



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:55 AM UTC

PDB ID : 6ZOG / pdb_00006zog
Title : Minocycline binding to the deep binding pocket of AcrB-I38F_I671T
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.75 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

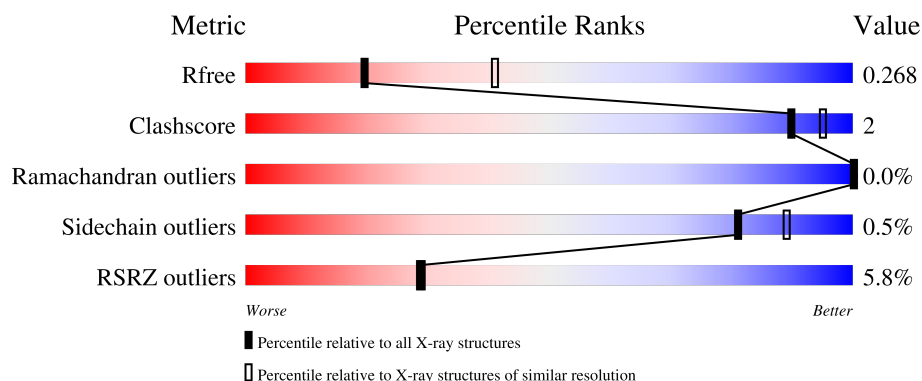
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	8% 92% 6%
1	B	1057	6% 92% 5%
1	C	1057	4% 92% 6%
2	D	169	4% 92% 7%
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
8	8K6	B	1104	-	-	-	X

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 26599 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
			7874	5066	1300	1464	44			
1	B	1034	Total	C	N	O	S	0	2	0
			7872	5065	1298	1464	45			
1	C	1034	Total	C	N	O	S	0	2	0
			7876	5069	1299	1464	44			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	PHE	ILE	engineered mutation	UNP P31224
A	671	THR	ILE	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	38	PHE	ILE	engineered mutation	UNP P31224
B	671	THR	ILE	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	38	PHE	ILE	engineered mutation	UNP P31224
C	671	THR	ILE	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224

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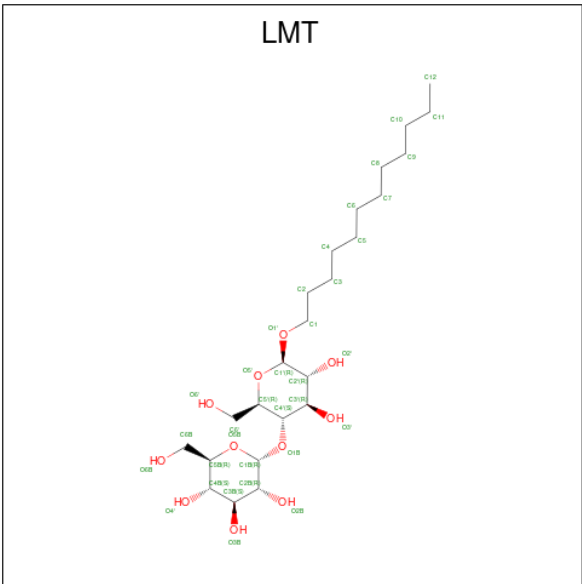
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056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

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	157	Total	C	N	O	S	0	0	0
			1186	747	208	230	1			
2	E	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



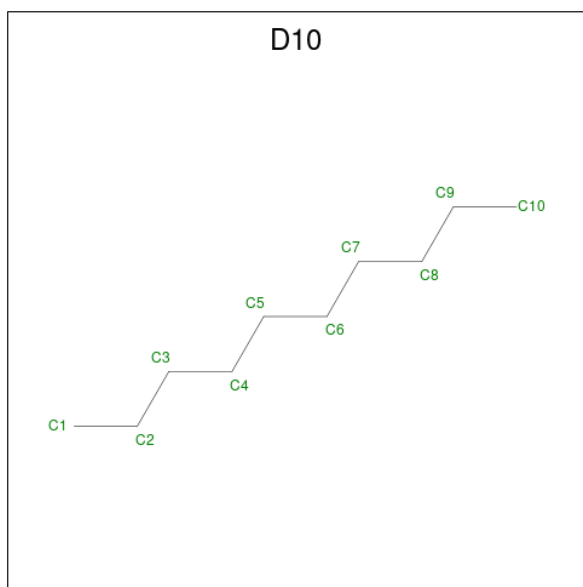
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

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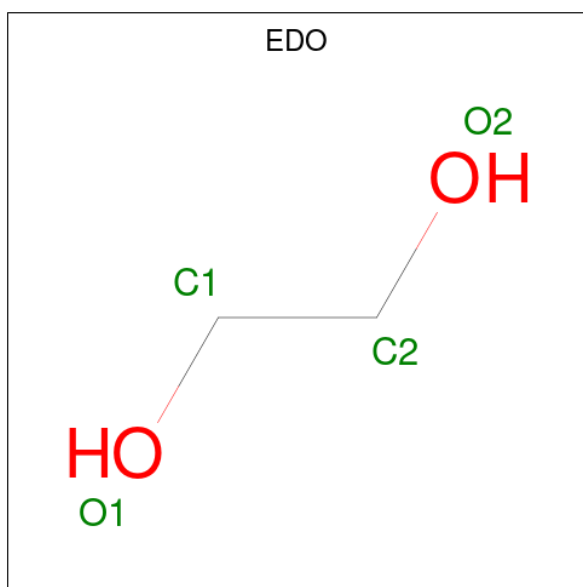
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

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



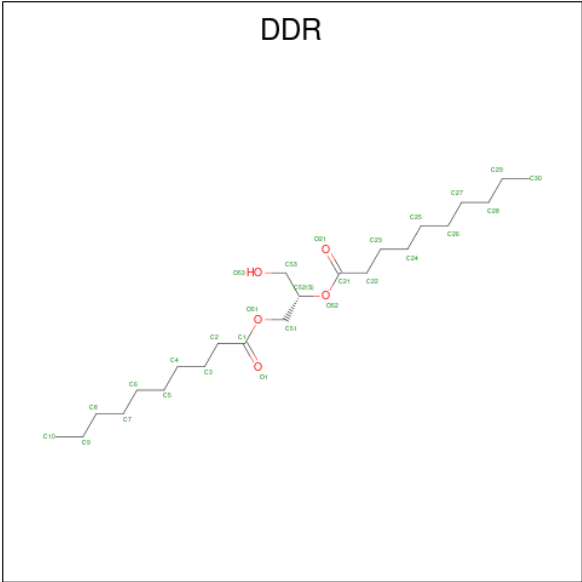
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		

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



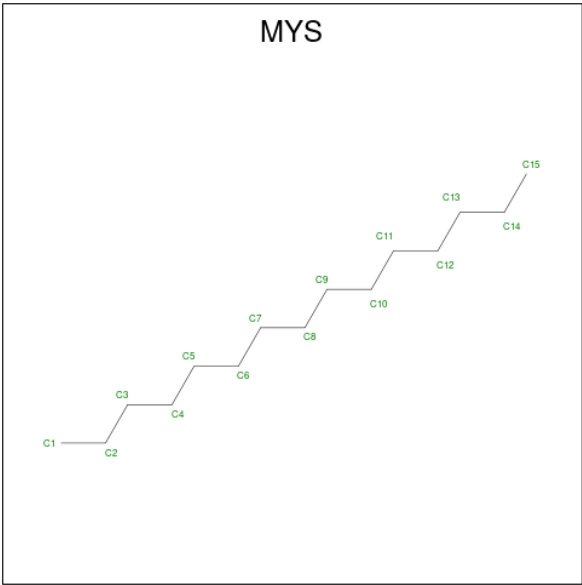
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



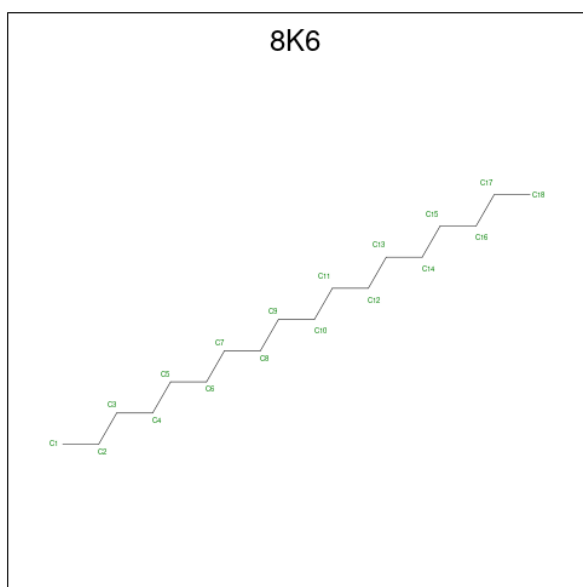
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 7 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



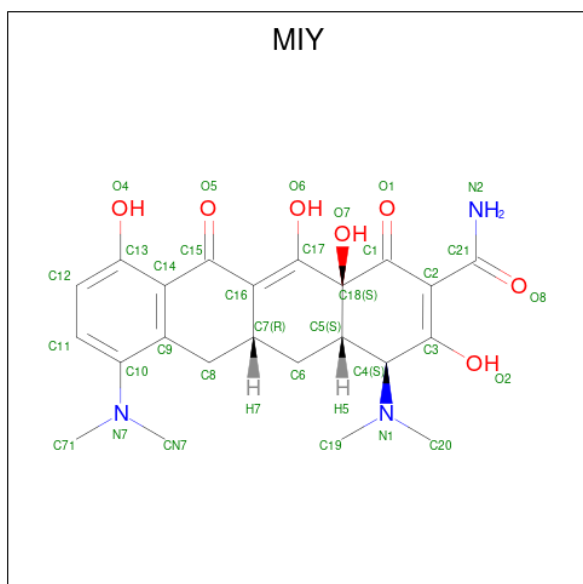
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C	0	0
			15	15		

- Molecule 8 is Octadecane (CCD ID: 8K6) (formula: C₁₈H₃₈).



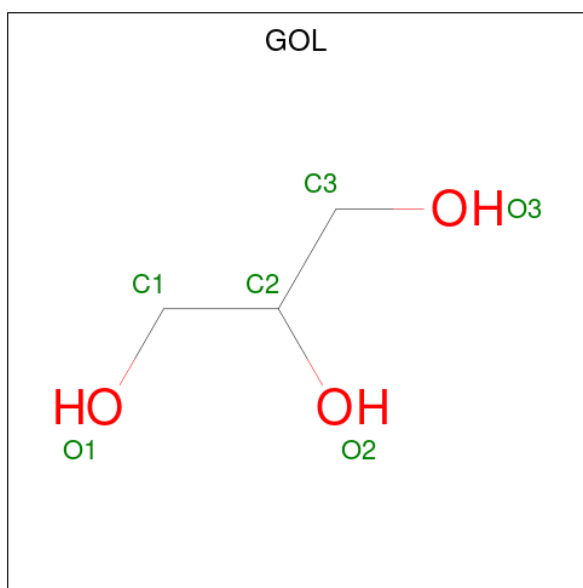
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	C	0	0
			18	18		

- Molecule 9 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$) (labeled as "Ligand of Interest" by depositor).



