



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2024 – 07:07 AM EST

PDB ID : 4DX7  
Title : Transport of drugs by the multidrug transporter AcrB involves an access and a deep binding pocket that are separated by a switch-loop  
Authors : Eicher, T.; Cha, H.; Seeger, M.A.; Brandstaetter, L.; El-Delik, J.; Bohnert, J.A.; Kern, W.V.; Verrey, F.; Gruetter, M.G.; Diederichs, K.; Pos, K.M.  
Deposited on : 2012-02-27  
Resolution : 2.25 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

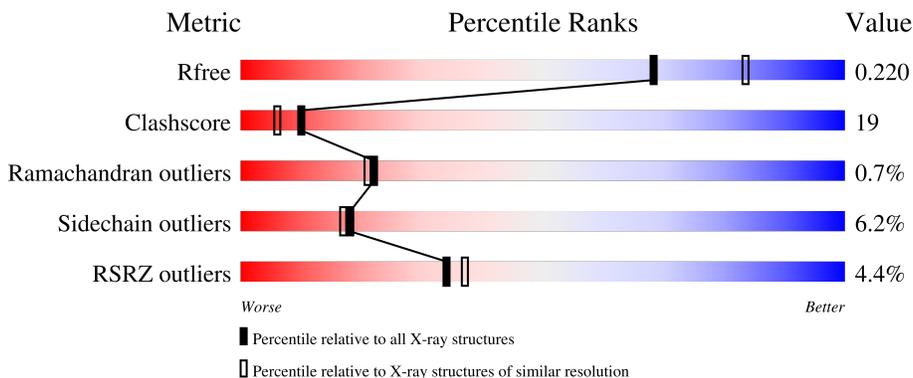
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	1057	
1	B	1057	
1	C	1057	
2	D	169	

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Mol	Chain	Length	Quality of chain
2	E	169	

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
4	DM2	A	1105	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28467 atoms, of which 273 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1042	7927	5097	1311	1475	44	0	0	0
1	B	1033	7849	5052	1295	1458	44	0	0	0
1	C	1036	7875	5067	1302	1462	44	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224

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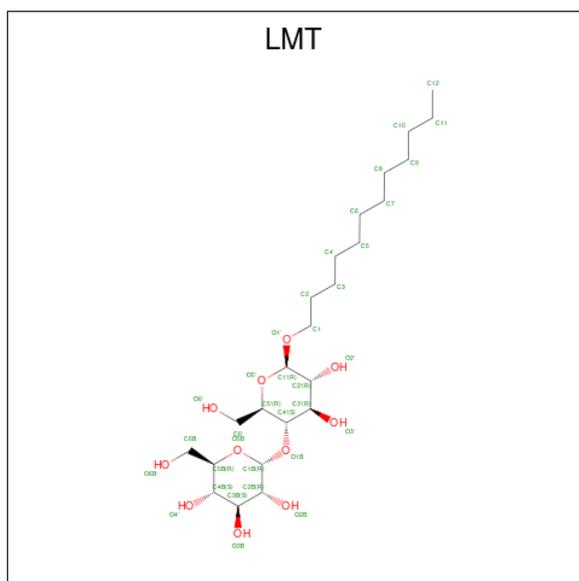
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1177	741	206	229	1	0	0	0
2	E	152	1151	726	202	222	1	0	0	0

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



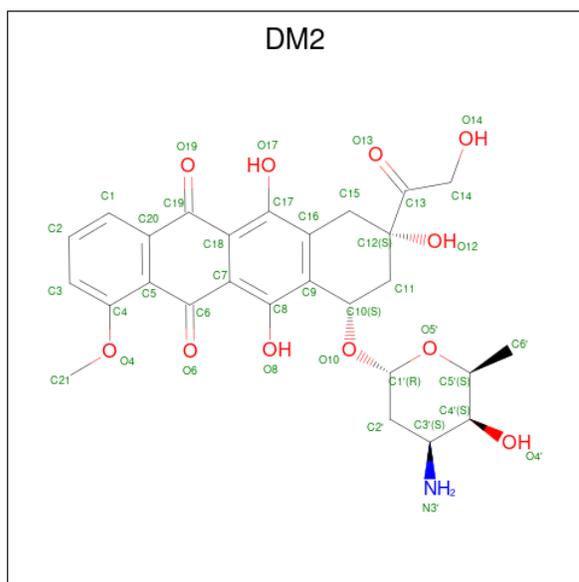
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

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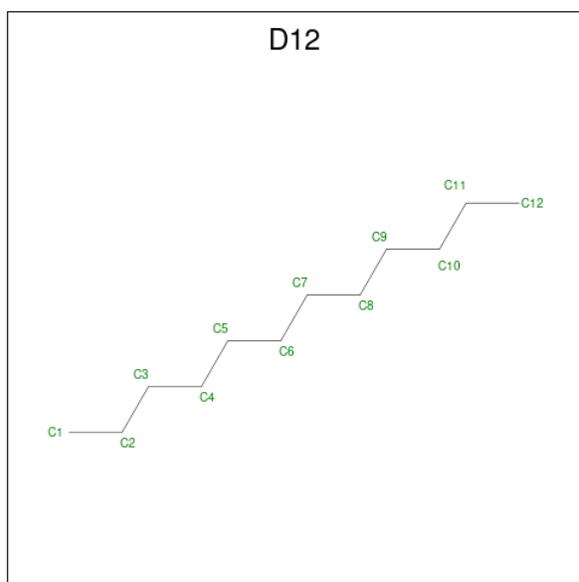
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is DOXORUBICIN (three-letter code: DM2) (formula:  $C_{27}H_{29}NO_{11}$ ).



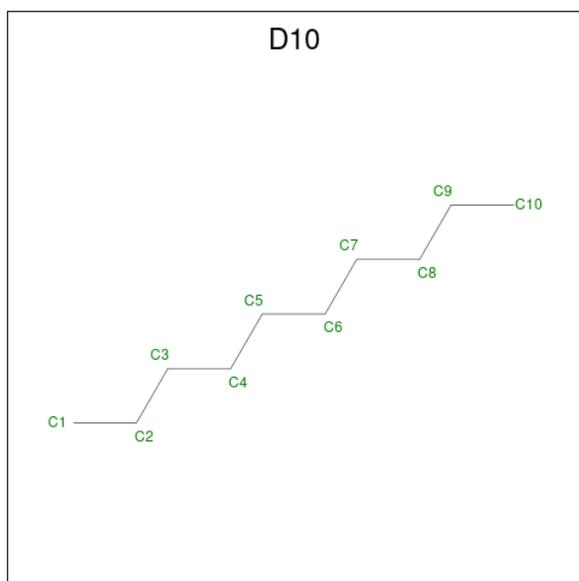
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	0	0	
			39	27	1	11			
4	A	1	Total	C	H	N	O	0	0
			68	27	29	1	11		
4	B	1	Total	C	N	O	0	0	
			39	27	1	11			

- Molecule 5 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ).



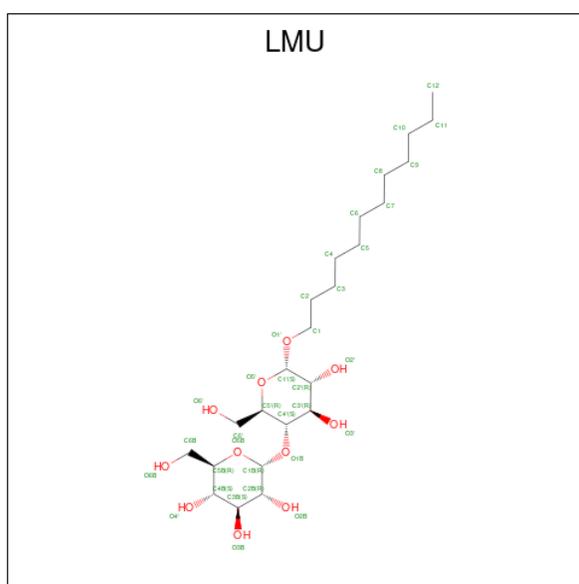
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C H	0	0
			38	12 26		
5	B	1	Total	C H	0	0
			38	12 26		
5	C	1	Total	C H	0	0
			38	12 26		
5	C	1	Total	C H	0	0
			38	12 26		

- Molecule 6 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ).



