	Total 37	O 37	0	0
38	U	27	Total 27	O 27	0	0

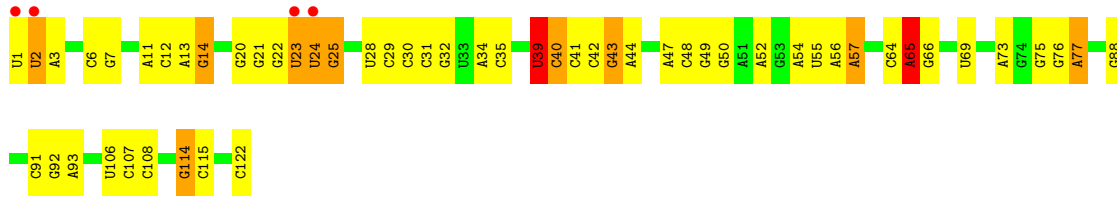
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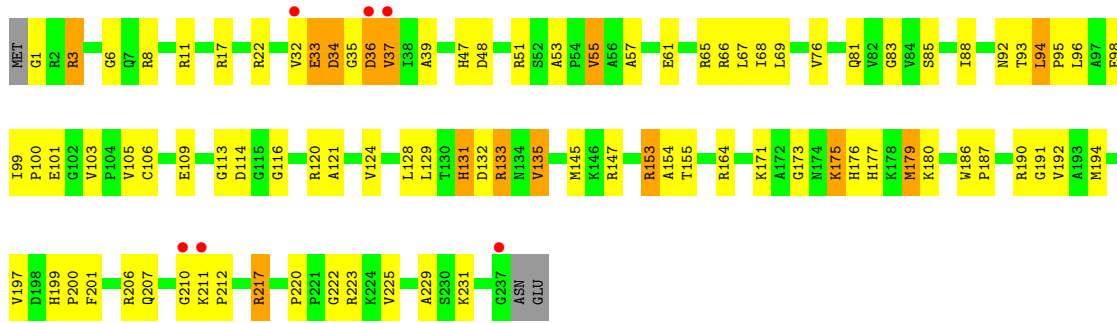
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	14	Total O 14 14	0	0
38	W	73	Total O 73 73	0	0
38	X	27	Total O 27 27	0	0
38	Y	94	Total O 94 94	0	0
38	Z	30	Total O 30 30	0	0
38	1	54	Total O 54 54	0	0
38	2	45	Total O 45 45	0	0
38	3	78	Total O 78 78	0	0