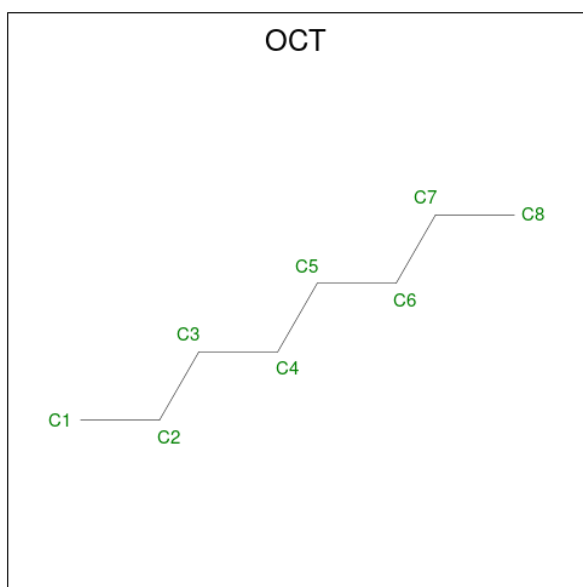
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			33	23	3	7		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



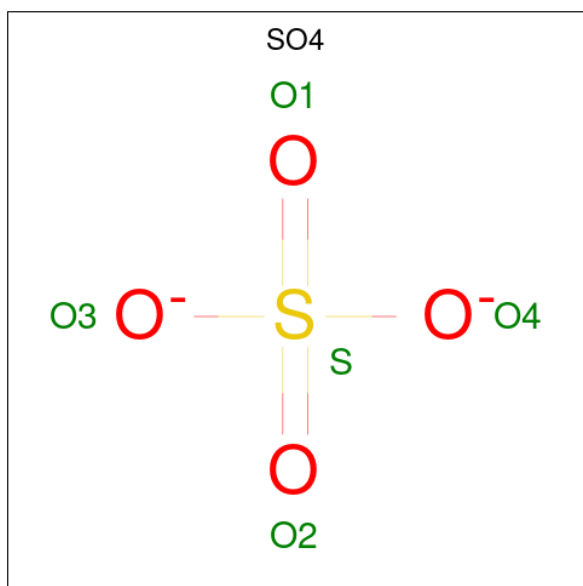
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



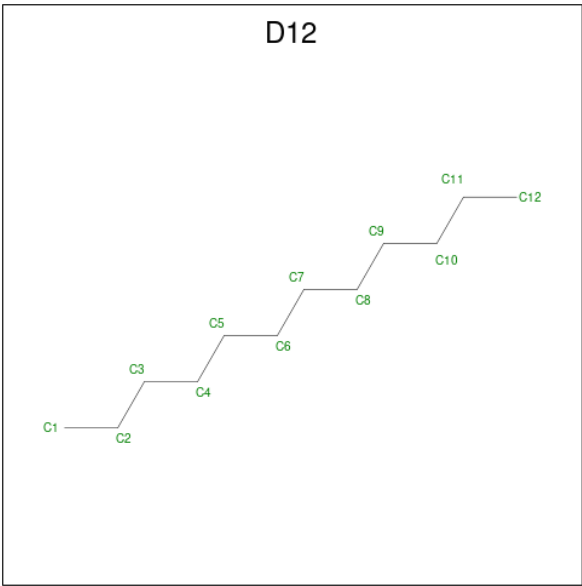
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total C 8 8	0	0

- Molecule 12 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



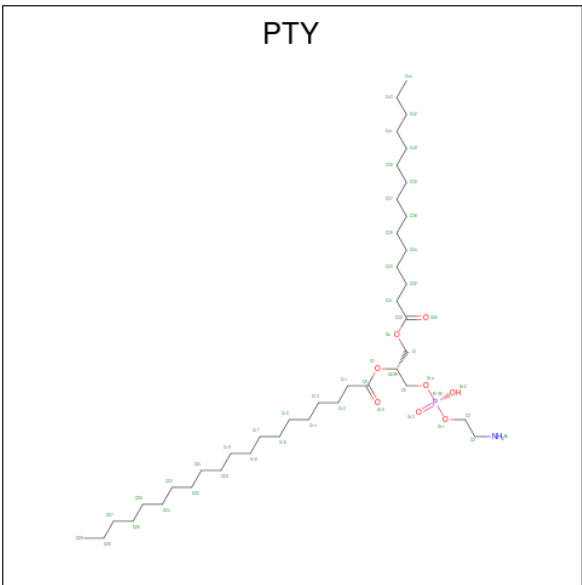
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	1	Total O S 5 4 1	0	0
12	B	1	Total O S 5 4 1	0	0
12	C	1	Total O S 5 4 1	0	0

- Molecule 13 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



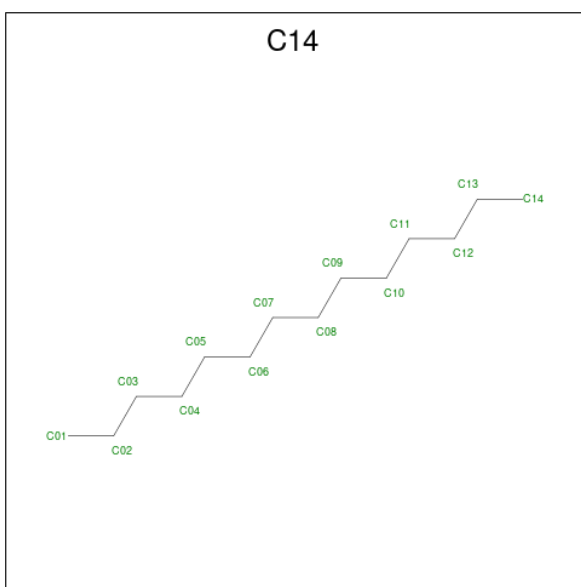
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C			0	0
			12	12				

- Molecule 14 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



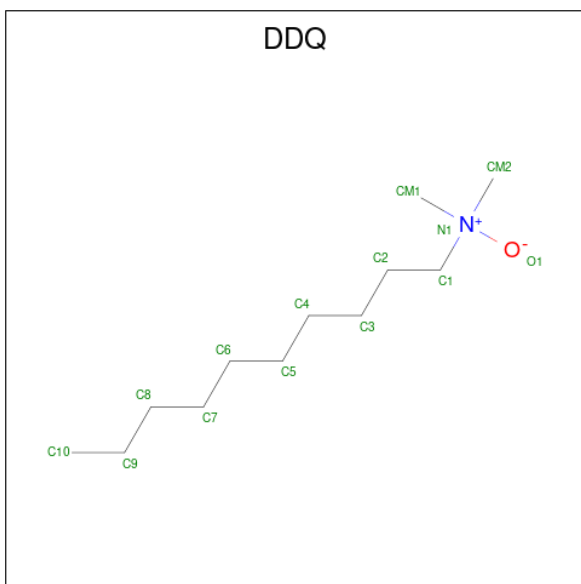
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
14	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 15 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total	C		0	0
			14	14			

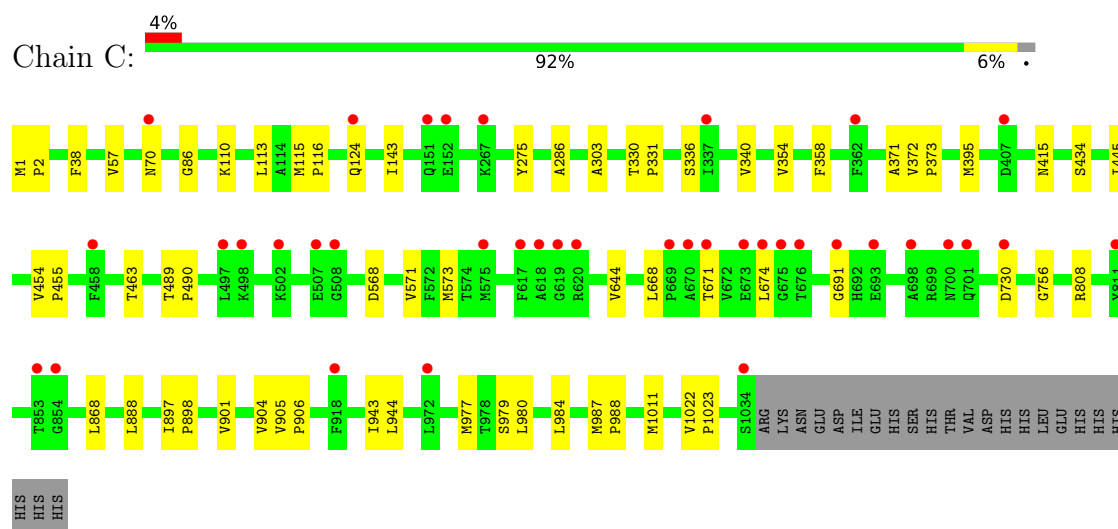
- Molecule 16 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



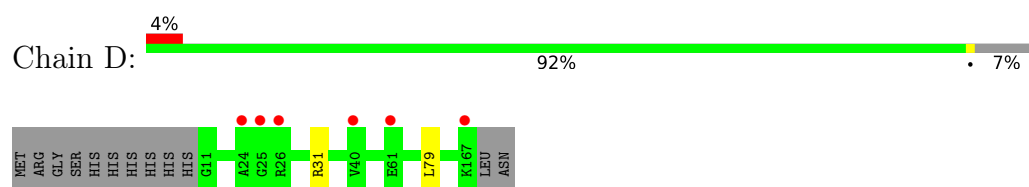
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	C	1	Total	C	N	O	0	0
			14	12	1	1		

- Molecule 17 is water.

