



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 06:57 AM UTC

PDB ID : 7OUM / pdb_00007oum
Title : BDM88855 inhibitor bound to the transmembrane domain of AcrB-R971A
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2021-06-12
Resolution : 2.45 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

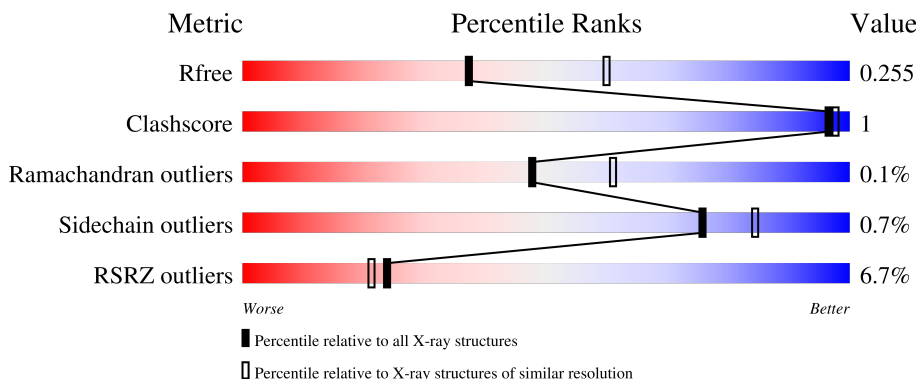
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	10% 94% ..
1	B	1057	8% 94% ..
1	C	1057	3% 93% ..
2	D	169	2% 92% 8%
2	E	169	3% 91% 9%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27129 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	1034	Total	C	N	O	S	0	2	0
			7881	5071	1302	1464	44			
1	B	1034	Total	C	N	O	S	0	2	0
			7866	5061	1298	1463	44			
1	C	1033	Total	C	N	O	S	0	1	0
			7852	5054	1294	1460	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	971	ALA	ARG	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	971	ALA	ARG	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	971	ALA	ARG	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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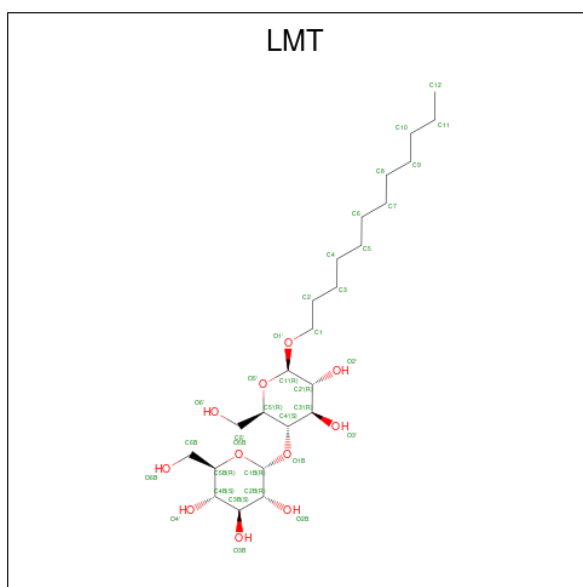
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

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

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



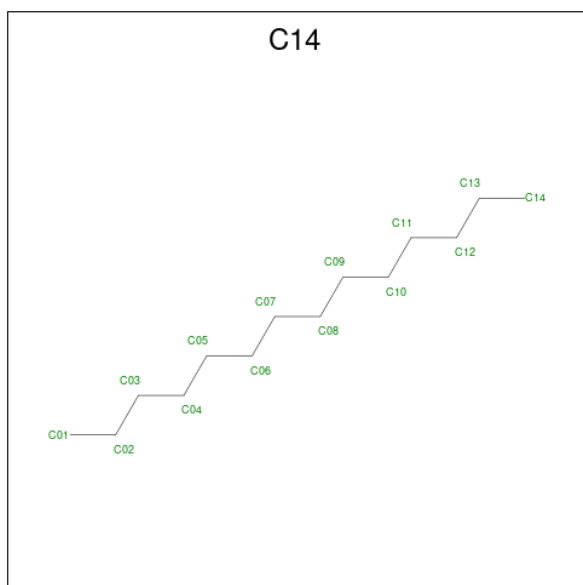
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

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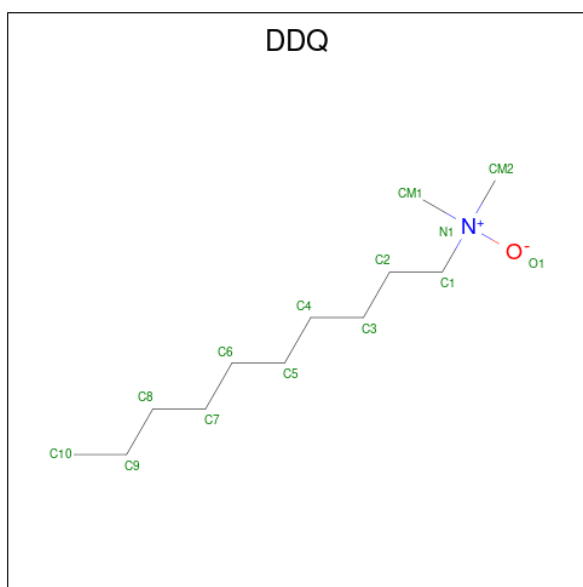
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



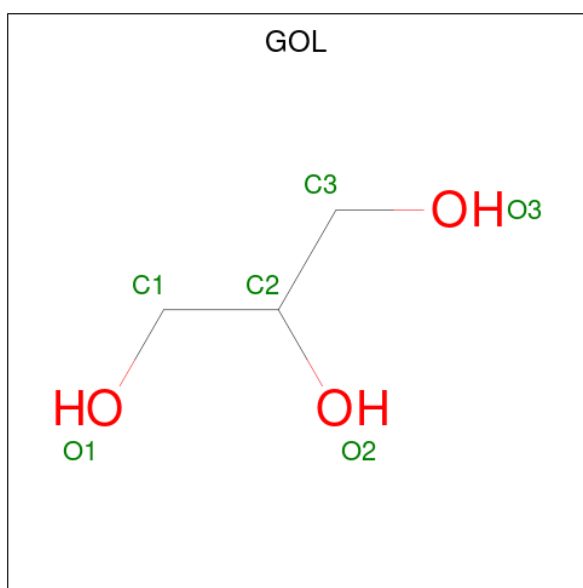
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			14	14		

- Molecule 5 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: C₁₂H₂₇NO).



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

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



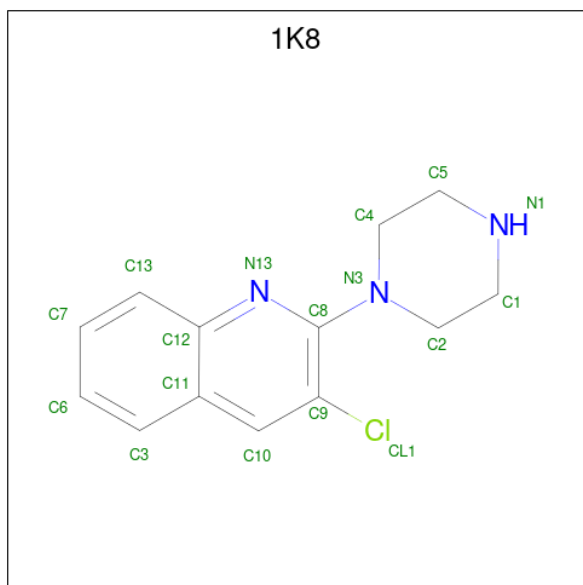
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

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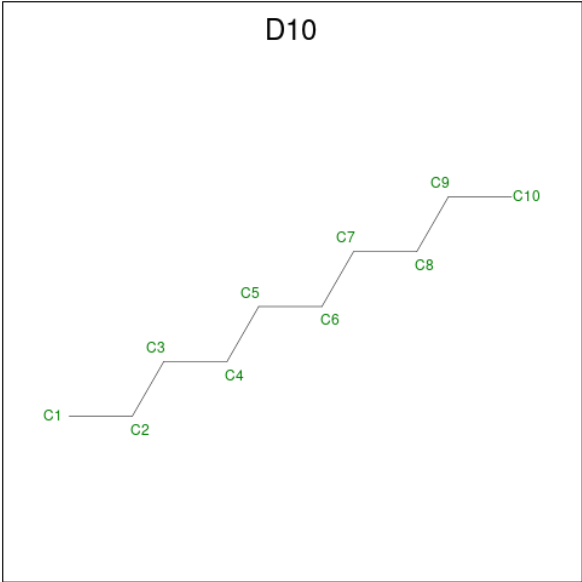
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 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).



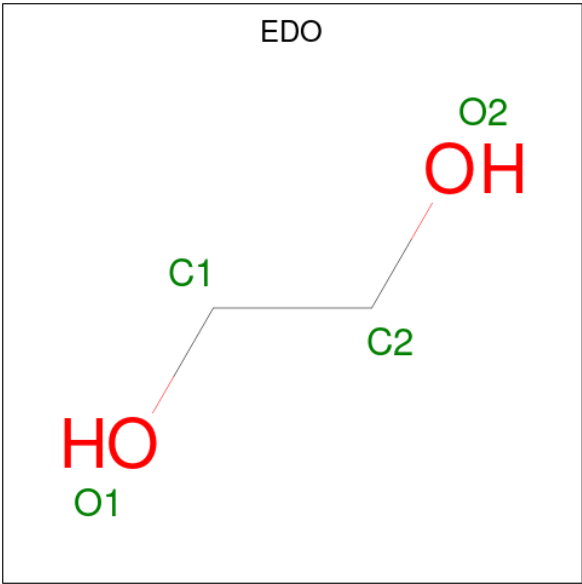
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Cl	N	0	0
			17	13	1	3		
7	B	1	Total	C	Cl	N	0	0
			17	13	1	3		

- Molecule 8 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



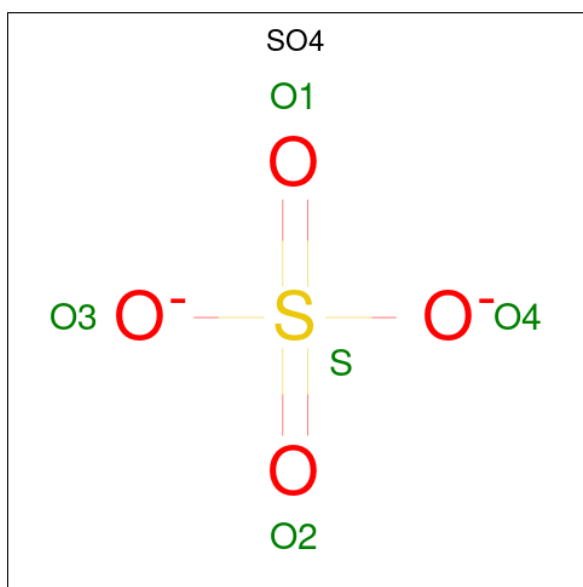
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 10 10	0	0
8	A	1	Total C 10 10	0	0
8	B	1	Total C 10 10	0	0
8	C	1	Total C 10 10	0	0