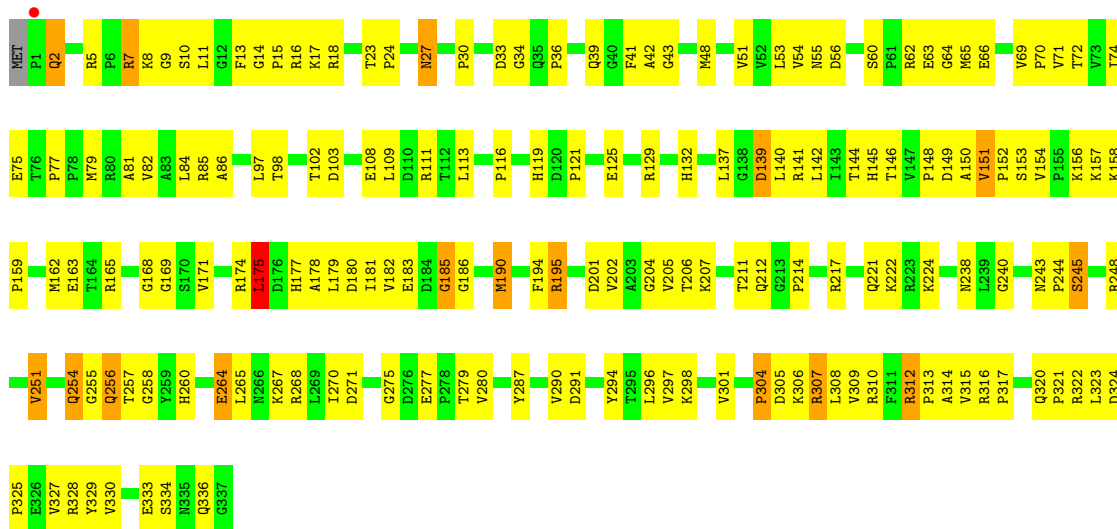
• Molecule 2: 5S Ribosomal RNA



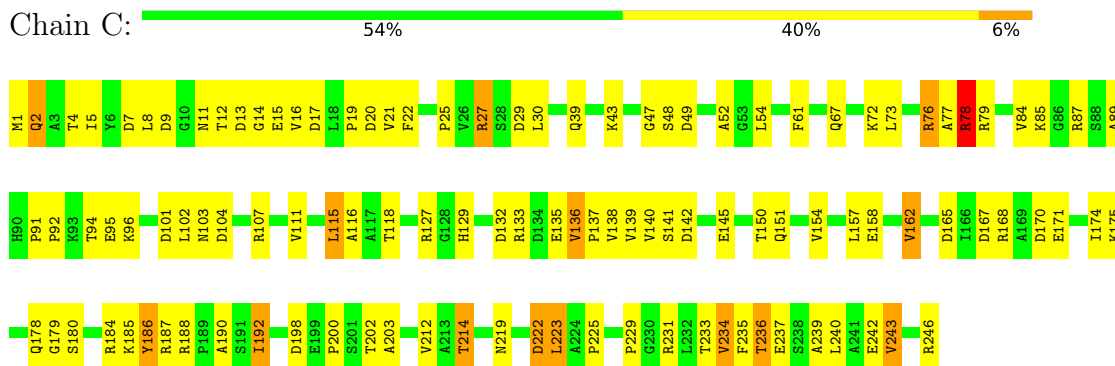
• Molecule 3: 50S ribosomal protein L2P



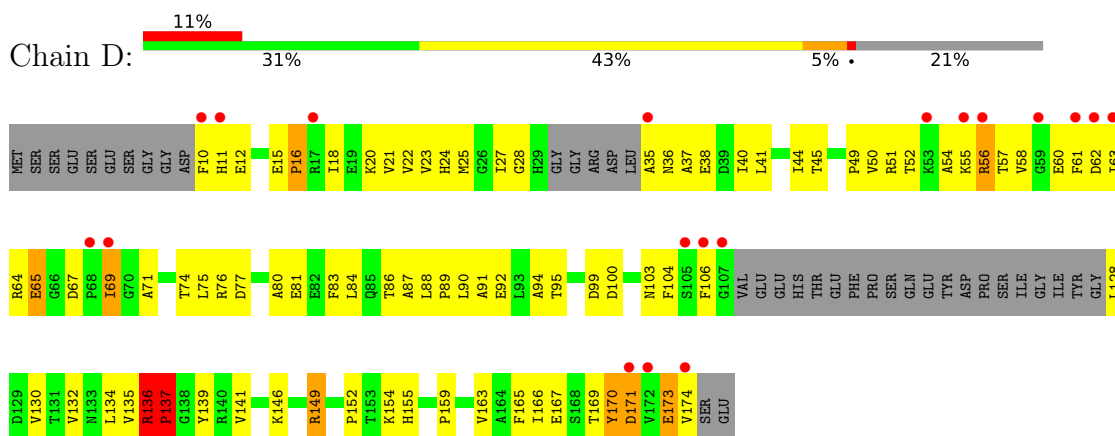
• Molecule 4: 50S ribosomal protein L3P



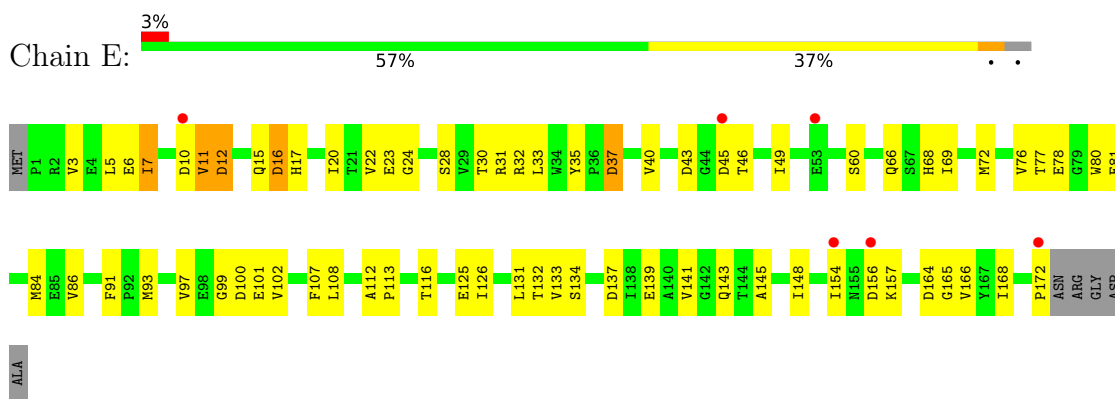
- Molecule 5: 50S ribosomal protein L4E



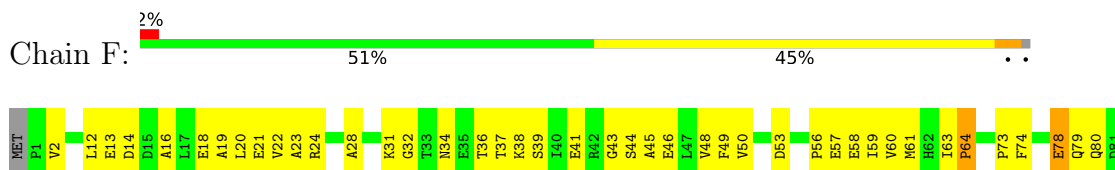
- Molecule 6: 50S ribosomal protein L5P



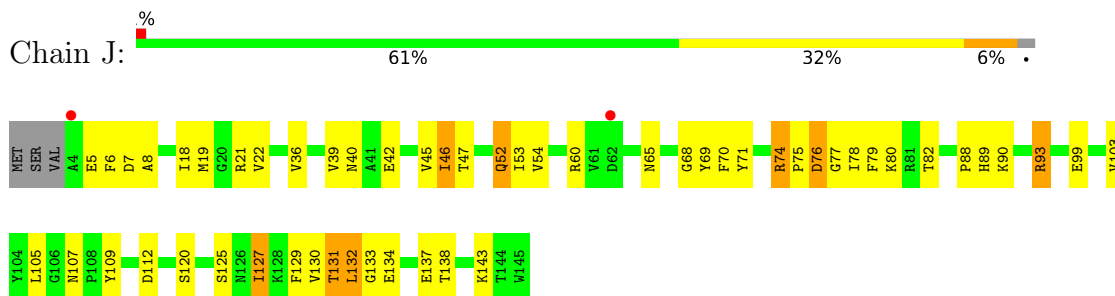
- Molecule 7: 50S ribosomal protein L6P



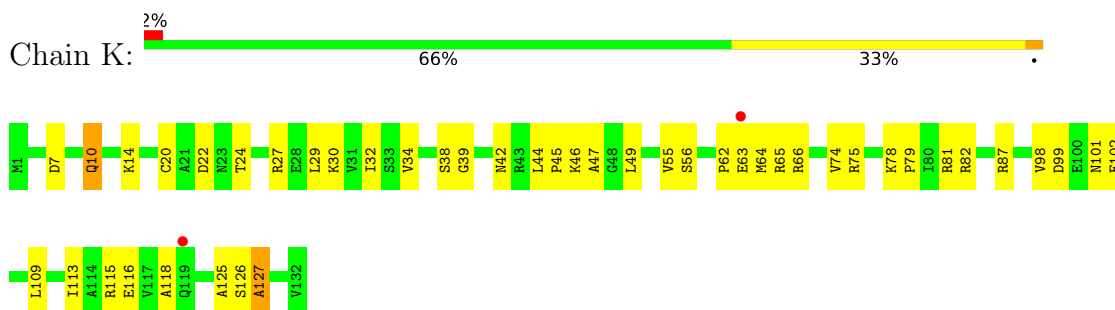
- Molecule 8: 50S ribosomal protein L7AE



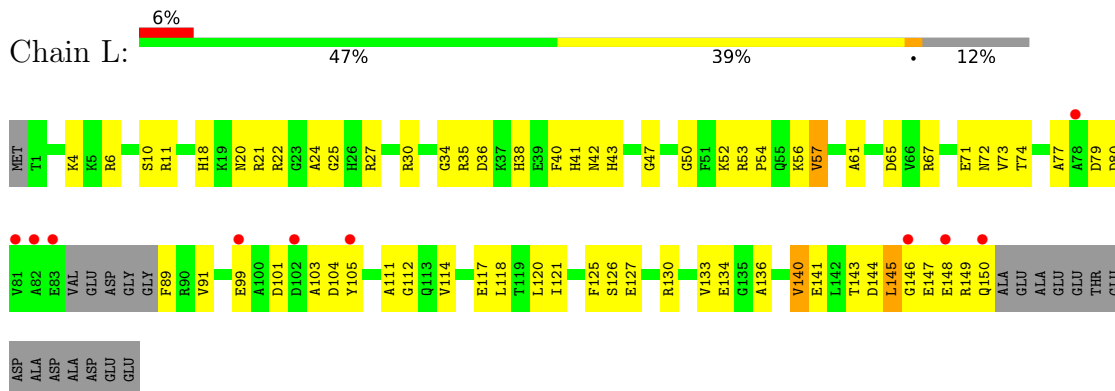
- Molecule 12: 50S ribosomal protein L13P



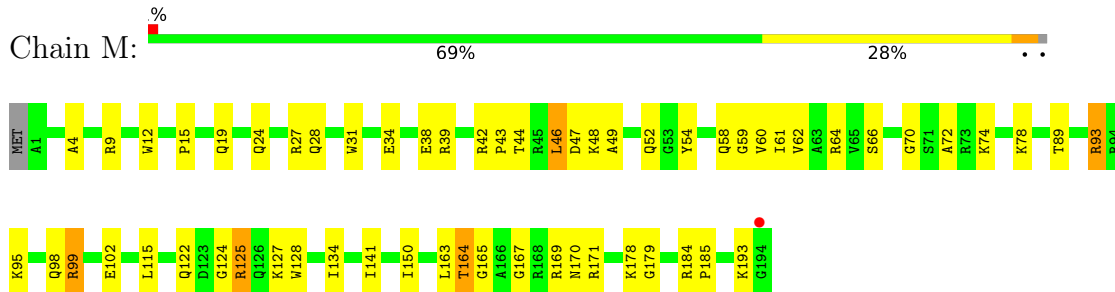
- Molecule 13: 50S ribosomal protein L14P



- Molecule 14: 50S ribosomal protein L15P



- Molecule 15: 50S Ribosomal Protein L15E

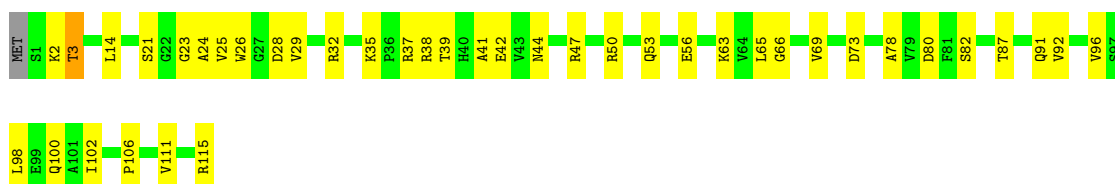


- Molecule 16: 50S ribosomal protein L18P

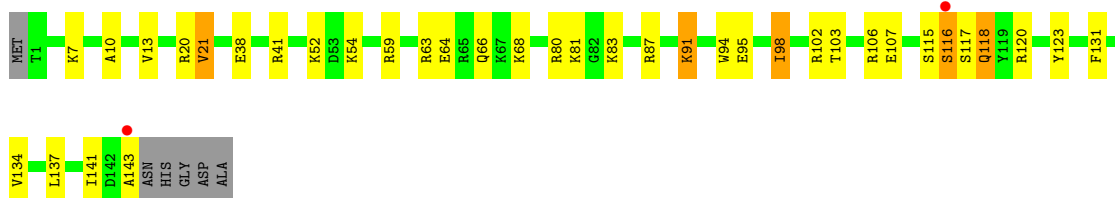




- Molecule 17: 50S ribosomal protein L18e



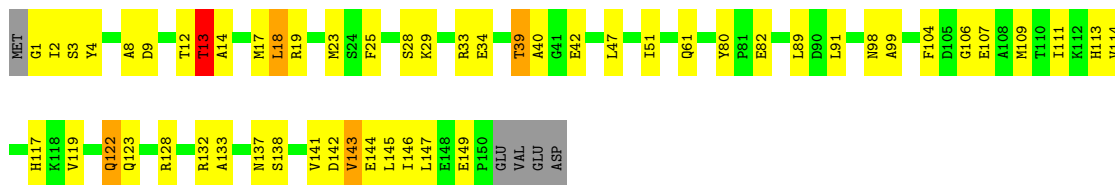
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e

