



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2024 – 08:23 AM EDT

PDB ID : 5NC5
Title : Crystal structure of AcrBZ in complex with antibiotic puromycin
Authors : Du, D.; Luisi, B.
Deposited on : 2017-03-03
Resolution : 3.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

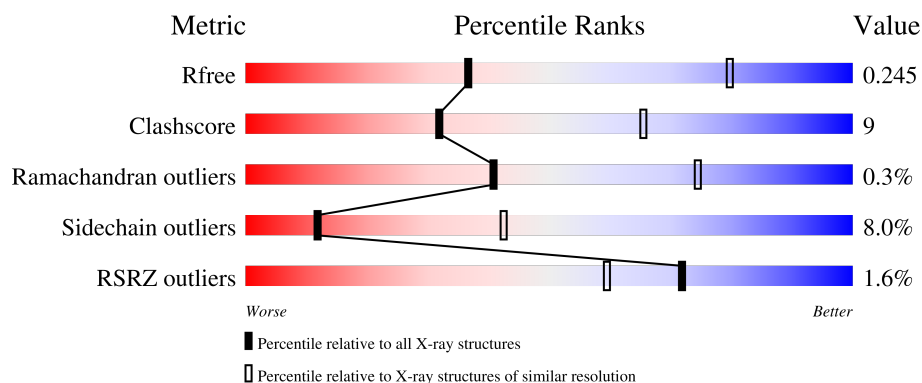
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



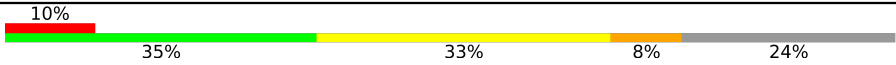
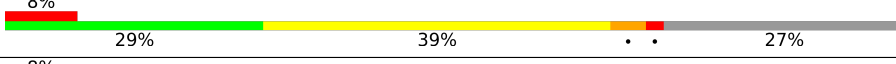
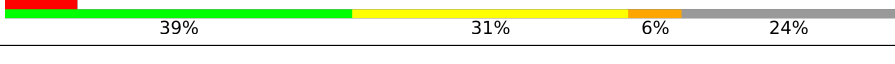
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	1049	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	B	1049	<div> <div>%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	C	1049	<div> <div>%</div> <div>71%</div> <div>24%</div> <div>..</div> </div>
2	D	169	<div> <div>%</div> <div>73%</div> <div>17%</div> <div>8%</div> </div>
2	E	169	<div> <div>%</div> <div>68%</div> <div>20%</div> <div>10%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	49	
3	G	49	
3	H	49	

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
5	D12	B	1104	-	-	-	X
6	D10	A	1105	-	-	-	X
6	D10	A	1109	-	-	-	X
6	D10	B	1114	-	-	-	X
6	D10	B	1122	-	-	-	X
6	D10	C	1111	-	-	-	X
6	D10	C	1114	-	-	-	X
6	D10	C	1115	-	-	-	X
6	D10	C	1116	-	-	-	X
6	D10	C	1117	-	-	-	X
7	DD9	A	1114	-	-	-	X
7	DD9	B	1106	-	-	-	X
7	DD9	B	1109	-	-	-	X
7	DD9	B	1112	-	-	-	X
8	PUY	B	1120	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 55690 atoms, of which 28293 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1044	Total	C	H	N	O	S	0	0	0
			15927	5086	8019	1308	1470	44			
1	B	1033	Total	C	H	N	O	S	0	0	0
			15835	5049	7990	1294	1458	44			
1	C	1033	Total	C	H	N	O	S	0	0	0
			15835	5049	7990	1294	1458	44			

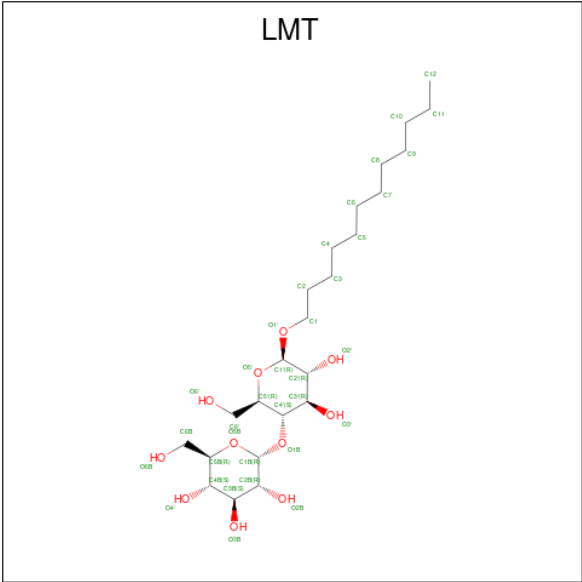
- Molecule 2 is a protein called DARPin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	156	Total	C	H	N	O	S	0	0	0
			2336	741	1159	206	229	1			
2	E	152	Total	C	H	N	O	S	0	0	0
			2287	726	1136	202	222	1			

- Molecule 3 is a protein called Multidrug efflux pump accessory protein AcrZ.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	37	Total	C	H	N	O	S	0	0	0
			601	196	318	39	45	3			
3	G	36	Total	C	H	N	O	S	0	0	0
			590	193	313	38	43	3			
3	H	37	Total	C	H	N	O	S	0	0	0
			601	196	318	39	45	3			

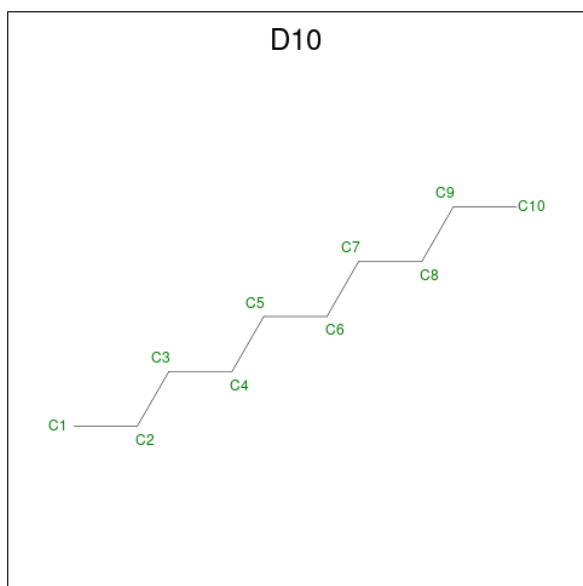
- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	H	0	0
			38	12	26		
5	B	1	Total	C	H	0	0
			28	9	19		
5	B	1	Total	C	H	0	0
			34	11	23		
5	C	1	Total	C	H	0	0
			38	12	26		
5	C	1	Total	C	H	0	0
			38	12	26		
5	C	1	Total	C	H	0	0
			38	12	26		
5	C	1	Total	C	H	0	0
			16	5	11		

- Molecule 6 is DECANE (three-letter code: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	0	0
			32	10	22		
6	A	1	Total	C	H	0	0
			32	10	22		
6	A	1	Total	C	H	0	0
			32	10	22		
6	A	1	Total	C	H	0	0
			32	10	22		

Continued on next page...

Continued from previous page...

