Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2021 – 03:10 pm GMT

PDB ID	:	7OUK
Title	:	BDM88855 inhibitor bound to the transmembrane domain of AcrB
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2021-06-12
Resolution	:	2.60 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:

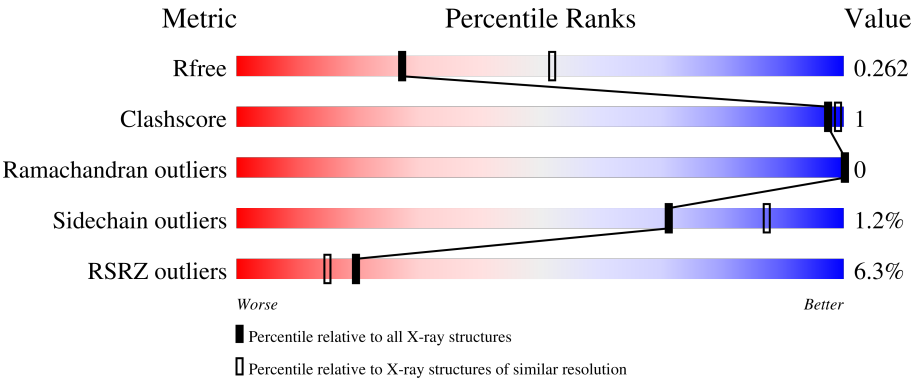
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	7% 95%
1	B	1057	5% 94%
1	C	1057	3% 94%
2	D	169	9% 91% 8%
2	E	169	21% 89% 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	EDO	C	1712	-	-	-	X
6	OCT	C	1704	-	-	-	X
8	GOL	B	1512	-	-	-	X

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 26935 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	1033	Total	C	N	O	S	0	1	0
			7873	5066	1299	1463	45			
1	B	1036	Total	C	N	O	S	0	1	0
			7883	5072	1303	1463	45			
1	C	1033	Total	C	N	O	S	0	3	0
			7874	5067	1303	1460	44			

There are 24 discrepancies between the modelled and reference sequences:

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

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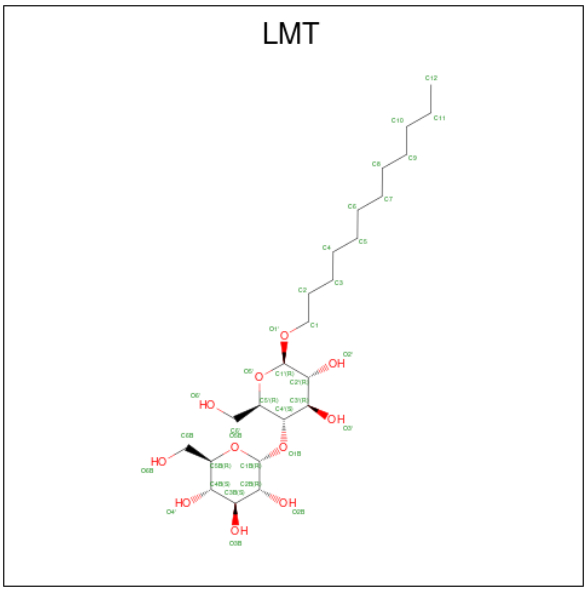
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1182	745	207	229	1			
2	E	153	Total	C	N	O	S	0	0	0
			1159	732	203	223	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		
3	B	1	Total	C	O	0	0
			35	24	11		

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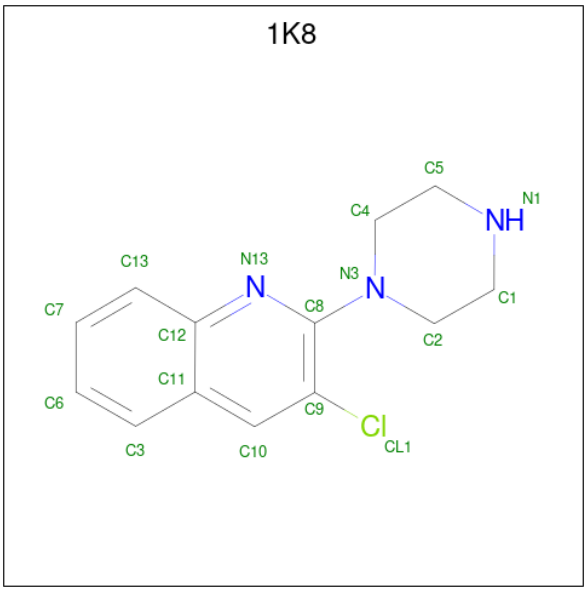
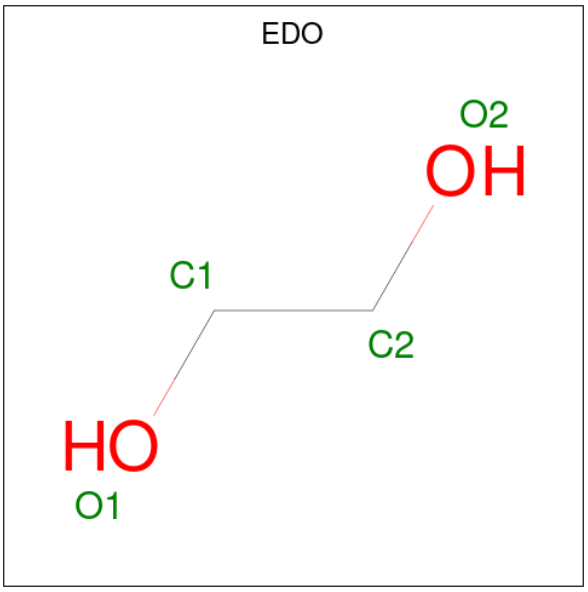
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0

- Molecule 4 is 3-chloranyl-2-piperazin-1-yl-quinoline (three-letter code: 1K8) (formula: $C_{13}H_{14}ClN_3$) (labeled as "Ligand of Interest" by depositor).



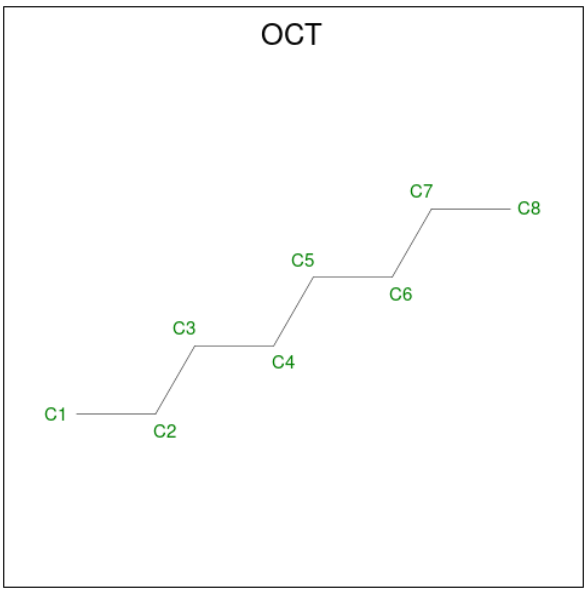
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C Cl N 17 13 1 3	0	0
4	B	1	Total C Cl N 17 13 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



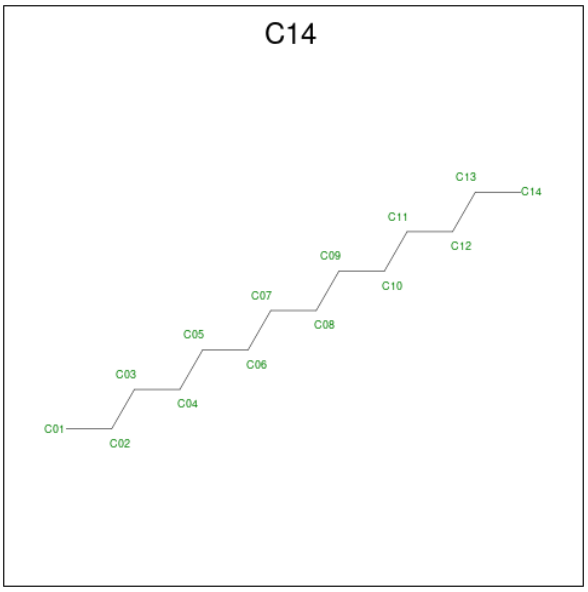
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

- Molecule 6 is N-OCTANE (three-letter code: OCT) (formula: C_8H_{18}).



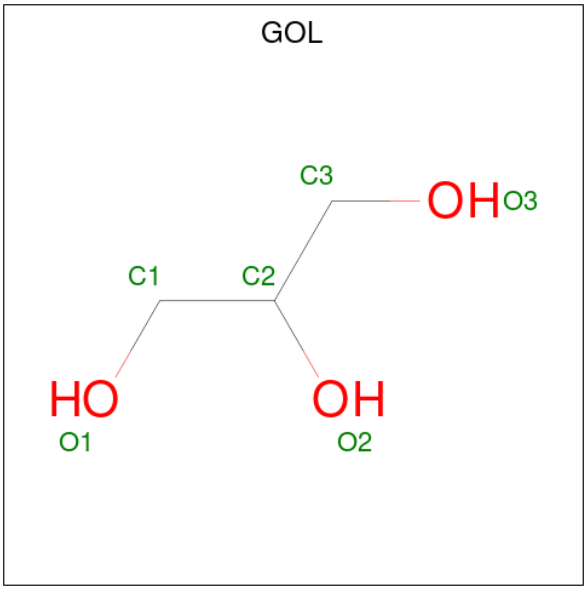
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0

- Molecule 7 is TETRADECANE (three-letter code: C14) (formula: $C_{14}H_{30}$).



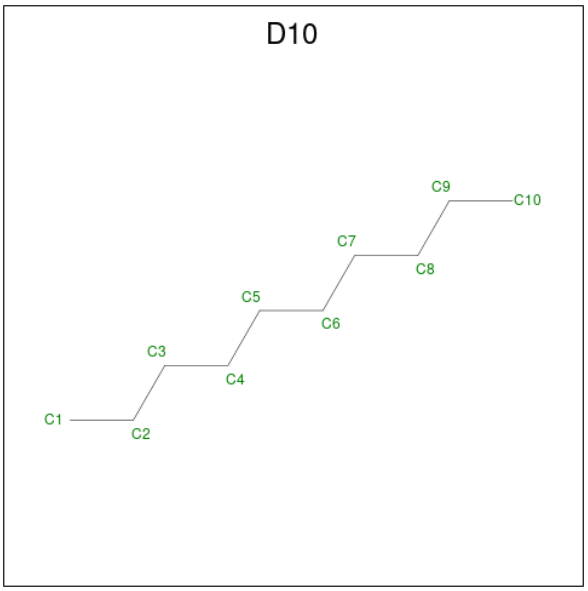
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 14 14	0	0
7	A	1	Total C 14 14	0	0
7	C	1	Total C 14 14	0	0

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



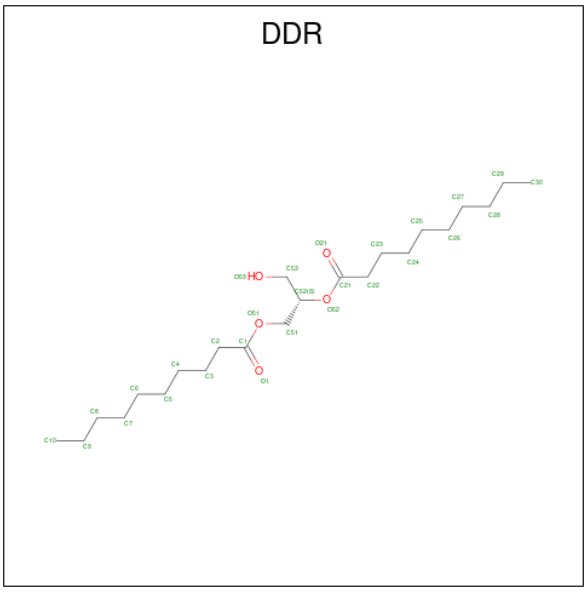
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



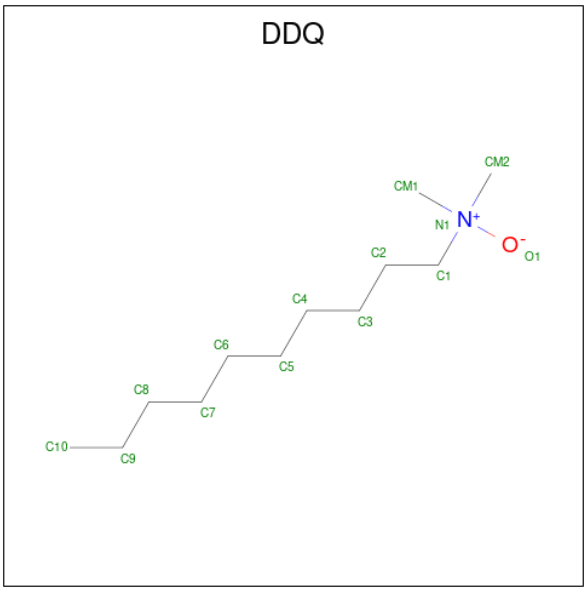
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C 10 10	0	0

- Molecule 10 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (three-letter code: DDR) (formula: $C_{23}H_{44}O_5$).



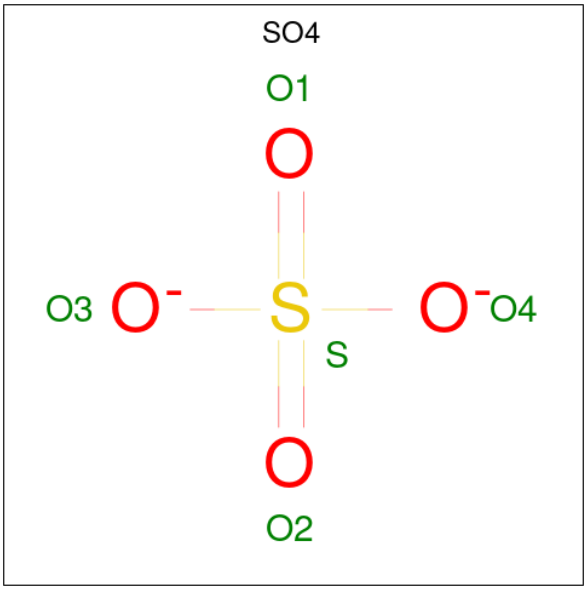
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 28 23 5	0	0

- Molecule 11 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



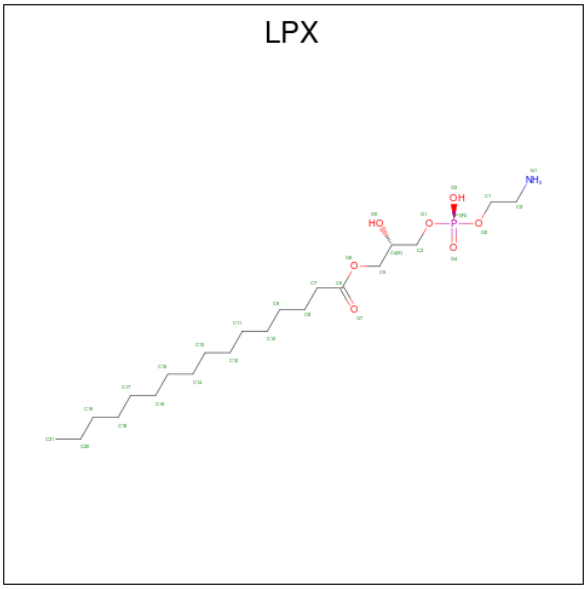
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 13 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
13	C	1	Total	C	N	O	P	0	0
			30	21	1	7	1		
13	C	1	Total	C	N	O	P	0	0
			30	21	1	7	1		

- Molecule 14 is water.

