



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:10 PM UTC

PDB ID : 7OUK / pdb_00007ouk
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 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

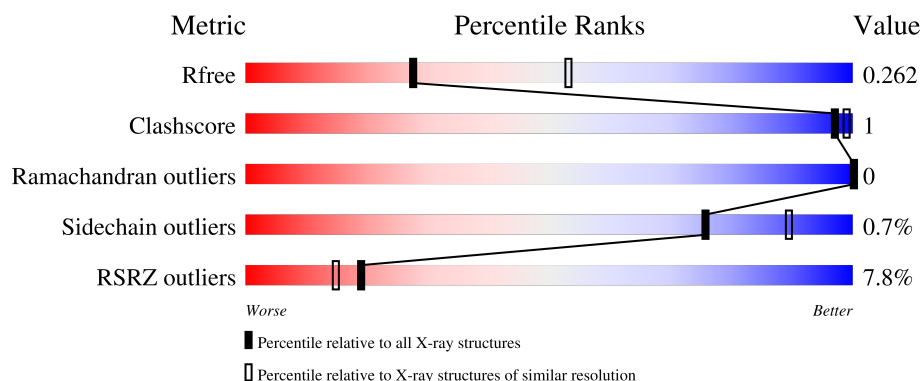
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	15% 95% ..
1	B	1057	6% 94% ..
1	C	1057	3% 95% ..
2	D	169	% 91% • 8%
2	E	169	5% 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
6	OCT	A	1105	-	-	-	X
6	OCT	C	1701	-	-	-	X
7	C14	A	1106	-	-	-	X

2 Entry composition

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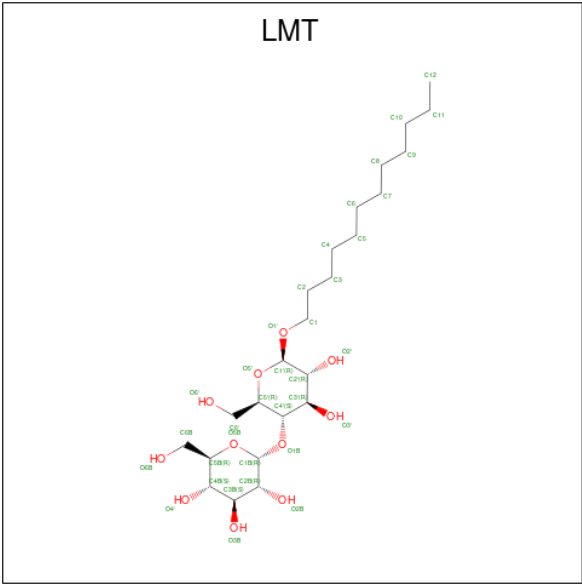
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- 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 (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



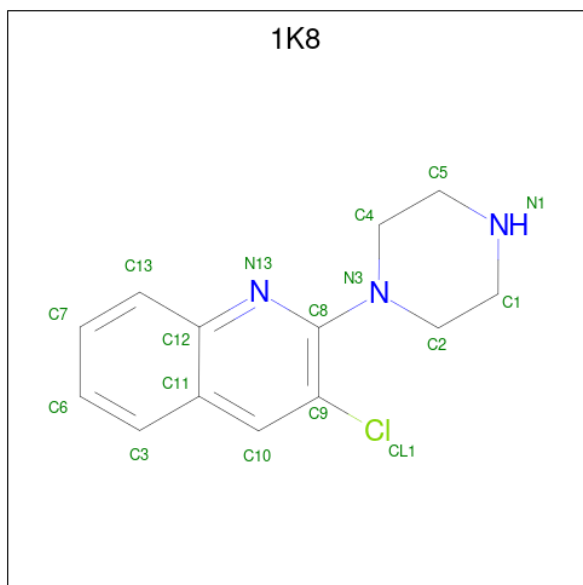
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

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

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



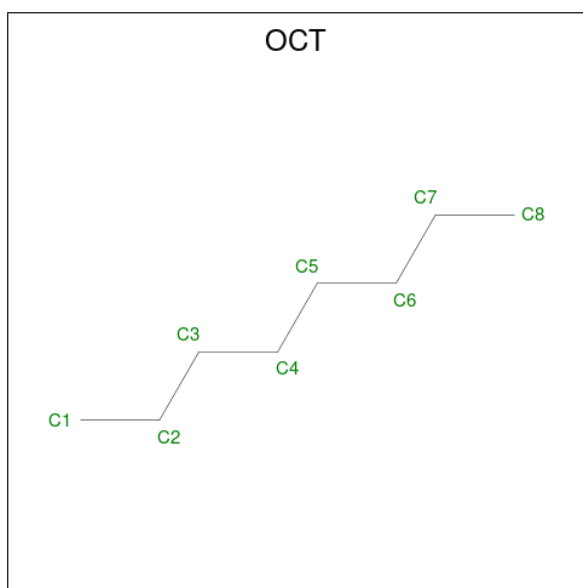
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			17	13	1	3		
4	B	1	Total	C	Cl	N	0	0
			17	13	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



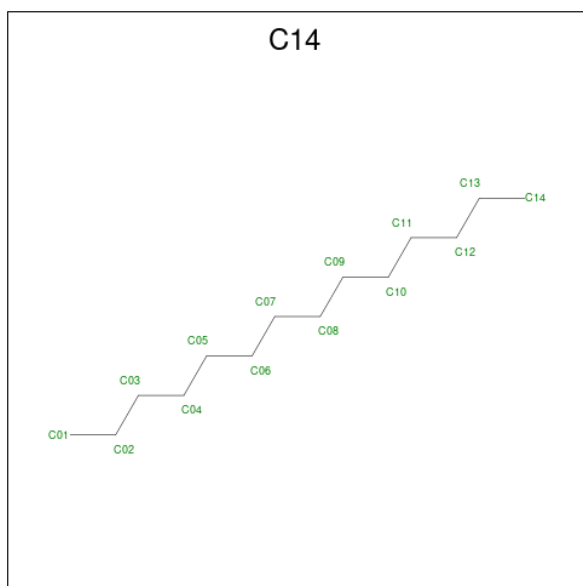
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	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 (CCD ID: OCT) (formula: C_8H_{18}).



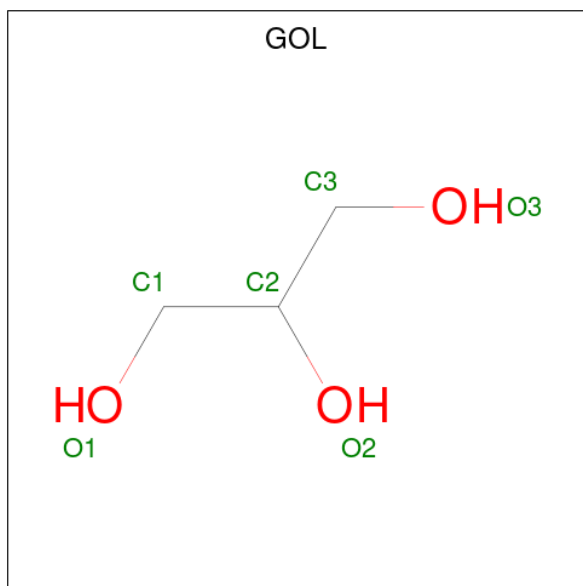
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0
6	C	1	Total C 8 8	0	0

- Molecule 7 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



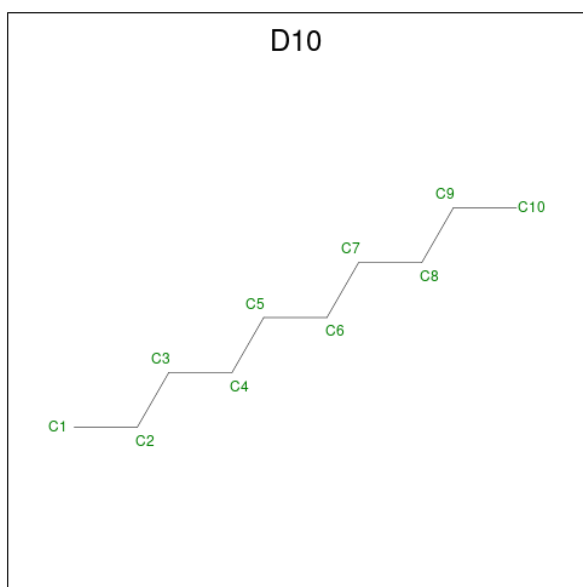
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C 14 14	0	0
7	A	1	Total C 14 14	0	0
7	C	1	Total C 14 14	0	0

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



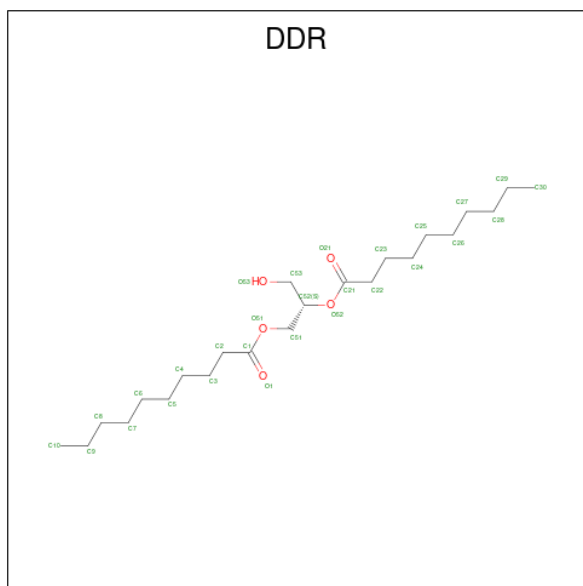
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	B	1	Total C O 6 3 3	0	0
8	C	1	Total C O 6 3 3	0	0

- Molecule 9 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



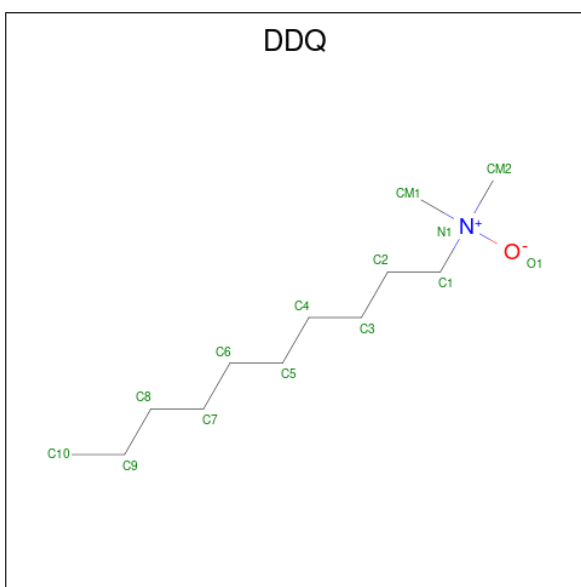
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			10	10		

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



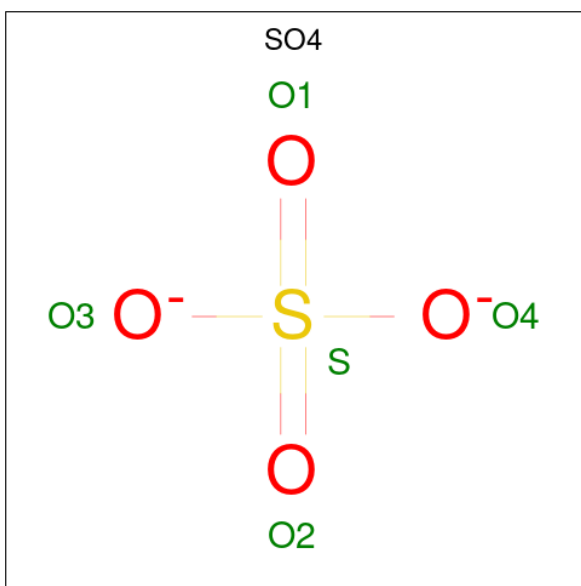
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			28	23	5		

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



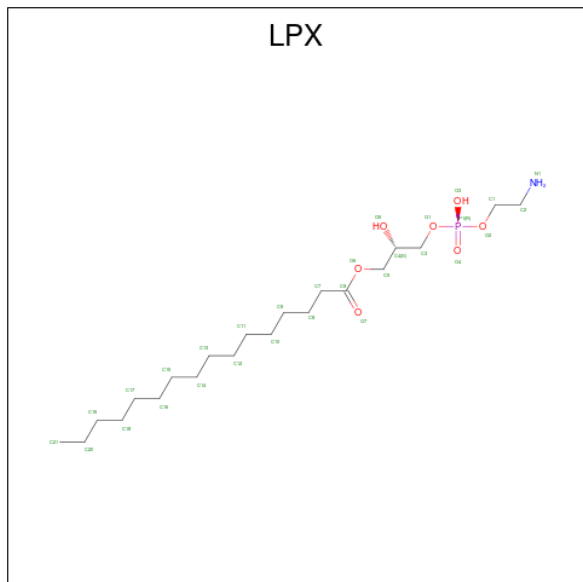
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 13 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



