Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 03:14 pm GMT

PDB ID	:	7OUL
Title	:	BDM88832 inhibitor bound to the transmembrane domain of AcrB-R971A
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2021-06-12
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

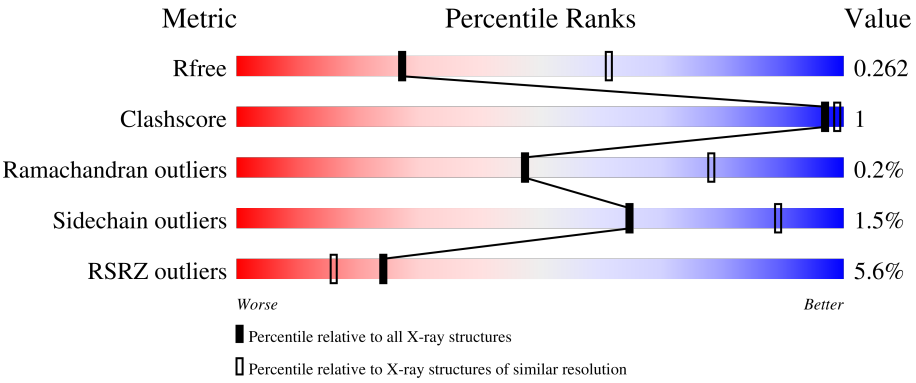
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	6% 94%
1	B	1057	5% 93%
1	C	1057	3% 94%
2	D	169	7% 92% 8%
2	E	169	22% 89% 9%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 26436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	2	0
			7866	5062	1297	1462	45			
1	B	1034	Total	C	N	O	S	0	0	0
			7849	5052	1293	1460	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7843	5049	1292	1458	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	971	ALA	ARG	engineered mutation	UNP P31224
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	971	ALA	ARG	engineered mutation	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	971	ALA	ARG	engineered mutation	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

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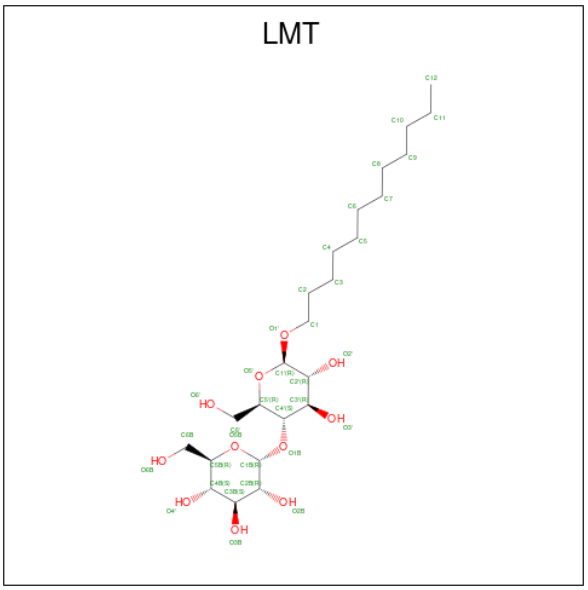
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	155	Total	C	N	O	S	0	0	0
			1173	739	205	228	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (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	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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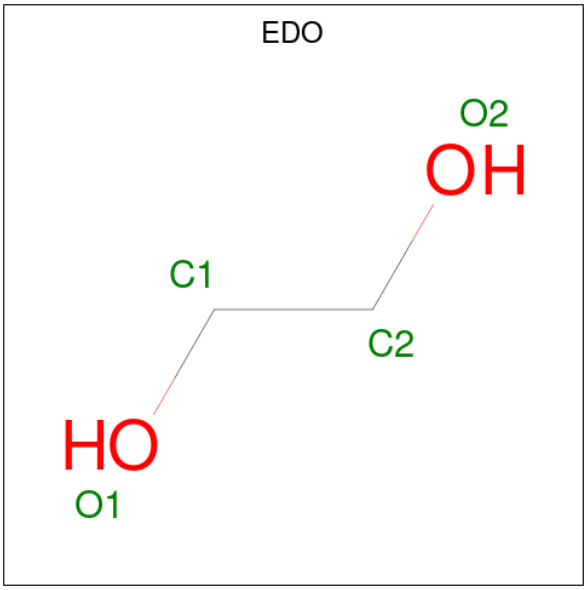
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 35 24 11	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

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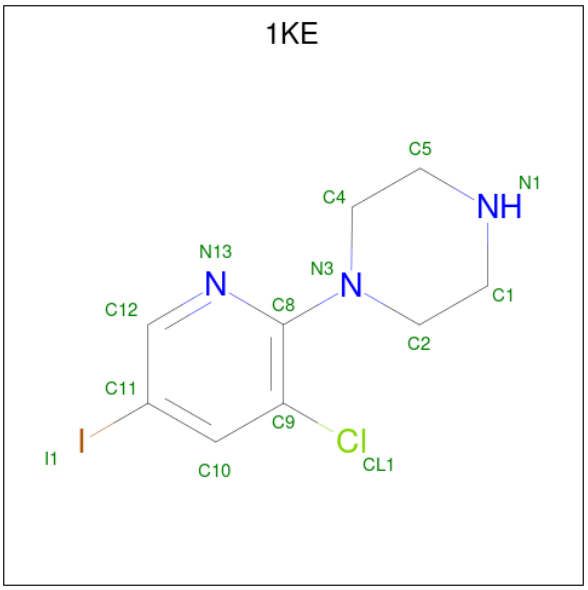
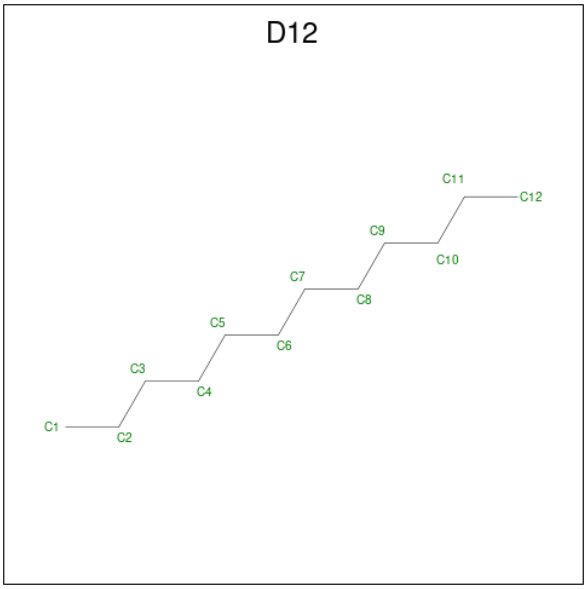
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C O 4 2 2	0	0

- Molecule 5 is 1-(3-chloranyl-5-iodanyl-pyridin-2-yl)piperazine (three-letter code: 1KE) (formula: $C_9H_{11}ClIN_3$) (labeled as "Ligand of Interest" by depositor).



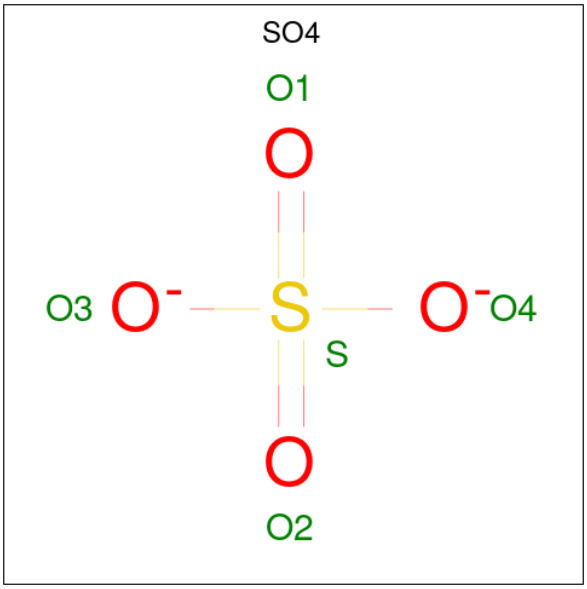
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C Cl I N 14 9 1 1 3	0	0

- Molecule 6 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



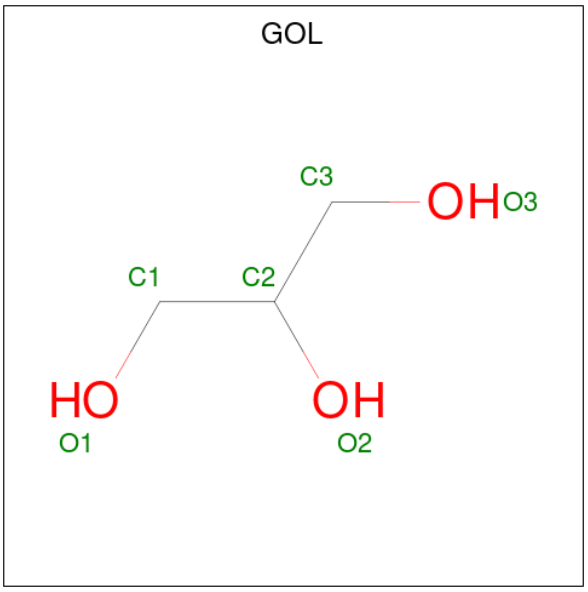
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 12 12	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



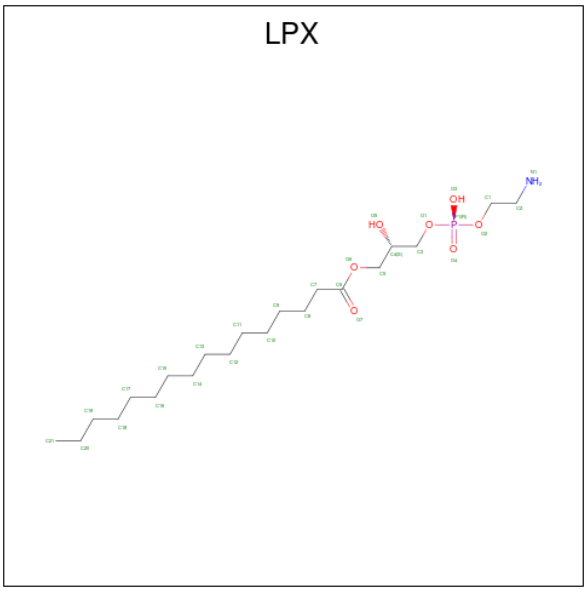
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	C	1	Total O S 5 4 1	0	0

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



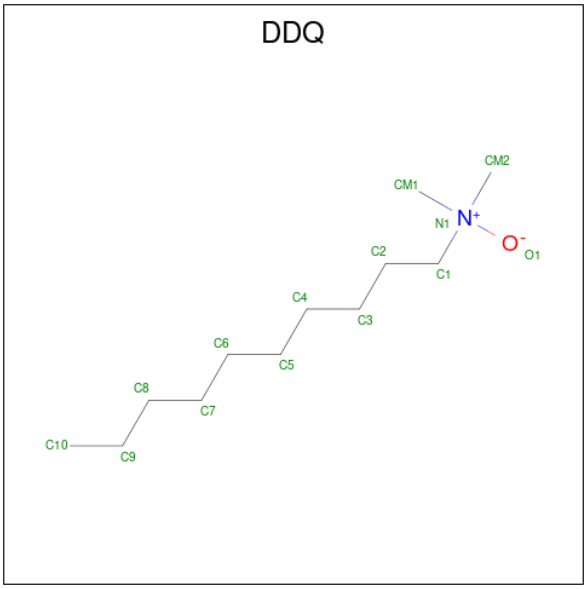
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: $C_{21}H_{44}NO_7P$).