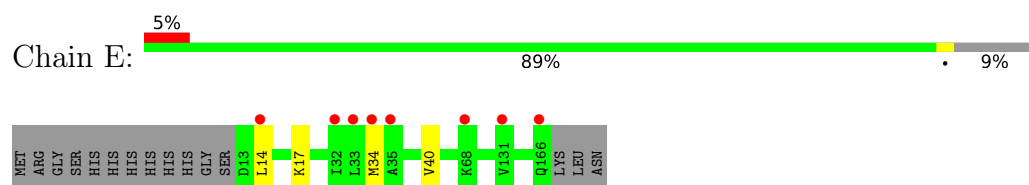
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	49	Total 49	O 49	0	0
17	B	35	Total 35	O 35	0	0
17	C	43	Total 43	O 43	0	0
17	D	5	Total 5	O 5	0	0
17	E	1	Total 1	O 1	0	0



• Molecule 2: DARPIN



• Molecule 2: DARPIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.97Å 161.95Å 245.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.75 49.59 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.59-2.75) 100.0 (49.59-2.75)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.230 , 0.268 0.232 , 0.268	Depositor DCC
R_{free} test set	7492 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.9	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	0.91	EDS
Total number of atoms	26599	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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: PTY, DDQ, LMT, D12, DDR, C14, MYS, EDO, MIY, 8K6, GOL, SO4, OCT, D10

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	0/8028	1.57	4/10901 (0.0%)
1	B	1.04	0/8023	1.58	5/10895 (0.0%)
1	C	1.04	0/8028	1.56	4/10902 (0.0%)
2	D	1.04	0/1205	1.59	0/1637
2	E	1.03	0/1186	1.62	0/1613
All	All	1.04	0/26470	1.57	13/35948 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	896	SER	CA-C-N	6.75	124.50	120.24
1	A	896	SER	C-N-CA	6.75	124.50	120.24
1	B	691	GLY	CA-C-O	-5.80	118.27	122.45
1	B	904	VAL	CA-C-N	5.67	124.87	120.33
1	B	904	VAL	C-N-CA	5.67	124.87	120.33
1	B	366	LEU	CA-C-N	5.46	124.70	120.33
1	B	366	LEU	C-N-CA	5.46	124.70	120.33
1	A	1021	PHE	CA-C-N	5.24	123.54	120.24
1	A	1021	PHE	C-N-CA	5.24	123.54	120.24
1	C	756	GLY	CA-C-O	-5.18	118.09	122.29
1	C	691	GLY	CA-C-O	-5.06	118.23	122.33
1	C	371	ALA	CA-C-N	5.05	124.37	120.33
1	C	371	ALA	C-N-CA	5.05	124.37	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	7874	0	8018	27	0
1	B	7872	0	8014	36	0
1	C	7876	0	8013	30	0
2	D	1186	0	1172	1	0
2	E	1167	0	1151	1	0
3	A	140	0	184	0	0
3	B	35	0	46	0	0
3	C	35	0	46	0	0
4	A	10	0	22	0	0
4	C	10	0	22	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	8	0	12	0	0
5	E	8	0	12	0	0
6	B	28	0	44	0	0
7	B	15	0	32	0	0
8	B	18	0	38	0	0
9	B	33	0	24	5	0
10	B	6	0	8	0	0
10	C	18	0	24	0	0
10	D	6	0	8	0	0
11	B	8	0	18	0	0
12	B	10	0	0	0	0
12	C	5	0	0	0	0
13	C	12	0	26	0	0
14	C	50	0	79	0	0
15	C	14	0	30	0	0
16	C	14	0	27	0	0
17	A	49	0	0	0	0
17	B	35	0	0	0	0
17	C	43	0	0	0	0
17	D	5	0	0	0	0
17	E	1	0	0	0	0
All	All	26599	0	27082	95	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (95) 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)
9:B:1105:MIY:H713	9:B:1105:MIY:H81	1.65	0.79
1:B:395[B]:MET:HA	1:B:395[B]:MET:HE2	1.75	0.67
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.80	0.64
1:B:303:ALA:HB2	1:B:330:THR:HG21	1.84	0.59
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.84	0.58
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.85	0.58
1:B:178:PHE:CD1	9:B:1105:MIY:H712	2.41	0.56
1:C:901:VAL:O	1:C:904:VAL:HG12	2.05	0.56
1:B:395[B]:MET:HE2	1:B:395[B]:MET:CA	2.34	0.56
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.88	0.54
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.90	0.53
1:C:979:SER:HA	1:C:1011:MET:HE3	1.91	0.53
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.25	0.52
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.92	0.52
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.92	0.51
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.92	0.51
1:C:445:ILE:HD11	1:C:944:LEU:HD21	1.92	0.51
1:B:739:LEU:HD13	1:B:799:VAL:HG11	1.93	0.51
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.42	0.50
1:B:340:VAL:HG21	1:B:395[A]:MET:HB3	1.92	0.50
1:B:340:VAL:HG21	1:B:395[B]:MET:HB3	1.92	0.50
9:B:1105:MIY:O7	9:B:1105:MIY:H192	2.11	0.50
1:C:336:SER:O	1:C:340:VAL:HG23	2.11	0.50
1:C:489:THR:HB	1:C:490:PRO:HD3	1.93	0.49
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.93	0.49
1:B:466:ILE:HD11	1:B:674:LEU:HD11	1.93	0.49
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.95	0.48
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.95	0.48
9:B:1105:MIY:H81	9:B:1105:MIY:C71	2.39	0.48
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.95	0.48
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.95	0.47
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.39	0.47
1:B:919:ARG:NH1	1:B:990:VAL:O	2.47	0.47
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.96	0.47
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.96	0.47
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.50	0.47
1:C:573:MET:HE2	1:C:668:LEU:HD22	1.97	0.46
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.51	0.46
1:A:777:ALA:O	1:A:781:MET:HG2	2.16	0.46
1:A:897:ILE:N	1:A:898:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395[B]:MET:HA	1:B:395[B]:MET:CE	2.38	0.46
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.46
1:B:367:ILE:N	1:B:368:PRO:HD2	2.31	0.45
1:B:973:ARG:N	1:B:974:PRO:HD2	2.31	0.45
1:B:447:MET:HA	1:B:447:MET:HE2	1.98	0.45
1:A:453:PHE:O	1:A:456:MET:HG2	2.17	0.45
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.99	0.45
1:A:178:PHE:HA	1:A:277:ILE:HG21	1.99	0.45
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:B:395[B]:MET:HE2	1:B:395[B]:MET:N	2.32	0.44
1:A:987:MET:N	1:A:988:PRO:CD	2.80	0.44
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.53	0.44
1:C:354:VAL:CG2	1:C:984:LEU:HD12	2.47	0.44
1:A:489:THR:HB	1:A:490:PRO:HD3	2.00	0.44
1:A:873:ALA:HB3	1:A:874:PRO:HD3	2.00	0.44
1:C:1:MET:HB3	1:C:2:PRO:HD3	2.00	0.44
1:A:901:VAL:O	1:A:904:VAL:HG22	2.17	0.44
1:C:571:VAL:HG23	1:C:668:LEU:HD11	2.00	0.43
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.00	0.43
1:C:115:MET:N	1:C:116:PRO:HD2	2.33	0.43
1:B:987:MET:N	1:B:988:PRO:CD	2.82	0.43
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.43
1:B:391:ASN:H	1:B:394:THR:HG1	1.67	0.43
1:B:897:ILE:N	1:B:898:PRO:HD2	2.32	0.43
1:A:350:LEU:HD22	1:A:984:LEU:HG	2.00	0.42
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.01	0.42
1:B:314:GLU:HB2	1:B:315:PRO:HD3	2.02	0.42
1:A:330:THR:N	1:A:331:PRO:CD	2.82	0.42
1:A:559:LEU:HD12	1:A:560:PRO:HD2	2.01	0.42
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.19	0.42
1:B:841:MET:HE1	1:B:867:ARG:HG3	2.02	0.42
1:C:143:ILE:HG22	1:C:286:ALA:HB2	2.02	0.42
1:B:178:PHE:CE1	9:B:1105:MIY:H712	2.55	0.42
1:C:1022:VAL:HB	1:C:1023:PRO:HD3	2.01	0.42
1:A:300:LEU:HD23	1:A:330:THR:HB	2.02	0.42
1:C:730:ASP:OD2	1:C:808:ARG:NH1	2.53	0.42
1:B:809:TRP:CD1	2:D:79:LEU:HD12	2.55	0.41
2:E:34:MET:SD	2:E:40:VAL:HG12	2.61	0.41
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.03	0.41
1:A:973:ARG:N	1:A:974:PRO:HD2	2.36	0.41
1:B:897:ILE:N	1:B:898:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:VAL:N	1:A:455:PRO:CD	2.84	0.41
1:C:987:MET:N	1:C:988:PRO:CD	2.83	0.41
1:A:184:MET:HG2	1:A:246:PHE:CD2	2.56	0.41
1:A:952:LEU:HA	1:A:956:GLU:HG2	2.03	0.41
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.83	0.41
1:B:130:GLU:HG2	1:C:113:LEU:HD21	2.02	0.41
1:C:358:PHE:CG	1:C:977:MET:HG2	2.56	0.41
1:C:395:MET:HA	1:C:395:MET:HE2	2.03	0.41
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.55	0.41
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	2.36	0.41
1:C:38:PHE:CZ	1:C:671:THR:HG21	2.56	0.40
1:C:415:ASN:HD22	1:C:434:SER:HB3	1.85	0.40
1:C:303:ALA:HB2	1:C:330:THR:HG21	2.04	0.40
1:C:980:LEU:HD23	1:C:980:LEU:HA	1.98	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	1034/1057 (98%)	1004 (97%)	29 (3%)	1 (0%)	48	71
1	B	1034/1057 (98%)	1004 (97%)	30 (3%)	0	100	100
1	C	1034/1057 (98%)	1010 (98%)	24 (2%)	0	100	100
2	D	155/169 (92%)	150 (97%)	5 (3%)	0	100	100
2	E	152/169 (90%)	146 (96%)	6 (4%)	0	100	100
All	All	3409/3509 (97%)	3314 (97%)	94 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	842/863 (98%)	839 (100%)	3 (0%)	84	91
1	B	842/863 (98%)	839 (100%)	3 (0%)	84	91
1	C	842/863 (98%)	835 (99%)	7 (1%)	73	84
2	D	121/132 (92%)	120 (99%)	1 (1%)	73	84
2	E	119/132 (90%)	117 (98%)	2 (2%)	53	71
All	All	2766/2853 (97%)	2750 (99%)	16 (1%)	81	88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	A	558	ARG
1	A	801	PHE
1	B	88	VAL
1	B	556	PHE
1	B	801	PHE
1	C	70[A]	ASN
1	C	70[B]	ASN
1	C	110	LYS
1	C	124	GLN
1	C	463	THR
1	C	674	LEU
1	C	868	LEU
2	D	31	ARG
2	E	14	LEU
2	E	17	LYS

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

Mol	Chain	Res	Type
1	A	89	GLN
1	A	194	ASN
1	A	526	HIS
1	A	588	GLN
1	A	923	ASN
1	B	58	GLN
1	B	70	ASN
1	B	194	ASN
1	B	218	GLN
1	B	231	ASN
1	B	361	ASN
1	B	469	GLN
1	B	642	ASN
1	B	687	GLN
1	B	1001	ASN
1	C	58	GLN
1	C	81	ASN
1	C	123	GLN
1	C	125	GLN
1	C	194	ASN
1	C	237	GLN
1	C	298	ASN
1	C	517	ASN
1	C	584	GLN
1	C	1001	ASN
2	D	92	HIS
2	D	102	ASN
2	D	125	HIS
2	E	102	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

