



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:24 AM UTC

PDB ID : 9HAO / pdb_00009hao
Title : BDM91531 inhibitor bound to the transmembrane domain of AcrB
Authors : Mueller, R.T.; Herrmann, A.; Pos, K.M.
Deposited on : 2024-11-04
Resolution : 1.94 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

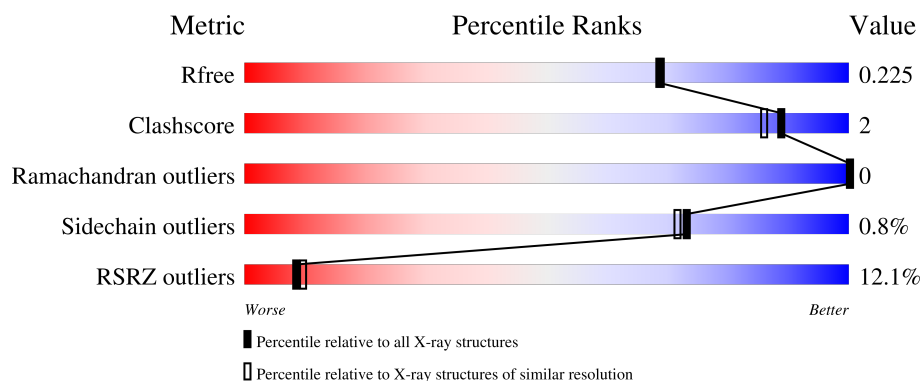
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	
1	B	1057	
1	C	1057	
2	D	169	
2	E	169	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 56249 atoms, of which 27795 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	1031	Total	C	H	N	O	S	0	2	0
			15866	5055	8012	1295	1459	45			
1	B	1034	Total	C	H	N	O	S	0	2	0
			15880	5060	8017	1297	1461	45			
1	C	1034	Total	C	H	N	O	S	0	2	0
			15907	5066	8033	1303	1461	44			

There are 24 discrepancies between the modelled and reference sequences:

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

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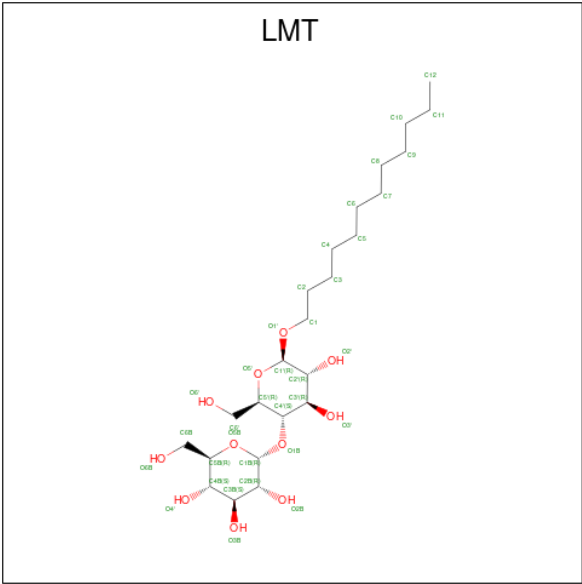
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	155	Total	C	H	N	O	S	0	0	0
			2329	739	1156	205	228	1			
2	E	153	Total	C	H	N	O	S	0	0	0
			2306	732	1147	203	223	1			

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



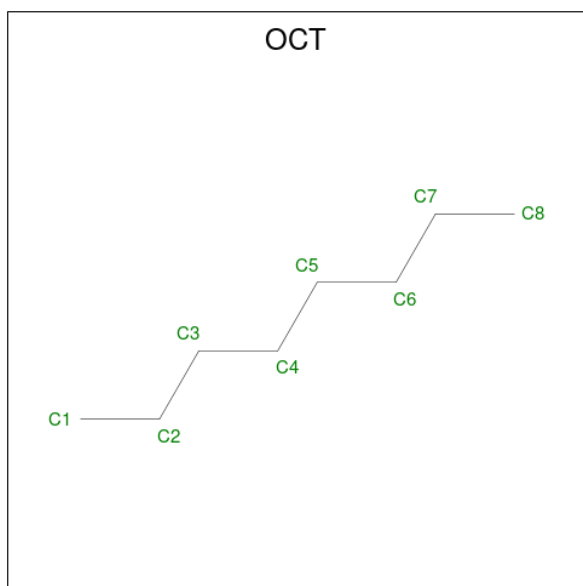
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	O		0	0
			81	24	46	11			
3	A	1	Total	C	H	O		0	0
			81	24	46	11			
3	A	1	Total	C	H	O		0	0
			81	24	46	11			
3	B	1	Total	C	H	O		0	0
			81	24	46	11			
3	B	1	Total	C	H	O		0	0
			81	24	46	11			
3	B	1	Total	C	H	O		0	0
			81	24	46	11			
3	C	1	Total	C	H	O		0	0
			81	24	46	11			