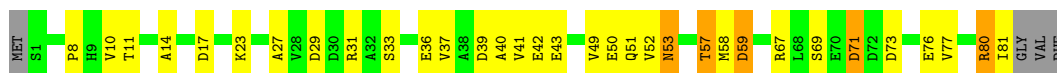


- Molecule 20: 50S ribosomal protein L22P



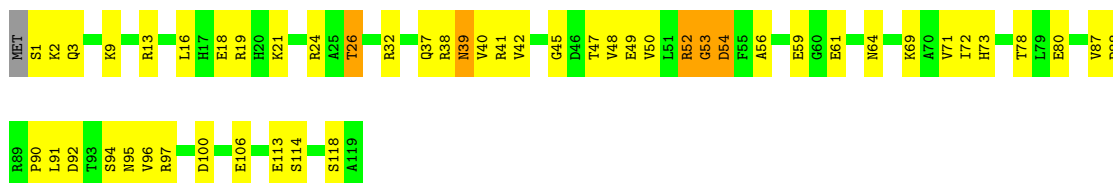
- Molecule 21: 50S ribosomal protein L23P

Chain S:  56% 33% 6% 5%



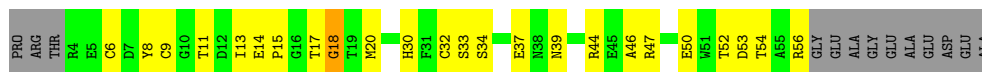
- Molecule 22: 50S ribosomal protein L24P

Chain T:  58% 38% 0% 0%



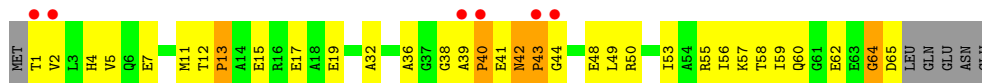
- Molecule 23: 50S ribosomal protein L24E

Chain U:  44% 35% 0% 20%



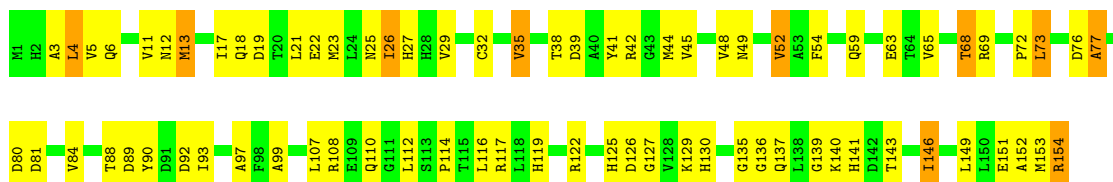
- Molecule 24: 50S ribosomal protein L29P

Chain V:  8% 45% 39% 7% 8%




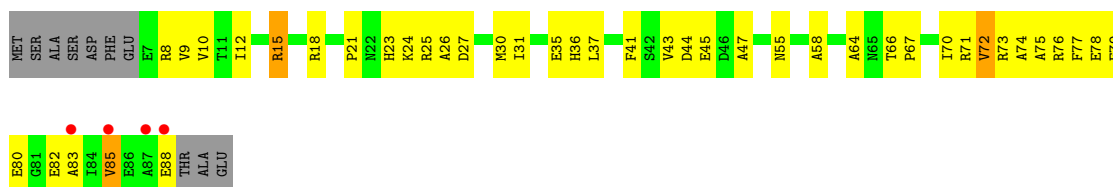
- Molecule 25: 50S ribosomal protein L30P

Chain W:  51% 42% 6%

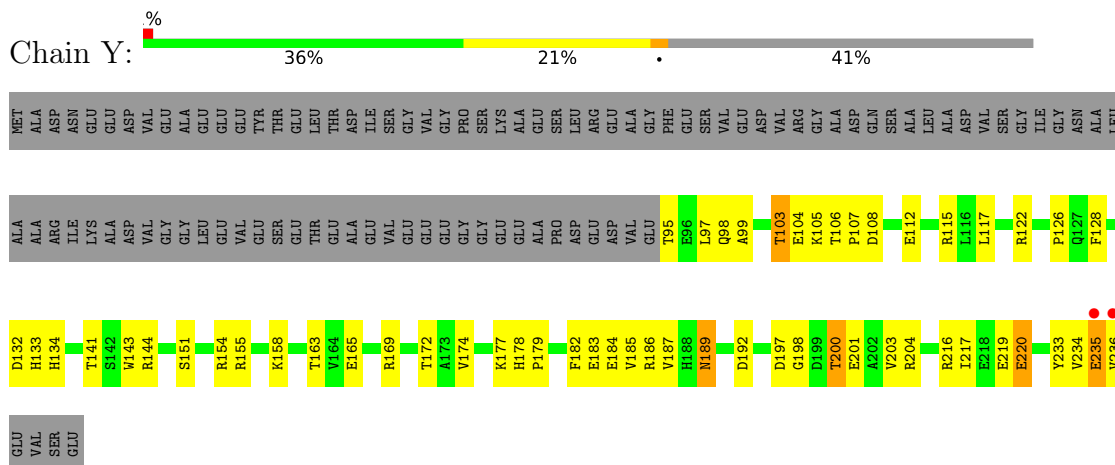


- Molecule 26: 50S ribosomal protein L31e

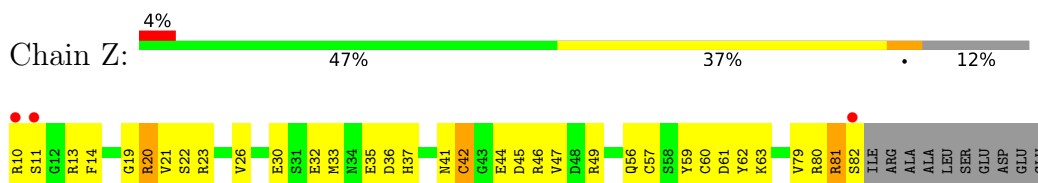
Chain X:  4% 43% 42% 0% 11%



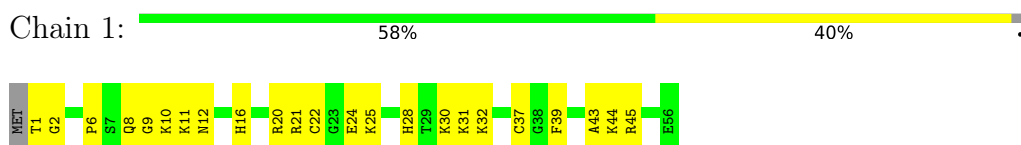
- Molecule 27: 50S ribosomal protein L32E



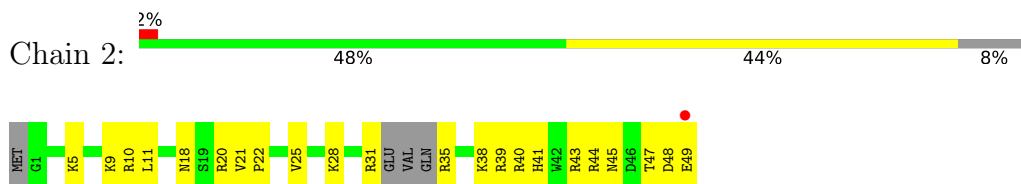
- Molecule 28: 50S ribosomal protein L37Ae