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		

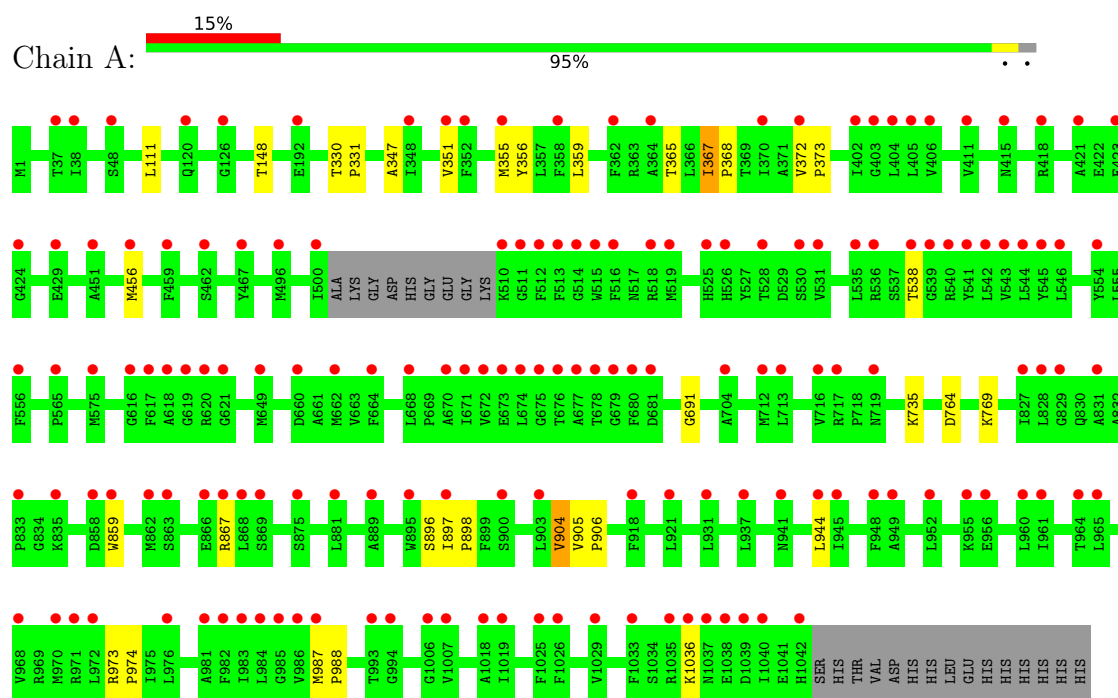
- Molecule 14 is water.

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		

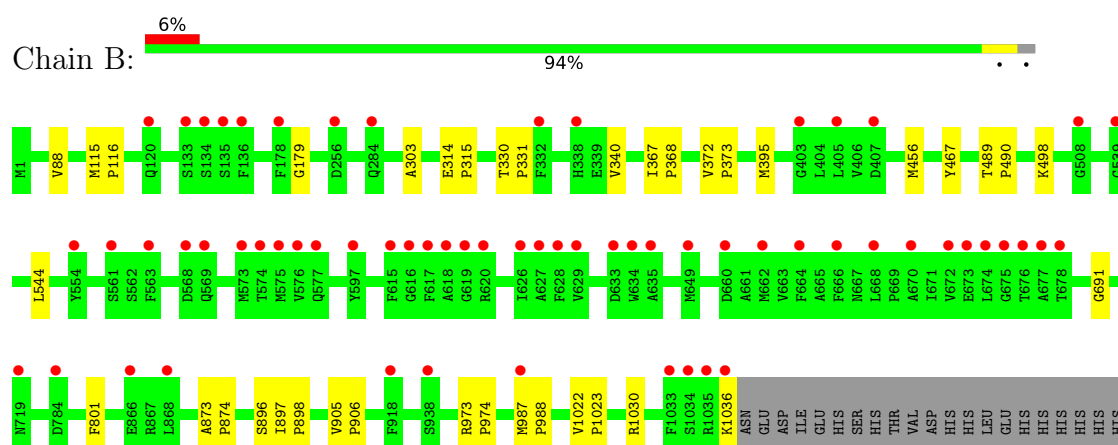
3 Residue-property plots

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.

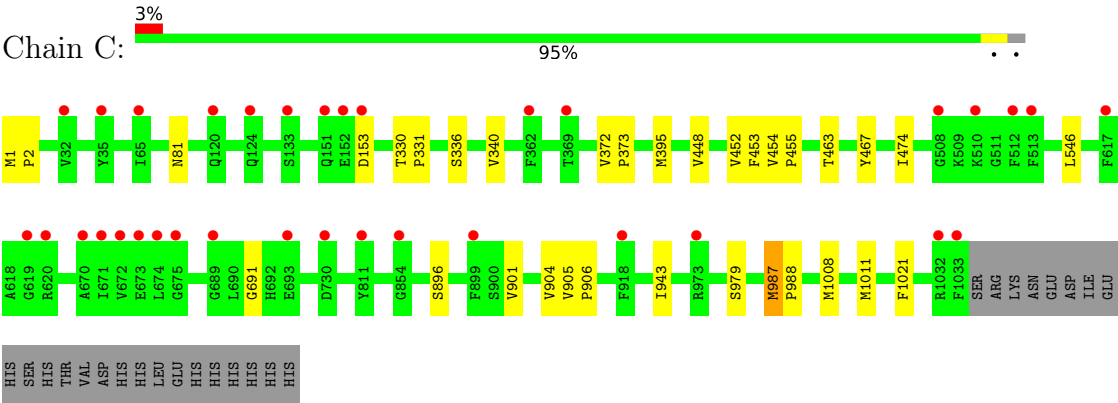
- Molecule 1: Multidrug efflux pump subunit AcrB



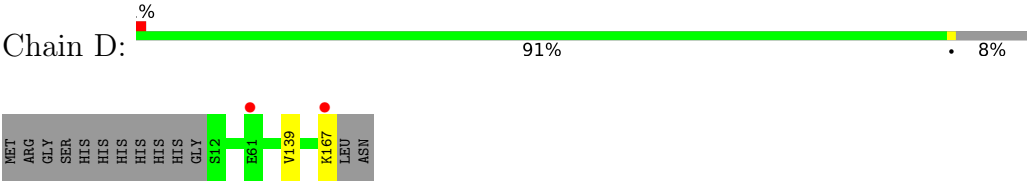
- Molecule 1: Multidrug efflux pump subunit AcrB



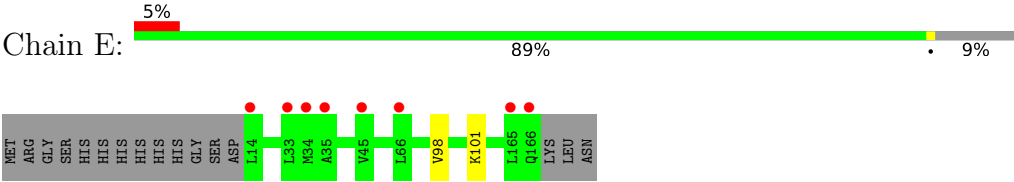
- Molecule 1: Multidrug efflux pump subunit AcrB



• 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	146.13Å 159.65Å 245.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.05 – 2.60 49.05 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.05-2.60) 99.9 (49.05-2.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.02%)	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)	0.30 , 18.1	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	0.91	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C14, EDO, LMT, DDQ, D10, LPX, 1K8, DDR, GOL, SO4, OCT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.04	0/8022	1.57	7/10893 (0.1%)
1	B	1.04	0/8033	1.57	4/10906 (0.0%)
1	C	1.03	0/8030	1.56	5/10904 (0.0%)
2	D	1.03	0/1201	1.59	0/1632
2	E	1.03	0/1178	1.60	0/1602
All	All	1.04	0/26464	1.57	16/35937 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	SER	CA-C-N	7.36	124.88	120.24
1	B	896	SER	C-N-CA	7.36	124.88	120.24
1	A	896	SER	CA-C-N	6.08	125.20	120.33
1	A	896	SER	C-N-CA	6.08	125.20	120.33
1	C	691	GLY	CA-C-O	-5.93	118.36	122.22
1	C	1021	PHE	CA-C-N	5.69	123.83	120.24
1	C	1021	PHE	C-N-CA	5.69	123.83	120.24
1	C	896	SER	CA-C-N	5.58	124.79	120.33
1	C	896	SER	C-N-CA	5.58	124.79	120.33
1	A	691	GLY	CA-C-O	-5.38	118.44	122.37
1	B	691	GLY	CA-C-O	-5.30	118.33	122.52
1	A	904	VAL	CA-C-N	5.29	124.56	120.33
1	A	904	VAL	C-N-CA	5.29	124.56	120.33
1	A	538	THR	CA-C-N	5.06	125.69	120.03
1	A	538	THR	C-N-CA	5.06	125.69	120.03
1	B	179	GLY	CA-C-O	-5.01	118.06	122.16

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	13	0
1	B	7883	0	8040	18	0
1	C	7874	0	8035	16	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
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	50	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:SER:HA	1:C:1011:MET:HE3	1.86	0.57
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:C:987:MET:HE3	1:C:1008:MET:HE1	1.93	0.50
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
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
1:C:987:MET:CE	1:C:1008:MET:HE1	2.47	0.44
1:C:395:MET:HA	1:C:395:MET:HE2	2.00	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:B:395[A]:MET:HA	1:B:395[A]:MET:HE2	2.00	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:351:VAL:HG12	1:A:355:MET:HE2	2.03	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%)	836 (99%)	8 (1%)	70	87
1	B	843/863 (98%)	837 (99%)	6 (1%)	76	89
1	C	842/863 (98%)	838 (100%)	4 (0%)	81	92
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%)	2750 (99%)	18 (1%)	76	89

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LEU
1	A	148	THR
1	A	367	ILE
1	A	456	MET
1	A	735	LYS
1	A	904	VAL
1	A	944	LEU
1	A	1036	LYS
1	B	88	VAL
1	B	498	LYS
1	B	544	LEU
1	B	801	PHE
1	B	1030	ARG
1	B	1036	LYS
1	C	81	ASN
1	C	153	ASP
1	C	546	LEU
1	C	987	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	89	GLN
1	A	194	ASN
1	A	237	GLN
1	A	284	GLN
1	A	298	ASN