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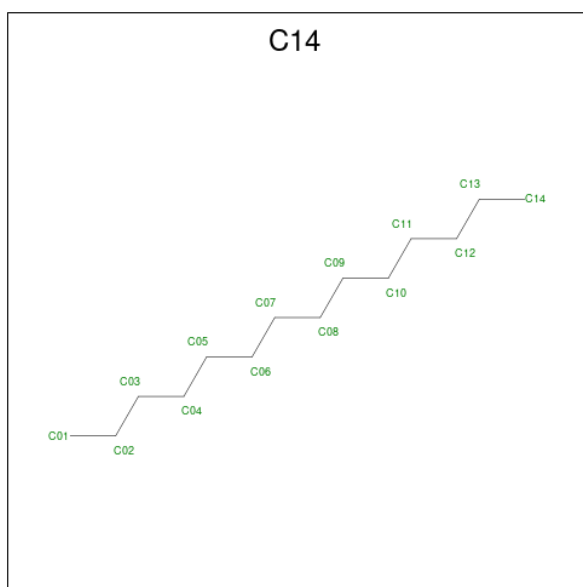
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 4 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	H	0	0
			26	8	18		
4	A	1	Total	C	H	0	0
			26	8	18		
4	B	1	Total	C	H	0	0
			26	8	18		
4	C	1	Total	C	H	0	0
			26	8	18		
4	C	1	Total	C	H	0	0
			26	8	18		
4	C	1	Total	C	H	0	0
			26	8	18		
4	C	1	Total	C	H	0	0
			26	8	18		

- Molecule 5 is TETRADECANE (CCD ID: C14) (formula: C₁₄H₃₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	H	0	0
			44	14	30		
5	C	1	Total	C	H	0	0
			44	14	30		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



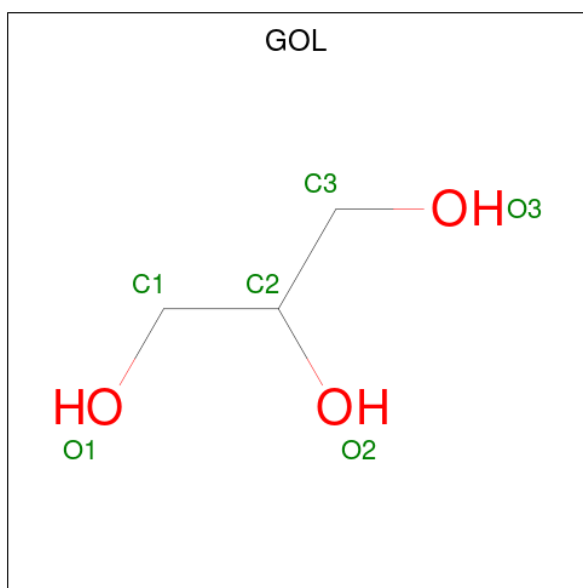
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		
6	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



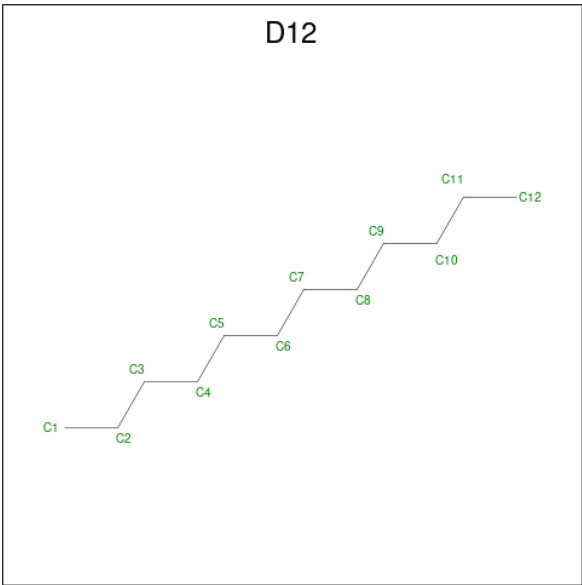
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			13	3	7	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	A	1	Total	C	H	O	0	0
			13	3	7	3		
7	A	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			13	3	7	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