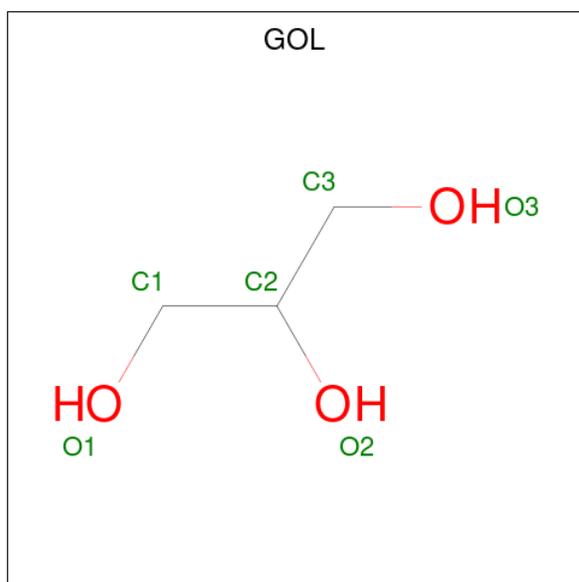
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	0	0
			32	10	22		
6	A	1	Total	C	H	0	0
			32	10	22		
6	B	1	Total	C	H	0	0
			32	10	22		
6	C	1	Total	C	H	0	0
			32	10	22		

- Molecule 7 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



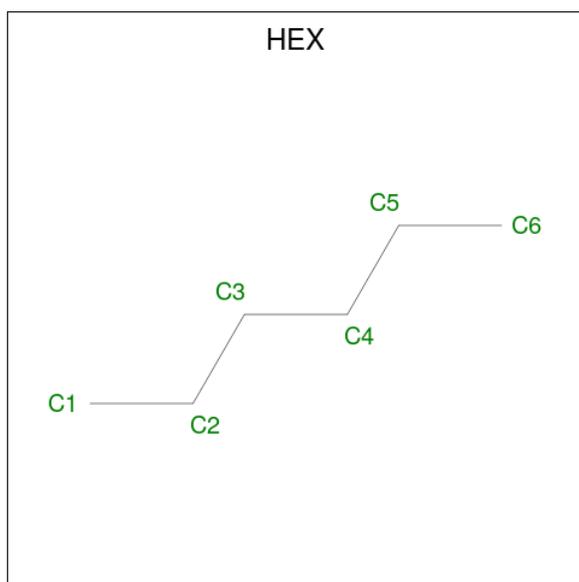
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
8	B	1	14	3	8	3	0	0
8	B	1	14	3	8	3	0	0
8	C	1	14	3	8	3	0	0

- Molecule 9 is HEXANE (three-letter code: HEX) (formula: C<sub>6</sub>H<sub>14</sub>).



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

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

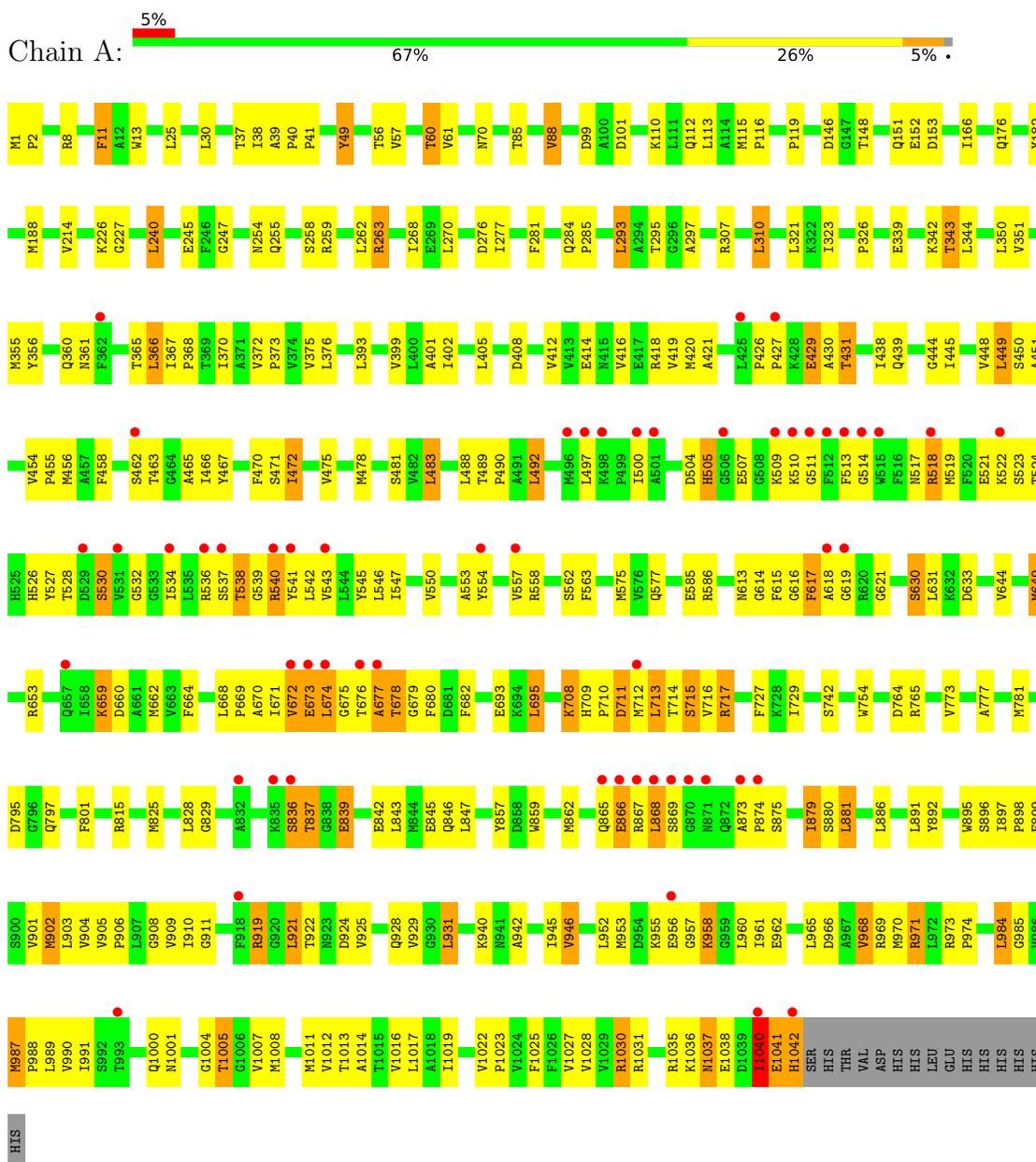
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	497	Total	O	0	0
			497	497		
10	B	494	Total	O	0	0
			494	494		
10	C	572	Total	O	0	0
			572	572		
10	D	81	Total	O	0	0
			81	81		
10	E	56	Total	O	0	0
			56	56		

### 3 Residue-property plots

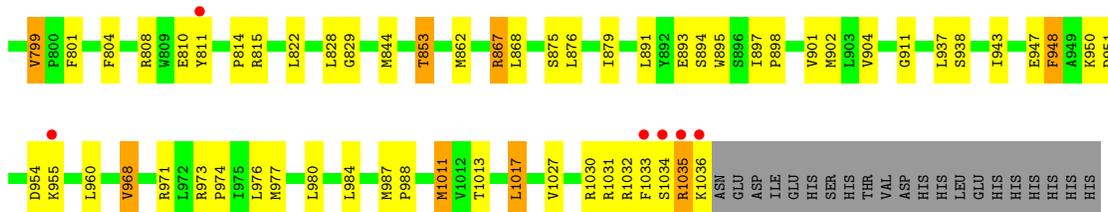
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Acriflavine resistance protein B

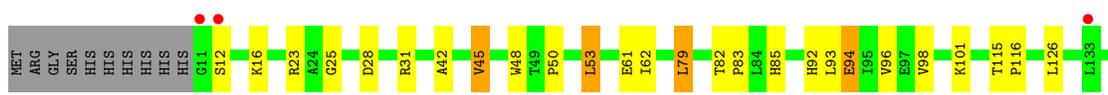
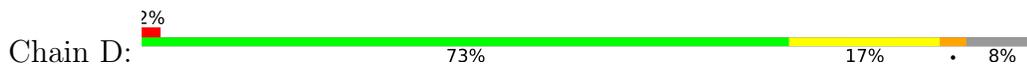


- Molecule 1: Acriflavine resistance protein B

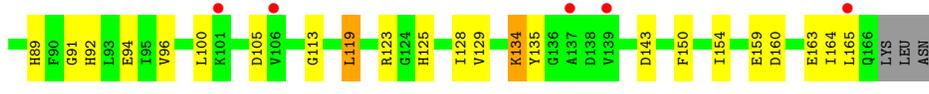
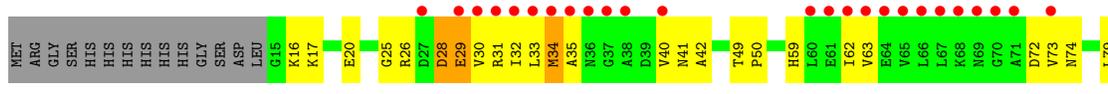




• Molecule 2: DARPIN



• Molecule 2: DARPIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.94Å 163.28Å 245.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.25 49.09 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.09-2.25) 99.5 (49.09-2.25)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.49 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, $R_{free}$	0.185 , 0.227 0.177 , 0.220	Depositor DCC
$R_{free}$ test set	13724 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtrriage
Anisotropy	0.514	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 55.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	28467	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: LMT, D10, LMU, HEX, GOL, DM2, 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	0.37	0/8078	0.53	1/10968 (0.0%)
1	B	0.37	0/7999	0.53	0/10863
1	C	0.39	0/8025	0.54	0/10896
2	D	0.35	0/1196	0.48	0/1626
2	E	0.32	0/1170	0.45	0/1591
All	All	0.37	0/26468	0.53	1/35944 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	CB-CA-C	-5.32	101.29	111.40

There are no chirality outliers.

