



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 07:03 PM UTC

PDB ID : 6ZOF / pdb_00006zof
Title : Fusidic acid binding to the TM7/TM8 groove of AcrB-F380A T protomer
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 3.30 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

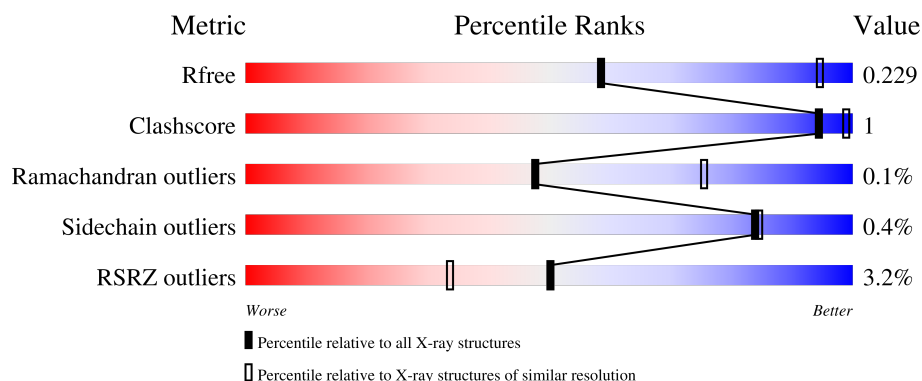
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	1057	4% 95% ..
1	B	1057	5% 93% 5% .
1	C	1057	2% 95% ..
2	D	169	% 92% 8%
2	E	169	2% 91% 9%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26308 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	1042	Total	C	N	O	S	0	0	0
			7921	5091	1311	1475	44			
1	B	1034	Total	C	N	O	S	0	0	0
			7849	5049	1296	1460	44			
1	C	1035	Total	C	N	O	S	0	0	0
			7860	5055	1300	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ALA	PHE	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	380	ALA	PHE	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	380	ALA	PHE	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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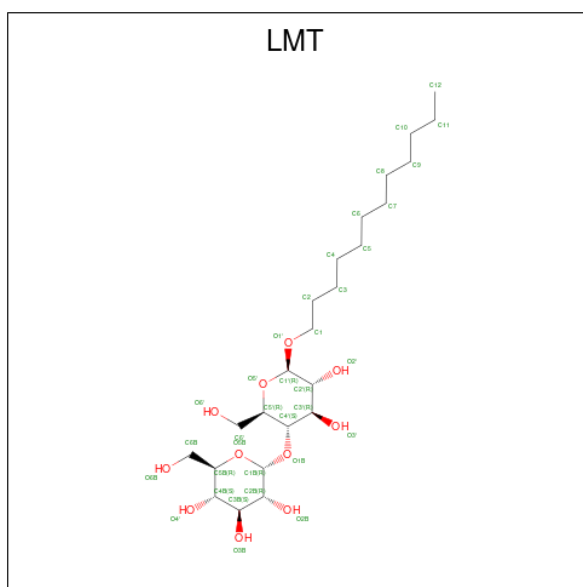
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

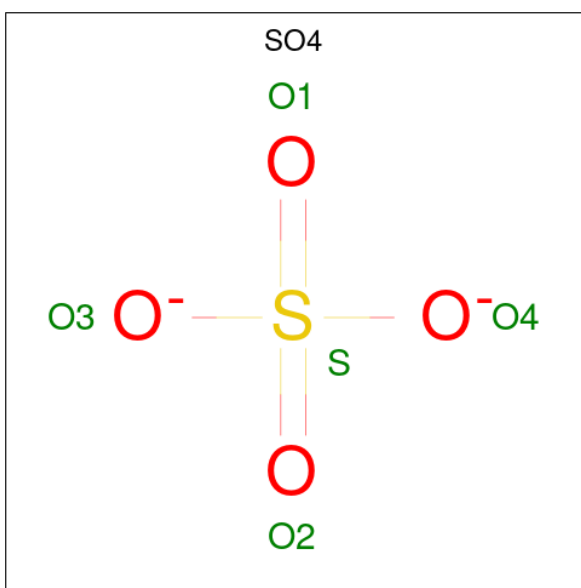
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	155	Total	C	N	O	S	0	0	0
			1173	739	205	228	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

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



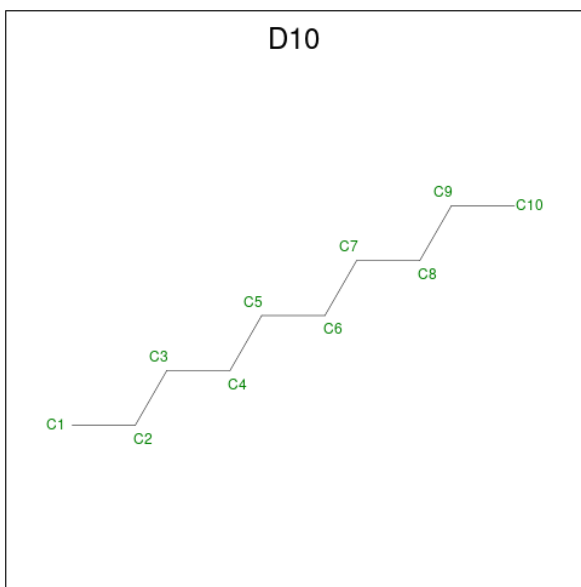
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



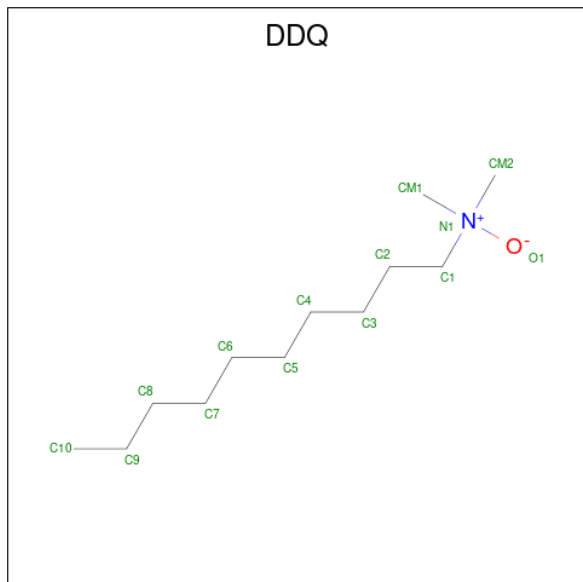
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



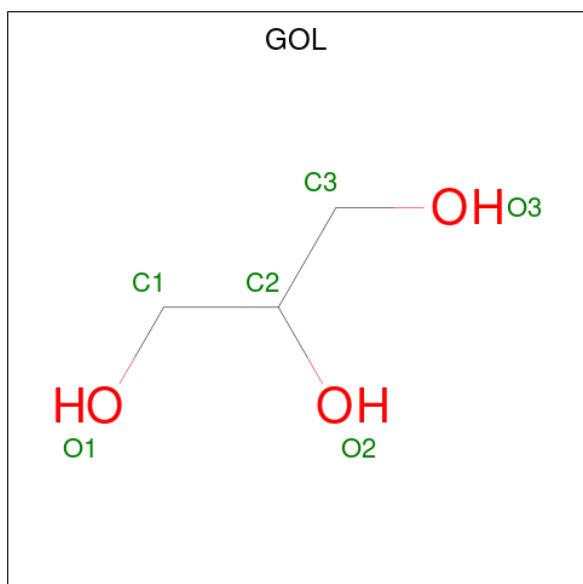
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	C	0	0
			10	10		