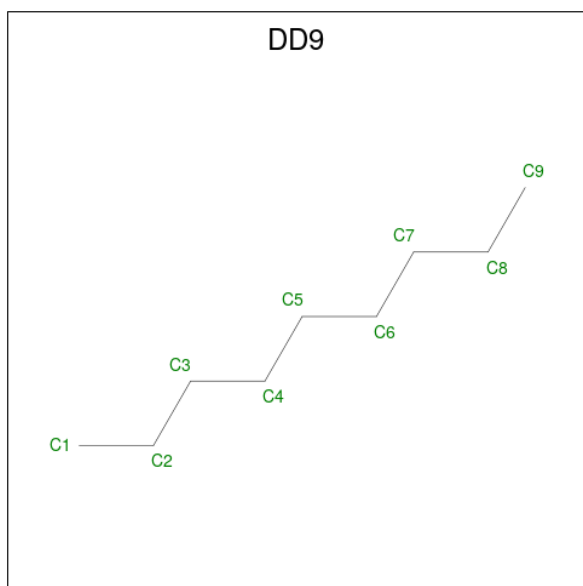
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0
6	C	1	Total 32	C 10	H 22	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	H	0	0
			32	10	22		

- Molecule 7 is nonane (three-letter code: DD9) (formula: C₉H₂₀).



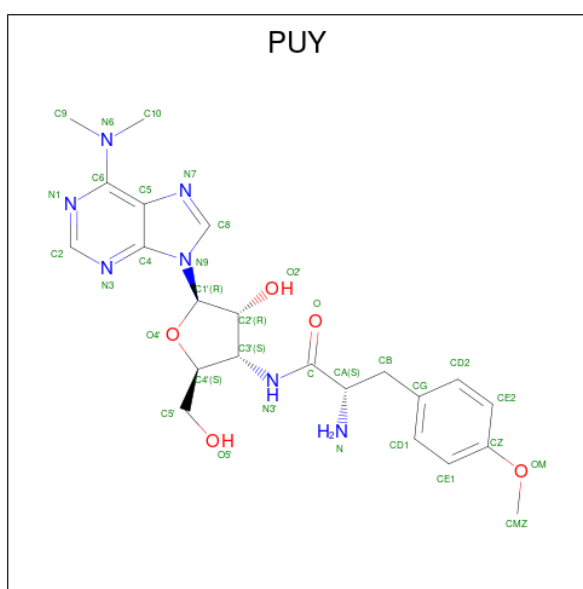
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	H	0	0
			28	9	19		
7	A	1	Total	C	H	0	0
			16	5	11		
7	A	1	Total	C	H	0	0
			22	7	15		
7	A	1	Total	C	H	0	0
			28	9	19		
7	B	1	Total	C	H	0	0
			16	5	11		
7	B	1	Total	C	H	0	0
			17	7	10		
7	B	1	Total	C	H	0	0
			19	6	13		
7	B	1	Total	C	H	0	0
			25	9	16		
7	B	1	Total	C	H	0	0
			22	7	15		
7	B	1	Total	C	H	0	0
			19	6	13		

Continued on next page...

Continued from previous page...

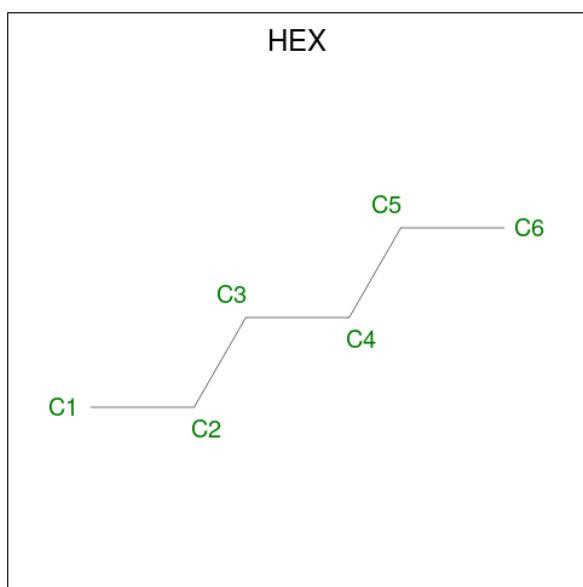
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	H	0	0
			28	9	19		
7	C	1	Total	C	H	0	0
			13	4	9		
7	C	1	Total	C	H	0	0
			19	6	13		
7	C	1	Total	C	H	0	0
			25	8	17		

- Molecule 8 is PUROMYCIN (three-letter code: PUY) (formula: $C_{22}H_{29}N_7O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			34	22	7	5		

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C_6H_{14}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	H	0	0
			20	6	14		

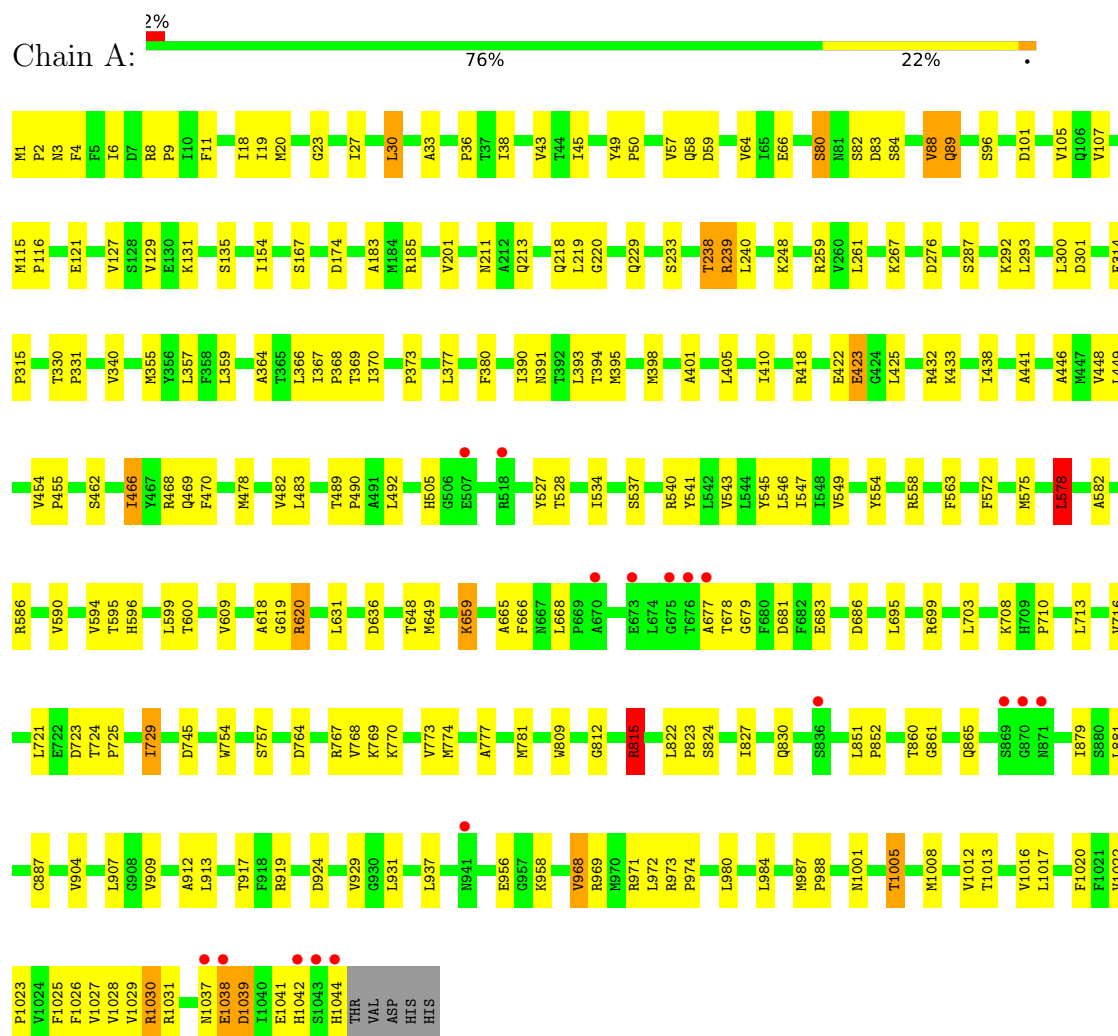
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total	O	0	0
			50	50		
10	B	26	Total	O	0	0
			26	26		
10	C	21	Total	O	0	0
			21	21		
10	D	1	Total	O	0	0
			1	1		