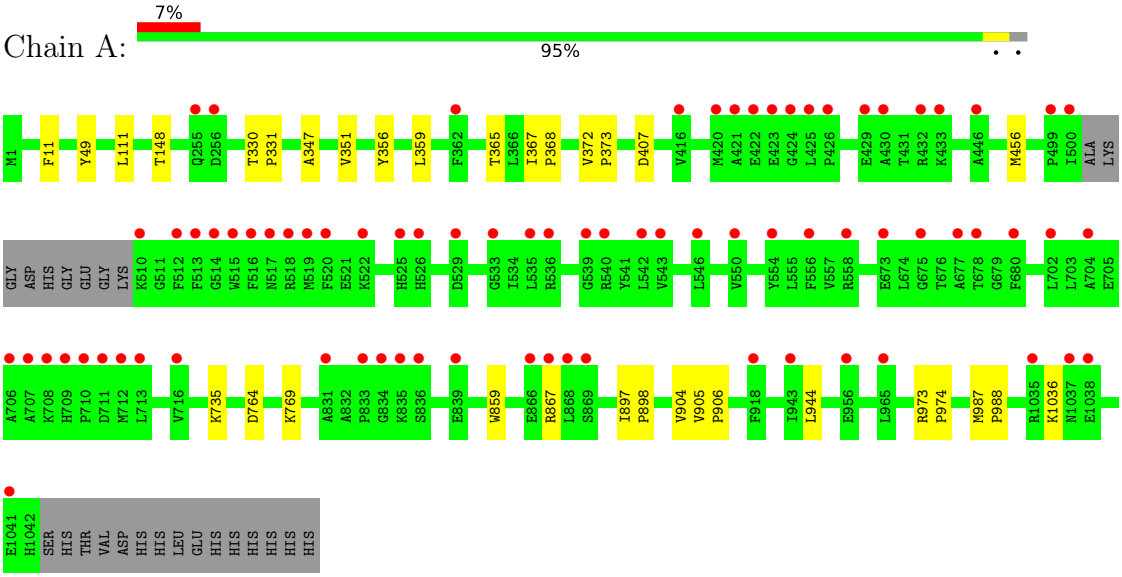
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	128	Total	O	0	0
			128	128		
14	B	94	Total	O	0	0
			94	94		
14	C	120	Total	O	0	0
			120	120		
14	D	14	Total	O	0	0
			14	14		
14	E	9	Total	O	0	0
			9	9		

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.

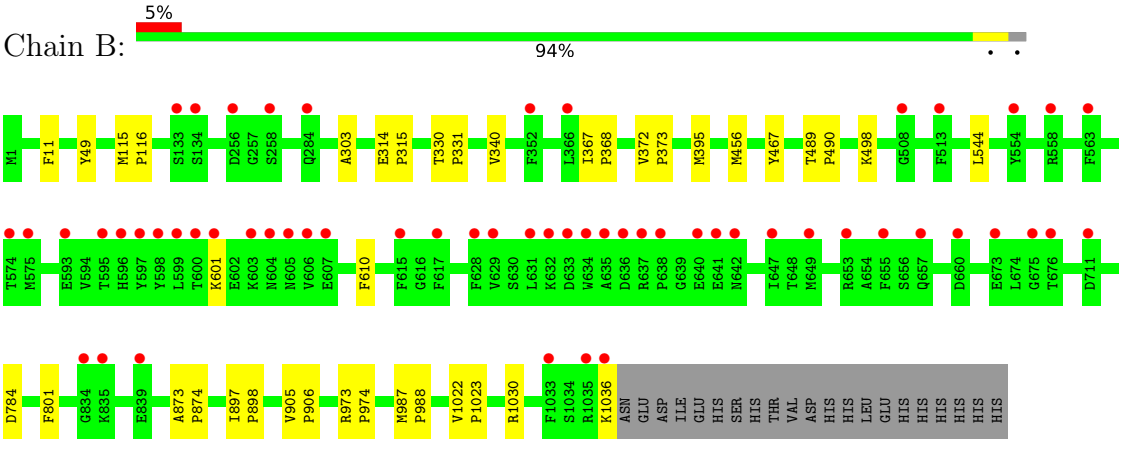
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain A:



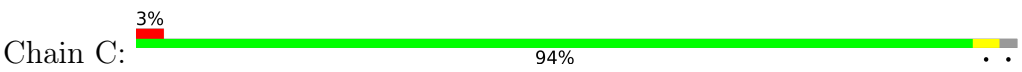
• Molecule 1: Multidrug efflux pump subunit AcrB

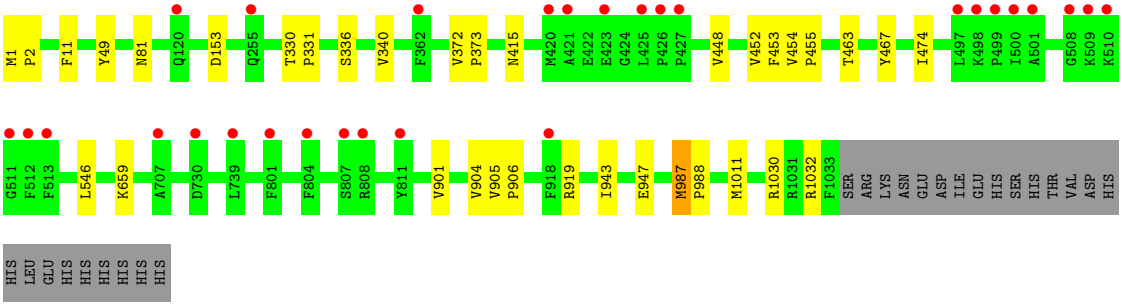
Chain B:



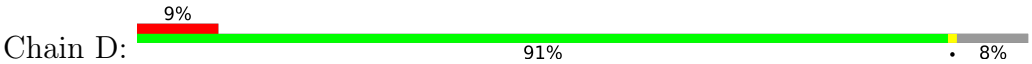
• Molecule 1: Multidrug efflux pump subunit AcrB

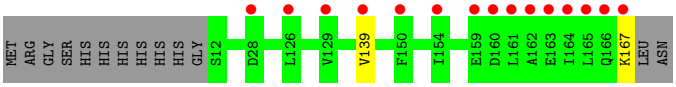
Chain C:



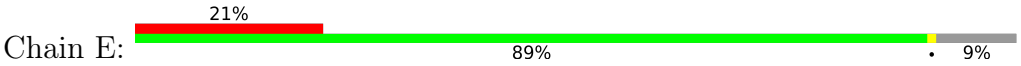


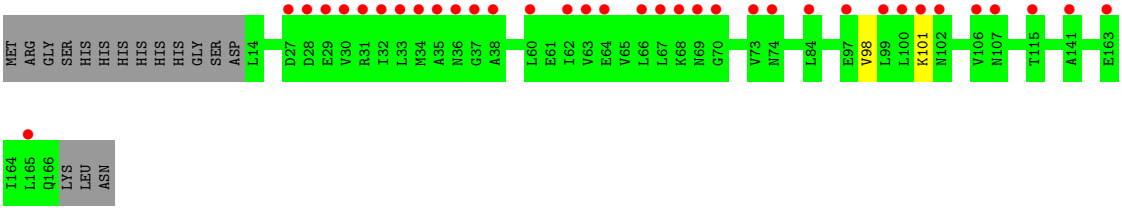
• Molecule 2: DARPIN





• 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	146.13Å 159.65Å 245.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 49.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-2.60) 99.9 (49.00-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.263 0.237 , 0.262	Depositor DCC
R_{free} test set	8846 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26935	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: D10, DDR, 1K8, LPX, OCT, GOL, DDQ, EDO, LMT, C14, SO4

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	0/8022	0.70	0/10893
1	B	0.67	0/8033	0.70	0/10906
1	C	0.67	0/8030	0.70	0/10904
2	D	0.68	0/1201	0.71	0/1632
2	E	0.68	0/1178	0.71	0/1602
All	All	0.67	0/26464	0.70	0/35937

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	7873	0	8022	12	0
1	B	7883	0	8040	17	0
1	C	7874	0	8035	12	0
2	D	1182	0	1169	1	0
2	E	1159	0	1147	1	0
3	A	105	0	138	0	0
3	B	105	0	138	0	0
3	C	70	0	92	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	17	0	0	0	0
4	B	17	0	0	1	0
5	A	20	0	30	0	0
5	B	20	0	30	0	0
5	C	16	0	24	0	0
6	A	8	0	18	0	0
6	C	16	0	36	0	0
7	A	28	0	60	0	0
7	C	14	0	30	0	0
8	A	6	0	8	0	0
8	B	24	0	32	0	0
8	C	6	0	8	0	0
9	B	10	0	22	0	0
10	B	28	0	44	0	0
11	B	14	0	27	0	0
12	B	10	0	0	0	0
12	C	5	0	0	0	0
13	C	60	0	86	0	0
14	A	128	0	0	0	0
14	B	94	0	0	0	0
14	C	120	0	0	0	0
14	D	14	0	0	0	0
14	E	9	0	0	0	0
All	All	26935	0	27236	44	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 (44) 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:372:VAL:HB	1:C:373:PRO:HD3	1.88	0.56
1:A:356:TYR:HA	1:A:365:THR:HG21	1.87	0.55
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.91	0.52
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.94	0.49
1:C:901:VAL:O	1:C:904:VAL:HG12	2.12	0.49
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49
2:E:98:VAL:HA	2:E:101:LYS:HE2	1.95	0.48
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.96	0.48
1:C:330:THR:N	1:C:331:PRO:CD	2.77	0.47
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.95	0.47
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.29	0.47
4:B:1516:1K8:C4	4:B:1516:1K8:CL1	3.00	0.47
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.97	0.47
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.97	0.47
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.98	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.99	0.45
1:A:987:MET:N	1:A:988:PRO:CD	2.80	0.44
1:B:330:THR:N	1:B:331:PRO:CD	2.81	0.44
1:B:115:MET:N	1:B:116:PRO:CD	2.81	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
2:D:139:VAL:HG11	2:D:167:LYS:HA	2.00	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43
1:B:897:ILE:N	1:B:898:PRO:CD	2.81	0.43
1:B:973:ARG:N	1:B:974:PRO:HD2	2.33	0.43
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.53	0.43
1:A:859:TRP:CD1	1:A:867:ARG:HD2	2.53	0.43
1:A:764:ASP:HB3	1:A:769:LYS:HD2	2.00	0.43
1:A:347:ALA:O	1:A:351:VAL:HG23	2.19	0.43
1:C:336:SER:O	1:C:340:VAL:HG23	2.19	0.43
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.55	0.42
1:A:359:LEU:HD12	1:A:365:THR:HG22	2.01	0.42
1:A:897:ILE:N	1:A:898:PRO:CD	2.83	0.42
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.42
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.55	0.42
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.02	0.41
1:B:340:VAL:HG21	1:B:395[B]:MET:HB3	2.02	0.41
1:B:905:VAL:HB	1:B:906:PRO:HD3	2.02	0.41
1:C:448:VAL:HG11	1:C:943:ILE:HD11	2.02	0.41
1:B:897:ILE:N	1:B:898:PRO:HD2	2.36	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.21	0.41
1:B:456:MET:HG2	1:B:467:TYR:HB3	2.03	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%)	989 (96%)	41 (4%)	0	100	100
1	B	1035/1057 (98%)	1011 (98%)	24 (2%)	0	100	100
1	C	1034/1057 (98%)	1007 (97%)	27 (3%)	0	100	100
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	151/169 (89%)	145 (96%)	6 (4%)	0	100	100
All	All	3404/3509 (97%)	3303 (97%)	101 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	844/863 (98%)	834 (99%)	10 (1%)	71	87
1	B	843/863 (98%)	833 (99%)	10 (1%)	71	87
1	C	842/863 (98%)	829 (98%)	13 (2%)	65	83
2	D	121/132 (92%)	121 (100%)	0	100	100
2	E	118/132 (89%)	118 (100%)	0	100	100
All	All	2768/2853 (97%)	2735 (99%)	33 (1%)	71	87

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	111	LEU
1	A	148	THR
1	A	407	ASP
1	A	456	MET
1	A	735	LYS
1	A	904	VAL
1	A	944	LEU
1	A	1036	LYS
1	B	11	PHE
1	B	49	TYR
1	B	498	LYS
1	B	544	LEU
1	B	601	LYS
1	B	610	PHE
1	B	784	ASP
1	B	801	PHE
1	B	1030	ARG
1	B	1036	LYS
1	C	11	PHE
1	C	49	TYR
1	C	81	ASN
1	C	153	ASP
1	C	415	ASN
1	C	546	LEU
1	C	659	LYS
1	C	919	ARG
1	C	947	GLU
1	C	987	MET
1	C	1011	MET
1	C	1030	ARG
1	C	1032	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

