



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:13 PM UTC

PDB ID : 6Q4O / pdb_00006q4o
Title : Fusidic acid bound AcrB_I27A
Authors : Tam, H.K.; Pos, K.M.
Deposited on : 2018-12-06
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

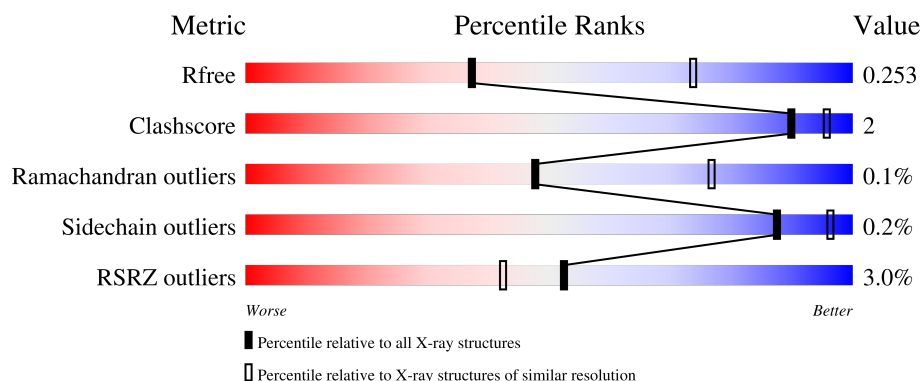
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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% 91% 7%
1	B	1057	3% 94% • •
1	C	1057	% 93% 5%
2	D	169	2% 92% 8%
2	E	169	5% 91% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DDQ	A	1108	-	-	-	X
5	DDQ	A	1109	-	-	-	X
7	HEX	A	1112	-	-	-	X
7	HEX	B	1117	-	-	-	X
7	HEX	C	1112	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 27628 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	4	0
			7952	5115	1314	1479	44			
1	B	1034	Total	C	N	O	S	0	1	0
			7860	5060	1296	1460	44			
1	C	1035	Total	C	N	O	S	0	1	0
			7871	5063	1303	1461	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	ILE	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	27	ALA	ILE	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	27	ALA	ILE	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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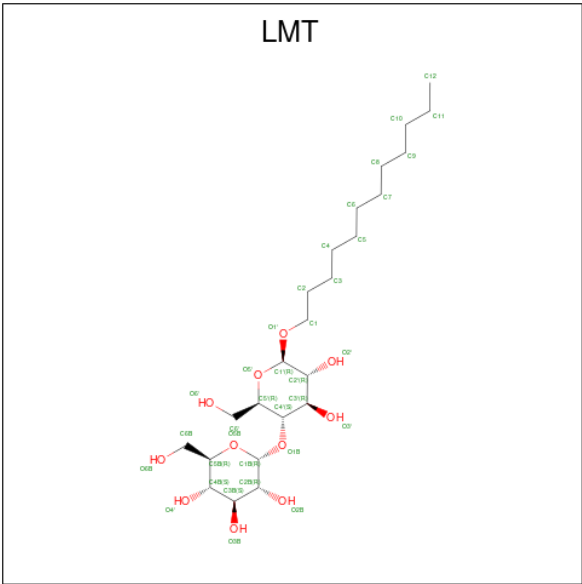
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1182	745	207	229	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: C₂₄H₄₆O₁₁).



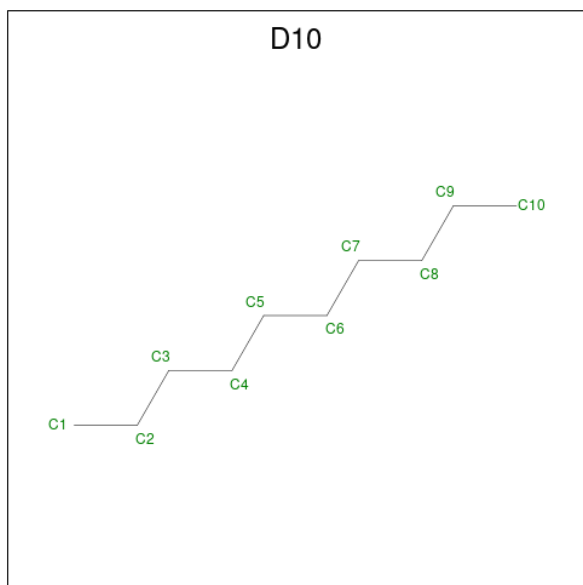
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

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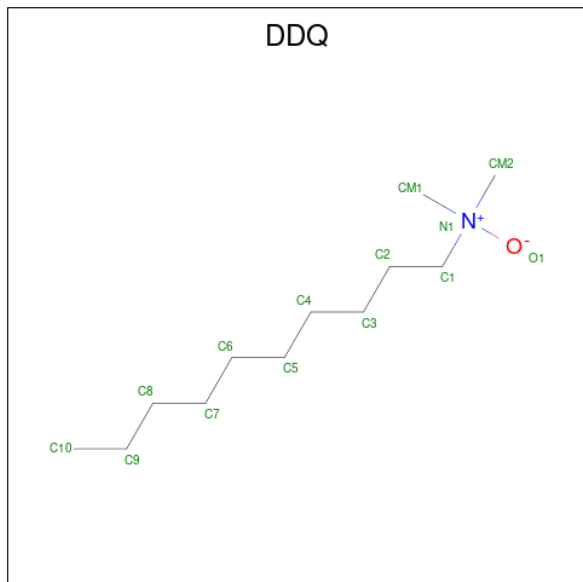
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



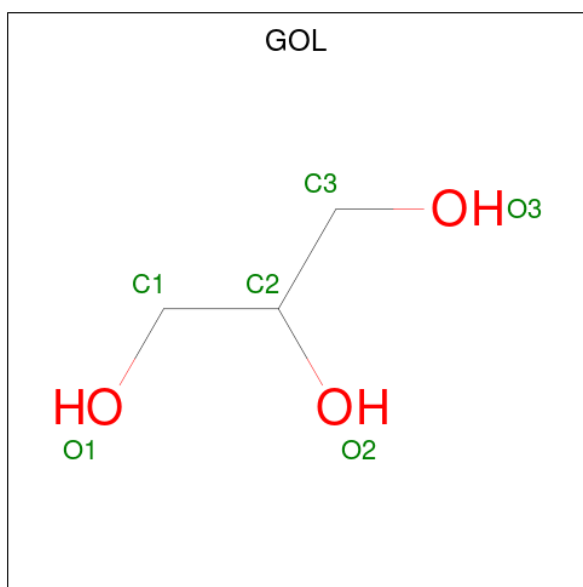
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			10	10		
4	A	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		

- Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



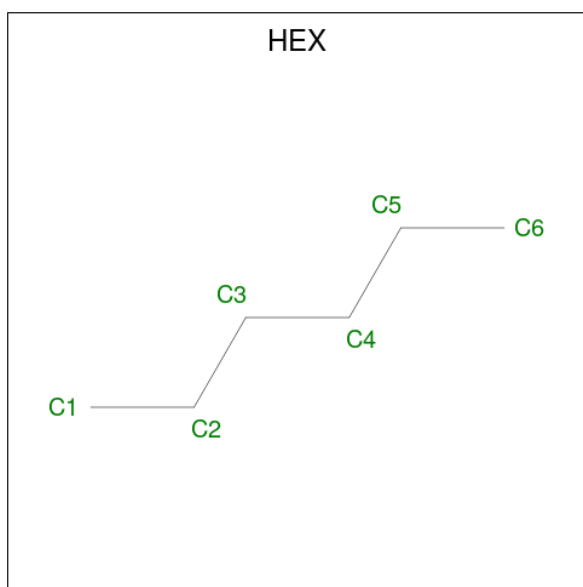
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	12	1	1		
5	A	1	Total	C	N	O	0	0
			14	12	1	1		
5	A	1	Total	C	N	O	0	0
			14	12	1	1		
5	B	1	Total	C	N	O	0	0
			14	12	1	1		
5	B	1	Total	C	N	O	0	0
			14	12	1	1		
5	B	1	Total	C	N	O	0	0
			14	12	1	1		
5	B	1	Total	C	N	O	0	0
			14	12	1	1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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



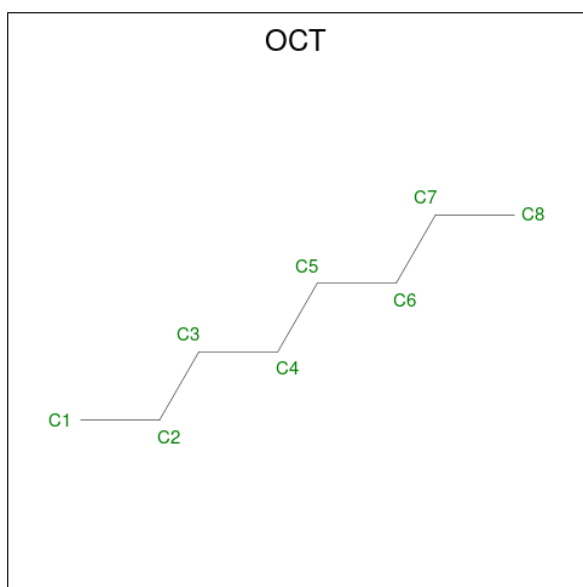
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



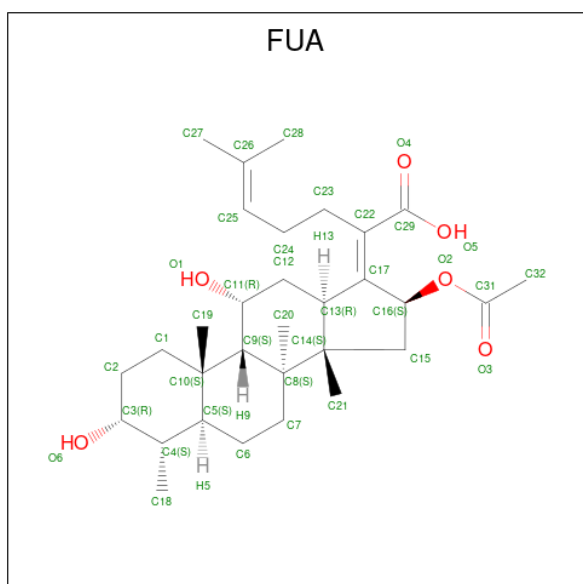
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	B	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0