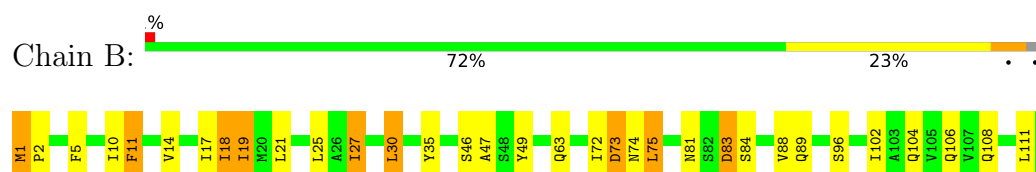
3 Residue-property plots

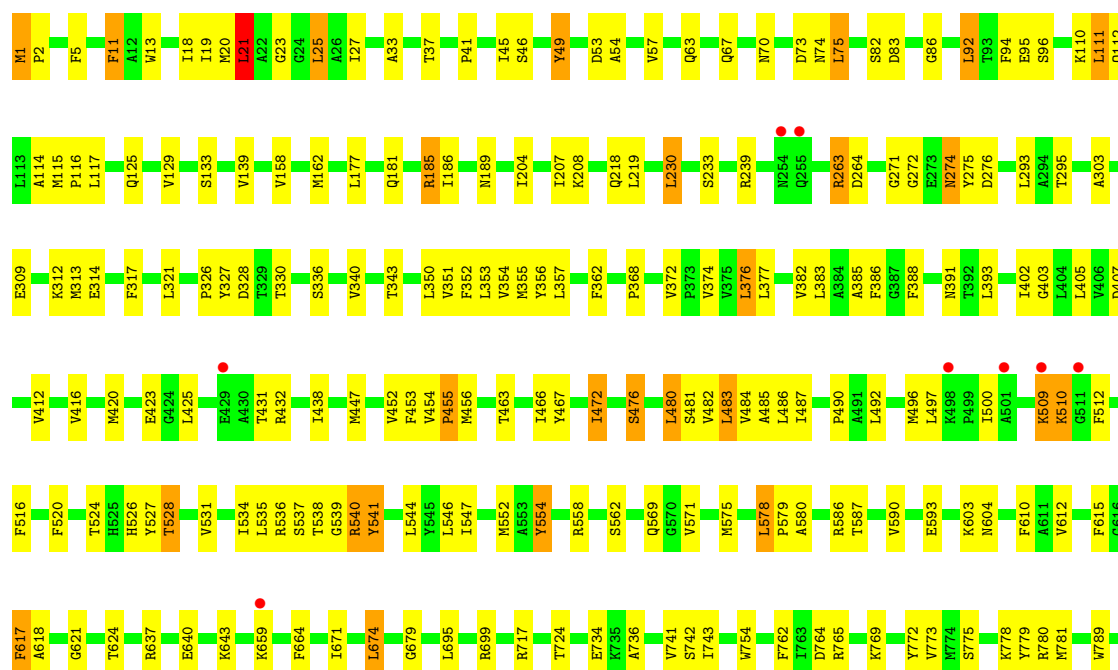
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

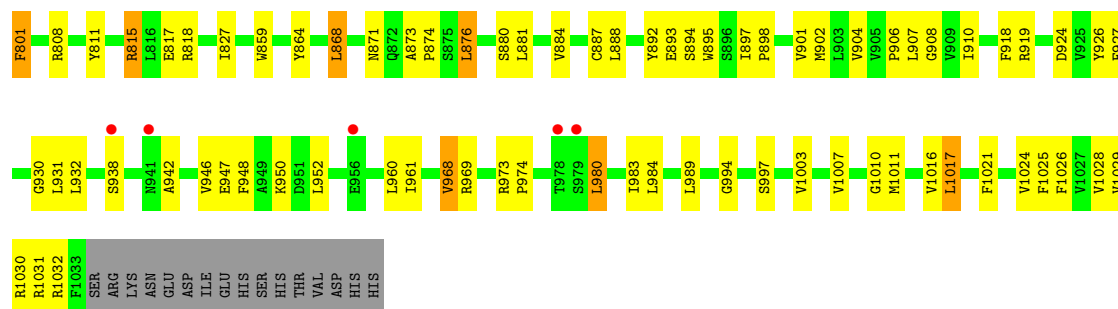
- Molecule 1: Multidrug efflux pump subunit AcrB



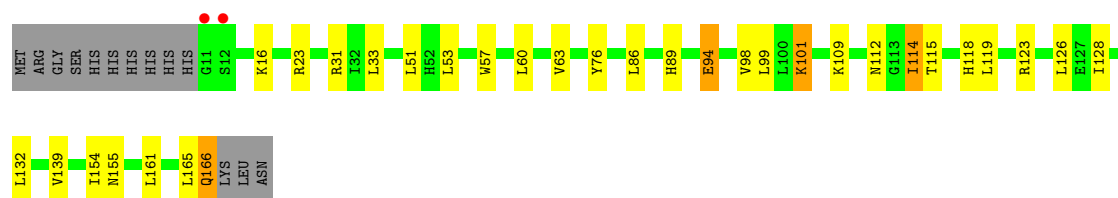
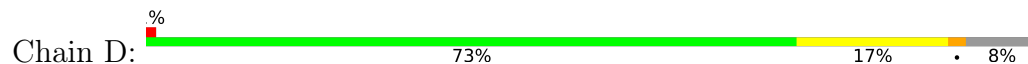
- Molecule 1: Multidrug efflux pump subunit AcrB