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Mol	Chain	Res	Type
1	A	1001	ASN
1	B	194	ASN
1	B	361	ASN
1	B	526	HIS
1	B	577	GLN
1	B	584	GLN
1	B	747	ASN
1	C	58	GLN
1	C	68	ASN
1	C	89	GLN
1	C	194	ASN
1	C	237	GLN
1	C	439	GLN
1	C	797	GLN
2	D	59	HIS
2	D	92	HIS
2	D	102	ASN
2	D	122	ASN
2	E	59	HIS
2	E	125	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1112	-	3,3,3	0.06	0	2,2,2	0.10	0
5	EDO	B	1506	-	3,3,3	0.07	0	2,2,2	0.13	0
8	GOL	B	1509	-	5,5,5	0.08	0	5,5,5	0.25	0
13	LPX	C	1705	-	29,29,29	0.29	0	31,33,33	0.36	0
3	LMT	B	1504	-	36,36,36	0.52	0	47,47,47	0.99	2 (4%)
10	DDR	B	1508	-	27,27,27	0.26	0	29,29,29	0.38	0
3	LMT	B	1510	-	36,36,36	0.51	1 (2%)	47,47,47	0.99	3 (6%)
4	1K8	B	1516	-	19,19,19	2.84	4 (21%)	24,26,26	1.49	4 (16%)
9	D10	B	1505	-	9,9,9	0.09	0	8,8,8	0.07	0
8	GOL	A	1107	-	5,5,5	0.10	0	5,5,5	0.28	0
11	DDQ	B	1515	-	11,13,13	0.17	0	12,15,15	0.25	0
8	GOL	C	1709	-	5,5,5	0.09	0	5,5,5	0.27	0
6	OCT	C	1701	-	7,7,7	0.10	0	6,6,6	0.08	0
3	LMT	C	1708	-	36,36,36	0.58	1 (2%)	47,47,47	0.95	3 (6%)
5	EDO	C	1712	-	3,3,3	0.08	0	2,2,2	0.23	0
5	EDO	A	1110	-	3,3,3	0.06	0	2,2,2	0.10	0
7	C14	C	1706	-	13,13,13	0.08	0	12,12,12	0.06	0
3	LMT	A	1111	-	36,36,36	0.50	1 (2%)	47,47,47	0.75	1 (2%)
12	SO4	B	1518	-	4,4,4	0.35	0	6,6,6	0.07	0
3	LMT	C	1703	-	36,36,36	0.45	0	47,47,47	0.50	0
12	SO4	C	1713	-	4,4,4	0.35	0	6,6,6	0.07	0
3	LMT	B	1503	-	36,36,36	0.47	0	47,47,47	0.58	0
7	C14	A	1108	-	13,13,13	0.08	0	12,12,12	0.08	0
5	EDO	A	1113	-	3,3,3	0.06	0	2,2,2	0.10	0
3	LMT	A	1101	-	36,36,36	0.45	0	47,47,47	0.62	0
8	GOL	B	1512	-	5,5,5	0.10	0	5,5,5	0.28	0
12	SO4	B	1517	-	4,4,4	0.35	0	6,6,6	0.08	0
5	EDO	A	1109	-	3,3,3	0.06	0	2,2,2	0.11	0
6	OCT	C	1704	-	7,7,7	0.11	0	6,6,6	0.07	0
8	GOL	B	1502	-	5,5,5	0.09	0	5,5,5	0.24	0
6	OCT	A	1105	-	7,7,7	0.11	0	6,6,6	0.07	0
3	LMT	A	1103	-	36,36,36	0.52	1 (2%)	47,47,47	0.84	2 (4%)
5	EDO	A	1104	-	3,3,3	0.07	0	2,2,2	0.06	0
5	EDO	B	1501	-	3,3,3	0.06	0	2,2,2	0.08	0
5	EDO	C	1702	-	3,3,3	0.07	0	2,2,2	0.12	0
7	C14	A	1106	-	13,13,13	0.08	0	12,12,12	0.06	0
5	EDO	B	1513	-	3,3,3	0.06	0	2,2,2	0.09	0
5	EDO	C	1711	-	3,3,3	0.06	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GOL	B	1511	-	5,5,5	0.09	0	5,5,5	0.31	0
5	EDO	B	1514	-	3,3,3	0.06	0	2,2,2	0.14	0
4	1K8	A	1102	-	19,19,19	2.70	4 (21%)	24,26,26	1.36	2 (8%)
13	LPX	C	1707	-	29,29,29	0.29	0	31,33,33	0.35	0
5	EDO	C	1710	-	3,3,3	0.06	0	2,2,2	0.09	0
5	EDO	B	1507	-	3,3,3	0.06	0	2,2,2	0.11	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	1112	-	-	0/1/1/1	-
5	EDO	B	1506	-	-	1/1/1/1	-
8	GOL	B	1509	-	-	0/4/4/4	-
13	LPX	C	1705	-	-	15/31/31/31	-
3	LMT	B	1504	-	-	12/21/61/61	0/2/2/2
10	DDR	B	1508	-	-	15/29/29/29	-
3	LMT	B	1510	-	-	10/21/61/61	0/2/2/2
4	1K8	B	1516	-	-	0/4/12/12	0/3/3/3
9	D10	B	1505	-	-	4/7/7/7	-
8	GOL	A	1107	-	-	2/4/4/4	-
11	DDQ	B	1515	-	-	5/11/11/11	-
8	GOL	C	1709	-	-	4/4/4/4	-
6	OCT	C	1701	-	-	1/5/5/5	-
3	LMT	C	1708	-	-	10/21/61/61	0/2/2/2
5	EDO	C	1712	-	-	1/1/1/1	-
5	EDO	A	1110	-	-	1/1/1/1	-
7	C14	C	1706	-	-	6/11/11/11	-
3	LMT	A	1111	-	-	10/21/61/61	0/2/2/2
3	LMT	C	1703	-	-	8/21/61/61	0/2/2/2
3	LMT	B	1503	-	-	9/21/61/61	0/2/2/2
7	C14	A	1108	-	-	5/11/11/11	-
5	EDO	A	1113	-	-	1/1/1/1	-
3	LMT	A	1101	-	-	7/21/61/61	0/2/2/2
8	GOL	B	1512	-	-	2/4/4/4	-
5	EDO	A	1109	-	-	0/1/1/1	-
6	OCT	C	1704	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	B	1502	-	-	2/4/4/4	-
6	OCT	A	1105	-	-	0/5/5/5	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
5	EDO	A	1104	-	-	1/1/1/1	-
5	EDO	B	1501	-	-	0/1/1/1	-
5	EDO	C	1702	-	-	1/1/1/1	-
7	C14	A	1106	-	-	3/11/11/11	-
5	EDO	B	1513	-	-	1/1/1/1	-
5	EDO	C	1711	-	-	1/1/1/1	-
8	GOL	B	1511	-	-	2/4/4/4	-
5	EDO	B	1514	-	-	0/1/1/1	-
4	1K8	A	1102	-	-	2/4/12/12	0/3/3/3
13	LPX	C	1707	-	-	14/31/31/31	-
5	EDO	C	1710	-	-	0/1/1/1	-
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	9.27	1.51	1.39
4	A	1102	1K8	C9-C8	8.63	1.50	1.39
4	A	1102	1K8	C11-C12	4.75	1.49	1.42
4	B	1516	1K8	C11-C12	4.70	1.49	1.42
4	B	1516	1K8	C8-N13	4.36	1.36	1.31
4	A	1102	1K8	C8-N13	3.98	1.36	1.31
4	A	1102	1K8	C9-CL1	2.82	1.80	1.73
4	B	1516	1K8	C9-CL1	2.62	1.79	1.73
3	C	1708	LMT	O1'-C1'	2.32	1.44	1.40
3	A	1103	LMT	O1'-C1'	2.30	1.44	1.40
3	A	1111	LMT	O1'-C1'	2.10	1.43	1.40
3	B	1510	LMT	O1'-C1'	2.02	1.43	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	1K8	C4-N3-C2	4.56	121.83	111.57
3	B	1510	LMT	O1B-C4'-C3'	3.54	116.24	107.23
3	C	1708	LMT	C1'-C2'-C3'	3.31	116.97	110.01
3	B	1504	LMT	C1'-C2'-C3'	2.97	116.25	110.01
4	B	1516	1K8	C8-N13-C12	2.96	122.51	116.11
3	B	1504	LMT	C2'-C3'-C4'	2.95	116.36	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1516	1K8	C5-C4-N3	-2.94	103.98	110.38
4	B	1516	1K8	C9-C8-N13	-2.84	118.11	122.81
4	B	1516	1K8	C10-C9-CL1	-2.68	116.52	119.19
3	B	1510	LMT	C1B-O5B-C5B	2.66	118.92	113.72
4	A	1102	1K8	C8-N13-C12	2.56	121.65	116.11
3	C	1708	LMT	C2'-C3'-C4'	2.54	115.45	109.68
3	A	1111	LMT	O1B-C4'-C3'	2.42	113.38	107.23
3	C	1708	LMT	O1B-C4'-C3'	2.41	113.37	107.23
3	B	1510	LMT	C1B-O1B-C4'	2.23	123.26	117.98
3	A	1103	LMT	O1'-C1'-C2'	2.15	111.54	108.27
3	A	1103	LMT	C3B-C4B-C5B	2.12	114.08	110.23

There are no chirality outliers.

All (169) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	1510	LMT	C3'-C4'-O1B-C1B
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
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	1510	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	C	1708	LMT	C3'-C4'-O1B-C1B
3	B	1503	LMT	O5'-C5'-C6'-O6'
10	B	1508	DDR	O1-C1-O51-C51
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5'-C1'-O1'-C1
3	B	1503	LMT	C4'-C5'-C6'-O6'
13	C	1705	LPX	C7-C6-O6-C5
3	C	1703	LMT	C4'-C5'-C6'-O6'
3	A	1101	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'
13	C	1705	LPX	O7-C6-O6-C5
3	A	1111	LMT	O5'-C1'-O1'-C1
3	C	1703	LMT	O1'-C1-C2-C3
13	C	1705	LPX	O5-C4-C5-O6
3	A	1111	LMT	O1'-C1-C2-C3
13	C	1705	LPX	C3-C4-C5-O6
3	B	1504	LMT	C2'-C1'-O1'-C1
3	C	1708	LMT	C2'-C1'-O1'-C1
8	A	1107	GOL	C1-C2-C3-O3
8	C	1709	GOL	O1-C1-C2-C3
3	B	1504	LMT	C2B-C1B-O1B-C4'
3	B	1510	LMT	O5B-C5B-C6B-O6B
3	B	1504	LMT	O5B-C1B-O1B-C4'
11	B	1515	DDQ	C2-C3-C4-C5
3	A	1111	LMT	C6-C7-C8-C9
3	C	1703	LMT	C2-C1-O1'-C1'
8	B	1512	GOL	O2-C2-C3-O3
3	B	1504	LMT	C5-C6-C7-C8
13	C	1707	LPX	C7-C6-O6-C5
7	A	1108	C14	C08-C09-C10-C11
7	A	1106	C14	C02-C03-C04-C05
3	C	1708	LMT	C1-C2-C3-C4
5	B	1506	EDO	O1-C1-C2-O2
5	C	1702	EDO	O1-C1-C2-O2
9	B	1505	D10	C4-C5-C6-C7
10	B	1508	DDR	C2-C3-C4-C5
13	C	1707	LPX	O7-C6-O6-C5
13	C	1707	LPX	C11-C12-C13-C14
3	B	1504	LMT	C3-C4-C5-C6
3	B	1503	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	C	1708	LMT	C3-C4-C5-C6
3	B	1504	LMT	C11-C10-C9-C8
3	B	1510	LMT	C1-C2-C3-C4
3	B	1503	LMT	C6-C7-C8-C9
11	B	1515	DDQ	C5-C6-C7-C8
3	C	1708	LMT	C7-C8-C9-C10
7	A	1108	C14	C06-C07-C08-C09
13	C	1705	LPX	C16-C17-C18-C19
3	C	1708	LMT	C5-C6-C7-C8
9	B	1505	D10	C3-C4-C5-C6
3	A	1101	LMT	C3-C4-C5-C6
3	B	1504	LMT	C4-C5-C6-C7
13	C	1705	LPX	C17-C18-C19-C20
3	A	1111	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	C7-C8-C9-C10
7	A	1108	C14	C03-C04-C05-C06
8	C	1709	GOL	O2-C2-C3-O3
3	C	1708	LMT	C4-C5-C6-C7
3	A	1103	LMT	C2'-C1'-O1'-C1
10	B	1508	DDR	O51-C51-C52-C53
13	C	1707	LPX	C17-C18-C19-C20
3	A	1103	LMT	C4'-C5'-C6'-O6'
5	A	1110	EDO	O1-C1-C2-O2
5	A	1113	EDO	O1-C1-C2-O2
5	B	1513	EDO	O1-C1-C2-O2
7	A	1108	C14	C07-C08-C09-C10
11	B	1515	DDQ	C6-C7-C8-C9
3	B	1510	LMT	C7-C8-C9-C10
7	A	1108	C14	C09-C10-C11-C12
13	C	1707	LPX	C13-C14-C15-C16
13	C	1707	LPX	C7-C8-C9-C10
10	B	1508	DDR	C7-C8-C9-C10
3	B	1504	LMT	C2-C1-O1'-C1'
3	C	1708	LMT	C5'-C4'-O1B-C1B
10	B	1508	DDR	C25-C26-C27-C28
10	B	1508	DDR	C4-C5-C6-C7
10	B	1508	DDR	C51-C52-C53-O53
7	A	1106	C14	C01-C02-C03-C04
5	B	1507	EDO	O1-C1-C2-O2
5	C	1712	EDO	O1-C1-C2-O2
3	A	1101	LMT	C1-C2-C3-C4
6	C	1701	OCT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	1504	LMT	O5'-C1'-O1'-C1
13	C	1705	LPX	C7-C8-C9-C10
13	C	1707	LPX	C18-C19-C20-C21
3	A	1111	LMT	C5'-C4'-O1B-C1B
3	A	1111	LMT	C11-C10-C9-C8
7	C	1706	C14	C10-C11-C12-C13
3	C	1703	LMT	C7-C8-C9-C10
3	A	1111	LMT	C9-C10-C11-C12
3	B	1510	LMT	C9-C10-C11-C12
3	B	1504	LMT	C1-C2-C3-C4
3	C	1703	LMT	C3-C4-C5-C6
7	C	1706	C14	C07-C08-C09-C10
3	C	1703	LMT	C9-C10-C11-C12
3	C	1708	LMT	C2-C1-O1'-C1'
3	C	1708	LMT	C11-C10-C9-C8
11	B	1515	DDQ	C3-C4-C5-C6
7	C	1706	C14	C09-C10-C11-C12
3	A	1101	LMT	C2-C3-C4-C5
13	C	1707	LPX	C16-C17-C18-C19
13	C	1705	LPX	C9-C10-C11-C12
10	B	1508	DDR	O51-C51-C52-O52
10	B	1508	DDR	C1-C2-C3-C4
13	C	1707	LPX	C3-O1-P1-O2
13	C	1707	LPX	C1-O2-P1-O1
3	B	1510	LMT	C3-C4-C5-C6
9	B	1505	D10	C5-C6-C7-C8
3	A	1103	LMT	C9-C10-C11-C12
3	A	1111	LMT	C4-C5-C6-C7
8	C	1709	GOL	O1-C1-C2-O2
10	B	1508	DDR	C51-C52-O52-C21
3	B	1503	LMT	C2-C3-C4-C5
13	C	1705	LPX	C11-C10-C9-C8
3	A	1103	LMT	C11-C10-C9-C8
3	B	1510	LMT	C4-C5-C6-C7
5	A	1104	EDO	O1-C1-C2-O2
7	C	1706	C14	C02-C03-C04-C05
3	B	1503	LMT	C2-C1-O1'-C1'
3	B	1503	LMT	O1'-C1-C2-C3
9	B	1505	D10	C1-C2-C3-C4
7	C	1706	C14	C04-C05-C06-C07
3	B	1504	LMT	C4B-C5B-C6B-O6B
10	B	1508	DDR	O52-C52-C53-O53