- Molecule 6 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



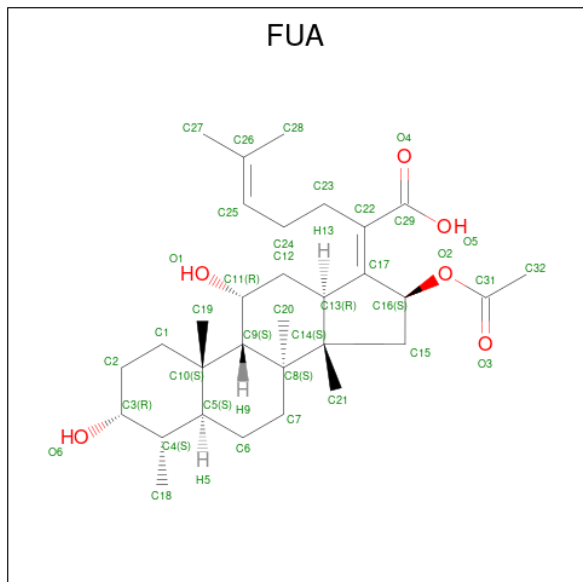
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



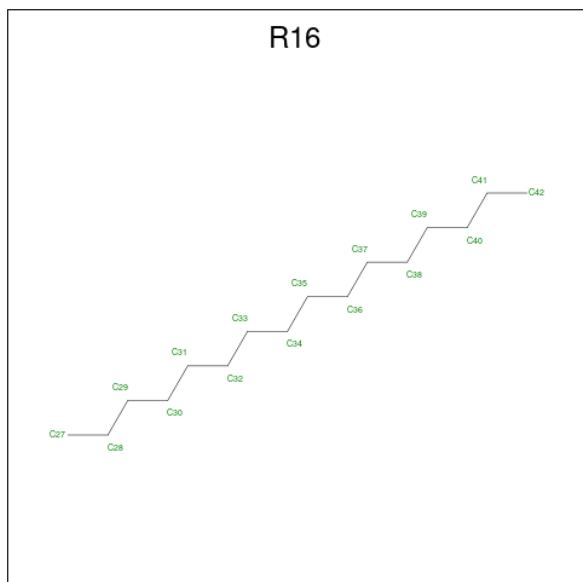
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



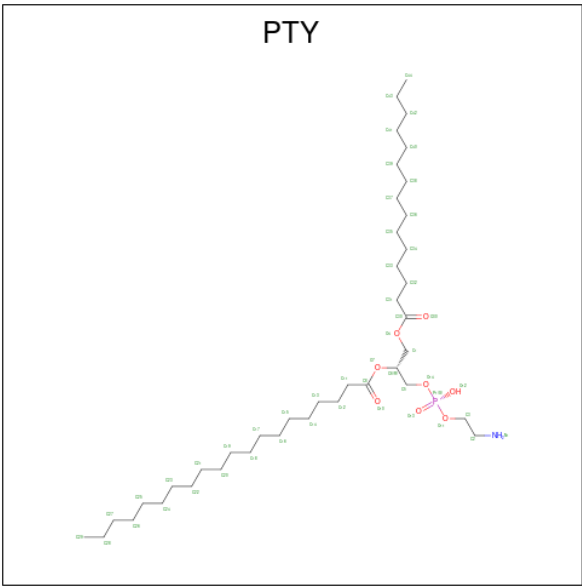
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C	O	0
			37	31	6	

- Molecule 9 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C		0
			16	16		

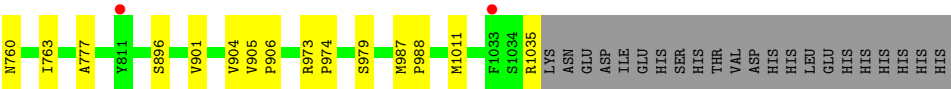
- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



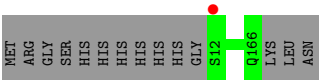
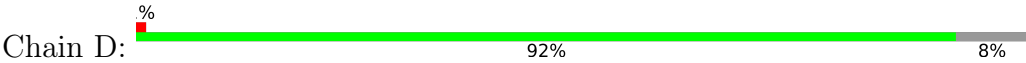
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 11 is water.

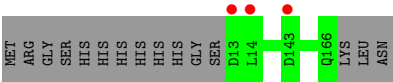
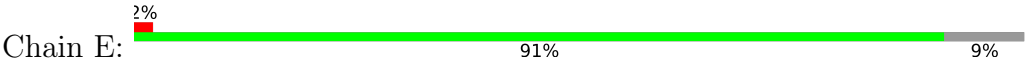
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	5	Total	O	0	0
			5	5		
11	B	9	Total	O	0	0
			9	9		
11	C	6	Total	O	0	0
			6	6		



• 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, α , β , γ	145.10Å 162.33Å 244.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 3.30 49.65 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.65-3.30) 99.9 (49.65-3.30)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.258 (Not available) , 0.229	Depositor DCC
R_{free} test set	4369 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	26308	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 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUA, LMT, R16, D10, SO4, GOL, DDQ, PTY

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	1.04	0/8071	1.57	2/10959 (0.0%)
1	B	1.04	0/7998	1.59	7/10862 (0.1%)
1	C	1.04	0/8009	1.57	4/10876 (0.0%)
2	D	1.03	0/1192	1.62	0/1621
2	E	1.03	0/1186	1.59	0/1613
All	All	1.04	0/26456	1.58	13/35931 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	7.31	124.85	120.24
1	A	896	SER	C-N-CA	7.31	124.85	120.24
1	B	896	SER	CA-C-N	7.29	124.83	120.24
1	B	896	SER	C-N-CA	7.29	124.83	120.24
1	B	179	GLY	CA-C-O	-6.08	117.93	122.37
1	B	1021	PHE	CA-C-N	5.64	123.79	120.24
1	B	1021	PHE	C-N-CA	5.64	123.79	120.24
1	C	126	GLY	CA-C-O	-5.62	118.35	122.23
1	B	126	GLY	CA-C-O	-5.51	118.43	122.23
1	C	896	SER	CA-C-N	5.46	124.70	120.33
1	C	896	SER	C-N-CA	5.46	124.70	120.33
1	B	756	GLY	CA-C-O	-5.13	118.14	122.29
1	C	691	GLY	CA-C-O	-5.07	118.22	122.33