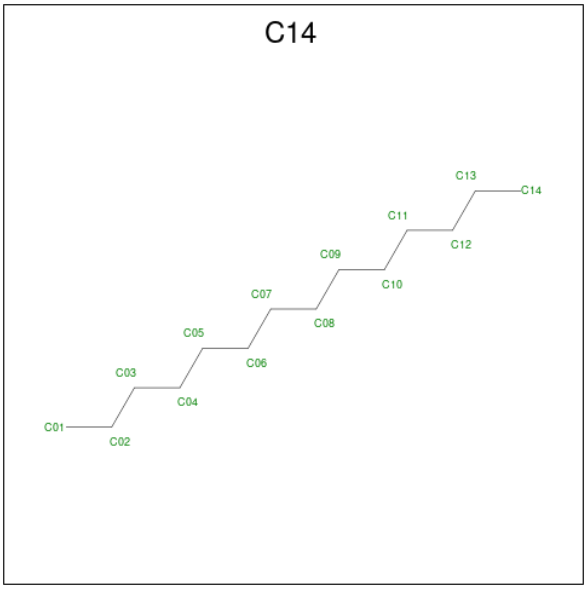
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C N O P 30 21 1 7 1	0	0

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 11 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	C	0	0
			14	14		

- Molecule 12 is water.

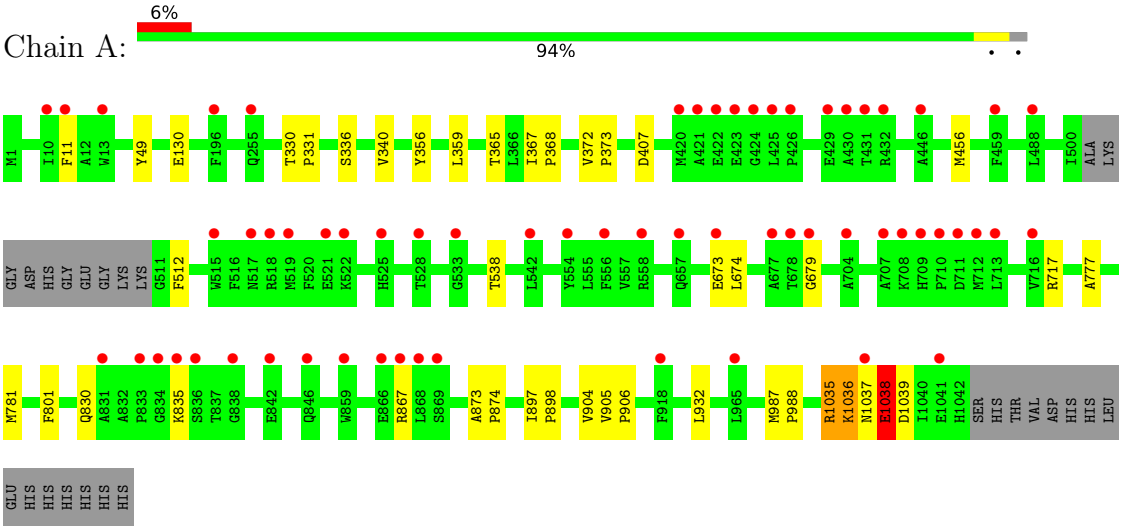
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	63	Total O 63 63	0	0
12	B	43	Total O 43 43	0	0
12	C	55	Total O 55 55	0	0
12	D	7	Total O 7 7	0	0
12	E	5	Total O 5 5	0	0

3 Residue-property plots (i)

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.

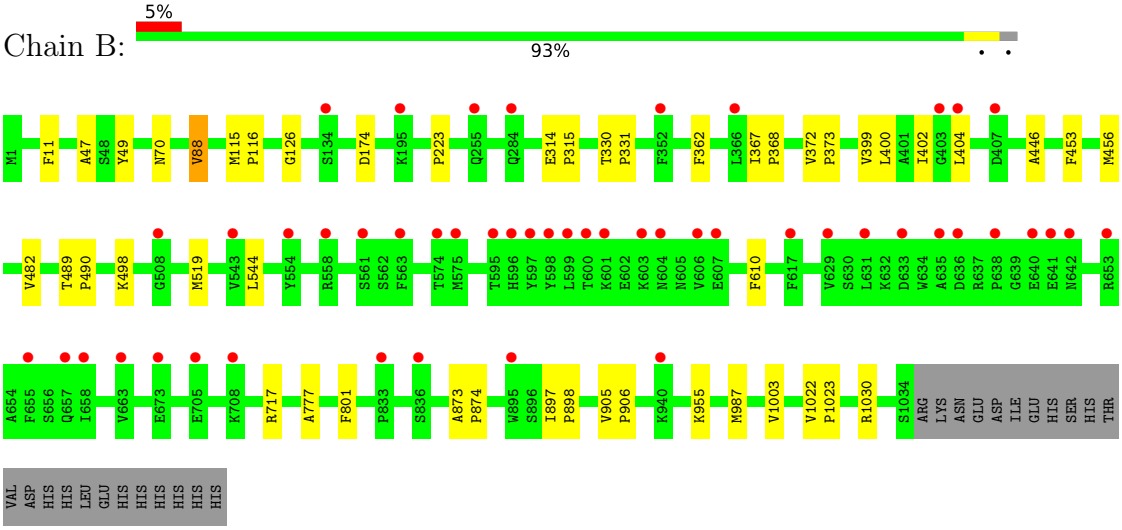
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



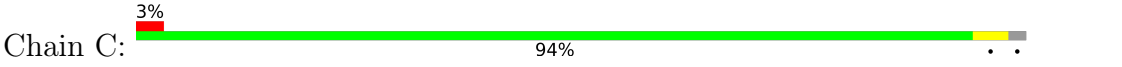
• Molecule 1: Multidrug efflux pump subunit AcrB

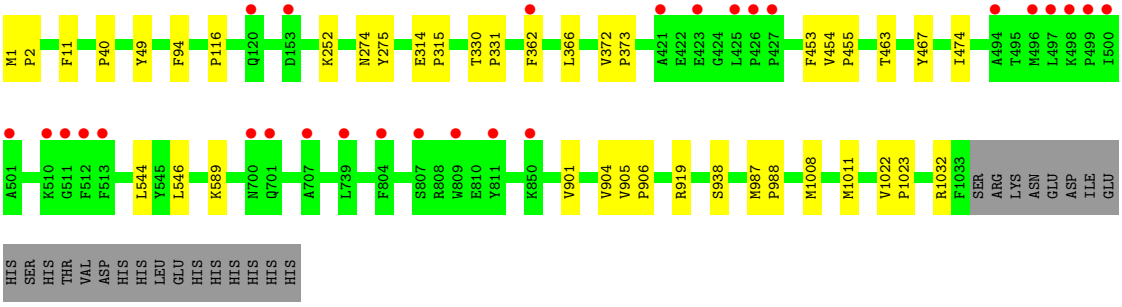
Chain B:



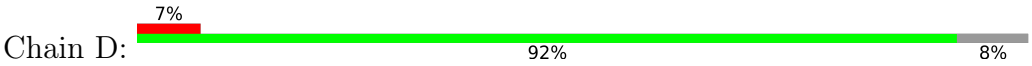
• Molecule 1: Multidrug efflux pump subunit AcrB

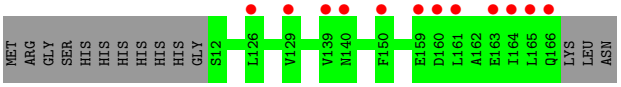
Chain C:



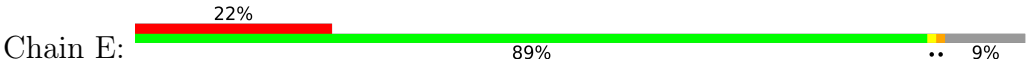


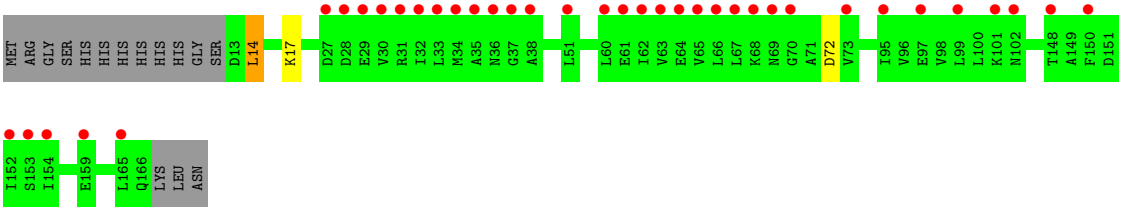
• Molecule 2: DARPIN





• Molecule 2: DARPIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	146.41Å 160.01Å 245.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 2.80 49.43 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.43-2.80) 100.0 (49.43-2.80)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.242 , 0.261 0.242 , 0.262	Depositor DCC
R_{free} test set	6989 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	26436	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 1KE, D12, LMT, C14, LPX, DDQ, EDO, GOL

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	0.67	0/8018	0.70	0/10889
1	B	0.67	0/7999	0.70	0/10864
1	C	0.67	0/7993	0.70	0/10856
2	D	0.68	0/1192	0.71	0/1621
2	E	0.68	0/1186	0.71	0/1613
All	All	0.67	0/26388	0.70	0/35843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	7866	0	8014	16	0
1	B	7849	0	7998	20	0
1	C	7843	0	7993	16	0
2	D	1173	0	1156	0	0
2	E	1167	0	1151	0	0
3	A	105	0	138	0	0
3	B	70	0	92	0	0
3	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	6	0	0
4	B	20	0	30	0	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
4	E	4	0	6	0	0
5	A	14	0	0	0	0
6	A	12	0	26	0	0
7	A	5	0	0	0	0
7	B	5	0	0	1	0
7	C	5	0	0	0	0
8	B	6	0	8	0	0
8	C	6	0	8	0	0
9	C	30	0	43	0	0
10	C	14	0	27	0	0
11	C	14	0	30	0	0
12	A	63	0	0	0	0
12	B	43	0	0	0	0
12	C	55	0	0	0	0
12	D	7	0	0	0	0
12	E	5	0	0	0	0
All	All	26436	0	26796	50	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 1.