31 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	1104	-	3,3,3	0.07	0	2,2,2	0.10	0
5	EDO	E	201	-	3,3,3	0.07	0	2,2,2	0.11	0
10	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.28	0
3	LMT	C	1302	-	36,36,36	0.44	0	47,47,47	0.49	0
12	SO4	B	1110	-	4,4,4	0.34	0	6,6,6	0.08	0
15	C14	C	1305	-	13,13,13	0.09	0	12,12,12	0.09	0
5	EDO	B	1108	-	3,3,3	0.08	0	2,2,2	0.07	0
10	GOL	C	1309	-	5,5,5	0.09	0	5,5,5	0.28	0
10	GOL	C	1308	-	5,5,5	0.08	0	5,5,5	0.27	0
4	D10	A	1102	-	9,9,9	0.10	0	8,8,8	0.09	0
11	OCT	B	1107	-	7,7,7	0.10	0	6,6,6	0.05	0
7	MYS	B	1103	-	14,14,14	0.09	0	13,13,13	0.06	0
3	LMT	B	1101	-	36,36,36	0.43	0	47,47,47	0.46	0
3	LMT	A	1105	-	36,36,36	0.51	0	47,47,47	1.08	3 (6%)
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.64	0
5	EDO	C	1306	-	3,3,3	0.08	0	2,2,2	0.06	0
9	MIY	B	1105	-	36,36,36	1.09	2 (5%)	42,58,58	1.16	4 (9%)
13	D12	C	1301	-	11,11,11	0.09	0	10,10,10	0.08	0
5	EDO	E	202	-	3,3,3	0.06	0	2,2,2	0.13	0
10	GOL	B	1106	-	5,5,5	0.10	0	5,5,5	0.26	0
14	PTY	C	1304	-	49,49,49	0.26	0	52,54,54	0.32	0
3	LMT	A	1106	-	36,36,36	0.49	0	47,47,47	0.61	0
6	DDR	B	1102	-	27,27,27	0.24	0	29,29,29	0.25	0
12	SO4	C	1312	-	4,4,4	0.34	0	6,6,6	0.08	0
10	GOL	C	1310	-	5,5,5	0.09	0	5,5,5	0.25	0
8	8K6	B	1104	-	17,17,17	0.07	0	16,16,16	0.06	0
12	SO4	B	1109	-	4,4,4	0.34	0	6,6,6	0.07	0
16	DDQ	C	1311	-	11,13,13	0.20	0	12,15,15	0.20	0
4	D10	C	1303	-	9,9,9	0.10	0	8,8,8	0.08	0
5	EDO	C	1307	-	3,3,3	0.06	0	2,2,2	0.10	0
3	LMT	A	1103	-	36,36,36	0.46	0	47,47,47	0.57	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	1104	-	-	0/1/1/1	-
5	EDO	E	201	-	-	0/1/1/1	-
10	GOL	D	201	-	-	2/4/4/4	-
3	LMT	C	1302	-	-	7/21/61/61	0/2/2/2
15	C14	C	1305	-	-	5/11/11/11	-
5	EDO	B	1108	-	-	1/1/1/1	-
10	GOL	C	1309	-	-	2/4/4/4	-
10	GOL	C	1308	-	-	0/4/4/4	-
4	D10	A	1102	-	-	1/7/7/7	-
11	OCT	B	1107	-	-	2/5/5/5	-
7	MYS	B	1103	-	-	2/12/12/12	-
3	LMT	B	1101	-	-	6/21/61/61	0/2/2/2
3	LMT	A	1105	-	-	13/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
5	EDO	C	1306	-	-	1/1/1/1	-
9	MIY	B	1105	-	-	0/12/70/70	0/4/4/4
13	D12	C	1301	-	-	3/9/9/9	-
5	EDO	E	202	-	-	0/1/1/1	-
10	GOL	B	1106	-	-	0/4/4/4	-
14	PTY	C	1304	-	-	30/53/53/53	-
3	LMT	A	1106	-	-	13/21/61/61	0/2/2/2
6	DDR	B	1102	-	-	14/29/29/29	-
10	GOL	C	1310	-	-	0/4/4/4	-
8	8K6	B	1104	-	-	8/15/15/15	-
16	DDQ	C	1311	-	-	2/11/11/11	-
4	D10	C	1303	-	-	0/7/7/7	-
5	EDO	C	1307	-	-	1/1/1/1	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1105	MIY	C21-N2	5.17	1.48	1.33
9	B	1105	MIY	O5-C15	2.27	1.28	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	LMT	C4B-C3B-C2B	3.98	117.82	110.83
3	A	1105	LMT	C3B-C4B-C5B	3.11	115.87	110.23
3	A	1105	LMT	C1B-C2B-C3B	2.94	116.20	110.01
9	B	1105	MIY	C19-N1-C4	2.65	120.14	114.10
9	B	1105	MIY	C18-C1-C2	2.41	119.58	115.75
9	B	1105	MIY	O7-C18-C17	-2.35	106.38	110.14
9	B	1105	MIY	C15-C16-C17	2.25	120.58	118.80

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1105	LMT	C2'-C1'-O1'-C1
3	A	1105	LMT	O5'-C1'-O1'-C1
10	C	1309	GOL	C1-C2-C3-O3
10	D	201	GOL	C1-C2-C3-O3
14	C	1304	PTY	N1-C2-C3-O11
14	C	1304	PTY	C3-O11-P1-O12
14	C	1304	PTY	C3-O11-P1-O14
14	C	1304	PTY	C31-C30-O4-C1
14	C	1304	PTY	O30-C30-O4-C1
3	A	1105	LMT	O5'-C5'-C6'-O6'
3	C	1302	LMT	O5'-C5'-C6'-O6'
6	B	1102	DDR	O1-C1-O51-C51
6	B	1102	DDR	C22-C21-O52-C52
3	A	1105	LMT	C4'-C5'-C6'-O6'
6	B	1102	DDR	C2-C1-O51-C51
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C4B-C5B-C6B-O6B
3	C	1302	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	O5'-C5'-C6'-O6'
6	B	1102	DDR	O21-C21-O52-C52
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	C4'-C5'-C6'-O6'
14	C	1304	PTY	C11-C8-O7-C6
3	A	1103	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	O5B-C5B-C6B-O6B
6	B	1102	DDR	C21-C22-C23-C24
3	A	1106	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
3	A	1105	LMT	O1'-C1-C2-C3
3	A	1106	LMT	O1'-C1-C2-C3
14	C	1304	PTY	O10-C8-O7-C6
3	A	1106	LMT	C3'-C4'-O1B-C1B
3	A	1106	LMT	C2'-C1'-O1'-C1
3	A	1106	LMT	C5'-C4'-O1B-C1B
3	A	1105	LMT	C6-C7-C8-C9
3	A	1106	LMT	C3-C4-C5-C6
14	C	1304	PTY	C32-C33-C34-C35
10	C	1309	GOL	O2-C2-C3-O3
10	D	201	GOL	O2-C2-C3-O3
3	A	1101	LMT	C11-C10-C9-C8
3	A	1105	LMT	O5B-C5B-C6B-O6B
3	A	1105	LMT	C1-C2-C3-C4
14	C	1304	PTY	C14-C15-C16-C17
3	A	1106	LMT	C1-C2-C3-C4
14	C	1304	PTY	C19-C20-C21-C22
14	C	1304	PTY	C24-C25-C26-C27
3	A	1106	LMT	C4-C5-C6-C7
14	C	1304	PTY	C39-C40-C41-C42
14	C	1304	PTY	C34-C35-C36-C37
3	C	1302	LMT	C5-C6-C7-C8
4	A	1102	D10	C5-C6-C7-C8
3	A	1101	LMT	C6-C7-C8-C9
14	C	1304	PTY	C33-C34-C35-C36
3	B	1101	LMT	O1'-C1-C2-C3
3	C	1302	LMT	C6-C7-C8-C9
14	C	1304	PTY	C38-C39-C40-C41
8	B	1104	8K6	C7-C8-C9-C10
3	A	1103	LMT	O5'-C5'-C6'-O6'
14	C	1304	PTY	C23-C24-C25-C26
14	C	1304	PTY	O14-C5-C6-C1
3	A	1101	LMT	C4-C5-C6-C7
14	C	1304	PTY	C31-C32-C33-C34
14	C	1304	PTY	O4-C1-C6-C5
13	C	1301	D12	C7-C8-C9-C10
6	B	1102	DDR	C5-C6-C7-C8
11	B	1107	OCT	C3-C4-C5-C6
8	B	1104	8K6	C2-C3-C4-C5
8	B	1104	8K6	C3-C4-C5-C6
3	A	1105	LMT	C9-C10-C11-C12
3	B	1101	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
3	A	1106	LMT	C6-C7-C8-C9
8	B	1104	8K6	C9-C10-C11-C12
16	C	1311	DDQ	C7-C8-C9-C10
14	C	1304	PTY	C13-C14-C15-C16
14	C	1304	PTY	C37-C38-C39-C40
11	B	1107	OCT	C1-C2-C3-C4
14	C	1304	PTY	C12-C13-C14-C15
3	A	1101	LMT	C4B-C5B-C6B-O6B
6	B	1102	DDR	C51-C52-C53-O53
8	B	1104	8K6	C4-C5-C6-C7
14	C	1304	PTY	O14-C5-C6-O7
3	A	1103	LMT	C1-C2-C3-C4
14	C	1304	PTY	O4-C1-C6-O7
6	B	1102	DDR	C2-C3-C4-C5
3	A	1105	LMT	C11-C10-C9-C8
15	C	1305	C14	C08-C09-C10-C11
15	C	1305	C14	C11-C12-C13-C14
14	C	1304	PTY	C25-C26-C27-C28
3	B	1101	LMT	C5-C6-C7-C8
3	A	1106	LMT	C2-C3-C4-C5
14	C	1304	PTY	C2-C3-O11-P1
3	A	1103	LMT	C3-C4-C5-C6
14	C	1304	PTY	C16-C17-C18-C19
3	C	1302	LMT	C2-C3-C4-C5
8	B	1104	8K6	C1-C2-C3-C4
3	A	1101	LMT	C3-C4-C5-C6
3	A	1106	LMT	C5-C6-C7-C8
14	C	1304	PTY	C5-O14-P1-O13
3	B	1101	LMT	C3-C4-C5-C6
14	C	1304	PTY	C6-C5-O14-P1
6	B	1102	DDR	C27-C28-C29-C30
3	A	1103	LMT	C4-C5-C6-C7
6	B	1102	DDR	C26-C27-C28-C29
8	B	1104	8K6	C14-C15-C16-C17
3	A	1106	LMT	C4'-C5'-C6'-O6'
3	C	1302	LMT	C9-C10-C11-C12
3	C	1302	LMT	C4-C5-C6-C7
6	B	1102	DDR	C25-C26-C27-C28
13	C	1301	D12	C6-C7-C8-C9
5	C	1307	EDO	O1-C1-C2-O2
14	C	1304	PTY	C41-C42-C43-C44
15	C	1305	C14	C03-C04-C05-C06