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	7921	0	8068	18	0
1	B	7849	0	8002	28	0
1	C	7860	0	8015	17	0
2	D	1173	0	1156	0	0
2	E	1167	0	1151	0	0
3	A	70	0	92	0	0
3	B	70	0	92	0	0
3	C	35	0	46	0	0
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	B	10	0	22	1	0
6	B	14	0	27	0	0
7	B	6	0	8	2	0
8	B	37	0	47	7	0
9	B	16	0	34	1	0
10	C	50	0	79	1	0
11	A	5	0	0	0	0
11	B	9	0	0	0	0
11	C	6	0	0	0	0
All	All	26308	0	26839	69	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 (69) 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:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.65	0.77
1:C:38:ILE:HD11	1:C:671:ILE:HD12	1.72	0.72
8:B:1104:FUA:H232	8:B:1104:FUA:H122	1.73	0.70
8:B:1104:FUA:H202	8:B:1104:FUA:H5	1.76	0.67
9:B:1105:R16:H382	9:B:1105:R16:H341	1.80	0.64
8:B:1104:FUA:O2	8:B:1104:FUA:H211	2.02	0.60
1:C:1035:ARG:NH2	10:C:1101:PTY:O13	2.37	0.58
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:LEU:HD12	1:A:402:ILE:HD11	1.87	0.57
8:B:1104:FUA:H232	8:B:1104:FUA:C12	2.34	0.56
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.87	0.55
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.89	0.55
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.90	0.54
1:C:38:ILE:HD11	1:C:671:ILE:CD1	2.39	0.52
1:C:979:SER:HA	1:C:1011:MET:HE3	1.93	0.51
1:A:435:MET:O	1:A:439:GLN:HB2	2.11	0.50
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.36	0.50
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.94	0.49
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.95	0.49
1:B:902:MET:HA	8:B:1104:FUA:H273	1.95	0.48
1:B:29:LYS:O	5:B:1101:D10:H101	2.13	0.48
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.95	0.48
8:B:1104:FUA:O4	8:B:1104:FUA:H16	2.14	0.48
7:B:1103:GOL:O3	7:B:1103:GOL:O1	2.21	0.47
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.96	0.47
1:B:677:ALA:O	1:B:678:THR:OG1	2.26	0.47
1:B:882:ILE:O	1:B:886:LEU:HG	2.14	0.47
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.97	0.46
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.96	0.46
1:B:686:ASP:HB2	1:B:695:LEU:HD22	1.97	0.46
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.97	0.46
1:A:987:MET:N	1:A:988:PRO:CD	2.80	0.45
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.45
8:B:1104:FUA:O4	8:B:1104:FUA:C16	2.64	0.45
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:C:108:GLN:O	1:C:112:GLN:HG2	2.17	0.44
1:A:457:ALA:O	1:A:468:ARG:NH1	2.51	0.44
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.99	0.44
1:B:489:THR:N	1:B:490:PRO:CD	2.81	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.99	0.44
1:A:344:LEU:CD1	1:A:402:ILE:HD11	2.47	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43
1:C:330:THR:N	1:C:331:PRO:CD	2.81	0.43
1:B:897:ILE:N	1:B:898:PRO:HD2	2.33	0.43
1:B:376:LEU:HD23	1:B:398:MET:HE1	1.99	0.43
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.53	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.00	0.43
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.18	0.43
1:A:454:VAL:N	1:A:455:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.43
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.42
1:B:760:ASN:HA	7:B:1103:GOL:H32	2.00	0.42
1:C:901:VAL:O	1:C:904:VAL:HG12	2.20	0.42
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.01	0.42
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.42
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.42
1:C:670:ALA:C	1:C:671:ILE:HD13	2.44	0.42
1:B:355:MET:HE1	1:B:413:VAL:HG11	2.02	0.42
1:B:375:VAL:HG11	1:B:405:LEU:HD22	2.01	0.41
1:B:314:GLU:N	1:B:315:PRO:CD	2.82	0.41
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.35	0.41
1:A:59:ASP:HB3	1:C:763:ILE:HD11	2.03	0.41
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.03	0.41
1:C:987:MET:N	1:C:988:PRO:CD	2.84	0.41
1:A:873:ALA:HB3	1:A:874:PRO:HD3	2.02	0.41
1:C:211:ASN:O	1:C:760:ASN:ND2	2.53	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.22	0.40
1:B:45:ILE:HD11	1:B:107:VAL:HG13	2.03	0.40
1:B:330:THR:N	1:B:331:PRO:CD	2.85	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	1032/1057 (98%)	986 (96%)	45 (4%)	1 (0%)	48	75
1	B	1032/1057 (98%)	996 (96%)	35 (3%)	1 (0%)	48	75
1	C	1033/1057 (98%)	989 (96%)	43 (4%)	1 (0%)	48	75
2	D	153/169 (90%)	147 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	152/169 (90%)	143 (94%)	9 (6%)	0	100	100
All	All	3402/3509 (97%)	3261 (96%)	138 (4%)	3 (0%)	48	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	B	678	THR
1	C	777	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	847/862 (98%)	844 (100%)	3 (0%)	84	84
1	B	839/862 (97%)	834 (99%)	5 (1%)	78	81
1	C	840/862 (97%)	838 (100%)	2 (0%)	87	88
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2765/2850 (97%)	2755 (100%)	10 (0%)	84	84

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	984	LEU
1	A	1041	GLU
1	B	88	VAL
1	B	398	MET
1	B	556	PHE
1	B	801	PHE
1	B	881	LEU
1	C	463	THR

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Mol	Chain	Res	Type
1	C	497	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	68	ASN
1	A	194	ASN
1	A	274	ASN
1	A	360	GLN
1	A	517	ASN
1	A	577	GLN
1	A	588	GLN
1	A	605	ASN
1	A	820	ASN
1	B	58	GLN
1	B	89	GLN
1	B	181	GLN
1	B	605	ASN
1	B	865	GLN
1	B	923	ASN
1	B	1001	ASN
1	C	58	GLN
1	C	68	ASN
1	C	274	ASN
1	C	391	ASN
1	C	577	GLN
1	C	584	GLN
1	C	797	GLN
1	C	1001	ASN
2	D	92	HIS
2	D	102	ASN
2	D	122	ASN
2	E	155	ASN

5.3.3 RNA ⓘ

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](#)

13 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	$\# Z > 2$
9	R16	B	1105	-	15,15,15	0.10	0	14,14,14	0.15	0
3	LMT	B	1106	-	36,36,36	0.43	0	47,47,47	0.50	0
3	LMT	B	1107	-	36,36,36	0.47	0	47,47,47	0.61	0
3	LMT	C	1102	-	36,36,36	0.43	0	47,47,47	0.55	0
4	SO4	C	1103	-	4,4,4	0.34	0	6,6,6	0.07	0
6	DDQ	B	1102	-	11,13,13	0.18	0	12,15,15	0.27	0
3	LMT	A	1102	-	36,36,36	0.43	0	47,47,47	0.48	0
5	D10	B	1101	-	9,9,9	0.09	0	8,8,8	0.09	0
8	FUA	B	1104	-	39,40,40	1.54	2 (5%)	50,64,64	0.85	1 (2%)
10	PTY	C	1101	-	49,49,49	0.26	0	52,54,54	0.39	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.64	1 (2%)
4	SO4	A	1103	-	4,4,4	0.34	0	6,6,6	0.07	0
7	GOL	B	1103	-	5,5,5	0.09	0	5,5,5	0.43	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
9	R16	B	1105	-	-	6/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	B	1106	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1107	-	-	11/21/61/61	0/2/2/2
3	LMT	C	1102	-	-	8/21/61/61	0/2/2/2
6	DDQ	B	1102	-	-	4/11/11/11	-
8	FUA	B	1104	-	-	6/16/92/92	0/4/4/4
3	LMT	A	1102	-	-	9/21/61/61	0/2/2/2
5	D10	B	1101	-	-	1/7/7/7	-
10	PTY	C	1101	-	-	21/53/53/53	-
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
7	GOL	B	1103	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1104	FUA	C29-C22	-8.73	1.35	1.47
8	B	1104	FUA	O5-C29	-2.68	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1104	FUA	C14-C8-C9	-2.61	104.72	109.30
3	A	1101	LMT	O1B-C4'-C5'	2.08	114.92	109.48