All (50) 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:C:901:VAL:O	1:C:904:VAL:HG12	2.03	0.58
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.86	0.57
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.87	0.55
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.90	0.53
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.93	0.51
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.27	0.50
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.94	0.50
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.50
1:A:456:MET:SD	1:A:932:LEU:HD13	2.52	0.49
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.96	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.95	0.47
1:C:330:THR:N	1:C:331:PRO:CD	2.77	0.47
1:B:330:THR:N	1:B:331:PRO:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.96	0.47
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.96	0.46
1:B:897:ILE:N	1:B:898:PRO:CD	2.79	0.46
1:A:356:TYR:HA	1:A:365:THR:HG21	1.97	0.45
1:A:1037:ASN:O	1:A:1038:GLU:HB3	2.16	0.44
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.99	0.44
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.44
1:A:897:ILE:N	1:A:898:PRO:CD	2.81	0.43
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:B:399:VAL:O	1:B:402:ILE:HG22	2.18	0.43
1:B:367:ILE:HB	1:B:368:PRO:HD3	2.00	0.43
1:A:987:MET:N	1:A:988:PRO:CD	2.81	0.43
1:B:400:LEU:HD21	1:B:1003:VAL:HG13	2.01	0.43
1:A:330:THR:N	1:A:331:PRO:CD	2.82	0.43
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.54	0.42
1:B:404:LEU:HD12	1:B:404:LEU:N	2.34	0.42
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.18	0.42
1:A:336:SER:O	1:A:340:VAL:HG23	2.19	0.42
1:A:1035:ARG:HB3	1:A:1036:LYS:HE3	2.01	0.42
1:C:314:GLU:N	1:C:315:PRO:CD	2.83	0.42
1:A:873:ALA:N	1:A:874:PRO:CD	2.83	0.42
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.55	0.42
1:C:362:PHE:CE2	1:C:366:LEU:HD11	2.54	0.42
1:A:1038:GLU:O	1:A:1039:ASP:HB2	2.21	0.41
1:B:362:PHE:N	7:B:1304:SO4:O4	2.53	0.41
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.20	0.41
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.02	0.41
1:C:40:PRO:HB2	1:C:94:PHE:O	2.21	0.41
1:A:679:GLY:HA2	1:A:830:GLN:HA	2.02	0.41
1:C:1:MET:HB3	1:C:2:PRO:HD3	2.02	0.41
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.55	0.41
1:B:314:GLU:N	1:B:315:PRO:CD	2.83	0.41
1:A:777:ALA:O	1:A:781:MET:HG2	2.21	0.40
1:B:897:ILE:N	1:B:898:PRO:HD2	2.37	0.40
1:B:47:ALA:HB3	1:B:88:VAL:HG13	2.02	0.40
1:B:453:PHE:O	1:B:456:MET:HB3	2.22	0.40
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.84	0.40

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	1030/1057 (97%)	991 (96%)	36 (4%)	3 (0%)	41 72
1	B	1032/1057 (98%)	1013 (98%)	18 (2%)	1 (0%)	51 81
1	C	1031/1057 (98%)	1001 (97%)	30 (3%)	0	100 100
2	D	153/169 (90%)	148 (97%)	5 (3%)	0	100 100
2	E	152/169 (90%)	143 (94%)	7 (5%)	2 (1%)	12 36
All	All	3398/3509 (97%)	3296 (97%)	96 (3%)	6 (0%)	47 78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1038	GLU
1	A	867	ARG
1	A	538	THR
1	B	777	ALA
2	E	14	LEU
2	E	72	ASP

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	843/862 (98%)	828 (98%)	15 (2%)	59 86
1	B	839/862 (97%)	825 (98%)	14 (2%)	60 87
1	C	838/862 (97%)	827 (99%)	11 (1%)	69 91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	120/132 (91%)	120 (100%)	0	100 100
2	E	119/132 (90%)	117 (98%)	2 (2%)	60 87
All	All	2759/2850 (97%)	2717 (98%)	42 (2%)	65 89

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	130	GLU
1	A	359	LEU
1	A	407	ASP
1	A	512	PHE
1	A	673	GLU
1	A	674	LEU
1	A	717	ARG
1	A	801	PHE
1	A	835	LYS
1	A	904	VAL
1	A	1035	ARG
1	A	1036	LYS
1	A	1038	GLU
1	B	11	PHE
1	B	49	TYR
1	B	70	ASN
1	B	88	VAL
1	B	174	ASP
1	B	498	LYS
1	B	519	MET
1	B	544	LEU
1	B	610	PHE
1	B	717	ARG
1	B	801	PHE
1	B	955	LYS
1	B	987	MET
1	B	1030	ARG
1	C	11	PHE
1	C	49	TYR
1	C	252	LYS
1	C	274	ASN
1	C	544	LEU

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Mol	Chain	Res	Type
1	C	546	LEU
1	C	589	LYS
1	C	919	ARG
1	C	1008	MET
1	C	1011	MET
1	C	1032	ARG
2	E	14	LEU
2	E	17	LYS

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)

27 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	$\#\|Z\| > 2$
8	GOL	B	1305	-	5,5,5	0.09	0	5,5,5	0.25	0
4	EDO	C	1607	-	3,3,3	0.06	0	2,2,2	0.22	0
11	C14	C	1605	-	13,13,13	0.08	0	12,12,12	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LMT	A	1101	-	36,36,36	0.53	1 (2%)	47,47,47	1.22	2 (4%)
4	EDO	A	1103	-	3,3,3	0.05	0	2,2,2	0.15	0
10	DDQ	C	1604	-	10,13,13	0.13	0	12,15,15	0.19	0
4	EDO	B	1309	-	3,3,3	0.06	0	2,2,2	0.16	0
3	LMT	A	1106	-	36,36,36	0.51	1 (2%)	47,47,47	0.78	1 (2%)
4	EDO	E	201	-	3,3,3	0.09	0	2,2,2	0.27	0
4	EDO	B	1307	-	3,3,3	0.06	0	2,2,2	0.22	0
6	D12	A	1105	-	11,11,11	0.09	0	10,10,10	0.07	0
4	EDO	C	1601	-	3,3,3	0.06	0	2,2,2	0.19	0
3	LMT	B	1302	-	36,36,36	0.47	0	47,47,47	0.59	0
4	EDO	D	202	-	3,3,3	0.06	0	2,2,2	0.18	0
5	1KE	A	1104	-	15,15,15	2.30	2 (13%)	16,20,20	1.63	3 (18%)
7	SO4	A	1107	-	4,4,4	0.38	0	6,6,6	0.05	0
7	SO4	C	1608	-	4,4,4	0.40	0	6,6,6	0.05	0
4	EDO	D	201	-	3,3,3	0.06	0	2,2,2	0.20	0
4	EDO	B	1308	-	3,3,3	0.06	0	2,2,2	0.17	0
8	GOL	C	1606	-	5,5,5	0.09	0	5,5,5	0.26	0
4	EDO	B	1306	-	3,3,3	0.07	0	2,2,2	0.24	0
7	SO4	B	1304	-	4,4,4	0.40	0	6,6,6	0.04	0
4	EDO	B	1301	-	3,3,3	0.05	0	2,2,2	0.15	0
3	LMT	B	1303	-	36,36,36	0.45	0	47,47,47	0.58	0
3	LMT	C	1603	-	36,36,36	0.44	0	47,47,47	0.55	0
3	LMT	A	1102	-	36,36,36	0.47	0	47,47,47	0.61	0
9	LPX	C	1602	-	29,29,29	0.29	0	31,33,33	0.35	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
8	GOL	B	1305	-	-	2/4/4/4	-
4	EDO	C	1607	-	-	1/1/1/1	-
11	C14	C	1605	-	-	6/11/11/11	-
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
4	EDO	A	1103	-	-	0/1/1/1	-
10	DDQ	C	1604	-	-	4/11/11/11	-
4	EDO	B	1309	-	-	0/1/1/1	-
3	LMT	A	1106	-	-	9/21/61/61	0/2/2/2
4	EDO	E	201	-	-	1/1/1/1	-
4	EDO	B	1307	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D12	A	1105	-	-	3/9/9/9	-
4	EDO	C	1601	-	-	1/1/1/1	-
3	LMT	B	1302	-	-	9/21/61/61	0/2/2/2
4	EDO	D	202	-	-	0/1/1/1	-
5	1KE	A	1104	-	-	2/4/12/12	0/2/2/2
4	EDO	D	201	-	-	0/1/1/1	-
4	EDO	B	1308	-	-	1/1/1/1	-
8	GOL	C	1606	-	-	2/4/4/4	-
4	EDO	B	1306	-	-	1/1/1/1	-
4	EDO	B	1301	-	-	0/1/1/1	-
3	LMT	B	1303	-	-	11/21/61/61	0/2/2/2
3	LMT	C	1603	-	-	6/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	10/21/61/61	0/2/2/2
9	LPX	C	1602	-	-	14/31/31/31	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1104	1KE	C9-C8	8.10	1.49	1.39
5	A	1104	1KE	C9-CL1	2.71	1.80	1.73
3	A	1101	LMT	O1'-C1'	2.39	1.44	1.40
3	A	1106	LMT	O1'-C1'	2.19	1.43	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	LMT	O1'-C1'-C2'	5.28	116.55	108.30
5	A	1104	1KE	C4-N3-C2	4.99	122.54	111.52
3	A	1101	LMT	C1-O1'-C1'	4.72	121.67	113.84
5	A	1104	1KE	C9-C8-N13	-2.79	118.41	122.91
5	A	1104	1KE	C12-N13-C8	2.24	122.28	115.17
3	A	1106	LMT	O1'-C1'-C2'	2.16	111.67	108.30