There are no planarity outliers.

### 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	7927	0	8072	451	0
1	B	7849	0	8001	238	0
1	C	7875	0	8032	232	0
2	D	1177	0	1159	23	0
2	E	1151	0	1136	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	140	0	184	28	0
3	B	70	0	92	14	0
3	C	35	0	46	1	0
4	A	78	29	58	43	0
4	B	39	0	29	9	0
5	A	12	26	26	3	0
5	B	12	26	26	0	0
5	C	24	52	52	2	0
6	A	20	44	44	2	0
6	B	10	22	22	1	0
6	C	10	22	22	0	0
7	B	35	0	46	4	0
8	B	12	16	16	1	0
8	C	6	8	8	1	0
9	B	6	14	14	0	0
9	C	6	14	14	0	0
10	A	497	0	0	25	0
10	B	494	0	0	20	0
10	C	572	0	0	29	0
10	D	81	0	0	1	0
10	E	56	0	0	4	0
All	All	28194	273	27099	1016	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 19.

The worst 5 of 1016 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)
1:A:867:ARG:N	1:A:868:LEU:HB2	1.40	1.33
1:C:509:LYS:CA	1:C:510:LYS:HB2	1.72	1.20
1:A:146:ASP:HB2	10:A:1514:HOH:O	1.45	1.14
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.33	1.11
1:A:866:GLU:HG2	1:A:867:ARG:HA	1.21	1.11

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	1040/1057 (98%)	979 (94%)	47 (4%)	14 (1%)	12	8
1	B	1031/1057 (98%)	997 (97%)	29 (3%)	5 (0%)	29	29
1	C	1034/1057 (98%)	997 (96%)	35 (3%)	2 (0%)	47	55
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	150/169 (89%)	141 (94%)	7 (5%)	2 (1%)	12	8
All	All	3409/3509 (97%)	3265 (96%)	121 (4%)	23 (1%)	22	21

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	617	PHE
1	A	672	VAL
1	A	677	ALA
1	B	659	LYS

### 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	848/863 (98%)	786 (93%)	62 (7%)	14	12
1	B	839/863 (97%)	788 (94%)	51 (6%)	18	18
1	C	842/863 (98%)	795 (94%)	47 (6%)	21	21
2	D	120/132 (91%)	114 (95%)	6 (5%)	24	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	117/132 (89%)	111 (95%)	6 (5%)	24	25
All	All	2766/2853 (97%)	2594 (94%)	172 (6%)	18	17

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	49	TYR
1	C	784	ASP
1	C	121	GLU
1	C	404	LEU
1	C	867	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	255	GLN
2	E	69	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

24 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$
5	D12	C	1106	-	11,11,11	0.31	0	10,10,10	0.86	0
8	GOL	B	1106	-	5,5,5	0.33	0	5,5,5	0.52	0
3	LMT	A	1104	-	36,36,36	1.25	4 (11%)	47,47,47	0.97	4 (8%)
5	D12	B	1109	-	11,11,11	0.24	0	10,10,10	0.73	0
6	D10	A	1108	-	9,9,9	0.28	0	8,8,8	0.76	0
8	GOL	C	1103	-	5,5,5	0.44	0	5,5,5	0.52	0
3	LMT	C	1101	-	36,36,36	1.19	4 (11%)	47,47,47	1.07	3 (6%)
3	LMT	A	1102	-	36,36,36	1.23	4 (11%)	47,47,47	1.14	4 (8%)
3	LMT	A	1101	-	36,36,36	1.24	4 (11%)	47,47,47	1.26	6 (12%)
6	D10	B	1105	-	9,9,9	0.32	0	8,8,8	0.84	0
3	LMT	B	1102	-	36,36,36	1.21	4 (11%)	47,47,47	1.15	4 (8%)
4	DM2	A	1105	-	41,43,43	2.52	12 (29%)	55,67,67	1.39	7 (12%)
6	D10	C	1104	-	9,9,9	0.25	0	8,8,8	0.73	0
8	GOL	B	1107	-	5,5,5	0.37	0	5,5,5	0.14	0
4	DM2	B	1104	-	41,43,43	2.55	11 (26%)	55,67,67	1.44	7 (12%)
7	LMU	B	1103	-	36,36,36	1.27	4 (11%)	47,47,47	1.21	8 (17%)
9	HEX	B	1108	-	5,5,5	0.20	0	4,4,4	0.54	0
9	HEX	C	1105	-	5,5,5	0.22	0	4,4,4	0.57	0
3	LMT	A	1103	-	36,36,36	1.18	3 (8%)	47,47,47	1.21	4 (8%)
5	D12	A	1107	-	11,11,11	0.30	0	10,10,10	0.85	0
5	D12	C	1102	-	11,11,11	0.17	0	10,10,10	0.56	0
4	DM2	A	1106	-	41,43,43	2.54	13 (31%)	55,67,67	1.71	10 (18%)
3	LMT	B	1101	-	36,36,36	1.26	4 (11%)	47,47,47	1.31	5 (10%)
6	D10	A	1109	-	9,9,9	0.25	0	8,8,8	0.69	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
5	D12	C	1106	-	-	2/9/9/9	-
8	GOL	B	1106	-	-	4/4/4/4	-
3	LMT	A	1104	-	-	14/21/61/61	0/2/2/2
5	D12	B	1109	-	-	0/9/9/9	-
6	D10	A	1108	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	1103	-	-	3/4/4/4	-
3	LMT	C	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
6	D10	B	1105	-	-	1/7/7/7	-
3	LMT	B	1102	-	-	12/21/61/61	0/2/2/2
4	DM2	A	1105	-	-	6/13/60/60	0/5/5/5
6	D10	C	1104	-	-	0/7/7/7	-
8	GOL	B	1107	-	-	3/4/4/4	-
4	DM2	B	1104	-	-	6/13/60/60	0/5/5/5
7	LMU	B	1103	-	-	6/21/61/61	0/2/2/2
9	HEX	B	1108	-	-	0/3/3/3	-
9	HEX	C	1105	-	-	0/3/3/3	-
3	LMT	A	1103	-	-	15/21/61/61	0/2/2/2
5	D12	A	1107	-	-	2/9/9/9	-
5	D12	C	1102	-	-	1/9/9/9	-
4	DM2	A	1106	-	-	1/13/60/60	0/5/5/5
3	LMT	B	1101	-	-	11/21/61/61	0/2/2/2
6	D10	A	1109	-	-	0/7/7/7	-

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	DM2	O6-C6	8.51	1.38	1.22
4	A	1105	DM2	O6-C6	8.43	1.38	1.22
4	A	1106	DM2	O6-C6	8.38	1.38	1.22
4	B	1104	DM2	O19-C19	7.60	1.36	1.22
4	A	1105	DM2	O19-C19	7.54	1.36	1.22

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1106	DM2	O4-C4-C5	4.90	122.67	115.85
3	B	1101	LMT	C1-O1'-C1'	4.53	121.36	113.84
4	A	1106	DM2	O4-C4-C3	-4.10	117.33	124.37
4	A	1106	DM2	C4-C5-C6	4.07	127.83	122.21
4	B	1104	DM2	O4-C4-C5	4.01	121.44	115.85