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1106	LMT	C2-C1-O1'-C1'
7	B	1103	GOL	O1-C1-C2-O2
7	B	1103	GOL	O1-C1-C2-C3
10	C	1101	PTY	N1-C2-C3-O11
10	C	1101	PTY	C11-C8-O7-C6
10	C	1101	PTY	O30-C30-O4-C1
3	A	1101	LMT	C5'-C4'-O1B-C1B
10	C	1101	PTY	O10-C8-O7-C6
10	C	1101	PTY	C31-C30-O4-C1
3	B	1107	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	O5'-C1'-O1'-C1
3	C	1102	LMT	O5'-C5'-C6'-O6'
9	B	1105	R16	C38-C39-C40-C41
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	C	1102	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	B	1106	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	B	1107	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	O1'-C1-C2-C3
9	B	1105	R16	C34-C35-C36-C37
8	B	1104	FUA	C32-C31-O2-C16
3	B	1106	LMT	C2'-C1'-O1'-C1
7	B	1103	GOL	C1-C2-C3-O3
5	B	1101	D10	C4-C5-C6-C7
3	B	1106	LMT	O5'-C1'-O1'-C1
10	C	1101	PTY	C11-C12-C13-C14
3	A	1102	LMT	C3-C4-C5-C6
3	A	1102	LMT	C11-C10-C9-C8
3	B	1106	LMT	C11-C10-C9-C8
10	C	1101	PTY	C35-C36-C37-C38
10	C	1101	PTY	C30-C31-C32-C33
6	B	1102	DDQ	C5-C6-C7-C8
3	B	1107	LMT	C1-C2-C3-C4
3	A	1102	LMT	C7-C8-C9-C10
3	B	1107	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	C3-C4-C5-C6
10	C	1101	PTY	C39-C40-C41-C42
8	B	1104	FUA	C22-C23-C24-C25
3	B	1106	LMT	C6-C7-C8-C9
3	C	1102	LMT	C1-C2-C3-C4
3	B	1107	LMT	C6-C7-C8-C9
3	C	1102	LMT	O1'-C1-C2-C3
3	B	1106	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	C9-C10-C11-C12
10	C	1101	PTY	C36-C37-C38-C39
3	B	1107	LMT	C9-C10-C11-C12
3	B	1107	LMT	C2-C1-O1'-C1'
3	C	1102	LMT	C2-C1-O1'-C1'
8	B	1104	FUA	O3-C31-O2-C16

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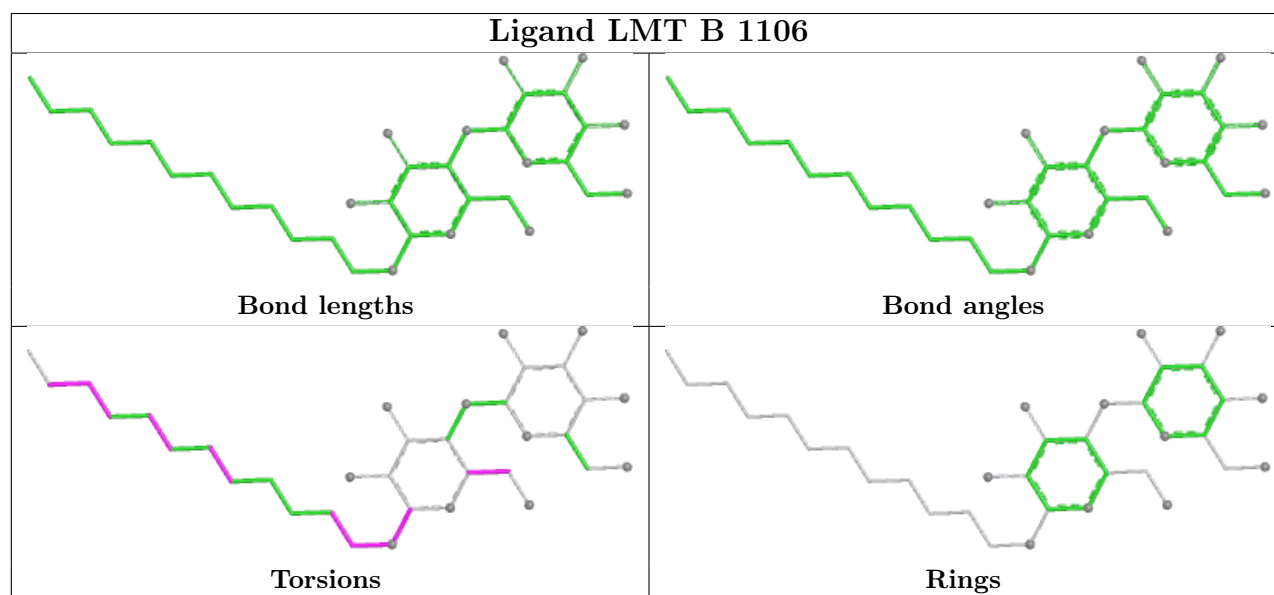
Mol	Chain	Res	Type	Atoms
3	C	1102	LMT	C4-C5-C6-C7
10	C	1101	PTY	C26-C27-C28-C29
10	C	1101	PTY	C19-C20-C21-C22
8	B	1104	FUA	C15-C16-O2-C31
9	B	1105	R16	C32-C33-C34-C35
7	B	1103	GOL	O2-C2-C3-O3
10	C	1101	PTY	C12-C11-C8-O7
10	C	1101	PTY	O14-C5-C6-C1
3	A	1102	LMT	C4-C5-C6-C7
6	B	1102	DDQ	C2-C1-N1-CM2
3	B	1107	LMT	O1'-C1-C2-C3
3	C	1102	LMT	C9-C10-C11-C12
9	B	1105	R16	C35-C36-C37-C38
10	C	1101	PTY	C34-C35-C36-C37
10	C	1101	PTY	O14-C5-C6-O7
10	C	1101	PTY	C25-C26-C27-C28
6	B	1102	DDQ	C2-C1-N1-O1
3	B	1106	LMT	C4-C5-C6-C7
3	B	1107	LMT	C4-C5-C6-C7
10	C	1101	PTY	C23-C24-C25-C26
10	C	1101	PTY	C31-C32-C33-C34
6	B	1102	DDQ	C7-C8-C9-C10
3	A	1102	LMT	C6-C7-C8-C9
3	B	1107	LMT	C3-C4-C5-C6
3	B	1107	LMT	C2-C3-C4-C5
3	A	1101	LMT	C9-C10-C11-C12
3	C	1102	LMT	C11-C10-C9-C8
3	B	1106	LMT	C9-C10-C11-C12
10	C	1101	PTY	C33-C34-C35-C36
3	A	1101	LMT	C3'-C4'-O1B-C1B
3	B	1106	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	C2-C3-C4-C5
3	A	1101	LMT	C7-C8-C9-C10
9	B	1105	R16	C28-C29-C30-C31
9	B	1105	R16	C37-C38-C39-C40
8	B	1104	FUA	C24-C25-C26-C27
10	C	1101	PTY	C12-C11-C8-O10
8	B	1104	FUA	C24-C25-C26-C28