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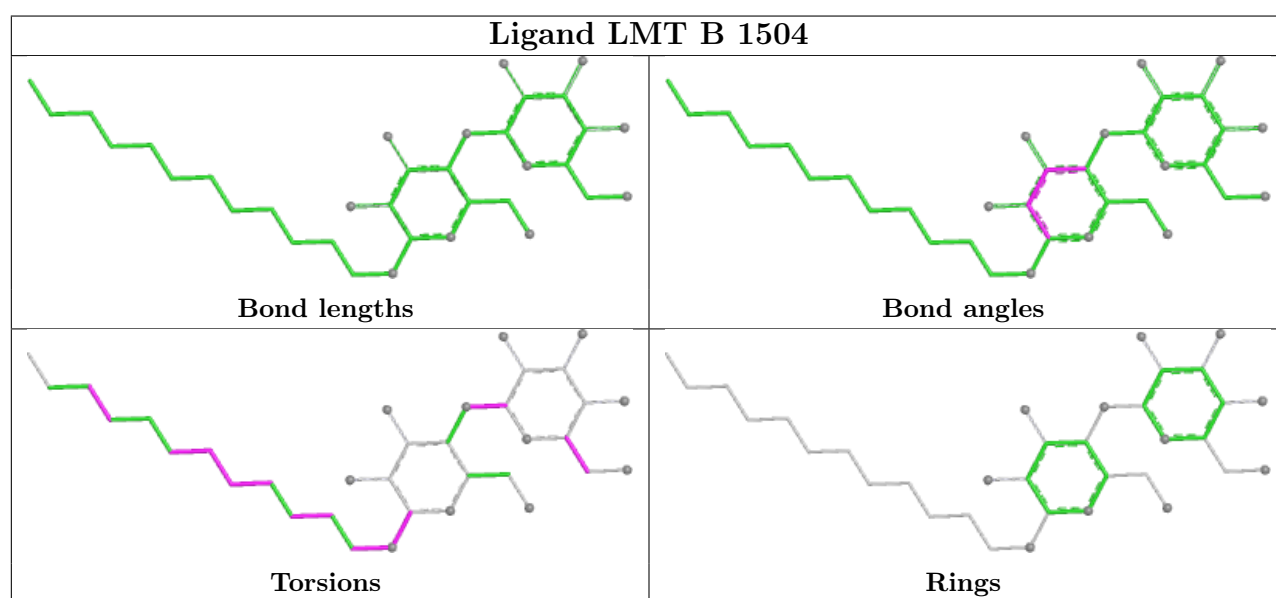
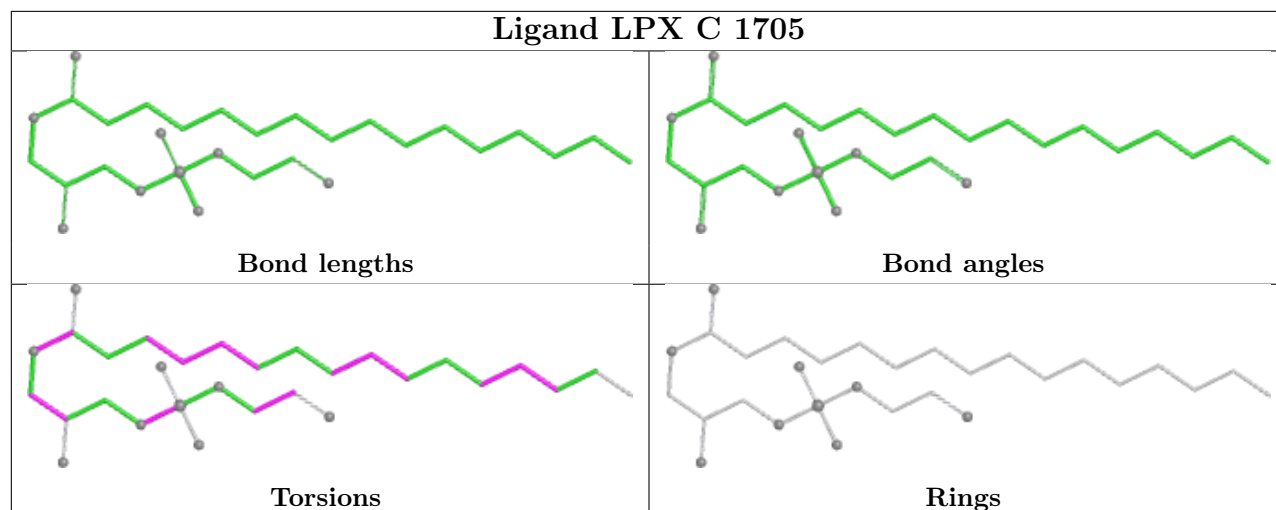
Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C11-C10-C9-C8
13	C	1707	LPX	C15-C16-C17-C18
3	B	1510	LMT	C11-C10-C9-C8
6	C	1704	OCT	C1-C2-C3-C4
7	C	1706	C14	C08-C09-C10-C11
3	A	1103	LMT	C1-C2-C3-C4
3	A	1103	LMT	C2-C3-C4-C5
3	A	1103	LMT	C2-C1-O1'-C1'
13	C	1705	LPX	C13-C14-C15-C16
5	C	1711	EDO	O1-C1-C2-O2
7	A	1106	C14	C09-C10-C11-C12
3	A	1103	LMT	C6-C7-C8-C9
3	C	1703	LMT	C2-C3-C4-C5
11	B	1515	DDQ	C2-C1-N1-O1
13	C	1705	LPX	C12-C13-C14-C15
3	A	1101	LMT	C4-C5-C6-C7
10	B	1508	DDR	C3-C4-C5-C6

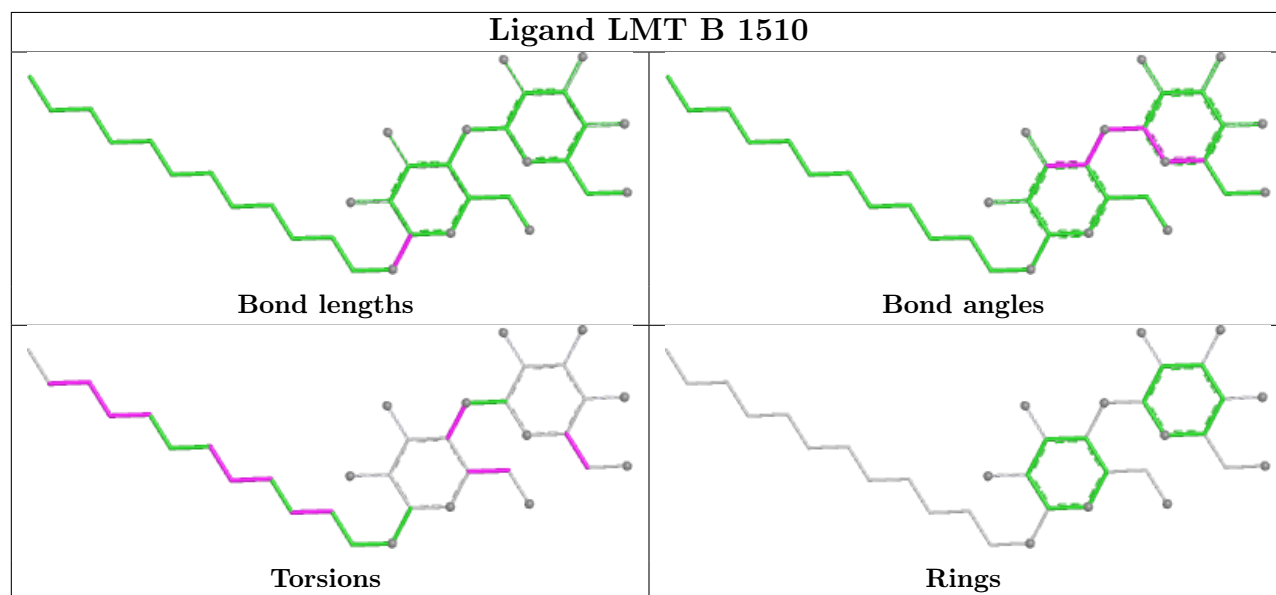
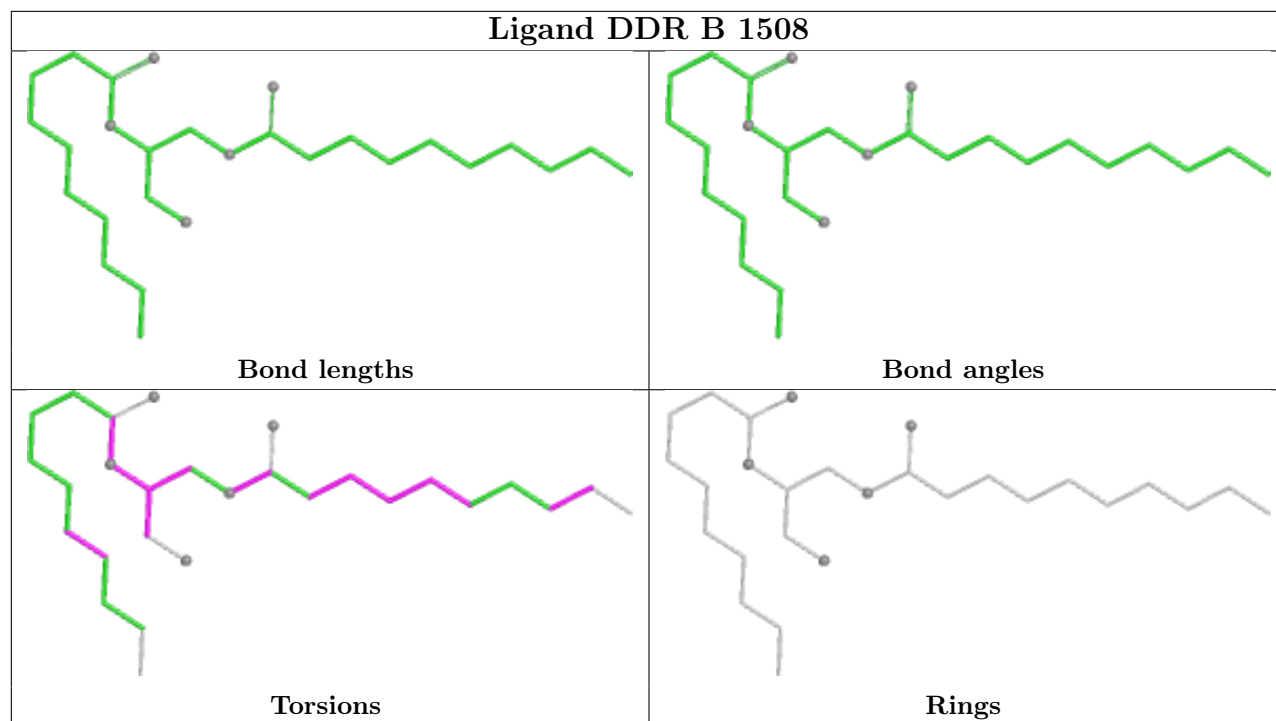
There are no ring outliers.