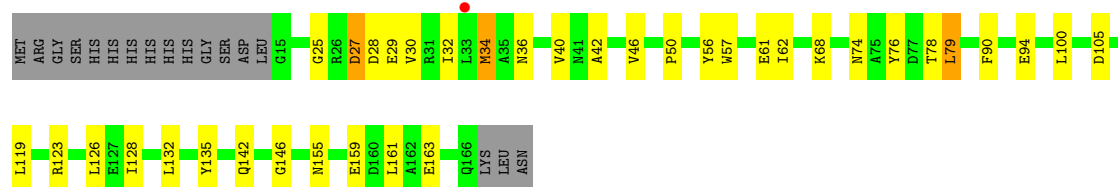




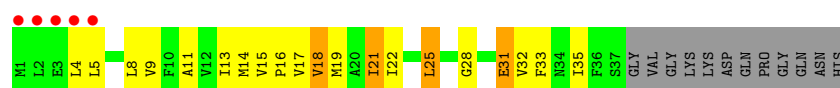
- Molecule 2: DARPin



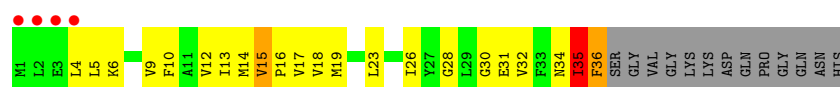
- Molecule 2: DARPin



- Molecule 3: Multidrug efflux pump accessory protein AcrZ

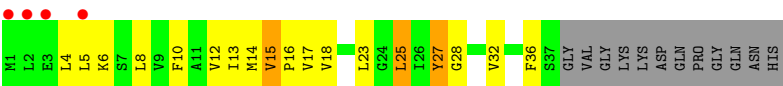


- Molecule 3: Multidrug efflux pump accessory protein AcrZ



- Molecule 3: Multidrug efflux pump accessory protein AcrZ





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	147.25Å 167.65Å 249.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.20 34.97 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (34.93-3.20) 92.0 (34.97-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 3.18Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.183 , 0.245 0.183 , 0.245	Depositor DCC
R_{free} test set	4696 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	55690	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, D10, PUY, DD9, HEX, D12

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	10/8060 (0.1%)	0.92	17/10947 (0.2%)
1	B	0.91	10/7995 (0.1%)	1.00	20/10859 (0.2%)
1	C	0.94	9/7995 (0.1%)	1.23	76/10859 (0.7%)
2	D	0.83	1/1196 (0.1%)	1.14	7/1626 (0.4%)
2	E	0.78	1/1170 (0.1%)	0.80	0/1591
3	F	0.82	0/287	0.86	0/388
3	G	0.76	0/281	1.28	1/380 (0.3%)
3	H	0.83	0/287	1.38	5/388 (1.3%)
All	All	0.90	31/27271 (0.1%)	1.06	126/37038 (0.3%)

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	A	0	1
1	B	0	4
1	C	0	5
All	All	0	10

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	GLY	C-N	-8.34	1.14	1.34
1	A	88	VAL	CB-CG2	-6.89	1.38	1.52
1	A	64	VAL	CB-CG2	-6.77	1.38	1.52
1	C	497	LEU	C-N	6.72	1.49	1.34
1	B	771	VAL	CB-CG2	-6.70	1.38	1.52

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	C	610	PHE	CB-CG-CD1	9.36	127.35	120.80
1	C	927	PHE	CB-CG-CD1	-9.27	114.31	120.80
1	C	610	PHE	CB-CG-CD2	-9.22	114.35	120.80
2	D	33	LEU	CB-CG-CD2	-8.71	96.20	111.00

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1037	ASN	Peptide
1	B	138	MET	Mainchain
1	B	326	PRO	Mainchain
1	B	328	ASP	Mainchain
1	B	572	PHE	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7908	8019	8019	136	0
1	B	7845	7990	7989	152	0
1	C	7845	7990	7990	144	0
2	D	1177	1159	1159	12	0
2	E	1151	1136	1136	19	0
3	F	283	318	318	15	0
3	G	277	313	313	20	0
3	H	283	318	318	13	0
4	A	48	81	81	3	0
5	A	24	52	52	0	0
5	B	20	42	38	1	0
5	C	41	89	87	0	0
6	A	50	110	110	2	0
6	B	120	264	264	3	0
6	C	90	198	198	1	0
7	A	30	64	62	2	0
7	B	49	97	97	3	0
7	C	18	39	33	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	34	0	28	5	0
9	C	6	14	14	0	0
10	A	50	0	0	3	0
10	B	26	0	0	0	0
10	C	21	0	0	0	0
10	D	1	0	0	0	0
All	All	27397	28293	28306	492	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 9.

The worst 5 of 492 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)
3:F:14:MET:O	3:F:18:VAL:HG12	1.78	0.83
1:B:600:THR:HG22	1:B:601:LYS:HD2	1.59	0.83
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.66	0.76
3:F:28:GLY:O	3:F:32:VAL:HG23	1.85	0.76
1:A:618:ALA:H	1:A:619:GLY:HA2	1.52	0.75

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1049 (99%)	1003 (96%)	36 (4%)	3 (0%)	41	74
1	B	1031/1049 (98%)	1005 (98%)	24 (2%)	2 (0%)	47	79
1	C	1031/1049 (98%)	1003 (97%)	24 (2%)	4 (0%)	34	69
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100	100
2	E	150/169 (89%)	148 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	35/49 (71%)	34 (97%)	1 (3%)	0	100	100
3	G	34/49 (69%)	33 (97%)	0	1 (3%)	4	28
3	H	35/49 (71%)	35 (100%)	0	0	100	100
All	All	3512/3632 (97%)	3413 (97%)	89 (2%)	10 (0%)	41	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	620	ARG
1	B	18	ILE
1	C	510	LYS
3	G	35	ILE
1	A	1041	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	
1	A	840/855 (98%)	792 (94%)	48 (6%)	20	56
1	B	838/855 (98%)	742 (88%)	96 (12%)	5	24
1	C	838/855 (98%)	791 (94%)	47 (6%)	21	57
2	D	120/132 (91%)	114 (95%)	6 (5%)	24	60
2	E	117/132 (89%)	104 (89%)	13 (11%)	6	25
3	F	32/41 (78%)	25 (78%)	7 (22%)	1	5
3	G	31/41 (76%)	25 (81%)	6 (19%)	1	7
3	H	32/41 (78%)	28 (88%)	4 (12%)	4	21
All	All	2848/2952 (96%)	2621 (92%)	227 (8%)	12	42

5 of 227 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	748	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	35	ILE
1	B	1030	ARG
3	G	18	VAL
2	E	29	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