- Molecule 8 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



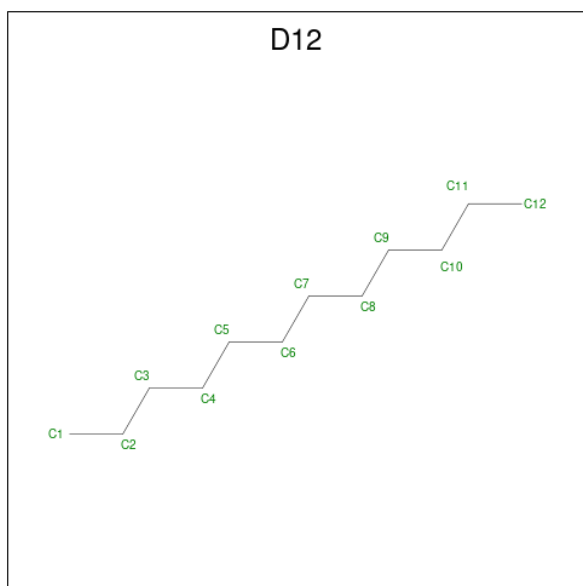
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 8 8	0	0
8	A	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0
8	B	1	Total C 8 8	0	0

- Molecule 9 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



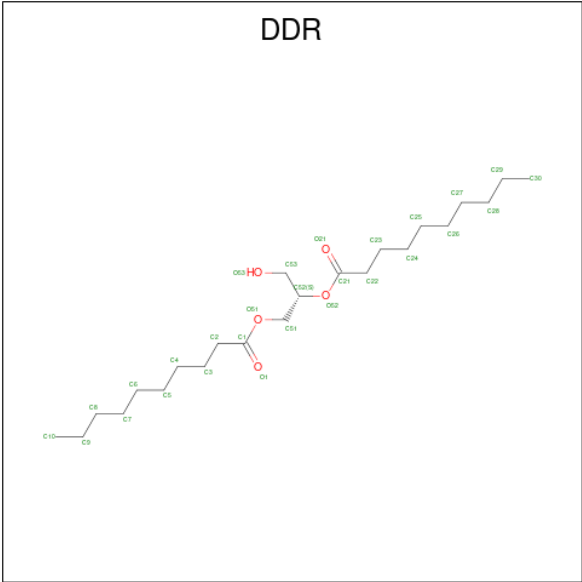
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C O	0	0
			37	31 6		

- Molecule 10 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



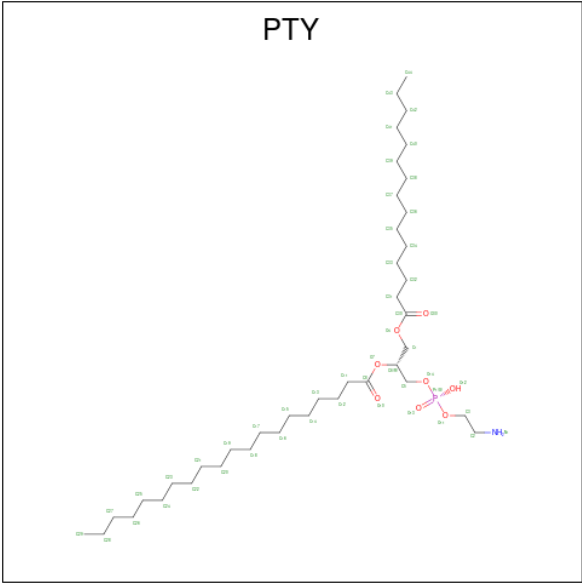
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		
10	C	1	Total	C	0	0
			12	12		

- Molecule 11 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 12 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



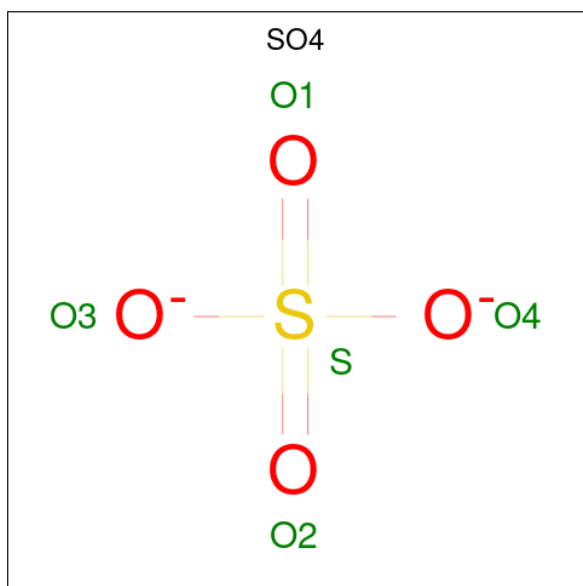
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
12	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
12	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

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

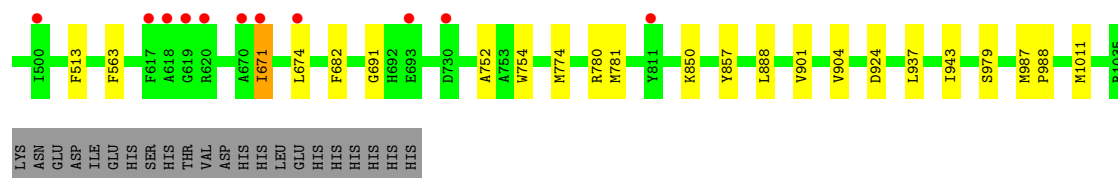
- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



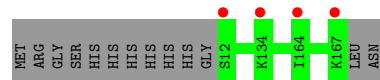
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is water.

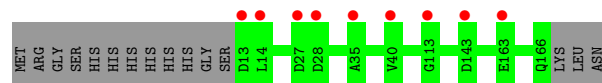
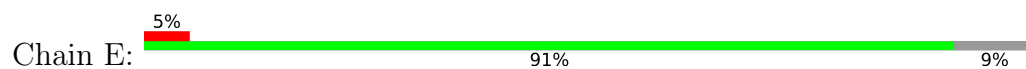
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	197	Total	O	0	0
			197	197		
14	B	173	Total	O	0	0
			173	173		
14	C	227	Total	O	0	0
			227	227		
14	D	34	Total	O	0	0
			34	34		
14	E	9	Total	O	0	0
			9	9		



- 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	145.20Å 162.57Å 243.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.52 – 2.80 47.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.52-2.80) 98.7 (47.52-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.212 , 0.256 0.213 , 0.253	Depositor DCC
R_{free} test set	6961 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27628	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PTY, DDQ, D12, GOL, DDR, OCT, FUA, D10, LMT, HEX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	0/8116	1.50	3/11018 (0.0%)
1	B	1.00	0/8014	1.52	2/10883 (0.0%)
1	C	1.00	0/8024	1.50	1/10895 (0.0%)
2	D	1.02	0/1201	1.53	0/1632
2	E	1.02	0/1186	1.55	0/1613
All	All	1.00	0/26541	1.51	6/36041 (0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	639	GLY	CA-C-O	-6.40	118.06	122.22
1	B	896	SER	CA-C-N	6.04	124.05	120.24
1	B	896	SER	C-N-CA	6.04	124.05	120.24
1	A	896	SER	CA-C-N	5.49	123.70	120.24
1	A	896	SER	C-N-CA	5.49	123.70	120.24

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	7952	0	8100	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7860	0	8009	24	0
1	C	7871	0	8026	34	0
2	D	1182	0	1169	0	0
2	E	1167	0	1151	0	0
3	A	140	0	184	0	0
3	B	70	0	92	1	0
3	C	70	0	92	0	0
4	A	20	0	44	0	0
4	B	30	0	66	0	0
4	C	30	0	66	0	0
5	A	42	0	81	0	0
5	B	56	0	108	0	0
5	C	28	0	54	0	0
6	A	12	0	16	0	0
6	B	18	0	24	0	0
6	C	24	0	32	0	0
6	D	6	0	8	0	0
6	E	6	0	8	0	0
7	A	6	0	14	0	0
7	B	24	0	56	0	0
7	C	24	0	56	0	0
8	A	16	0	36	0	0
8	B	16	0	36	1	0
9	B	37	0	47	6	0
10	B	12	0	26	0	0
10	C	36	0	78	0	0
11	B	28	0	44	0	0
12	C	200	0	316	2	0
13	C	5	0	0	0	0
14	A	197	0	0	0	0
14	B	173	0	0	0	0
14	C	227	0	0	0	0
14	D	34	0	0	0	0
14	E	9	0	0	0	0
All	All	27628	0	28039	99	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 2.

The worst 5 of 99 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:671:ILE:HD11	1:C:674:LEU:HD12	1.64	0.80
9:B:1101:FUA:H202	9:B:1101:FUA:H5	1.66	0.76
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.68	0.75
1:C:360:GLN:HG2	1:C:513:PHE:CG	2.32	0.65
1:A:837:THR:HG22	1:A:841:MET:HE3	1.79	0.65

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	1044/1057 (99%)	1014 (97%)	27 (3%)	3 (0%)	36	66
1	B	1033/1057 (98%)	1012 (98%)	21 (2%)	0	100	100
1	C	1034/1057 (98%)	1014 (98%)	20 (2%)	0	100	100
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100	100
2	E	152/169 (90%)	150 (99%)	2 (1%)	0	100	100
All	All	3417/3509 (97%)	3342 (98%)	72 (2%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER
1	A	126	GLY
1	A	1037	ASN

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	851/862 (99%)	850 (100%)	1 (0%)	88	97
1	B	840/862 (97%)	839 (100%)	1 (0%)	88	97
1	C	841/862 (98%)	838 (100%)	3 (0%)	84	94
2	D	121/132 (92%)	121 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2772/2850 (97%)	2767 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	B	556	PHE
1	C	239	ARG
1	C	671	ILE
1	C	850	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	81	ASN
1	C	1001	ASN
1	C	124	GLN
2	D	69	ASN
1	B	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