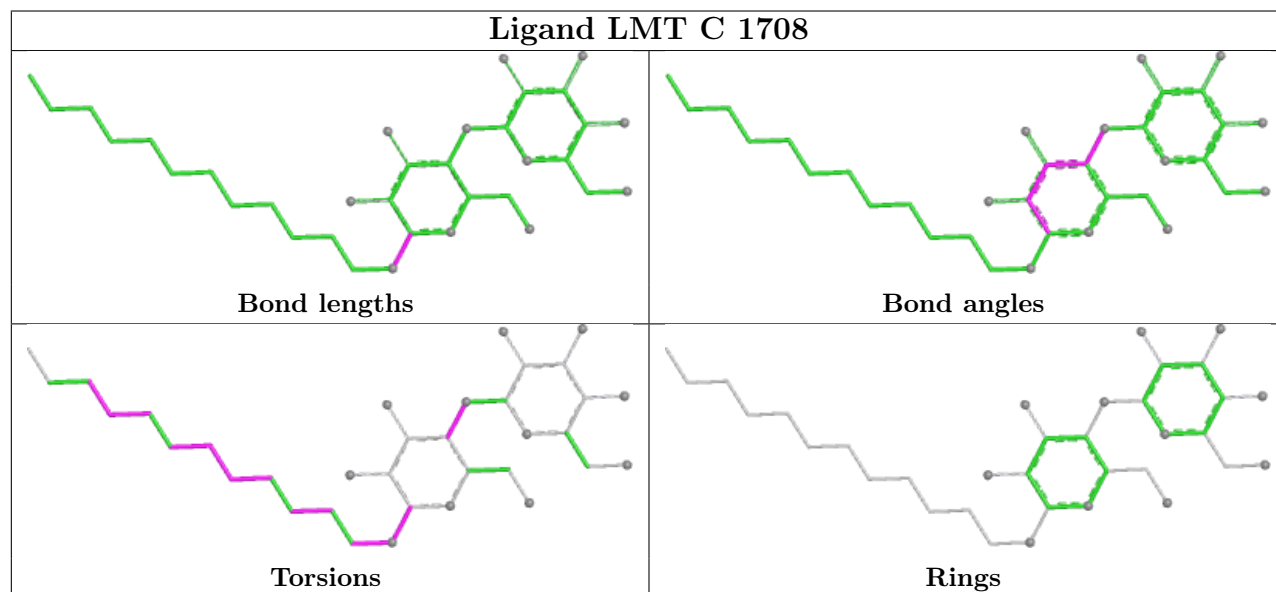
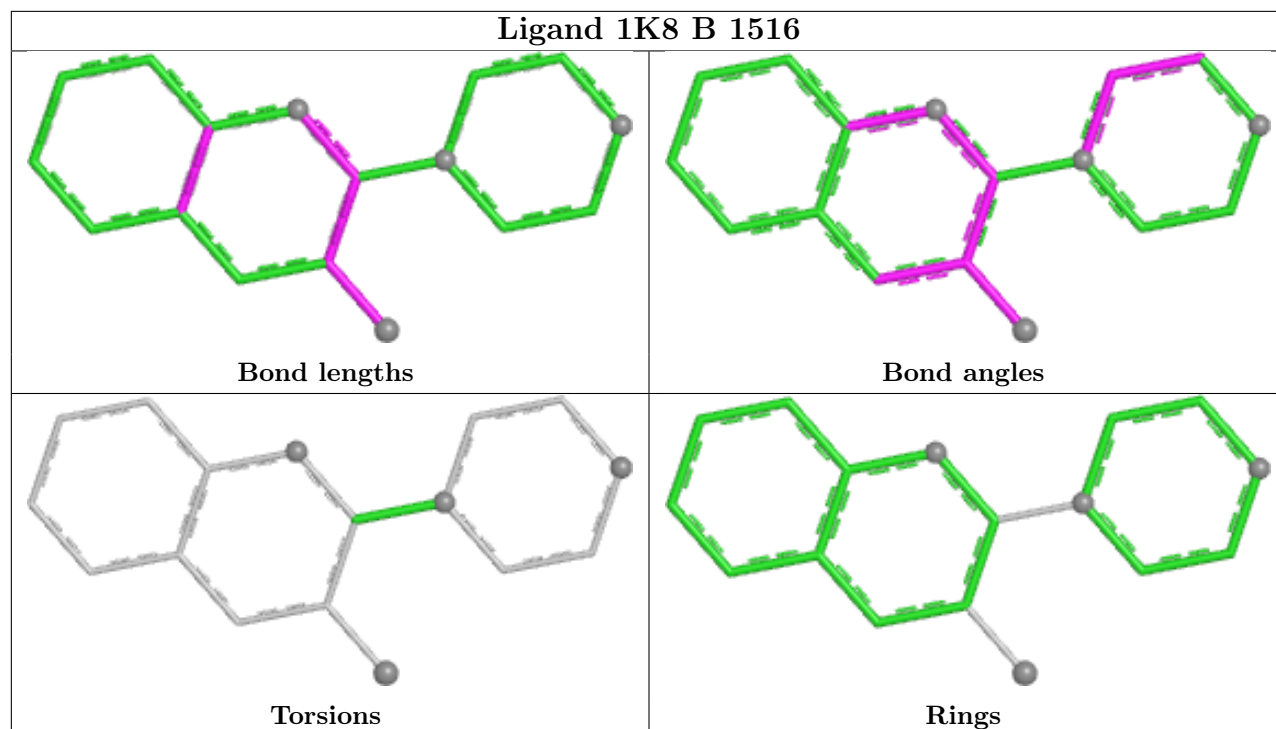
1 monomer is involved in 1 short contact:

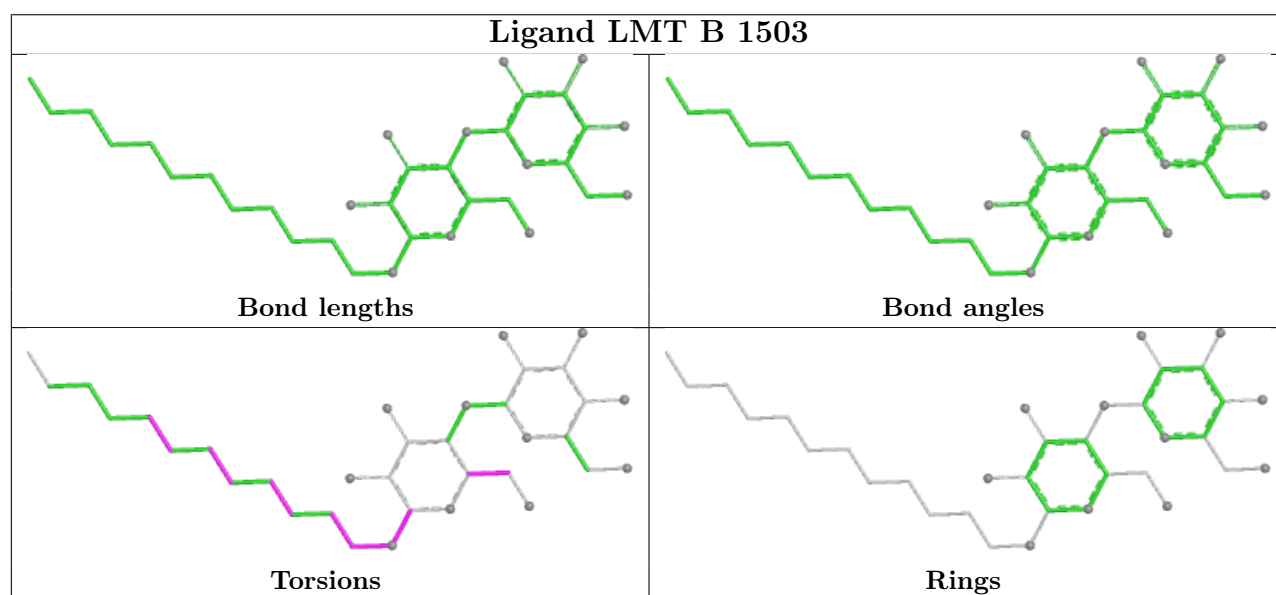
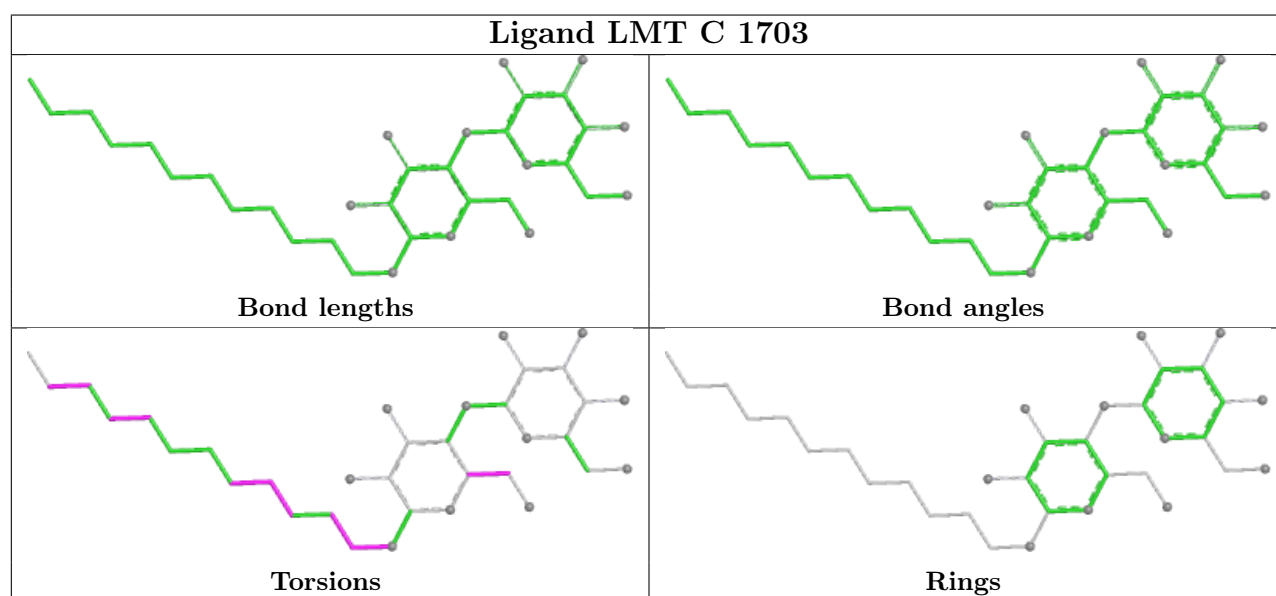
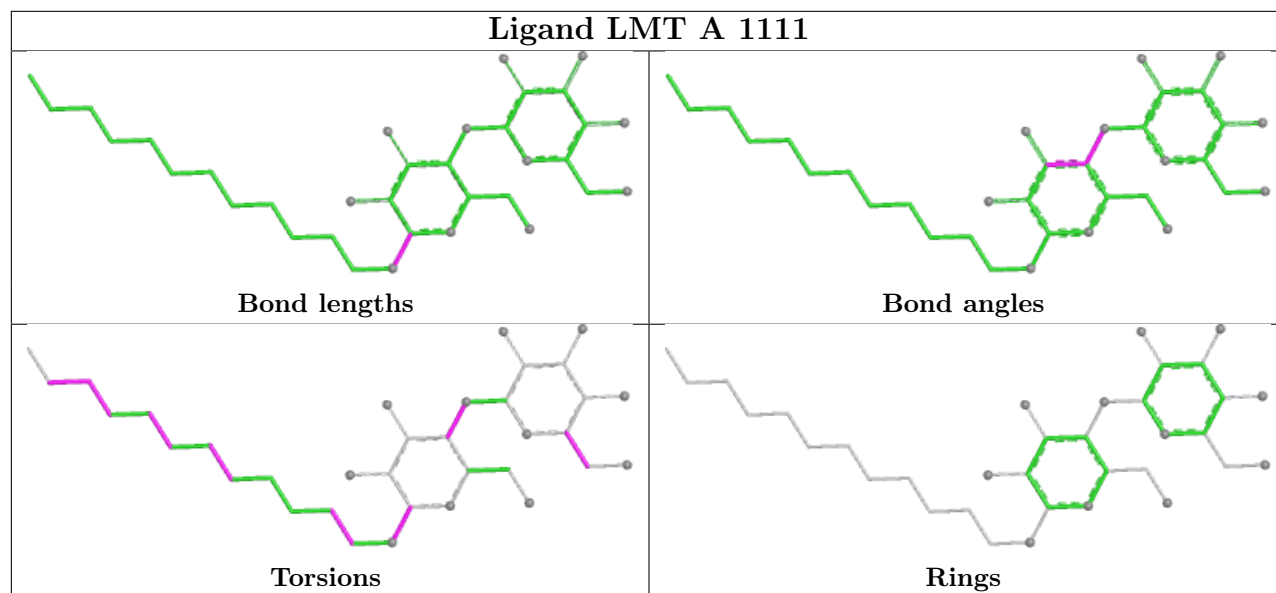
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1516	1K8	1	0