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

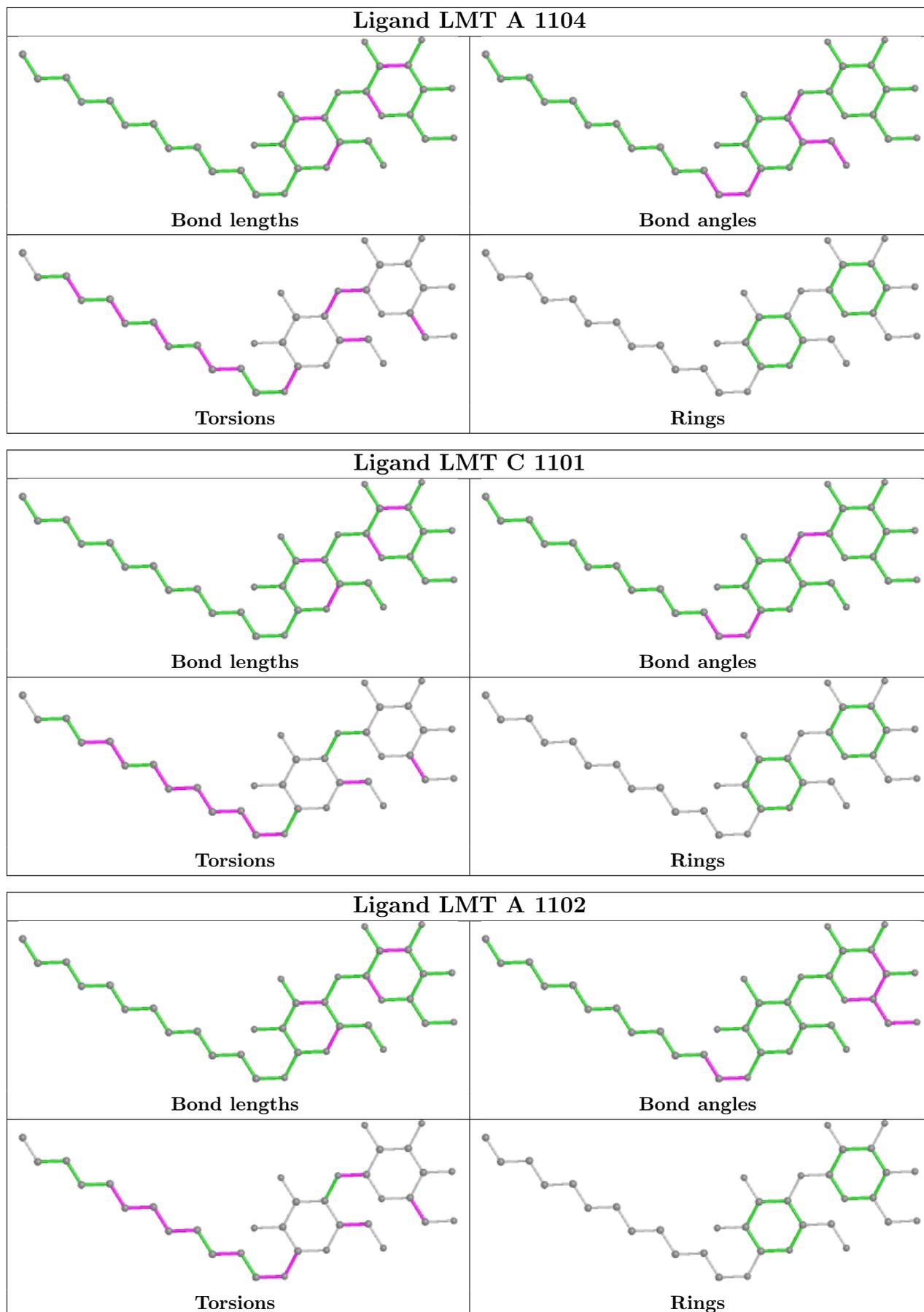
Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1104	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1

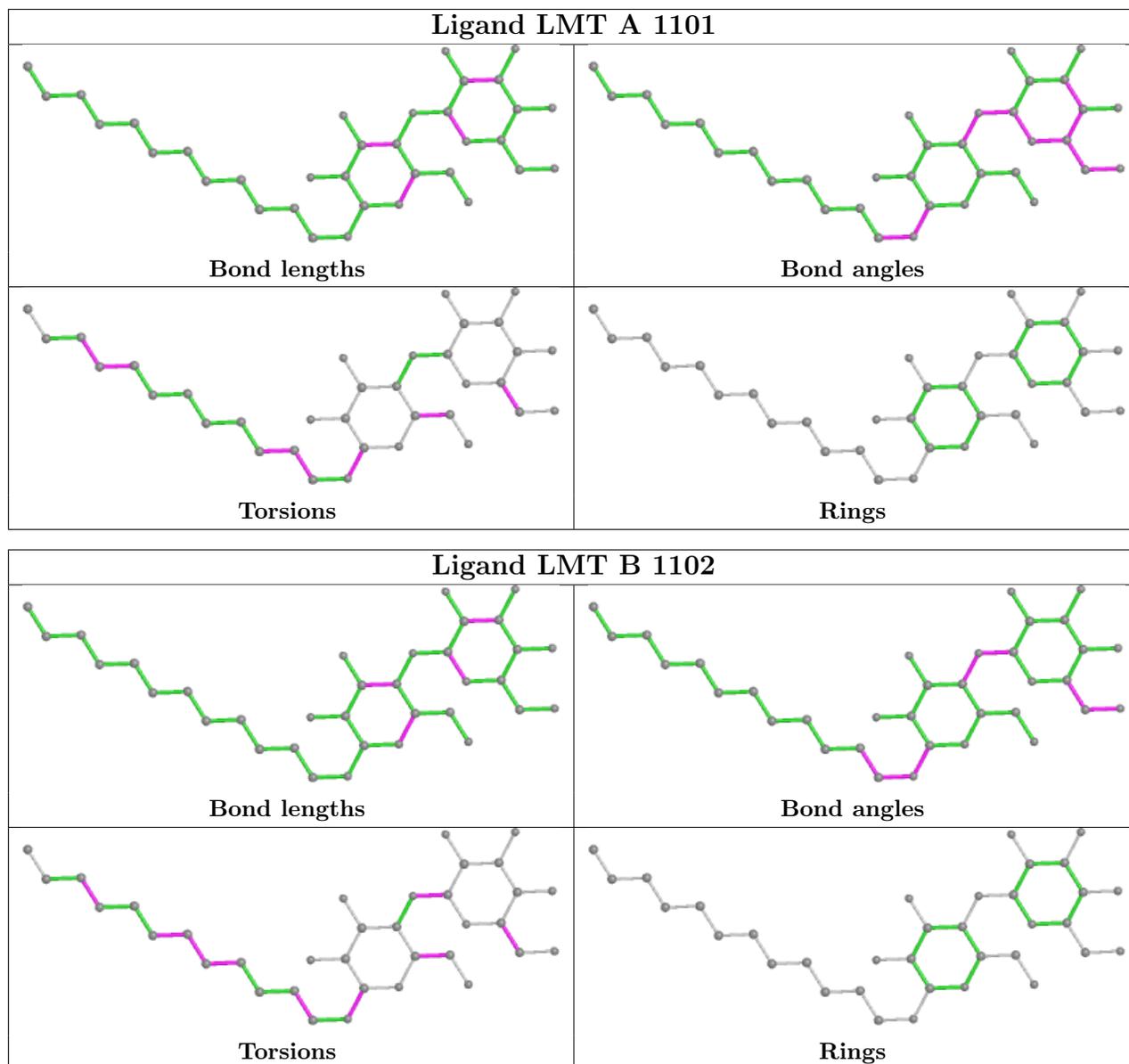
There are no ring outliers.