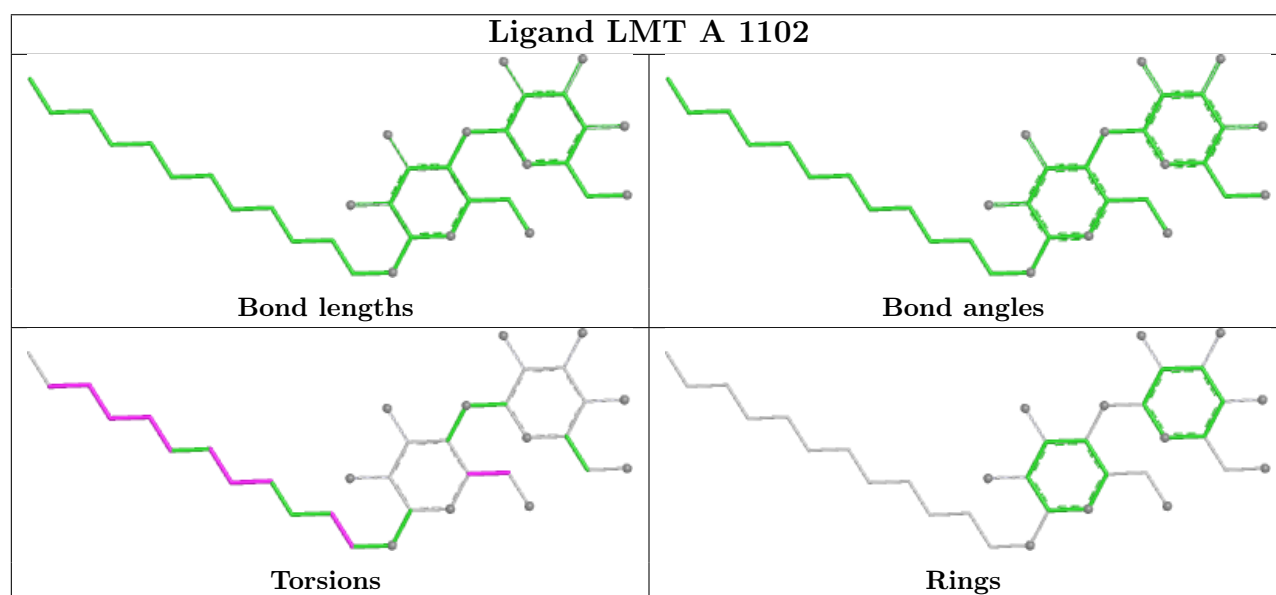
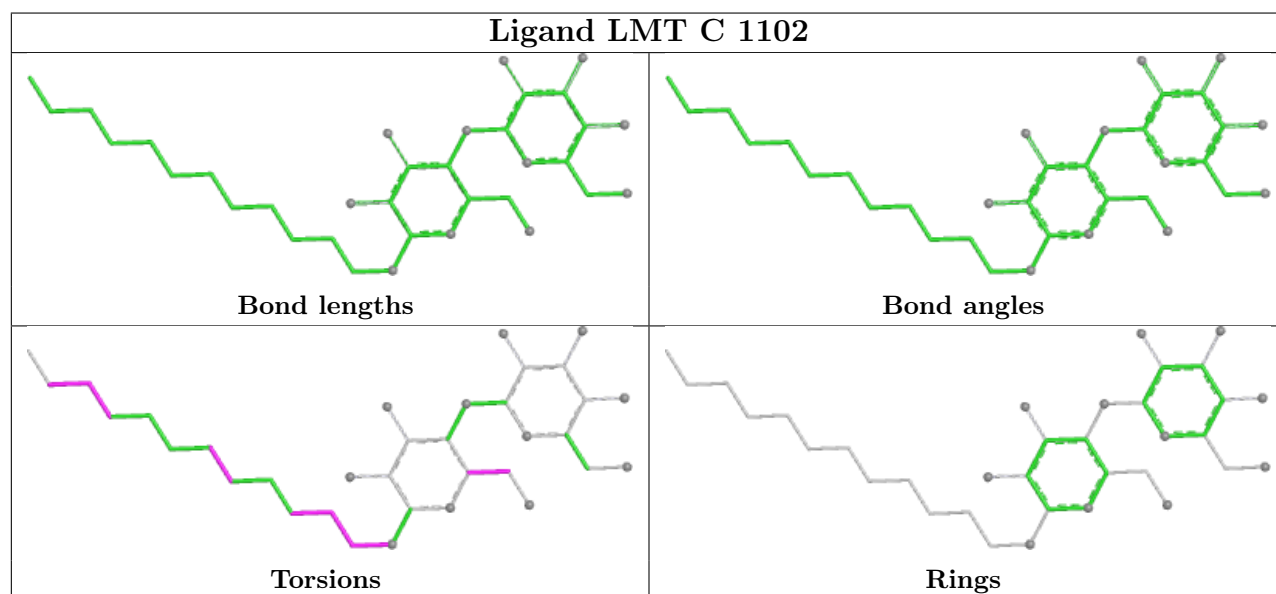
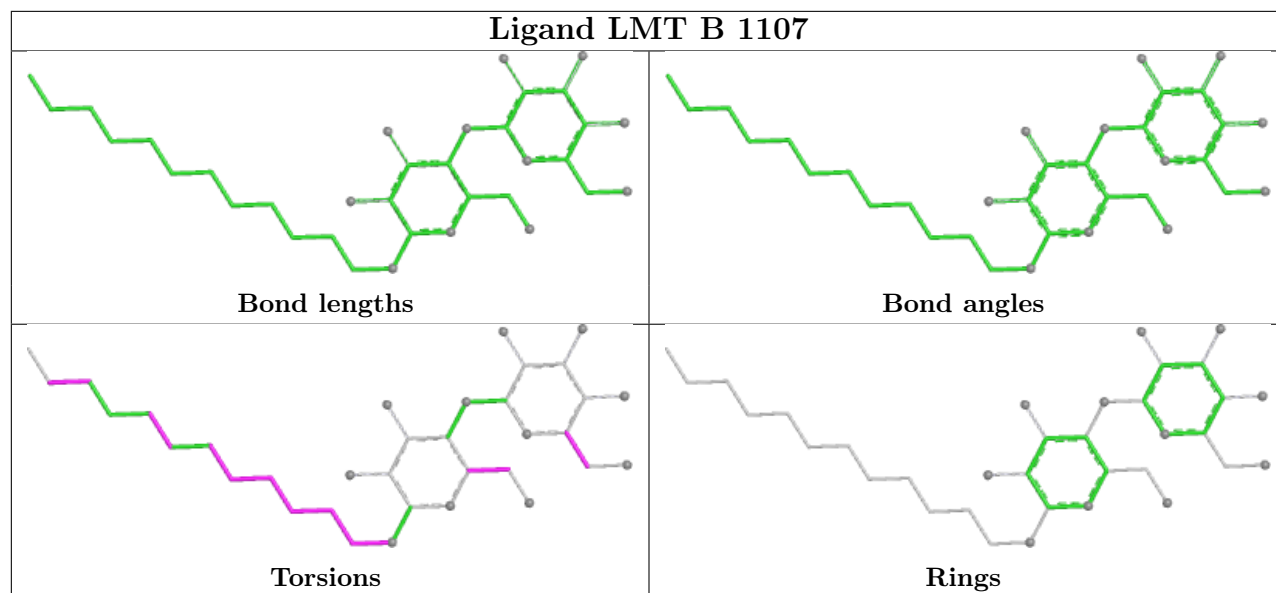
There are no ring outliers.