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



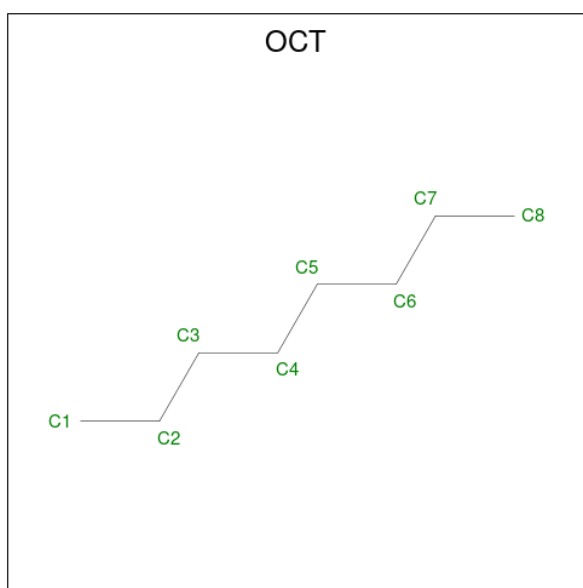
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	A	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0
9	B	1	Total C O 4 2 2	0	0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

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 11 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



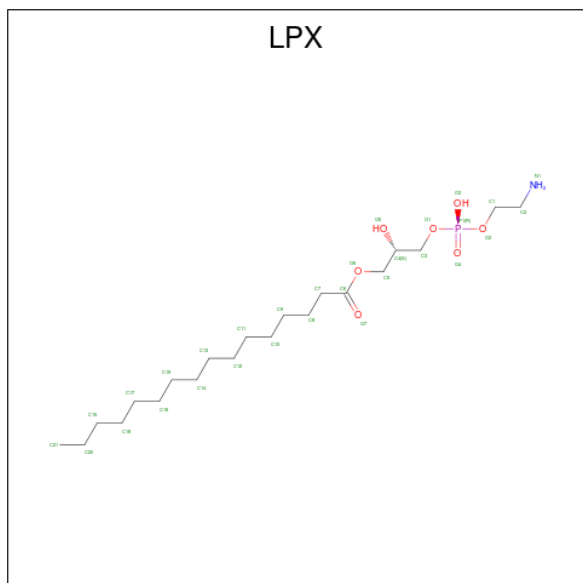
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	1	Total	C	0	0
			8	8		
11	C	1	Total	C	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C 8 8	0	0
11	C	1	Total C 8 8	0	0

- Molecule 12 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



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

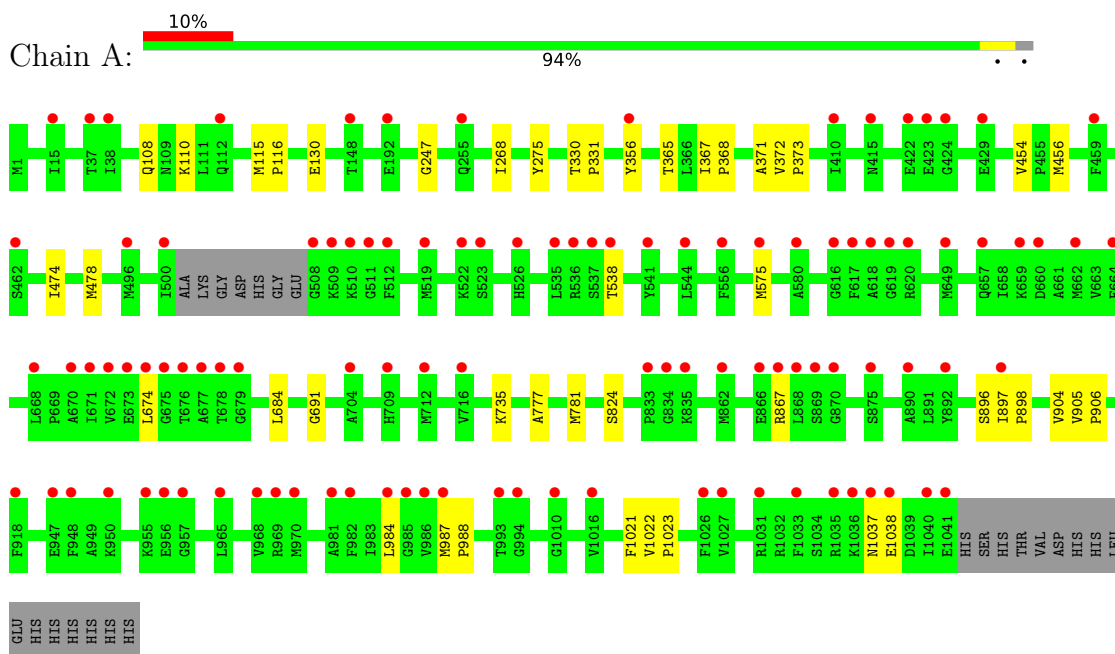
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	220	Total O 220 220	0	0
13	B	180	Total O 180 180	0	0
13	C	239	Total O 239 239	0	0
13	D	24	Total O 24 24	0	0
13	E	8	Total O 8 8	0	0

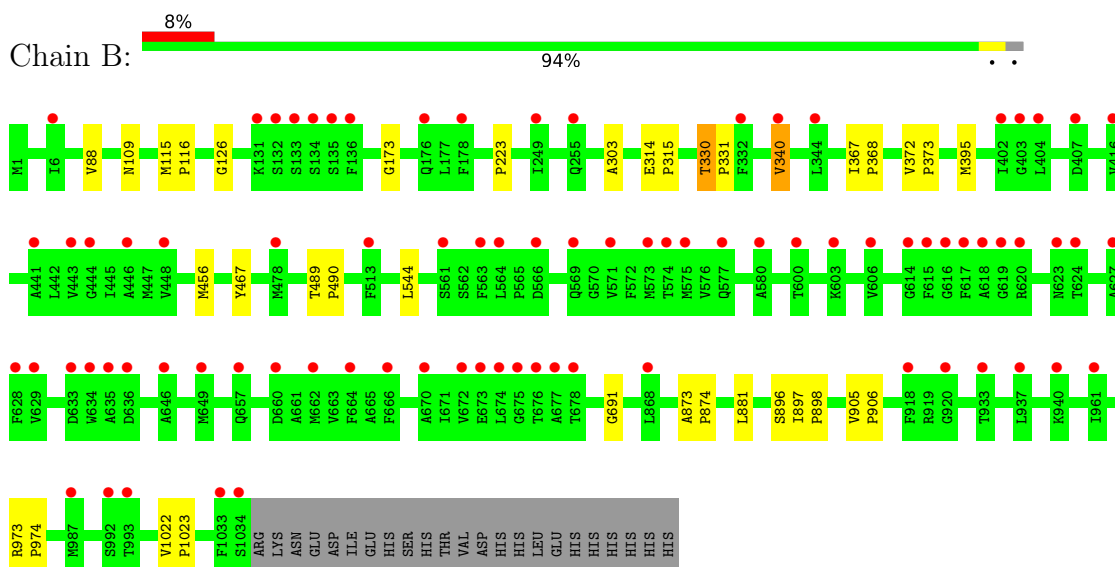
3 Residue-property plots

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.

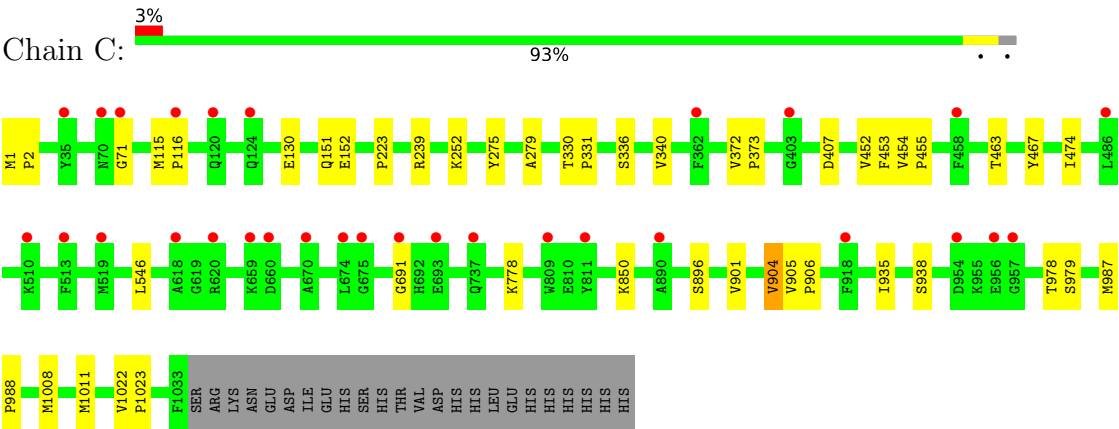
• Molecule 1: Multidrug efflux pump subunit AcrB



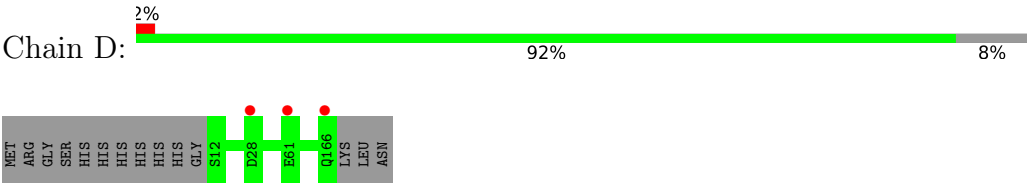
• Molecule 1: Multidrug efflux pump subunit AcrB



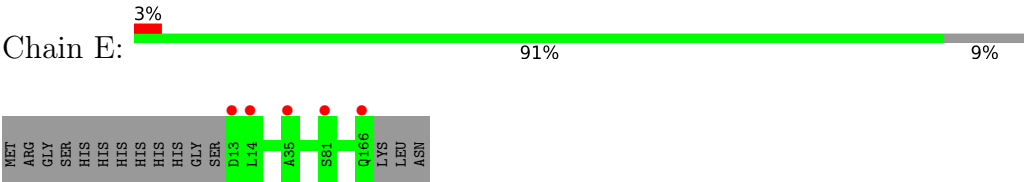
● Molecule 1: Multidrug efflux pump subunit AcrB



● 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	146.21Å 161.63Å 244.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 2.45 49.51 – 2.45	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.51-2.45) 100.0 (49.51-2.45)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.228 , 0.256 0.230 , 0.255	Depositor DCC
R_{free} test set	10468 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27129	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: OCT, SO4, 1K8, DDQ, D10, GOL, C14, LMT, LPX, EDO

