



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 08:01 AM UTC

PDB ID : 5NC5 / pdb\_00005nc5  
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](mailto: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>.

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

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

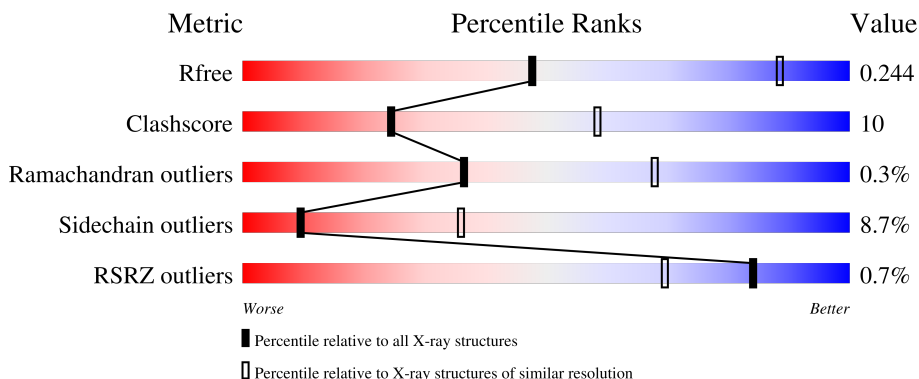
# 1 Overall quality at a glance

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))
$R_{free}$	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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  $\geq 3$ , 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	
1	B	1049	
1	C	1049	
2	D	169	
2	E	169	

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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
8	PUY	B	1120	-	-	-	X

## 2 Entry composition [i](#)

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	
			Total	C	H	N	O				S
1	A	1044	Total 15927	C 5086	H 8019	N 1308	O 1470	S 44	0	0	0
1	B	1033	Total 15835	C 5049	H 7990	N 1294	O 1458	S 44	0	0	0
1	C	1033	Total 15835	C 5049	H 7990	N 1294	O 1458	S 44	0	0	0

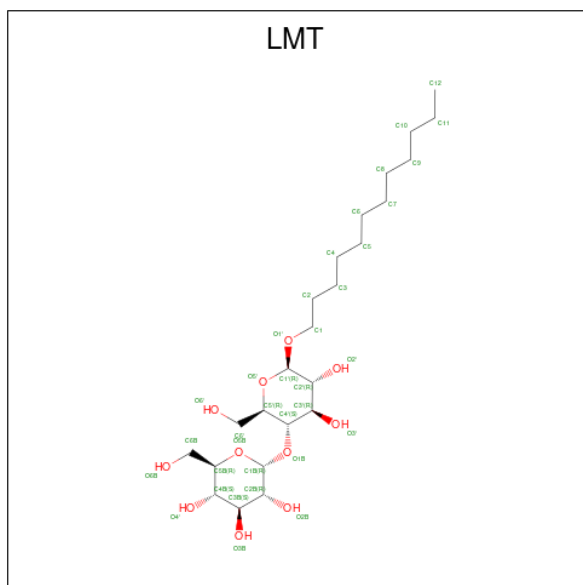
- Molecule 2 is a protein called DARPin.

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

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

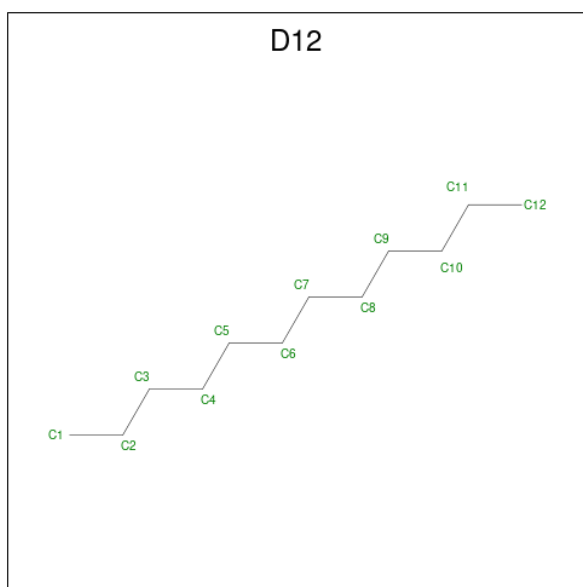
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	F	37	Total 601	C 196	H 318	N 39	O 45	S 3	0	0	0
3	G	36	Total 590	C 193	H 313	N 38	O 43	S 3	0	0	0
3	H	37	Total 601	C 196	H 318	N 39	O 45	S 3	0	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	A	1	Total	C	H	O	0	0
			59	18	35	6		
4	A	1	Total	C	H		0	0
			35	12	23			
4	A	1	Total	C	H		0	0
			35	12	23			

- Molecule 5 is DODECANE (CCD ID: D12) (formula:  $C_{12}H_{26}$ ).



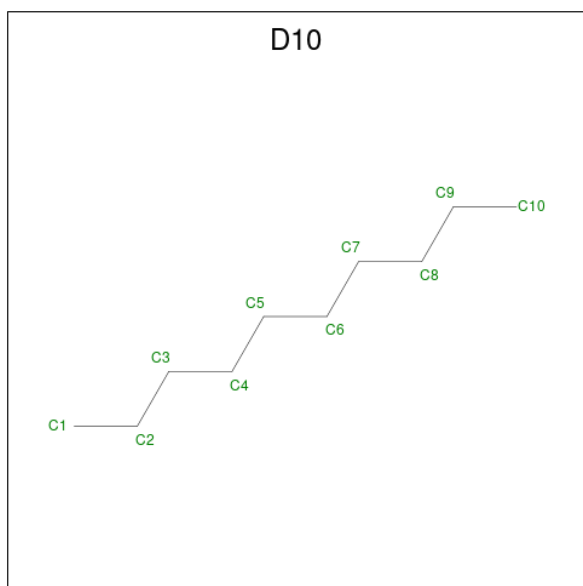
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
5	A	1	Total	C	H		0	0
			38	12	26			

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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 (CCD ID: D10) (formula: C<sub>10</sub>H<sub>22</sub>).