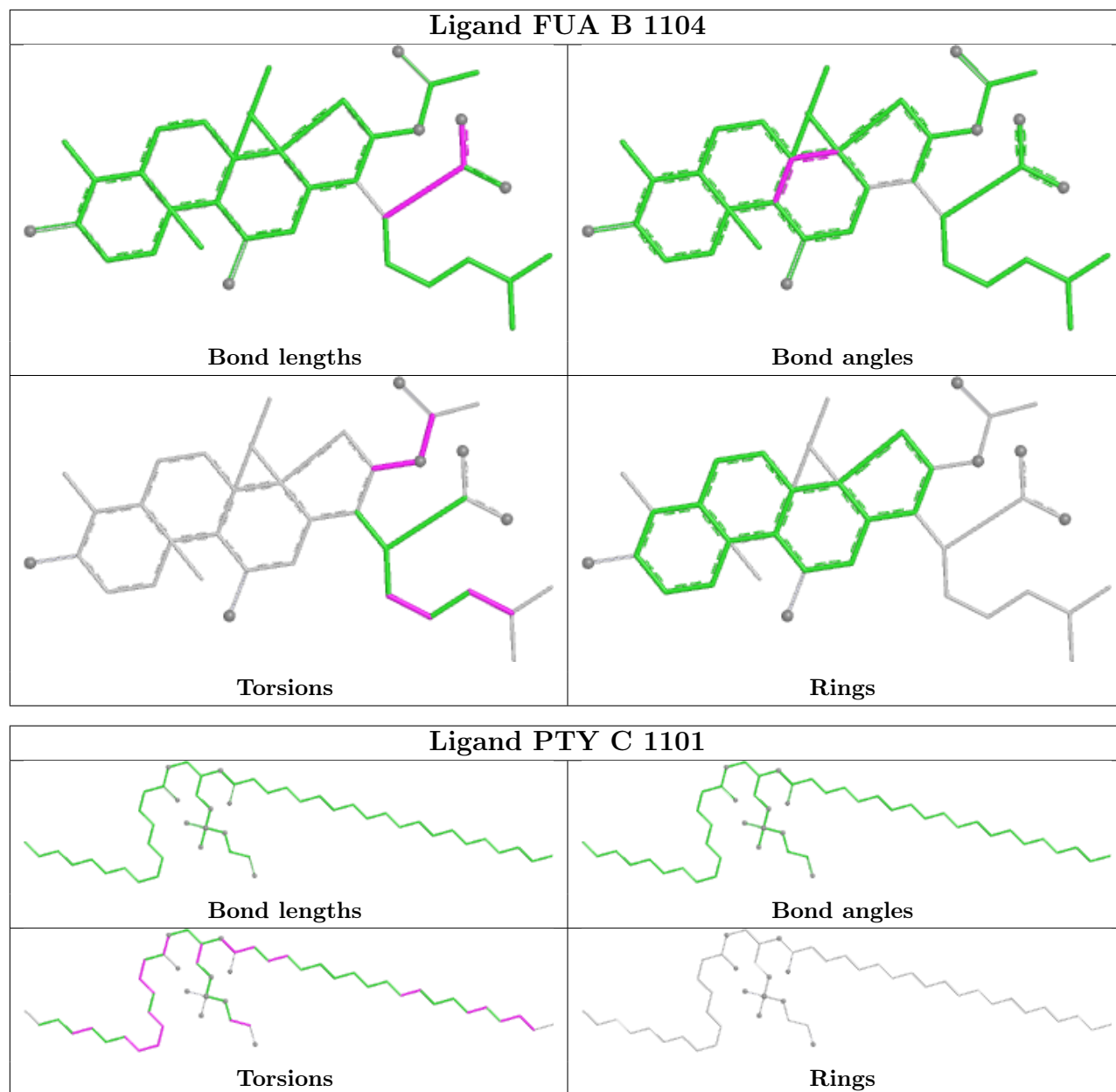
5 monomers are involved in 12 short contacts:

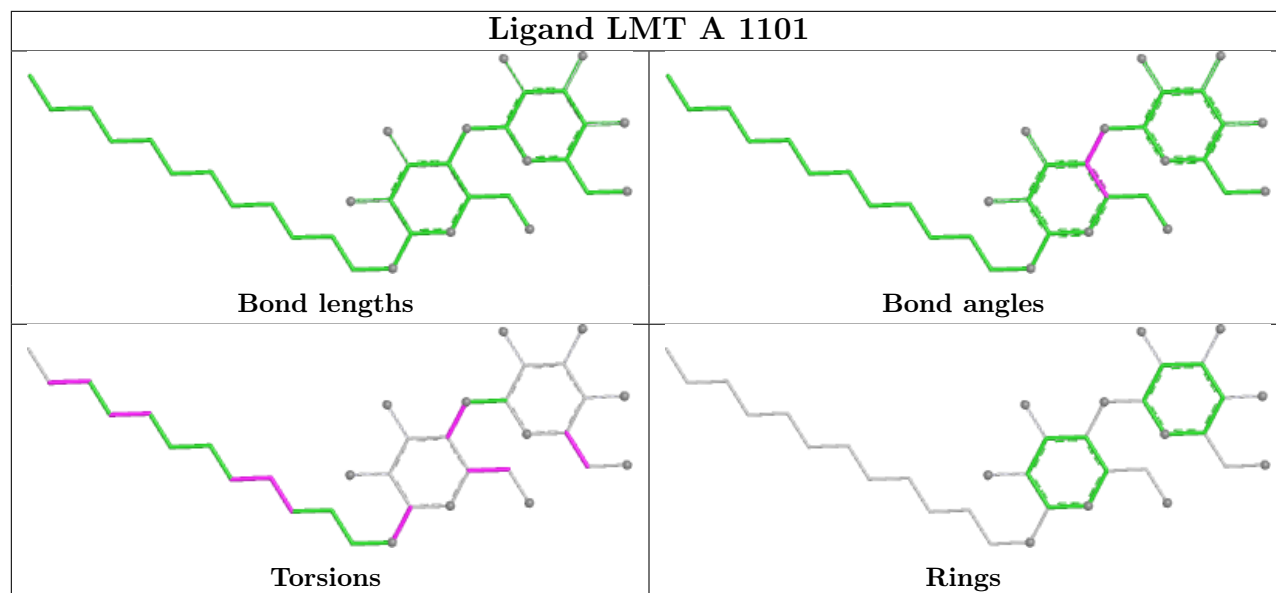
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1105	R16	1	0
5	B	1101	D10	1	0
8	B	1104	FUA	7	0
10	C	1101	PTY	1	0
7	B	1103	GOL	2	0