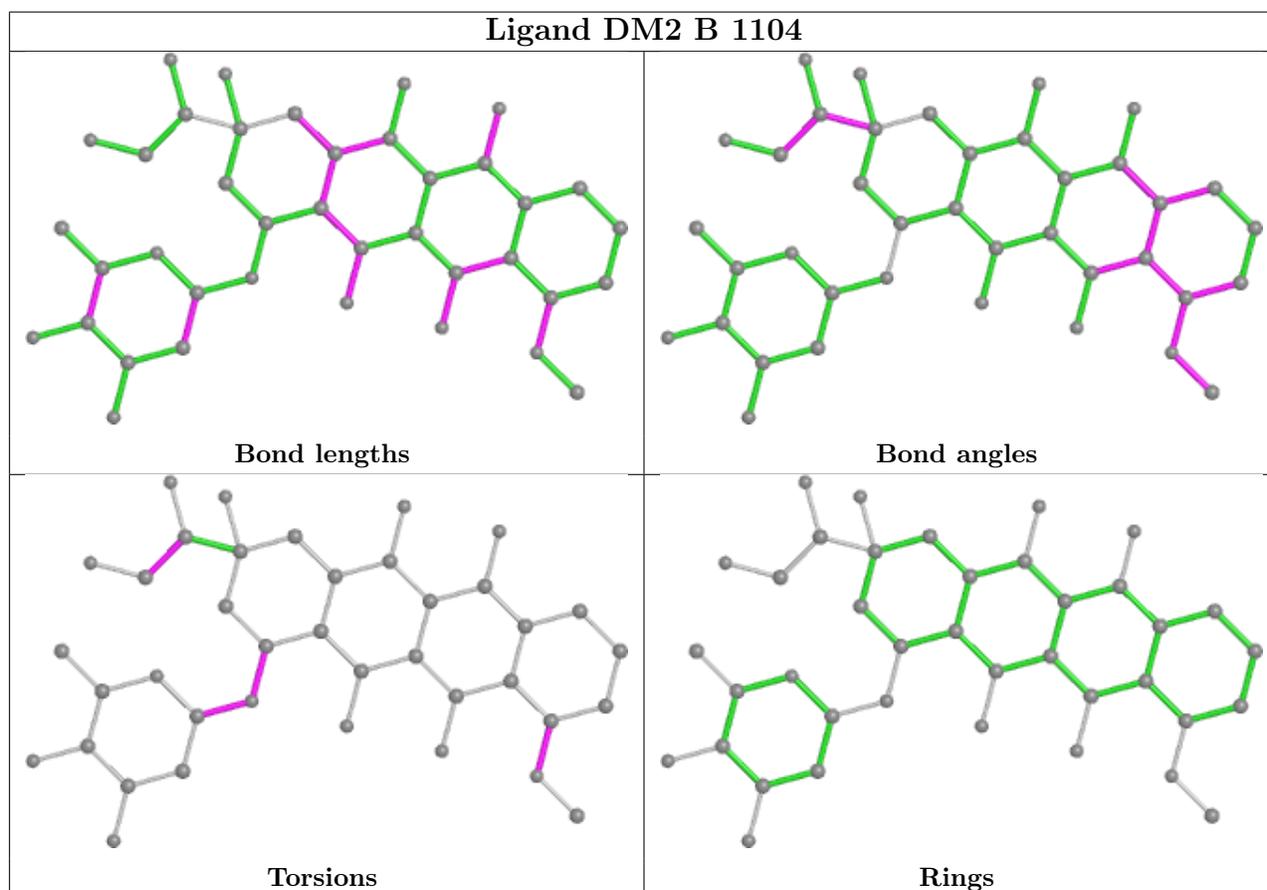
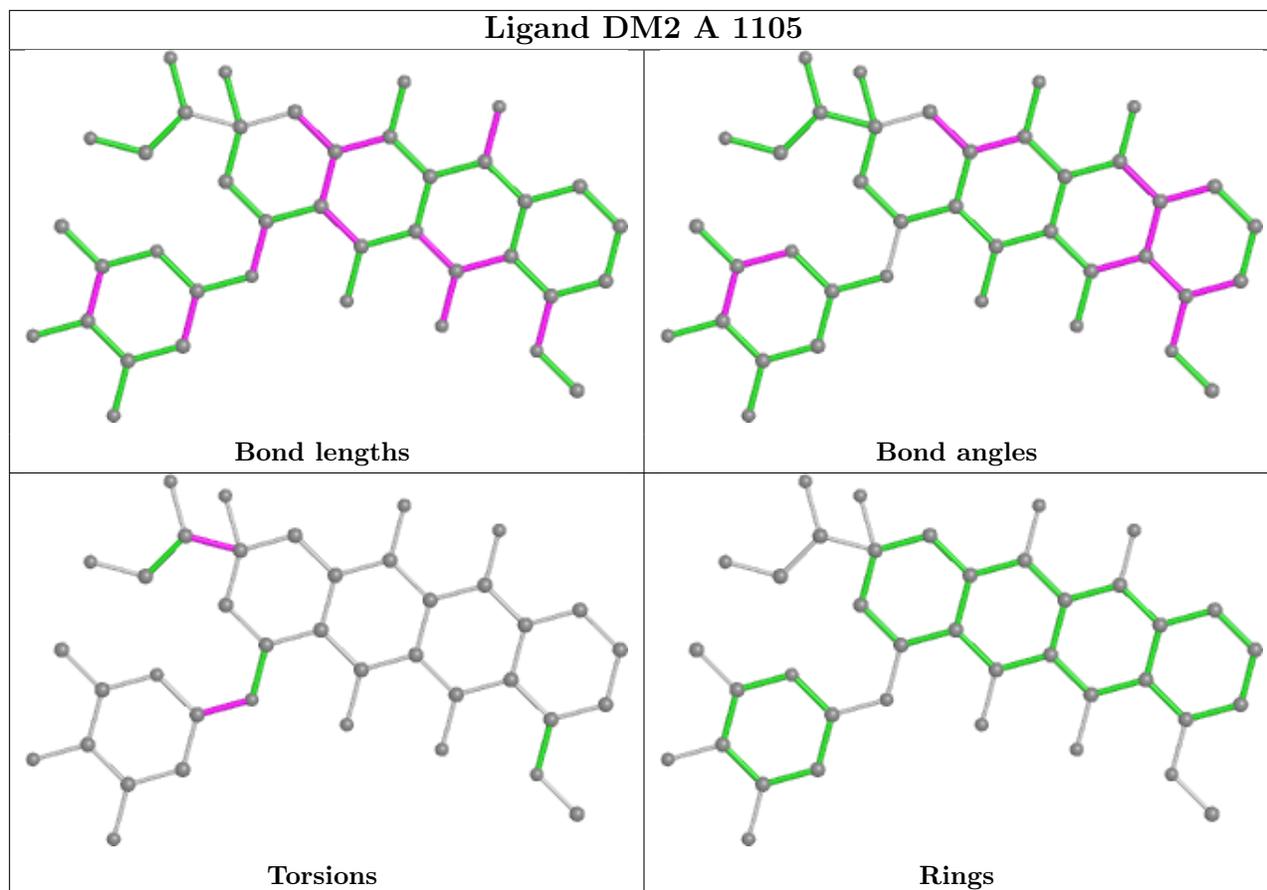
17 monomers are involved in 107 short contacts:

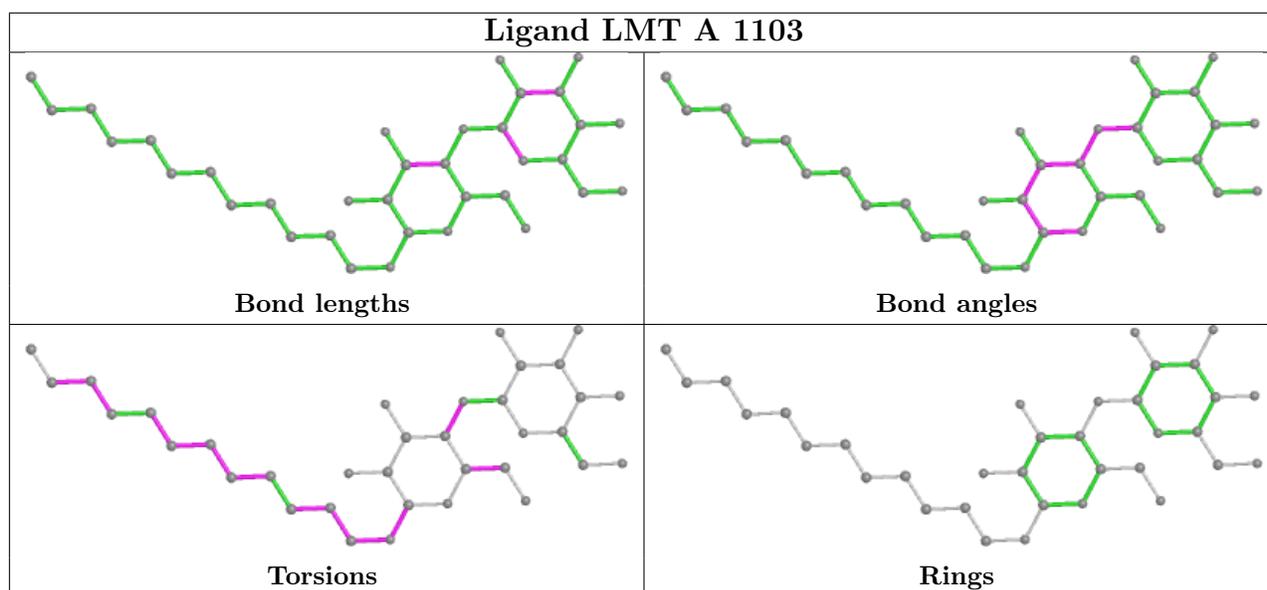
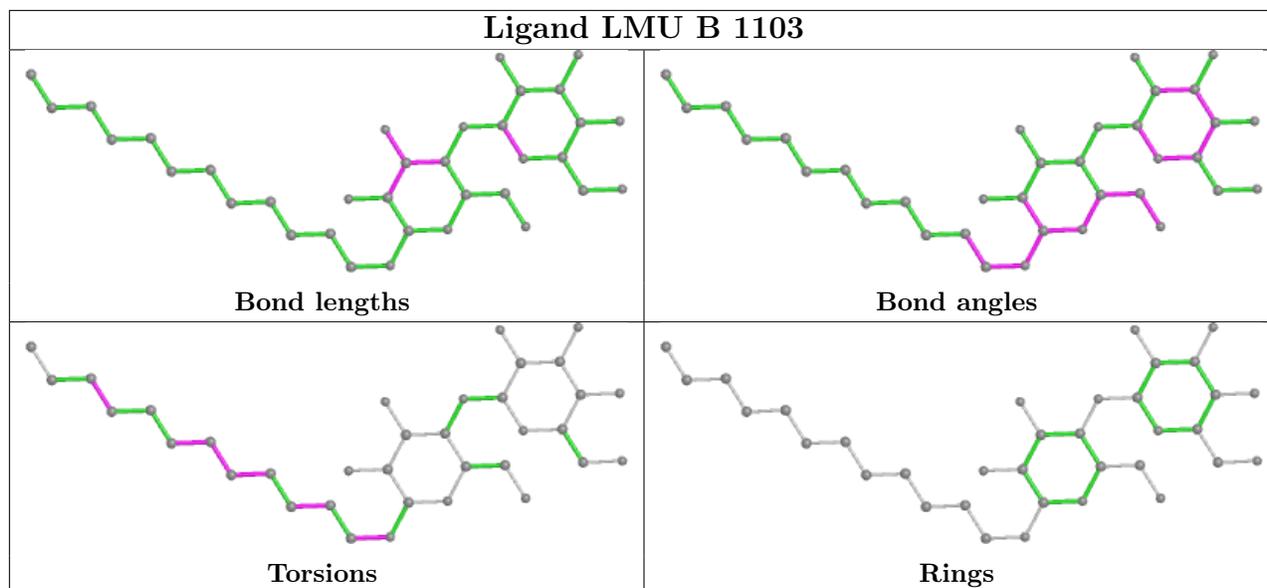
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1106	GOL	1	0
3	A	1104	LMT	6	0
6	A	1108	D10	2	0
8	C	1103	GOL	1	0
3	C	1101	LMT	1	0
3	A	1102	LMT	8	0
3	A	1101	LMT	3	0
6	B	1105	D10	1	0
3	B	1102	LMT	4	0
4	A	1105	DM2	33	0
4	B	1104	DM2	9	0
7	B	1103	LMU	4	0
3	A	1103	LMT	11	0
5	A	1107	D12	3	0
5	C	1102	D12	2	0
4	A	1106	DM2	12	0
3	B	1101	LMT	10	0