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1106	LMT	O5'-C1'-O1'-C1
3	A	1106	LMT	C2-C1-O1'-C1'
3	B	1303	LMT	C2'-C1'-O1'-C1
3	B	1303	LMT	O5'-C1'-O1'-C1
3	B	1303	LMT	C2-C1-O1'-C1'
5	A	1104	1KE	C9-C8-N3-C4
5	A	1104	1KE	N13-C8-N3-C4
8	B	1305	GOL	O1-C1-C2-C3
9	C	1602	LPX	C3-O1-P1-O3
9	C	1602	LPX	C3-O1-P1-O2
9	C	1602	LPX	C3-O1-P1-O4
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C5'-C4'-O1B-C1B
3	B	1302	LMT	O5B-C1B-O1B-C4'
3	B	1303	LMT	O5'-C5'-C6'-O6'
3	B	1302	LMT	C2B-C1B-O1B-C4'
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	A	1106	LMT	O5'-C5'-C6'-O6'
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C4B-C5B-C6B-O6B
8	C	1606	GOL	O1-C1-C2-O2
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	B	1303	LMT	C4'-C5'-C6'-O6'
3	C	1603	LMT	O1'-C1-C2-C3
9	C	1602	LPX	C7-C6-O6-C5
3	A	1102	LMT	C11-C10-C9-C8
3	B	1303	LMT	C6-C7-C8-C9
9	C	1602	LPX	C9-C10-C11-C12
9	C	1602	LPX	C7-C8-C9-C10
9	C	1602	LPX	O7-C6-O6-C5
8	C	1606	GOL	O1-C1-C2-C3
3	C	1603	LMT	C5-C6-C7-C8
3	A	1101	LMT	C2-C3-C4-C5
3	B	1303	LMT	C11-C10-C9-C8
3	B	1303	LMT	O5B-C1B-O1B-C4'
10	C	1604	DDQ	C3-C4-C5-C6
8	B	1305	GOL	O1-C1-C2-O2
10	C	1604	DDQ	C6-C7-C8-C9
3	B	1302	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
4	E	201	EDO	O1-C1-C2-O2
3	B	1302	LMT	C4-C5-C6-C7
6	A	1105	D12	C2-C3-C4-C5
3	B	1303	LMT	C2B-C1B-O1B-C4'
3	C	1603	LMT	C1-C2-C3-C4
3	B	1303	LMT	C3-C4-C5-C6
3	A	1101	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C6-C7-C8-C9
3	A	1106	LMT	C2-C3-C4-C5
3	A	1106	LMT	C2'-C1'-O1'-C1
9	C	1602	LPX	C1-O2-P1-O1
3	A	1101	LMT	C11-C10-C9-C8
3	C	1603	LMT	C7-C8-C9-C10
3	A	1102	LMT	C2-C3-C4-C5
3	A	1106	LMT	C5-C6-C7-C8
3	B	1302	LMT	O5B-C5B-C6B-O6B
3	B	1302	LMT	C9-C10-C11-C12
6	A	1105	D12	C3-C4-C5-C6
10	C	1604	DDQ	C1-C2-C3-C4
4	B	1306	EDO	O1-C1-C2-O2
3	B	1302	LMT	C3-C4-C5-C6
9	C	1602	LPX	C14-C15-C16-C17
11	C	1605	C14	C08-C09-C10-C11
3	A	1101	LMT	C9-C10-C11-C12
9	C	1602	LPX	C11-C12-C13-C14
3	A	1102	LMT	C3-C4-C5-C6
3	A	1106	LMT	C6-C7-C8-C9
9	C	1602	LPX	C10-C11-C12-C13
11	C	1605	C14	C06-C07-C08-C09
9	C	1602	LPX	C4-C3-O1-P1
9	C	1602	LPX	C1-O2-P1-O3
3	A	1102	LMT	C3'-C4'-O1B-C1B
3	A	1106	LMT	C4'-C5'-C6'-O6'
11	C	1605	C14	C02-C03-C04-C05
3	C	1603	LMT	C9-C10-C11-C12
3	B	1302	LMT	C2-C3-C4-C5
9	C	1602	LPX	C16-C17-C18-C19
3	B	1303	LMT	O1'-C1-C2-C3
4	B	1308	EDO	O1-C1-C2-O2
11	C	1605	C14	C10-C11-C12-C13
3	A	1106	LMT	C3-C4-C5-C6
11	C	1605	C14	C05-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
3	C	1603	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C5-C6-C7-C8
4	C	1607	EDO	O1-C1-C2-O2
10	C	1604	DDQ	C2-C1-N1-CM1
6	A	1105	D12	C4-C5-C6-C7
11	C	1605	C14	C04-C05-C06-C07
3	A	1102	LMT	C7-C8-C9-C10
4	C	1601	EDO	O1-C1-C2-O2
3	B	1302	LMT	C2-C1-O1'-C1'

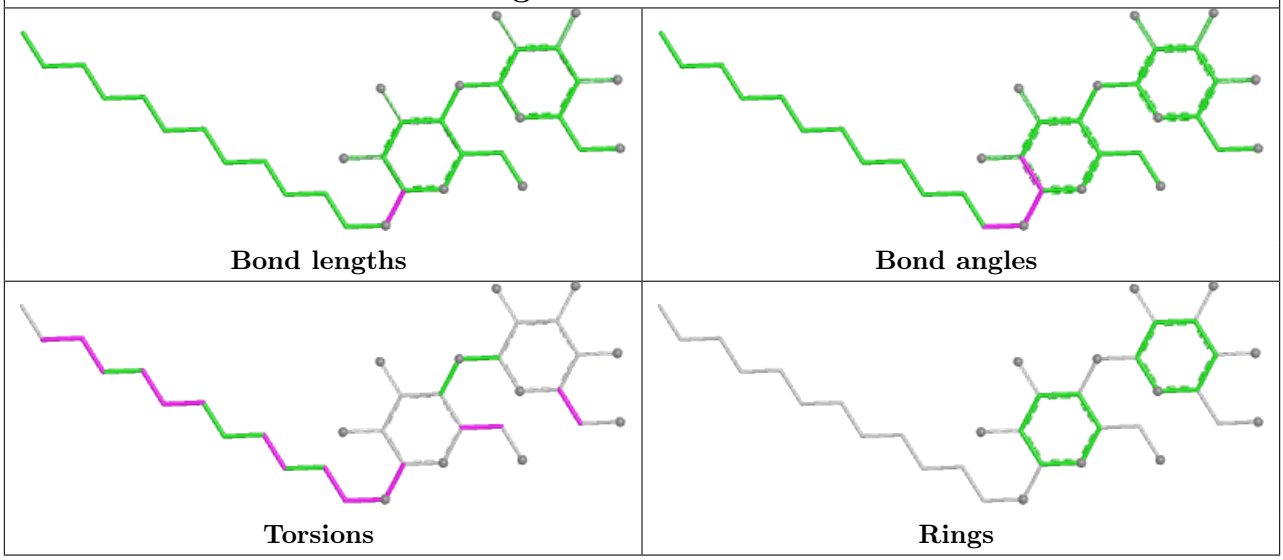
There are no ring outliers.

1 monomer is involved in 1 short contact:

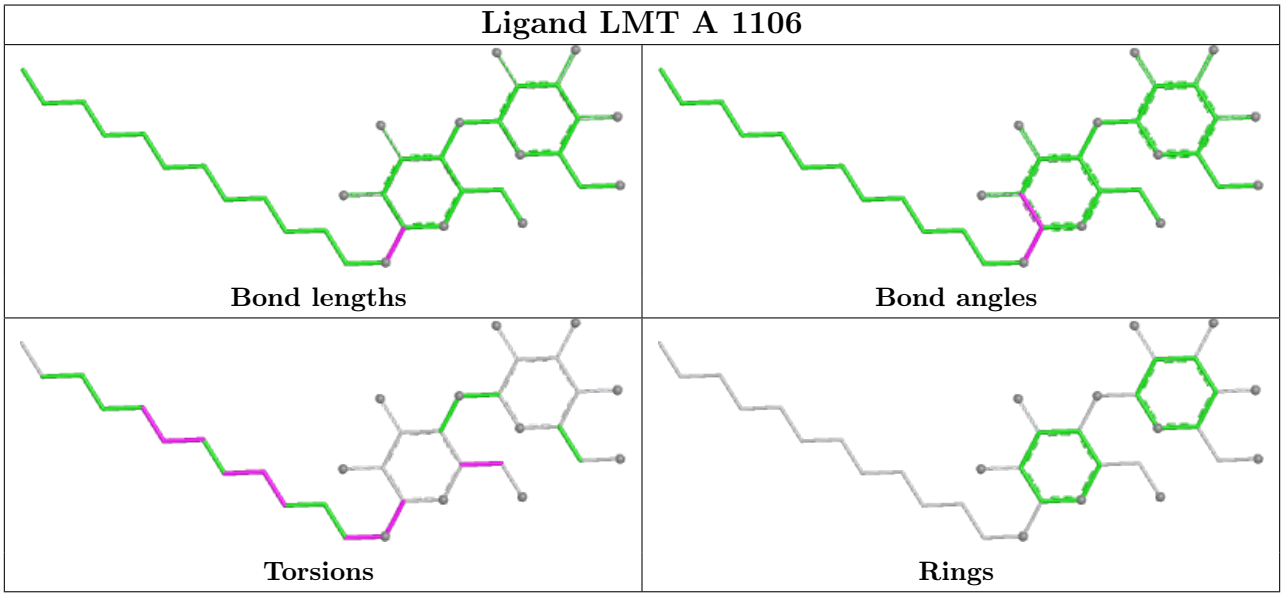
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1304	SO4	1	0

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 then 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.