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		

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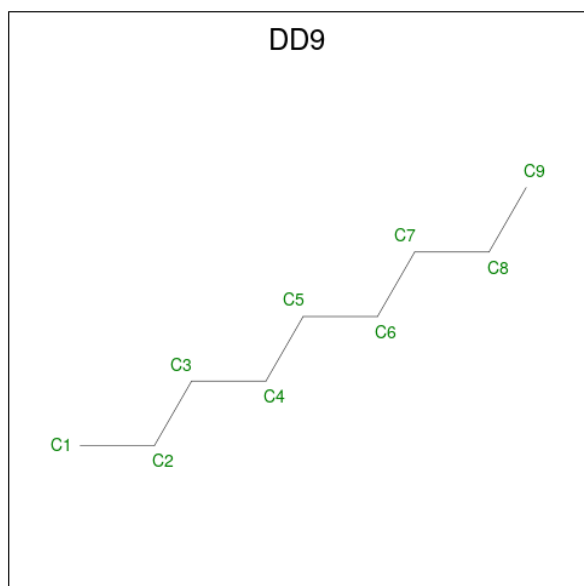
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0	0
6	B	1	Total 32	C 10	H 22	0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

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

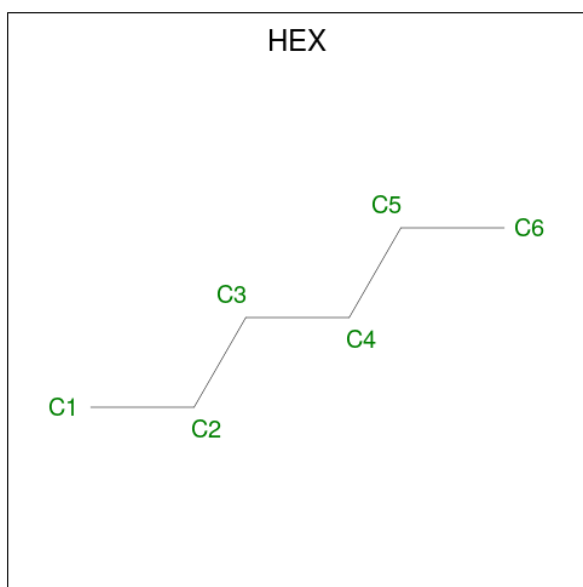
- Molecule 7 is nonane (CCD ID: DD9) (formula: C<sub>9</sub>H<sub>20</sub>).



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		

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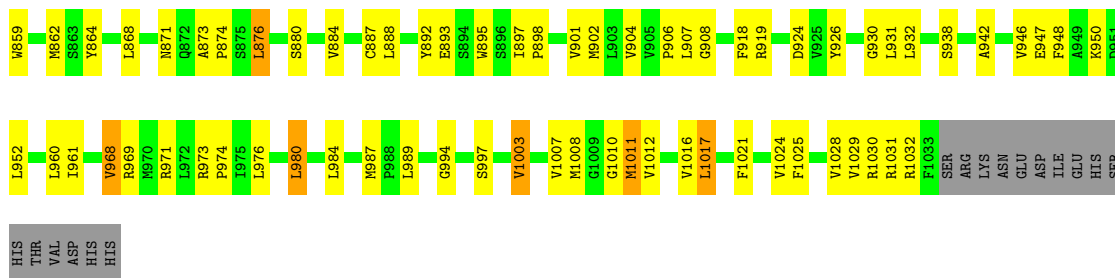
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	H	0	0
			20	6	14		

- Molecule 10 is water.

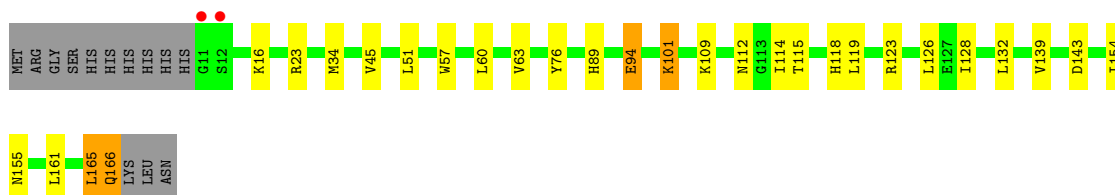
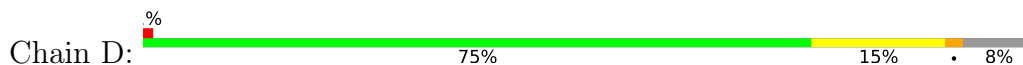
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total	O	0	0
			50	50		
10	B	26	Total	O	0	0
			26	26		
10	C	21	Total	O	0	0
			21	21		
10	D	1	Total	O	0	0
			1	1		