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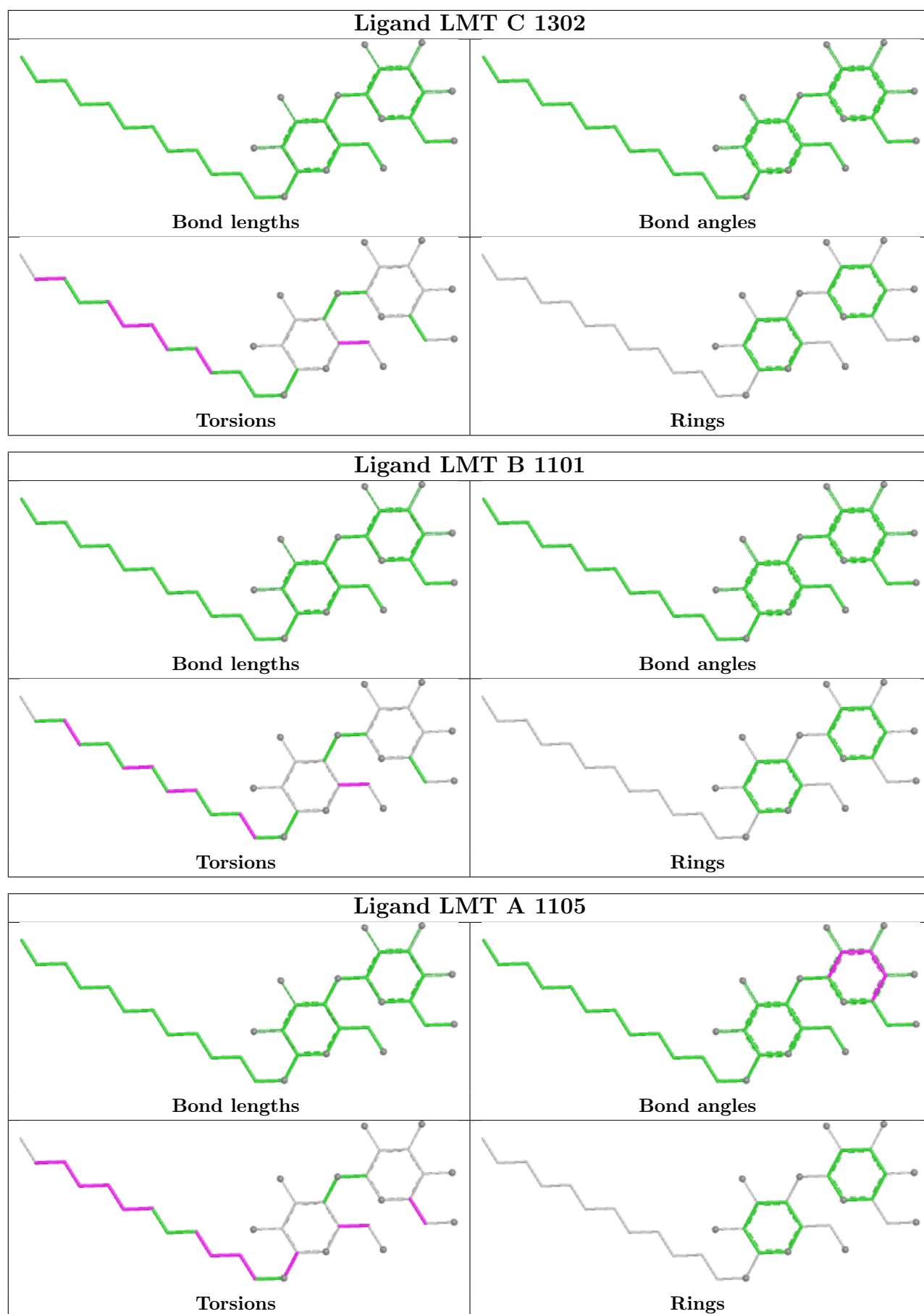
Mol	Chain	Res	Type	Atoms
8	B	1104	8K6	C5-C6-C7-C8
15	C	1305	C14	C07-C08-C09-C10
6	B	1102	DDR	O52-C52-C53-O53
5	B	1108	EDO	O1-C1-C2-O2
5	C	1306	EDO	O1-C1-C2-O2
16	C	1311	DDQ	C6-C7-C8-C9
7	B	1103	MYS	C9-C10-C11-C12
7	B	1103	MYS	C7-C8-C9-C10
3	A	1105	LMT	C2-C3-C4-C5
13	C	1301	D12	C11-C10-C9-C8
3	A	1106	LMT	O5'-C5'-C6'-O6'
3	A	1105	LMT	C5-C6-C7-C8
6	B	1102	DDR	C1-C2-C3-C4
3	A	1105	LMT	C7-C8-C9-C10
15	C	1305	C14	C09-C10-C11-C12
3	A	1103	LMT	C5'-C4'-O1B-C1B
3	A	1103	LMT	C3'-C4'-O1B-C1B
6	B	1102	DDR	O51-C51-C52-C53
3	A	1103	LMT	C5-C6-C7-C8

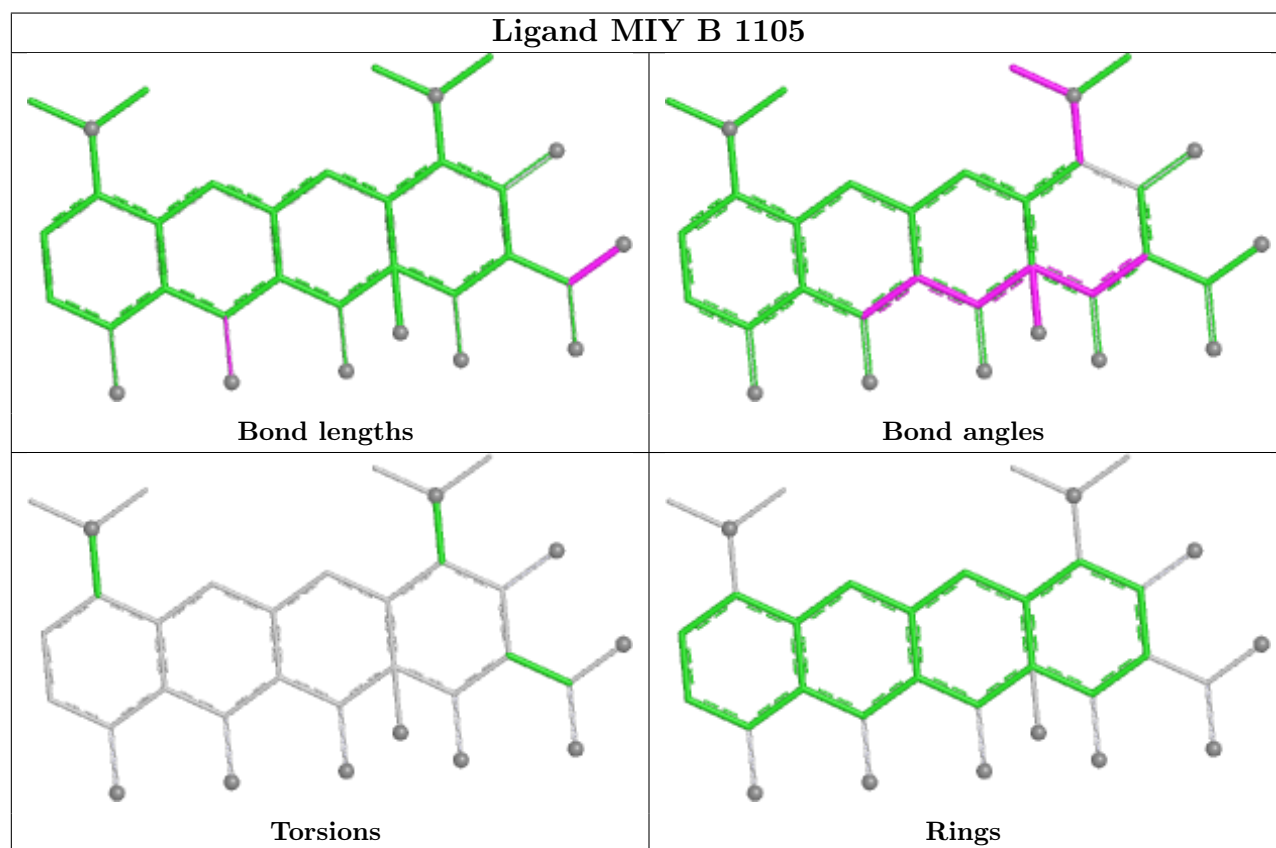
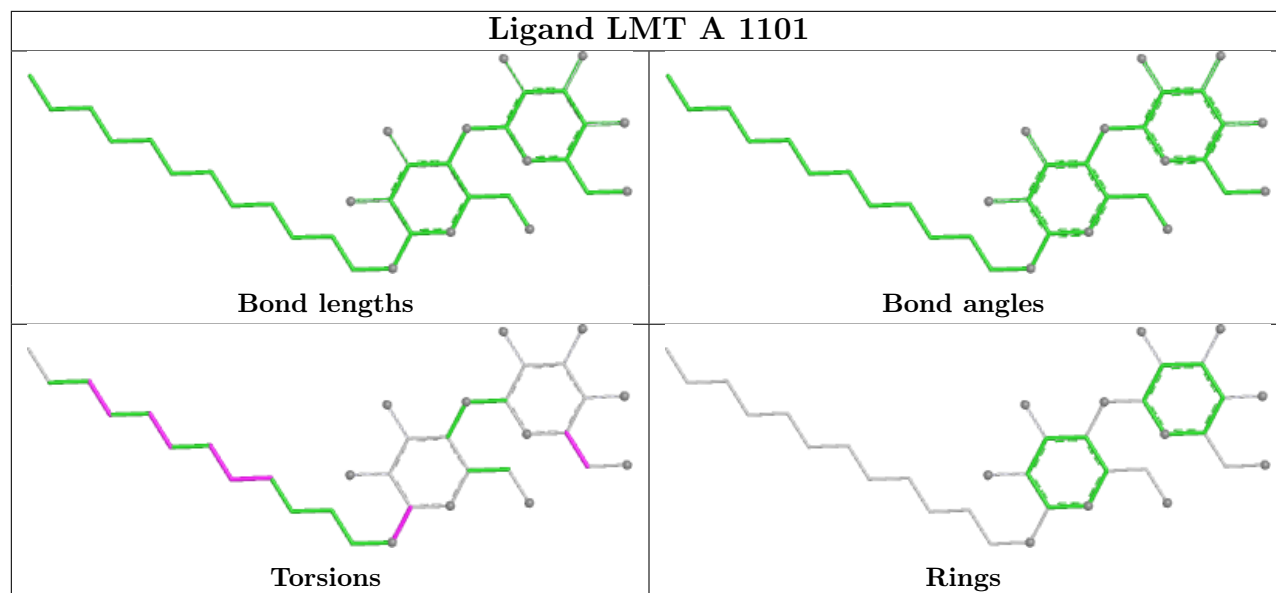
There are no ring outliers.