60 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
7	HEX	C	1115	-	5,5,5	0.14	0	4,4,4	0.11	0
5	DDQ	B	1107	-	11,13,13	2.22	2 (18%)	12,15,15	0.39	0
12	PTY	C	1116	-	49,49,49	0.28	0	52,54,54	0.32	0
4	D10	C	1104	-	9,9,9	0.10	0	8,8,8	0.08	0
7	HEX	C	1114	-	5,5,5	0.13	0	4,4,4	0.11	0
7	HEX	B	1115	-	5,5,5	0.13	0	4,4,4	0.12	0
6	GOL	C	1109	-	5,5,5	0.10	0	5,5,5	0.30	0
7	HEX	B	1114	-	5,5,5	0.14	0	4,4,4	0.08	0
7	HEX	B	1117	-	5,5,5	0.13	0	4,4,4	0.13	0
10	D12	C	1121	-	11,11,11	0.30	0	10,10,10	0.46	0
3	LMT	A	1103	-	36,36,36	0.55	0	47,47,47	1.08	5 (10%)
3	LMT	C	1101	-	36,36,36	0.48	1 (2%)	47,47,47	0.72	0
10	D12	C	1122	-	11,11,11	0.27	0	10,10,10	0.46	0
5	DDQ	B	1110	-	11,13,13	2.22	2 (18%)	12,15,15	0.55	0
8	OCT	B	1118	-	7,7,7	0.10	0	6,6,6	0.06	0
6	GOL	A	1111	-	5,5,5	0.09	0	5,5,5	0.25	0
4	D10	A	1106	-	9,9,9	0.11	0	8,8,8	0.07	0
12	PTY	C	1118	-	49,49,49	0.27	0	52,54,54	0.32	0
6	GOL	D	201	-	5,5,5	0.10	0	5,5,5	0.29	0
6	GOL	B	1111	-	5,5,5	0.09	0	5,5,5	0.23	0
4	D10	B	1106	-	9,9,9	0.10	0	8,8,8	0.06	0
6	GOL	B	1112	-	5,5,5	0.09	0	5,5,5	0.26	0
5	DDQ	A	1109	-	11,13,13	2.32	2 (18%)	12,15,15	0.43	0
4	D10	A	1105	-	9,9,9	0.09	0	8,8,8	0.08	0
3	LMT	A	1102	-	36,36,36	0.52	1 (2%)	47,47,47	0.72	1 (2%)
4	D10	B	1105	-	9,9,9	0.11	0	8,8,8	0.09	0
13	SO4	C	1123	-	4,4,4	0.33	0	6,6,6	0.07	0
5	DDQ	B	1109	-	11,13,13	2.23	2 (18%)	12,15,15	0.43	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.58	0
3	LMT	B	1102	-	36,36,36	0.45	0	47,47,47	0.69	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OCT	A	1114	-	7,7,7	0.11	0	6,6,6	0.08	0
4	D10	C	1105	-	9,9,9	0.10	0	8,8,8	0.12	0
6	GOL	E	201	-	5,5,5	0.09	0	5,5,5	0.23	0
4	D10	C	1103	-	9,9,9	0.09	0	8,8,8	0.06	0
5	DDQ	A	1108	-	11,13,13	2.27	2 (18%)	12,15,15	0.54	0
5	DDQ	B	1108	-	11,13,13	2.25	2 (18%)	12,15,15	0.45	0
9	FUA	B	1101	-	39,40,40	1.68	2 (5%)	50,64,64	0.96	2 (4%)
3	LMT	C	1102	-	36,36,36	0.63	1 (2%)	47,47,47	1.19	7 (14%)
4	D10	B	1104	-	9,9,9	0.10	0	8,8,8	0.07	0
6	GOL	C	1108	-	5,5,5	0.08	0	5,5,5	0.23	0
7	HEX	C	1113	-	5,5,5	0.12	0	4,4,4	0.09	0
3	LMT	A	1104	-	36,36,36	0.50	0	47,47,47	0.66	0
3	LMT	B	1103	-	36,36,36	0.47	1 (2%)	47,47,47	0.62	0
7	HEX	B	1116	-	5,5,5	0.13	0	4,4,4	0.11	0
10	D12	C	1120	-	11,11,11	0.32	0	10,10,10	0.39	0
7	HEX	C	1112	-	5,5,5	0.13	0	4,4,4	0.09	0
6	GOL	C	1111	-	5,5,5	0.08	0	5,5,5	0.24	0
6	GOL	C	1110	-	5,5,5	0.09	0	5,5,5	0.31	0
10	D12	B	1120	-	11,11,11	0.30	0	10,10,10	0.42	0
5	DDQ	C	1107	-	11,13,13	2.25	2 (18%)	12,15,15	0.45	0
8	OCT	B	1119	-	7,7,7	0.10	0	6,6,6	0.10	0
6	GOL	A	1110	-	5,5,5	0.10	0	5,5,5	0.28	0
11	DDR	B	1121	-	27,27,27	1.24	2 (7%)	29,29,29	1.25	2 (6%)
5	DDQ	C	1106	-	11,13,13	2.25	2 (18%)	12,15,15	0.38	0
12	PTY	C	1117	-	49,49,49	0.27	0	52,54,54	0.36	0
12	PTY	C	1119	-	49,49,49	0.27	0	52,54,54	0.35	0
7	HEX	A	1112	-	5,5,5	0.12	0	4,4,4	0.09	0
5	DDQ	A	1107	-	11,13,13	2.24	2 (18%)	12,15,15	0.50	0
6	GOL	B	1113	-	5,5,5	0.11	0	5,5,5	0.30	0
8	OCT	A	1113	-	7,7,7	0.11	0	6,6,6	0.10	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
7	HEX	C	1115	-	-	0/3/3/3	-
5	DDQ	B	1107	-	-	5/11/11/11	-
12	PTY	C	1116	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	D10	C	1104	-	-	3/7/7/7	-
7	HEX	C	1114	-	-	0/3/3/3	-
7	HEX	B	1115	-	-	0/3/3/3	-
6	GOL	C	1109	-	-	2/4/4/4	-
7	HEX	B	1114	-	-	0/3/3/3	-
7	HEX	B	1117	-	-	1/3/3/3	-
10	D12	C	1121	-	-	3/9/9/9	-
3	LMT	A	1103	-	-	10/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	10/21/61/61	0/2/2/2
10	D12	C	1122	-	-	3/9/9/9	-
5	DDQ	B	1110	-	-	5/11/11/11	-
8	OCT	B	1118	-	-	2/5/5/5	-
6	GOL	A	1111	-	-	1/4/4/4	-
4	D10	A	1106	-	-	3/7/7/7	-
12	PTY	C	1118	-	-	29/53/53/53	-
6	GOL	D	201	-	-	4/4/4/4	-
6	GOL	B	1111	-	-	0/4/4/4	-
4	D10	B	1106	-	-	2/7/7/7	-
6	GOL	B	1112	-	-	0/4/4/4	-
5	DDQ	A	1109	-	-	1/11/11/11	-
4	D10	A	1105	-	-	0/7/7/7	-
3	LMT	A	1102	-	-	14/21/61/61	0/2/2/2
4	D10	B	1105	-	-	2/7/7/7	-
5	DDQ	B	1109	-	-	1/11/11/11	-
3	LMT	A	1101	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	6/21/61/61	0/2/2/2
8	OCT	A	1114	-	-	0/5/5/5	-
4	D10	C	1105	-	-	4/7/7/7	-
6	GOL	E	201	-	-	0/4/4/4	-
4	D10	C	1103	-	-	2/7/7/7	-
5	DDQ	A	1108	-	-	1/11/11/11	-
5	DDQ	B	1108	-	-	3/11/11/11	-
9	FUA	B	1101	-	-	5/16/92/92	0/4/4/4
3	LMT	C	1102	-	-	8/21/61/61	0/2/2/2
4	D10	B	1104	-	-	1/7/7/7	-
6	GOL	C	1108	-	-	1/4/4/4	-
7	HEX	C	1113	-	-	0/3/3/3	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1104	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1103	-	-	5/21/61/61	0/2/2/2
7	HEX	B	1116	-	-	0/3/3/3	-
10	D12	C	1120	-	-	2/9/9/9	-
7	HEX	C	1112	-	-	1/3/3/3	-
6	GOL	C	1111	-	-	0/4/4/4	-
6	GOL	C	1110	-	-	2/4/4/4	-
10	D12	B	1120	-	-	3/9/9/9	-
5	DDQ	C	1107	-	-	6/11/11/11	-
8	OCT	B	1119	-	-	4/5/5/5	-
6	GOL	A	1110	-	-	0/4/4/4	-
11	DDR	B	1121	-	-	17/29/29/29	-
5	DDQ	C	1106	-	-	2/11/11/11	-
12	PTY	C	1117	-	-	24/53/53/53	-
12	PTY	C	1119	-	-	19/53/53/53	-
7	HEX	A	1112	-	-	1/3/3/3	-
5	DDQ	A	1107	-	-	3/11/11/11	-
6	GOL	B	1113	-	-	2/4/4/4	-
8	OCT	A	1113	-	-	0/5/5/5	-

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1101	FUA	C29-C22	-9.74	1.34	1.47
5	A	1109	DDQ	O1-N1	-6.94	1.25	1.42
5	C	1107	DDQ	O1-N1	-6.87	1.25	1.42
5	B	1108	DDQ	O1-N1	-6.84	1.25	1.42
5	B	1109	DDQ	O1-N1	-6.81	1.25	1.42

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	1121	DDR	O52-C21-C22	4.33	120.84	111.48
3	A	1103	LMT	O1B-C4'-C3'	3.49	116.11	107.23
3	C	1102	LMT	C1B-O5B-C5B	3.19	119.95	113.72
3	C	1102	LMT	O5'-C1'-C2'	-2.87	104.47	110.37
3	C	1102	LMT	O5B-C1B-C2B	2.82	116.17	110.37

There are no chirality outliers.