44 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	EDO	A	1110	-	3,3,3	0.06	0	2,2,2	0.17	0
8	GOL	B	1509	-	5,5,5	0.09	0	5,5,5	0.26	0
3	LMT	C	1708	-	36,36,36	0.58	1 (2%)	47,47,47	0.94	3 (6%)
5	EDO	C	1710	-	3,3,3	0.06	0	2,2,2	0.16	0
5	EDO	C	1702	-	3,3,3	0.07	0	2,2,2	0.19	0
8	GOL	A	1107	-	5,5,5	0.11	0	5,5,5	0.29	0
4	1K8	B	1516	-	19,19,19	2.79	4 (21%)	24,26,26	1.49	5 (20%)
5	EDO	C	1711	-	3,3,3	0.05	0	2,2,2	0.21	0
9	D10	B	1505	-	9,9,9	0.10	0	8,8,8	0.06	0
8	GOL	B	1511	-	5,5,5	0.09	0	5,5,5	0.31	0
4	1K8	A	1102	-	19,19,19	2.66	5 (26%)	24,26,26	1.37	2 (8%)
11	DDQ	B	1515	-	10,13,13	0.12	0	12,15,15	0.25	0
5	EDO	A	1109	-	3,3,3	0.05	0	2,2,2	0.18	0
10	DDR	B	1508	-	27,27,27	0.26	0	29,29,29	0.37	0
5	EDO	B	1513	-	3,3,3	0.06	0	2,2,2	0.17	0
5	EDO	A	1104	-	3,3,3	0.07	0	2,2,2	0.14	0
5	EDO	C	1712	-	3,3,3	0.08	0	2,2,2	0.30	0
8	GOL	C	1709	-	5,5,5	0.09	0	5,5,5	0.28	0
3	LMT	C	1703	-	36,36,36	0.45	0	47,47,47	0.49	0
6	OCT	C	1704	-	7,7,7	0.11	0	6,6,6	0.07	0
13	LPX	C	1707	-	29,29,29	0.29	0	31,33,33	0.35	0
7	C14	A	1106	-	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	$\#\|Z\|>2$
8	GOL	B	1512	-	5,5,5	0.10	0	5,5,5	0.29	0
12	SO4	B	1518	-	4,4,4	0.40	0	6,6,6	0.04	0
5	EDO	B	1501	-	3,3,3	0.06	0	2,2,2	0.15	0
3	LMT	B	1510	-	36,36,36	0.51	0	47,47,47	0.97	3 (6%)
7	C14	C	1706	-	13,13,13	0.08	0	12,12,12	0.05	0
3	LMT	B	1503	-	36,36,36	0.46	0	47,47,47	0.57	0
5	EDO	A	1113	-	3,3,3	0.06	0	2,2,2	0.18	0
13	LPX	C	1705	-	29,29,29	0.28	0	31,33,33	0.35	0
5	EDO	B	1506	-	3,3,3	0.07	0	2,2,2	0.20	0
5	EDO	A	1112	-	3,3,3	0.06	0	2,2,2	0.17	0
6	OCT	C	1701	-	7,7,7	0.11	0	6,6,6	0.07	0
6	OCT	A	1105	-	7,7,7	0.11	0	6,6,6	0.07	0
3	LMT	A	1101	-	36,36,36	0.44	0	47,47,47	0.61	0
8	GOL	B	1502	-	5,5,5	0.10	0	5,5,5	0.26	0
12	SO4	C	1713	-	4,4,4	0.39	0	6,6,6	0.05	0
5	EDO	B	1514	-	3,3,3	0.06	0	2,2,2	0.21	0
7	C14	A	1108	-	13,13,13	0.09	0	12,12,12	0.07	0
3	LMT	A	1103	-	36,36,36	0.52	1 (2%)	47,47,47	0.83	2 (4%)
3	LMT	A	1111	-	36,36,36	0.50	1 (2%)	47,47,47	0.73	1 (2%)
12	SO4	B	1517	-	4,4,4	0.40	0	6,6,6	0.05	0
3	LMT	B	1504	-	36,36,36	0.52	0	47,47,47	0.98	2 (4%)
5	EDO	B	1507	-	3,3,3	0.06	0	2,2,2	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1110	-	-	1/1/1/1	-
8	GOL	B	1509	-	-	0/4/4/4	-
3	LMT	C	1708	-	-	11/21/61/61	0/2/2/2
5	EDO	C	1710	-	-	0/1/1/1	-
5	EDO	C	1702	-	-	1/1/1/1	-
8	GOL	A	1107	-	-	2/4/4/4	-
4	1K8	B	1516	-	-	0/4/12/12	0/3/3/3
5	EDO	C	1711	-	-	1/1/1/1	-
9	D10	B	1505	-	-	4/7/7/7	-
8	GOL	B	1511	-	-	2/4/4/4	-
4	1K8	A	1102	-	-	2/4/12/12	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	DDQ	B	1515	-	-	5/11/11/11	-
5	EDO	A	1109	-	-	0/1/1/1	-
10	DDR	B	1508	-	-	15/29/29/29	-
5	EDO	B	1513	-	-	1/1/1/1	-
5	EDO	A	1104	-	-	1/1/1/1	-
5	EDO	C	1712	-	-	1/1/1/1	-
8	GOL	C	1709	-	-	4/4/4/4	-
3	LMT	C	1703	-	-	8/21/61/61	0/2/2/2
6	OCT	C	1704	-	-	1/5/5/5	-
13	LPX	C	1707	-	-	17/31/31/31	-
7	C14	A	1106	-	-	3/11/11/11	-
8	GOL	B	1512	-	-	2/4/4/4	-
5	EDO	B	1501	-	-	0/1/1/1	-
3	LMT	B	1510	-	-	10/21/61/61	0/2/2/2
7	C14	C	1706	-	-	6/11/11/11	-
3	LMT	B	1503	-	-	9/21/61/61	0/2/2/2
5	EDO	A	1113	-	-	1/1/1/1	-
13	LPX	C	1705	-	-	15/31/31/31	-
5	EDO	B	1506	-	-	1/1/1/1	-
5	EDO	A	1112	-	-	0/1/1/1	-
6	OCT	C	1701	-	-	1/5/5/5	-
6	OCT	A	1105	-	-	0/5/5/5	-
3	LMT	A	1101	-	-	7/21/61/61	0/2/2/2
8	GOL	B	1502	-	-	2/4/4/4	-
5	EDO	B	1514	-	-	0/1/1/1	-
7	C14	A	1108	-	-	5/11/11/11	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1111	-	-	10/21/61/61	0/2/2/2
3	LMT	B	1504	-	-	12/21/61/61	0/2/2/2
5	EDO	B	1507	-	-	1/1/1/1	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1516	1K8	C9-C8	9.09	1.51	1.39
4	A	1102	1K8	C9-C8	8.46	1.50	1.39
4	A	1102	1K8	C11-C12	4.57	1.49	1.42
4	B	1516	1K8	C11-C12	4.52	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1516	1K8	C8-N13	4.41	1.36	1.31
4	A	1102	1K8	C8-N13	4.03	1.36	1.31
4	A	1102	1K8	C9-CL1	2.80	1.80	1.73
4	B	1516	1K8	C9-CL1	2.60	1.79	1.73
3	C	1708	LMT	O1'-C1'	2.27	1.44	1.40
3	A	1103	LMT	O1'-C1'	2.25	1.44	1.40
3	A	1111	LMT	O1'-C1'	2.06	1.43	1.40
4	A	1102	1K8	C10-C9	2.04	1.39	1.36

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	1K8	C4-N3-C2	4.67	121.83	111.52
3	B	1510	LMT	O1B-C4'-C3'	3.37	116.24	107.28
3	C	1708	LMT	C1'-C2'-C3'	3.35	116.97	110.00
4	B	1516	1K8	C8-N13-C12	3.03	122.51	116.11
4	B	1516	1K8	C5-C4-N3	-3.00	103.98	110.48
3	B	1504	LMT	C1'-C2'-C3'	3.00	116.25	110.00
3	B	1504	LMT	C2'-C3'-C4'	2.93	116.36	109.68
4	B	1516	1K8	C10-C9-CL1	-2.70	116.52	119.20
4	B	1516	1K8	C9-C8-N13	-2.70	118.11	122.70
3	B	1510	LMT	C1B-O5B-C5B	2.66	118.92	113.69
4	A	1102	1K8	C8-N13-C12	2.62	121.65	116.11
3	C	1708	LMT	C2'-C3'-C4'	2.53	115.45	109.68
3	A	1111	LMT	O1B-C4'-C3'	2.29	113.38	107.28
3	C	1708	LMT	O1B-C4'-C3'	2.29	113.37	107.28
4	B	1516	1K8	C8-C9-CL1	2.19	123.32	121.43
3	A	1103	LMT	C3B-C4B-C5B	2.15	114.08	110.24
3	B	1510	LMT	C1B-O1B-C4'	2.14	123.26	117.96
3	A	1103	LMT	O1'-C1'-C2'	2.07	111.54	108.30

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1111	LMT	C2'-C1'-O1'-C1
3	B	1503	LMT	C2'-C1'-O1'-C1
3	B	1503	LMT	O5'-C1'-O1'-C1
3	C	1703	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
4	A	1102	1K8	C9-C8-N3-C2
4	A	1102	1K8	N13-C8-N3-C2
8	A	1107	GOL	O2-C2-C3-O3
8	B	1502	GOL	O1-C1-C2-C3
8	B	1511	GOL	O1-C1-C2-O2
8	B	1511	GOL	O1-C1-C2-C3
8	B	1512	GOL	C1-C2-C3-O3
8	C	1709	GOL	C1-C2-C3-O3
10	B	1508	DDR	C22-C21-O52-C52
13	C	1705	LPX	C3-O1-P1-O3
13	C	1705	LPX	C3-O1-P1-O2
13	C	1705	LPX	C3-O1-P1-O4
13	C	1705	LPX	O2-C1-C2-N1
13	C	1707	LPX	O5-C4-C5-O6
13	C	1707	LPX	C3-C4-C5-O6
13	C	1707	LPX	C1-O2-P1-O3
3	B	1510	LMT	C3'-C4'-O1B-C1B
10	B	1508	DDR	O21-C21-O52-C52
3	A	1111	LMT	C3'-C4'-O1B-C1B
10	B	1508	DDR	C2-C1-O51-C51
3	B	1510	LMT	O5'-C5'-C6'-O6'
3	B	1503	LMT	O5'-C5'-C6'-O6'
3	B	1510	LMT	C4'-C5'-C6'-O6'
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	C	1708	LMT	C3'-C4'-O1B-C1B
10	B	1508	DDR	O1-C1-O51-C51
3	C	1703	LMT	C4'-C5'-C6'-O6'
3	B	1503	LMT	C4'-C5'-C6'-O6'
13	C	1705	LPX	C7-C6-O6-C5
3	C	1708	LMT	C2'-C1'-O1'-C1
3	B	1504	LMT	O5B-C5B-C6B-O6B
8	B	1502	GOL	O1-C1-C2-O2
3	C	1703	LMT	O5'-C5'-C6'-O6'
3	B	1504	LMT	C2B-C1B-O1B-C4'
13	C	1705	LPX	O7-C6-O6-C5
3	A	1111	LMT	O5'-C1'-O1'-C1
3	C	1703	LMT	O1'-C1-C2-C3
3	B	1504	LMT	O5B-C1B-O1B-C4'
3	A	1111	LMT	O1'-C1-C2-C3
13	C	1705	LPX	O5-C4-C5-O6
3	A	1111	LMT	C6-C7-C8-C9
11	B	1515	DDQ	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
13	C	1705	LPX	C3-C4-C5-O6
7	A	1108	C14	C08-C09-C10-C11
7	A	1106	C14	C02-C03-C04-C05
3	B	1504	LMT	C2'-C1'-O1'-C1
3	B	1504	LMT	C5-C6-C7-C8
3	C	1708	LMT	C3-C4-C5-C6
10	B	1508	DDR	C2-C3-C4-C5
3	B	1504	LMT	C3-C4-C5-C6
13	C	1707	LPX	C11-C12-C13-C14
8	A	1107	GOL	C1-C2-C3-O3
8	C	1709	GOL	O1-C1-C2-C3
3	B	1510	LMT	O5B-C5B-C6B-O6B
3	B	1503	LMT	C6-C7-C8-C9
3	B	1504	LMT	C11-C10-C9-C8
11	B	1515	DDQ	C5-C6-C7-C8
3	A	1101	LMT	C3-C4-C5-C6
9	B	1505	D10	C4-C5-C6-C7
3	C	1708	LMT	C2-C1-O1'-C1'
13	C	1705	LPX	C17-C18-C19-C20
8	B	1512	GOL	O2-C2-C3-O3
3	B	1503	LMT	C4-C5-C6-C7
13	C	1707	LPX	C7-C6-O6-C5
3	C	1708	LMT	C7-C8-C9-C10
7	A	1108	C14	C03-C04-C05-C06
7	A	1108	C14	C06-C07-C08-C09
3	C	1708	LMT	C1-C2-C3-C4
5	A	1113	EDO	O1-C1-C2-O2
5	B	1506	EDO	O1-C1-C2-O2
5	B	1513	EDO	O1-C1-C2-O2
5	C	1702	EDO	O1-C1-C2-O2
13	C	1705	LPX	C16-C17-C18-C19
3	C	1708	LMT	C5-C6-C7-C8
9	B	1505	D10	C3-C4-C5-C6
13	C	1707	LPX	O7-C6-O6-C5
3	B	1510	LMT	C1-C2-C3-C4
3	B	1504	LMT	C4-C5-C6-C7
3	A	1103	LMT	C7-C8-C9-C10
3	C	1708	LMT	C4-C5-C6-C7
3	A	1103	LMT	C2'-C1'-O1'-C1
3	A	1111	LMT	O5B-C5B-C6B-O6B
11	B	1515	DDQ	C6-C7-C8-C9
13	C	1707	LPX	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
7	A	1108	C14	C07-C08-C09-C10
10	B	1508	DDR	O51-C51-C52-C53
3	B	1510	LMT	C7-C8-C9-C10
8	C	1709	GOL	O2-C2-C3-O3
7	A	1108	C14	C09-C10-C11-C12
13	C	1707	LPX	C13-C14-C15-C16
3	A	1103	LMT	C4'-C5'-C6'-O6'
13	C	1707	LPX	C7-C8-C9-C10
10	B	1508	DDR	C7-C8-C9-C10
5	A	1110	EDO	O1-C1-C2-O2
10	B	1508	DDR	C25-C26-C27-C28
10	B	1508	DDR	C4-C5-C6-C7
6	C	1701	OCT	C2-C3-C4-C5
3	A	1103	LMT	C2-C1-O1'-C1'
3	B	1503	LMT	C2-C1-O1'-C1'
3	B	1504	LMT	C2-C1-O1'-C1'
7	A	1106	C14	C01-C02-C03-C04
3	C	1708	LMT	C5'-C4'-O1B-C1B
13	C	1707	LPX	C3-O1-P1-O2
3	A	1101	LMT	C1-C2-C3-C4
13	C	1705	LPX	C7-C8-C9-C10
3	B	1504	LMT	O5'-C1'-O1'-C1
10	B	1508	DDR	C51-C52-C53-O53
3	A	1111	LMT	C11-C10-C9-C8
7	C	1706	C14	C10-C11-C12-C13
3	C	1703	LMT	C7-C8-C9-C10
5	B	1507	EDO	O1-C1-C2-O2
5	C	1712	EDO	O1-C1-C2-O2
13	C	1707	LPX	C18-C19-C20-C21
7	C	1706	C14	C07-C08-C09-C10
3	A	1111	LMT	C9-C10-C11-C12
3	B	1510	LMT	C9-C10-C11-C12
3	C	1703	LMT	C3-C4-C5-C6
3	B	1504	LMT	C1-C2-C3-C4
3	A	1111	LMT	C5'-C4'-O1B-C1B
3	C	1703	LMT	C9-C10-C11-C12
3	C	1708	LMT	C11-C10-C9-C8
11	B	1515	DDQ	C3-C4-C5-C6
10	B	1508	DDR	C1-C2-C3-C4
7	C	1706	C14	C09-C10-C11-C12
3	A	1101	LMT	C2-C3-C4-C5
13	C	1707	LPX	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	C	1705	LPX	C9-C10-C11-C12
3	B	1510	LMT	C3-C4-C5-C6
10	B	1508	DDR	O51-C51-C52-O52
3	A	1111	LMT	C4-C5-C6-C7
9	B	1505	D10	C5-C6-C7-C8
3	A	1103	LMT	C9-C10-C11-C12
3	B	1503	LMT	C2-C3-C4-C5
13	C	1705	LPX	C11-C10-C9-C8
3	A	1103	LMT	C11-C10-C9-C8
10	B	1508	DDR	C51-C52-O52-C21
3	B	1510	LMT	C4-C5-C6-C7
7	C	1706	C14	C02-C03-C04-C05
5	A	1104	EDO	O1-C1-C2-O2
13	C	1707	LPX	C1-O2-P1-O1
3	B	1503	LMT	O1'-C1-C2-C3
8	C	1709	GOL	O1-C1-C2-O2
7	C	1706	C14	C04-C05-C06-C07
9	B	1505	D10	C1-C2-C3-C4
3	A	1101	LMT	C11-C10-C9-C8
3	B	1504	LMT	C4B-C5B-C6B-O6B
13	C	1707	LPX	C15-C16-C17-C18
3	A	1103	LMT	C1-C2-C3-C4
3	B	1510	LMT	C11-C10-C9-C8
6	C	1704	OCT	C1-C2-C3-C4
10	B	1508	DDR	O52-C52-C53-O53
7	C	1706	C14	C08-C09-C10-C11
5	C	1711	EDO	O1-C1-C2-O2
3	C	1708	LMT	O5'-C1'-O1'-C1
13	C	1705	LPX	C13-C14-C15-C16
3	A	1103	LMT	C2-C3-C4-C5
7	A	1106	C14	C09-C10-C11-C12
13	C	1707	LPX	C3-O1-P1-O4
13	C	1707	LPX	C1-O2-P1-O4
3	C	1703	LMT	C2-C3-C4-C5
3	A	1103	LMT	C6-C7-C8-C9
11	B	1515	DDQ	C2-C1-N1-O1
3	A	1101	LMT	C4-C5-C6-C7
10	B	1508	DDR	C3-C4-C5-C6
13	C	1707	LPX	O6-C6-C7-C8
13	C	1705	LPX	C12-C13-C14-C15