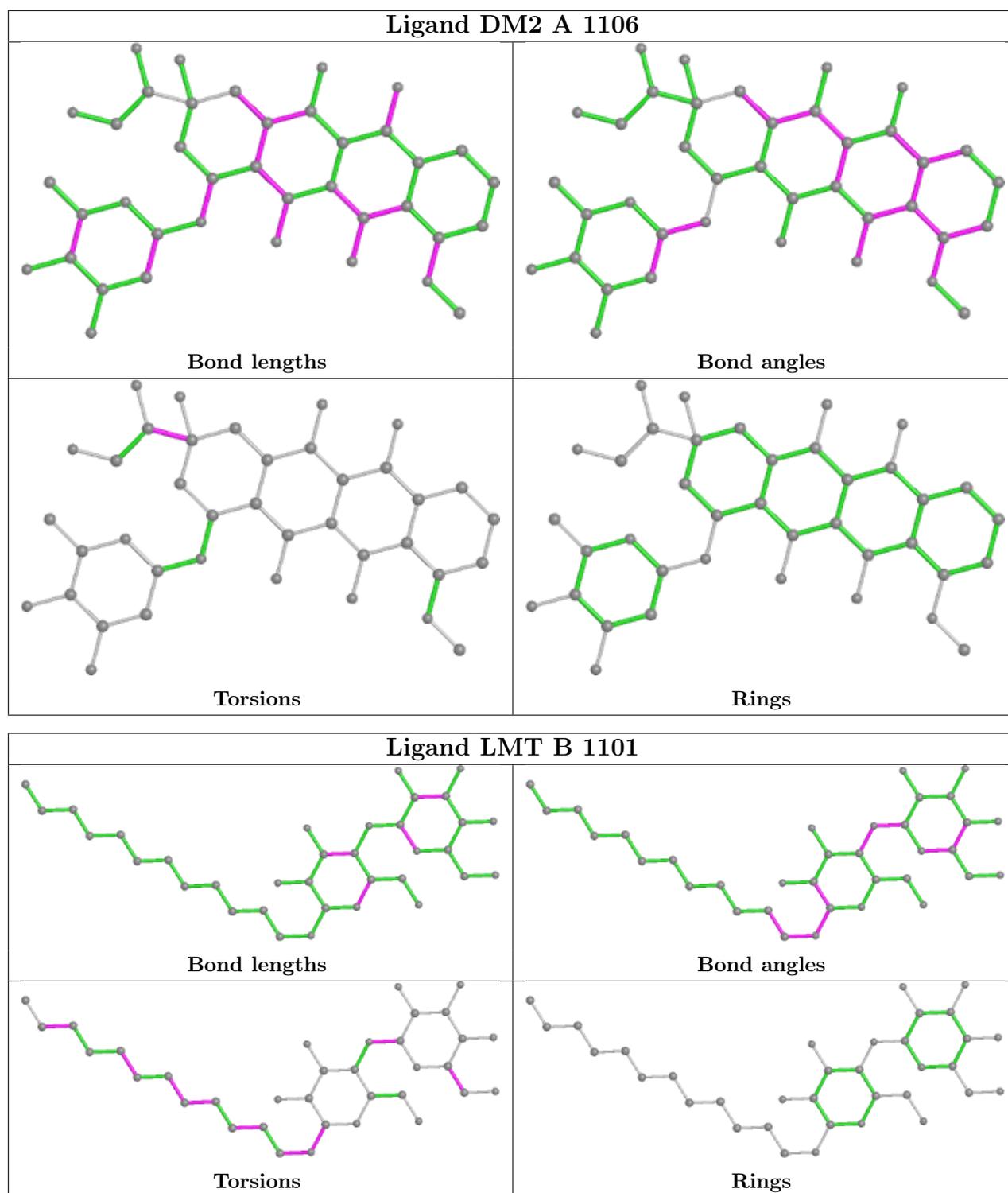
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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	1042/1057 (98%)	0.02	55 (5%) 26 29	23, 48, 95, 151	0
1	B	1033/1057 (97%)	-0.17	32 (3%) 49 52	23, 46, 75, 131	0
1	C	1036/1057 (98%)	-0.13	28 (2%) 54 57	25, 43, 74, 151	0
2	D	156/169 (92%)	-0.16	4 (2%) 56 59	33, 45, 74, 110	0
2	E	152/169 (89%)	0.92	30 (19%) 1 1	38, 56, 87, 104	0
All	All	3419/3509 (97%)	-0.05	149 (4%) 34 37	23, 46, 83, 151	0

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	11	GLY	9.0
1	C	1036	LYS	8.5
1	B	678	THR	6.9
2	E	34	MET	6.8
1	A	868	LEU	5.4

### 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 [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,

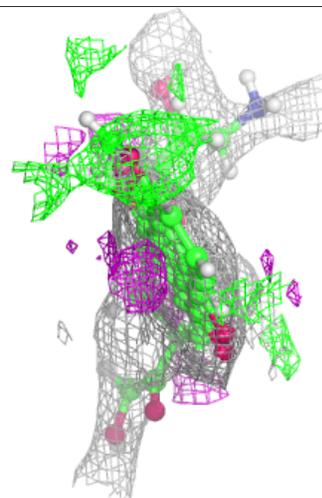
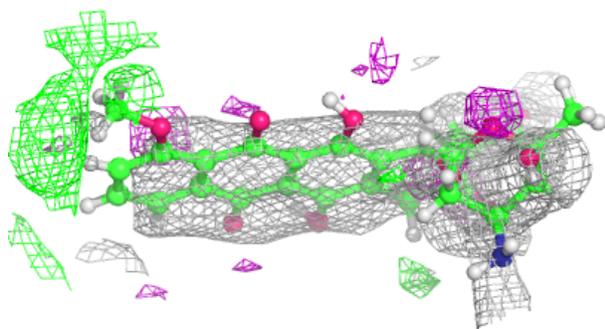
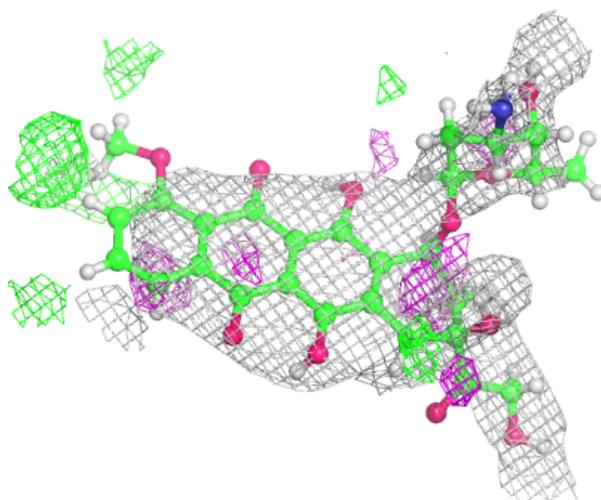
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	D10	A	1109	10/10	0.55	0.29	83,107,121,121	0
5	D12	C	1102	12/12	0.56	0.17	58,91,99,100	0
9	HEX	B	1108	6/6	0.69	0.15	84,101,109,109	0
4	DM2	A	1106	39/39	0.70	0.24	81,141,174,176	0
5	D12	B	1109	12/12	0.71	0.19	52,73,88,91	0
9	HEX	C	1105	6/6	0.71	0.20	84,101,105,105	0
5	D12	A	1107	12/12	0.72	0.20	58,82,125,125	0
6	D10	A	1108	10/10	0.73	0.18	85,103,113,113	0
8	GOL	B	1107	6/6	0.74	0.39	95,119,134,143	0
7	LMU	B	1103	35/35	0.75	0.22	65,84,96,105	0
4	DM2	B	1104	39/39	0.75	0.26	93,121,139,142	0
5	D12	C	1106	12/12	0.75	0.13	81,98,109,109	0
6	D10	C	1104	10/10	0.75	0.18	80,97,104,107	0
6	D10	B	1105	10/10	0.76	0.18	75,97,109,110	0
3	LMT	B	1101	35/35	0.79	0.27	73,114,134,136	0
3	LMT	A	1102	35/35	0.80	0.27	73,105,119,120	0
4	DM2	A	1105	39/39	0.82	0.18	75,91,110,115	0
3	LMT	A	1103	35/35	0.86	0.16	59,95,115,119	0
8	GOL	B	1106	6/6	0.89	0.27	73,88,107,114	0
3	LMT	A	1104	35/35	0.90	0.31	74,94,100,104	0
3	LMT	B	1102	35/35	0.90	0.21	63,77,111,112	0
3	LMT	C	1101	35/35	0.93	0.14	62,74,93,97	0
8	GOL	C	1103	6/6	0.93	0.15	37,48,59,68	0
3	LMT	A	1101	35/35	0.94	0.13	49,74,107,108	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.