5 of 274 torsion outliers are listed below:

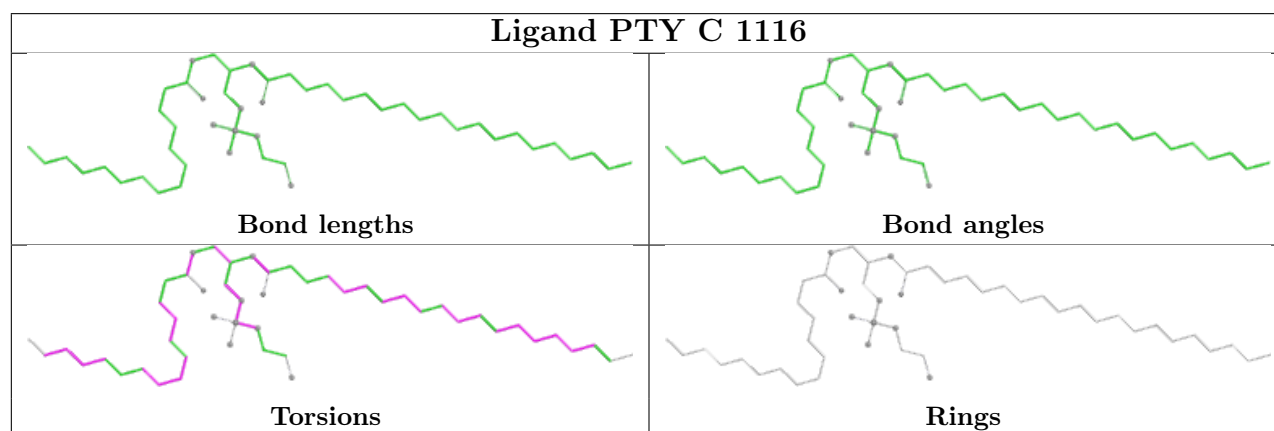
Mol	Chain	Res	Type	Atoms
3	C	1102	LMT	C2'-C1'-O1'-C1
5	A	1107	DDQ	N1-C1-C2-C3
5	B	1107	DDQ	C2-C1-N1-CM2
5	C	1107	DDQ	C2-C1-N1-CM2
6	C	1109	GOL	O1-C1-C2-C3

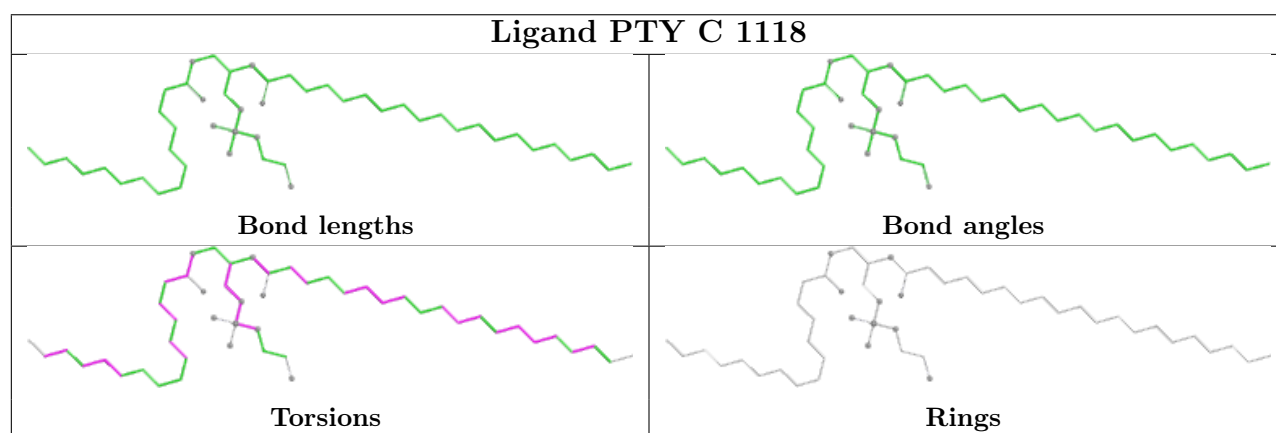
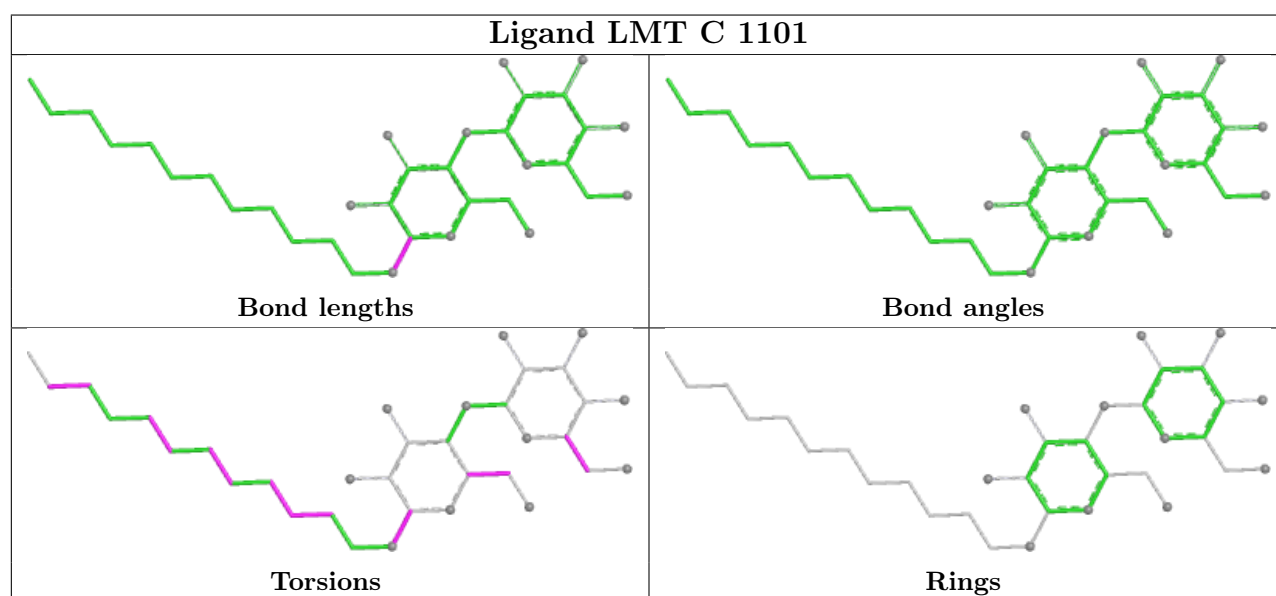
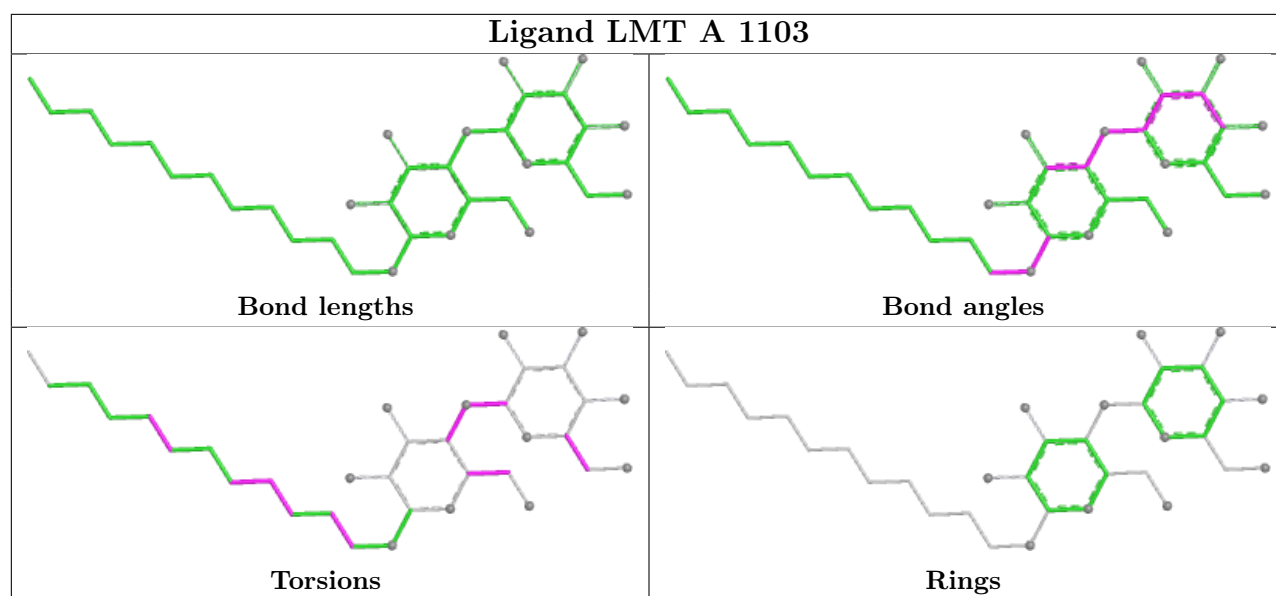
There are no ring outliers.