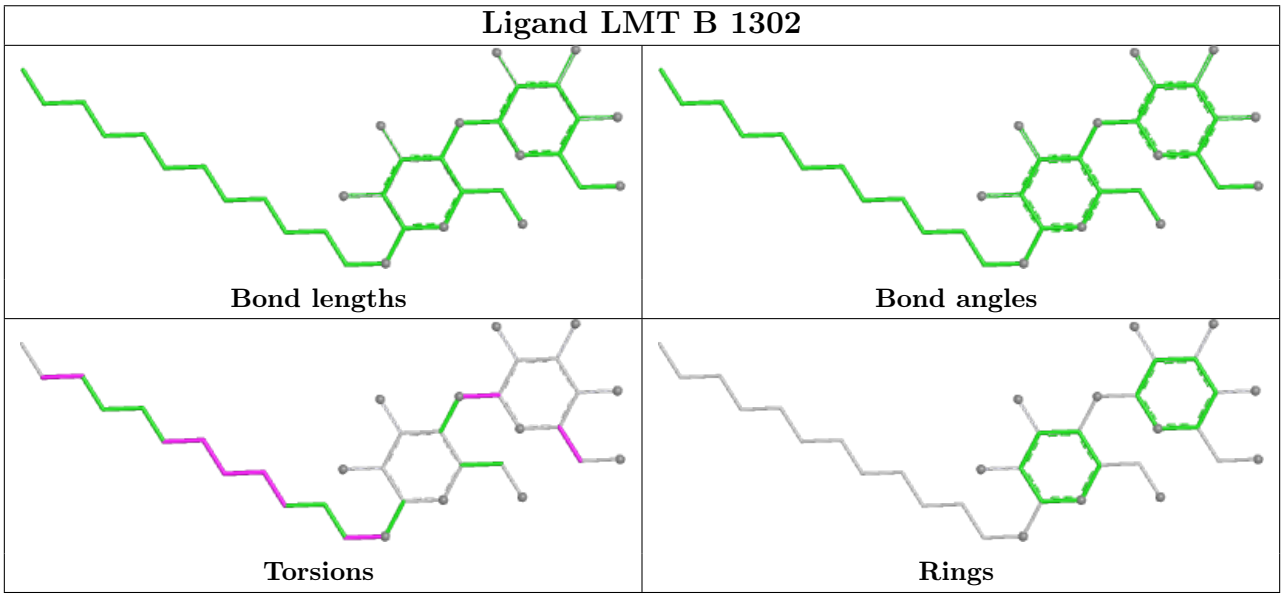
Ligand LMT A 1101



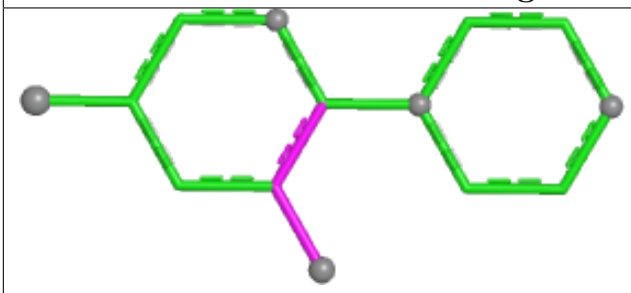
Ligand LMT A 1106



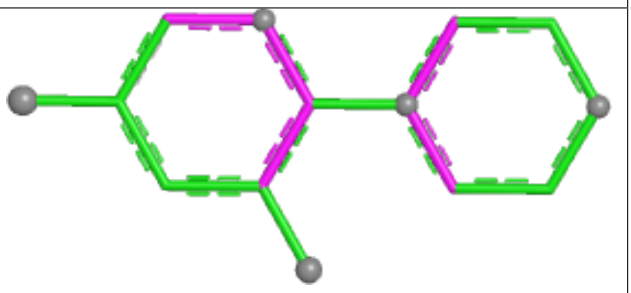
Ligand LMT B 1302



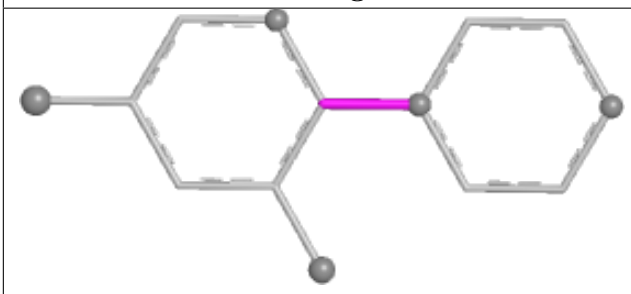
Ligand 1KE A 1104



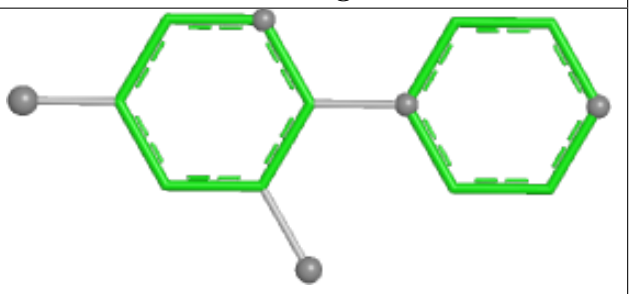
Bond lengths



Bond angles

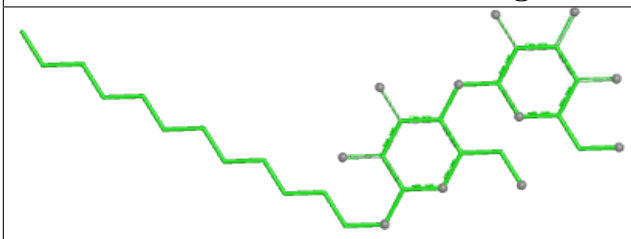


Torsions

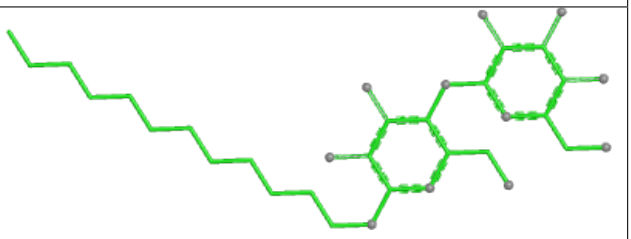


Rings

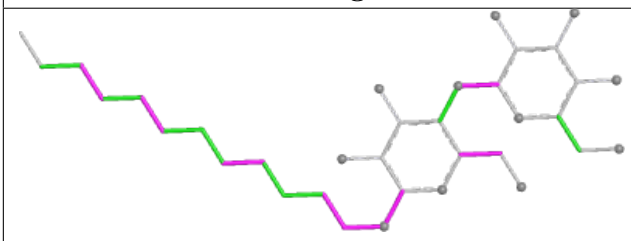
Ligand LMT B 1303



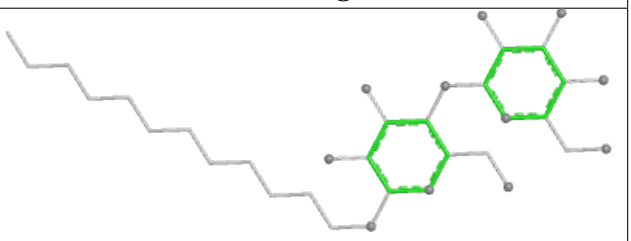
Bond lengths



Bond angles

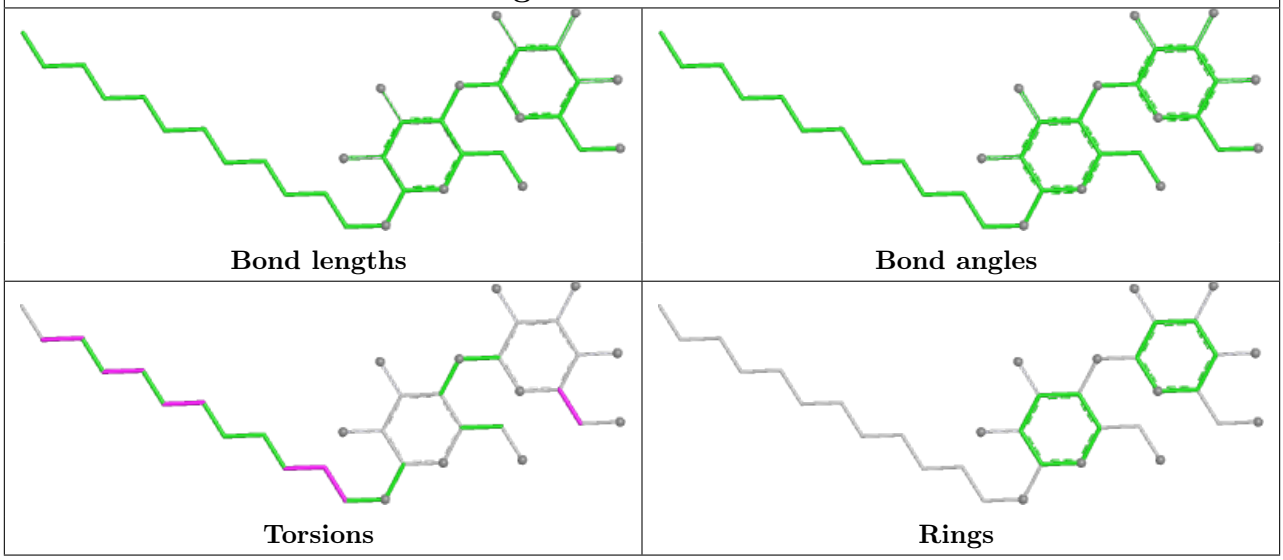


Torsions

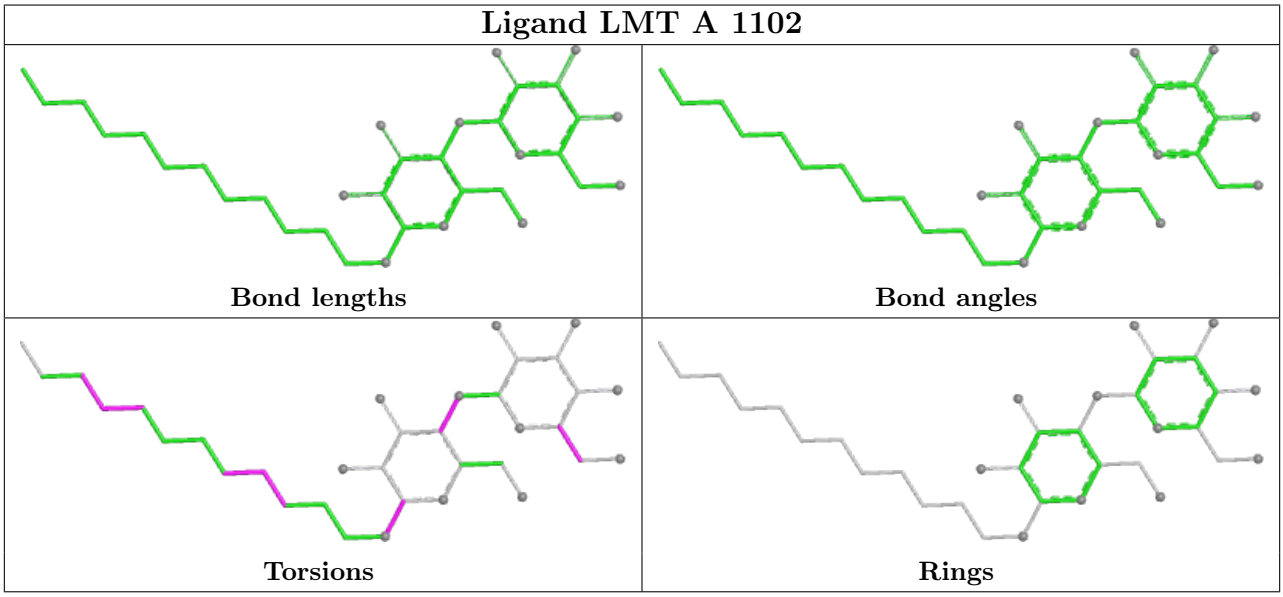


Rings

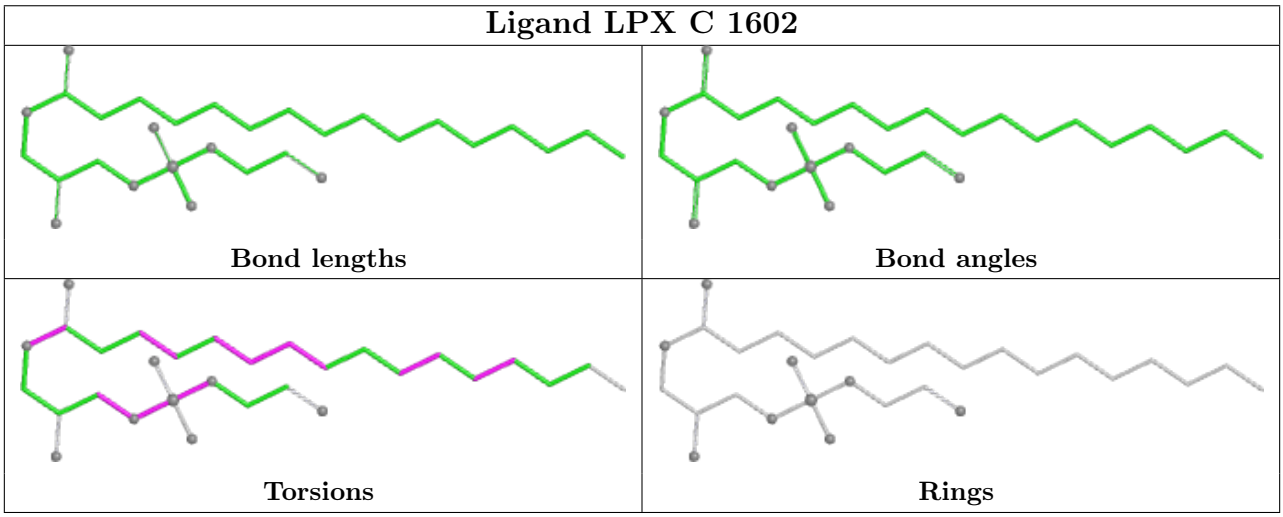
Ligand LMT C 1603



Ligand LMT A 1102



Ligand LPX C 1602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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	1032/1057 (97%)	0.36	63 (6%)	21	13	41, 63, 111, 129	0
1	B	1034/1057 (97%)	0.21	50 (4%)	30	21	42, 63, 79, 91	0
1	C	1033/1057 (97%)	0.08	28 (2%)	54	44	40, 51, 71, 81	0
2	D	155/169 (91%)	0.36	12 (7%)	13	7	49, 59, 73, 81	0
2	E	154/169 (91%)	1.05	37 (24%)	0	0	53, 69, 88, 95	0
All	All	3408/3509 (97%)	0.26	190 (5%)	24	16	40, 59, 90, 129	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1037	ASN	7.9
1	A	713	LEU	6.5
2	E	66	LEU	5.5
1	A	712	MET	5.2
2	E	34	MET	5.0
2	E	68	LYS	5.0
1	A	833	PRO	4.9
1	A	421	ALA	4.8
2	E	36	ASN	4.8
1	A	423	GLU	4.7
1	A	678	THR	4.7
1	A	869	SER	4.6
1	C	497	LEU	4.6
2	E	35	ALA	4.5
1	A	711	ASP	4.5
2	E	64	GLU	4.5
1	A	716	VAL	4.5
2	E	67	LEU	4.4
1	B	574	THR	4.3
1	A	868	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	835	LYS	4.0
1	B	655	PHE	4.0
2	E	31	ARG	4.0
2	D	126	LEU	4.0
1	A	965	LEU	3.9
1	A	834	GLY	3.9
2	E	99	LEU	3.8
1	C	362	PHE	3.8
1	C	513	PHE	3.8
2	E	60	LEU	3.7
1	B	599	LEU	3.7
1	B	600	THR	3.7
2	E	28	ASP	3.7
2	E	69	ASN	3.6
1	C	425	LEU	3.6
1	B	508	GLY	3.6
2	E	32	ILE	3.5
1	B	657	GLN	3.5
1	A	515	TRP	3.5
1	B	284	GLN	3.5
1	A	429	GLU	3.4
1	C	498	LYS	3.4
1	B	597	TYR	3.3
1	B	641	GLU	3.3
2	E	33	LEU	3.3
2	E	27	ASP	3.3
2	D	164	ILE	3.2
1	A	1041	GLU	3.2
1	A	831	ALA	3.2
1	B	705	GLU	3.2
1	A	709	HIS	3.2
2	D	165	LEU	3.2
2	E	30	VAL	3.2
1	A	255	GLN	3.2
1	A	710	PRO	3.2
1	C	427	PRO	3.2
1	C	804	PHE	3.2
1	B	607	GLU	3.2
1	B	629	VAL	3.1
2	E	70	GLY	3.1