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	0/8032	1.57	9/10905 (0.1%)
1	B	1.03	0/8016	1.57	3/10886 (0.0%)
1	C	1.03	0/8002	1.55	5/10868 (0.0%)
2	D	1.03	0/1192	1.59	0/1621
2	E	1.04	0/1186	1.61	0/1613
All	All	1.03	0/26428	1.57	17/35893 (0.0%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	7.61	125.03	120.24
1	A	896	SER	C-N-CA	7.61	125.03	120.24
1	B	896	SER	CA-C-N	6.97	124.63	120.24
1	B	896	SER	C-N-CA	6.97	124.63	120.24
1	A	1021	PHE	CA-C-N	5.92	123.97	120.24
1	A	1021	PHE	C-N-CA	5.92	123.97	120.24
1	A	691	GLY	CA-C-O	-5.67	118.37	122.45
1	A	371	ALA	CA-C-N	5.53	124.75	120.33
1	A	371	ALA	C-N-CA	5.53	124.75	120.33
1	C	691	GLY	CA-C-O	-5.51	118.48	122.45
1	A	904	VAL	CA-C-N	5.39	124.64	120.33
1	A	904	VAL	C-N-CA	5.39	124.64	120.33
1	C	896	SER	CA-C-N	5.21	124.50	120.33
1	C	896	SER	C-N-CA	5.21	124.50	120.33
1	B	691	GLY	CA-C-O	-5.16	118.45	122.52
1	C	904	VAL	CA-C-N	5.12	124.42	120.33
1	C	904	VAL	C-N-CA	5.12	124.42	120.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7881	0	8040	16	0
1	B	7866	0	8014	19	0
1	C	7852	0	8000	24	0
2	D	1173	0	1156	0	0
2	E	1167	0	1151	0	0
3	A	105	0	138	0	0
3	B	105	0	138	0	0
3	C	35	0	46	0	0
4	A	14	0	30	0	0
5	A	14	0	27	0	0
5	C	14	0	27	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	A	17	0	0	0	0
7	B	17	0	0	0	0
8	A	20	0	44	0	0
8	B	10	0	22	0	0
8	C	10	0	22	0	0
9	A	12	0	18	0	0
9	B	28	0	42	0	0
9	C	20	0	30	0	0
9	D	4	0	6	0	0
9	E	4	0	6	0	0
10	B	5	0	0	0	0
10	C	5	0	0	0	0
11	C	32	0	72	1	0
12	C	30	0	43	0	0
13	A	220	0	0	0	0
13	B	180	0	0	0	0
13	C	239	0	0	0	0
13	D	24	0	0	0	0
13	E	8	0	0	0	0
All	All	27129	0	27096	53	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 (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.83	0.61
1:C:901:VAL:O	1:C:904:VAL:HG12	2.01	0.61
1:A:356:TYR:HA	1:A:365:THR:HG21	1.83	0.61
1:C:151:GLN:NE2	1:C:279:ALA:O	2.35	0.59
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.84	0.59
1:C:979:SER:HA	1:C:1011:MET:HE3	1.85	0.58
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.88	0.54
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.89	0.54
1:C:935:ILE:HD11	11:C:1108:OCT:H81	1.91	0.52
1:A:474:ILE:HG22	1:A:478:MET:HE2	1.93	0.51
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.94	0.49
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.28	0.48
1:B:173:GLY:O	1:C:71:GLY:HA3	2.13	0.48
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.96	0.47
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.96	0.47
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.95	0.47
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.95	0.47
1:A:108:GLN:NE2	1:B:109:ASN:O	2.48	0.46
1:B:897:ILE:N	1:B:898:PRO:CD	2.78	0.46
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.46
1:C:115:MET:HB2	1:C:116:PRO:HD3	1.98	0.46
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.98	0.46
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.98	0.45
1:C:336:SER:O	1:C:340:VAL:HG23	2.16	0.45
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.98	0.45
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.98	0.45
1:C:987:MET:HA	1:C:1008:MET:CE	2.47	0.44
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.52	0.44
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.53	0.44
1:B:330:THR:N	1:B:331:PRO:CD	2.81	0.44
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.99	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.53	0.43
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.01	0.43
1:B:489:THR:N	1:B:490:PRO:CD	2.82	0.43
1:B:126:GLY:HA3	1:C:116:PRO:HB3	2.01	0.43
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.01	0.43
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.48	0.43
1:A:987:MET:N	1:A:988:PRO:CD	2.82	0.43
1:A:777:ALA:O	1:A:781:MET:HG2	2.20	0.42
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.82	0.42
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.42
1:A:897:ILE:N	1:A:898:PRO:CD	2.83	0.41
1:B:115:MET:N	1:B:116:PRO:CD	2.83	0.41
1:B:873:ALA:HB3	1:B:874:PRO:HD3	2.02	0.41
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.41
1:C:407:ASP:HA	1:C:978:THR:HG22	2.02	0.41
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.56	0.41
1:A:110:LYS:NZ	1:C:130:GLU:OE1	2.53	0.40
1:B:303:ALA:CB	1:B:330:THR:HG21	2.52	0.40
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.56	0.40
1:A:684:LEU:O	1:A:824:SER:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1032/1057 (98%)	997 (97%)	31 (3%)	4 (0%)	30	37
1	B	1034/1057 (98%)	1013 (98%)	21 (2%)	0	100	100
1	C	1032/1057 (98%)	1008 (98%)	24 (2%)	0	100	100
2	D	153/169 (90%)	150 (98%)	3 (2%)	0	100	100
2	E	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
All	All	3403/3509 (97%)	3315 (97%)	84 (2%)	4 (0%)	48	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1038	GLU
1	A	1037	ASN
1	A	867	ARG
1	A	538	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	844/862 (98%)	837 (99%)	7 (1%)	73	83
1	B	841/862 (98%)	836 (99%)	5 (1%)	78	86
1	C	839/862 (97%)	833 (99%)	6 (1%)	76	84
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2763/2850 (97%)	2745 (99%)	18 (1%)	76	84

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

Mol	Chain	Res	Type
1	A	130	GLU
1	A	454	VAL
1	A	456	MET
1	A	575	MET
1	A	674	LEU
1	A	735	LYS
1	A	984	LEU
1	B	88	VAL
1	B	330	THR
1	B	340	VAL
1	B	544	LEU
1	B	881	LEU
1	C	152	GLU
1	C	239	ARG
1	C	252	LYS
1	C	546	LEU

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Mol	Chain	Res	Type
1	C	778	LYS
1	C	850	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	194	ASN
1	A	415	ASN
1	A	437	GLN
1	A	525	HIS
1	B	120	GLN
1	B	124	GLN
1	B	194	ASN
1	B	229	GLN
1	B	254	ASN
1	B	577	GLN
1	B	584	GLN
1	C	89	GLN
1	C	505	HIS
1	C	584	GLN
1	C	797	GLN
2	D	59	HIS
2	E	59	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

43 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	D10	C	1103	-	9,9,9	0.10	0	8,8,8	0.06	0
9	EDO	C	1105	-	3,3,3	0.06	0	2,2,2	0.10	0
5	DDQ	A	1104	-	11,13,13	0.18	0	12,15,15	0.19	0
6	GOL	B	1105	-	5,5,5	0.09	0	5,5,5	0.24	0
3	LMT	B	1101	-	36,36,36	0.45	0	47,47,47	0.57	0
9	EDO	B	1108	-	3,3,3	0.05	0	2,2,2	0.10	0
4	C14	A	1103	-	13,13,13	0.08	0	12,12,12	0.07	0
3	LMT	A	1107	-	36,36,36	0.49	1 (2%)	47,47,47	0.67	1 (2%)
6	GOL	C	1111	-	5,5,5	0.10	0	5,5,5	0.29	0
9	EDO	B	1104	-	3,3,3	0.06	0	2,2,2	0.09	0
11	OCT	C	1108	-	7,7,7	0.11	0	6,6,6	0.07	0
9	EDO	A	1110	-	3,3,3	0.07	0	2,2,2	0.13	0
9	EDO	C	1107	-	3,3,3	0.06	0	2,2,2	0.11	0
9	EDO	C	1114	-	3,3,3	0.07	0	2,2,2	0.09	0
11	OCT	C	1109	-	7,7,7	0.11	0	6,6,6	0.06	0
9	EDO	B	1106	-	3,3,3	0.06	0	2,2,2	0.16	0
10	SO4	B	1114	-	4,4,4	0.34	0	6,6,6	0.08	0
3	LMT	C	1101	-	36,36,36	0.43	0	47,47,47	0.48	0
11	OCT	C	1112	-	7,7,7	0.10	0	6,6,6	0.08	0
9	EDO	B	1110	-	3,3,3	0.07	0	2,2,2	0.10	0
12	LPX	C	1106	-	29,29,29	0.30	0	31,33,33	0.37	0
8	D10	A	1108	-	9,9,9	0.10	0	8,8,8	0.08	0
8	D10	A	1111	-	9,9,9	0.09	0	8,8,8	0.07	0
9	EDO	A	1112	-	3,3,3	0.07	0	2,2,2	0.13	0
9	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.11	0
8	D10	B	1111	-	9,9,9	0.10	0	8,8,8	0.09	0
9	EDO	B	1112	-	3,3,3	0.06	0	2,2,2	0.12	0
3	LMT	A	1102	-	36,36,36	0.45	0	47,47,47	0.59	0
3	LMT	B	1107	-	36,36,36	0.51	1 (2%)	47,47,47	0.79	1 (2%)
9	EDO	C	1113	-	3,3,3	0.07	0	2,2,2	0.13	0
11	OCT	C	1104	-	7,7,7	0.10	0	6,6,6	0.10	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	A	1105	-	5,5,5	0.09	0	5,5,5	0.28	0
9	EDO	C	1110	-	3,3,3	0.06	0	2,2,2	0.12	0
7	1K8	A	1106	-	19,19,19	2.71	4 (21%)	24,26,26	1.28	2 (8%)
9	EDO	D	201	-	3,3,3	0.07	0	2,2,2	0.10	0
7	1K8	B	1113	-	19,19,19	2.76	4 (21%)	24,26,26	1.29	3 (12%)
9	EDO	A	1109	-	3,3,3	0.07	0	2,2,2	0.10	0
9	EDO	B	1103	-	3,3,3	0.06	0	2,2,2	0.11	0
3	LMT	B	1102	-	36,36,36	0.46	0	47,47,47	0.73	0
10	SO4	C	1115	-	4,4,4	0.34	0	6,6,6	0.08	0
9	EDO	B	1109	-	3,3,3	0.07	0	2,2,2	0.09	0
5	DDQ	C	1102	-	11,13,13	0.15	0	12,15,15	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D10	C	1103	-	-	1/7/7/7	-
9	EDO	C	1105	-	-	0/1/1/1	-
5	DDQ	A	1104	-	-	3/11/11/11	-
6	GOL	B	1105	-	-	2/4/4/4	-
3	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
9	EDO	B	1108	-	-	0/1/1/1	-
4	C14	A	1103	-	-	4/11/11/11	-
3	LMT	A	1107	-	-	15/21/61/61	0/2/2/2
6	GOL	C	1111	-	-	2/4/4/4	-
9	EDO	B	1104	-	-	1/1/1/1	-
11	OCT	C	1108	-	-	1/5/5/5	-
9	EDO	A	1110	-	-	1/1/1/1	-
9	EDO	C	1107	-	-	1/1/1/1	-
9	EDO	C	1114	-	-	1/1/1/1	-
11	OCT	C	1109	-	-	2/5/5/5	-
9	EDO	B	1106	-	-	1/1/1/1	-
3	LMT	C	1101	-	-	7/21/61/61	0/2/2/2
11	OCT	C	1112	-	-	4/5/5/5	-
9	EDO	B	1110	-	-	1/1/1/1	-
12	LPX	C	1106	-	-	15/31/31/31	-
8	D10	A	1108	-	-	1/7/7/7	-
8	D10	A	1111	-	-	5/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	EDO	A	1112	-	-	1/1/1/1	-
9	EDO	E	201	-	-	1/1/1/1	-
8	D10	B	1111	-	-	4/7/7/7	-
9	EDO	B	1112	-	-	0/1/1/1	-
3	LMT	A	1102	-	-	12/21/61/61	0/2/2/2
3	LMT	B	1107	-	-	10/21/61/61	0/2/2/2
9	EDO	C	1113	-	-	0/1/1/1	-
11	OCT	C	1104	-	-	2/5/5/5	-
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
6	GOL	A	1105	-	-	0/4/4/4	-
9	EDO	C	1110	-	-	1/1/1/1	-
7	1K8	A	1106	-	-	2/4/12/12	0/3/3/3
9	EDO	D	201	-	-	0/1/1/1	-
7	1K8	B	1113	-	-	2/4/12/12	0/3/3/3
9	EDO	A	1109	-	-	0/1/1/1	-
9	EDO	B	1103	-	-	1/1/1/1	-
3	LMT	B	1102	-	-	7/21/61/61	0/2/2/2
9	EDO	B	1109	-	-	1/1/1/1	-
5	DDQ	C	1102	-	-	5/11/11/11	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1113	1K8	C9-C8	8.91	1.50	1.39
7	A	1106	1K8	C9-C8	8.80	1.50	1.39
7	B	1113	1K8	C11-C12	4.77	1.49	1.42
7	A	1106	1K8	C11-C12	4.68	1.49	1.42
7	B	1113	1K8	C8-N13	4.11	1.36	1.31
7	A	1106	1K8	C8-N13	3.88	1.35	1.31
7	A	1106	1K8	C9-CL1	2.73	1.80	1.73
7	B	1113	1K8	C9-CL1	2.65	1.79	1.73
3	A	1107	LMT	O1'-C1'	2.11	1.43	1.40
3	B	1107	LMT	O1'-C1'	2.07	1.43	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1106	1K8	C4-N3-C2	3.89	120.31	111.57
7	B	1113	1K8	C4-N3-C2	3.24	118.86	111.57
7	A	1106	1K8	C8-N13-C12	2.65	121.84	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1113	1K8	C8-N13-C12	2.63	121.80	116.11
7	B	1113	1K8	C9-C8-N13	-2.21	119.16	122.81
3	B	1107	LMT	C1B-O5B-C5B	2.08	117.79	113.72
3	A	1107	LMT	C1'-O5'-C5'	2.06	117.75	113.72