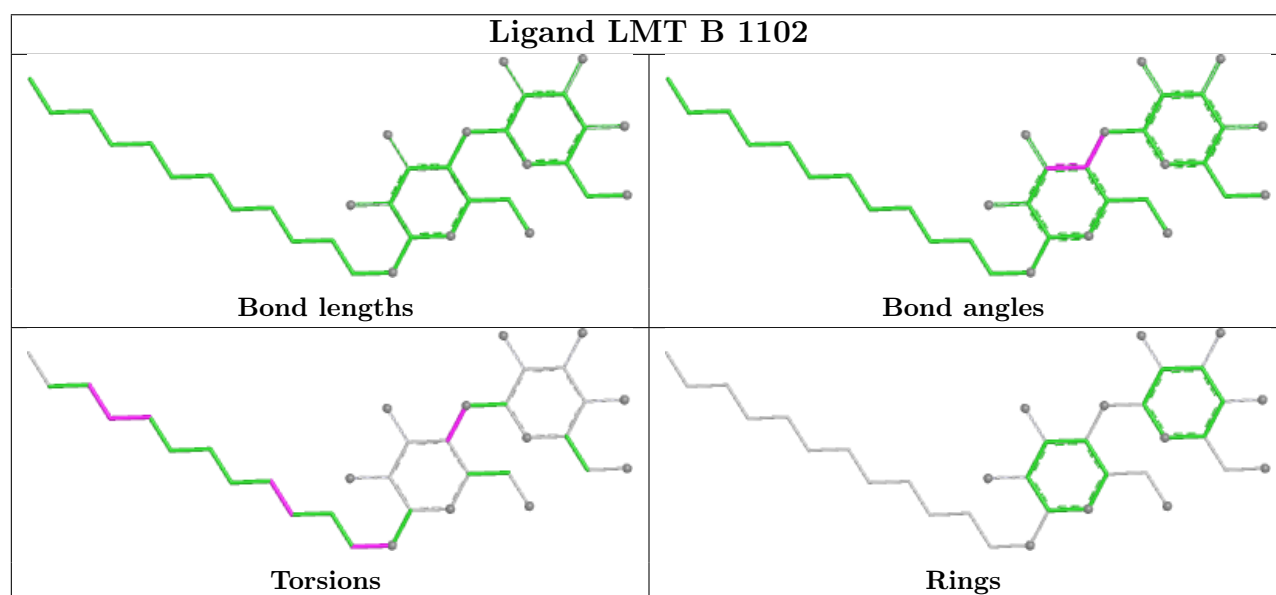
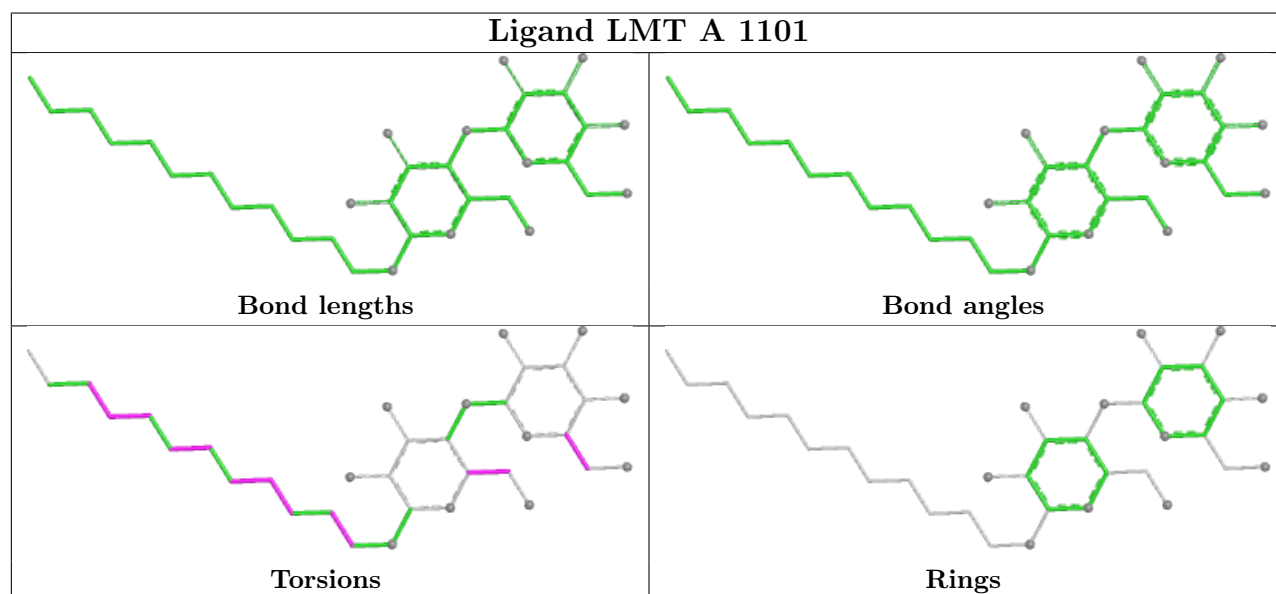
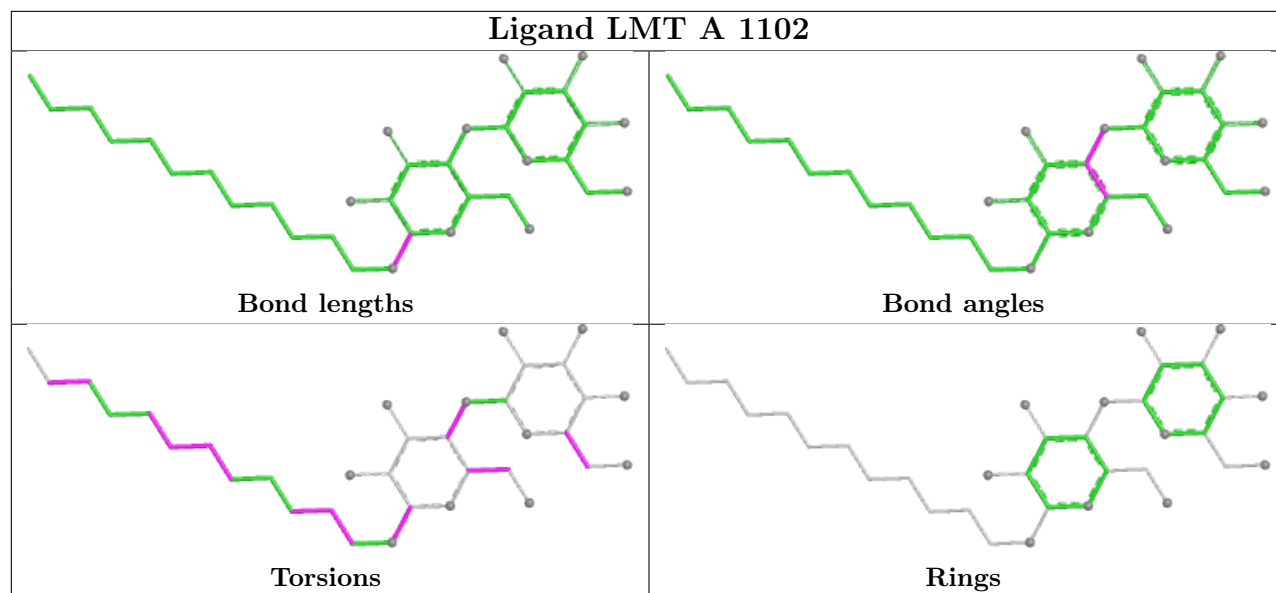
4 monomers are involved in 8 short contacts:

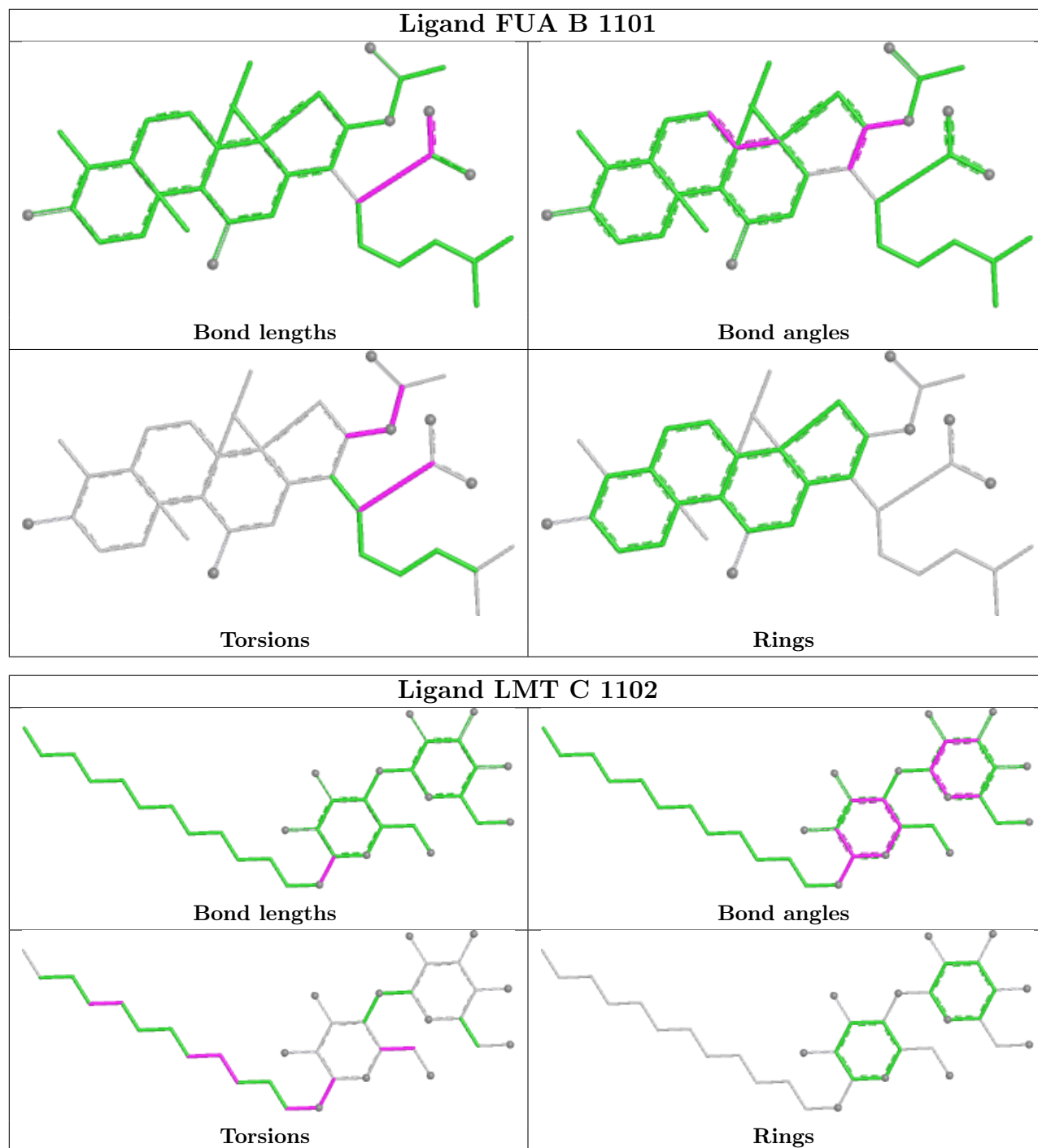
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	1116	PTY	2	0
3	B	1102	LMT	1	0
9	B	1101	FUA	6	0
8	B	1119	OCT	1	0