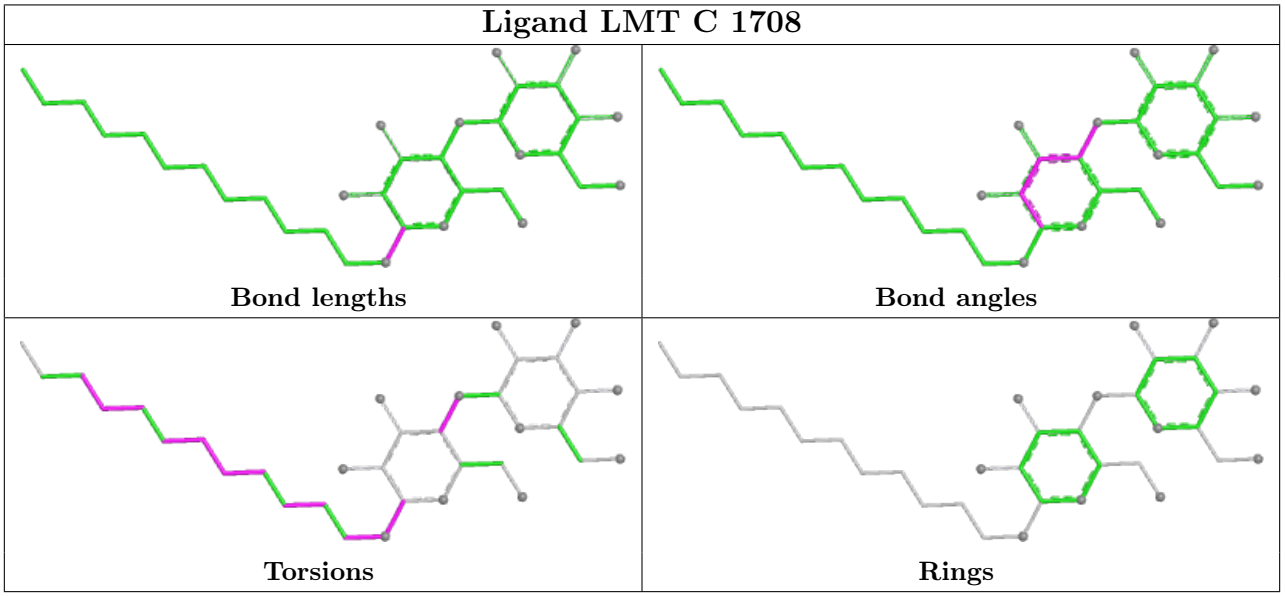
There are no ring outliers.

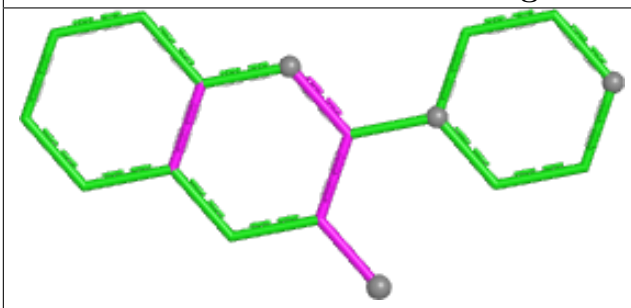
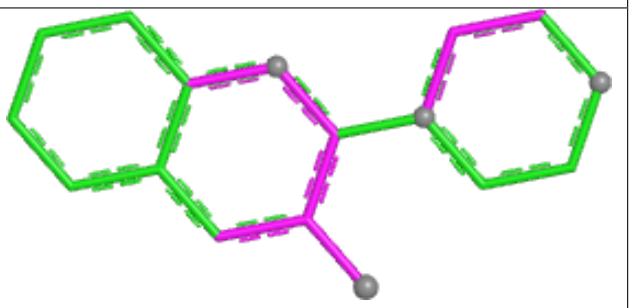
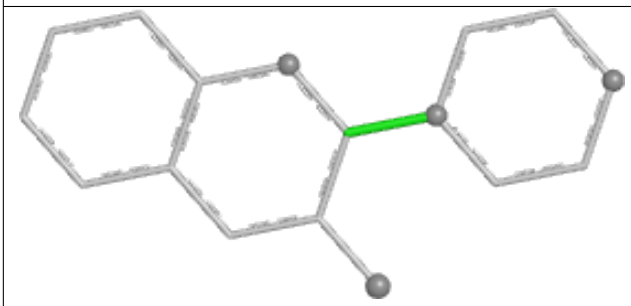
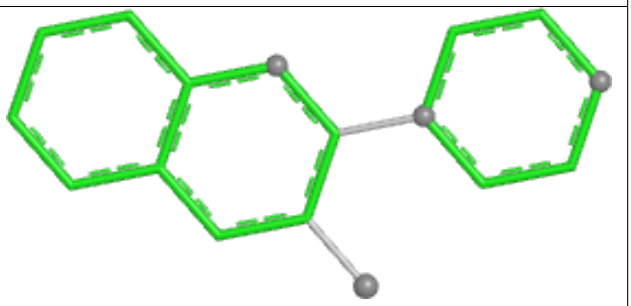
1 monomer is involved in 1 short contact:

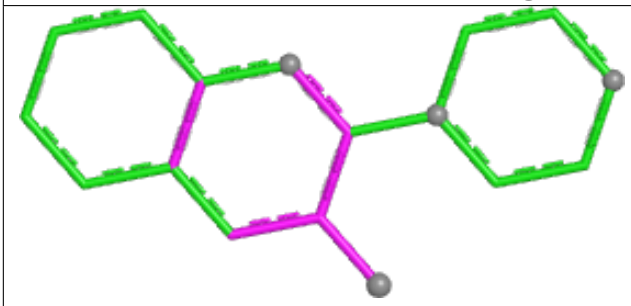
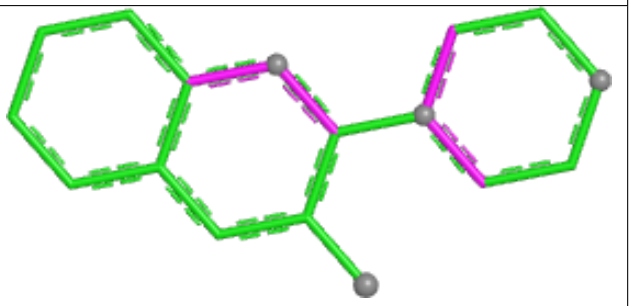
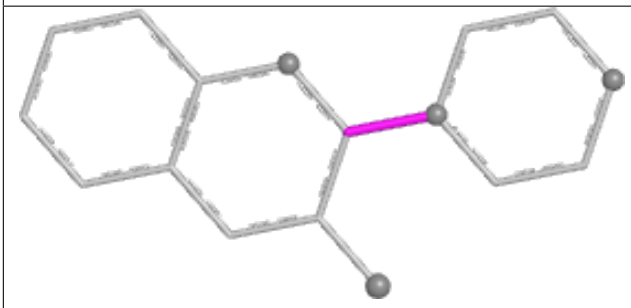
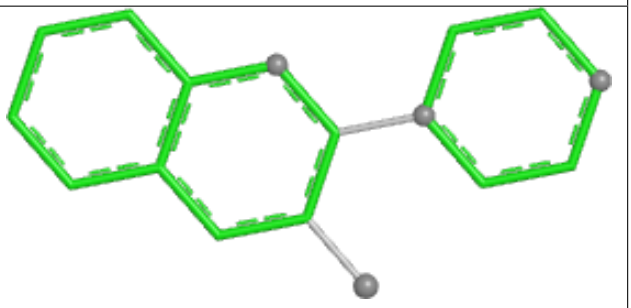
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1516	1K8	1	0

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.

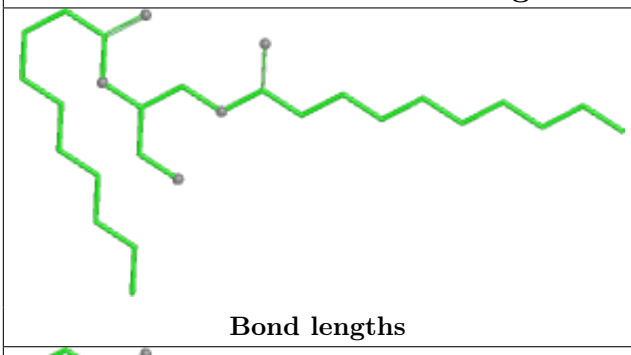
Ligand LMT C 1708



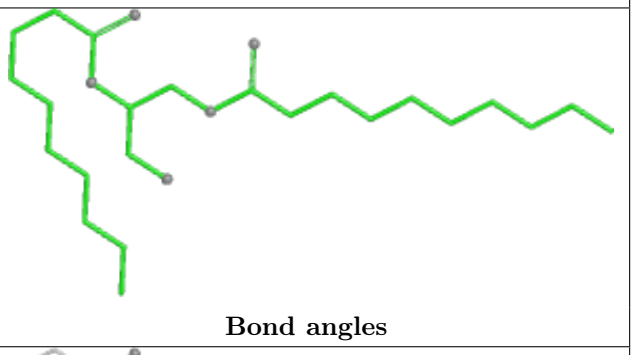
Ligand 1K8 B 1516	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 1K8 A 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