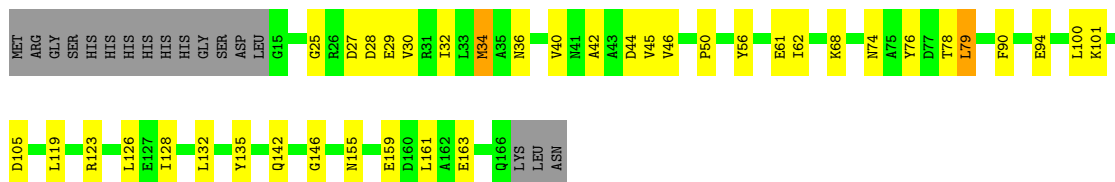




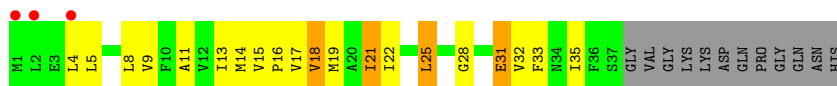
• Molecule 2: DARPin



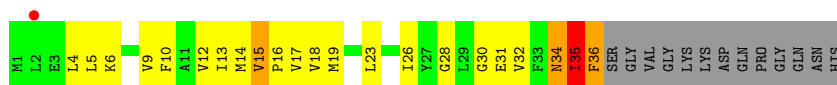
• Molecule 2: DARPin



• Molecule 3: Multidrug efflux pump accessory protein AcrZ

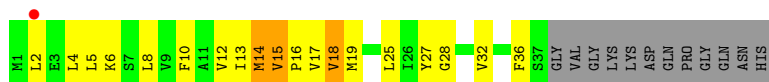


• Molecule 3: Multidrug efflux pump accessory protein AcrZ



• 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, $\alpha$ , $\beta$ , $\gamma$	147.25Å 167.65Å 249.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.93 – 3.20 34.93 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.0 (34.93-3.20) 91.9 (34.93-3.20)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.18Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.183 , 0.245 0.186 , 0.244	Depositor DCC
$R_{free}$ test set	4696 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.6	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	55690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: D12, PUY, LMT, D10, DD9, HEX

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	0.87	1/8060 (0.0%)	0.97	5/10947 (0.0%)
1	B	0.95	24/7995 (0.3%)	1.09	46/10859 (0.4%)
1	C	0.93	0/7995	1.30	30/10859 (0.3%)
2	D	0.84	0/1196	1.15	3/1626 (0.2%)
2	E	0.77	0/1170	0.89	0/1591
3	F	0.82	0/287	0.95	0/388
3	G	0.78	0/281	1.40	2/380 (0.5%)
3	H	0.84	0/287	1.42	3/388 (0.8%)
All	All	0.90	25/27271 (0.1%)	1.12	89/37038 (0.2%)

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 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	139	VAL	C-O	-10.57	1.12	1.24
1	B	136	PHE	C-O	-10.16	1.11	1.24
1	B	283	GLY	C-N	-9.02	1.14	1.33
1	B	277	ILE	C-N	8.79	1.44	1.33
1	B	664	PHE	C-O	-8.23	1.13	1.24

The worst 5 of 89 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	509	LYS	N-CA-C	-12.64	91.78	110.48
1	B	615	PHE	CA-C-N	9.89	131.27	122.47
1	B	615	PHE	C-N-CA	9.89	131.27	122.47
1	B	139	VAL	CA-C-O	-9.56	109.47	120.66
1	B	277	ILE	CA-C-O	-9.50	109.16	120.75

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 [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	A	7908	8019	8019	151	0
1	B	7845	7990	7990	171	0
1	C	7845	7990	7990	162	0
2	D	1177	1159	1159	15	0
2	E	1151	1136	1136	21	0
3	F	283	318	318	18	0
3	G	277	313	313	21	0
3	H	283	318	318	19	0
4	A	48	81	81	3	0
5	A	24	52	52	1	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

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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	28307	551	0

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

The worst 5 of 551 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%)	36 68
1	B	1031/1049 (98%)	1005 (98%)	24 (2%)	2 (0%)	43 73
1	C	1031/1049 (98%)	1003 (97%)	24 (2%)	4 (0%)	30 62
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100 100
2	E	150/169 (89%)	148 (99%)	2 (1%)	0	100 100

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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%)	3	24
3	H	35/49 (71%)	35 (100%)	0	0	100	100
All	All	3512/3632 (97%)	3413 (97%)	89 (2%)	10 (0%)	36	68

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 [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	
1	A	840/855 (98%)	792 (94%)	48 (6%)	18	51
1	B	838/855 (98%)	729 (87%)	109 (13%)	4	20
1	C	838/855 (98%)	784 (94%)	54 (6%)	16	48
2	D	120/132 (91%)	114 (95%)	6 (5%)	22	55
2	E	117/132 (89%)	103 (88%)	14 (12%)	5	23
3	F	32/41 (78%)	25 (78%)	7 (22%)	1	5
3	G	31/41 (76%)	25 (81%)	6 (19%)	1	8
3	H	32/41 (78%)	27 (84%)	5 (16%)	2	13
All	All	2848/2952 (96%)	2599 (91%)	249 (9%)	9	36

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	600	THR

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Mol	Chain	Res	Type
2	E	36	ASN
1	B	955	LYS
2	E	32	ILE
3	F	25	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	726	GLN
1	B	830	GLN
2	E	125	HIS
2	E	74	ASN
2	E	112	ASN