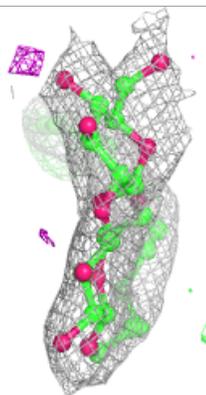
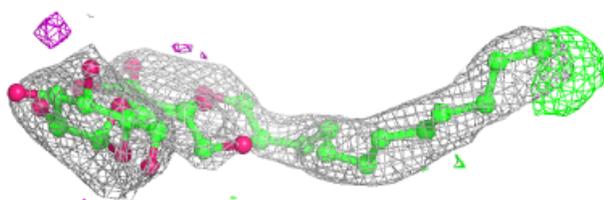
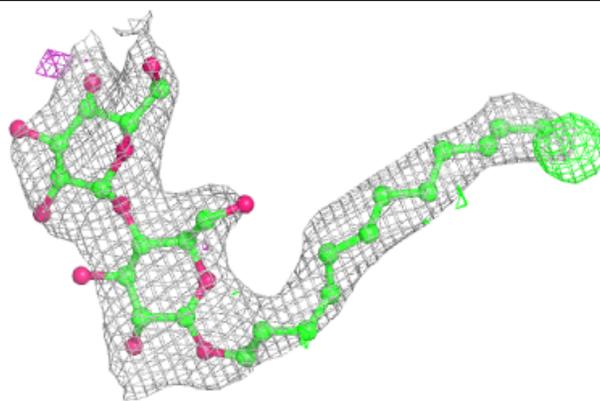
**Electron density around DM2 A 1106:**

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

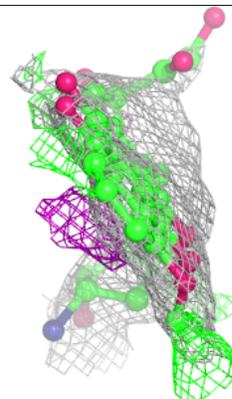
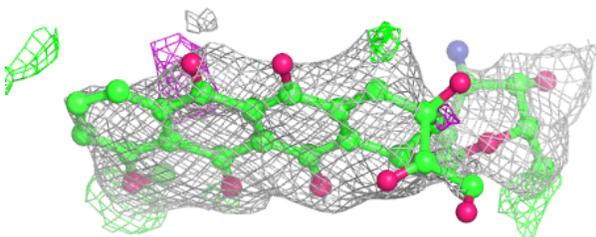
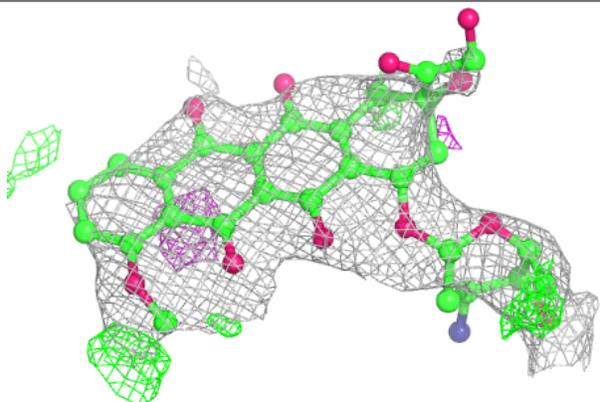


**Electron density around LMU B 1103:**

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

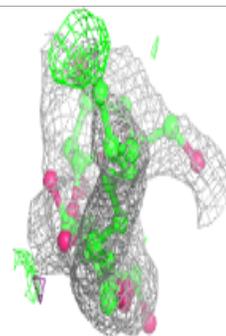
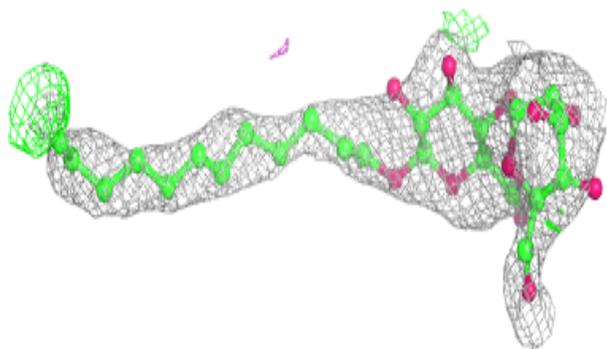
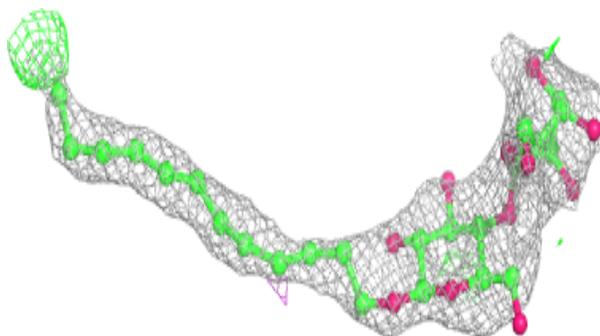
**Electron density around DM2 B 1104:**

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

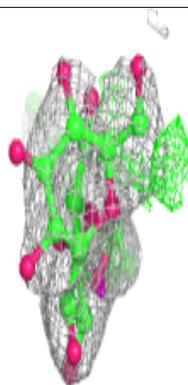
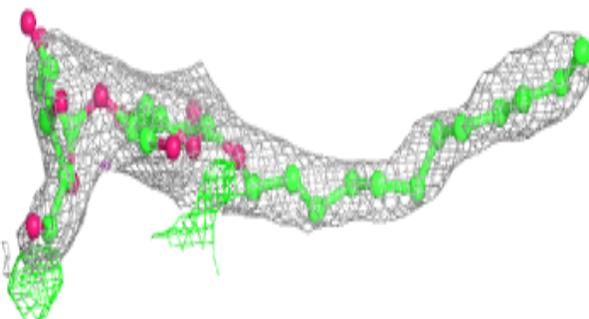
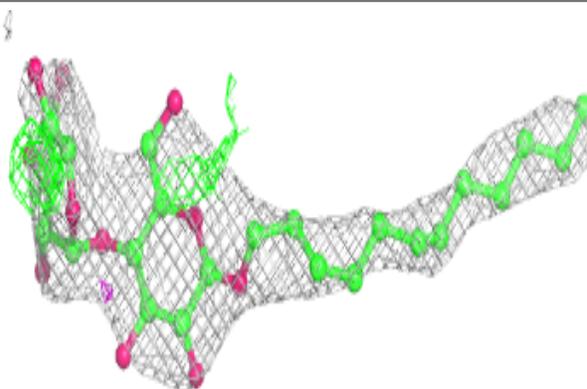


**Electron density around LMT B 1101:**

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

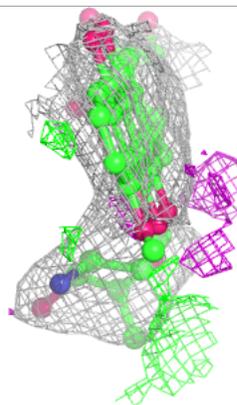
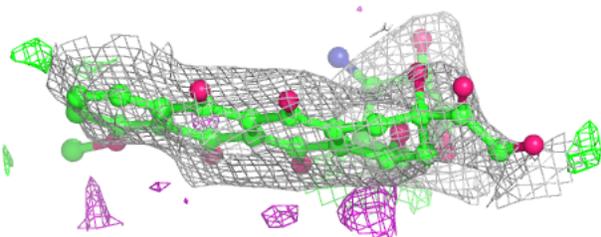
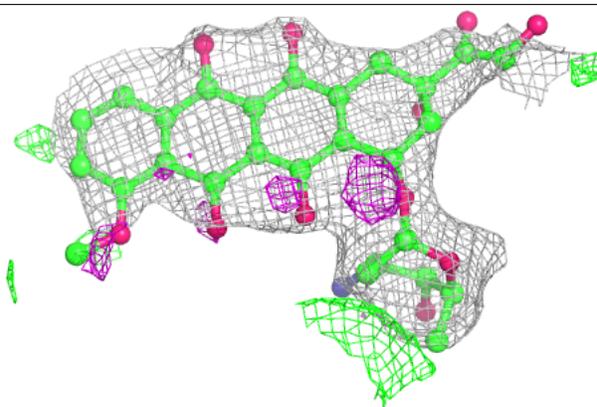
**Electron density around LMT A 1102:**