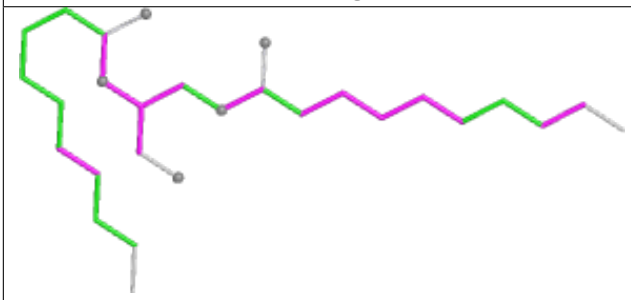
Ligand DDR B 1508



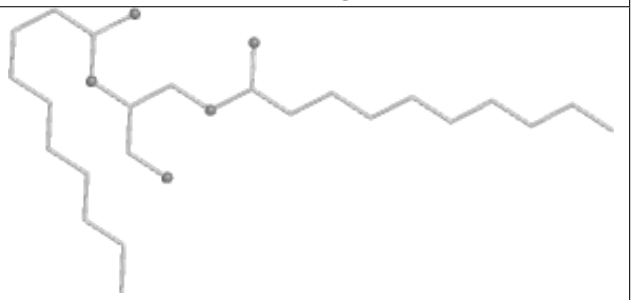
Bond lengths



Bond angles

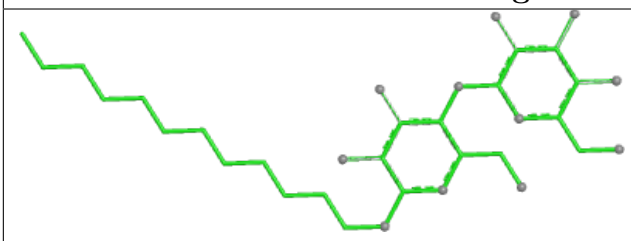


Torsions

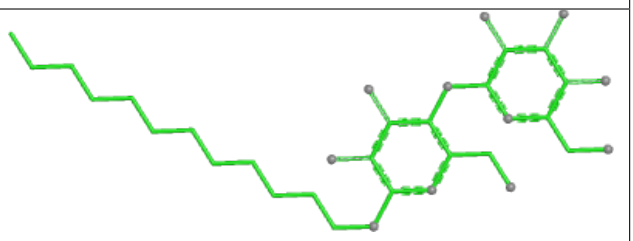


Rings

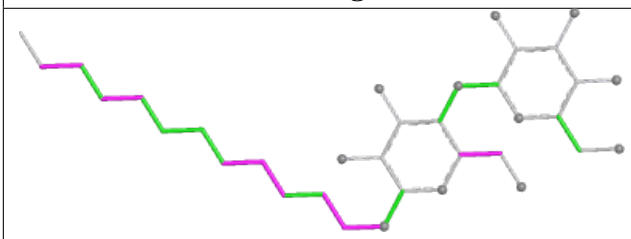
Ligand LMT C 1703



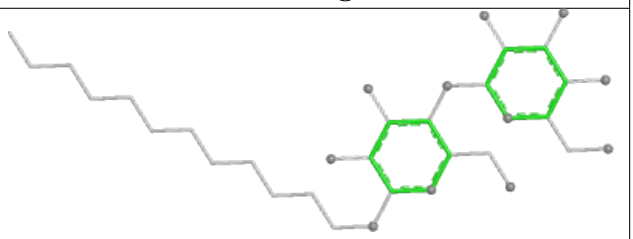
Bond lengths



Bond angles

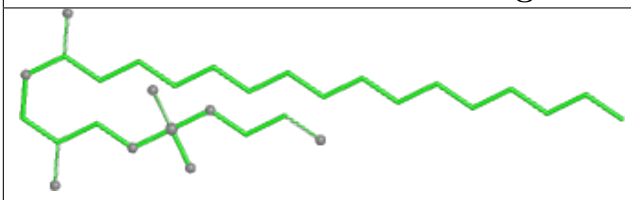


Torsions

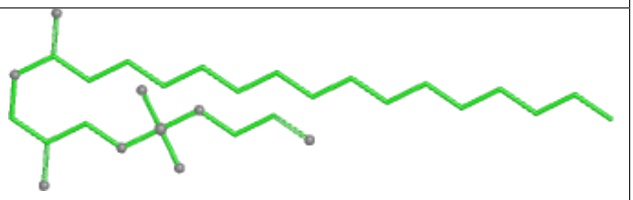


Rings

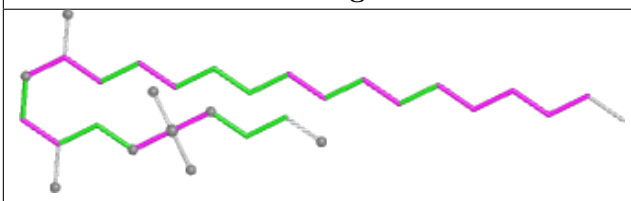
Ligand LPX C 1707



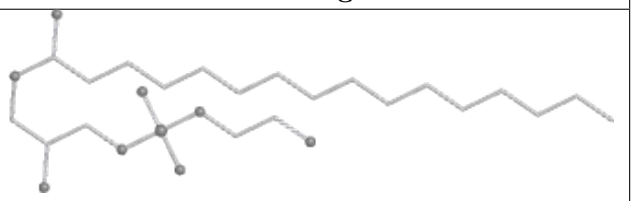
Bond lengths



Bond angles

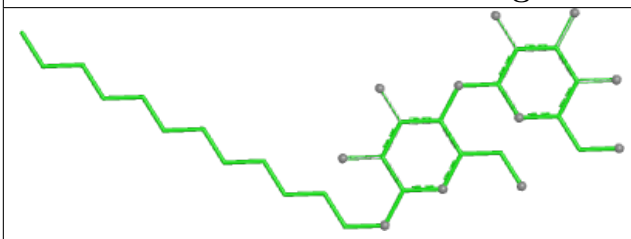


Torsions

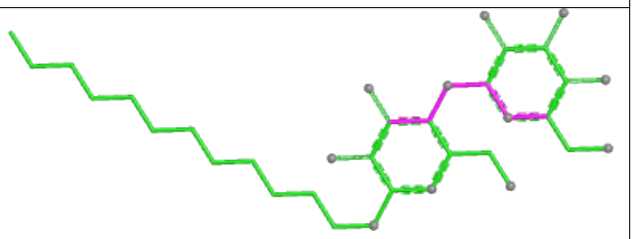


Rings

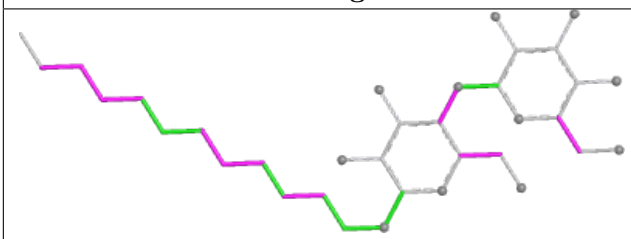
Ligand LMT B 1510



Bond lengths



Bond angles



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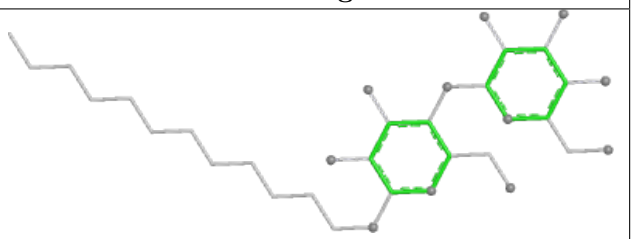
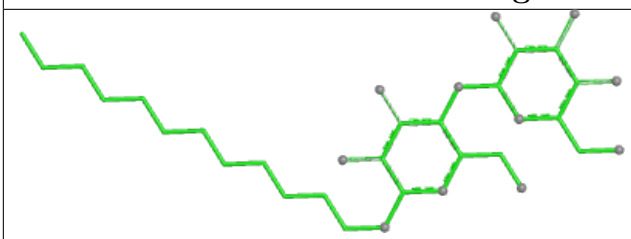
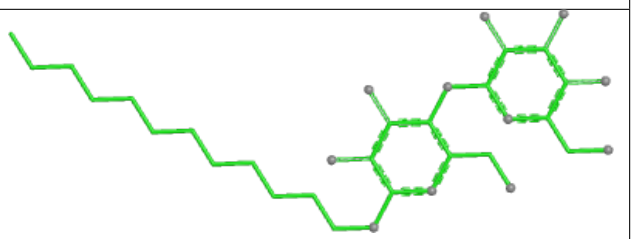


Rings

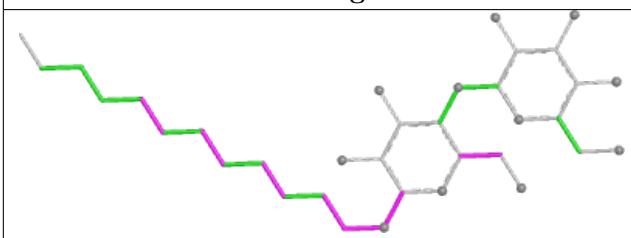
Ligand LMT B 1503



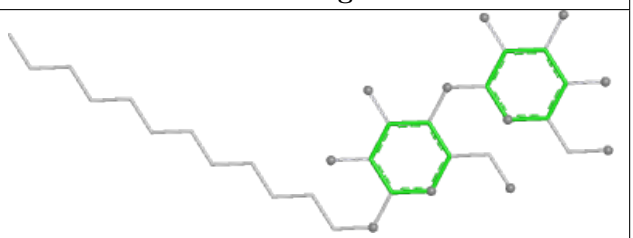
Bond lengths



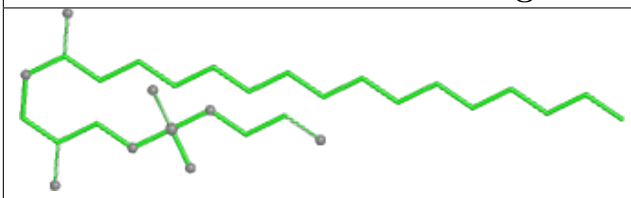
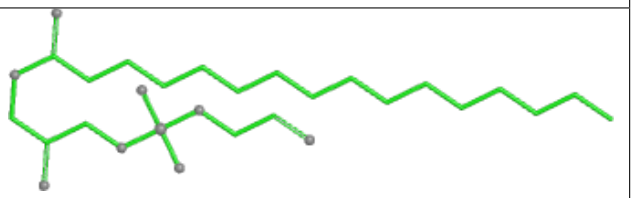
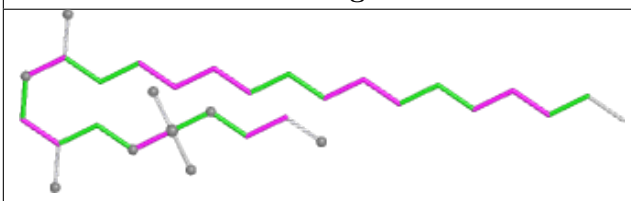
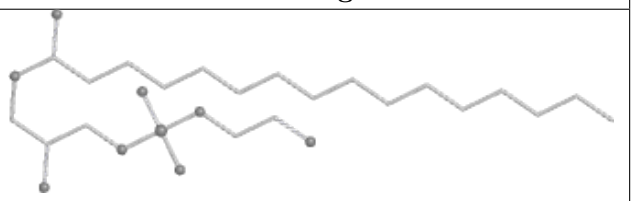
Bond angles

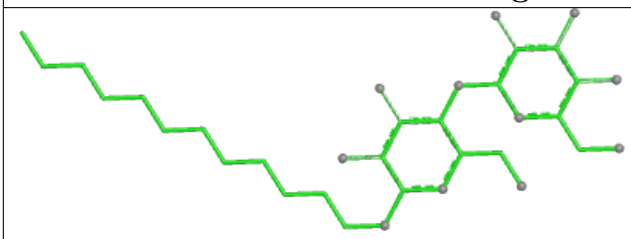
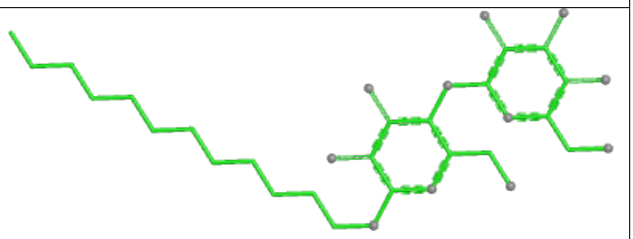
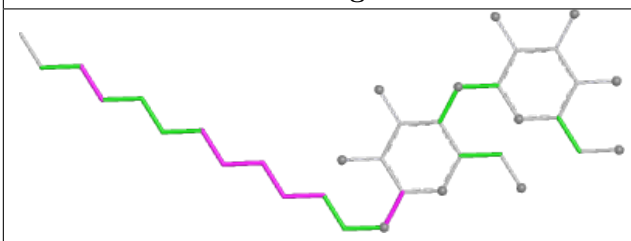
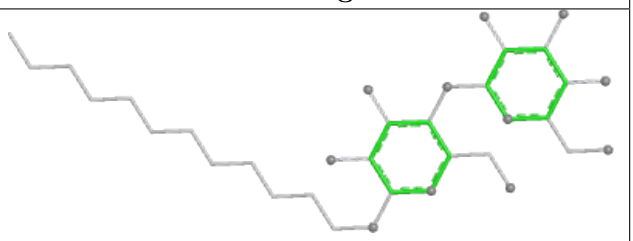


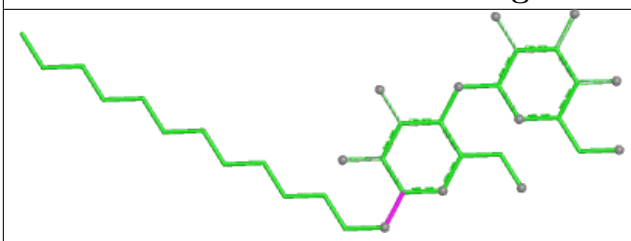
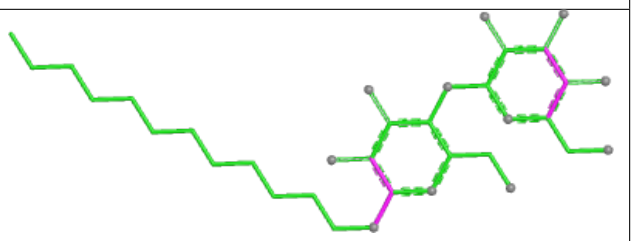
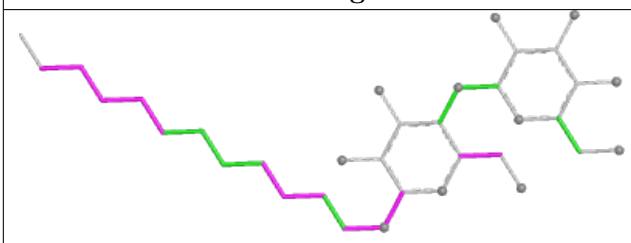
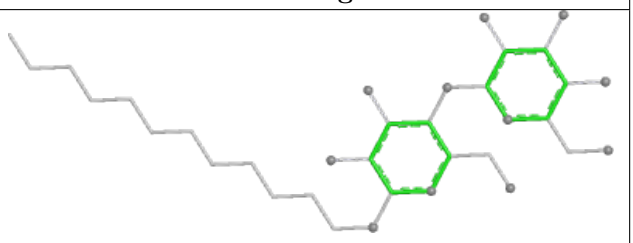
Torsions



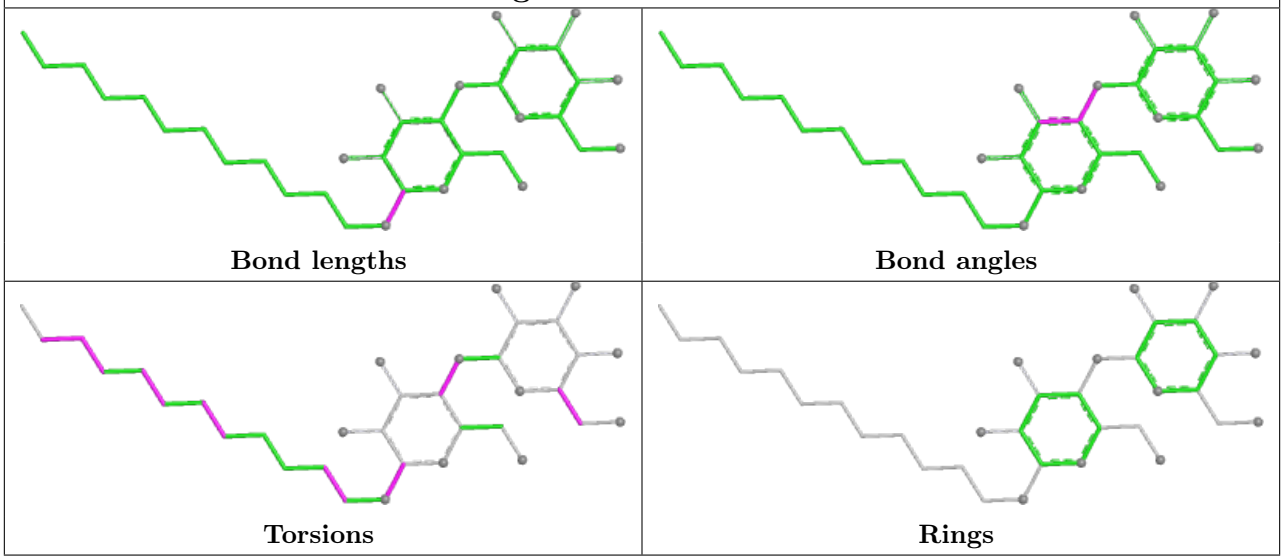
Rings

Ligand LPX C 1705	
 Bond lengths	 Bond angles
 Torsions	 Rings

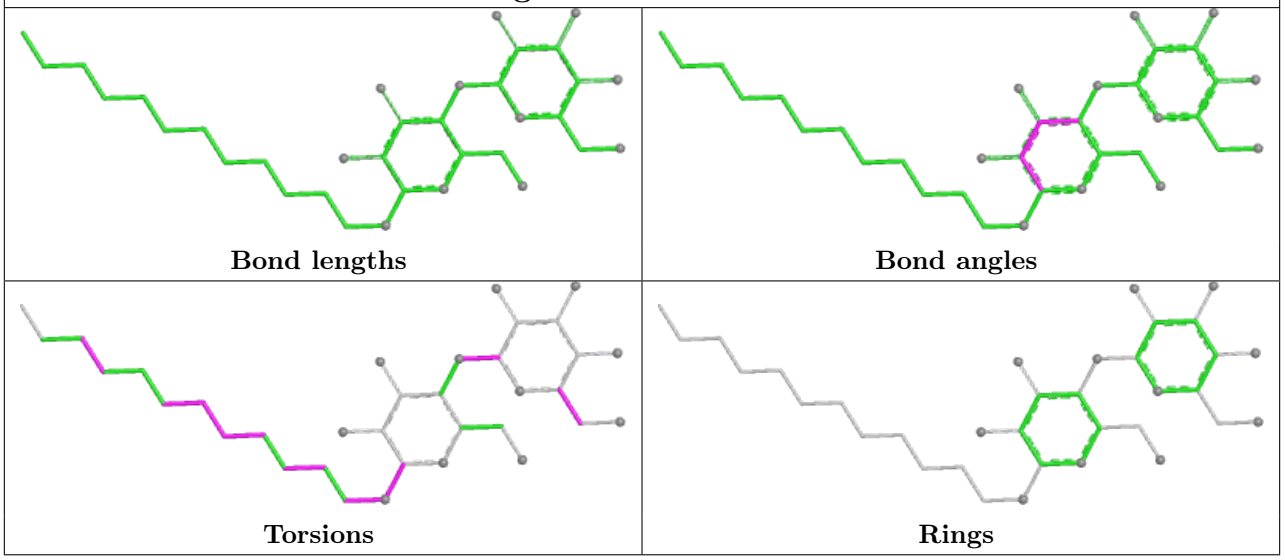
Ligand LMT A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 1103	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMT A 1111