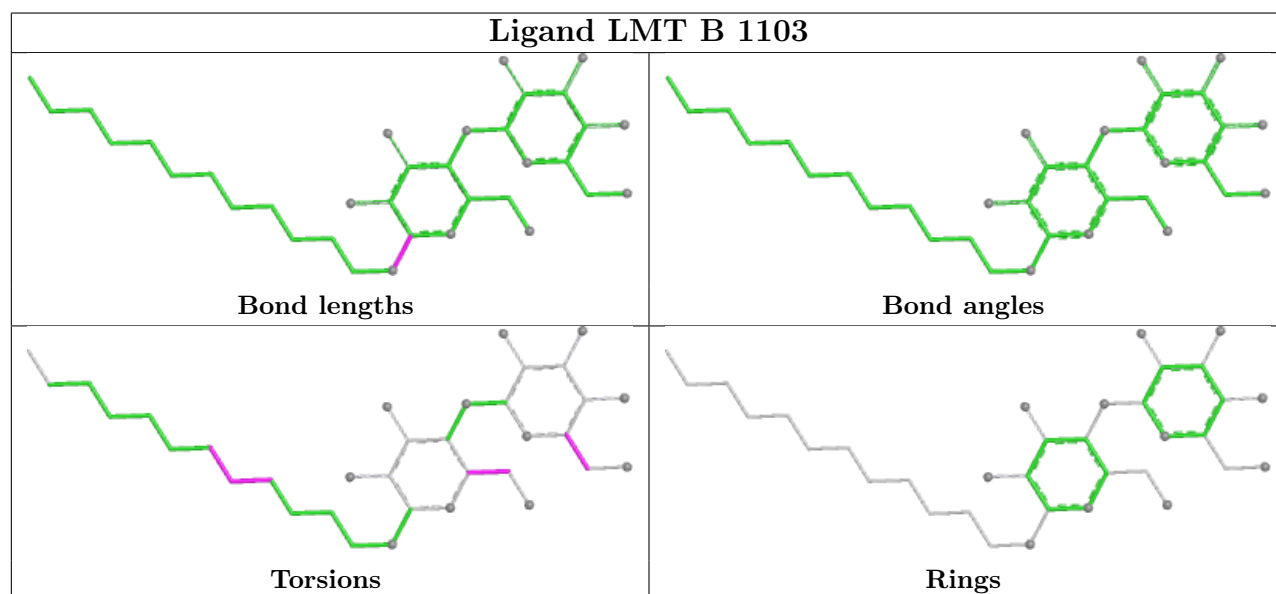
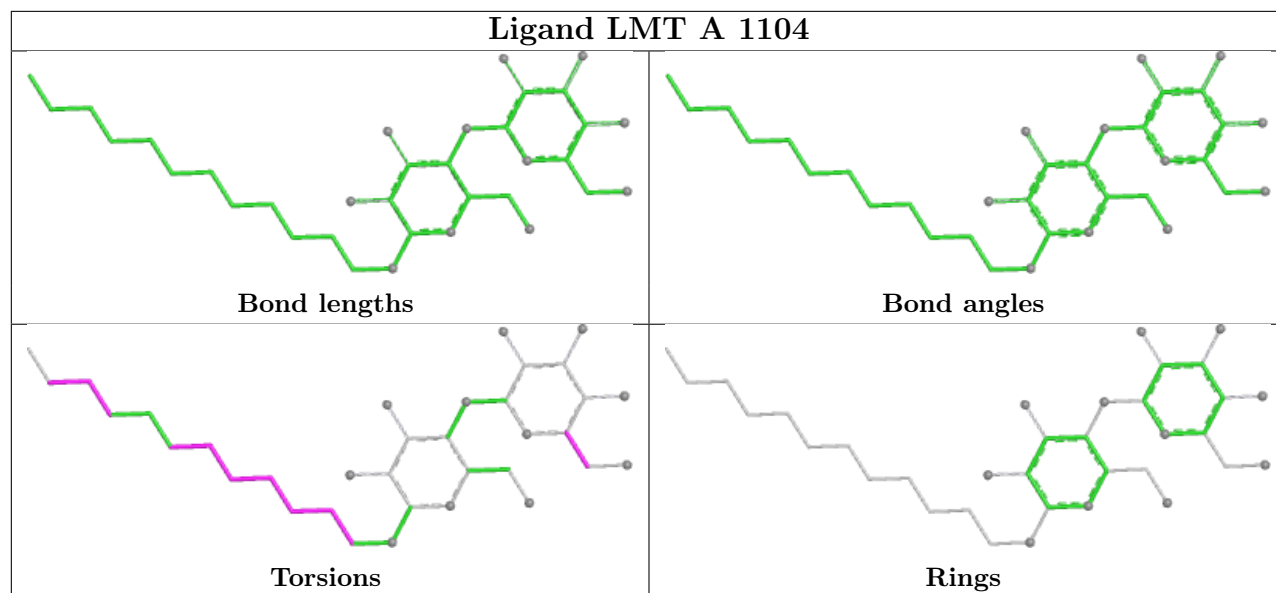
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

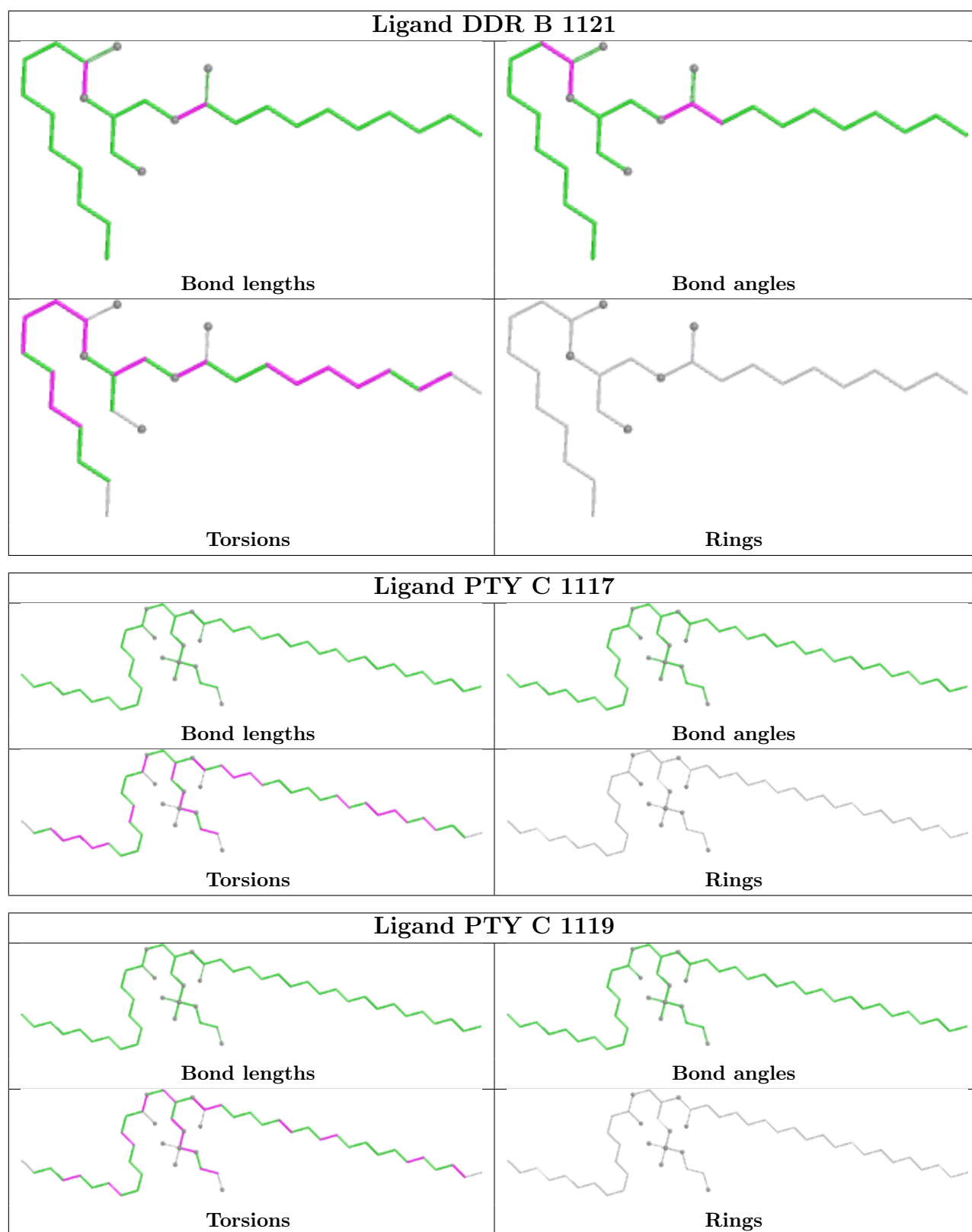












5.7 Other polymers [i](#)

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, 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%)	0.30	42 (4%)	42	33	20, 50, 87, 138	4 (0%)
1	B	1034/1057 (97%)	0.20	34 (3%)	49	39	27, 47, 73, 92	1 (0%)
1	C	1035/1057 (97%)	-0.00	13 (1%)	75	66	23, 42, 66, 100	1 (0%)
2	D	156/169 (92%)	0.23	4 (2%)	57	47	39, 48, 80, 105	0
2	E	154/169 (91%)	0.67	9 (5%)	29	22	42, 63, 88, 98	0
All	All	3421/3509 (97%)	0.19	102 (2%)	52	42	20, 47, 79, 138	6 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	618	ALA	6.8
1	A	672	VAL	6.8
1	A	868	LEU	6.3
1	A	676	THR	4.8
1	A	617	PHE	4.8

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(Å ²)	Q<0.9
7	HEX	B	1115	6/6	0.60	0.33	63,65,66,66	0
7	HEX	B	1117	6/6	0.61	0.47	69,69,70,70	0
7	HEX	A	1112	6/6	0.63	0.47	79,80,81,82	0
7	HEX	C	1114	6/6	0.65	0.36	69,72,73,73	0
7	HEX	C	1112	6/6	0.67	0.42	72,73,74,74	0
8	OCT	A	1114	8/8	0.67	0.26	65,66,67,67	0
5	DDQ	A	1108	14/14	0.70	0.40	104,113,120,121	0
5	DDQ	A	1109	14/14	0.72	0.41	97,100,100,100	0
7	HEX	B	1116	6/6	0.73	0.29	63,64,65,65	0
5	DDQ	B	1110	14/14	0.74	0.33	99,103,114,114	0
4	D10	C	1105	10/10	0.74	0.38	76,80,83,83	0
3	LMT	A	1101	35/35	0.75	0.23	80,107,125,126	0
7	HEX	C	1113	6/6	0.75	0.38	74,75,75,75	0
12	PTY	C	1119	50/50	0.75	0.31	99,115,144,151	0
10	D12	C	1120	12/12	0.76	0.31	62,69,74,74	0
6	GOL	B	1111	6/6	0.76	0.24	61,63,64,65	0
5	DDQ	C	1107	14/14	0.77	0.29	82,86,90,91	0
7	HEX	B	1114	6/6	0.78	0.24	67,67,68,68	0
3	LMT	C	1102	35/35	0.78	0.22	74,91,104,106	0
4	D10	A	1106	10/10	0.79	0.27	61,63,64,64	0
3	LMT	A	1103	35/35	0.79	0.23	78,110,135,135	0
7	HEX	C	1115	6/6	0.80	0.23	57,58,59,59	0
5	DDQ	B	1109	14/14	0.80	0.29	78,90,102,105	0
3	LMT	A	1104	35/35	0.80	0.19	79,91,102,103	0
12	PTY	C	1118	50/50	0.80	0.30	88,112,129,132	0
5	DDQ	A	1107	14/14	0.80	0.30	92,102,112,112	0
12	PTY	C	1116	50/50	0.81	0.25	65,95,115,125	0
12	PTY	C	1117	50/50	0.81	0.26	73,84,97,102	0
5	DDQ	B	1108	14/14	0.81	0.26	82,87,92,93	0
10	D12	C	1121	12/12	0.81	0.28	58,67,69,69	0
6	GOL	A	1111	6/6	0.82	0.18	72,73,73,74	0
4	D10	C	1103	10/10	0.82	0.26	68,69,69,70	0
10	D12	B	1120	12/12	0.82	0.24	69,70,70,71	0
6	GOL	E	201	6/6	0.83	0.15	61,62,63,64	0
4	D10	B	1106	10/10	0.83	0.26	56,56,57,57	0
8	OCT	A	1113	8/8	0.83	0.28	73,75,76,76	0
3	LMT	A	1102	35/35	0.83	0.18	64,81,98,99	0
8	OCT	B	1118	8/8	0.83	0.31	69,71,72,72	0
6	GOL	D	201	6/6	0.83	0.20	63,65,66,68	0
4	D10	B	1104	10/10	0.84	0.22	60,62,62,63	0
5	DDQ	B	1107	14/14	0.84	0.24	70,76,92,93	0