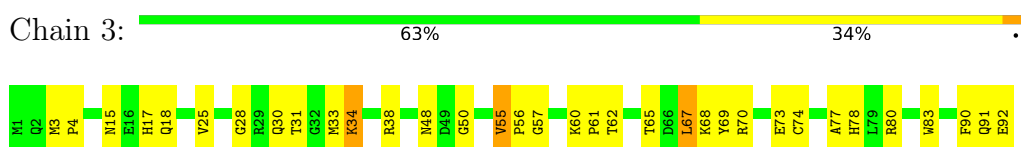
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 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	212.44Å 299.99Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.65) 94.4 (30.00-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.65Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.176 , 0.214 0.174 , 0.212	Depositor DCC
R_{free} test set	4879 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtrriage
Anisotropy	0.185	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99086	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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: CL, OMG, K, UR3, CD, MG, OMU, ERY, NA, PSU, 1MA

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	0.37	0/65957	0.61	25/102867 (0.0%)
2	9	0.37	0/2904	0.61	3/4526 (0.1%)
3	A	0.41	0/1786	1.00	5/2408 (0.2%)
4	B	0.40	0/2690	0.98	6/3652 (0.2%)
5	C	0.45	0/1884	0.99	9/2551 (0.4%)
6	D	0.35	0/1111	0.92	7/1498 (0.5%)
7	E	0.38	0/1382	0.89	2/1880 (0.1%)
8	F	0.36	0/901	0.87	0/1224
9	G	0.34	0/241	0.73	0/324
10	H	0.43	0/1302	0.95	4/1743 (0.2%)
11	I	0.38	0/526	0.99	5/716 (0.7%)
12	J	0.42	0/1136	0.95	7/1530 (0.5%)
13	K	0.40	0/1001	1.01	1/1347 (0.1%)
14	L	0.36	0/1130	0.97	6/1509 (0.4%)
15	M	0.40	0/1582	0.92	4/2117 (0.2%)
16	N	0.37	0/1474	1.03	9/1999 (0.5%)
17	O	0.42	0/874	0.93	6/1181 (0.5%)
18	P	0.40	0/1147	0.85	1/1528 (0.1%)
19	Q	0.42	0/749	1.06	4/1005 (0.4%)
20	R	0.44	0/1172	0.95	8/1578 (0.5%)
21	S	0.37	0/648	0.88	3/875 (0.3%)
22	T	0.37	0/958	0.96	5/1289 (0.4%)
23	U	0.37	0/417	0.89	2/562 (0.4%)
24	V	0.37	0/502	0.97	3/675 (0.4%)
25	W	0.47	0/1219	1.00	4/1655 (0.2%)
26	X	0.43	0/664	0.94	1/895 (0.1%)
27	Y	0.44	0/1146	0.92	2/1536 (0.1%)
28	Z	0.38	0/589	0.93	0/787
29	1	0.42	0/438	0.92	1/578 (0.2%)
30	2	0.40	0/401	0.77	0/529
31	3	0.40	0/771	0.89	3/1024 (0.3%)
All	All	0.38	0/98702	0.72	136/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	45
2	9	0	2
All	All	1	47

There are no bond length outliers.

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	0	1563	G	C2'-C3'-O3'	13.57	129.85	109.50
16	N	135	VAL	N-CA-C	-10.09	103.32	113.10
1	0	1563	G	C4'-C3'-O3'	8.79	122.58	109.40
19	Q	17	LYS	N-CA-C	-8.70	98.78	109.83
6	D	136	ARG	CA-C-N	8.53	130.50	119.84

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	26	U	Sidechain
1	0	270	U	Sidechain
1	0	396	U	Sidechain
1	0	470	U	Sidechain

5.2 Too-close contacts [i](#)

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	59020	0	29810	812	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	2599	0	1325	63	0
3	A	1753	0	1766	116	0
4	B	2625	0	2533	178	0
5	C	1859	0	1816	124	0
6	D	1094	0	1085	91	0
7	E	1357	0	1266	79	0
8	F	890	0	843	61	0
9	G	240	0	231	19	0
10	H	1282	0	1292	72	0
11	I	519	0	500	61	0
12	J	1120	0	1098	58	0
13	K	992	0	1031	54	0
14	L	1118	0	1076	65	0
15	M	1558	0	1566	58	0
16	N	1445	0	1401	114	0
17	O	865	0	873	29	0
18	P	1136	0	1123	42	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	52	0
21	S	641	0	605	28	0
22	T	950	0	923	47	0
23	U	410	0	364	31	0
24	V	499	0	511	36	0
25	W	1196	0	1137	102	0
26	X	654	0	653	48	0
27	Y	1130	0	1133	65	0
28	Z	578	0	539	28	0
29	1	431	0	426	33	0
30	2	396	0	413	32	0
31	3	755	0	728	30	0
32	0	51	0	67	0	0
33	0	108	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	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
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5869	0	0	163	0
38	1	54	0	0	3	0
38	2	45	0	0	6	0
38	3	78	0	0	10	0
38	9	138	0	0	9	0
38	A	121	0	0	16	0
38	B	151	0	0	20	0
38	C	168	0	0	27	0
38	D	50	0	0	17	0
38	E	42	0	0	11	0
38	F	28	0	0	8	0
38	G	19	0	0	1	0
38	H	71	0	0	17	0
38	I	9	0	0	4	0
38	J	55	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	K	61	0	0	11	0
38	L	81	0	0	23	0
38	M	124	0	0	11	0
38	N	67	0	0	13	0
38	O	43	0	0	6	0
38	P	66	0	0	2	0
38	Q	49	0	0	6	0
38	R	80	0	0	6	0
38	S	37	0	0	5	0
38	T	37	0	0	7	0
38	U	27	0	0	4	0
38	V	14	0	0	3	0
38	W	73	0	0	12	0
38	X	27	0	0	9	0
38	Y	94	0	0	14	0
38	Z	30	0	0	1	0
All	All	99086	0	59985	2416	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 16.

The worst 5 of 2416 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)
10:H:172:GLU:HB2	38:H:8591:HOH:O	1.34	1.21
1:O:1160:G:H5'	1:O:1161:A:H5'	1.24	1.17
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.16
10:H:174:LEU:HA	38:H:8571:HOH:O	1.50	1.11
2:9:6:C:H5''	16:N:37:ARG:NH1	1.66	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	213 (91%)	20 (8%)	2 (1%)	14	24
4	B	335/338 (99%)	300 (90%)	30 (9%)	5 (2%)	8	13
5	C	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	30	45
6	D	134/177 (76%)	98 (73%)	27 (20%)	9 (7%)	1	0
7	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
8	F	117/120 (98%)	101 (86%)	12 (10%)	4 (3%)	3	4
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	9	16
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100	100
12	J	140/145 (97%)	130 (93%)	5 (4%)	5 (4%)	2	4
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	16	27
14	L	141/165 (86%)	121 (86%)	19 (14%)	1 (1%)	18	30
15	M	192/195 (98%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	4	6
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	133 (94%)	7 (5%)	1 (1%)	18	30
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	14	24
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	3	4
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	16
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	1	1
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	11	19
All	All	3705/4437 (84%)	3374 (91%)	285 (8%)	46 (1%)	10	17

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
6	D	173	GLU
8	F	101	ALA
14	L	80	ASP
16	N	154	LEU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/182 (98%)	168 (94%)	11 (6%)	17	30
4	B	282/283 (100%)	264 (94%)	18 (6%)	16	28
5	C	193/193 (100%)	174 (90%)	19 (10%)	7	11
6	D	117/148 (79%)	113 (97%)	4 (3%)	32	53
7	E	152/156 (97%)	147 (97%)	5 (3%)	33	55
8	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
9	G	27/283 (10%)	26 (96%)	1 (4%)	30	50
10	H	134/145 (92%)	127 (95%)	7 (5%)	21	36
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	108 (92%)	10 (8%)	10	17
13	K	106/106 (100%)	103 (97%)	3 (3%)	38	60
14	L	113/127 (89%)	111 (98%)	2 (2%)	51	72
15	M	158/159 (99%)	154 (98%)	4 (2%)	42	64
16	N	149/150 (99%)	142 (95%)	7 (5%)	23	40
17	O	93/94 (99%)	90 (97%)	3 (3%)	34	55
18	P	113/117 (97%)	109 (96%)	4 (4%)	32	52
19	Q	79/80 (99%)	75 (95%)	4 (5%)	21	36
20	R	117/122 (96%)	113 (97%)	4 (3%)	32	53
21	S	71/74 (96%)	68 (96%)	3 (4%)	26	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	T	105/106 (99%)	101 (96%)	4 (4%)	29	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	48
25	W	130/130 (100%)	121 (93%)	9 (7%)	14	24
26	X	66/74 (89%)	63 (96%)	3 (4%)	24	42
27	Y	120/196 (61%)	112 (93%)	8 (7%)	15	25
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	78 (99%)	1 (1%)	61	77
All	All	3095/3619 (86%)	2957 (96%)	138 (4%)	24	42