53 ligands 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	$\# Z > 2$
6	D10	C	1116	-	9,9,9	0.55	0	8,8,8	0.34	0
6	D10	B	1110	-	9,9,9	0.63	0	8,8,8	0.31	0
6	D10	B	1116	-	9,9,9	0.61	0	8,8,8	0.50	0
6	D10	B	1103	-	9,9,9	0.65	0	8,8,8	0.40	0
7	DD9	B	1119	-	8,8,8	0.60	0	7,7,7	0.27	0
8	PUY	B	1120	-	32,37,37	3.58	12 (37%)	33,53,53	6.44	12 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	D10	B	1117	-	9,9,9	0.56	0	8,8,8	0.57	0
6	D10	C	1114	-	9,9,9	0.55	0	8,8,8	0.55	0
5	D12	C	1108	-	4,4,11	0.51	0	3,3,10	0.44	0
6	D10	C	1115	-	9,9,9	0.48	0	8,8,8	0.62	0
6	D10	B	1118	-	9,9,9	0.67	0	8,8,8	0.41	0
6	D10	A	1108	-	9,9,9	0.65	0	8,8,8	0.29	0
6	D10	B	1108	-	9,9,9	0.60	0	8,8,8	0.37	0
6	D10	C	1104	-	9,9,9	0.53	0	8,8,8	0.58	0
9	HEX	C	1105	-	5,5,5	0.62	0	4,4,4	0.19	0
7	DD9	A	1114	-	8,8,8	0.56	0	7,7,7	0.37	0
7	DD9	B	1102	-	4,4,8	0.44	0	3,3,7	0.44	0
6	D10	B	1105	-	9,9,9	0.61	0	8,8,8	0.47	0
6	D10	C	1113	-	9,9,9	0.65	0	8,8,8	0.32	0
6	D10	B	1101	-	9,9,9	0.65	0	8,8,8	0.39	0
6	D10	A	1105	-	9,9,9	0.56	0	8,8,8	0.39	0
5	D12	C	1103	-	11,11,11	0.61	0	10,10,10	0.66	0
7	DD9	A	1110	-	4,4,8	0.49	0	3,3,7	0.32	0
5	D12	B	1121	-	10,10,11	0.69	0	9,9,10	0.33	0
6	D10	C	1117	-	9,9,9	0.53	0	8,8,8	0.41	0
4	LMT	A	1111	-	11,11,36	0.46	0	10,10,47	0.36	0
5	D12	C	1107	-	11,11,11	0.79	0	10,10,10	0.29	0
5	D12	A	1103	-	11,11,11	0.50	0	10,10,10	0.65	0
7	DD9	C	1109	-	5,5,8	0.58	0	4,4,7	0.20	0
7	DD9	B	1106	-	6,6,8	0.70	0	5,5,7	0.14	0
6	D10	A	1104	-	9,9,9	0.56	0	8,8,8	0.52	0
6	D10	B	1114	-	9,9,9	0.51	0	8,8,8	0.53	0
6	D10	C	1102	-	9,9,9	0.74	0	8,8,8	0.35	0
5	D12	B	1104	-	8,8,11	0.50	0	7,7,10	0.43	0
7	DD9	C	1110	-	7,7,8	0.55	0	6,6,7	0.41	0
6	D10	B	1122	-	9,9,9	0.60	0	8,8,8	0.35	0
6	D10	B	1113	-	9,9,9	0.45	0	8,8,8	0.52	0
7	DD9	C	1101	-	3,3,8	0.54	0	2,2,7	0.65	0
7	DD9	B	1109	-	8,8,8	0.60	0	7,7,7	0.42	0
7	DD9	B	1107	-	5,5,8	0.55	0	4,4,7	0.19	0
4	LMT	A	1102	-	11,11,36	0.46	0	10,10,47	0.40	0
5	D12	A	1112	-	11,11,11	0.62	0	10,10,10	0.43	0
6	D10	A	1106	-	9,9,9	0.64	0	8,8,8	0.42	0
7	DD9	A	1107	-	8,8,8	0.72	0	7,7,7	0.32	0
4	LMT	A	1101	-	24,24,36	1.18	3 (12%)	29,29,47	1.30	3 (10%)
5	D12	C	1106	-	11,11,11	0.39	0	10,10,10	0.70	0
7	DD9	A	1113	-	6,6,8	0.60	0	5,5,7	0.38	0
6	D10	A	1109	-	9,9,9	0.66	0	8,8,8	0.26	0
6	D10	C	1112	-	9,9,9	0.42	0	8,8,8	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	DD9	B	1112	-	6,6,8	0.41	0	5,5,7	0.56	0
7	DD9	B	1115	-	5,5,8	0.47	0	4,4,7	0.29	0
6	D10	B	1111	-	9,9,9	0.71	0	8,8,8	0.33	0
6	D10	C	1111	-	9,9,9	0.56	0	8,8,8	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	C	1116	-	-	6/7/7/7	-
6	D10	B	1110	-	-	4/7/7/7	-
6	D10	B	1116	-	-	2/7/7/7	-
6	D10	B	1103	-	-	3/7/7/7	-
7	DD9	B	1119	-	-	3/6/6/6	-
8	PUY	B	1120	-	-	13/20/40/40	0/4/4/4
6	D10	B	1117	-	-	3/7/7/7	-
6	D10	C	1114	-	-	1/7/7/7	-
5	D12	C	1108	-	-	0/2/2/9	-
6	D10	C	1115	-	-	2/7/7/7	-
6	D10	B	1118	-	-	6/7/7/7	-
6	D10	A	1108	-	-	4/7/7/7	-
6	D10	B	1108	-	-	3/7/7/7	-
6	D10	C	1104	-	-	4/7/7/7	-
9	HEX	C	1105	-	-	3/3/3/3	-
7	DD9	A	1114	-	-	4/6/6/6	-
7	DD9	B	1102	-	-	1/2/2/6	-
6	D10	B	1105	-	-	5/7/7/7	-
6	D10	C	1113	-	-	0/7/7/7	-
6	D10	B	1101	-	-	2/7/7/7	-
6	D10	A	1105	-	-	2/7/7/7	-
5	D12	C	1103	-	-	4/9/9/9	-
7	DD9	A	1110	-	-	1/2/2/6	-
5	D12	B	1121	-	-	4/8/8/9	-
6	D10	C	1117	-	-	4/7/7/7	-
4	LMT	A	1111	-	-	6/9/9/61	-
5	D12	C	1107	-	-	5/9/9/9	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	D12	A	1103	-	-	6/9/9/9	-
7	DD9	C	1109	-	-	2/3/3/6	-
7	DD9	B	1106	-	-	2/4/4/6	-
6	D10	A	1104	-	-	1/7/7/7	-
6	D10	B	1114	-	-	3/7/7/7	-
6	D10	C	1102	-	-	4/7/7/7	-
5	D12	B	1104	-	-	4/6/6/9	-
7	DD9	C	1110	-	-	3/5/5/6	-
6	D10	B	1122	-	-	1/7/7/7	-
6	D10	B	1113	-	-	4/7/7/7	-
7	DD9	C	1101	-	-	0/1/1/6	-
7	DD9	B	1109	-	-	0/6/6/6	-
7	DD9	B	1107	-	-	2/3/3/6	-
4	LMT	A	1102	-	-	1/9/9/61	-
5	D12	A	1112	-	-	5/9/9/9	-
6	D10	A	1106	-	-	2/7/7/7	-
7	DD9	A	1107	-	-	4/6/6/6	-
4	LMT	A	1101	-	-	5/15/35/61	0/1/1/2
5	D12	C	1106	-	-	4/9/9/9	-
7	DD9	A	1113	-	-	3/4/4/6	-
6	D10	A	1109	-	-	4/7/7/7	-
6	D10	C	1112	-	-	2/7/7/7	-
7	DD9	B	1112	-	-	1/4/4/6	-
7	DD9	B	1115	-	-	2/3/3/6	-
6	D10	B	1111	-	-	3/7/7/7	-
6	D10	C	1111	-	-	4/7/7/7	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1120	PUY	O4'-C1'	11.81	1.57	1.41
8	B	1120	PUY	C2'-C1'	-11.08	1.37	1.53
8	B	1120	PUY	C-N3'	6.72	1.48	1.34
8	B	1120	PUY	O4'-C4'	-4.63	1.34	1.45
8	B	1120	PUY	O-C	-4.22	1.15	1.23

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1120	PUY	N1-C6-N6	-30.24	85.23	117.06
8	B	1120	PUY	CA-C-N3'	11.63	132.28	116.15
8	B	1120	PUY	CG-CB-CA	7.77	130.28	114.13
8	B	1120	PUY	C4-C5-N7	-7.40	101.69	109.40
8	B	1120	PUY	CB-CA-C	6.88	125.07	108.97

There are no chirality outliers.