There are no chirality outliers.

All (131) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	O5B-C1B-O1B-C4'
5	A	1104	DDQ	N1-C1-C2-C3
7	A	1106	1K8	C9-C8-N3-C2
7	A	1106	1K8	N13-C8-N3-C2
7	B	1113	1K8	C9-C8-N3-C2
12	C	1106	LPX	C3-O1-P1-O3
12	C	1106	LPX	C3-O1-P1-O2
12	C	1106	LPX	O7-C6-O6-C5
3	A	1101	LMT	C5'-C4'-O1B-C1B
12	C	1106	LPX	C7-C6-O6-C5
3	C	1101	LMT	O5'-C5'-C6'-O6'
3	B	1107	LMT	C2B-C1B-O1B-C4'
12	C	1106	LPX	O1-C3-C4-O5
3	A	1102	LMT	O5'-C5'-C6'-O6'
3	A	1107	LMT	O5'-C5'-C6'-O6'
3	B	1107	LMT	O5B-C1B-O1B-C4'
3	C	1101	LMT	C4'-C5'-C6'-O6'
7	B	1113	1K8	N13-C8-N3-C2
3	A	1107	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1107	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	A	1107	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C2'-C1'-O1'-C1
3	A	1107	LMT	C2'-C1'-O1'-C1
12	C	1106	LPX	C6-C7-C8-C9
12	C	1106	LPX	C4-C5-O6-C6
3	C	1101	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
12	C	1106	LPX	O5-C4-C5-O6
3	B	1107	LMT	O5B-C5B-C6B-O6B
12	C	1106	LPX	C3-C4-C5-O6
6	B	1105	GOL	O1-C1-C2-C3
6	C	1111	GOL	O1-C1-C2-C3
12	C	1106	LPX	C10-C11-C12-C13
5	C	1102	DDQ	C2-C3-C4-C5
6	B	1105	GOL	O1-C1-C2-O2
3	B	1107	LMT	C4-C5-C6-C7
5	A	1104	DDQ	C6-C7-C8-C9
3	A	1107	LMT	C7-C8-C9-C10
3	B	1107	LMT	C5-C6-C7-C8
3	B	1102	LMT	C6-C7-C8-C9
8	B	1111	D10	C6-C7-C8-C9
3	C	1101	LMT	C1-C2-C3-C4
3	A	1107	LMT	C4'-C5'-C6'-O6'
8	B	1111	D10	C2-C3-C4-C5
9	A	1110	EDO	O1-C1-C2-O2
9	B	1109	EDO	O1-C1-C2-O2
9	E	201	EDO	O1-C1-C2-O2
11	C	1109	OCT	C2-C3-C4-C5
3	B	1102	LMT	C11-C10-C9-C8
3	C	1101	LMT	C5-C6-C7-C8
5	C	1102	DDQ	C3-C4-C5-C6
3	A	1101	LMT	C3-C4-C5-C6
3	A	1107	LMT	C3-C4-C5-C6
3	B	1102	LMT	C5'-C4'-O1B-C1B
8	A	1111	D10	C2-C3-C4-C5
12	C	1106	LPX	C11-C12-C13-C14
3	B	1102	LMT	C3-C4-C5-C6
3	A	1102	LMT	C11-C10-C9-C8
8	A	1111	D10	C3-C4-C5-C6
5	A	1104	DDQ	C3-C4-C5-C6
12	C	1106	LPX	O1-C3-C4-C5
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	B	1102	LMT	C3'-C4'-O1B-C1B
3	B	1102	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C4-C5-C6-C7
4	A	1103	C14	C09-C10-C11-C12
3	B	1107	LMT	O1'-C1-C2-C3
9	B	1104	EDO	O1-C1-C2-O2
3	A	1102	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1103	C14	C06-C07-C08-C09
3	A	1101	LMT	C9-C10-C11-C12
3	A	1102	LMT	C9-C10-C11-C12
3	B	1107	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C2-C1-O1'-C1'
11	C	1104	OCT	C5-C6-C7-C8
8	A	1111	D10	C5-C6-C7-C8
11	C	1112	OCT	C1-C2-C3-C4
11	C	1112	OCT	C2-C3-C4-C5
3	A	1102	LMT	C3-C4-C5-C6
3	A	1102	LMT	C4B-C5B-C6B-O6B
8	B	1111	D10	C7-C8-C9-C10
3	C	1101	LMT	C9-C10-C11-C12
11	C	1109	OCT	C4-C5-C6-C7
3	B	1107	LMT	C11-C10-C9-C8
3	A	1107	LMT	C2-C3-C4-C5
11	C	1112	OCT	C4-C5-C6-C7
12	C	1106	LPX	C16-C17-C18-C19
3	A	1107	LMT	C5-C6-C7-C8
3	A	1107	LMT	O1'-C1-C2-C3
8	C	1103	D10	C6-C7-C8-C9
11	C	1104	OCT	C2-C3-C4-C5
3	A	1107	LMT	C6-C7-C8-C9
9	C	1107	EDO	O1-C1-C2-O2
8	A	1111	D10	C1-C2-C3-C4
3	B	1107	LMT	C3-C4-C5-C6
12	C	1106	LPX	C4-C3-O1-P1
4	A	1103	C14	C10-C11-C12-C13
3	B	1107	LMT	C1-C2-C3-C4
8	B	1111	D10	C3-C4-C5-C6
3	B	1101	LMT	O1'-C1-C2-C3
5	C	1102	DDQ	N1-C1-C2-C3
11	C	1108	OCT	C4-C5-C6-C7
9	C	1114	EDO	O1-C1-C2-O2
3	A	1102	LMT	C2-C1-O1'-C1'
3	A	1107	LMT	C2-C1-O1'-C1'
12	C	1106	LPX	C14-C15-C16-C17
4	A	1103	C14	C01-C02-C03-C04
3	A	1101	LMT	C2-C3-C4-C5
8	A	1111	D10	C6-C7-C8-C9
9	C	1110	EDO	O1-C1-C2-O2
3	A	1102	LMT	C2-C3-C4-C5