Ligand LMT B 1504



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	1033/1057 (97%)	0.44	78 (7%)	13	10	39, 61, 115, 137	0
1	B	1036/1057 (98%)	0.21	58 (5%)	24	19	40, 59, 73, 80	0
1	C	1033/1057 (97%)	0.10	29 (2%)	53	46	39, 49, 67, 76	0
2	D	156/169 (92%)	0.37	15 (9%)	8	5	46, 58, 75, 83	0
2	E	153/169 (90%)	1.08	35 (22%)	0	0	52, 65, 85, 93	0
All	All	3411/3509 (97%)	0.29	215 (6%)	20	15	39, 56, 91, 137	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424	GLY	7.5
2	E	66	LEU	6.7
1	A	868	LEU	6.0
2	E	33	LEU	6.0
1	C	510	LYS	5.8
2	E	34	MET	5.6
1	A	867	ARG	5.6
1	B	508	GLY	5.5
1	A	543	VAL	5.4
1	A	713	LEU	5.2
2	E	67	LEU	5.1
1	A	712	MET	5.1
2	D	165	LEU	5.1
1	A	833	PRO	5.1
1	A	421	ALA	5.0
2	E	35	ALA	4.9
1	B	606	VAL	4.9
1	B	600	THR	4.8
1	A	536	ARG	4.7
1	C	499	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	597	TYR	4.6
1	B	599	LEU	4.6
2	D	163	GLU	4.6
1	A	542	LEU	4.5
1	B	617	PHE	4.4
1	A	554	TYR	4.3
2	E	64	GLU	4.3
1	B	635	ALA	4.2
1	A	425	LEU	4.1
1	A	835	LYS	4.1
1	B	633	ASP	4.1
1	A	515	TRP	4.0
2	E	28	ASP	4.0
1	B	603	LYS	4.0
1	A	518	ARG	4.0
1	A	512	PHE	4.0
1	C	497	LEU	3.9
2	D	166	GLN	3.9
1	A	529	ASP	3.9
2	E	36	ASN	3.9
1	C	513	PHE	3.9
1	C	362	PHE	3.8
2	D	150	PHE	3.8
1	A	869	SER	3.8
1	C	421	ALA	3.8
1	B	575	MET	3.8
1	A	675	GLY	3.8
2	E	38	ALA	3.7
1	B	675	GLY	3.7
2	D	126	LEU	3.7
1	B	605	ASN	3.7
2	E	73	VAL	3.7
1	A	834	GLY	3.6
1	C	811	TYR	3.6
1	A	831	ALA	3.6
1	B	1035	ARG	3.6
1	A	513	PHE	3.6
2	D	167	LYS	3.6
1	B	628	PHE	3.5
1	A	678	THR	3.5
2	E	31	ARG	3.5
1	A	423	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	32	ILE	3.5
1	A	1037	ASN	3.5
1	A	707	ALA	3.4
1	A	362	PHE	3.4
2	E	68	LYS	3.4
1	C	498	LYS	3.4
2	E	37	GLY	3.4
2	E	27	ASP	3.4
1	A	516	PHE	3.4
2	E	60	LEU	3.3
2	E	97	GLU	3.3
1	C	501	ALA	3.3
1	A	539	GLY	3.3
2	E	101	LYS	3.3
1	C	425	LEU	3.3
1	B	637	ARG	3.3
1	B	634	TRP	3.2
1	B	676	THR	3.2
1	B	134	SER	3.2
1	B	660	ASP	3.2
1	A	429	GLU	3.2
1	B	638	PRO	3.2
1	C	508	GLY	3.2
2	D	161	LEU	3.1
1	B	636	ASP	3.1
1	A	1035	ARG	3.1
2	D	139	VAL	3.1
2	D	164	ILE	3.1
2	D	159	GLU	3.1
1	A	709	HIS	3.1
1	B	655	PHE	3.1
1	A	420	MET	3.0
1	C	500	ILE	3.0
1	A	426	PRO	3.0
2	E	30	VAL	3.0
1	B	641	GLU	3.0
1	B	604	ASN	3.0
1	B	574	THR	3.0
1	A	866	GLU	3.0
1	B	607	GLU	3.0
1	A	255	GLN	2.9
1	B	640	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	550	VAL	2.9
2	E	102	ASN	2.9
1	A	526	HIS	2.9
1	B	673	GLU	2.9
1	B	1033	PHE	2.9
1	B	366	LEU	2.9
2	D	162	ALA	2.9
1	C	730	ASP	2.9
2	E	74	ASN	2.9
1	A	710	PRO	2.8
2	E	69	ASN	2.8
1	A	956	GLU	2.8
1	B	256	ASP	2.8
1	B	596	HIS	2.8
1	B	631	LEU	2.8
1	A	704	ALA	2.8
1	C	739	LEU	2.7
2	E	62	ILE	2.7
1	B	595	THR	2.7
1	A	711	ASP	2.7
1	B	629	VAL	2.7
2	E	99	LEU	2.7
1	A	432	ARG	2.6
1	B	601	LYS	2.6
1	A	433	LYS	2.6
1	A	558	ARG	2.6
1	A	533	GLY	2.6
1	A	525	HIS	2.6
2	D	129	VAL	2.6
1	A	422	GLU	2.6
1	B	653	ARG	2.6
1	B	1036	LYS	2.6
1	C	808	ARG	2.6
2	D	154	ILE	2.6
2	E	107	ASN	2.6
1	C	511	GLY	2.6
2	E	165	LEU	2.5
1	A	673	GLU	2.5
1	B	554	TYR	2.5
2	E	115	THR	2.5
1	A	1038	GLU	2.5
1	A	556	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	420	MET	2.5
2	E	63	VAL	2.4
1	B	642	ASN	2.4
1	C	427	PRO	2.4
1	B	258	SER	2.4
1	B	615	PHE	2.4
1	B	632	LYS	2.4
1	A	680	PHE	2.4
1	B	647	ILE	2.4
1	C	807	SER	2.4
1	A	918	PHE	2.4
2	E	106	VAL	2.4
1	C	426	PRO	2.4
1	B	284	GLN	2.3
1	C	120	GLN	2.3
1	A	517	ASN	2.3
1	C	707	ALA	2.3
2	E	84	LEU	2.3
1	B	558	ARG	2.3
1	C	255	GLN	2.3
1	A	706	ALA	2.3
1	B	598	TYR	2.3
1	A	499	PRO	2.3
1	B	657	GLN	2.3
1	C	423	GLU	2.3
1	A	708	LYS	2.3
1	A	430	ALA	2.3
1	B	593	GLU	2.2
1	A	546	LEU	2.2
1	A	965	LEU	2.2
1	A	446	ALA	2.2
1	A	519	MET	2.2
1	B	563	PHE	2.2
1	C	804	PHE	2.2
2	D	28	ASP	2.2
1	A	500	ILE	2.2
1	A	514	GLY	2.2
1	A	943	ILE	2.2
1	A	510	LYS	2.2
1	B	834	GLY	2.2
1	A	535	LEU	2.2
1	A	677	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1041	GLU	2.2
1	C	801	PHE	2.2
1	A	702	LEU	2.2
2	E	29	GLU	2.2
1	A	716	VAL	2.2
1	B	133	SER	2.2
2	E	163	GLU	2.2
1	C	918	PHE	2.2
1	A	416	VAL	2.1
1	C	512	PHE	2.1
2	D	160	ASP	2.1
1	B	649	MET	2.1
1	A	522	LYS	2.1
2	E	100	LEU	2.1
1	B	839	GLU	2.1
2	E	141	ALA	2.1
1	B	711	ASP	2.1
1	A	256	ASP	2.1
1	A	839	GLU	2.0
2	E	70	GLY	2.0
1	A	520	PHE	2.0
1	B	352	PHE	2.0
1	A	836	SER	2.0
1	B	513	PHE	2.0
1	A	540	ARG	2.0
1	B	835	LYS	2.0
1	C	509	LYS	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
5	EDO	C	1712	4/4	0.58	0.40	59,59,59,60	0
10	DDR	B	1508	28/28	0.59	0.28	69,73,74,74	0
3	LMT	B	1504	35/35	0.72	0.29	71,75,80,80	0
6	OCT	C	1704	8/8	0.74	0.41	60,61,62,62	0
3	LMT	C	1708	35/35	0.74	0.25	66,77,79,80	0
5	EDO	A	1109	4/4	0.75	0.18	67,68,68,68	0
3	LMT	B	1510	35/35	0.76	0.38	69,76,79,80	0
7	C14	A	1106	14/14	0.76	0.18	75,83,91,93	0
8	GOL	B	1512	6/6	0.76	0.46	68,69,70,70	0
6	OCT	C	1701	8/8	0.76	0.28	83,87,92,92	0
11	DDQ	B	1515	14/14	0.76	0.25	62,64,66,67	0
9	D10	B	1505	10/10	0.77	0.19	66,68,69,69	0
4	1K8	A	1102	17/17	0.81	0.30	80,86,91,91	0
8	GOL	A	1107	6/6	0.81	0.31	66,67,67,67	0
6	OCT	A	1105	8/8	0.82	0.30	86,91,96,98	0
3	LMT	A	1101	35/35	0.82	0.30	66,69,72,73	0
3	LMT	A	1111	35/35	0.82	0.22	61,76,82,83	0
13	LPX	C	1705	30/30	0.82	0.37	66,70,75,76	0
4	1K8	B	1516	17/17	0.83	0.32	51,53,55,55	17
3	LMT	A	1103	35/35	0.84	0.32	73,76,81,83	0
5	EDO	A	1112	4/4	0.85	0.18	60,60,61,61	0
5	EDO	B	1501	4/4	0.85	0.26	58,58,59,60	0
5	EDO	B	1507	4/4	0.85	0.30	56,56,56,57	0
5	EDO	B	1514	4/4	0.85	0.13	75,75,75,76	0
3	LMT	B	1503	35/35	0.85	0.35	75,78,81,82	0
5	EDO	C	1702	4/4	0.86	0.23	63,64,64,64	0
5	EDO	B	1506	4/4	0.86	0.26	61,61,62,62	0
7	C14	A	1108	14/14	0.86	0.23	62,66,68,68	0
8	GOL	B	1511	6/6	0.87	0.23	61,61,61,62	0
5	EDO	A	1110	4/4	0.88	0.21	73,73,74,74	0
5	EDO	A	1113	4/4	0.88	0.20	63,63,64,65	0
12	SO4	B	1518	5/5	0.88	0.48	111,111,111,112	0
8	GOL	B	1509	6/6	0.88	0.34	70,70,71,71	0
8	GOL	B	1502	6/6	0.89	0.26	62,62,63,63	0
3	LMT	C	1703	35/35	0.90	0.22	60,65,68,68	0
7	C14	C	1706	14/14	0.90	0.18	57,58,59,59	0
5	EDO	A	1104	4/4	0.90	0.26	53,53,53,53	0
5	EDO	B	1513	4/4	0.91	0.16	78,78,78,78	0
13	LPX	C	1707	30/30	0.91	0.28	63,68,73,74	0
8	GOL	C	1709	6/6	0.92	0.19	52,52,53,53	0
12	SO4	C	1713	5/5	0.93	0.18	76,76,76,77	0

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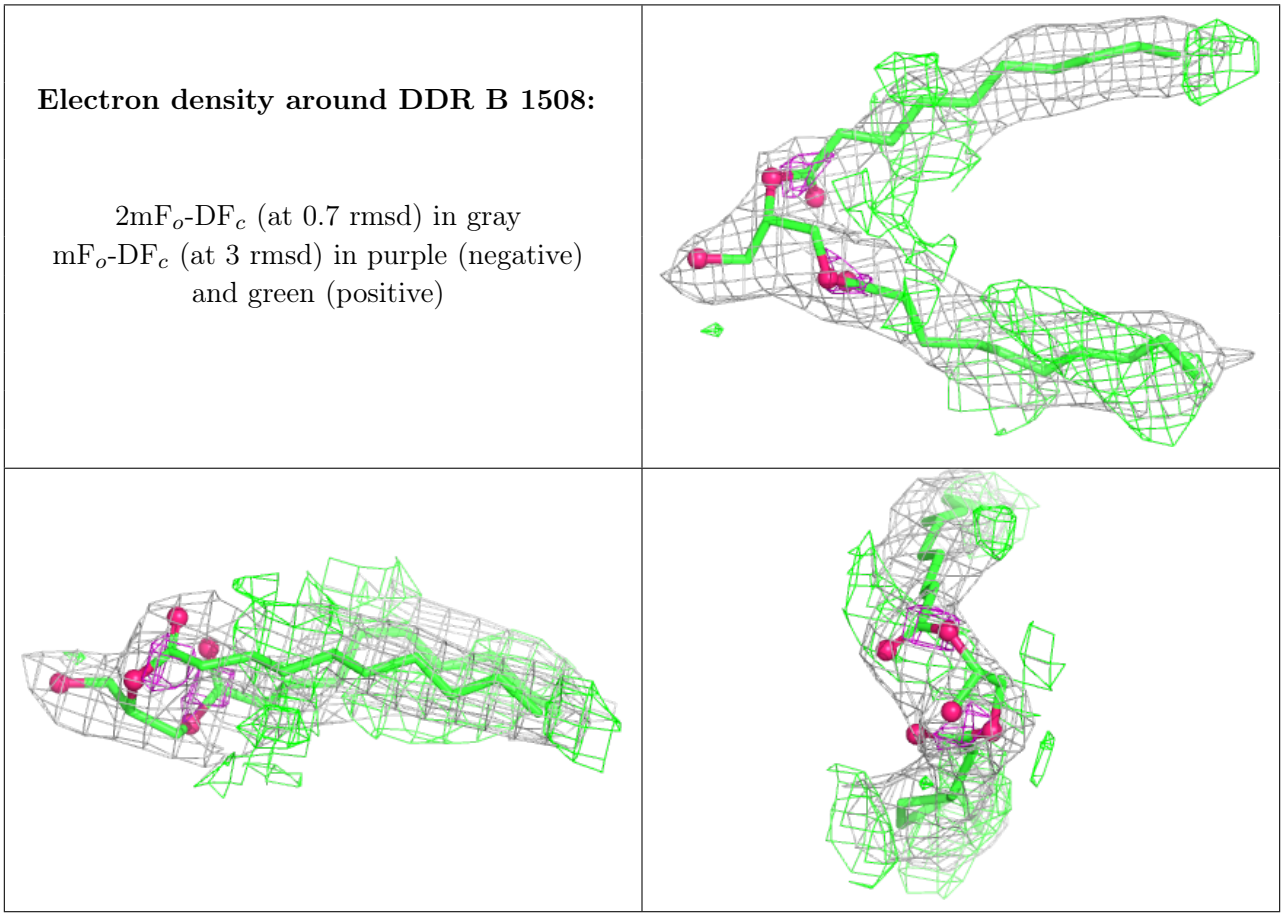
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	C	1711	4/4	0.94	0.26	57,57,57,58	0
12	SO4	B	1517	5/5	0.95	0.28	81,81,82,82	0
5	EDO	C	1710	4/4	0.96	0.36	56,56,56,57	0

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.