### 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 oligosaccharides 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	B	1113	-	9,9,9	0.48	0	8,8,8	0.53	0
6	D10	B	1103	-	9,9,9	0.70	0	8,8,8	0.41	0
5	D12	C	1107	-	11,11,11	0.86	0	10,10,10	0.29	0
6	D10	B	1110	-	9,9,9	0.68	0	8,8,8	0.31	0
6	D10	B	1108	-	9,9,9	0.65	0	8,8,8	0.39	0
5	D12	B	1121	-	10,10,11	0.75	0	9,9,10	0.37	0
7	DD9	A	1110	-	4,4,8	0.53	0	3,3,7	0.33	0
6	D10	C	1116	-	9,9,9	0.59	0	8,8,8	0.36	0
6	D10	C	1112	-	9,9,9	0.45	0	8,8,8	0.67	0
6	D10	B	1101	-	9,9,9	0.70	0	8,8,8	0.39	0
6	D10	B	1111	-	9,9,9	0.78	0	8,8,8	0.35	0
6	D10	A	1104	-	9,9,9	0.61	0	8,8,8	0.52	0
5	D12	B	1104	-	8,8,11	0.53	0	7,7,10	0.44	0
7	DD9	C	1109	-	5,5,8	0.64	0	4,4,7	0.21	0
7	DD9	A	1107	-	8,8,8	0.79	0	7,7,7	0.33	0
6	D10	C	1117	-	9,9,9	0.56	0	8,8,8	0.43	0
7	DD9	B	1112	-	6,6,8	0.44	0	5,5,7	0.58	0
6	D10	C	1102	-	9,9,9	0.81	0	8,8,8	0.36	0
6	D10	C	1114	-	9,9,9	0.59	0	8,8,8	0.55	0
6	D10	B	1116	-	9,9,9	0.66	0	8,8,8	0.52	0
6	D10	B	1105	-	9,9,9	0.66	0	8,8,8	0.48	0
6	D10	B	1118	-	9,9,9	0.73	0	8,8,8	0.43	0
6	D10	C	1104	-	9,9,9	0.56	0	8,8,8	0.63	0
6	D10	B	1117	-	9,9,9	0.61	0	8,8,8	0.58	0
6	D10	C	1113	-	9,9,9	0.70	0	8,8,8	0.33	0
5	D12	A	1103	-	11,11,11	0.53	0	10,10,10	0.67	0
7	DD9	B	1106	-	6,6,8	0.76	0	5,5,7	0.15	0
5	D12	A	1112	-	11,11,11	0.66	0	10,10,10	0.44	0
6	D10	C	1111	-	9,9,9	0.60	0	8,8,8	0.29	0
7	DD9	B	1119	-	8,8,8	0.65	0	7,7,7	0.28	0
7	DD9	B	1109	-	8,8,8	0.66	0	7,7,7	0.43	0
4	LMT	A	1111	-	11,11,36	0.49	0	10,10,47	0.37	0
5	D12	C	1108	-	4,4,11	0.55	0	3,3,10	0.47	0
7	DD9	A	1113	-	6,6,8	0.65	0	5,5,7	0.40	0
7	DD9	C	1101	-	3,3,8	0.54	0	2,2,7	0.66	0
7	DD9	A	1114	-	8,8,8	0.61	0	7,7,7	0.38	0
7	DD9	B	1107	-	5,5,8	0.60	0	4,4,7	0.20	0
6	D10	B	1114	-	9,9,9	0.55	0	8,8,8	0.53	0
6	D10	A	1108	-	9,9,9	0.70	0	8,8,8	0.30	0
6	D10	A	1106	-	9,9,9	0.69	0	8,8,8	0.43	0
6	D10	C	1115	-	9,9,9	0.51	0	8,8,8	0.64	0
9	HEX	C	1105	-	5,5,5	0.67	0	4,4,4	0.21	0
6	D10	A	1105	-	9,9,9	0.60	0	8,8,8	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	D12	C	1103	-	11,11,11	0.65	0	10,10,10	0.68	0
4	LMT	A	1102	-	11,11,36	0.49	0	10,10,47	0.42	0
6	D10	B	1122	-	9,9,9	0.64	0	8,8,8	0.35	0
7	DD9	B	1102	-	4,4,8	0.47	0	3,3,7	0.47	0
4	LMT	A	1101	-	24,24,36	1.16	3 (12%)	29,29,47	1.30	3 (10%)
7	DD9	C	1110	-	7,7,8	0.59	0	6,6,7	0.42	0
7	DD9	B	1115	-	5,5,8	0.50	0	4,4,7	0.31	0
5	D12	C	1106	-	11,11,11	0.41	0	10,10,10	0.70	0
6	D10	A	1109	-	9,9,9	0.71	0	8,8,8	0.27	0
8	PUY	B	1120	-	37,37,37	2.75	15 (40%)	48,53,53	5.91	22 (45%)

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	B	1113	-	-	4/7/7/7	-
6	D10	B	1103	-	-	3/7/7/7	-
5	D12	C	1107	-	-	5/9/9/9	-
6	D10	B	1110	-	-	4/7/7/7	-
6	D10	B	1108	-	-	3/7/7/7	-
5	D12	B	1121	-	-	4/8/8/9	-
7	DD9	A	1110	-	-	1/2/2/6	-
6	D10	C	1116	-	-	6/7/7/7	-
6	D10	C	1112	-	-	2/7/7/7	-
6	D10	B	1101	-	-	2/7/7/7	-
6	D10	B	1111	-	-	3/7/7/7	-
6	D10	A	1104	-	-	1/7/7/7	-
5	D12	B	1104	-	-	4/6/6/9	-
7	DD9	C	1109	-	-	2/3/3/6	-
7	DD9	A	1107	-	-	4/6/6/6	-
6	D10	C	1117	-	-	4/7/7/7	-
7	DD9	B	1112	-	-	1/4/4/6	-
6	D10	C	1102	-	-	4/7/7/7	-
6	D10	C	1114	-	-	1/7/7/7	-
6	D10	B	1116	-	-	2/7/7/7	-
6	D10	B	1105	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	B	1118	-	-	6/7/7/7	-
6	D10	C	1104	-	-	4/7/7/7	-
6	D10	B	1117	-	-	3/7/7/7	-
6	D10	C	1113	-	-	0/7/7/7	-
5	D12	A	1103	-	-	6/9/9/9	-
7	DD9	B	1106	-	-	2/4/4/6	-
5	D12	A	1112	-	-	5/9/9/9	-
6	D10	C	1111	-	-	4/7/7/7	-
7	DD9	B	1119	-	-	3/6/6/6	-
7	DD9	B	1109	-	-	0/6/6/6	-
4	LMT	A	1111	-	-	6/9/9/61	-
5	D12	C	1108	-	-	0/2/2/9	-
7	DD9	A	1113	-	-	3/4/4/6	-
7	DD9	C	1101	-	-	0/1/1/6	-
7	DD9	A	1114	-	-	4/6/6/6	-
7	DD9	B	1107	-	-	2/3/3/6	-
6	D10	B	1114	-	-	3/7/7/7	-
6	D10	A	1108	-	-	4/7/7/7	-
6	D10	A	1106	-	-	2/7/7/7	-
6	D10	C	1115	-	-	2/7/7/7	-
9	HEX	C	1105	-	-	3/3/3/3	-
6	D10	A	1105	-	-	2/7/7/7	-
5	D12	C	1103	-	-	4/9/9/9	-
4	LMT	A	1102	-	-	1/9/9/61	-
6	D10	B	1122	-	-	1/7/7/7	-
7	DD9	B	1102	-	-	1/2/2/6	-
4	LMT	A	1101	-	-	5/15/35/61	0/1/1/2
7	DD9	C	1110	-	-	3/5/5/6	-
7	DD9	B	1115	-	-	2/3/3/6	-
5	D12	C	1106	-	-	4/9/9/9	-
6	D10	A	1109	-	-	4/7/7/7	-
8	PUY	B	1120	-	-	15/24/40/40	0/4/4/4