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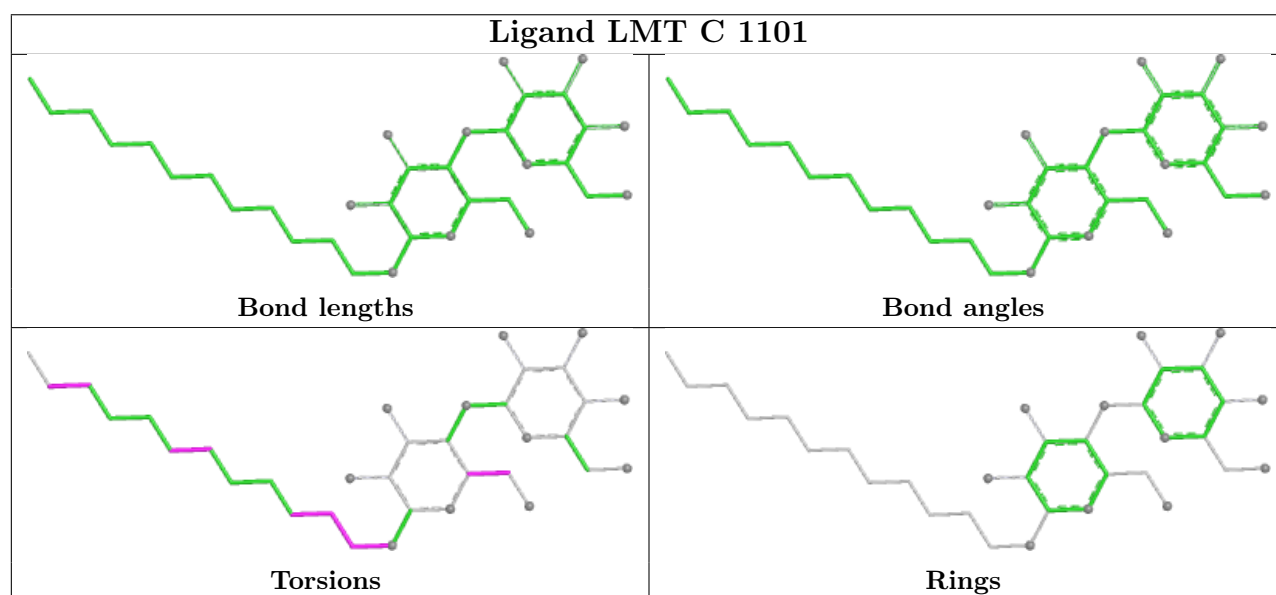
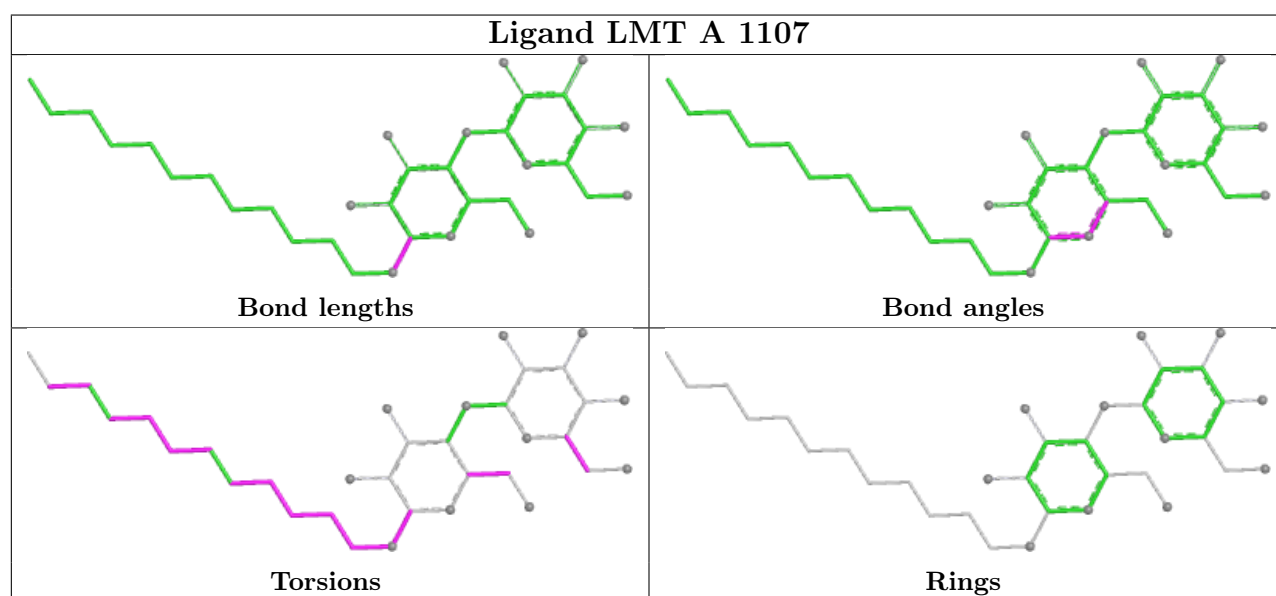
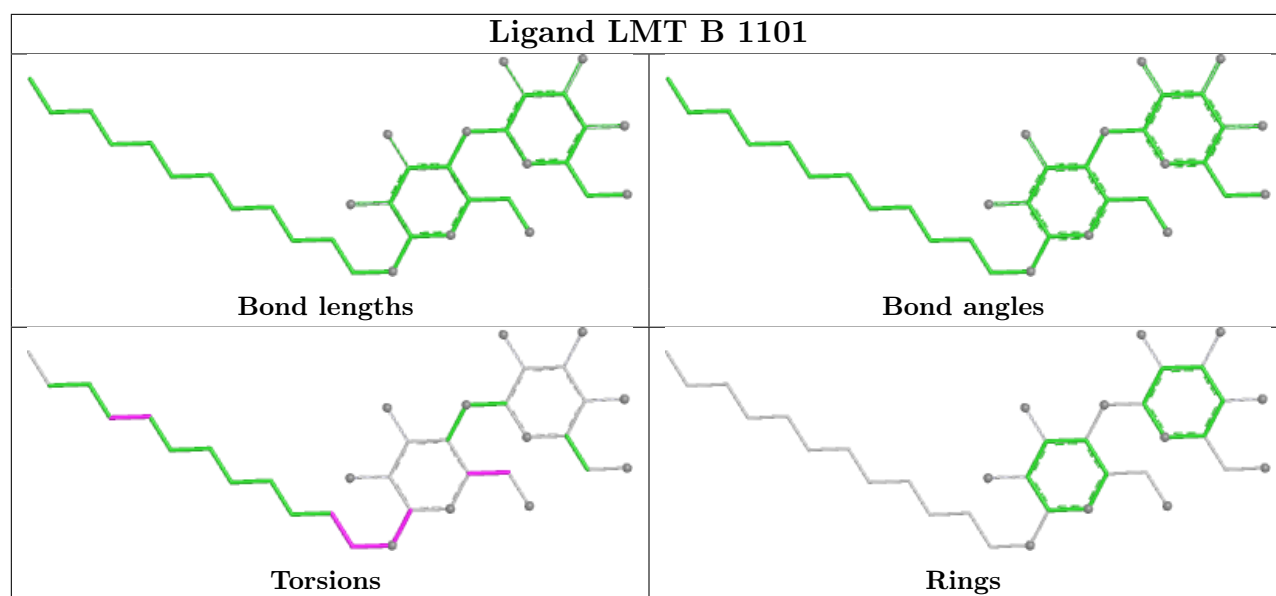
Mol	Chain	Res	Type	Atoms
8	A	1108	D10	C7-C8-C9-C10
3	B	1101	LMT	C7-C8-C9-C10
11	C	1112	OCT	C3-C4-C5-C6
9	A	1112	EDO	O1-C1-C2-O2
9	B	1103	EDO	O1-C1-C2-O2
3	A	1101	LMT	C3'-C4'-O1B-C1B
3	A	1107	LMT	C9-C10-C11-C12
5	C	1102	DDQ	C7-C8-C9-C10
3	A	1101	LMT	O1'-C1-C2-C3
9	B	1106	EDO	O1-C1-C2-O2
5	C	1102	DDQ	C5-C6-C7-C8
9	B	1110	EDO	O1-C1-C2-O2
3	A	1107	LMT	C1-C2-C3-C4
6	C	1111	GOL	O1-C1-C2-O2

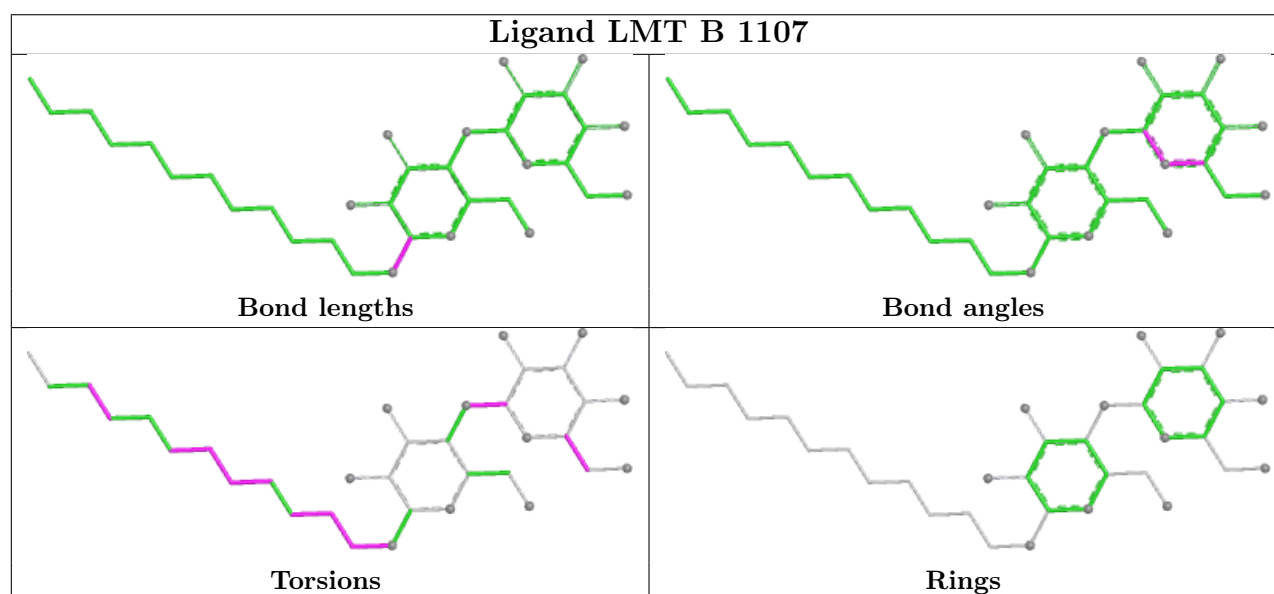
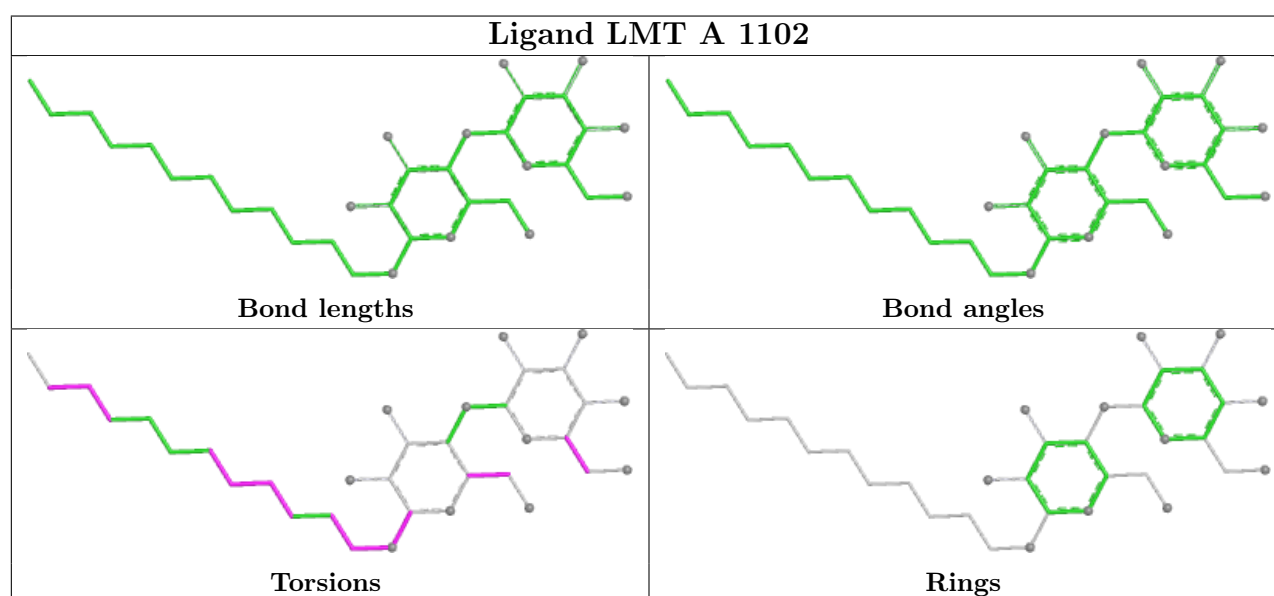
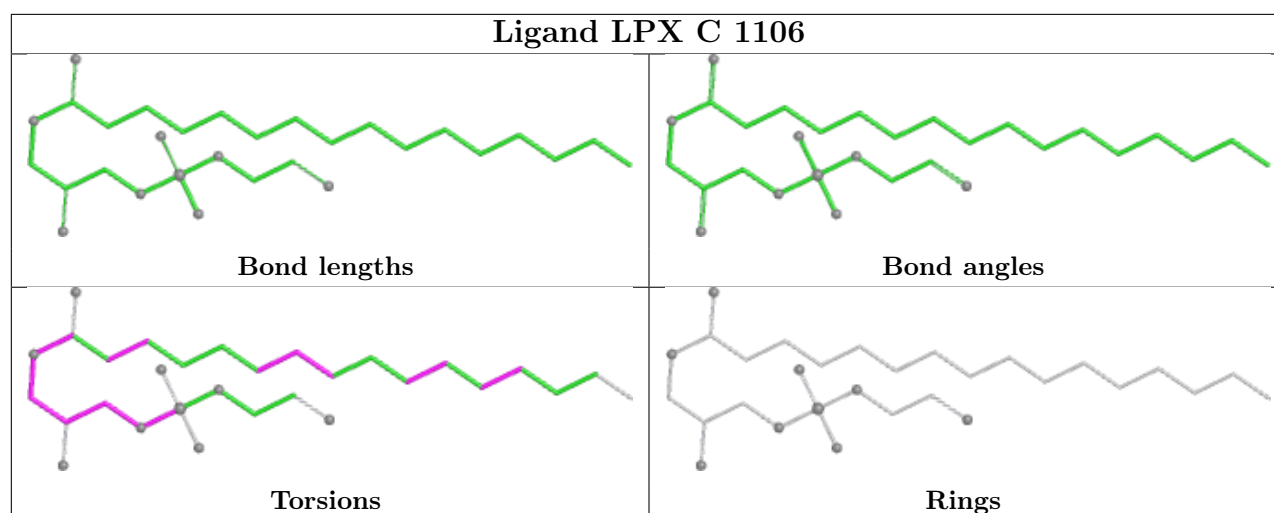
There are no ring outliers.