1	C	499	PRO	3.1
2	E	101	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	422	GLU	3.1
1	A	704	ALA	3.1
1	B	635	ALA	3.0
1	A	432	ARG	3.0
1	B	606	VAL	3.0
1	A	838	GLY	3.0
1	A	525	HIS	3.0
1	B	595	THR	3.0
1	B	575	MET	3.0
1	C	739	LEU	3.0
1	B	407	ASP	2.9
1	A	554	TYR	2.9
1	C	807	SER	2.9
2	D	139	VAL	2.9
1	A	425	LEU	2.9
2	D	163	GLU	2.9
2	D	129	VAL	2.9
1	A	431	THR	2.8
1	B	558	ARG	2.8
2	E	159	GLU	2.8
1	C	512	PHE	2.8
2	E	102	ASN	2.8
2	E	148	THR	2.8
1	B	617	PHE	2.8
2	D	150	PHE	2.8
2	E	97	GLU	2.8
1	C	421	ALA	2.8
1	B	255	GLN	2.8
1	B	640	GLU	2.8
2	D	161	LEU	2.8
1	C	511	GLY	2.7
1	A	836	SER	2.7
2	E	73	VAL	2.7
1	A	424	GLY	2.7
1	A	679	GLY	2.7
1	C	426	PRO	2.7
2	E	62	ILE	2.7
1	B	554	TYR	2.7
1	B	658	ILE	2.7
1	B	543	VAL	2.7
1	C	510	LYS	2.7
1	C	811	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	596	HIS	2.7
1	C	700	ASN	2.6
1	A	677	ALA	2.6
1	B	833	PRO	2.6
1	C	701	GLN	2.6
1	B	603	LYS	2.6
1	A	426	PRO	2.6
1	C	707	ALA	2.6
1	A	842	GLU	2.6
1	C	500	ILE	2.6
1	B	708	LYS	2.6
1	C	809	TRP	2.6
1	A	11	PHE	2.6
1	A	707	ALA	2.6
2	E	95	ILE	2.5
1	A	519	MET	2.5
2	D	160	ASP	2.5
1	A	459	PHE	2.5
1	B	636	ASP	2.5
1	A	866	GLU	2.5
1	C	496	MET	2.5
2	D	166	GLN	2.5
1	B	604	ASN	2.5
1	B	633	ASP	2.5
1	A	13	TRP	2.5
1	B	895	TRP	2.5
2	D	159	GLU	2.4
1	C	423	GLU	2.4
1	B	940	LYS	2.4
1	B	403	GLY	2.4
2	E	150	PHE	2.4
1	A	556	PHE	2.4
1	A	533	GLY	2.4
2	E	38	ALA	2.4
2	E	37	GLY	2.3
1	A	846	GLN	2.3
1	C	153	ASP	2.3
1	C	501	ALA	2.3
1	B	134	SER	2.3
2	E	154	ILE	2.3
1	B	601	LYS	2.3
1	B	631	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	165	LEU	2.3
2	E	63	VAL	2.3
2	E	153	SER	2.3
1	A	708	LYS	2.3
1	B	352	PHE	2.3
1	A	518	ARG	2.3
1	C	494	ALA	2.3
1	B	561	SER	2.2
1	A	430	ALA	2.2
1	B	366	LEU	2.2
1	A	673	GLU	2.2
1	A	867	ARG	2.2
1	C	850	LYS	2.2
2	E	61	GLU	2.2
1	A	420	MET	2.2
1	A	446	ALA	2.2
1	A	521	GLU	2.2
1	B	195	LYS	2.2
2	E	152	ILE	2.1
2	E	29	GLU	2.1
1	A	488	LEU	2.1
1	B	836	SER	2.1
1	B	563	PHE	2.1
1	A	517	ASN	2.1
1	B	663	VAL	2.1
1	A	528	THR	2.1
1	B	653	ARG	2.1
1	B	598	TYR	2.1
1	A	522	LYS	2.1
1	B	404	LEU	2.1
1	A	657	GLN	2.1
1	A	10	ILE	2.1
1	B	638	PRO	2.1
1	A	542	LEU	2.1
1	A	859	TRP	2.1
1	C	120	GLN	2.1
2	D	140	ASN	2.1
1	A	558	ARG	2.0
2	E	65	VAL	2.0
1	A	918	PHE	2.0
1	B	642	ASN	2.0
2	E	51	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	673	GLU	2.0
1	A	196	PHE	2.0