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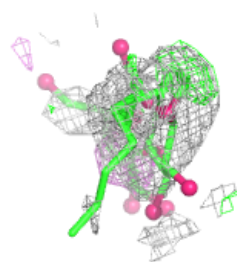
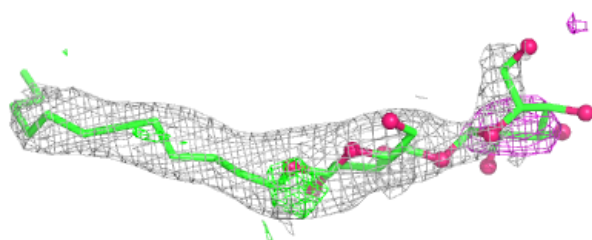
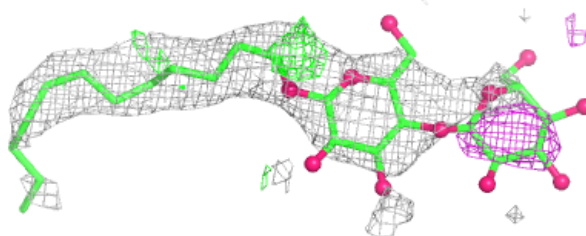
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	B	1113	6/6	0.84	0.22	69,70,71,72	0
4	D10	B	1105	10/10	0.85	0.23	63,65,68,68	0
10	D12	C	1122	12/12	0.85	0.28	78,79,81,81	0
8	OCT	B	1119	8/8	0.85	0.30	83,85,86,86	0
6	GOL	C	1111	6/6	0.86	0.20	71,73,74,74	0
4	D10	A	1105	10/10	0.87	0.23	71,74,74,75	0
6	GOL	B	1112	6/6	0.88	0.14	52,54,56,59	0
5	DDQ	C	1106	14/14	0.88	0.23	76,78,81,82	0
3	LMT	B	1102	35/35	0.89	0.14	64,67,69,71	0
6	GOL	A	1110	6/6	0.89	0.19	63,63,64,64	0
4	D10	C	1104	10/10	0.90	0.19	57,61,63,63	0
6	GOL	C	1110	6/6	0.91	0.18	65,67,67,68	0
3	LMT	B	1103	35/35	0.91	0.14	61,68,89,90	0
6	GOL	C	1109	6/6	0.91	0.14	58,60,62,62	0
11	DDR	B	1121	28/28	0.91	0.22	75,88,99,101	0
9	FUA	B	1101	37/37	0.92	0.12	64,66,71,72	0
3	LMT	C	1101	35/35	0.93	0.12	52,60,76,76	0
13	SO4	C	1123	5/5	0.94	0.17	67,67,67,68	0
6	GOL	C	1108	6/6	0.96	0.09	37,39,39,40	0

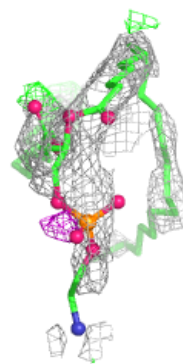
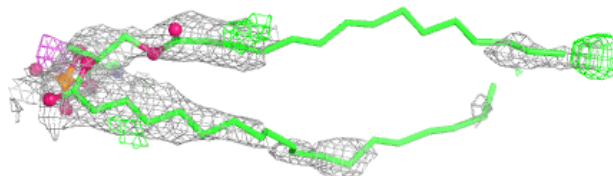
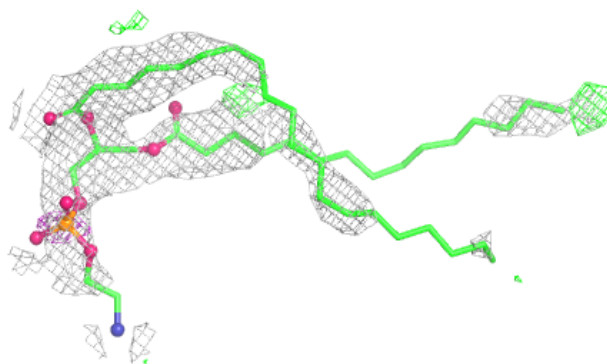
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1101:

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

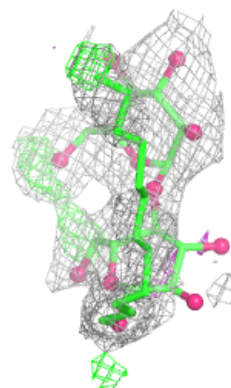
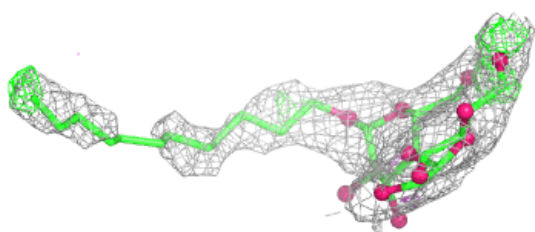
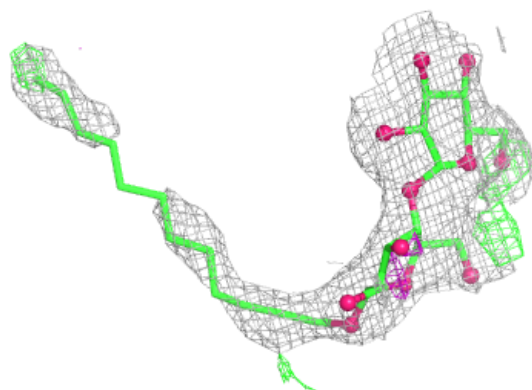
**Electron density around PTY C 1119:**

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

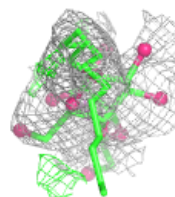
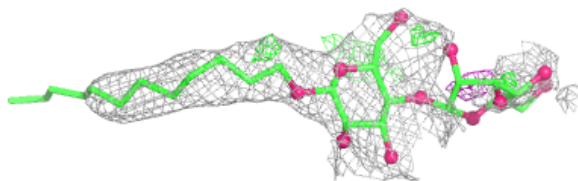
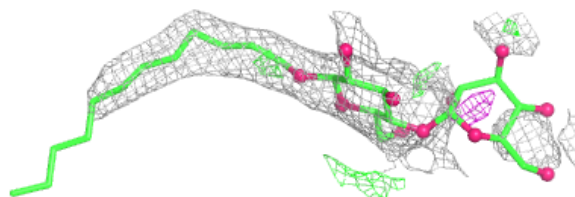


Electron density around LMT C 1102:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

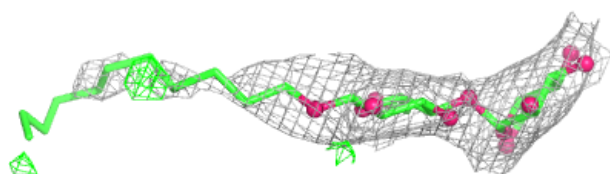
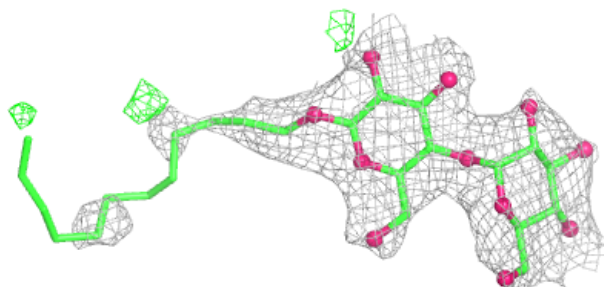
**Electron density around LMT A 1103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

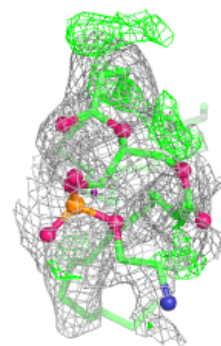
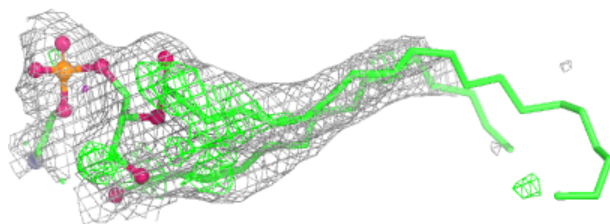
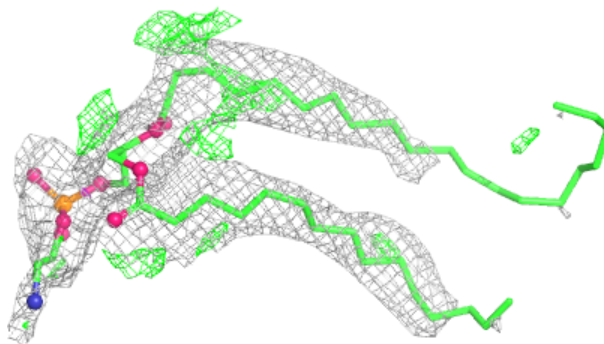