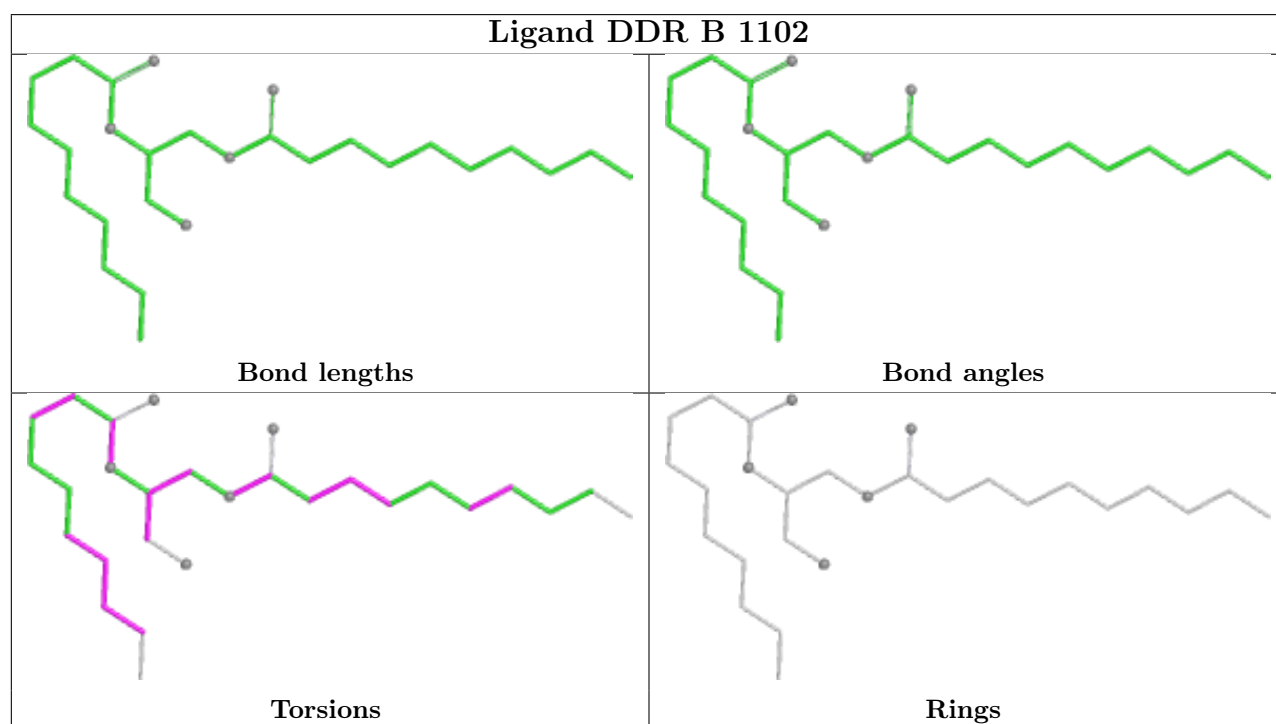
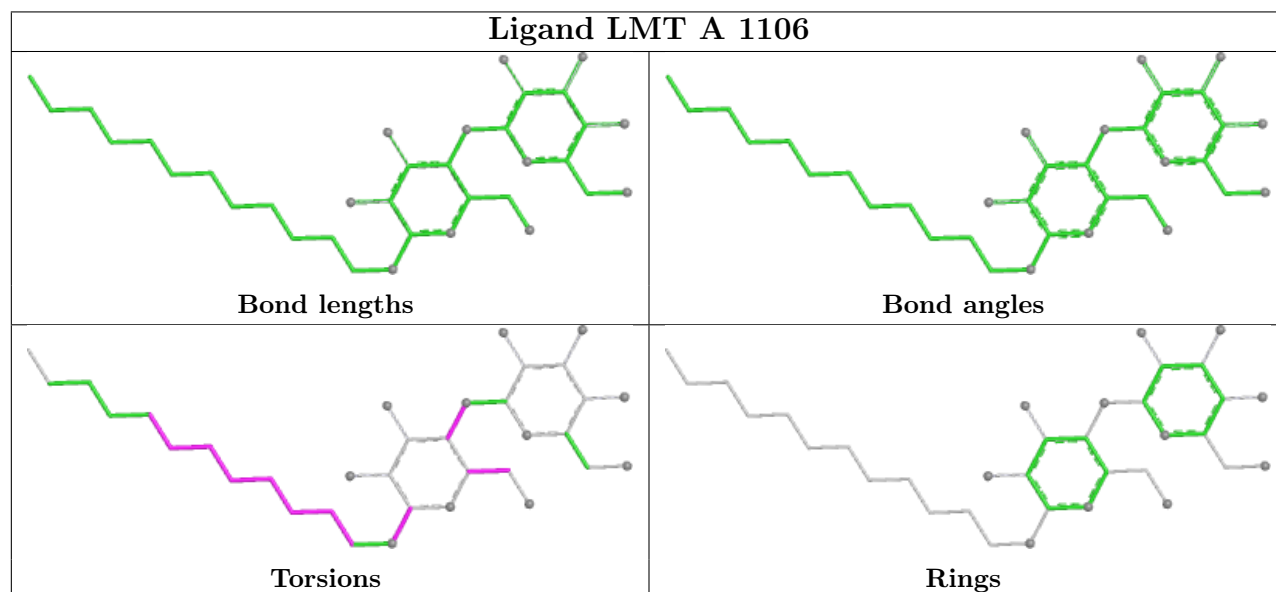
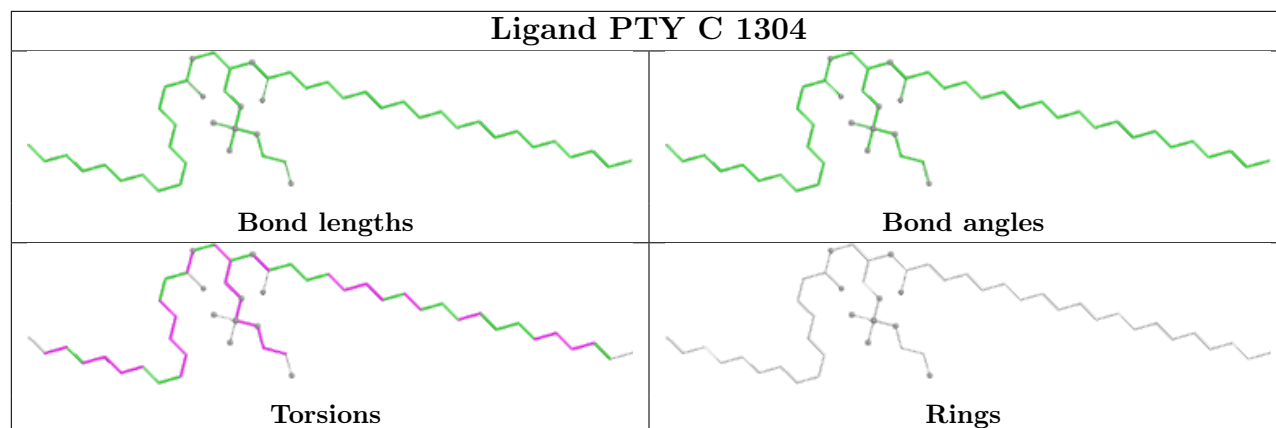
1 monomer is involved in 5 short contacts:

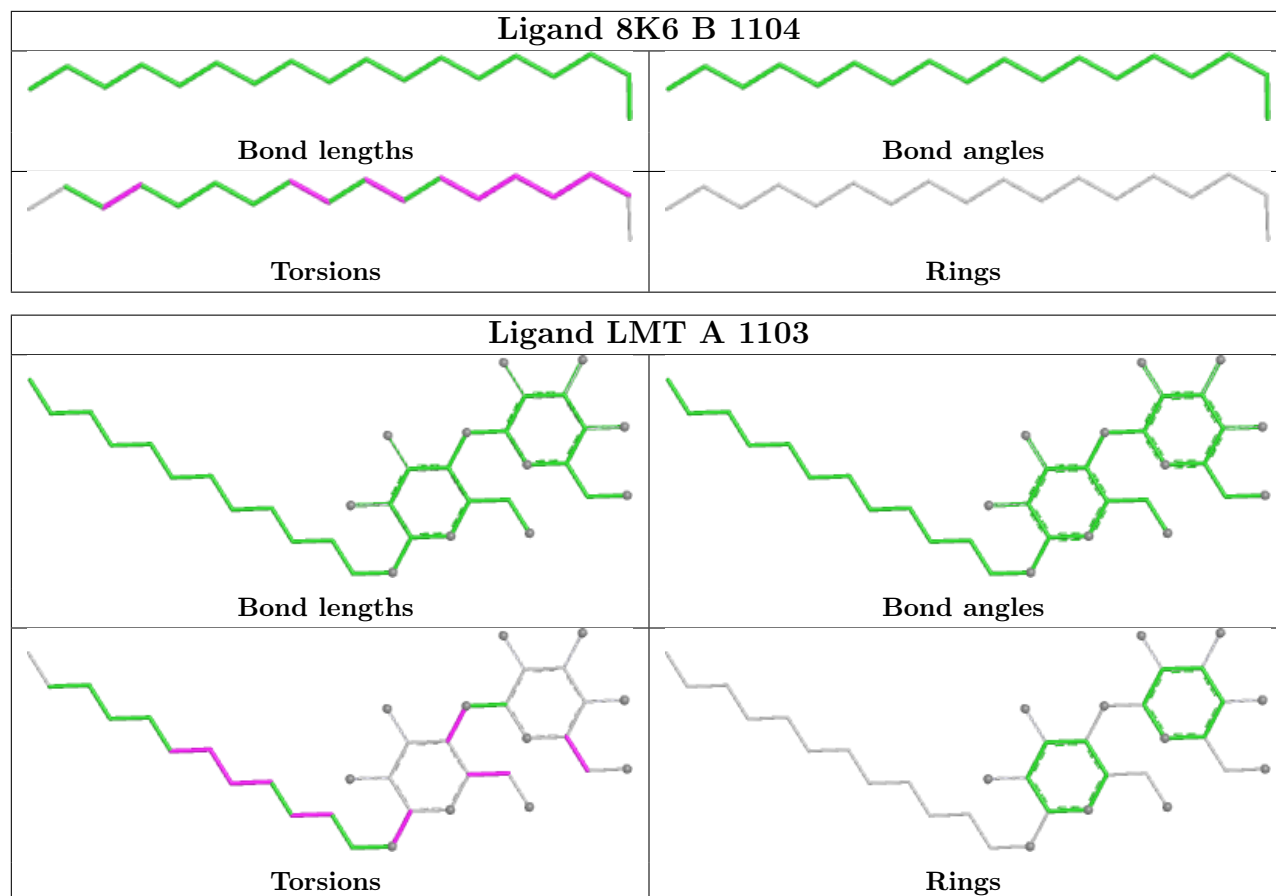
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1105	MIY	5	0