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 (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^{th} 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
3	LMT	A	1102	35/35	0.78	0.25	75,90,95,97	0
10	DDQ	C	1604	14/14	0.80	0.27	64,71,75,76	0
7	SO4	A	1107	5/5	0.81	0.26	107,107,107,108	0
3	LMT	B	1302	35/35	0.82	0.38	67,70,73,74	0
9	LPX	C	1602	30/30	0.82	0.40	63,75,81,82	0
6	D12	A	1105	12/12	0.82	0.30	63,66,67,68	0
3	LMT	B	1303	35/35	0.83	0.44	82,87,91,92	0
4	EDO	B	1307	4/4	0.85	0.32	64,65,65,65	0
3	LMT	A	1106	35/35	0.86	0.34	69,73,78,81	0
8	GOL	B	1305	6/6	0.86	0.23	58,58,58,58	0
11	C14	C	1605	14/14	0.86	0.20	56,57,57,57	0
3	LMT	A	1101	35/35	0.87	0.25	61,64,69,71	0
3	LMT	C	1603	35/35	0.88	0.24	62,67,71,72	0
4	EDO	B	1309	4/4	0.88	0.19	58,58,58,58	0
4	EDO	D	202	4/4	0.88	0.25	64,65,65,65	0
4	EDO	E	201	4/4	0.89	0.22	63,64,64,66	0
4	EDO	B	1306	4/4	0.90	0.21	62,62,63,63	0
4	EDO	B	1301	4/4	0.91	0.23	54,54,54,55	0
4	EDO	B	1308	4/4	0.92	0.28	57,57,58,59	0
4	EDO	C	1607	4/4	0.92	0.20	57,58,58,59	0
4	EDO	A	1103	4/4	0.93	0.22	46,46,47,47	0

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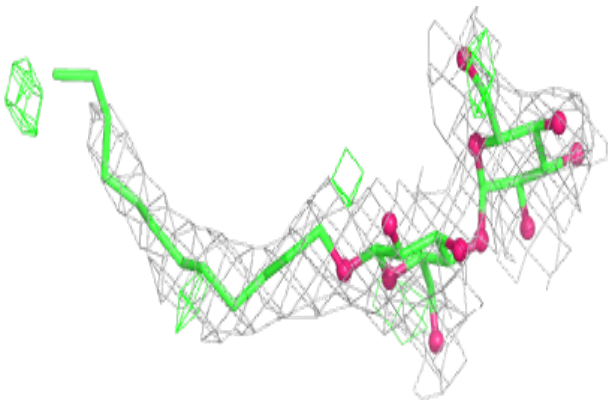
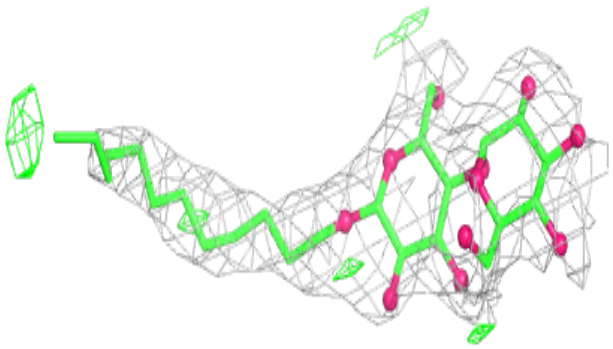
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	1KE	A	1104	14/14	0.93	0.20	87,93,97,101	0
8	GOL	C	1606	6/6	0.94	0.29	55,55,56,56	0
7	SO4	C	1608	5/5	0.94	0.18	80,80,80,80	0
4	EDO	D	201	4/4	0.95	0.18	63,63,64,64	0
4	EDO	C	1601	4/4	0.95	0.34	51,51,52,52	0
7	SO4	B	1304	5/5	0.96	0.26	90,91,92,92	0

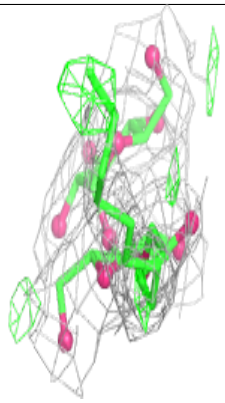
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

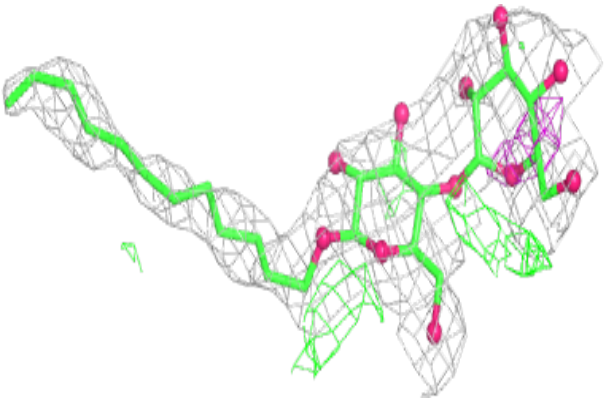


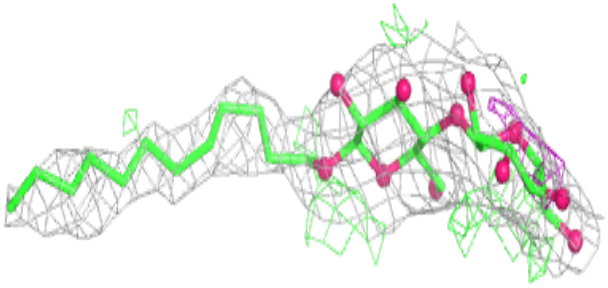


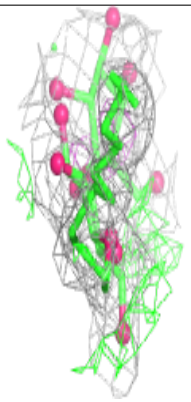


Electron density around LMT B 1302:

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

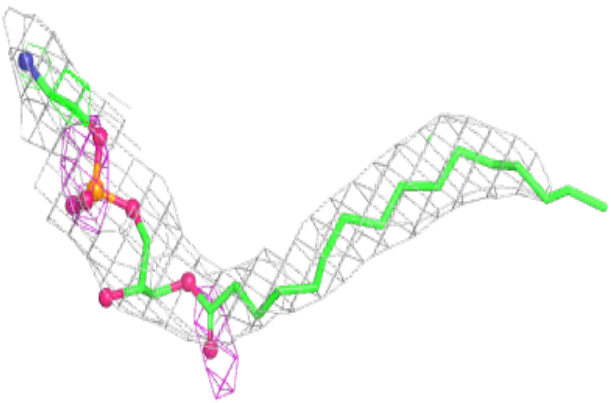


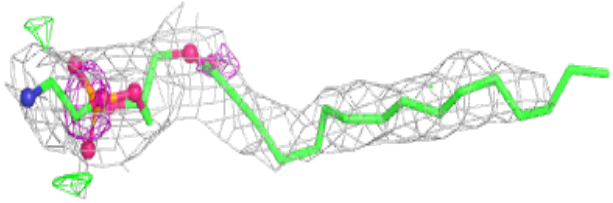


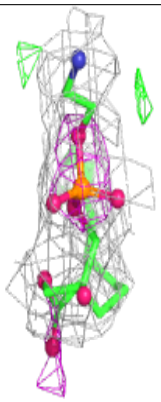


Electron density around LPX C 1602:

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

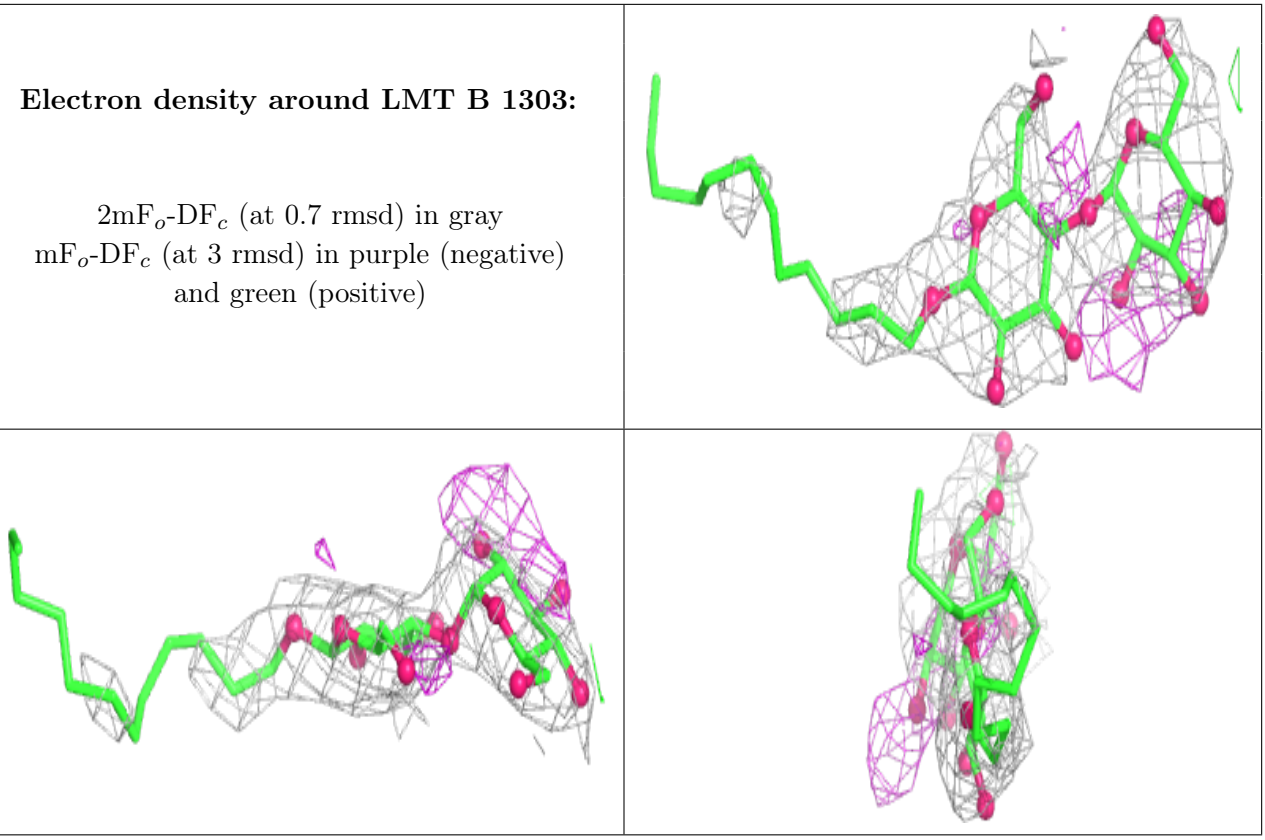






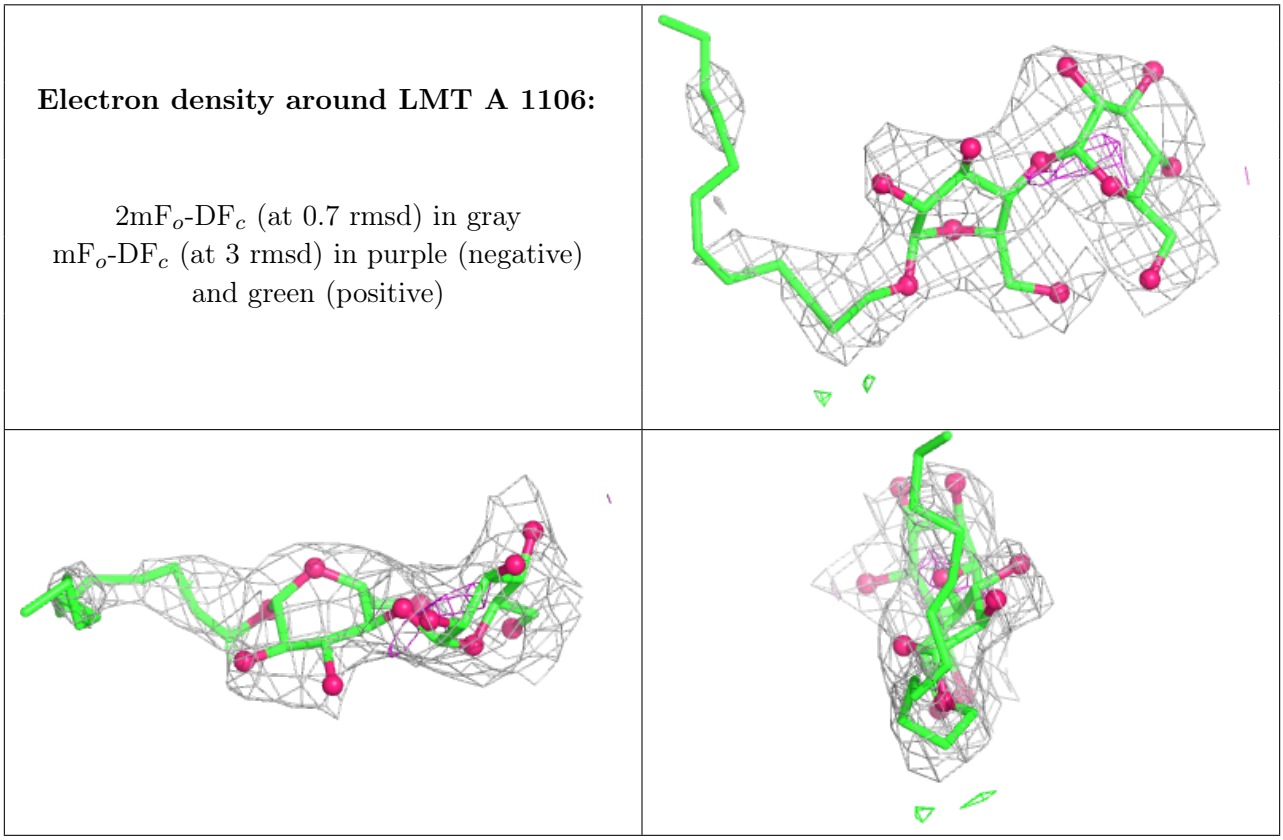
Electron density around LMT B 1303:

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



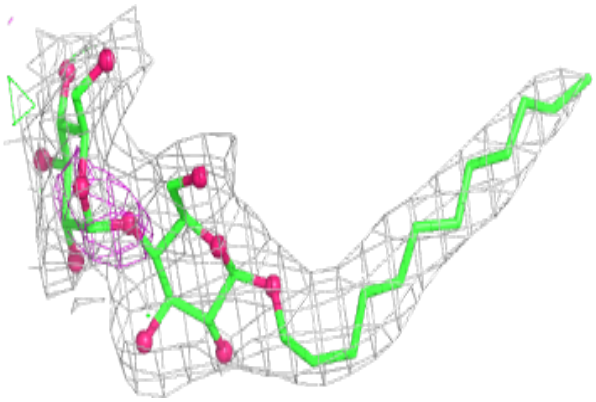
Electron density around LMT A 1106:

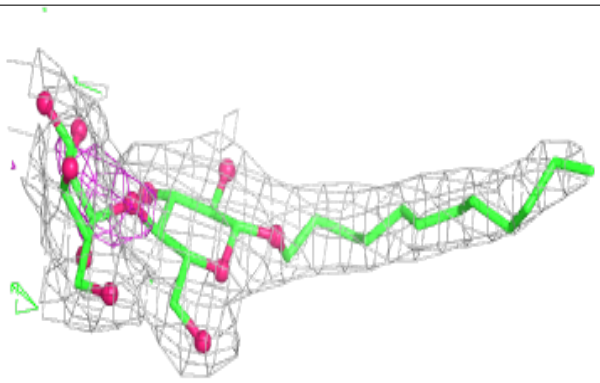
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

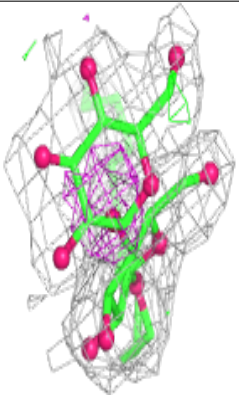


Electron density around LMT A 1101:

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

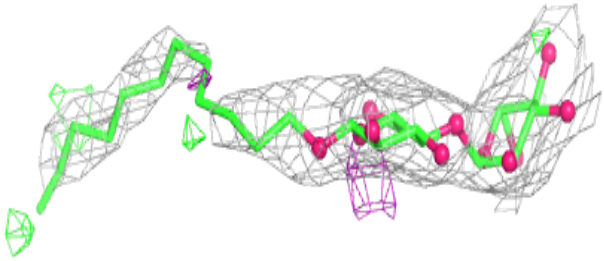


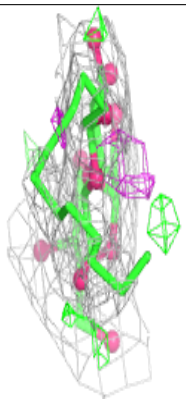




Electron density around LMT C 1603:

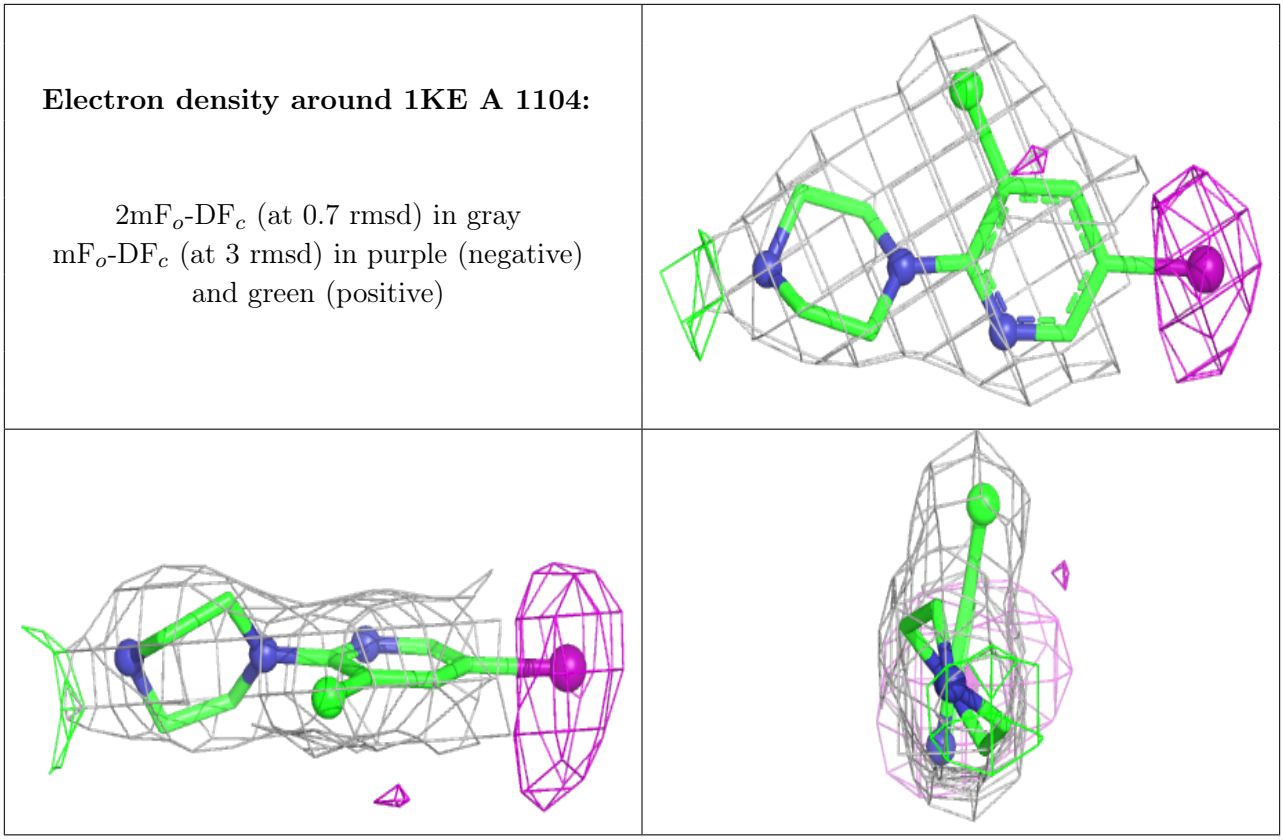
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around 1KE 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)



6.5 Other polymers

There are no such residues in this entry.