5 of 167 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	1120	PUY	O-C-CA-CB
8	B	1120	PUY	N3'-C-CA-CB
8	B	1120	PUY	C3'-C4'-C5'-O5'
8	B	1120	PUY	N1-C6-N6-C9
8	B	1120	PUY	N1-C6-N6-C10

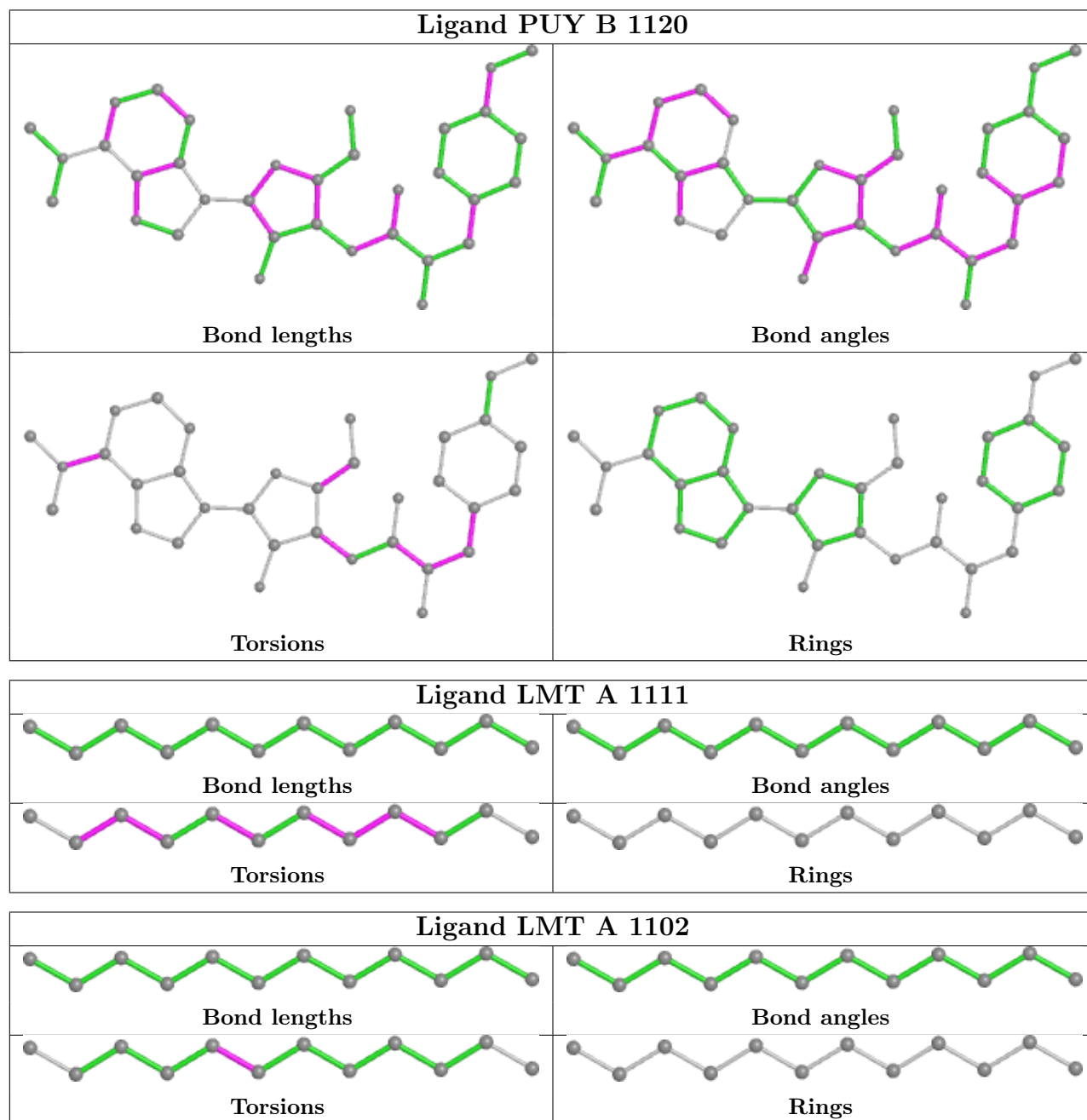
There are no ring outliers.

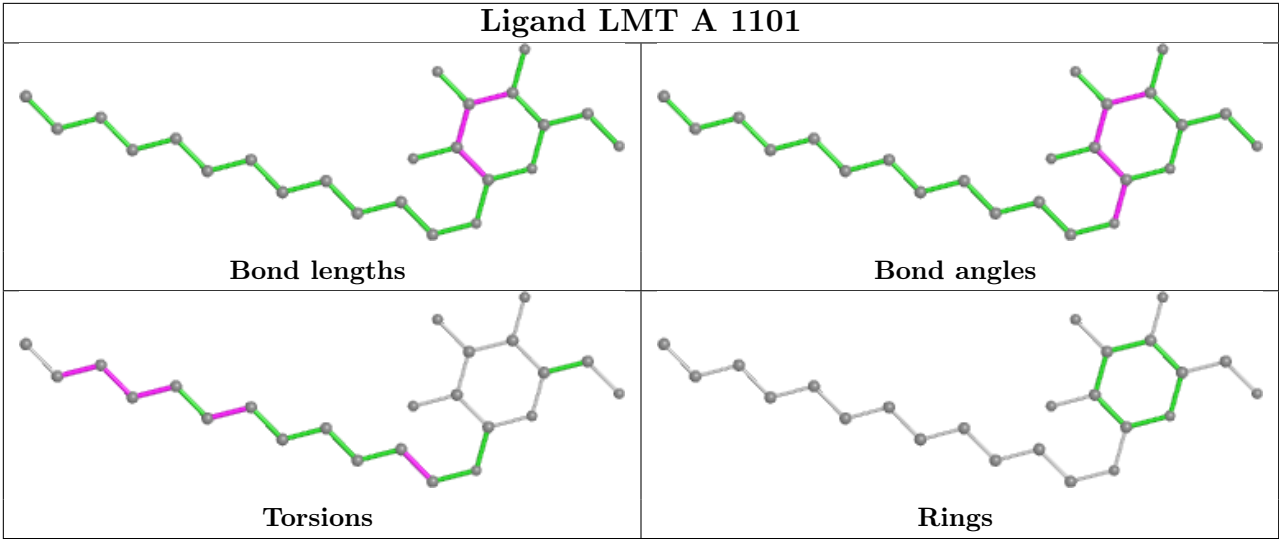
14 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1116	D10	1	0
7	B	1119	DD9	3	0
8	B	1120	PUY	5	0
6	B	1118	D10	1	0
5	B	1121	D12	1	0
4	A	1111	LMT	2	0
7	C	1109	DD9	2	0
7	C	1110	DD9	2	0
6	B	1113	D10	1	0
6	A	1106	D10	2	0
4	A	1101	LMT	1	0
7	A	1113	DD9	2	0
6	C	1112	D10	1	0
7	B	1112	DD9	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	283:GLY	C	284:GLN	N	1.14