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	V	13	PRO
25	W	26	ILE
27	Y	163	THR
6	D	24	HIS
5	C	243	VAL

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

Mol	Chain	Res	Type
16	N	140	GLN
21	S	9	HIS
30	2	18	ASN
18	P	66	GLN
20	R	61	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	249 (9%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2867/3044 (94%)	265 (9%)	36 (1%)

5 of 265 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2526	C
2	9	65	A
1	0	2536	C
1	0	2726	U
1	0	898	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PSU	0	2621	1	18,21,22	1.49	2 (11%)	21,30,33	1.26	3 (14%)
1	1MA	0	628	1	21,25,26	0.69	1 (4%)	30,37,40	0.79	1 (3%)
1	OMU	0	2587	1	19,22,23	0.31	0	25,31,34	0.38	0
1	OMG	0	2588	1	23,26,27	0.29	0	32,38,41	0.34	0
1	UR3	0	2619	1	19,22,23	0.46	0	26,32,35	0.71	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	2/7/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.98	1.43	1.36
1	0	2621	PSU	C6-C5	3.04	1.38	1.35
1	0	628	1MA	C6-N6	2.39	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	2.88	120.12	118.17
1	0	2621	PSU	C6-N1-C2	-2.88	120.02	122.69
1	0	2621	PSU	O2-C2-N1	2.85	125.72	122.79
1	0	628	1MA	N1-C2-N3	2.82	129.34	126.00
1	0	2619	UR3	C4-N3-C2	2.73	126.77	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2588	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ERY	0	9000	-	53,53,53	1.26	5 (9%)	82,82,82	0.99	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ERY	0	9000	-	-	4/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	ERY	C6-C5	3.44	1.61	1.55
32	0	9000	ERY	C7-C6	2.56	1.58	1.54
32	0	9000	ERY	O2-C13	2.25	1.50	1.46
32	0	9000	ERY	C2-C3	2.22	1.60	1.54
32	0	9000	ERY	O4-C18	2.07	1.49	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	ERY	C3-C2-C1	-2.58	104.71	109.93
32	0	9000	ERY	C25-C24-C23	-2.45	106.50	110.02
32	0	9000	ERY	O5-C16-C17	2.09	106.88	103.86
32	0	9000	ERY	O13-C12-C35	-2.05	103.65	107.84
32	0	9000	ERY	C6-C5-C4	-2.04	110.94	113.89

There are no chirality outliers.

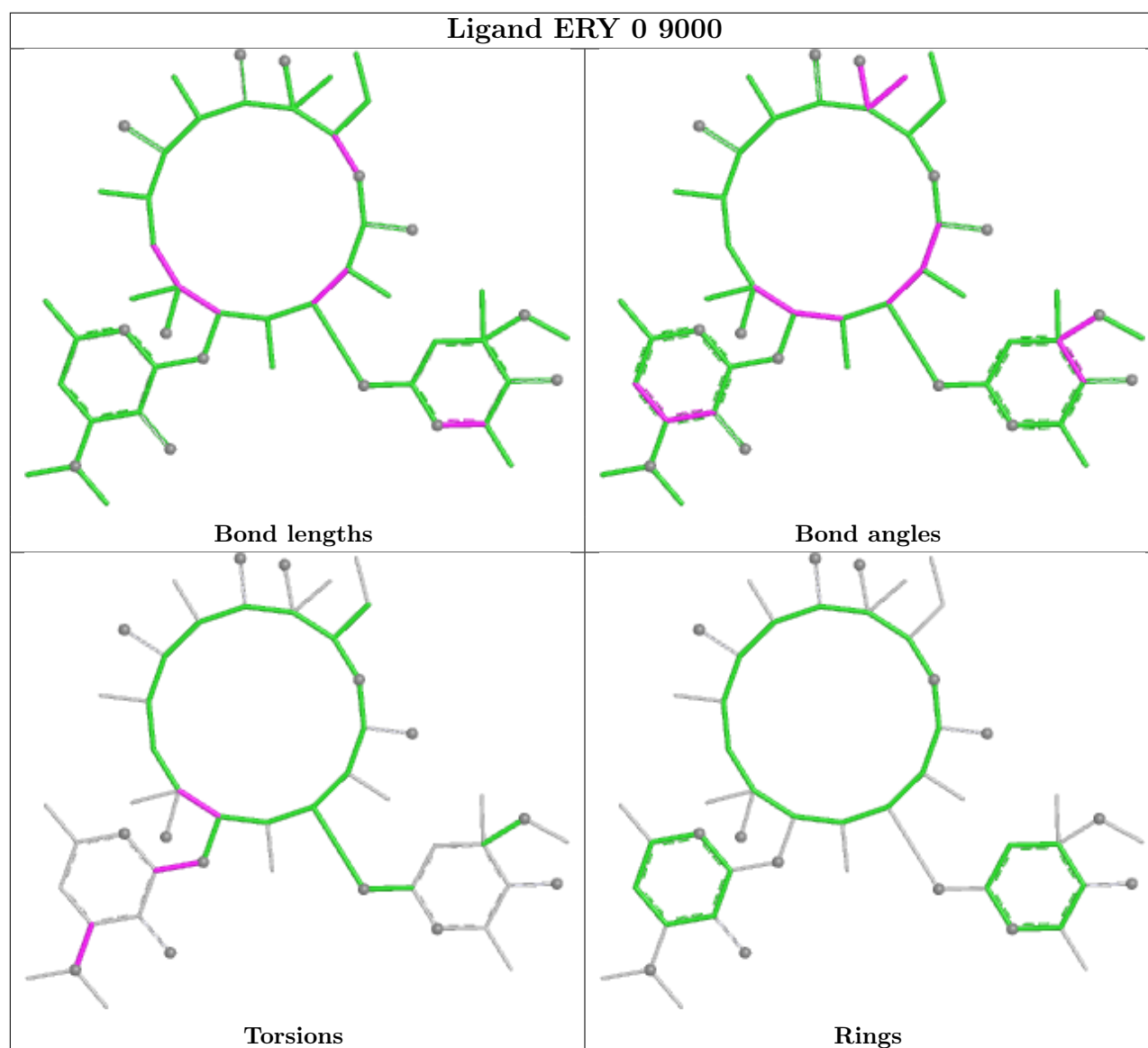
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	9000	ERY	O9-C22-O7-C5
32	0	9000	ERY	O7-C5-C6-C7
32	0	9000	ERY	C23-C22-O7-C5
32	0	9000	ERY	C25-C24-N1-C29