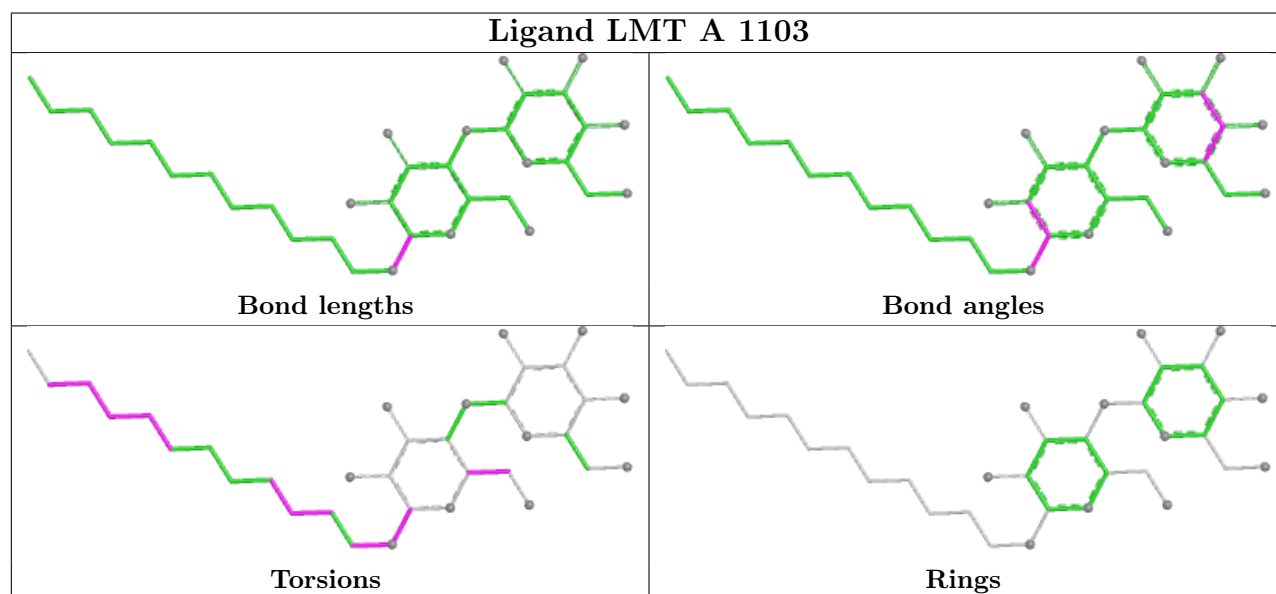
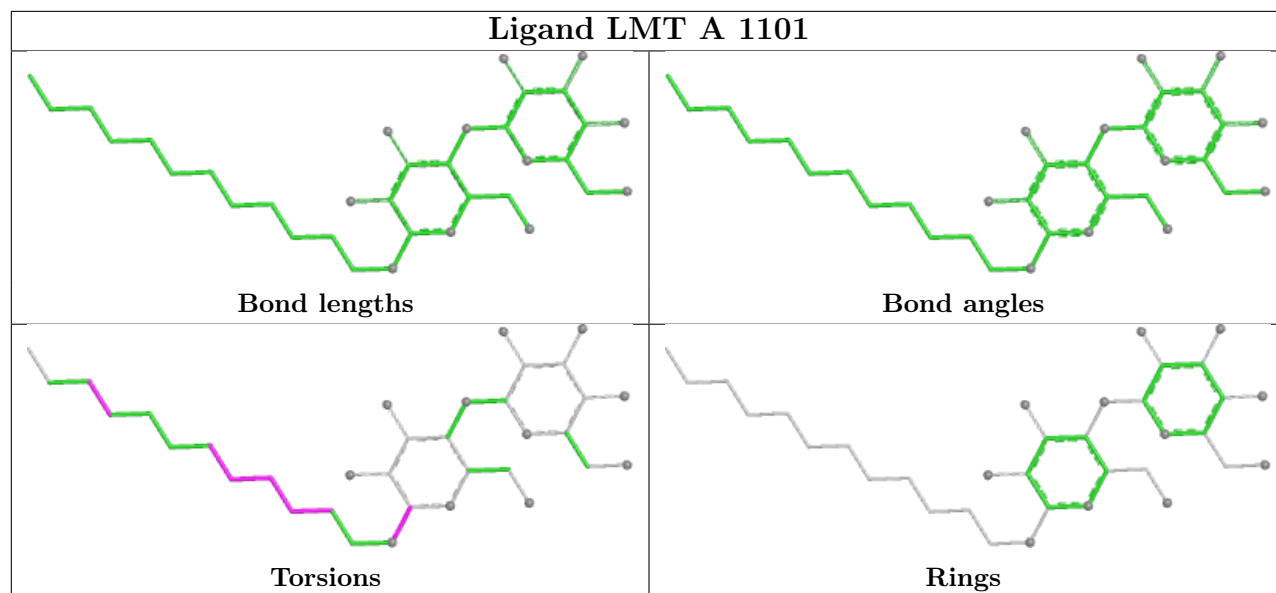
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

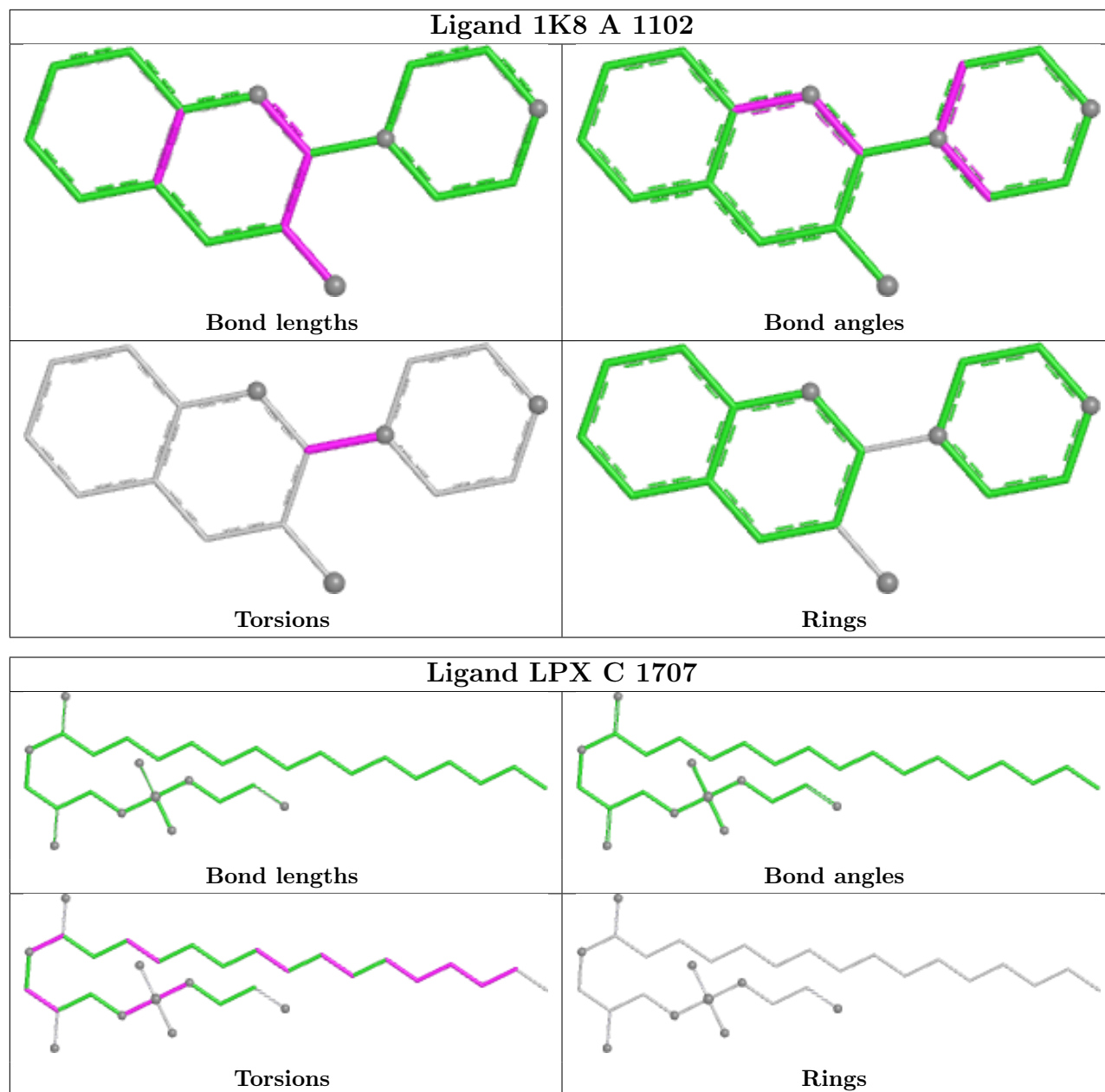












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1033/1057 (97%)	0.96	158 (15%) 5 4	32, 61, 115, 137	1 (0%)
1	B	1036/1057 (98%)	0.55	64 (6%) 26 21	28, 59, 73, 80	1 (0%)
1	C	1033/1057 (97%)	0.30	34 (3%) 49 43	24, 49, 67, 76	3 (0%)
2	D	156/169 (92%)	0.34	2 (1%) 75 71	46, 58, 75, 83	0
2	E	153/169 (90%)	0.72	8 (5%) 33 27	52, 65, 85, 93	0
All	All	3411/3509 (97%)	0.60	266 (7%) 19 15	24, 56, 91, 137	5 (0%)