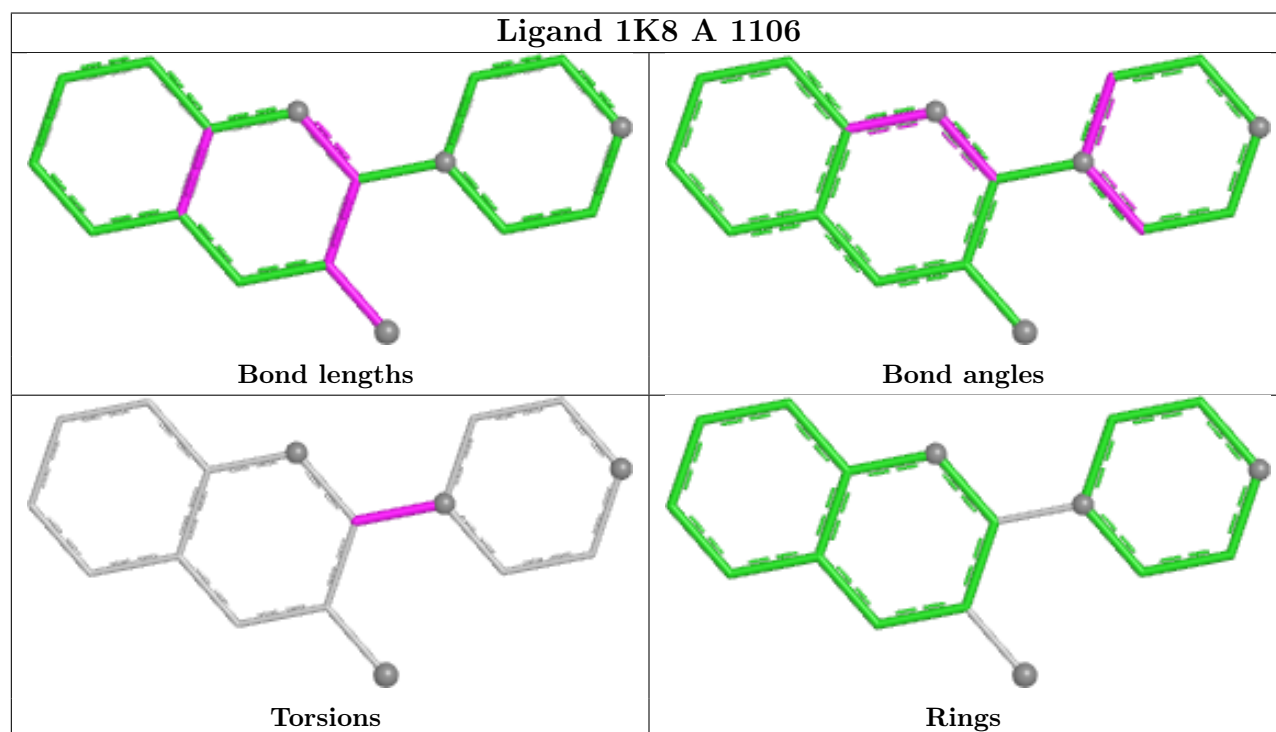
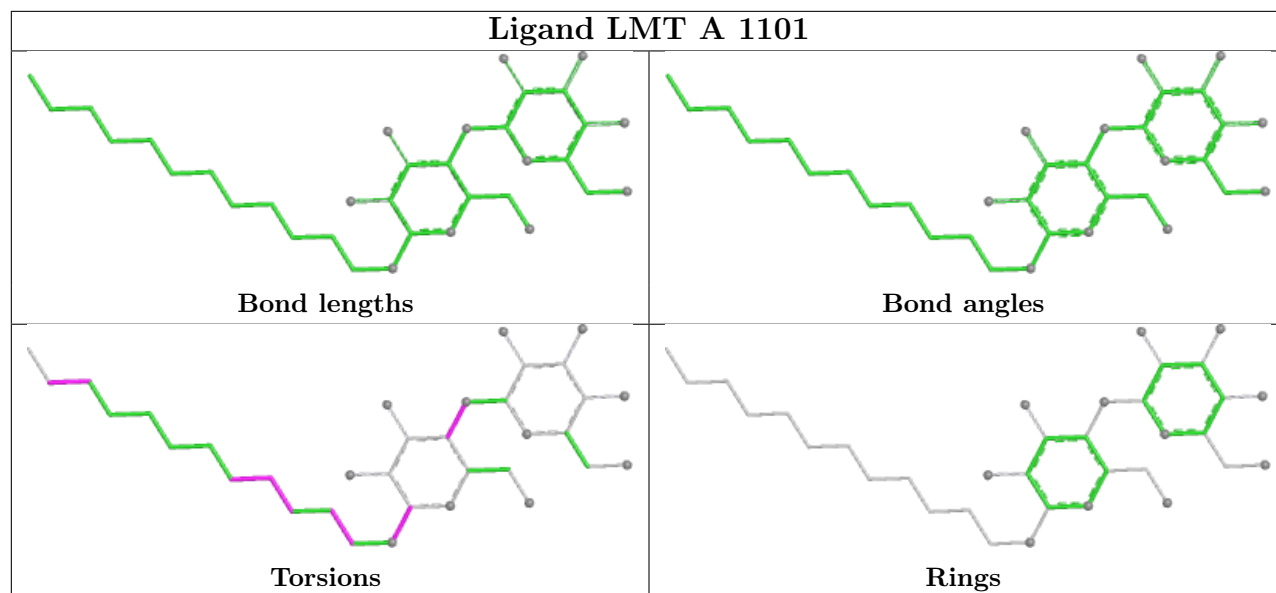
1 monomer is involved in 1 short contact:

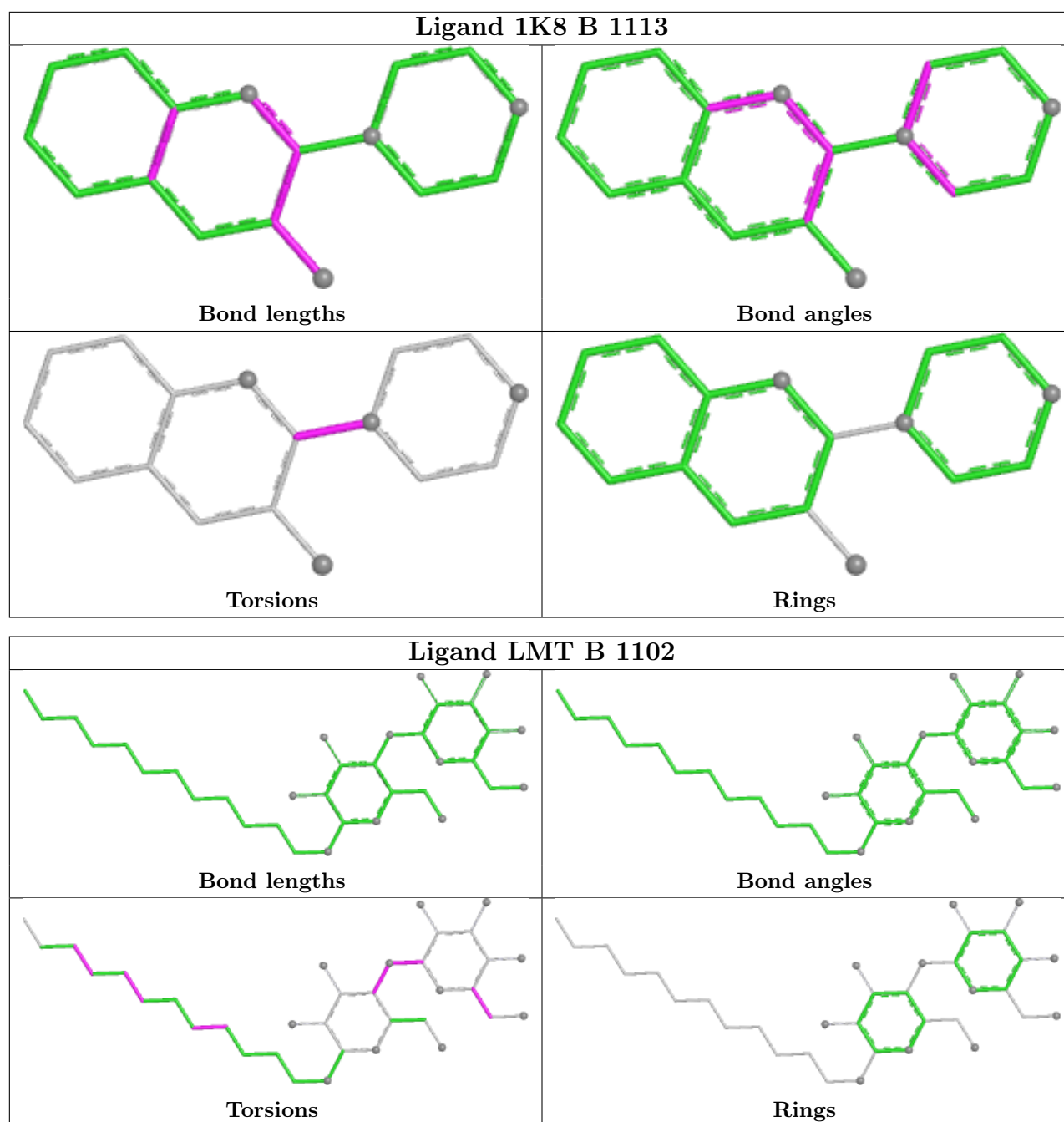
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	1108	OCT	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1034/1057 (97%)	0.79	106 (10%)	12 9	21, 53, 98, 114	2 (0%)
1	B	1034/1057 (97%)	0.68	83 (8%)	18 16	22, 54, 68, 78	2 (0%)
1	C	1033/1057 (97%)	0.30	30 (2%)	53 55	19, 43, 61, 69	1 (0%)
2	D	155/169 (91%)	0.33	3 (1%)	66 67	41, 52, 67, 77	0
2	E	154/169 (91%)	0.78	5 (3%)	50 51	50, 64, 84, 93	0
All	All	3410/3509 (97%)	0.59	227 (6%)	24 21	19, 50, 79, 114	5 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	LEU	7.5
1	A	677	ALA	6.2
1	A	508	GLY	6.2
1	A	674	LEU	6.0
1	A	1040	ILE	6.0
1	A	678	THR	5.9
1	B	617	PHE	5.8
1	B	618	ALA	5.6
1	A	676	THR	5.3
1	A	981	ALA	5.2
1	A	675	GLY	5.0
1	B	628	PHE	4.9
1	B	575	MET	4.8
1	B	615	PHE	4.8
1	A	500	ILE	4.8
1	C	811	TYR	4.7
1	A	618	ALA	4.7
1	B	674	LEU	4.7
1	B	672	VAL	4.5
1	B	133	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	673	GLU	4.3
1	B	633	ASP	4.3
1	C	124	GLN	4.1
1	A	869	SER	4.1
1	A	672	VAL	4.1
1	B	675	GLY	4.0
1	A	982	PHE	4.0
1	A	580	ALA	4.0
1	A	664	PHE	3.9
1	B	332	PHE	3.9
1	B	635	ALA	3.9
1	B	676	THR	3.9
1	A	617	PHE	3.8
1	B	662	MET	3.8
1	B	403	GLY	3.8
2	E	14	LEU	3.8
1	A	510	LYS	3.7
1	A	509	LYS	3.7
1	A	1036	LYS	3.7
1	C	362	PHE	3.6
1	A	955	LYS	3.6
1	B	134	SER	3.6
1	A	956	GLU	3.5
1	A	1038	GLU	3.5
1	B	573	MET	3.5
1	A	462	SER	3.5
1	A	662	MET	3.5
1	A	575	MET	3.5
1	B	629	VAL	3.5
1	B	580	ALA	3.4
1	A	993	THR	3.4
1	B	404	LEU	3.4
1	B	616	GLY	3.4
1	A	526	HIS	3.4
1	B	135	SER	3.4
1	B	634	TRP	3.3
1	B	666	PHE	3.3
2	E	13	ASP	3.3
1	A	968	VAL	3.3
1	B	937	LEU	3.3
1	B	446	ALA	3.2
1	A	833	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	519	MET	3.2
1	B	677	ALA	3.1
1	C	918	PHE	3.1
1	A	423	GLU	3.1
1	B	563	PHE	3.1
1	A	538	THR	3.0
1	A	1041	GLU	3.0
1	A	459	PHE	3.0
1	A	867	ARG	3.0
2	E	166	GLN	3.0
1	A	1027	VAL	2.9
1	A	994	GLY	2.9
1	A	522	LYS	2.9
1	A	429	GLU	2.9
1	A	1035	ARG	2.9
1	B	868	LEU	2.9
1	B	178	PHE	2.9
1	B	606	VAL	2.9
2	E	35	ALA	2.8
1	A	712	MET	2.8
1	A	918	PHE	2.8
1	A	965	LEU	2.8
1	A	192	GLU	2.8
1	A	866	GLU	2.8
1	A	671	ILE	2.8
1	B	561	SER	2.8
1	C	659	LYS	2.8
1	B	407	ASP	2.8
1	A	512	PHE	2.8
1	A	673	GLU	2.8
1	C	660	ASP	2.8
1	A	556	PHE	2.8
1	B	620	ARG	2.7
1	A	657	GLN	2.7
1	B	660	ASP	2.7
2	D	28	ASP	2.7
1	B	444	GLY	2.7
1	C	675	GLY	2.7
1	A	897	ILE	2.7
1	A	986	VAL	2.7
1	C	620	ARG	2.7
1	B	918	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	623	ASN	2.7
1	B	993	THR	2.7
1	A	1026	PHE	2.6
1	A	537	SER	2.6
1	A	37	THR	2.6
1	A	38	ILE	2.6
1	B	176	GLN	2.6
1	C	120	GLN	2.6
1	A	424	GLY	2.6
1	A	536	ARG	2.6
1	B	619	GLY	2.6
1	B	132	SER	2.6
1	A	679	GLY	2.5
1	A	985	GLY	2.5
1	B	478	MET	2.5
1	B	657	GLN	2.5
1	C	957	GLY	2.5
1	A	255	GLN	2.5
1	A	511	GLY	2.5
1	C	809	TRP	2.5
1	A	890	ALA	2.5
1	C	618	ALA	2.5
1	C	116	PRO	2.5
1	A	616	GLY	2.5
1	A	541	TYR	2.5
1	B	564	LEU	2.5
1	C	670	ALA	2.5
1	A	535	LEU	2.4
1	B	577	GLN	2.4
1	A	957	GLY	2.4
1	C	403	GLY	2.4
1	B	6	ILE	2.4
1	B	636	ASP	2.4
1	B	569	GLN	2.4
1	B	443	VAL	2.4
1	A	987	MET	2.4
1	A	704	ALA	2.4
1	B	1034	SER	2.4
1	C	458	PHE	2.4
1	A	544	LEU	2.4
1	B	136	PHE	2.4
1	B	678	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	969	ARG	2.3
2	D	166	GLN	2.3
2	D	61	GLU	2.3
1	B	664	PHE	2.3
1	A	716	VAL	2.3
1	A	422	GLU	2.3
1	B	614	GLY	2.3
1	B	344	LEU	2.3
1	C	954	ASP	2.3
1	B	603	LYS	2.3
1	A	356	TYR	2.3
1	A	1037	ASN	2.3
1	A	709	HIS	2.3
1	C	674	LEU	2.3
1	A	496	MET	2.3
1	A	970	MET	2.3
1	B	1033	PHE	2.3
1	C	693	GLU	2.3
1	B	920	GLY	2.2
1	C	691	GLY	2.2
1	A	660	ASP	2.2
1	A	948	PHE	2.2
1	B	255	GLN	2.2
1	A	834	GLY	2.2
1	B	649	MET	2.2
1	B	513	PHE	2.2
1	B	670	ALA	2.2
1	B	940	LYS	2.2
1	C	737	GLN	2.2
1	A	649	MET	2.2
1	A	668	LEU	2.2
1	A	870	GLY	2.2
1	B	249	ILE	2.2
1	B	961	ILE	2.2
1	A	947	GLU	2.2
1	A	835	LYS	2.2
1	A	875	SER	2.2
1	C	956	GLU	2.2
1	B	448	VAL	2.1
1	A	415	ASN	2.1
1	A	670	ALA	2.1
1	B	987	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	624	THR	2.1
1	A	15	ILE	2.1
1	C	510	LYS	2.1
1	A	112	GLN	2.1
1	B	600	THR	2.1
1	C	35	TYR	2.1
2	E	81	SER	2.1
1	A	862	MET	2.1
1	B	340	VAL	2.1
1	B	571	VAL	2.1
1	B	646	ALA	2.1
1	A	619	GLY	2.1
1	A	1010	GLY	2.1
1	A	892	TYR	2.1
1	A	950	LYS	2.1
1	A	523	SER	2.1
1	B	566	ASP	2.1
1	A	1016	VAL	2.1
1	A	1033	PHE	2.1
1	B	416	VAL	2.1
1	C	890	ALA	2.1
1	A	1031	ARG	2.1
1	B	574	THR	2.1
1	C	519	MET	2.1
1	C	513	PHE	2.0
1	C	70	ASN	2.0
1	C	71	GLY	2.0
1	A	410	ILE	2.0
1	B	402	ILE	2.0
1	B	992	SER	2.0
1	A	620	ARG	2.0
1	A	984	LEU	2.0
1	B	441	ALA	2.0
1	B	627	ALA	2.0
1	C	486	LEU	2.0
1	A	659	LYS	2.0
1	B	131	LYS	2.0
1	A	148	THR	2.0
1	B	933	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DDQ	A	1104	14/14	0.64	0.33	66,73,80,80	0
8	D10	B	1111	10/10	0.70	0.37	66,68,70,71	0
3	LMT	B	1102	35/35	0.71	0.20	64,66,71,72	0
3	LMT	B	1107	35/35	0.74	0.18	59,64,68,68	0
4	C14	A	1103	14/14	0.74	0.26	55,57,60,60	0
9	EDO	C	1114	4/4	0.74	0.29	57,57,57,57	0
5	DDQ	C	1102	14/14	0.75	0.26	58,64,66,67	0
8	D10	A	1108	10/10	0.76	0.28	59,60,61,62	0
9	EDO	B	1109	4/4	0.77	0.23	57,57,58,58	0
9	EDO	B	1104	4/4	0.77	0.23	55,55,56,56	0
11	OCT	C	1104	8/8	0.78	0.23	49,50,51,51	0
11	OCT	C	1109	8/8	0.78	0.26	55,56,58,58	0
12	LPX	C	1106	30/30	0.78	0.21	57,68,75,75	0
9	EDO	C	1113	4/4	0.79	0.20	56,56,56,56	0
8	D10	A	1111	10/10	0.81	0.32	69,74,80,81	0
9	EDO	B	1110	4/4	0.81	0.28	75,76,76,76	0
10	SO4	B	1114	5/5	0.81	0.13	85,85,85,85	0
3	LMT	A	1101	35/35	0.82	0.17	65,78,83,85	0
9	EDO	A	1112	4/4	0.82	0.18	42,42,42,42	0
7	1K8	B	1113	17/17	0.82	0.23	45,47,48,49	17
9	EDO	B	1106	4/4	0.82	0.18	53,54,54,54	0
3	LMT	A	1107	35/35	0.83	0.17	64,67,71,73	0
9	EDO	B	1103	4/4	0.83	0.21	49,49,49,50	0
9	EDO	E	201	4/4	0.84	0.27	61,62,62,64	0
8	D10	C	1103	10/10	0.84	0.18	49,49,50,51	0
9	EDO	A	1109	4/4	0.84	0.16	59,60,60,61	0
3	LMT	A	1102	35/35	0.84	0.16	56,59,62,63	0

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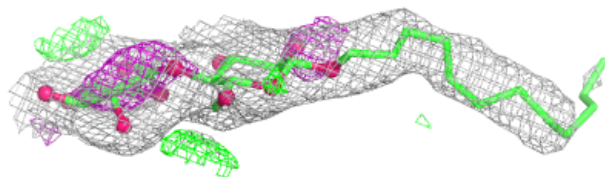
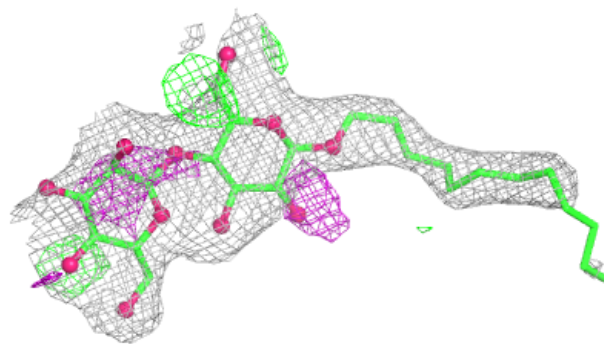
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	EDO	B	1108	4/4	0.84	0.21	53,53,53,54	0
9	EDO	A	1110	4/4	0.87	0.17	60,60,61,61	0
11	OCT	C	1108	8/8	0.87	0.17	48,49,50,50	0
3	LMT	B	1101	35/35	0.87	0.16	70,72,75,75	0
6	GOL	A	1105	6/6	0.87	0.16	48,48,48,49	0
6	GOL	B	1105	6/6	0.88	0.17	58,59,59,59	0
9	EDO	C	1105	4/4	0.89	0.26	57,57,57,57	0
9	EDO	D	201	4/4	0.89	0.18	55,56,56,56	0
9	EDO	C	1110	4/4	0.89	0.13	52,52,52,53	0
9	EDO	B	1112	4/4	0.89	0.13	59,59,59,60	0
3	LMT	C	1101	35/35	0.90	0.13	57,61,63,64	0
11	OCT	C	1112	8/8	0.91	0.16	51,52,53,54	0
9	EDO	C	1107	4/4	0.91	0.17	47,47,47,47	0
7	1K8	A	1106	17/17	0.92	0.15	67,72,77,77	0
10	SO4	C	1115	5/5	0.93	0.19	75,75,75,76	0
6	GOL	C	1111	6/6	0.94	0.11	43,44,44,44	0