Electron density around LMT A 1104:

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

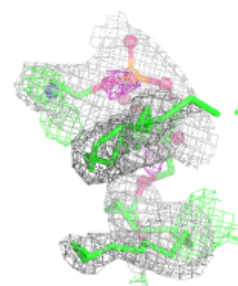
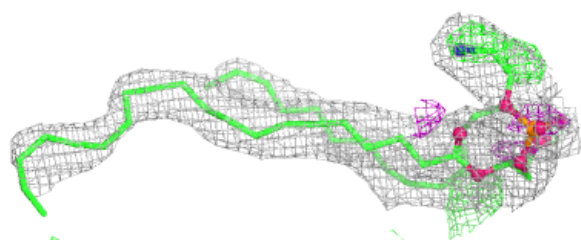
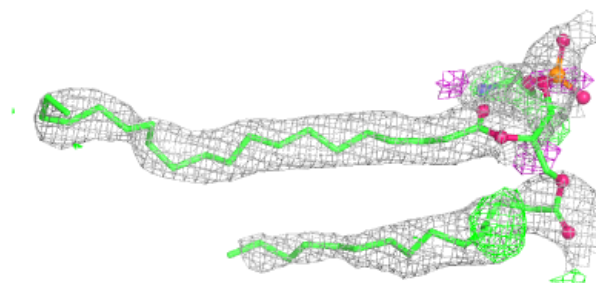
**Electron density around PTY C 1118:**

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and green (positive)

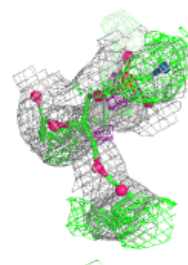
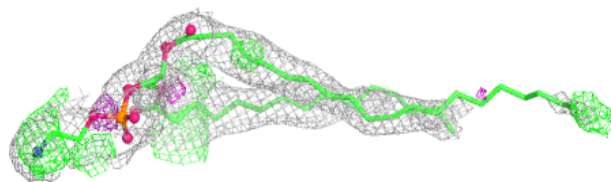
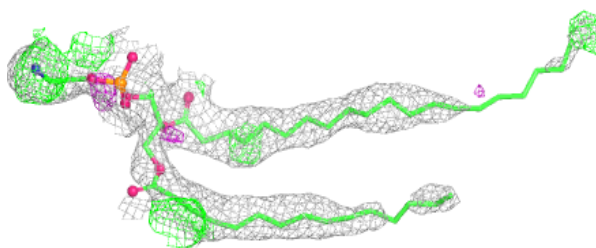


Electron density around PTY C 1116:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

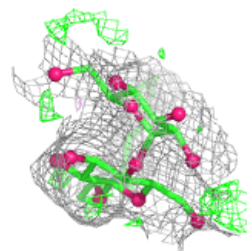
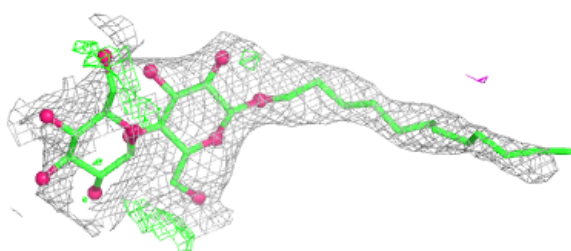
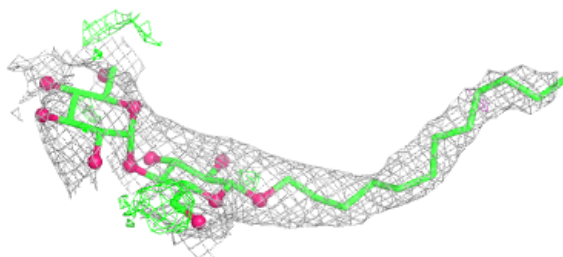
**Electron density around PTY C 1117:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

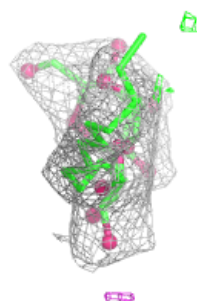
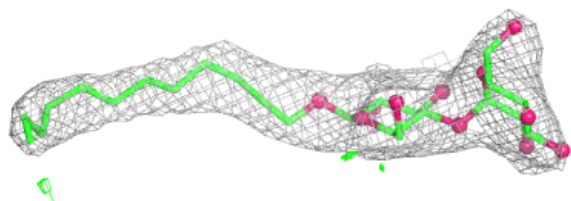
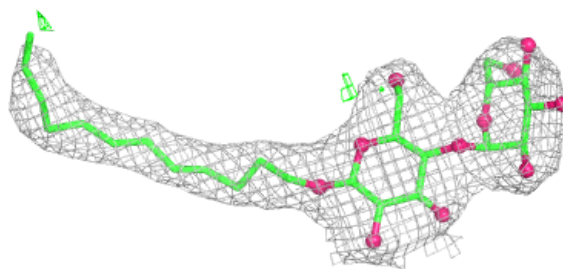


Electron density around LMT A 1102:

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

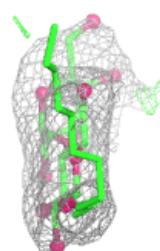
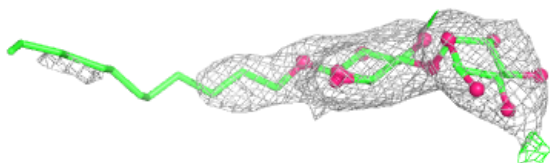
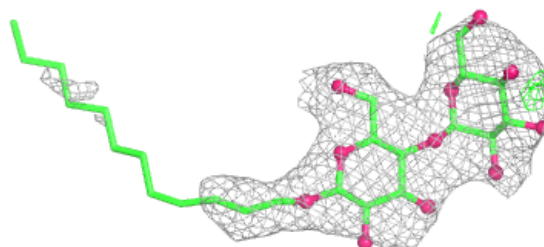
**Electron density around LMT B 1102:**

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



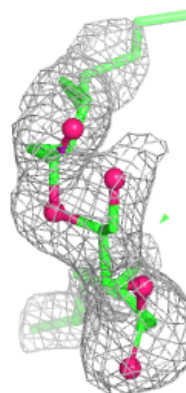
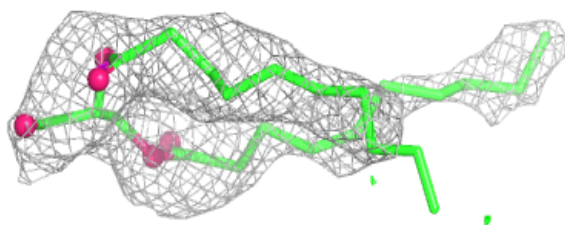
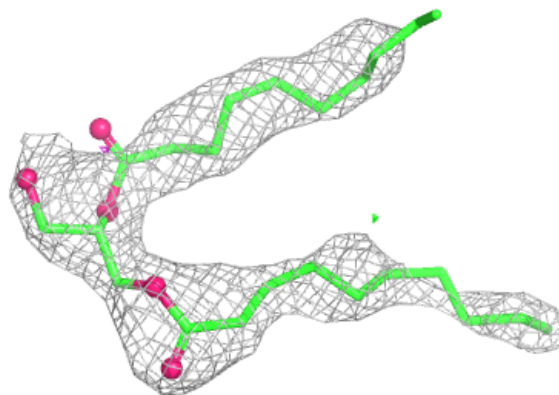
Electron density around LMT B 1103:

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



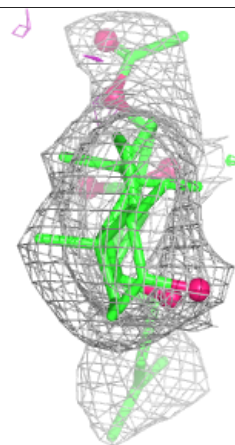
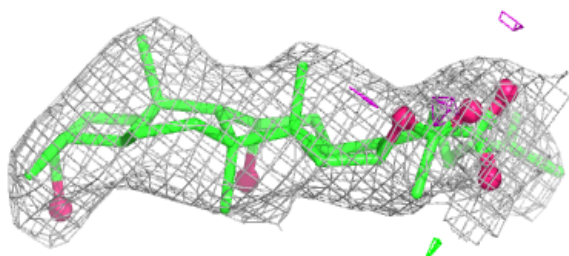
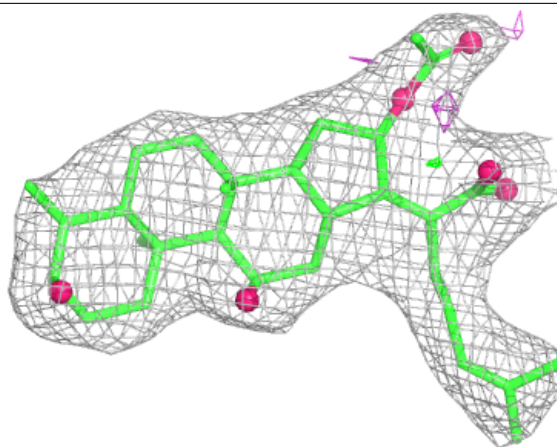
Electron density around DDR B 1121:

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



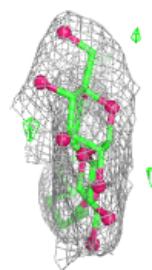
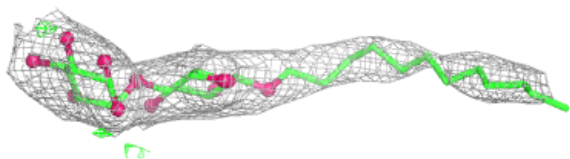
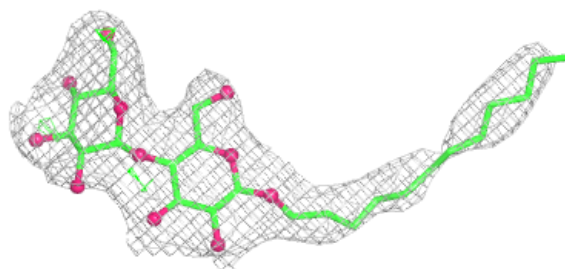
Electron density around FUA B 1101:

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



Electron density around LMT C 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 ⓘ

There are no such residues in this entry.