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.65	30 (1%) 78 75	26, 49, 94, 152	0
2	9	122/122 (100%)	-0.20	4 (3%) 49 40	40, 65, 90, 154	0
3	A	237/240 (98%)	-0.08	6 (2%) 58 52	31, 54, 88, 109	0
4	B	337/338 (99%)	-0.05	1 (0%) 90 89	30, 58, 83, 92	0
5	C	246/246 (100%)	-0.17	0 100 100	26, 48, 73, 82	0
6	D	140/177 (79%)	1.07	19 (13%) 7 5	56, 101, 125, 132	0
7	E	172/178 (96%)	0.24	6 (3%) 47 38	49, 71, 90, 94	0
8	F	119/120 (99%)	0.39	2 (1%) 69 64	51, 76, 95, 111	0
9	G	29/348 (8%)	1.01	7 (24%) 2 1	77, 93, 102, 104	0
10	H	160/177 (90%)	0.01	6 (3%) 44 36	39, 59, 92, 99	0
11	I	70/162 (43%)	1.88	27 (38%) 1 0	109, 122, 139, 141	0
12	J	142/145 (97%)	-0.12	2 (1%) 73 69	38, 53, 75, 95	0
13	K	132/132 (100%)	-0.03	2 (1%) 72 67	34, 55, 75, 86	0
14	L	145/165 (87%)	0.35	10 (6%) 23 17	27, 68, 109, 122	0
15	M	194/195 (99%)	-0.36	1 (0%) 87 85	34, 46, 61, 70	0
16	N	186/187 (99%)	0.29	5 (2%) 56 49	41, 64, 108, 119	0
17	O	115/116 (99%)	0.07	0 100 100	39, 57, 74, 78	0
18	P	143/149 (95%)	0.03	2 (1%) 73 69	41, 58, 71, 80	0
19	Q	95/96 (98%)	-0.36	1 (1%) 78 75	38, 46, 62, 76	0
20	R	150/155 (96%)	-0.46	0 100 100	35, 48, 67, 77	0
21	S	81/85 (95%)	-0.11	0 100 100	47, 63, 83, 88	0
22	T	119/120 (99%)	0.05	0 100 100	40, 61, 85, 97	0
23	U	53/66 (80%)	0.07	0 100 100	46, 59, 76, 86	0
24	V	65/71 (91%)	0.63	6 (9%) 14 11	58, 77, 114, 118	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.30	0 100 100	35, 50, 67, 78	0
26	X	82/92 (89%)	0.16	4 (4%) 35 27	48, 61, 85, 101	0
27	Y	142/241 (58%)	-0.26	2 (1%) 73 69	28, 47, 71, 89	0
28	Z	73/83 (87%)	0.35	3 (4%) 41 33	52, 64, 80, 95	0
29	1	56/57 (98%)	-0.70	0 100 100	29, 36, 42, 52	0
30	2	46/50 (92%)	0.21	1 (2%) 62 56	37, 61, 87, 102	0
31	3	92/92 (100%)	-0.05	0 100 100	37, 56, 70, 83	0
All	All	6646/7481 (88%)	-0.24	147 (2%) 62 56	26, 55, 99, 154	0