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1120	PUY	C-N3'	6.90	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1120	PUY	O4'-C1'	6.73	1.57	1.42
8	B	1120	PUY	C2'-C1'	-5.26	1.37	1.53
8	B	1120	PUY	O4'-C4'	-4.65	1.34	1.45
8	B	1120	PUY	C8-N9	-4.50	1.29	1.37

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1120	PUY	N1-C6-N6	-25.96	85.23	116.86
8	B	1120	PUY	C5-C6-N6	18.47	154.57	125.33
8	B	1120	PUY	CA-C-N3'	11.87	132.28	116.21
8	B	1120	PUY	CG-CB-CA	7.89	130.28	114.13
8	B	1120	PUY	C4-C5-N7	-7.78	101.69	110.58

There are no chirality outliers.

5 of 169 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.

15 monomers are involved in 19 short contacts:

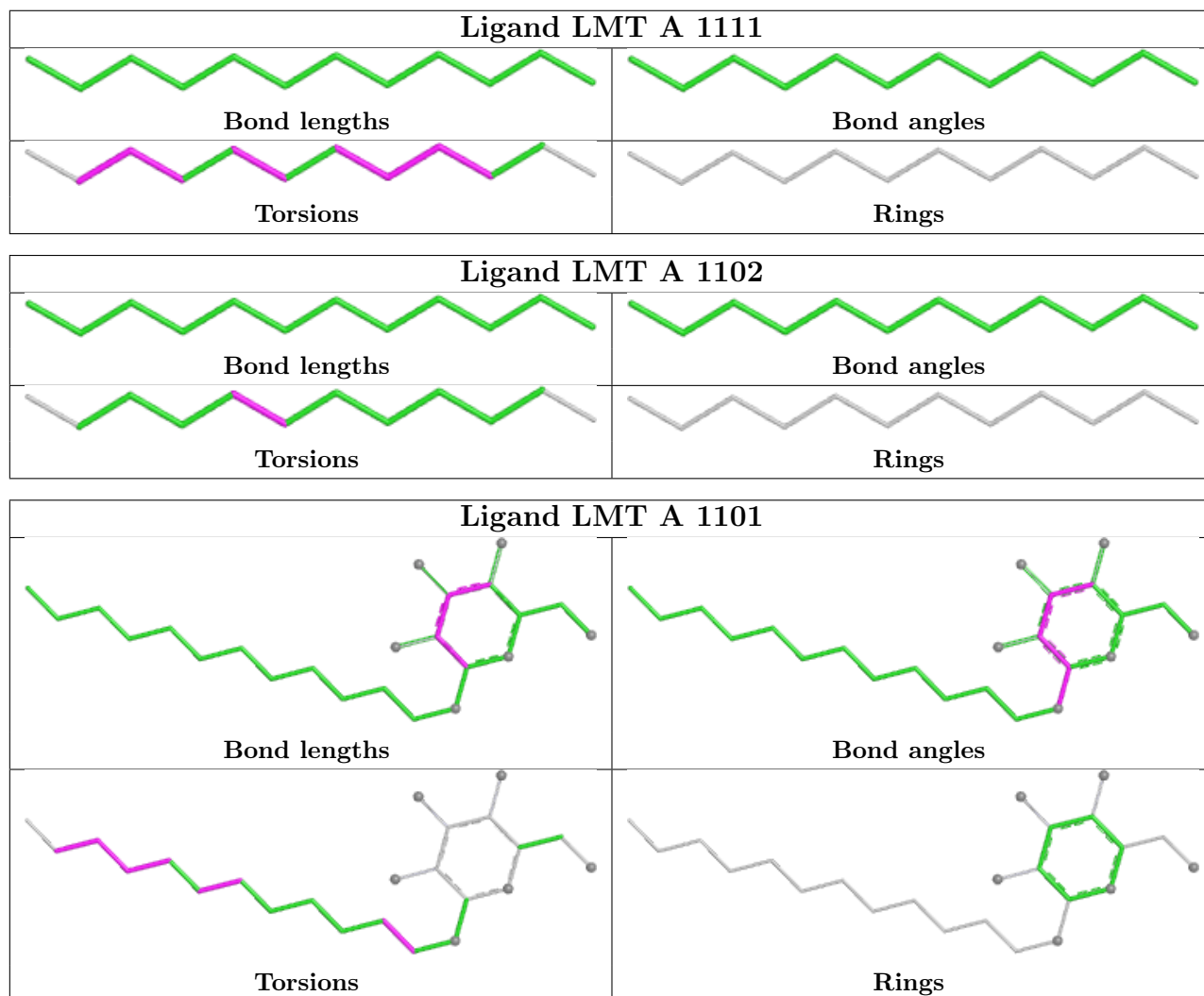
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1113	D10	1	0
5	B	1121	D12	1	0
6	C	1112	D10	1	0
7	C	1109	DD9	2	0
7	B	1112	DD9	2	0
6	B	1116	D10	1	0
6	B	1118	D10	1	0
5	A	1103	D12	1	0
7	B	1119	DD9	3	0
4	A	1111	LMT	2	0
7	A	1113	DD9	2	0
6	A	1106	D10	2	0
4	A	1101	LMT	1	0