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

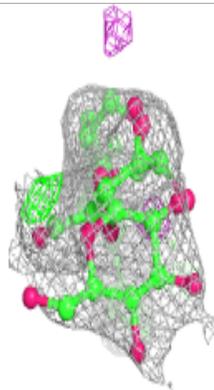
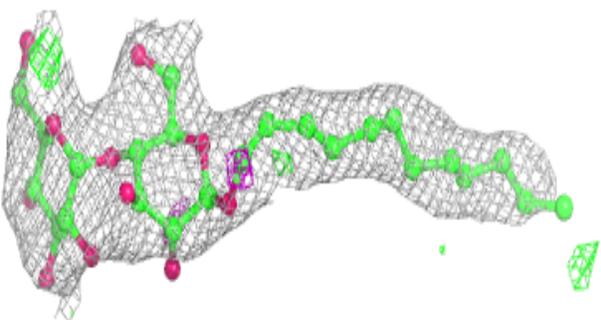
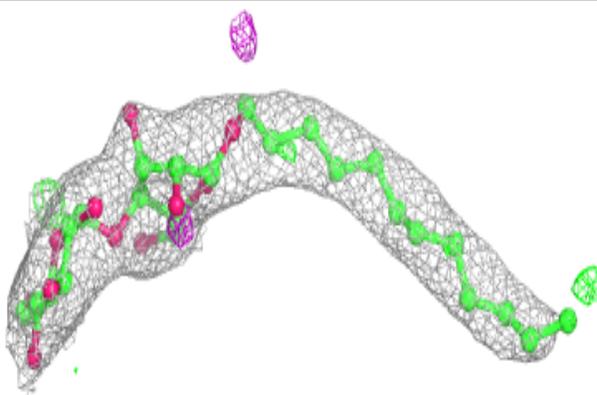


**Electron density around DM2 A 1105:**

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

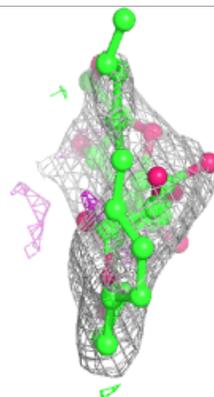
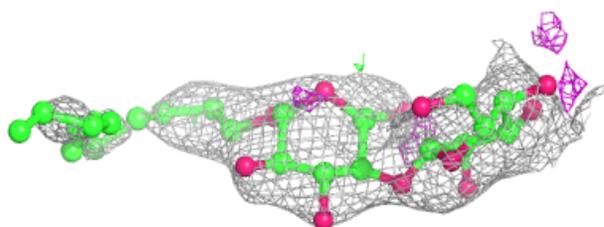
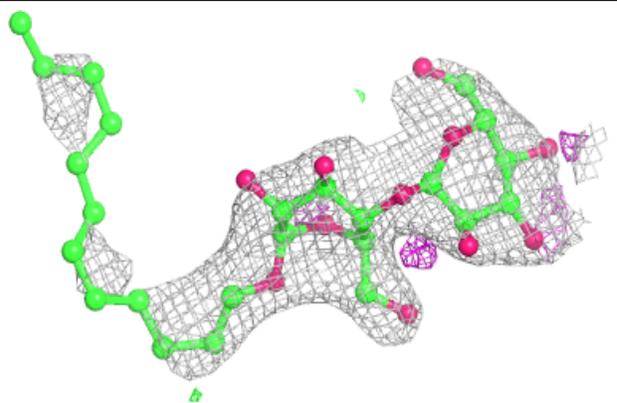
**Electron density around LMT A 1103:**

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

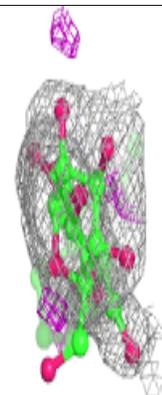
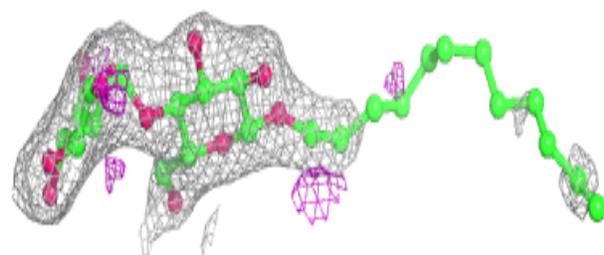
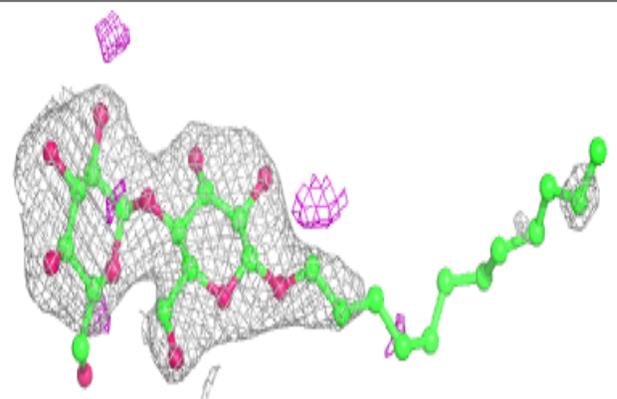


**Electron density around LMT A 1104:**

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

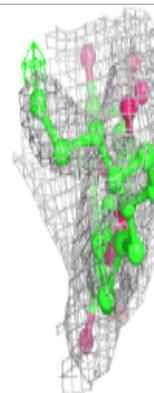
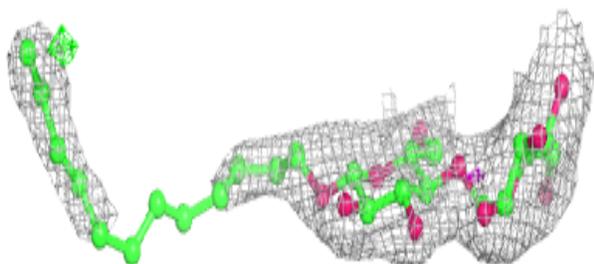
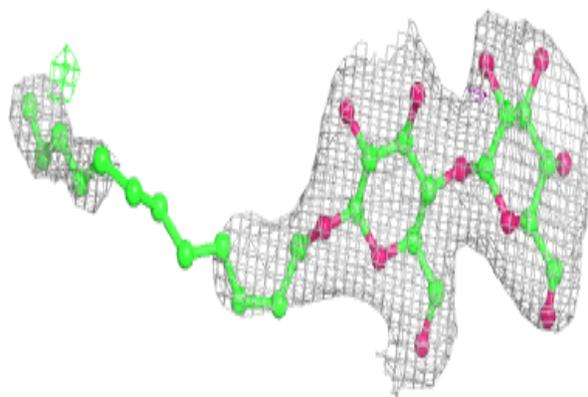
**Electron density around LMT B 1102:**

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

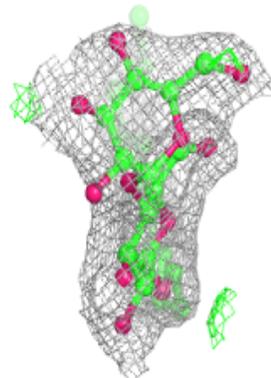
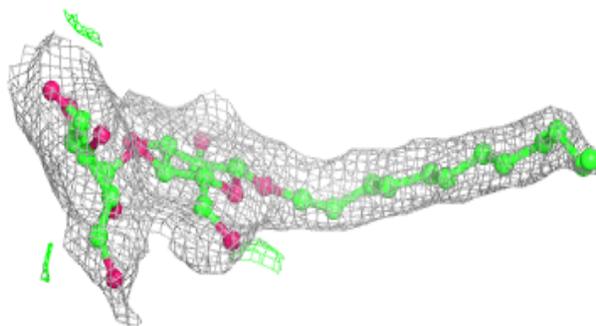
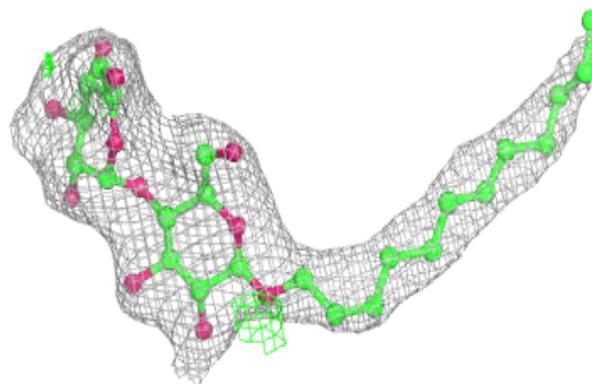


**Electron density around LMT C 1101:**

$2mF_o-DF_c$  (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.