The worst 5 of 147 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	1	U	7.0
6	D	10	PHE	6.9
11	I	128	THR	6.4
24	V	1	THR	6.3
24	V	2	VAL	5.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	1MA	0	628	23/24	0.98	0.06	30,33,34,36	0
1	OMU	0	2587	21/22	0.98	0.06	35,37,40,43	0
1	OMG	0	2588	24/25	0.98	0.06	34,36,38,40	0
1	PSU	0	2621	20/21	0.98	0.05	28,31,35,36	0
1	UR3	0	2619	21/22	0.99	0.05	35,37,41,45	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands 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
35	NA	0	8529	1/1	0.56	0.18	76,76,76,76	0
35	NA	R	8586	1/1	0.68	0.58	87,87,87,87	0
35	NA	0	8571	1/1	0.75	0.20	58,58,58,58	0
35	NA	0	8582	1/1	0.77	0.17	80,80,80,80	0
33	MG	0	8087	1/1	0.79	0.21	63,63,63,63	0
33	MG	0	8049	1/1	0.80	0.16	74,74,74,74	0
33	MG	0	8092	1/1	0.81	0.15	83,83,83,83	0
35	NA	0	8584	1/1	0.82	0.14	54,54,54,54	0
35	NA	0	8524	1/1	0.83	0.31	62,62,62,62	0
35	NA	9	8551	1/1	0.85	0.29	39,39,39,39	0
35	NA	0	8541	1/1	0.86	0.15	53,53,53,53	0
33	MG	0	8050	1/1	0.86	0.08	71,71,71,71	0
33	MG	0	8088	1/1	0.87	0.07	38,38,38,38	0
35	NA	0	8564	1/1	0.87	0.15	49,49,49,49	0
35	NA	0	8568	1/1	0.87	0.24	76,76,76,76	0
35	NA	0	8540	1/1	0.87	0.14	52,52,52,52	0
35	NA	0	8566	1/1	0.88	0.12	59,59,59,59	0
33	MG	2	8076	1/1	0.88	0.08	53,53,53,53	0
35	NA	0	8570	1/1	0.88	0.27	63,63,63,63	0
35	NA	9	8583	1/1	0.88	0.13	58,58,58,58	0
33	MG	9	8095	1/1	0.88	0.15	72,72,72,72	0
35	NA	0	8562	1/1	0.89	0.19	63,63,63,63	0
35	NA	0	8563	1/1	0.89	0.21	63,63,63,63	0
35	NA	0	8533	1/1	0.89	0.11	38,38,38,38	0
35	NA	0	8526	1/1	0.89	0.13	55,55,55,55	0
33	MG	0	8112	1/1	0.89	0.09	47,47,47,47	0
35	NA	0	8557	1/1	0.89	0.16	60,60,60,60	0
35	NA	0	8514	1/1	0.90	0.14	40,40,40,40	0
35	NA	0	8569	1/1	0.90	0.16	57,57,57,57	0
35	NA	0	8585	1/1	0.90	0.27	53,53,53,53	0
32	ERY	0	9000	51/51	0.91	0.16	69,75,79,80	0
35	NA	0	8581	1/1	0.91	0.08	51,51,51,51	0
35	NA	0	8508	1/1	0.92	0.14	68,68,68,68	0
33	MG	0	8102	1/1	0.92	0.07	55,55,55,55	0
33	MG	0	8094	1/1	0.92	0.15	72,72,72,72	0
35	NA	0	8559	1/1	0.92	0.16	64,64,64,64	0
35	NA	0	8560	1/1	0.92	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8567	1/1	0.93	0.10	50,50,50,50	0
35	NA	0	8511	1/1	0.93	0.10	58,58,58,58	0
35	NA	0	8542	1/1	0.93	0.17	52,52,52,52	0
35	NA	0	8552	1/1	0.93	0.21	57,57,57,57	0
35	NA	0	8555	1/1	0.93	0.11	72,72,72,72	0
35	NA	0	8579	1/1	0.93	0.11	58,58,58,58	0
33	MG	0	8082	1/1	0.93	0.13	64,64,64,64	0
33	MG	0	8045	1/1	0.93	0.10	60,60,60,60	0
33	MG	0	8101	1/1	0.93	0.10	58,58,58,58	0
35	NA	0	8502	1/1	0.93	0.09	56,56,56,56	0
35	NA	0	8532	1/1	0.93	0.10	40,40,40,40	0
35	NA	0	8507	1/1	0.93	0.11	54,54,54,54	0
35	NA	L	8580	1/1	0.93	0.30	60,60,60,60	0
33	MG	0	8070	1/1	0.93	0.06	50,50,50,50	0
35	NA	0	8572	1/1	0.94	0.13	64,64,64,64	0
35	NA	0	8573	1/1	0.94	0.06	58,58,58,58	0
35	NA	0	8577	1/1	0.94	0.20	62,62,62,62	0
35	NA	0	8518	1/1	0.94	0.08	39,39,39,39	0
33	MG	0	8053	1/1	0.94	0.07	45,45,45,45	0
35	NA	0	8565	1/1	0.94	0.20	46,46,46,46	0
33	MG	0	8062	1/1	0.94	0.07	66,66,66,66	0
35	NA	0	8527	1/1	0.94	0.07	45,45,45,45	0
33	MG	0	8066	1/1	0.94	0.08	96,96,96,96	0
33	MG	0	8114	1/1	0.94	0.06	55,55,55,55	0
33	MG	0	8099	1/1	0.94	0.09	55,55,55,55	0
35	NA	R	8537	1/1	0.94	0.06	42,42,42,42	0
33	MG	T	8073	1/1	0.94	0.05	61,61,61,61	0
36	CL	0	8815	1/1	0.94	0.18	81,81,81,81	0
36	CL	3	8804	1/1	0.94	0.08	63,63,63,63	0
35	NA	0	8574	1/1	0.95	0.16	65,65,65,65	0
33	MG	0	8051	1/1	0.95	0.06	71,71,71,71	0
35	NA	0	8510	1/1	0.95	0.09	45,45,45,45	0
33	MG	0	8047	1/1	0.95	0.10	77,77,77,77	0
35	NA	0	8513	1/1	0.95	0.06	54,54,54,54	0
33	MG	0	8085	1/1	0.95	0.06	50,50,50,50	0
35	NA	0	8516	1/1	0.95	0.09	51,51,51,51	0
35	NA	0	8549	1/1	0.95	0.06	46,46,46,46	0
35	NA	0	8550	1/1	0.95	0.09	47,47,47,47	0
35	NA	H	8522	1/1	0.95	0.22	56,56,56,56	0
33	MG	0	8100	1/1	0.95	0.13	69,69,69,69	0
35	NA	Q	8548	1/1	0.95	0.05	47,47,47,47	0
33	MG	0	8041	1/1	0.95	0.07	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8046	1/1	0.95	0.04	43,43,43,43	0
35	NA	S	8512	1/1	0.95	0.11	22,22,22,22	0
36	CL	0	8805	1/1	0.95	0.09	63,63,63,63	0
35	NA	0	8558	1/1	0.95	0.26	102,102,102,102	0
36	CL	0	8822	1/1	0.95	0.27	83,83,83,83	0
36	CL	L	8810	1/1	0.95	0.07	60,60,60,60	0
33	MG	0	8105	1/1	0.95	0.05	54,54,54,54	0
33	MG	0	8063	1/1	0.96	0.04	68,68,68,68	0
35	NA	0	8535	1/1	0.96	0.08	49,49,49,49	0
35	NA	A	8545	1/1	0.96	0.07	50,50,50,50	0
35	NA	C	8504	1/1	0.96	0.08	46,46,46,46	0
33	MG	0	8064	1/1	0.96	0.07	34,34,34,34	0
33	MG	0	8103	1/1	0.96	0.08	67,67,67,67	0
35	NA	0	8520	1/1	0.96	0.08	37,37,37,37	0
35	NA	0	8575	1/1	0.96	0.18	50,50,50,50	0
35	NA	0	8576	1/1	0.96	0.09	52,52,52,52	0
33	MG	0	8104	1/1	0.96	0.06	53,53,53,53	0
33	MG	0	8096	1/1	0.96	0.05	45,45,45,45	0
36	CL	0	8813	1/1	0.96	0.09	57,57,57,57	0
33	MG	0	8098	1/1	0.96	0.08	34,34,34,34	0
36	CL	0	8816	1/1	0.96	0.09	60,60,60,60	0
33	MG	0	8048	1/1	0.96	0.06	71,71,71,71	0
36	CL	A	8809	1/1	0.96	0.08	66,66,66,66	0
35	NA	0	8556	1/1	0.96	0.17	44,44,44,44	0
33	MG	0	8043	1/1	0.96	0.05	49,49,49,49	0
35	NA	0	8530	1/1	0.97	0.07	49,49,49,49	0
35	NA	0	8561	1/1	0.97	0.07	58,58,58,58	0
33	MG	0	8113	1/1	0.97	0.07	51,51,51,51	0
34	K	0	8402	1/1	0.97	0.15	59,59,59,59	0
35	NA	0	8534	1/1	0.97	0.14	44,44,44,44	0
35	NA	0	8515	1/1	0.97	0.10	48,48,48,48	0
35	NA	0	8539	1/1	0.97	0.04	28,28,28,28	0
35	NA	H	8509	1/1	0.97	0.04	34,34,34,34	0
33	MG	0	8057	1/1	0.97	0.06	49,49,49,49	0
35	NA	0	8517	1/1	0.97	0.06	46,46,46,46	0
35	NA	M	8547	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8505	1/1	0.97	0.05	33,33,33,33	0
35	NA	0	8544	1/1	0.97	0.04	32,32,32,32	0
35	NA	0	8506	1/1	0.97	0.19	42,42,42,42	0
35	NA	0	8521	1/1	0.97	0.11	57,57,57,57	0
35	NA	0	8523	1/1	0.97	0.10	38,38,38,38	0
35	NA	0	8554	1/1	0.97	0.11	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8115	1/1	0.97	0.04	55,55,55,55	0
35	NA	0	8525	1/1	0.97	0.07	59,59,59,59	0
36	CL	0	8817	1/1	0.97	0.05	63,63,63,63	0
33	MG	0	8042	1/1	0.97	0.07	40,40,40,40	0
35	NA	0	8578	1/1	0.97	0.14	52,52,52,52	0
36	CL	J	8801	1/1	0.97	0.13	65,65,65,65	0
36	CL	J	8802	1/1	0.97	0.05	63,63,63,63	0
33	MG	K	8069	1/1	0.97	0.03	57,57,57,57	0
36	CL	N	8807	1/1	0.97	0.07	63,63,63,63	0
36	CL	O	8808	1/1	0.97	0.07	72,72,72,72	0
36	CL	Y	8820	1/1	0.97	0.06	46,46,46,46	0
33	MG	0	8090	1/1	0.97	0.09	60,60,60,60	0
33	MG	0	8107	1/1	0.98	0.07	68,68,68,68	0
33	MG	0	8111	1/1	0.98	0.10	34,34,34,34	0
33	MG	0	8075	1/1	0.98	0.03	44,44,44,44	0
35	NA	R	8538	1/1	0.98	0.04	57,57,57,57	0
33	MG	0	8097	1/1	0.98	0.05	36,36,36,36	0
35	NA	0	8531	1/1	0.98	0.05	40,40,40,40	0
35	NA	T	8543	1/1	0.98	0.07	39,39,39,39	0
36	CL	0	8803	1/1	0.98	0.07	59,59,59,59	0
33	MG	0	8039	1/1	0.98	0.04	50,50,50,50	0
33	MG	0	8044	1/1	0.98	0.06	49,49,49,49	0
36	CL	0	8814	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	8116	1/1	0.98	0.04	37,37,37,37	0
33	MG	0	8040	1/1	0.98	0.03	61,61,61,61	0
33	MG	B	8055	1/1	0.98	0.04	52,52,52,52	0
33	MG	0	8014	1/1	0.98	0.07	34,34,34,34	0
33	MG	0	8052	1/1	0.98	0.04	58,58,58,58	0
36	CL	B	8819	1/1	0.98	0.08	54,54,54,54	0
33	MG	0	8067	1/1	0.98	0.06	49,49,49,49	0
33	MG	3	8078	1/1	0.98	0.09	47,47,47,47	0
36	CL	J	8821	1/1	0.98	0.05	55,55,55,55	0
34	K	0	8401	1/1	0.98	0.17	75,75,75,75	0
33	MG	0	8093	1/1	0.98	0.06	48,48,48,48	0
35	NA	0	8501	1/1	0.98	0.10	35,35,35,35	0
36	CL	R	8806	1/1	0.98	0.06	50,50,50,50	0
35	NA	J	8546	1/1	0.98	0.06	55,55,55,55	0
33	MG	0	8024	1/1	0.98	0.03	23,23,23,23	0
33	MG	A	8065	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8091	1/1	0.99	0.03	59,59,59,59	0
33	MG	0	8004	1/1	0.99	0.03	27,27,27,27	0
33	MG	0	8016	1/1	0.99	0.03	35,35,35,35	0