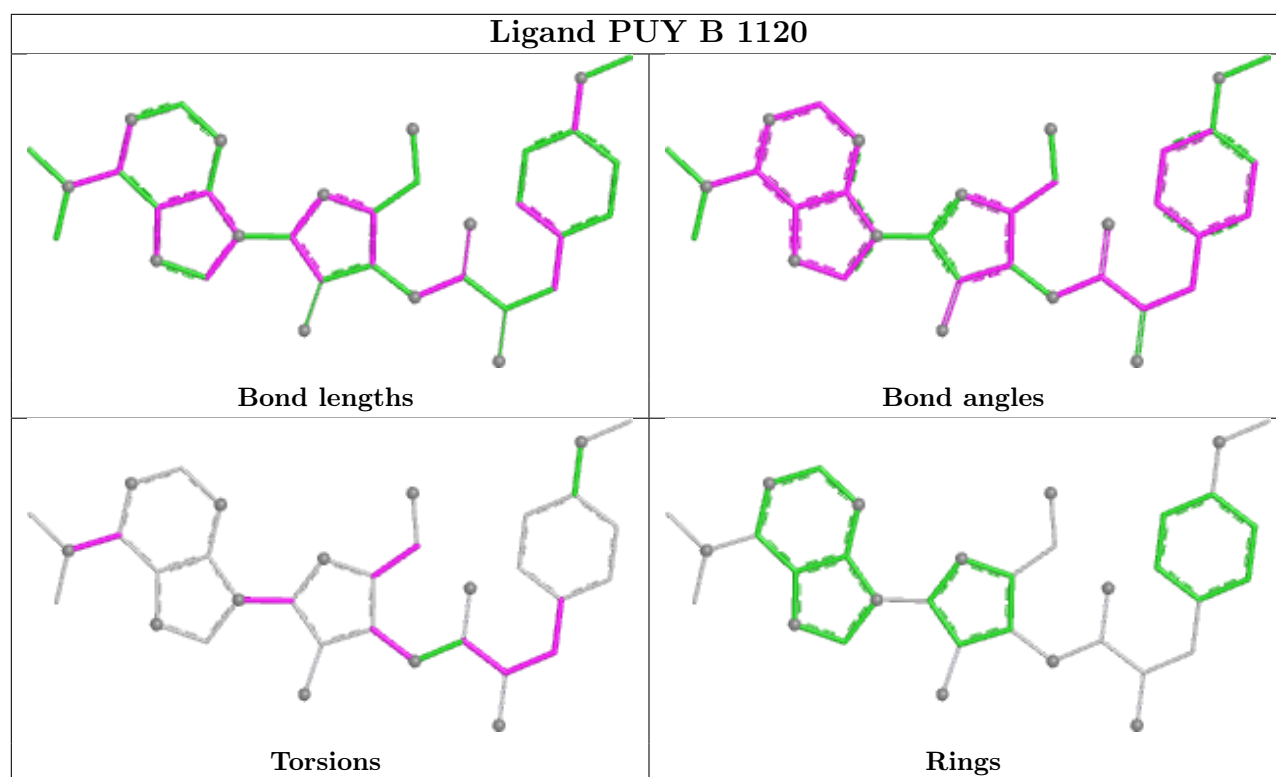
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1110	DD9	2	0
8	B	1120	PUY	5	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1044/1049 (99%)	-0.53	13 (1%) 76 58	26, 63, 120, 181	0
1	B	1033/1049 (98%)	-0.57	3 (0%) 90 81	28, 62, 92, 124	0
1	C	1033/1049 (98%)	-0.57	1 (0%) 92 89	30, 57, 103, 144	0
2	D	156/169 (92%)	-0.54	2 (1%) 75 55	45, 62, 91, 135	0
2	E	152/169 (89%)	-0.38	0 100 100	45, 70, 101, 117	0
3	F	37/49 (75%)	0.33	3 (8%) 18 11	67, 93, 177, 192	0
3	G	36/49 (73%)	-0.15	1 (2%) 55 35	92, 117, 154, 178	0
3	H	37/49 (75%)	-0.00	1 (2%) 56 36	75, 98, 165, 181	0
All	All	3528/3632 (97%)	-0.53	24 (0%) 84 69	26, 62, 111, 192	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	4	LEU	4.3
1	A	617	PHE	4.2
3	F	1	MET	4.1
1	A	670	ALA	4.1
3	F	2	LEU	4.0

### 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 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, 95<sup>th</sup> 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.