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	A	1044/1049 (99%)	-0.33	17 (1%) 72 59	23, 58, 112, 164	0
1	B	1033/1049 (98%)	-0.36	10 (0%) 82 72	26, 56, 83, 110	0
1	C	1033/1049 (98%)	-0.27	13 (1%) 77 65	27, 52, 94, 134	0
2	D	156/169 (92%)	-0.21	2 (1%) 77 65	40, 56, 84, 124	0
2	E	152/169 (89%)	-0.03	1 (0%) 87 81	40, 65, 92, 112	0
3	F	37/49 (75%)	0.21	5 (13%) 3 2	62, 85, 165, 178	0
3	G	36/49 (73%)	0.16	4 (11%) 5 3	86, 106, 138, 164	0
3	H	37/49 (75%)	0.34	4 (10%) 5 3	68, 89, 149, 167	0
All	All	3528/3632 (97%)	-0.29	56 (1%) 72 59	23, 57, 101, 178	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1	MET	7.0
2	D	11	GLY	5.8
2	D	12	SER	5.3
1	A	676	THR	5.2
3	H	2	LEU	5.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

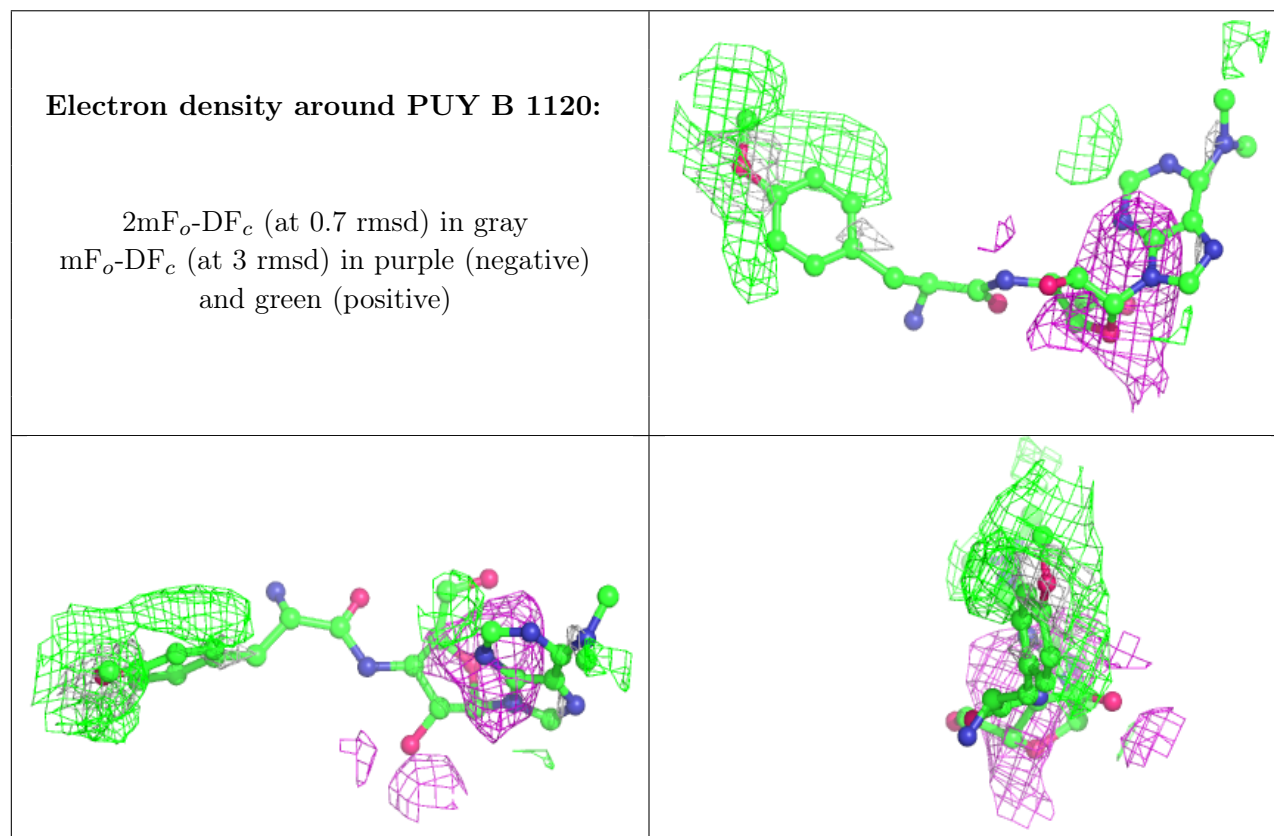
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	D10	C	1116	10/10	0.43	0.63	76,109,133,139	0
8	PUY	B	1120	34/34	0.50	0.57	96,159,207,234	0
6	D10	A	1105	10/10	0.60	0.85	68,99,129,130	0
7	DD9	B	1109	9/9	0.70	0.61	86,113,126,126	0
6	D10	C	1115	10/10	0.70	0.70	82,104,124,125	0
6	D10	B	1122	10/10	0.71	0.58	73,110,128,130	0
6	D10	C	1111	10/10	0.74	0.54	75,108,132,134	0
6	D10	C	1117	10/10	0.74	0.95	75,96,113,113	0
7	DD9	B	1106	7/9	0.75	0.41	65,90,110,110	0
5	D12	C	1103	12/12	0.77	0.33	51,81,98,104	0
6	D10	C	1114	10/10	0.77	0.54	68,97,112,116	0
7	DD9	B	1112	7/9	0.78	0.55	81,97,108,113	0
6	D10	A	1109	10/10	0.78	0.54	66,91,103,105	0
5	D12	B	1104	9/12	0.79	0.44	79,98,109,111	0
6	D10	B	1114	10/10	0.79	0.46	69,92,106,111	0
7	DD9	A	1114	9/9	0.80	0.63	72,95,113,116	0
6	D10	B	1118	10/10	0.81	0.37	63,91,108,112	0
9	HEX	C	1105	6/6	0.81	0.22	61,77,99,99	0
7	DD9	A	1107	9/9	0.83	0.34	54,74,88,90	0
7	DD9	B	1119	9/9	0.83	0.51	68,86,103,104	0
6	D10	B	1110	10/10	0.84	0.54	69,90,104,105	0
6	D10	C	1113	10/10	0.84	0.61	58,82,102,111	0
6	D10	C	1112	10/10	0.85	0.30	81,106,121,126	0
6	D10	A	1104	10/10	0.85	0.47	66,93,111,111	0
5	D12	C	1106	12/12	0.86	0.47	80,97,107,110	0
6	D10	C	1102	10/10	0.86	0.43	52,71,88,91	0
7	DD9	A	1113	7/9	0.86	0.28	65,83,96,100	0
6	D10	A	1106	10/10	0.86	0.35	60,84,100,105	0
4	LMT	A	1102	12/35	0.86	0.37	59,84,101,103	0
7	DD9	B	1115	6/9	0.87	0.55	60,74,87,87	0
6	D10	B	1113	10/10	0.87	0.57	73,100,113,115	0
7	DD9	C	1109	6/9	0.87	0.49	73,88,108,108	0
5	D12	C	1108	5/12	0.87	0.43	77,97,105,105	0
4	LMT	A	1111	12/35	0.87	0.24	63,85,101,102	0
5	D12	B	1121	11/12	0.88	0.45	57,88,105,110	0
6	D10	B	1116	10/10	0.89	0.30	46,71,86,90	0

Continued on next page...