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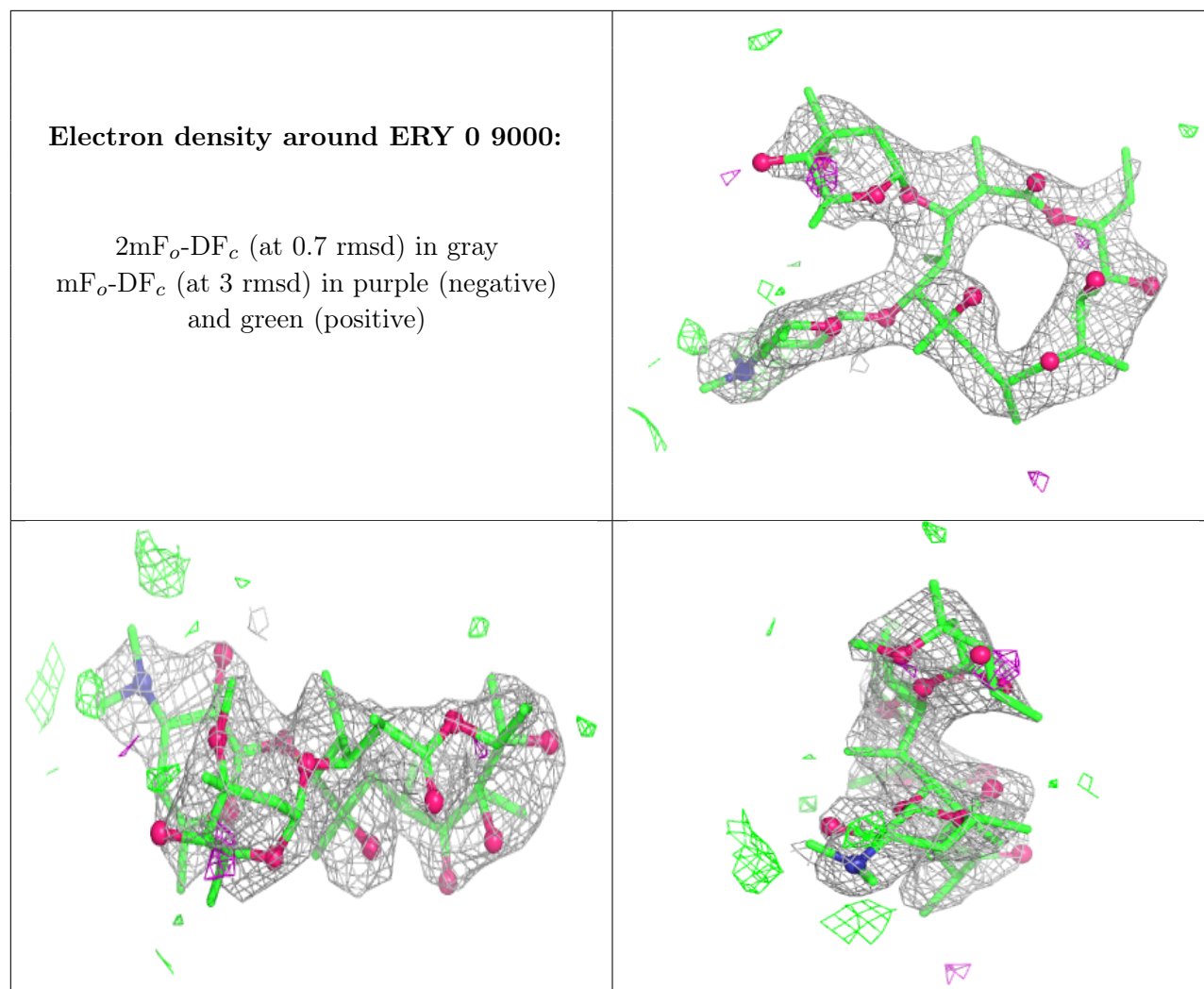
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	Y	8108	1/1	0.99	0.04	40,40,40,40	0
35	NA	0	8528	1/1	0.99	0.15	49,49,49,49	0
33	MG	0	8019	1/1	0.99	0.02	37,37,37,37	0
33	MG	0	8022	1/1	0.99	0.02	41,41,41,41	0
33	MG	0	8012	1/1	0.99	0.03	34,34,34,34	0
33	MG	0	8068	1/1	0.99	0.02	68,68,68,68	0
33	MG	0	8025	1/1	0.99	0.02	46,46,46,46	0
33	MG	0	8071	1/1	0.99	0.03	72,72,72,72	0
36	CL	0	8811	1/1	0.99	0.05	54,54,54,54	0
36	CL	0	8812	1/1	0.99	0.05	54,54,54,54	0
35	NA	0	8503	1/1	0.99	0.05	39,39,39,39	0
35	NA	0	8536	1/1	0.99	0.02	47,47,47,47	0
33	MG	0	8072	1/1	0.99	0.03	56,56,56,56	0
33	MG	0	8027	1/1	0.99	0.04	49,49,49,49	0
33	MG	0	8080	1/1	0.99	0.03	46,46,46,46	0
33	MG	0	8081	1/1	0.99	0.03	53,53,53,53	0
33	MG	0	8028	1/1	0.99	0.02	37,37,37,37	0
33	MG	0	8083	1/1	0.99	0.05	41,41,41,41	0
33	MG	0	8110	1/1	0.99	0.02	41,41,41,41	0
33	MG	0	8084	1/1	0.99	0.06	48,48,48,48	0
35	NA	0	8553	1/1	0.99	0.05	30,30,30,30	0
33	MG	0	8058	1/1	0.99	0.05	44,44,44,44	0
36	CL	M	8818	1/1	0.99	0.03	48,48,48,48	0
33	MG	0	8086	1/1	0.99	0.05	48,48,48,48	0
33	MG	0	8059	1/1	0.99	0.04	33,33,33,33	0
33	MG	0	8060	1/1	0.99	0.05	42,42,42,42	0
33	MG	0	8089	1/1	0.99	0.10	56,56,56,56	0
33	MG	0	8061	1/1	0.99	0.03	40,40,40,40	0
37	CD	O	8705	1/1	0.99	0.02	74,74,74,74	0
37	CD	1	8702	1/1	0.99	0.03	63,63,63,63	0
33	MG	0	8008	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8054	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8056	1/1	1.00	0.02	53,53,53,53	0
33	MG	0	8026	1/1	1.00	0.01	29,29,29,29	0
33	MG	0	8009	1/1	1.00	0.02	33,33,33,33	0
33	MG	0	8010	1/1	1.00	0.02	37,37,37,37	0
33	MG	0	8029	1/1	1.00	0.01	49,49,49,49	0
33	MG	0	8030	1/1	1.00	0.01	29,29,29,29	0
33	MG	0	8031	1/1	1.00	0.01	34,34,34,34	0
33	MG	0	8032	1/1	1.00	0.07	39,39,39,39	0
33	MG	0	8033	1/1	1.00	0.02	32,32,32,32	0
33	MG	0	8034	1/1	1.00	0.02	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8035	1/1	1.00	0.01	49,49,49,49	0
35	NA	0	8519	1/1	1.00	0.04	36,36,36,36	0
33	MG	0	8106	1/1	1.00	0.01	42,42,42,42	0
33	MG	0	8036	1/1	1.00	0.03	35,35,35,35	0
33	MG	0	8109	1/1	1.00	0.02	23,23,23,23	0
33	MG	0	8037	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8038	1/1	1.00	0.01	32,32,32,32	0
33	MG	0	8011	1/1	1.00	0.05	25,25,25,25	0
33	MG	0	8074	1/1	1.00	0.01	38,38,38,38	0
33	MG	0	8002	1/1	1.00	0.06	33,33,33,33	0
33	MG	0	8077	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8079	1/1	1.00	0.02	30,30,30,30	0
33	MG	0	8013	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8003	1/1	1.00	0.01	32,32,32,32	0
33	MG	0	8015	1/1	1.00	0.02	35,35,35,35	0
33	MG	0	8001	1/1	1.00	0.03	33,33,33,33	0
33	MG	0	8017	1/1	1.00	0.04	25,25,25,25	0
33	MG	0	8018	1/1	1.00	0.02	45,45,45,45	0
33	MG	0	8005	1/1	1.00	0.01	30,30,30,30	0
33	MG	0	8020	1/1	1.00	0.01	36,36,36,36	0
33	MG	0	8021	1/1	1.00	0.01	35,35,35,35	0
33	MG	0	8006	1/1	1.00	0.02	38,38,38,38	0
33	MG	0	8023	1/1	1.00	0.02	39,39,39,39	0
37	CD	U	8701	1/1	1.00	0.01	67,67,67,67	0
37	CD	Z	8703	1/1	1.00	0.01	63,63,63,63	0
33	MG	0	8007	1/1	1.00	0.03	27,27,27,27	0
37	CD	3	8704	1/1	1.00	0.02	62,62,62,62	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.



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.