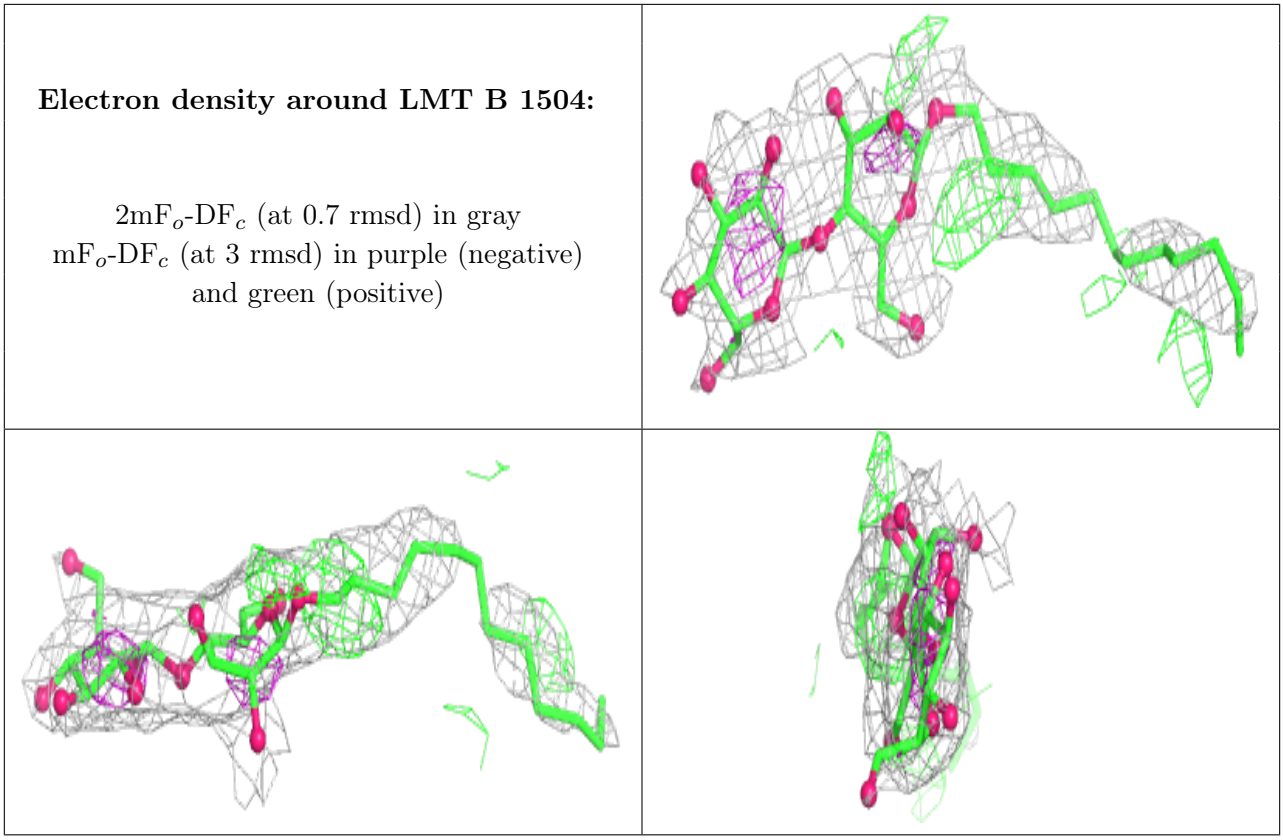
Electron density around DDR B 1508:

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



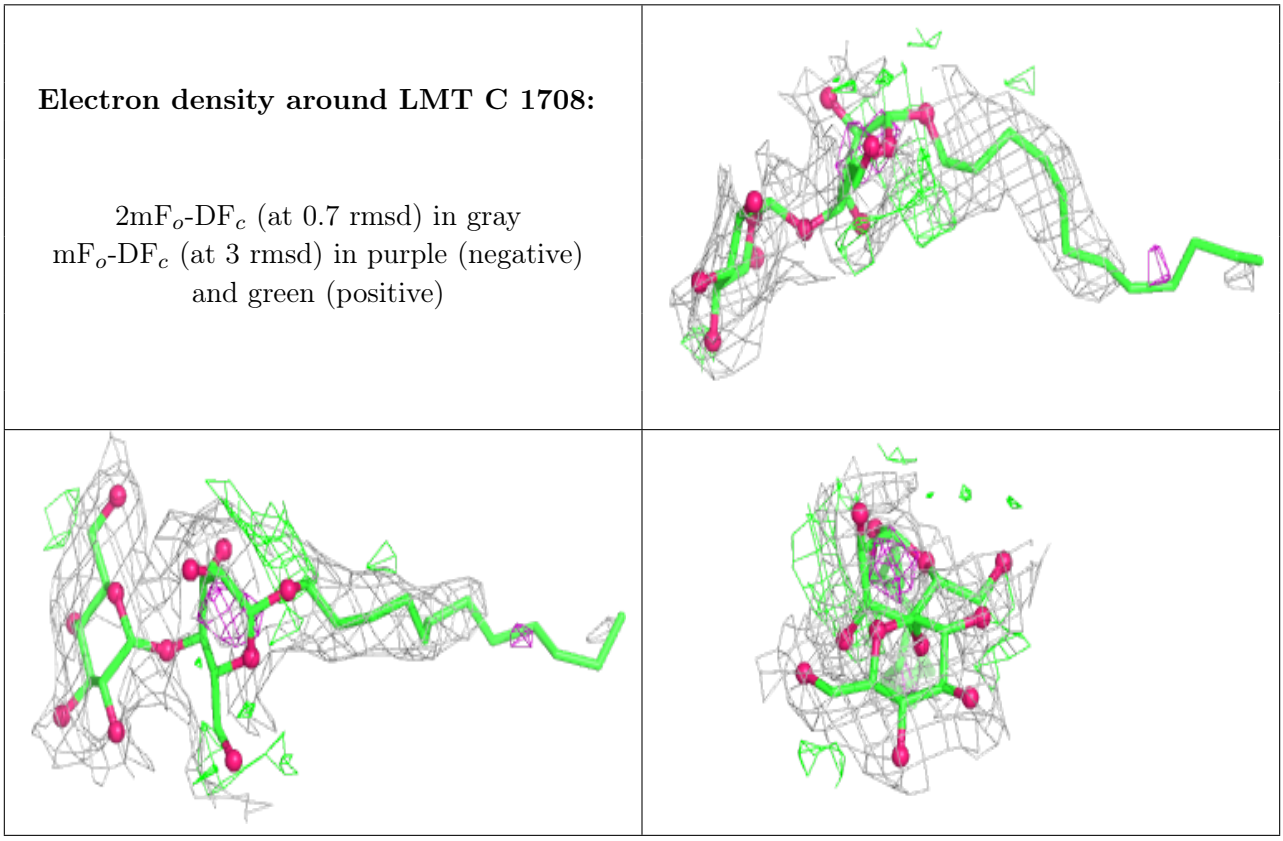
Electron density around LMT B 1504:

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



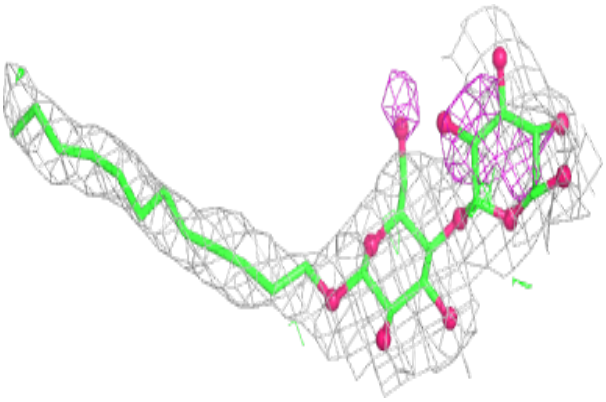
Electron density around LMT C 1708:

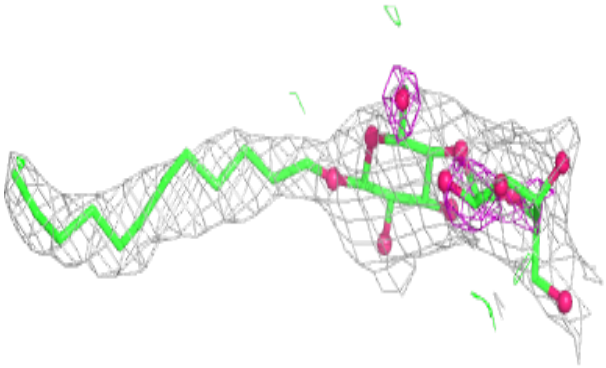
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

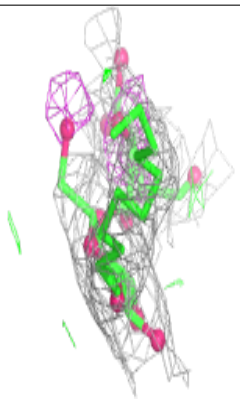


Electron density around LMT B 1510:

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

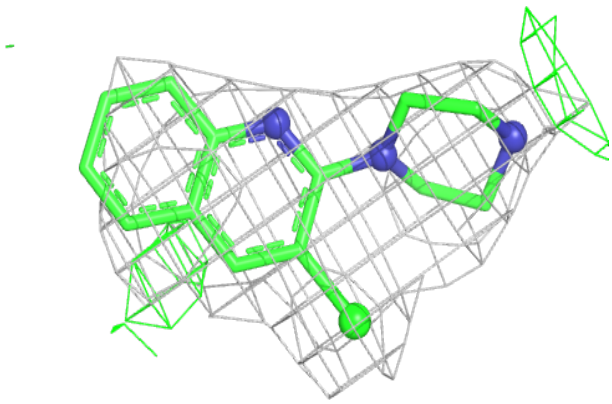


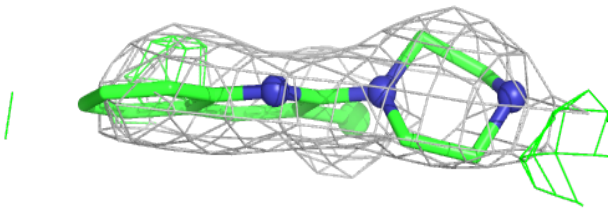


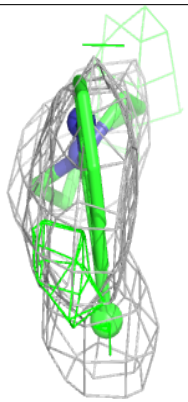


Electron density around 1K8 A 1102:

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

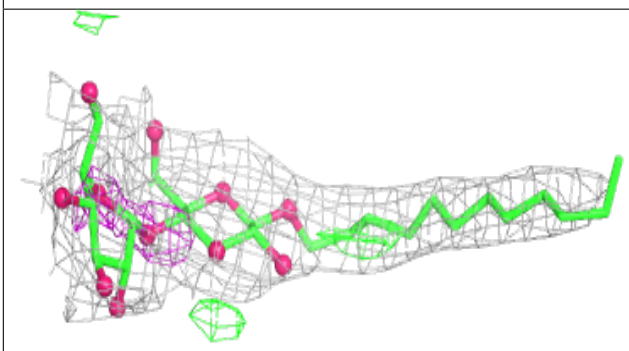


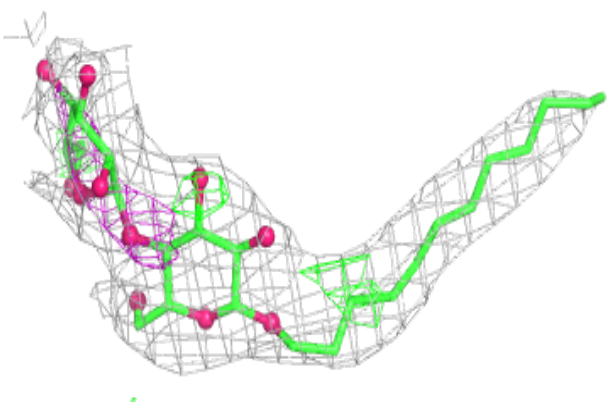


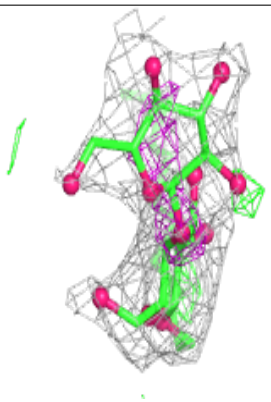


Electron density around LMT A 1101:

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

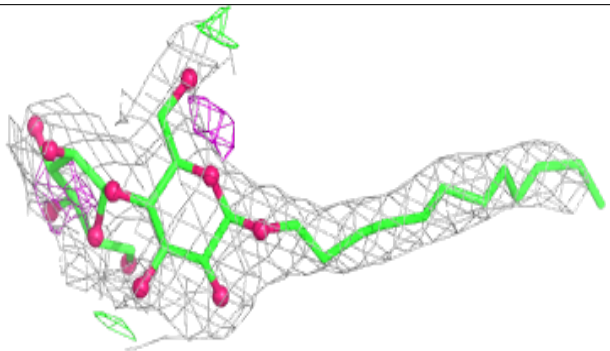


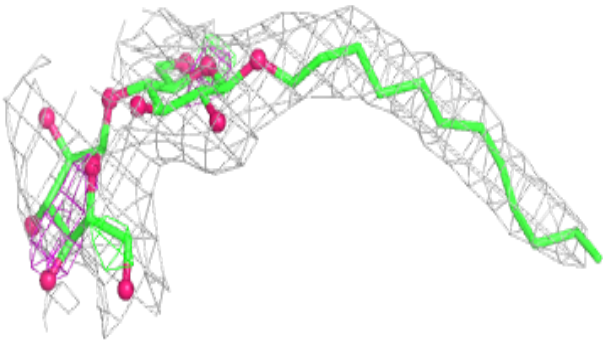




Electron density around LMT A 1111:

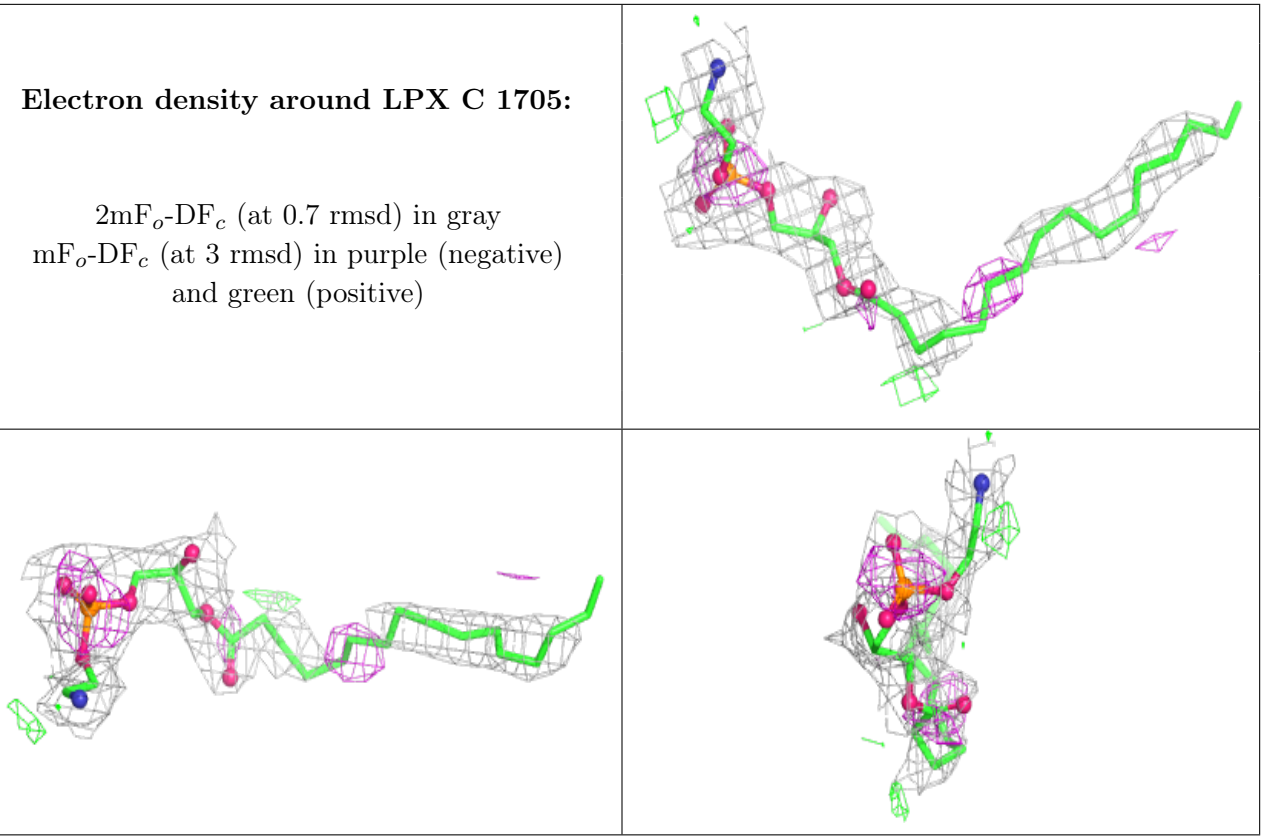
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