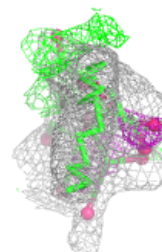
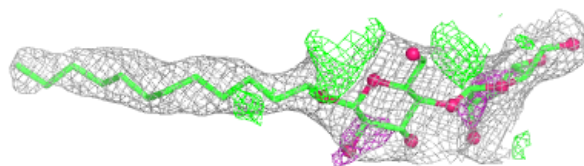
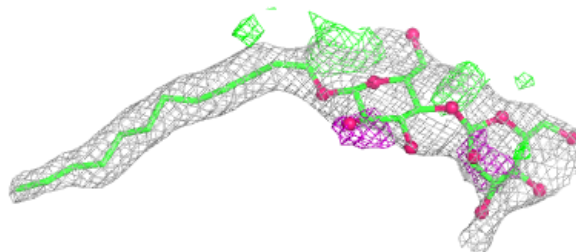
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 1102:

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

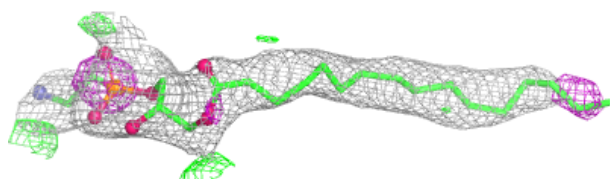
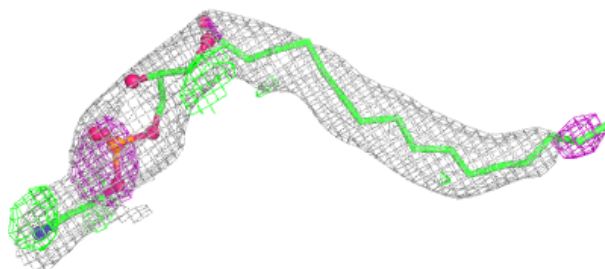
**Electron density around LMT B 1107:**

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

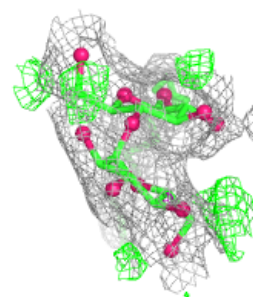
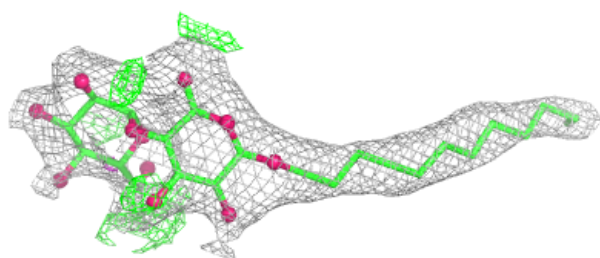
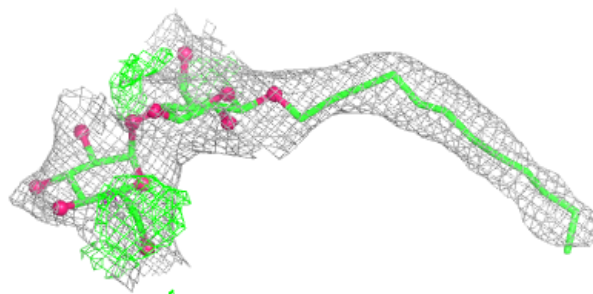


Electron density around LPX C 1106:

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

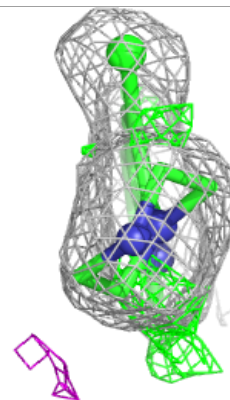
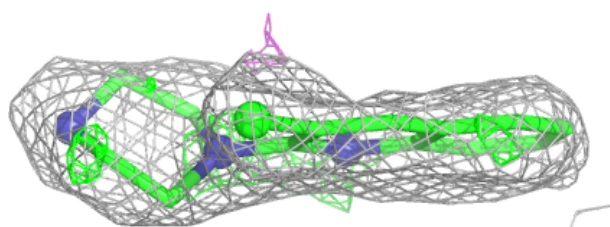
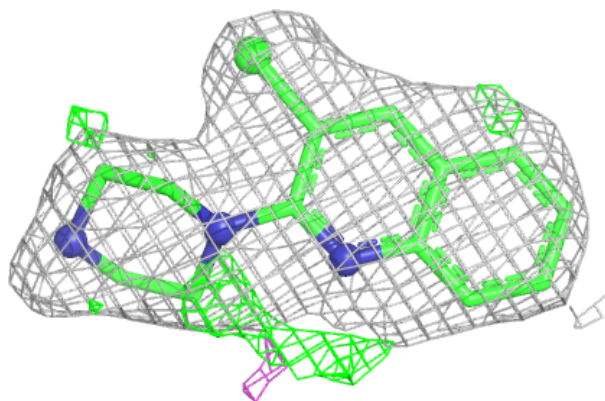
**Electron density around LMT A 1101:**

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

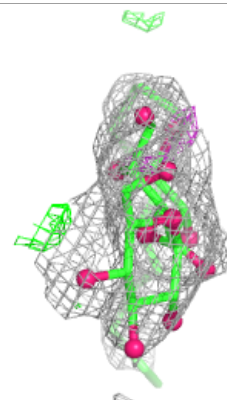
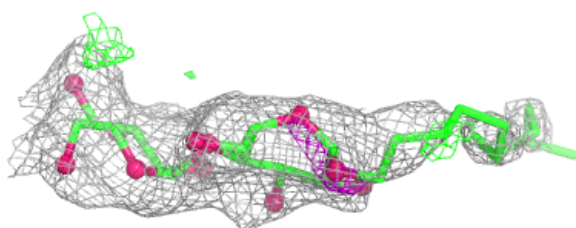
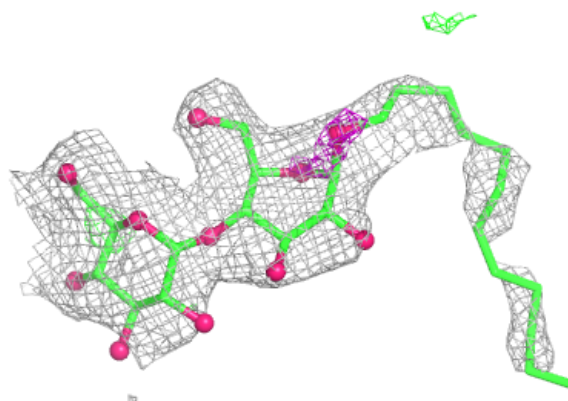


Electron density around 1K8 B 1113:

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

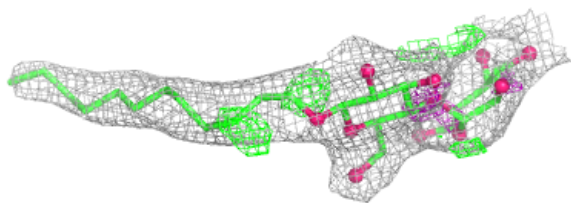
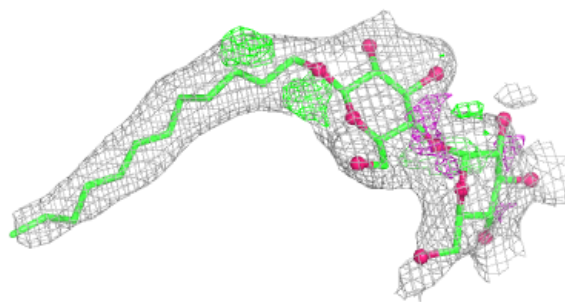
**Electron density around LMT A 1107:**

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

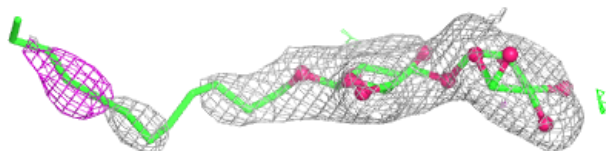
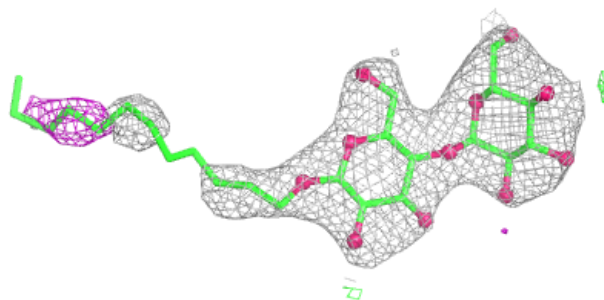


Electron density around LMT A 1102:

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

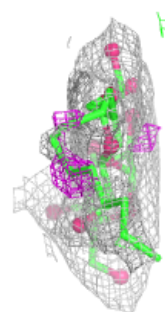
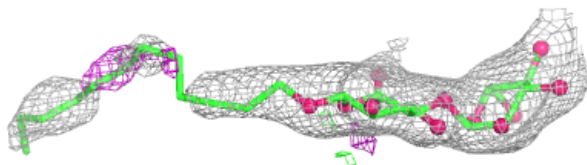
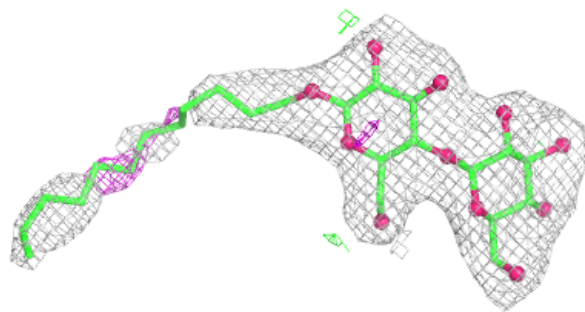
**Electron density around LMT B 1101:**

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

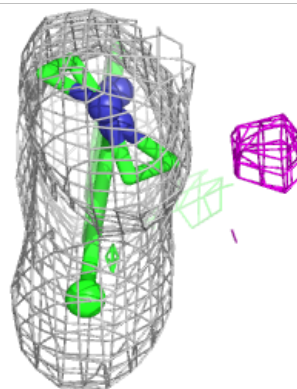
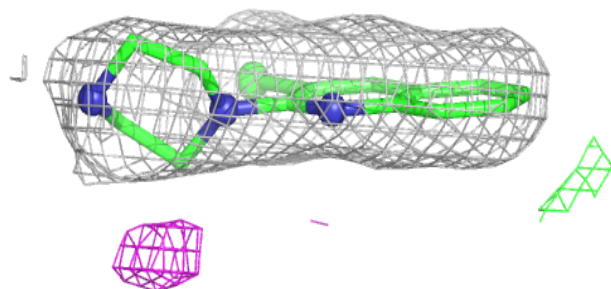
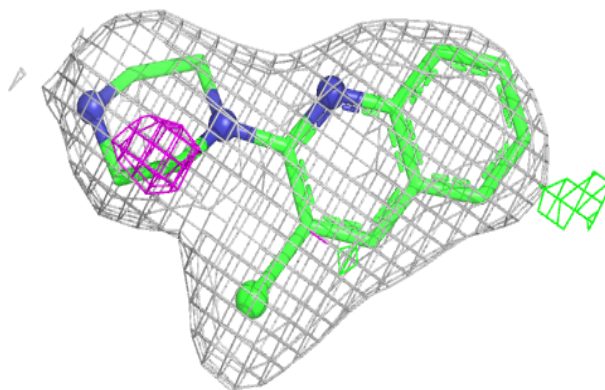


Electron density around LMT C 1101:

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

**Electron density around 1K8 A 1106:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.