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	617	PHE	10.6
1	B	628	PHE	7.7
1	A	868	LEU	7.1
1	B	675	GLY	6.9
1	A	672	VAL	6.8
1	A	674	LEU	6.7
1	A	675	GLY	6.6
1	B	676	THR	6.5
1	B	615	PHE	6.4
1	B	618	ALA	6.4
1	B	673	GLU	6.3
2	E	14	LEU	6.3
1	A	948	PHE	6.3
1	A	673	GLU	6.1
1	A	982	PHE	6.0
1	B	575	MET	6.0
1	B	616	GLY	5.6
1	A	424	GLY	5.4
1	A	617	PHE	5.3
1	B	672	VAL	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	37	THR	5.0
1	B	573	MET	4.8
1	B	133	SER	4.7
1	A	500	ILE	4.5
1	A	678	THR	4.5
1	A	716	VAL	4.4
1	B	674	LEU	4.3
1	C	120	GLN	4.3
1	A	542	LEU	4.3
1	A	677	ALA	4.3
1	B	135	SER	4.2
1	A	867	ARG	4.2
1	A	351	VAL	4.2
1	B	677	ALA	4.2
1	A	1040	ILE	4.1
1	B	626	ILE	4.1
1	A	985	GLY	4.0
1	A	680	PHE	4.0
1	C	811	TYR	4.0
1	A	719	ASN	4.0
1	A	971	ARG	4.0
1	A	429	GLU	3.9
1	A	649[A]	MET	3.9
1	A	421	ALA	3.8
1	A	970	MET	3.8
1	B	134	SER	3.8
1	A	540	ARG	3.7
1	B	670	ALA	3.7
1	C	675	GLY	3.7
1	A	662	MET	3.7
1	A	984	LEU	3.6
1	C	670	ALA	3.6
1	A	38	ILE	3.6
1	A	192	GLU	3.6
1	A	1019	ILE	3.5
1	A	713	LEU	3.5
1	A	575	MET	3.5
1	A	510	LYS	3.5
1	A	866	GLU	3.5
1	A	1036	LYS	3.4
1	A	987	MET	3.4
1	A	676	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	362	PHE	3.4
1	A	679	GLY	3.4
1	B	178	PHE	3.4
1	A	671	ILE	3.3
1	A	404	LEU	3.3
1	A	1042	HIS	3.3
1	A	531	VAL	3.3
1	B	666	PHE	3.3
1	A	983	ILE	3.3
1	C	124	GLN	3.2
1	A	829	GLY	3.2
1	B	563	PHE	3.2
1	B	719	ASN	3.2
1	B	120	GLN	3.2
1	A	968	VAL	3.2
1	B	284	GLN	3.2
1	C	513	PHE	3.2
1	A	1039	ASP	3.1
1	A	668	LEU	3.1
1	B	136	PHE	3.1
1	A	362	PHE	3.1
1	A	618	ALA	3.1
1	A	965	LEU	3.0
1	A	828	LEU	3.0
1	C	510	LYS	3.0
1	B	577	GLN	3.0
1	A	712	MET	3.0
1	A	538	THR	3.0
1	A	949	ALA	3.0
1	A	869	SER	3.0
1	A	862	MET	3.0
1	B	629	VAL	3.0
1	A	565	PRO	2.9
1	A	681	ASP	2.9
1	A	664	PHE	2.9
1	B	668	LEU	2.9
1	A	1037	ASN	2.9
1	B	662	MET	2.9
1	B	633	ASP	2.9
1	A	994	GLY	2.9
1	A	459	PHE	2.9
1	A	986	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	462	SER	2.9
1	B	627	ALA	2.9
1	B	635	ALA	2.9
2	E	166	GLN	2.9
1	A	539	GLY	2.9
1	A	554	TYR	2.9
1	A	405	LEU	2.9
1	A	403	GLY	2.8
1	B	508	GLY	2.8
2	E	35	ALA	2.8
1	A	536	ARG	2.8
1	B	619	GLY	2.8
1	A	556	PHE	2.8
1	C	673	GLU	2.8
1	A	372	VAL	2.8
1	A	526	HIS	2.8
1	A	918	PHE	2.8
1	A	859	TRP	2.8
1	B	634	TRP	2.8
1	B	868	LEU	2.8
1	A	355	MET	2.8
1	B	784	ASP	2.7
1	B	664	PHE	2.7
1	C	899	PHE	2.7
1	A	402	ILE	2.7
1	A	952	LEU	2.7
1	A	616	GLY	2.7
1	A	406	VAL	2.7
1	A	704	ALA	2.7
2	D	167	LYS	2.7
1	B	405	LEU	2.7
1	B	338	HIS	2.7
1	B	561	SER	2.7
1	A	981	ALA	2.7
1	A	543	VAL	2.6
1	A	670	ALA	2.6
1	A	972	LEU	2.6
2	E	33	LEU	2.6
1	B	574	THR	2.6
1	A	423	GLU	2.6
1	A	364	ALA	2.6
1	A	863	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	256	ASP	2.6
1	C	153	ASP	2.6
1	A	370	ILE	2.6
1	C	671	ILE	2.6
1	A	535	LEU	2.6
1	A	931	LEU	2.6
1	A	544	LEU	2.5
1	A	1026	PHE	2.5
1	A	519	MET	2.5
1	B	678	THR	2.5
1	A	541	TYR	2.5
1	C	32	VAL	2.5
1	A	418	ARG	2.5
1	C	620	ARG	2.5
1	B	569	GLN	2.5
1	C	1033	PHE	2.5
1	C	674	LEU	2.4
1	A	511	GLY	2.4
1	B	1036	LYS	2.4
1	C	973[A]	ARG	2.4
1	A	530	SER	2.4
1	B	403	GLY	2.4
1	B	332	PHE	2.4
1	B	1033	PHE	2.4
1	C	617	PHE	2.4
1	A	525	HIS	2.4
1	B	407	ASP	2.4
1	A	496	MET	2.4
1	A	120	GLN	2.4
1	A	411	VAL	2.4
1	B	554	TYR	2.4
1	A	546	LEU	2.4
1	A	937	LEU	2.4
1	C	133	SER	2.4
1	A	1018	ALA	2.4
1	A	875	SER	2.3
1	A	900	SER	2.3
1	A	955	LYS	2.3
1	C	689	GLY	2.3
1	A	513	PHE	2.3
1	A	944	LEU	2.3
1	A	961	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1038	GLU	2.3
1	A	514	GLY	2.3
1	A	518	ARG	2.3
1	B	1035	ARG	2.3
1	C	512	PHE	2.3
1	A	831	ALA	2.3
1	A	945	ILE	2.3
1	C	35	TYR	2.3
1	A	515	TRP	2.3
1	A	621	GLY	2.3
2	E	66	LEU	2.3
1	C	369	THR	2.3
1	C	693	GLU	2.3
1	A	941	ASN	2.3
1	A	833	PRO	2.3
1	B	576	VAL	2.3
2	E	165	LEU	2.3
1	A	352	PHE	2.3
2	D	61	GLU	2.2
1	C	508	GLY	2.2
1	A	897	ILE	2.2
2	E	34	MET	2.2
1	B	649	MET	2.2
1	A	993	THR	2.2
1	C	854	GLY	2.2
2	E	45	VAL	2.2
1	A	1025	PHE	2.2
1	A	1035	ARG	2.2
1	A	976	LEU	2.2
1	A	1006	GLY	2.2
1	C	619	GLY	2.2
1	B	987	MET	2.2
1	B	938	SER	2.2
1	B	918	PHE	2.2
1	A	528	THR	2.1
1	A	467	TYR	2.1
1	C	151	GLN	2.1
1	A	456	MET	2.1
1	A	881	LEU	2.1
1	A	921	LEU	2.1
1	A	619	GLY	2.1
1	A	660	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1007	VAL	2.1
1	B	568	ASP	2.1
1	B	866	GLU	2.1
1	A	835	LYS	2.1
1	A	348	ILE	2.1
1	C	672	VAL	2.1
1	A	48	SER	2.1
1	A	358	PHE	2.1
1	A	1033	PHE	2.1
1	C	918	PHE	2.1
1	A	889	ALA	2.1
1	C	1032	ARG	2.1
1	B	539	GLY	2.1
1	B	597	TYR	2.1
1	C	65	ILE	2.1
1	A	512	PHE	2.1
1	C	730	ASP	2.1
1	B	620	ARG	2.1
1	A	895	TRP	2.1
1	A	964	THR	2.1
1	A	545	TYR	2.1
1	A	620	ARG	2.0
1	B	660	ASP	2.0
1	A	451	ALA	2.0
1	C	152	GLU	2.0
1	B	1034	SER	2.0
1	A	903	LEU	2.0
1	A	960	LEU	2.0
1	A	415	ASN	2.0
1	A	126	GLY	2.0
1	A	827	ILE	2.0
1	A	1029	VAL	2.0
1	A	516	PHE	2.0
1	A	717	ARG	2.0
1	A	858	ASP	2.0
1	A	956	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	1712	4/4	0.63	0.32	59,59,59,60	0
6	OCT	C	1704	8/8	0.65	0.39	60,61,62,62	0
5	EDO	A	1109	4/4	0.68	0.30	67,68,68,68	0
5	EDO	C	1702	4/4	0.71	0.23	63,64,64,64	0
3	LMT	C	1708	35/35	0.72	0.22	66,77,79,80	0
7	C14	A	1106	14/14	0.72	0.42	75,83,91,93	0
10	DDR	B	1508	28/28	0.72	0.27	69,73,74,74	0
8	GOL	A	1107	6/6	0.73	0.22	66,67,67,67	0
3	LMT	B	1510	35/35	0.73	0.19	69,76,79,80	0
11	DDQ	B	1515	14/14	0.73	0.26	62,64,66,67	0
6	OCT	C	1701	8/8	0.74	0.50	83,87,92,92	0
8	GOL	B	1509	6/6	0.74	0.18	70,70,71,71	0
3	LMT	B	1504	35/35	0.75	0.21	71,75,80,80	0
5	EDO	B	1501	4/4	0.76	0.21	58,58,59,60	0
9	D10	B	1505	10/10	0.77	0.28	66,68,69,69	0
6	OCT	A	1105	8/8	0.79	0.52	86,91,96,98	0
5	EDO	A	1110	4/4	0.79	0.26	73,73,74,74	0
4	1K8	B	1516	17/17	0.79	0.24	51,53,55,55	17
5	EDO	A	1104	4/4	0.80	0.23	53,53,53,53	0
8	GOL	B	1512	6/6	0.81	0.18	68,69,70,70	0
3	LMT	A	1103	35/35	0.81	0.18	73,76,81,83	0
4	1K8	A	1102	17/17	0.81	0.24	80,86,91,91	0
3	LMT	A	1111	35/35	0.81	0.17	61,76,82,83	0
7	C14	A	1108	14/14	0.83	0.23	62,66,68,68	0
7	C14	C	1706	14/14	0.83	0.23	57,58,59,59	0
13	LPX	C	1705	30/30	0.83	0.20	66,70,75,76	0
5	EDO	B	1513	4/4	0.84	0.26	78,78,78,78	0
12	SO4	B	1517	5/5	0.84	0.16	81,81,82,82	0
12	SO4	B	1518	5/5	0.84	0.16	111,111,111,112	0
3	LMT	A	1101	35/35	0.84	0.17	66,69,72,73	0
5	EDO	C	1711	4/4	0.86	0.18	57,57,57,58	0
5	EDO	A	1113	4/4	0.86	0.22	63,63,64,65	0

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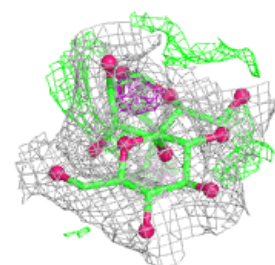
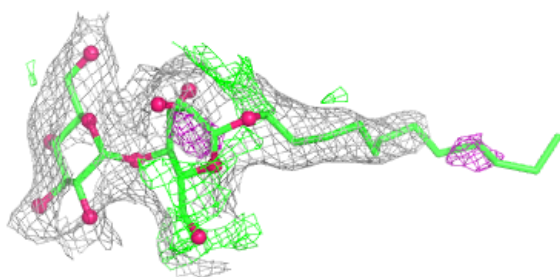
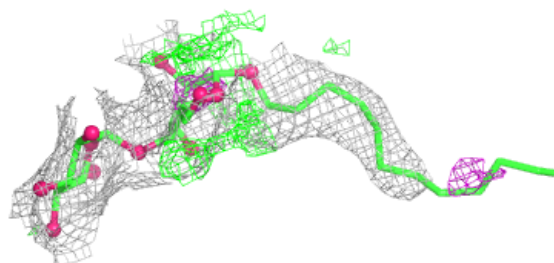
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	1507	4/4	0.86	0.15	56,56,56,57	0
8	GOL	B	1502	6/6	0.86	0.19	62,62,63,63	0
5	EDO	A	1112	4/4	0.87	0.16	60,60,61,61	0
3	LMT	B	1503	35/35	0.87	0.16	75,78,81,82	0
12	SO4	C	1713	5/5	0.88	0.21	76,76,76,77	0
5	EDO	B	1514	4/4	0.88	0.20	75,75,75,76	0
13	LPX	C	1707	30/30	0.88	0.16	63,68,73,74	0
8	GOL	B	1511	6/6	0.89	0.14	61,61,61,62	0
5	EDO	B	1506	4/4	0.90	0.22	61,61,62,62	0
3	LMT	C	1703	35/35	0.91	0.13	60,65,68,68	0
5	EDO	C	1710	4/4	0.93	0.21	56,56,56,57	0
8	GOL	C	1709	6/6	0.93	0.11	52,52,53,53	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.

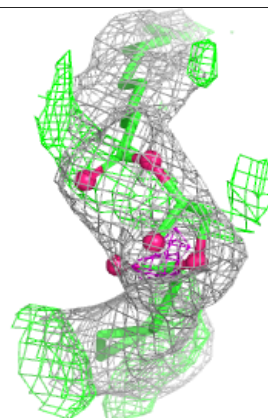
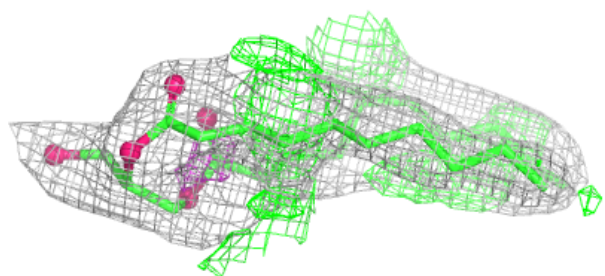
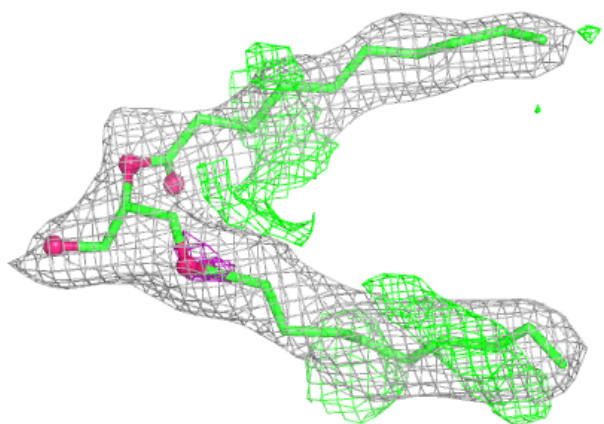
Electron density around LMT C 1708:

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

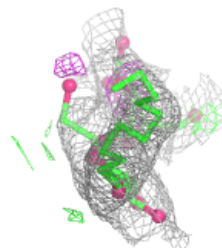
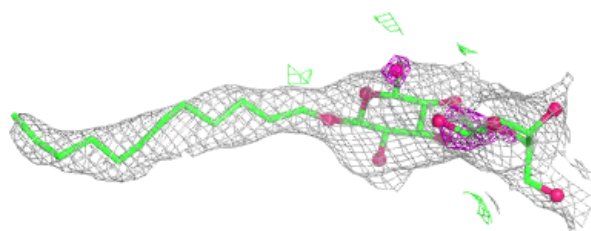
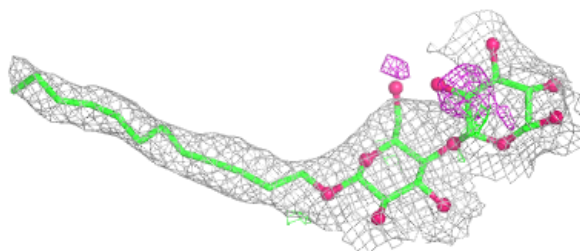


Electron density around DDR B 1508:

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

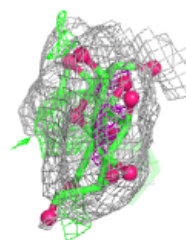
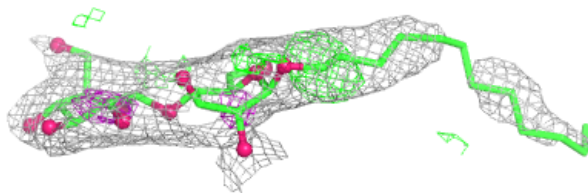
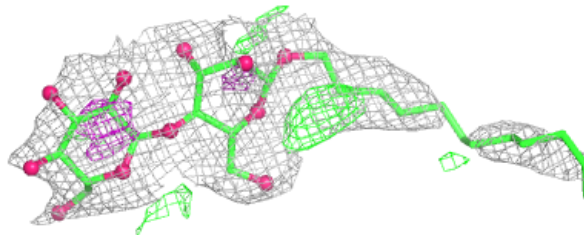
**Electron density around LMT B 1510:**

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

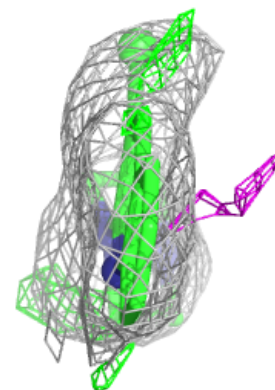
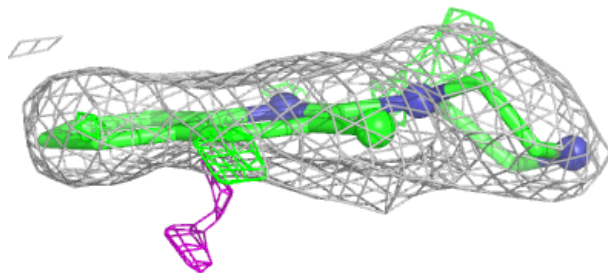
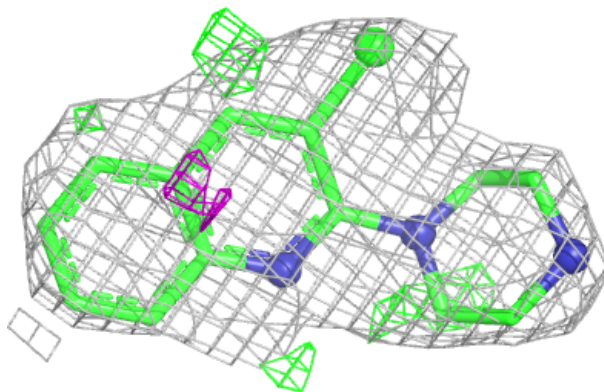


Electron density around LMT B 1504:

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

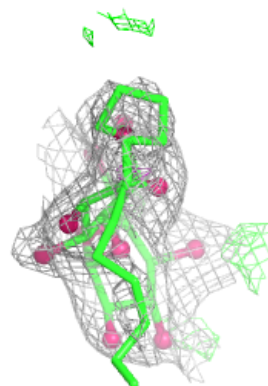
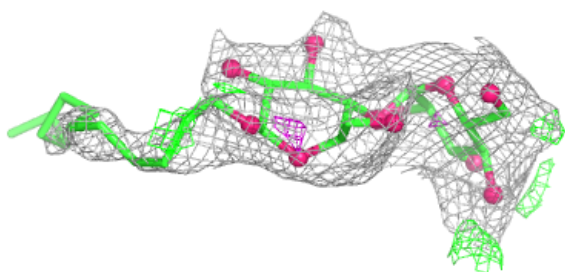
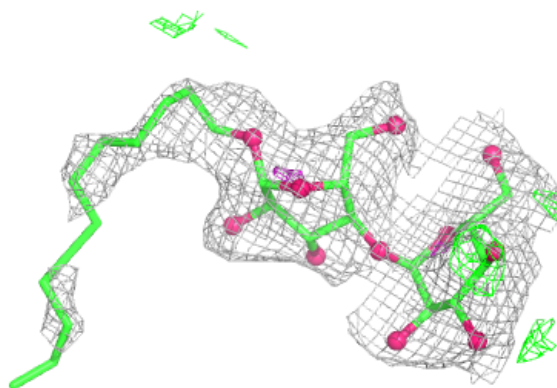
**Electron density around 1K8 B 1516:**

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

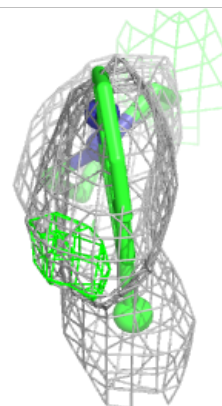
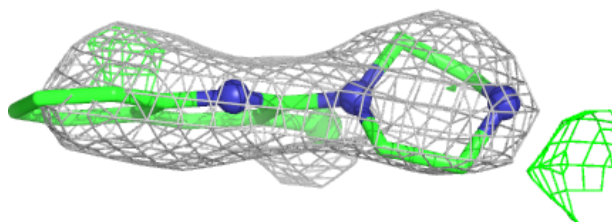
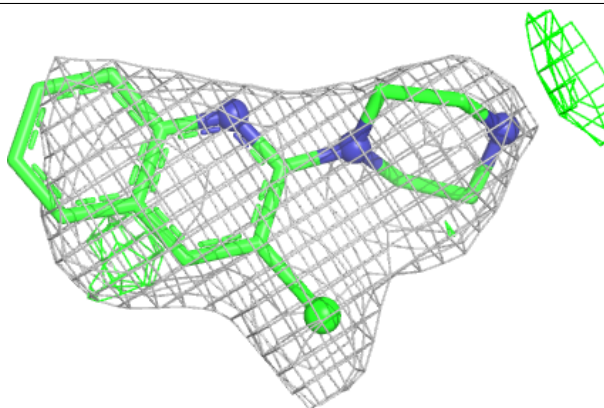


Electron density around LMT A 1103:

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

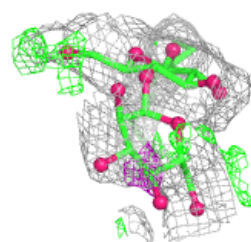
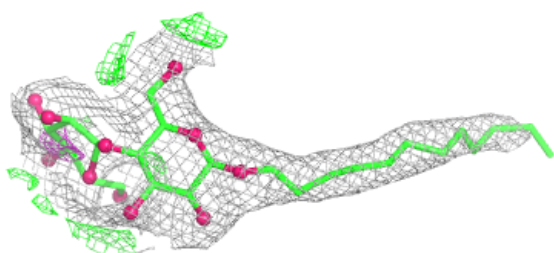
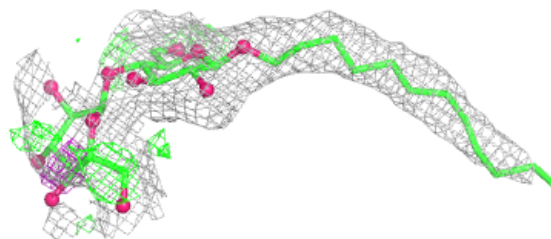
**Electron density around 1K8 A 1102:**

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

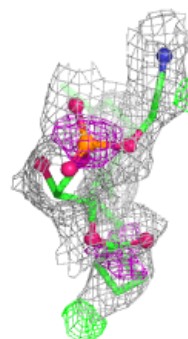
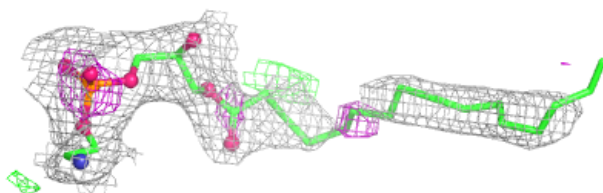
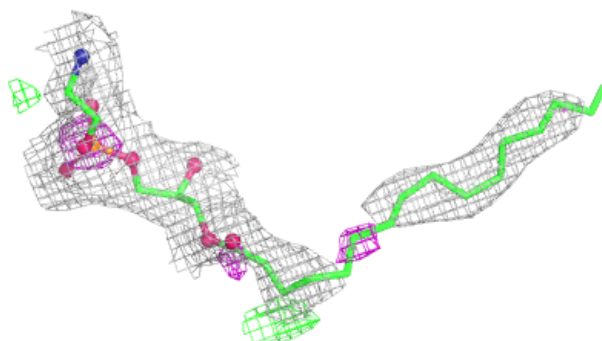


Electron density around LMT A 1111:

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

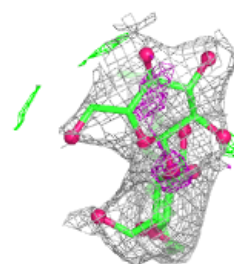
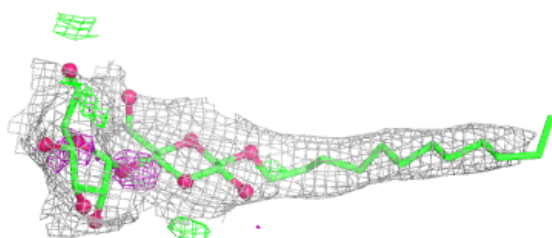
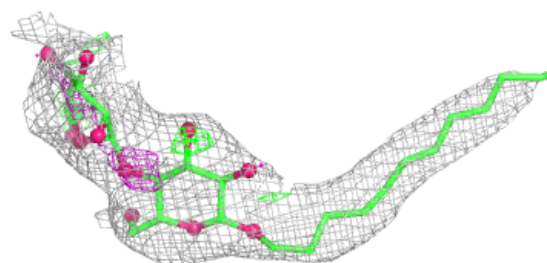
**Electron density around LPX C 1705:**

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

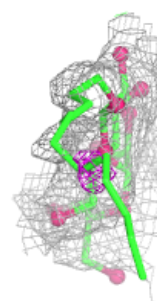
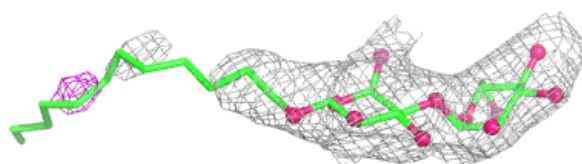
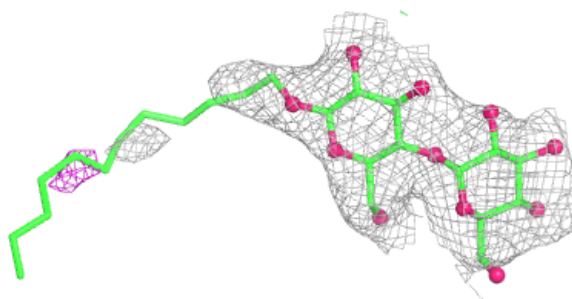


Electron density around LMT A 1101:

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

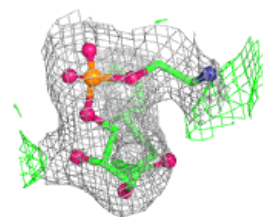
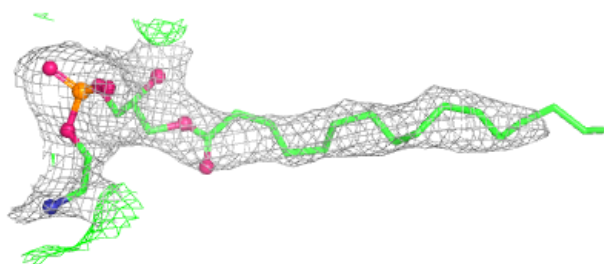
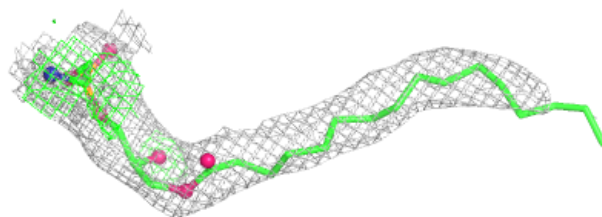
**Electron density around LMT B 1503:**

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

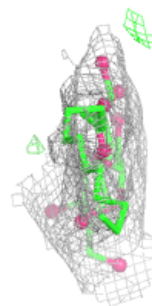
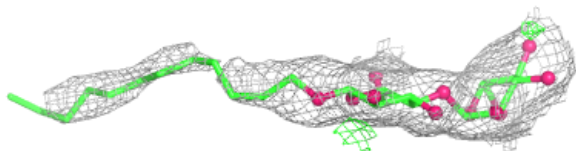
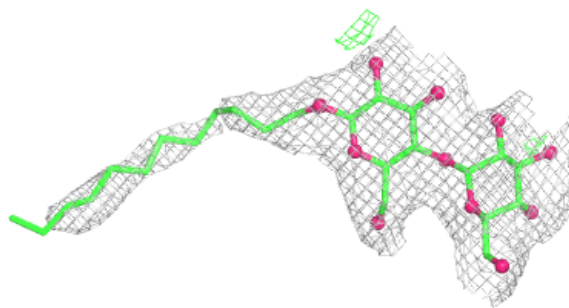


Electron density around LPX C 1707:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.