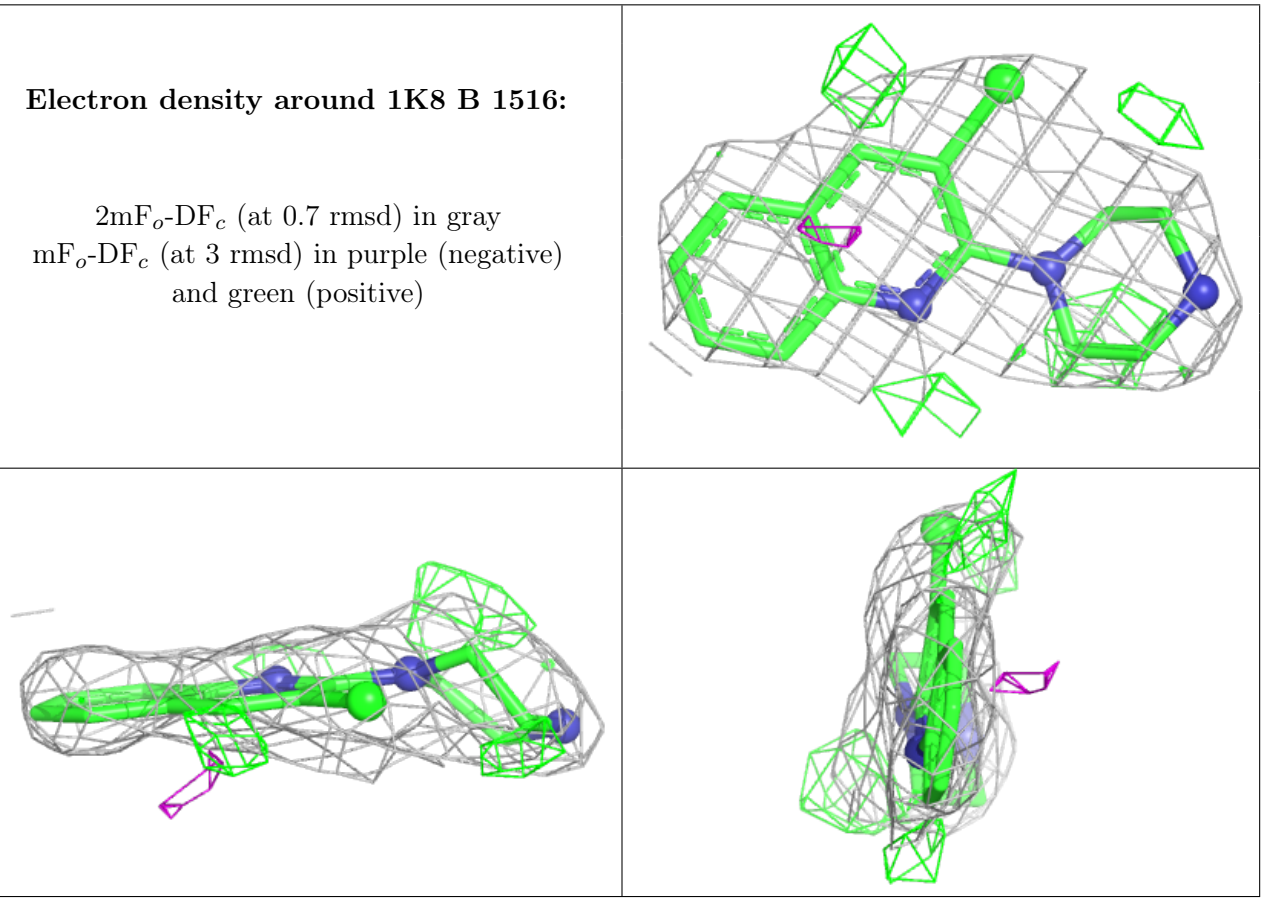
Electron density around LPX C 1705:

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



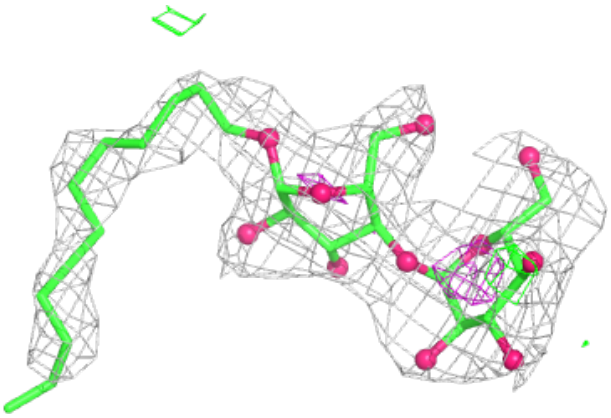
Electron density around 1K8 B 1516:

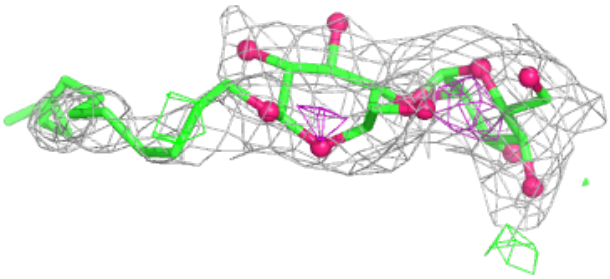
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

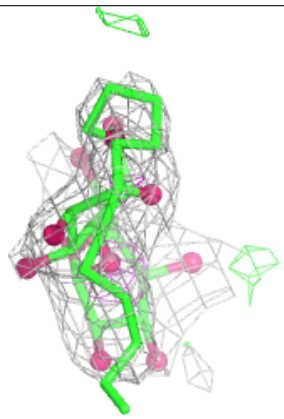


Electron density around LMT A 1103:

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

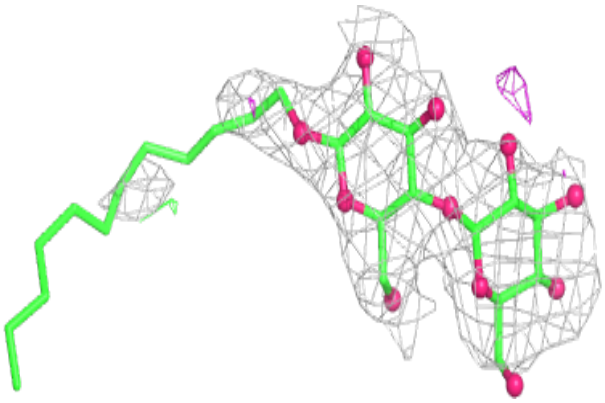


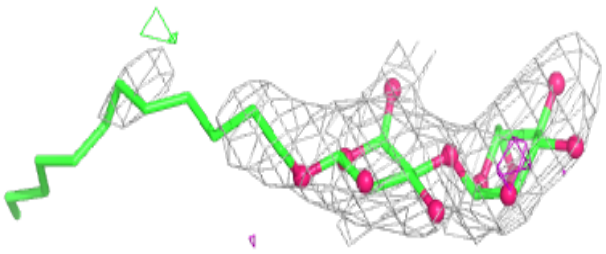




Electron density around LMT B 1503:

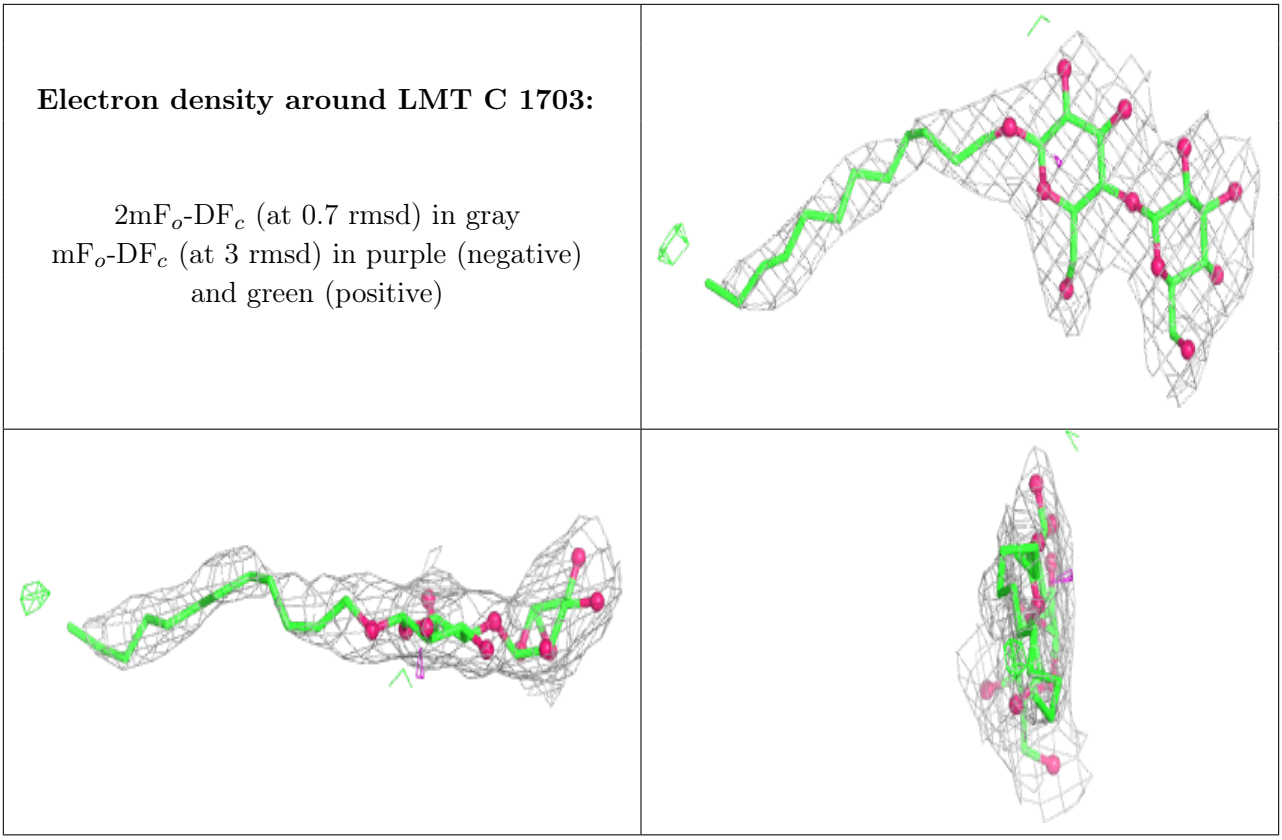
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





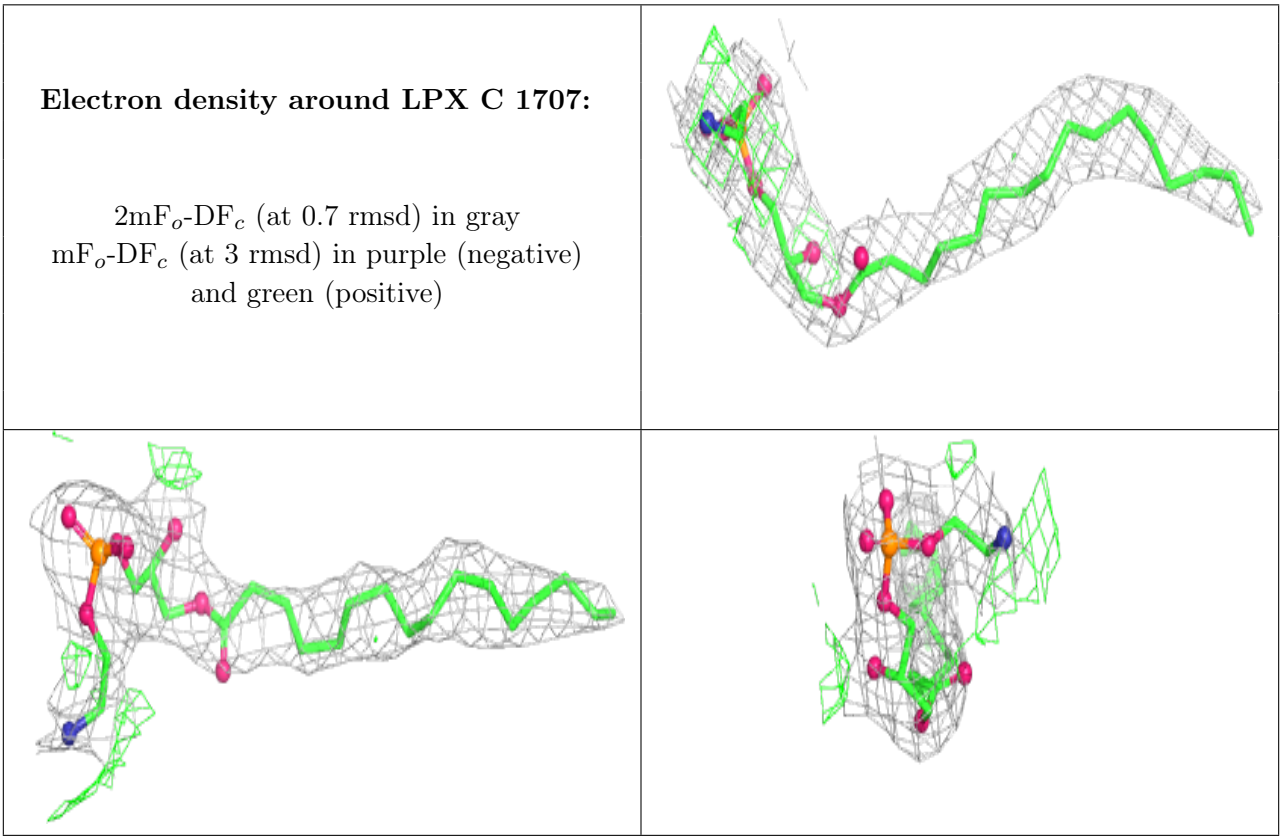
Electron density around LMT C 1703:

$2mF_o$-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 1707:

$2mF_o$-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.