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









5.7 Other polymers [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1042/1057 (98%)	0.47	37 (3%)	46	31	33, 61, 96, 131	0
1	B	1034/1057 (97%)	0.46	49 (4%)	36	24	35, 59, 86, 110	0
1	C	1035/1057 (97%)	0.29	19 (1%)	67	49	40, 52, 73, 97	0
2	D	155/169 (91%)	0.39	1 (0%)	85	73	49, 62, 77, 86	0
2	E	154/169 (91%)	0.61	3 (1%)	66	48	57, 71, 91, 101	0
All	All	3420/3509 (97%)	0.42	109 (3%)	50	34	33, 58, 87, 131	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	134	SER	6.3
1	A	672	VAL	5.1
1	A	868	LEU	4.9
1	B	678	THR	4.7
1	B	677	ALA	4.6
1	B	615	PHE	4.6
1	A	674	LEU	4.5
1	B	672	VAL	4.4
1	B	671	ILE	4.4
1	B	617	PHE	4.3
1	B	634	TRP	4.2
1	B	674	LEU	4.0
1	B	577	GLN	4.0
1	B	662	MET	4.0
1	B	628	PHE	4.0
1	B	1015	THR	4.0
1	B	133	SER	3.9
1	A	617	PHE	3.7
1	B	575	MET	3.6
1	B	618	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	664	PHE	3.5
1	A	406	VAL	3.4
1	C	674	LEU	3.4
1	A	673	GLU	3.3
1	C	89	GLN	3.3
1	A	802	SER	3.3
1	A	676	THR	3.3
1	A	1040	ILE	3.2
1	B	403	GLY	3.2
1	C	1033	PHE	3.2
1	C	620	ARG	3.2
1	B	676	THR	3.2
1	B	669	PRO	3.1
1	A	362	PHE	3.1
1	B	627	ALA	3.0
1	B	332	PHE	3.0
1	A	678	THR	3.0
1	B	573	MET	3.0
1	A	670	ALA	3.0
1	B	660	ASP	3.0
1	B	178	PHE	2.9
1	A	510	LYS	2.9
1	B	979	SER	2.9
1	A	664	PHE	2.8
1	C	617	PHE	2.8
1	A	677	ALA	2.8
1	B	407	ASP	2.8
1	B	666	PHE	2.7
1	B	626	ILE	2.6
1	C	676	THR	2.6
1	B	665	ALA	2.6
1	A	509	LYS	2.6
1	A	125	GLN	2.6
1	A	511	GLY	2.6
1	B	675	GLY	2.6
1	B	787	GLY	2.6
2	E	14	LEU	2.6
1	A	707	ALA	2.6
1	B	563	PHE	2.5
1	A	542	LEU	2.5
2	E	143	ASP	2.5
1	A	1036	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	865	GLN	2.5
1	A	575	MET	2.4
1	A	719	ASN	2.4
1	C	811	TYR	2.4
1	A	112	GLN	2.4
1	A	369	THR	2.4
1	B	132	SER	2.4
1	A	37	THR	2.3
1	C	264	ASP	2.3
1	A	869	SER	2.3
1	A	981	ALA	2.3
1	B	784	ASP	2.3
1	B	655	PHE	2.3
1	C	737	GLN	2.3
1	B	938	SER	2.3
1	B	1011	MET	2.3
1	A	968	VAL	2.3
1	B	670	ALA	2.3
1	B	405	LEU	2.3
1	B	663	VAL	2.3
1	B	408	ASP	2.2
1	A	828	LEU	2.2
1	C	266	ALA	2.2
1	C	403	GLY	2.2
1	B	620	ARG	2.2
1	C	619	GLY	2.2
2	D	12	SER	2.2
1	B	616	GLY	2.2
1	C	575	MET	2.1
1	A	866	GLU	2.1
1	C	134	SER	2.1
1	A	675	GLY	2.1
1	A	918	PHE	2.1
1	C	733	GLN	2.1
1	B	937	LEU	2.1
2	E	13	ASP	2.1
1	A	877	TYR	2.1
1	B	830	GLN	2.1
1	C	657	GLN	2.1
1	A	715	SER	2.0
1	B	574	THR	2.0
1	B	673	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	868	LEU	2.0
1	A	618	ALA	2.0
1	C	124	GLN	2.0
1	C	673	GLU	2.0
1	C	671	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

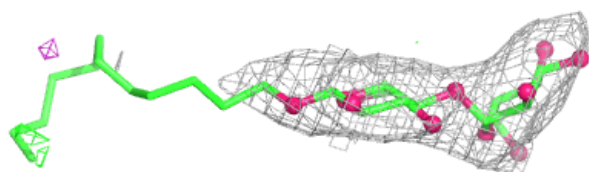
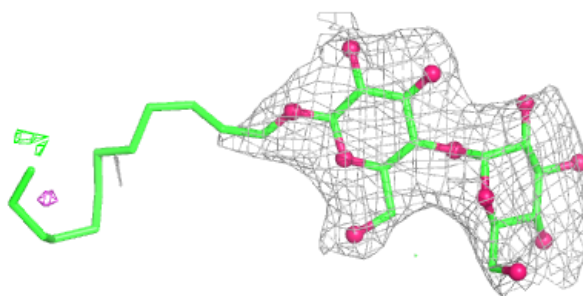
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	D10	B	1101	10/10	0.51	0.36	48,49,49,49	0
4	SO4	A	1103	5/5	0.72	0.20	140,140,141,141	0
6	DDQ	B	1102	14/14	0.76	0.28	64,68,73,74	0
3	LMT	A	1102	35/35	0.79	0.19	94,98,101,101	0
10	PTY	C	1101	50/50	0.82	0.25	81,87,105,106	0
9	R16	B	1105	16/16	0.83	0.28	58,61,61,61	0
3	LMT	B	1107	35/35	0.83	0.23	92,115,122,124	0
8	FUA	B	1104	37/37	0.87	0.20	74,76,91,93	0
3	LMT	A	1101	35/35	0.88	0.16	75,90,101,103	0
3	LMT	B	1106	35/35	0.88	0.17	86,88,92,92	0
7	GOL	B	1103	6/6	0.88	0.17	47,48,48,48	0
4	SO4	C	1103	5/5	0.92	0.13	75,75,75,75	0
3	LMT	C	1102	35/35	0.93	0.12	63,65,67,68	0

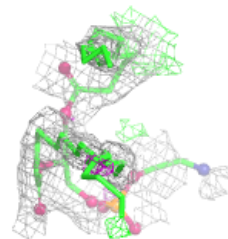
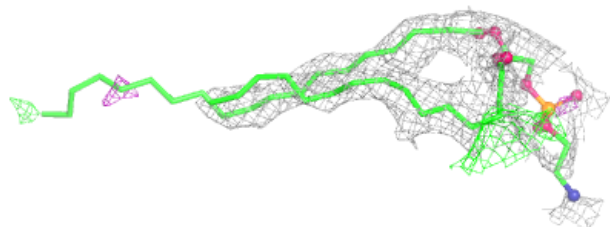
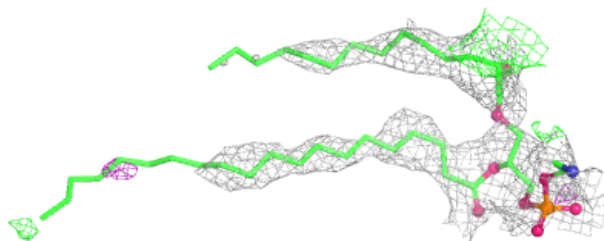
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