Continued from previous page...

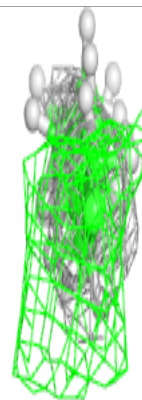
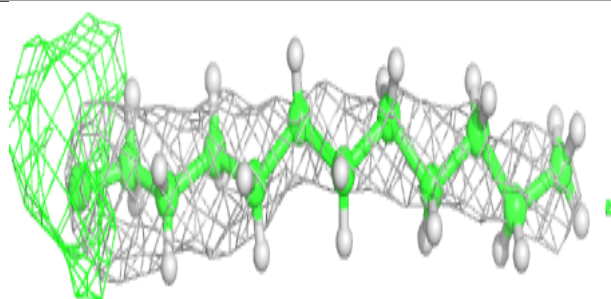
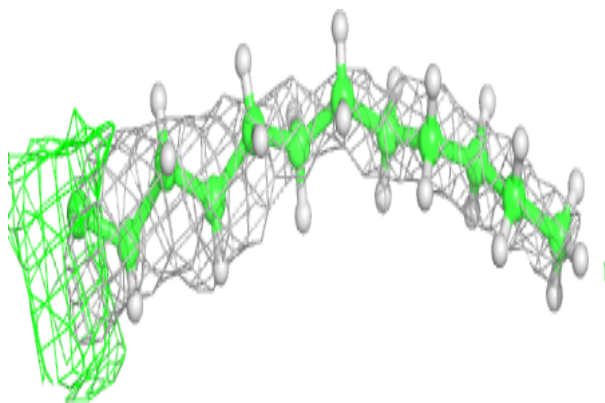
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	D10	B	1103	10/10	0.89	0.31	63,86,91,92	0
5	D12	C	1107	12/12	0.90	0.34	43,56,68,72	0
6	D10	B	1105	10/10	0.90	0.48	52,72,79,80	0
5	D12	A	1103	12/12	0.90	0.38	58,80,90,90	0
6	D10	B	1111	10/10	0.90	0.27	44,75,103,105	0
5	D12	A	1112	12/12	0.91	0.28	46,75,99,104	0
4	LMT	A	1101	24/35	0.91	0.24	53,80,116,124	0
6	D10	A	1108	10/10	0.91	0.61	52,67,76,77	0
7	DD9	C	1110	8/9	0.91	0.45	64,91,103,110	0
6	D10	B	1108	10/10	0.91	0.42	64,85,103,103	0
7	DD9	A	1110	5/9	0.91	0.60	56,67,80,80	0
7	DD9	B	1107	6/9	0.93	0.56	66,79,94,94	0
6	D10	B	1117	10/10	0.93	0.27	49,68,100,105	0
6	D10	B	1101	10/10	0.93	0.44	52,81,91,95	0
6	D10	C	1104	10/10	0.94	0.17	50,70,83,87	0
7	DD9	C	1101	4/9	0.95	0.34	62,75,83,83	0
7	DD9	B	1102	5/9	0.96	0.52	48,65,83,83	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

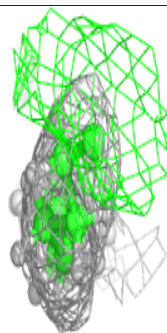
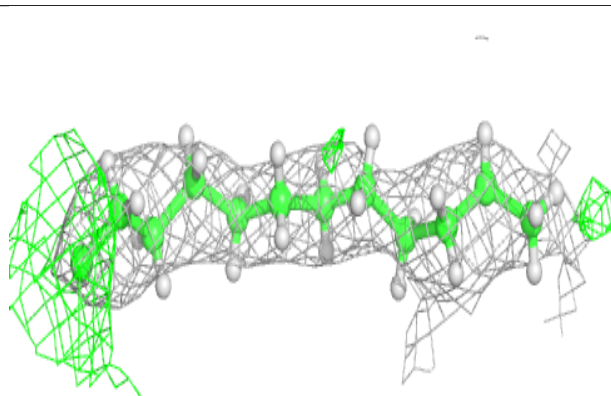
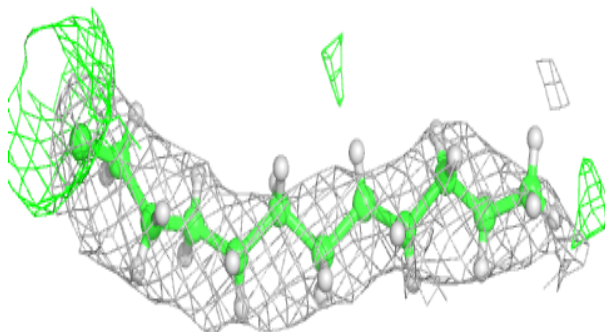


Electron density around LMT A 1102:

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

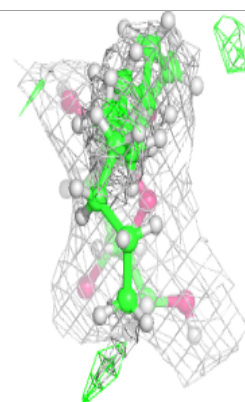
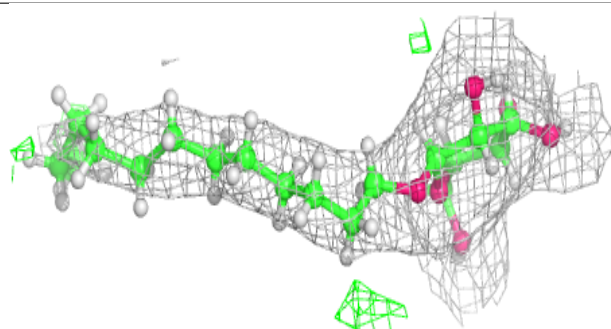
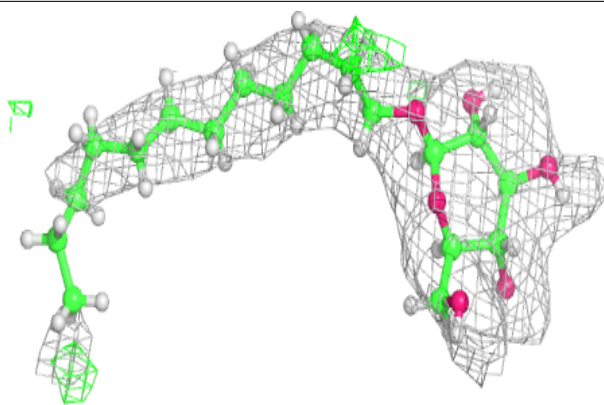
**Electron density around LMT A 1111:**

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



Electron density around LMT A 1101:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.