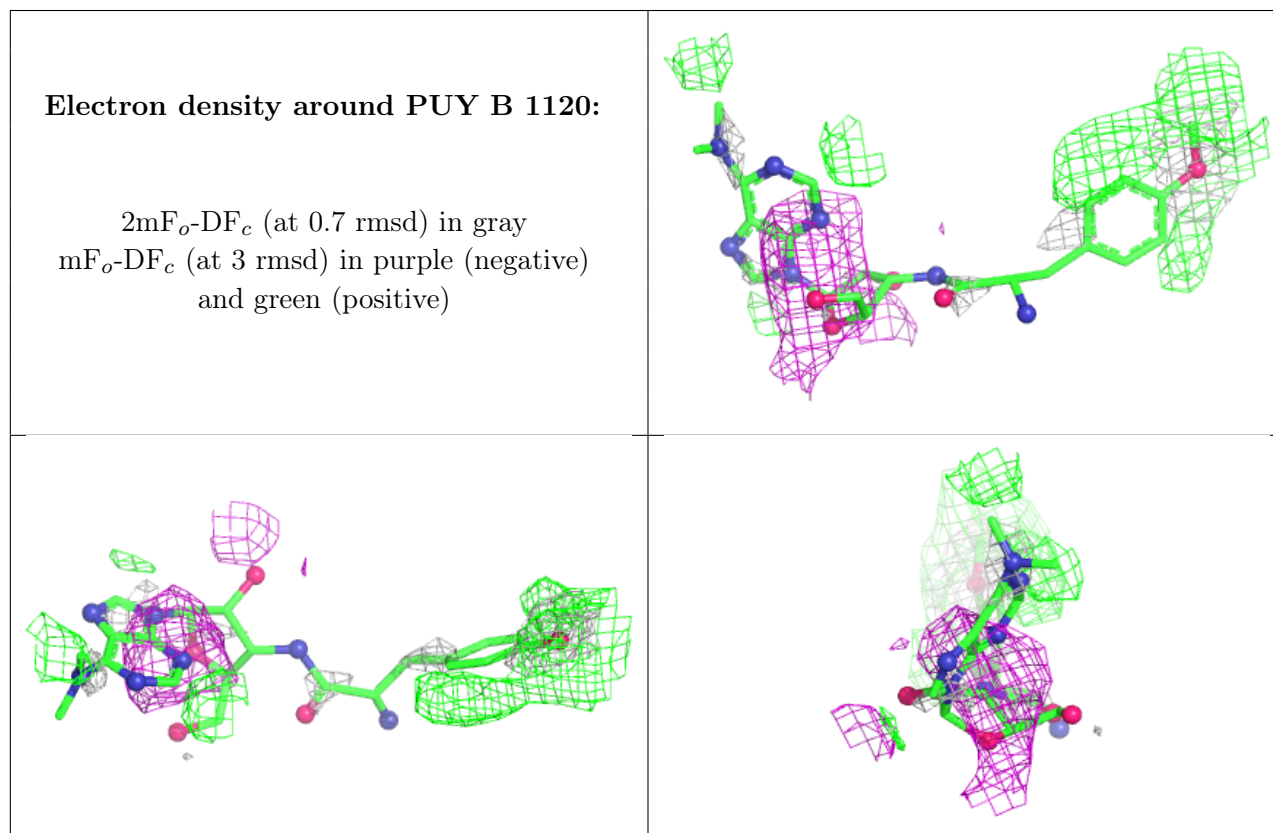
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
8	PUY	B	1120	34/34	0.58	0.44	96,159,207,234	0
6	D10	A	1105	10/10	0.62	0.28	68,99,129,130	0
5	D12	B	1104	9/12	0.66	0.20	79,98,109,111	0
7	DD9	C	1109	6/9	0.67	0.18	73,88,108,108	0
6	D10	A	1109	10/10	0.69	0.15	66,91,103,105	0
7	DD9	A	1114	9/9	0.71	0.15	72,95,113,116	0
6	D10	B	1114	10/10	0.72	0.20	69,92,106,111	0
6	D10	B	1122	10/10	0.72	0.18	73,110,128,130	0
6	D10	C	1114	10/10	0.72	0.26	68,97,112,116	0
6	D10	B	1118	10/10	0.73	0.21	63,91,108,112	0
5	D12	C	1103	12/12	0.73	0.24	51,81,98,104	0
5	D12	C	1108	5/12	0.74	0.29	77,97,105,105	0
6	D10	C	1113	10/10	0.75	0.15	58,82,102,111	0
6	D10	C	1116	10/10	0.76	0.27	76,109,133,139	0
7	DD9	B	1106	7/9	0.76	0.30	65,90,110,110	0
7	DD9	C	1110	8/9	0.77	0.15	64,91,103,110	0
7	DD9	A	1107	9/9	0.77	0.22	54,74,88,90	0
7	DD9	B	1119	9/9	0.80	0.16	68,86,103,104	0
5	D12	A	1112	12/12	0.80	0.21	46,75,99,104	0
6	D10	A	1106	10/10	0.80	0.20	60,84,100,105	0
7	DD9	B	1115	6/9	0.80	0.18	60,74,87,87	0
6	D10	B	1103	10/10	0.81	0.21	63,86,91,92	0
6	D10	C	1111	10/10	0.81	0.17	75,108,132,134	0
7	DD9	B	1112	7/9	0.81	0.14	81,97,108,113	0
6	D10	B	1110	10/10	0.81	0.22	69,90,104,105	0
6	D10	A	1104	10/10	0.82	0.21	66,93,111,111	0
4	LMT	A	1102	12/35	0.82	0.24	59,84,101,103	0
6	D10	B	1111	10/10	0.82	0.22	44,75,103,105	0
7	DD9	B	1109	9/9	0.82	0.32	86,113,126,126	0
6	D10	C	1102	10/10	0.82	0.22	52,71,88,91	0
9	HEX	C	1105	6/6	0.83	0.24	61,77,99,99	0
6	D10	C	1112	10/10	0.84	0.20	81,106,121,126	0
4	LMT	A	1111	12/35	0.84	0.16	63,85,101,102	0
5	D12	B	1121	11/12	0.84	0.22	57,88,105,110	0
6	D10	C	1117	10/10	0.85	0.22	75,96,113,113	0
5	D12	A	1103	12/12	0.85	0.17	58,80,90,90	0
6	D10	C	1104	10/10	0.86	0.23	50,70,83,87	0