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%)	0.68	80 (7%)	19 19	24, 67, 108, 151	2 (0%)
1	B	1034/1057 (97%)	0.60	67 (6%)	25 24	30, 64, 88, 101	2 (0%)
1	C	1034/1057 (97%)	0.41	38 (3%)	45 42	32, 59, 82, 98	2 (0%)
2	D	157/169 (92%)	0.56	6 (3%)	44 41	55, 66, 89, 105	0
2	E	154/169 (91%)	0.86	8 (5%)	33 32	58, 75, 100, 106	0
All	All	3413/3509 (97%)	0.58	199 (5%)	29 29	24, 63, 96, 151	6 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	617[A]	PHE	7.2
1	A	674	LEU	7.2
1	B	617	PHE	6.9
1	B	618	ALA	6.8
1	A	670	ALA	6.4
1	A	672	VAL	6.4
1	A	676	THR	6.2
1	A	673	GLU	5.9
1	A	677	ALA	5.6
1	C	811	TYR	5.3
1	B	134	SER	5.2
1	A	668	LEU	5.1
1	B	628	PHE	4.8
1	B	133	SER	4.7
1	A	675	GLY	4.6
1	B	868	LEU	4.6
1	B	615	PHE	4.6
1	C	671	THR	4.4
1	C	673	GLU	4.3
1	B	662	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	664	PHE	4.1
1	A	868	LEU	4.1
1	A	538	THR	4.0
1	A	565	PRO	4.0
1	A	918	PHE	4.0
1	A	968	VAL	3.9
1	A	617	PHE	3.9
2	D	167	LYS	3.9
1	B	573	MET	3.9
1	A	678	THR	3.8
1	B	853[A]	THR	3.8
1	A	980	LEU	3.7
2	D	24	ALA	3.7
1	C	362	PHE	3.7
1	A	987	MET	3.7
1	B	678	THR	3.7
2	E	35	ALA	3.7
1	B	619	GLY	3.7
1	A	982	PHE	3.7
1	A	362	PHE	3.6
1	A	719	ASN	3.6
1	A	510	LYS	3.6
1	A	37	THR	3.6
1	B	671	THR	3.6
1	C	853	THR	3.5
1	C	674	LEU	3.5
1	A	575	MET	3.5
1	B	132	SER	3.4
1	C	675	GLY	3.4
1	B	606	VAL	3.4
1	A	511	GLY	3.4
1	C	618	ALA	3.4
1	B	575	MET	3.3
1	A	866	GLU	3.3
1	B	577	GLN	3.2
1	A	877	TYR	3.2
1	A	983	ILE	3.2
1	B	136	PHE	3.2
1	B	620	ARG	3.2
1	B	677	ALA	3.2
1	B	178	PHE	3.2
2	E	68	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	407	ASP	3.1
1	C	691	GLY	3.1
1	B	408	ASP	3.0
1	A	865	GLN	3.0
1	B	659	LYS	3.0
1	B	616	GLY	3.0
1	A	948	PHE	3.0
1	C	701	GLN	2.9
1	C	575	MET	2.9
1	A	971	ARG	2.9
1	B	173	GLY	2.9
1	A	38	PHE	2.9
1	C	70[A]	ASN	2.9
1	B	674	LEU	2.9
1	C	620	ARG	2.8
1	B	831	ALA	2.8
1	C	124	GLN	2.8
1	B	676	THR	2.8
1	B	623	ASN	2.7
1	B	1015	THR	2.7
2	E	33	LEU	2.7
1	B	135	SER	2.7
1	B	666	PHE	2.7
1	B	120	GLN	2.7
1	C	698	ALA	2.7
1	B	508	GLY	2.6
1	B	705	GLU	2.6
1	A	411	VAL	2.6
1	A	1034	SER	2.6
1	A	512	PHE	2.6
1	A	1008	MET	2.6
1	C	972	LEU	2.6
1	A	956	GLU	2.6
1	A	681	ASP	2.6
1	C	619	GLY	2.6
1	A	495	THR	2.6
1	C	730	ASP	2.6
1	A	571	VAL	2.6
1	A	415	ASN	2.6
1	C	267	LYS	2.5
1	B	673	GLU	2.5
1	A	981	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	654	ALA	2.5
1	A	192	GLU	2.5
1	A	669	PRO	2.5
1	B	38	PHE	2.5
1	B	478	MET	2.5
1	B	174	ASP	2.5
1	A	413	VAL	2.5
1	A	663	VAL	2.5
1	A	618	ALA	2.5
1	B	332	PHE	2.5
1	B	624	THR	2.5
1	A	945	ILE	2.5
1	A	662	MET	2.5
1	A	540	ARG	2.4
1	A	403	GLY	2.4
1	B	635	ALA	2.4
1	B	720	GLY	2.4
1	C	854	GLY	2.4
1	B	569	GLN	2.4
1	A	1028	VAL	2.4
1	B	89	GLN	2.4
2	E	131	VAL	2.4
1	A	960	LEU	2.3
1	C	337	ILE	2.3
1	B	463	THR	2.3
1	B	574	THR	2.3
1	C	669	PRO	2.3
1	C	151	GLN	2.3
1	C	458	PHE	2.3
1	A	148	THR	2.3
1	B	621	GLY	2.3
1	B	649	MET	2.3
2	E	34	MET	2.3
1	C	152	GLU	2.3
1	A	537	SER	2.3
1	C	407	ASP	2.3
2	E	32	ILE	2.3
1	B	987	MET	2.3
1	A	462	SER	2.3
1	B	1009	GLY	2.3
1	A	952	LEU	2.3
1	A	556	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	660	ASP	2.2
1	B	1034	SER	2.2
1	A	957	GLY	2.2
1	B	563	PHE	2.2
1	C	918	PHE	2.2
1	B	866	GLU	2.2
2	D	26	ARG	2.2
1	A	146	ASP	2.2
1	C	1034	SER	2.2
1	B	629	VAL	2.2
1	A	418	ARG	2.2
1	A	833	PRO	2.2
1	A	539	GLY	2.2
1	B	675	GLY	2.2
1	A	543	VAL	2.2
1	A	862	MET	2.2
1	B	862	MET	2.2
2	D	40	VAL	2.2
1	A	915	ALA	2.2
1	A	671	THR	2.2
1	C	676	THR	2.2
1	A	509	LYS	2.2
1	B	631	LEU	2.2
1	C	508	GLY	2.2
2	E	166	GLN	2.1
2	D	25	GLY	2.1
1	A	406	VAL	2.1
1	A	660	ASP	2.1
1	C	670	ALA	2.1
1	C	693	GLU	2.1
1	A	1023	PRO	2.1
1	A	563	PHE	2.1
1	A	665	ALA	2.1
2	D	61	GLU	2.1
1	A	620	ARG	2.1
1	C	498	LYS	2.1
1	B	366	LEU	2.1
1	A	1022	VAL	2.1
1	B	571	VAL	2.1
1	B	664	PHE	2.1
2	E	14	LEU	2.1
1	A	338	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	362	PHE	2.1
1	A	873	ALA	2.0
1	B	665	ALA	2.0
1	C	507	GLU	2.0
1	A	955	LYS	2.0
1	C	502	LYS	2.0
1	A	505	HIS	2.0
1	B	655	PHE	2.0
1	A	369	THR	2.0
1	C	497	LEU	2.0
1	C	700	ASN	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(Å ²)	Q<0.9
10	GOL	C	1310	6/6	0.43	0.22	77,77,78,78	0
10	GOL	C	1309	6/6	0.70	0.25	82,82,83,83	0
8	8K6	B	1104	18/18	0.73	0.43	85,90,91,91	0
10	GOL	C	1308	6/6	0.73	0.20	81,82,82,82	0
16	DDQ	C	1311	14/14	0.74	0.29	70,70,70,70	0
5	EDO	E	201	4/4	0.77	0.29	82,82,82,82	0
5	EDO	C	1306	4/4	0.77	0.20	49,49,49,50	0
15	C14	C	1305	14/14	0.78	0.36	70,73,76,76	0
5	EDO	A	1104	4/4	0.78	0.20	63,63,64,64	0
5	EDO	C	1307	4/4	0.79	0.24	67,68,68,68	0
3	LMT	A	1105	35/35	0.79	0.21	89,117,121,122	0
5	EDO	B	1108	4/4	0.80	0.23	59,59,59,59	0

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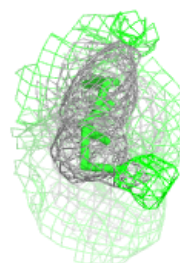
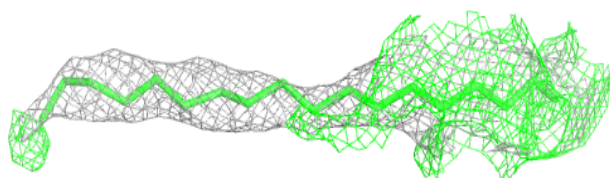
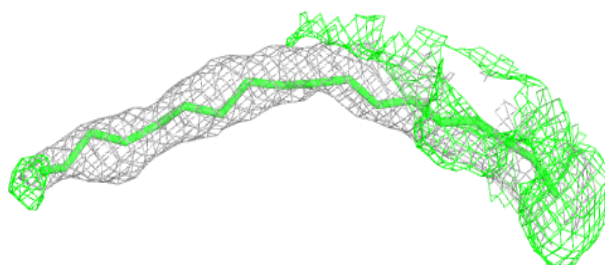
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	SO4	B	1109	5/5	0.80	0.16	120,121,121,121	0
13	D12	C	1301	12/12	0.81	0.36	81,83,84,85	0
11	OCT	B	1107	8/8	0.81	0.34	77,78,78,78	0
3	LMT	A	1101	35/35	0.81	0.19	121,123,125,125	0
9	MIY	B	1105	33/33	0.83	0.18	88,89,90,90	0
4	D10	A	1102	10/10	0.84	0.29	80,81,82,82	0
14	PTY	C	1304	50/50	0.85	0.26	93,97,102,103	0
3	LMT	A	1103	35/35	0.85	0.19	95,110,121,121	0
3	LMT	A	1106	35/35	0.85	0.18	92,101,112,112	0
7	MYS	B	1103	15/15	0.86	0.28	84,85,86,86	0
3	LMT	B	1101	35/35	0.86	0.19	94,98,113,113	0
10	GOL	D	201	6/6	0.86	0.22	88,88,89,89	0
5	EDO	E	202	4/4	0.87	0.19	61,61,61,61	0
12	SO4	B	1110	5/5	0.87	0.14	105,106,106,106	0
4	D10	C	1303	10/10	0.89	0.28	77,79,81,81	0
10	GOL	B	1106	6/6	0.92	0.14	65,65,66,66	0
6	DDR	B	1102	28/28	0.92	0.20	86,90,94,94	0
3	LMT	C	1302	35/35	0.93	0.13	75,79,90,90	0
12	SO4	C	1312	5/5	0.93	0.12	87,87,87,87	0

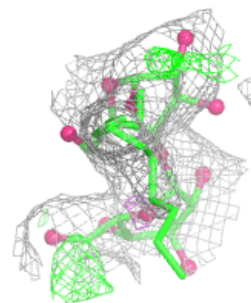
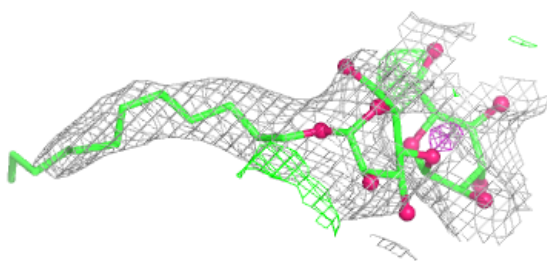
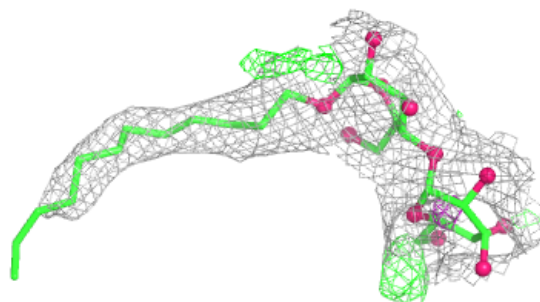
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8K6 B 1104:

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

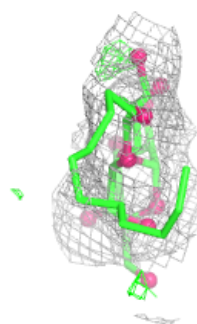
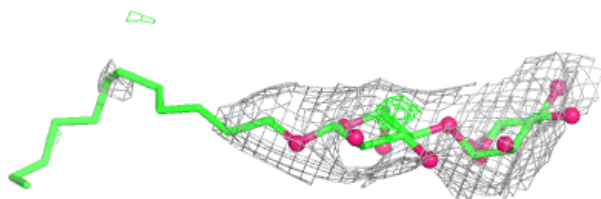
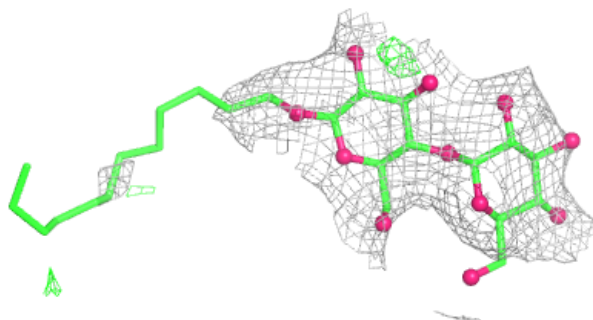
**Electron density around LMT A 1105:**

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

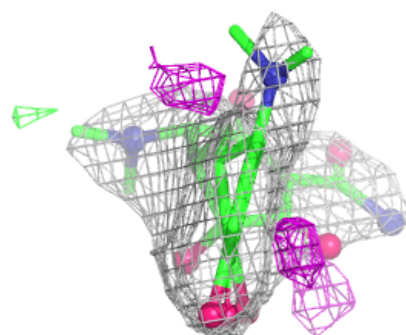
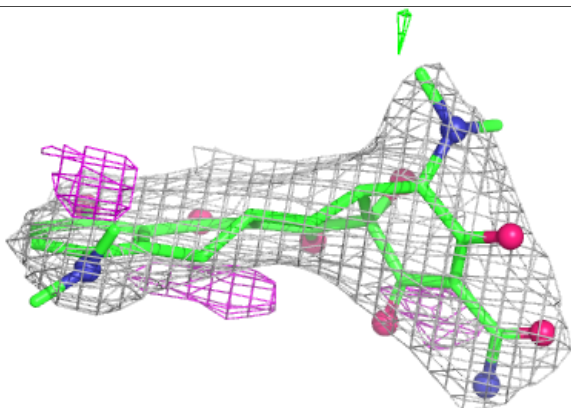
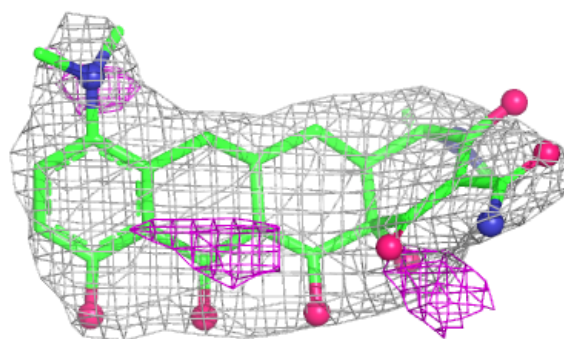


Electron density around LMT A 1101:

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

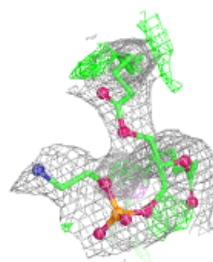
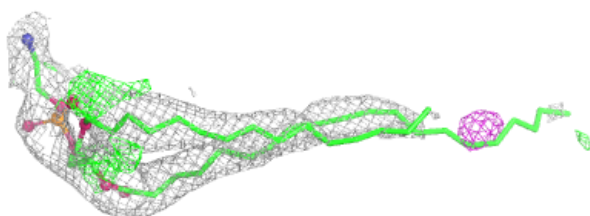
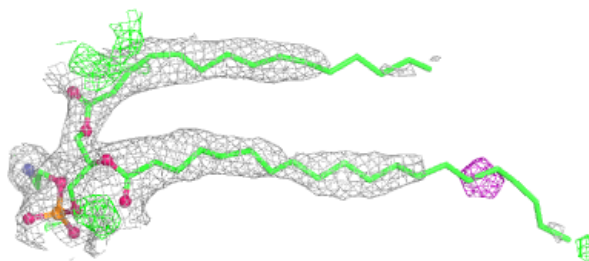
**Electron density around MIY B 1105:**

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

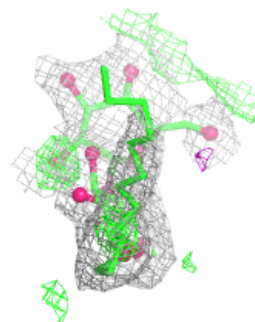
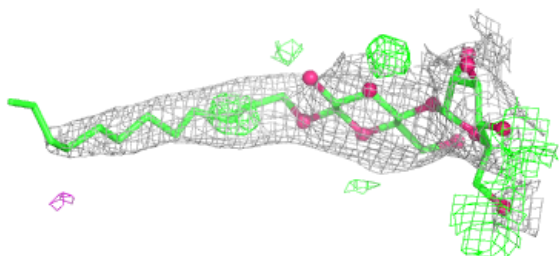
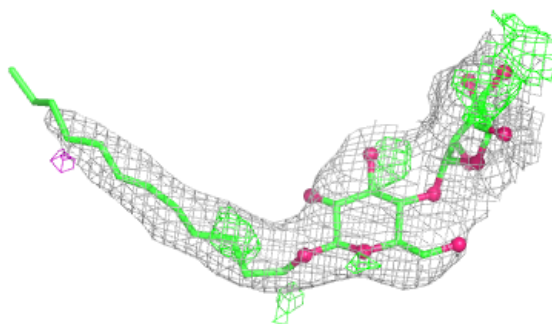


Electron density around PTY C 1304:

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

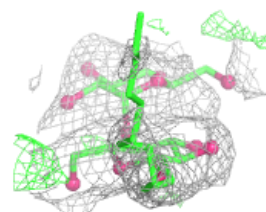
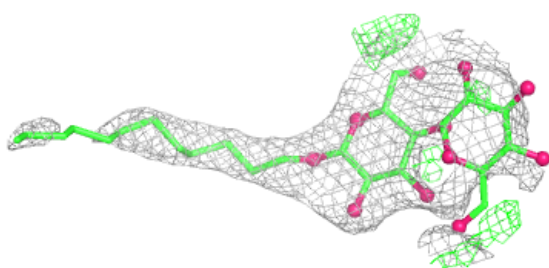
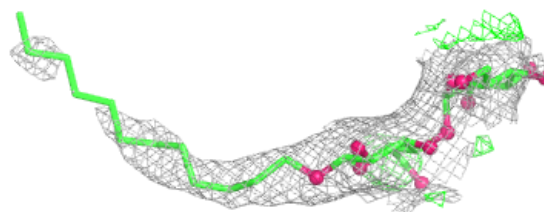
**Electron density around LMT A 1103:**

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

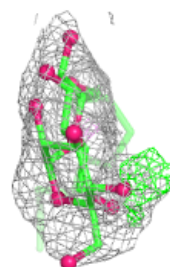
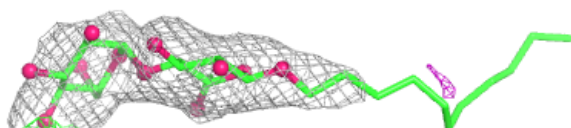
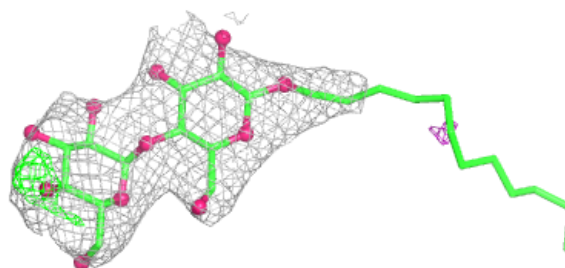


Electron density around LMT A 1106:

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

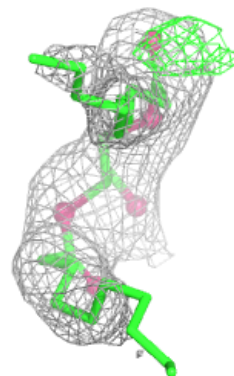
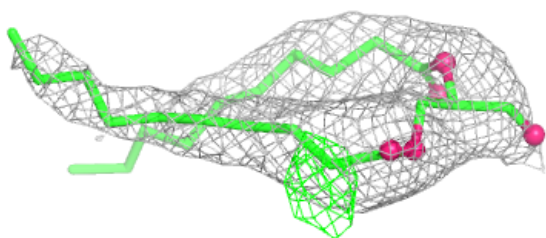
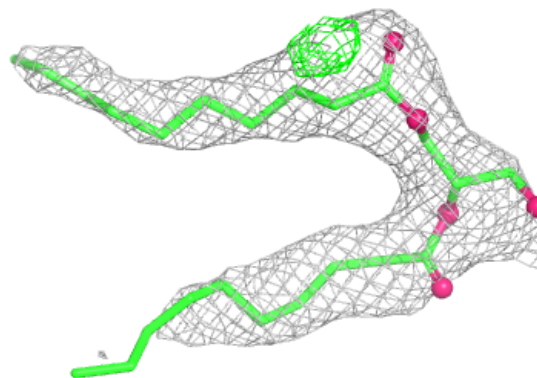
**Electron density around LMT B 1101:**

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

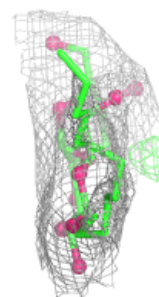
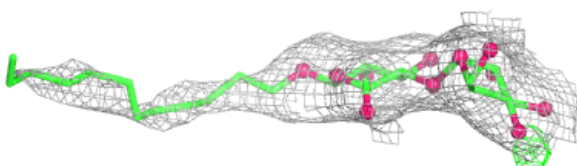
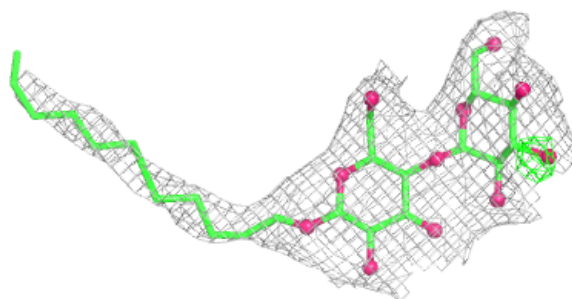


Electron density around DDR B 1102:

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

**Electron density around LMT C 1302:**

$2mF_o-DF_c$ (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.