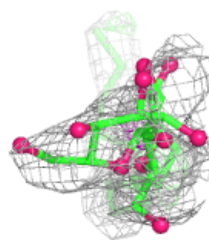
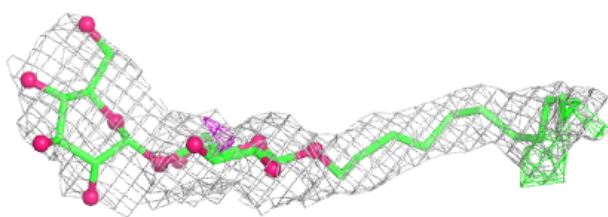
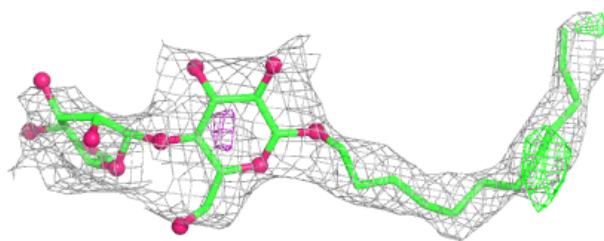
**Electron density around PTY C 1101:**

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



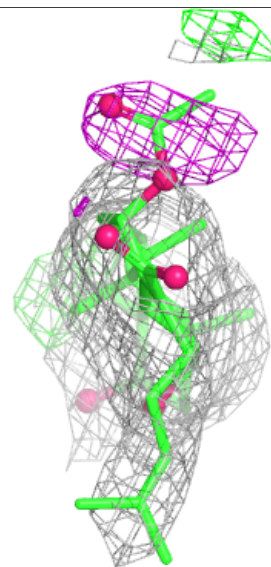
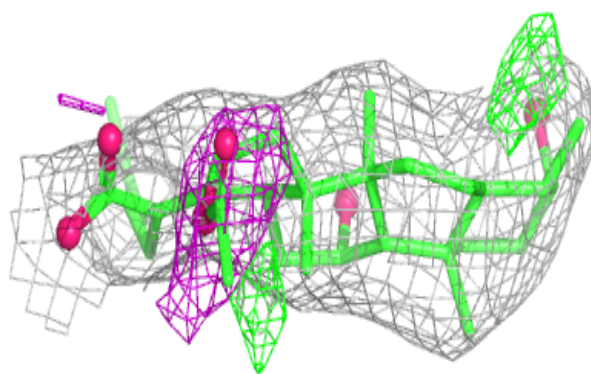
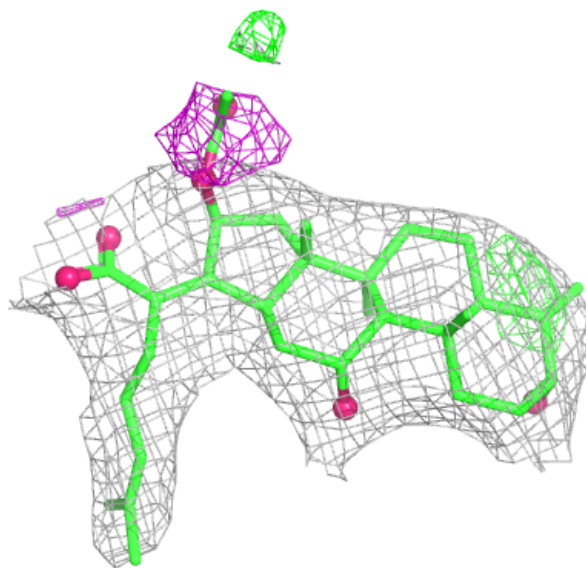
Electron density around LMT B 1107:

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



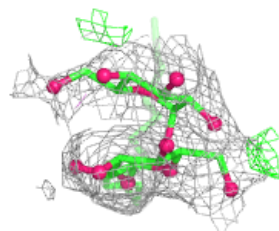
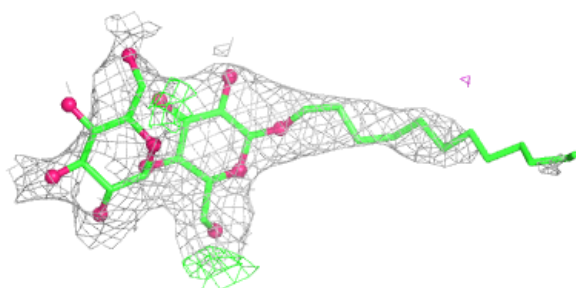
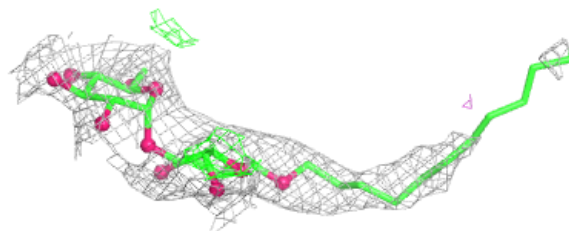
Electron density around FUA B 1104:

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

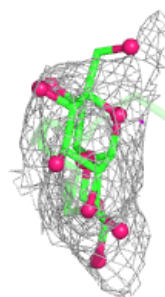
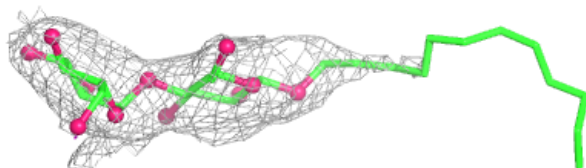
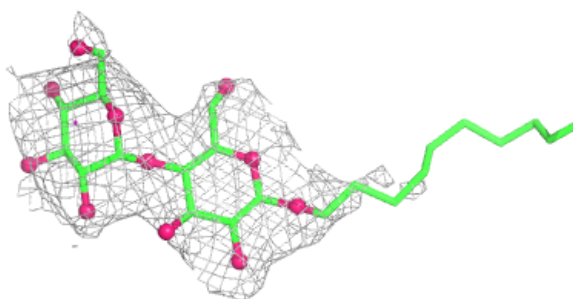


Electron density around LMT A 1101:

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

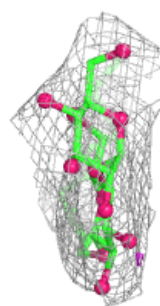
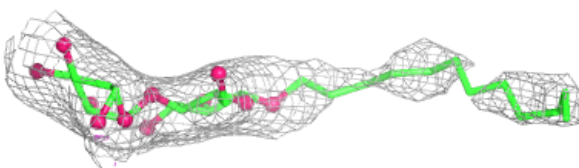
**Electron density around LMT B 1106:**

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



Electron density around LMT C 1102:

$2mF_o-DF_c$ (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.