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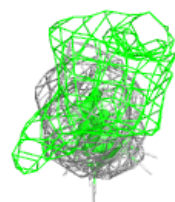
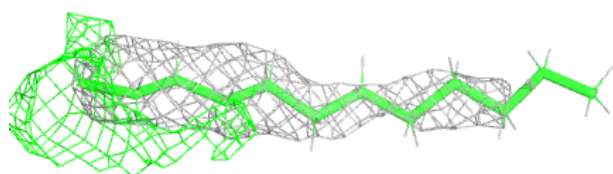
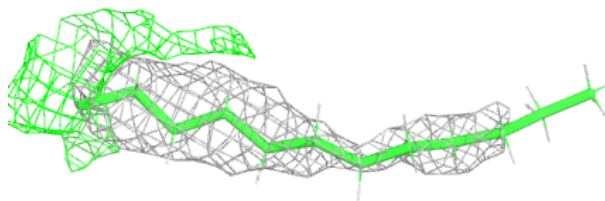
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	D10	B	1117	10/10	0.86	0.23	49,68,100,105	0
6	D10	B	1113	10/10	0.86	0.18	73,100,113,115	0
6	D10	B	1108	10/10	0.87	0.16	64,85,103,103	0
7	DD9	A	1113	7/9	0.87	0.20	65,83,96,100	0
6	D10	C	1115	10/10	0.87	0.21	82,104,124,125	0
6	D10	B	1116	10/10	0.88	0.16	46,71,86,90	0
5	D12	C	1106	12/12	0.89	0.21	80,97,107,110	0
5	D12	C	1107	12/12	0.89	0.13	43,56,68,72	0
6	D10	B	1105	10/10	0.89	0.16	52,72,79,80	0
6	D10	A	1108	10/10	0.90	0.12	52,67,76,77	0
6	D10	B	1101	10/10	0.91	0.14	52,81,91,95	0
7	DD9	C	1101	4/9	0.91	0.16	62,75,83,83	0
7	DD9	A	1110	5/9	0.91	0.15	56,67,80,80	0
4	LMT	A	1101	24/35	0.94	0.10	53,80,116,124	0
7	DD9	B	1102	5/9	0.94	0.13	48,65,83,83	0
7	DD9	B	1107	6/9	0.95	0.13	66,79,94,94	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.

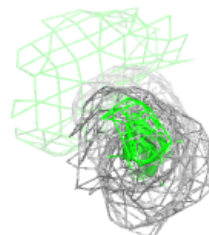
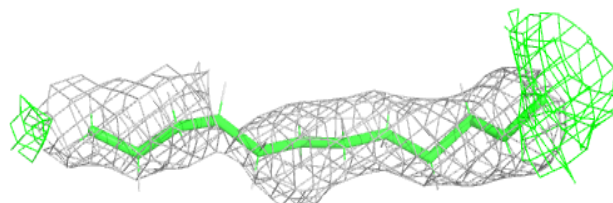
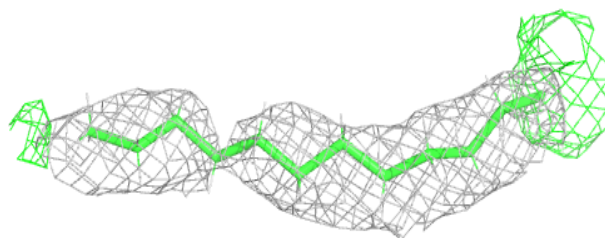


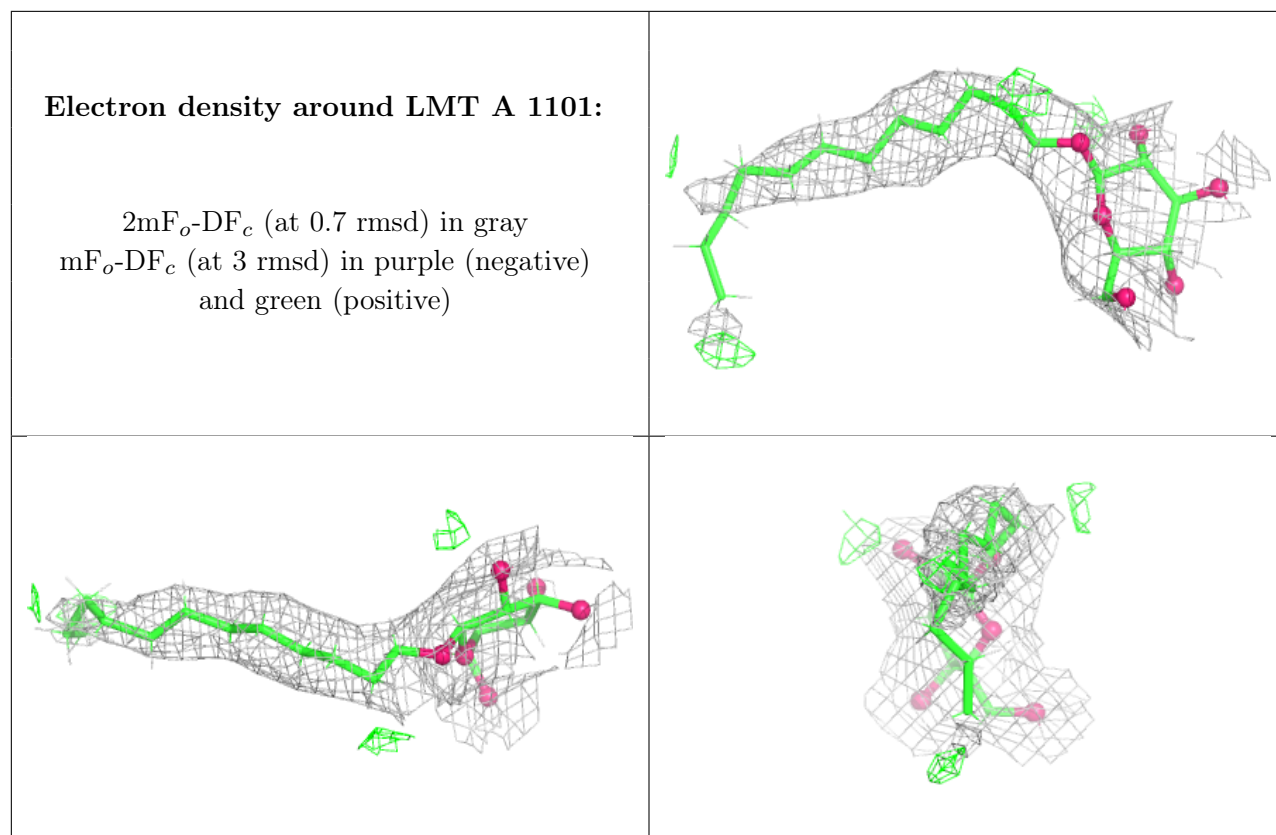
**Electron density around LMT A 1102:**

$2mF_o-DF_c$  (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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.