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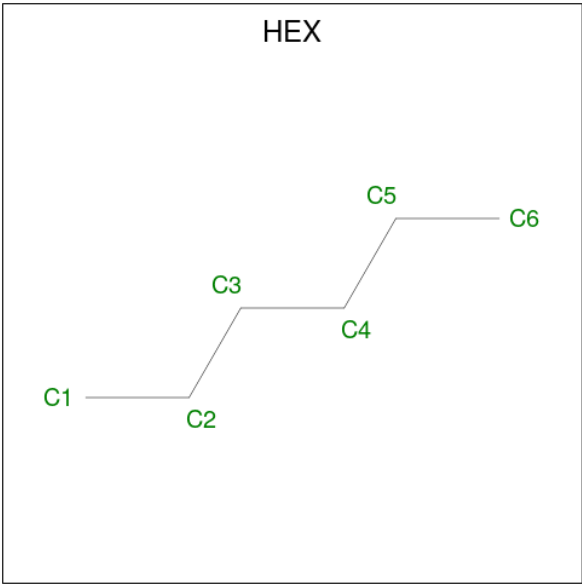
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			13	3	7	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	C	1	Total	C	H	O	0	0
			14	3	8	3		
7	D	1	Total	C	H	O	0	0
			13	3	7	3		
7	D	1	Total	C	H	O	0	0
			14	3	8	3		
7	D	1	Total	C	H	O	0	0
			14	3	8	3		
7	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆).



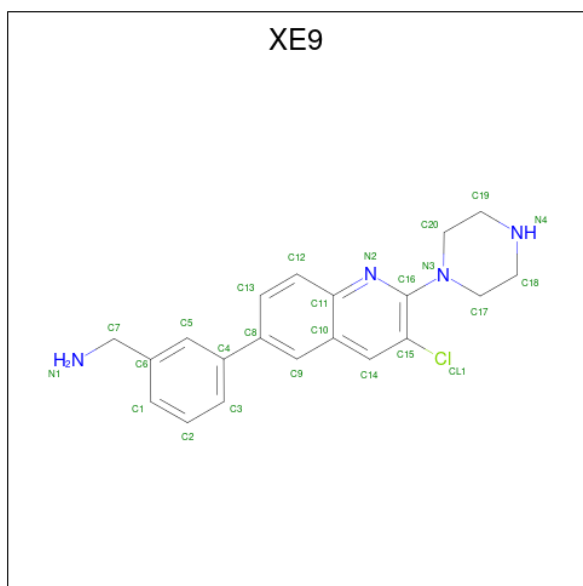
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	H	0	0
			38	12	26		
8	A	1	Total	C	H	0	0
			38	12	26		
8	B	1	Total	C	H	0	0
			38	12	26		
8	B	1	Total	C	H	0	0
			38	12	26		

- Molecule 9 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



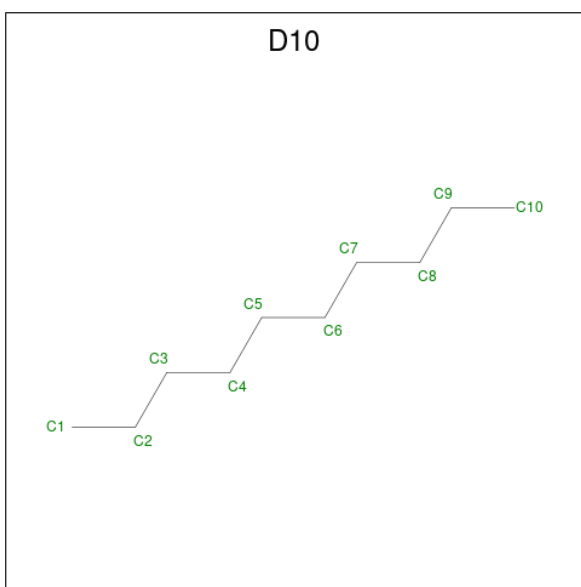
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	H	0	0
			20	6	14		
9	A	1	Total	C	H	0	0
			20	6	14		
9	B	1	Total	C	H	0	0
			20	6	14		
9	B	1	Total	C	H	0	0
			20	6	14		
9	B	1	Total	C	H	0	0
			20	6	14		
9	C	1	Total	C	H	0	0
			20	6	14		
9	C	1	Total	C	H	0	0
			20	6	14		
9	C	1	Total	C	H	0	0
			20	6	14		

- Molecule 10 is [3-(3-chloranyl-2-piperazin-1-yl-quinolin-6-yl)phenyl]methanamine (CCD ID: XE9) (formula: C₂₀H₂₁ClN₄) (labeled as "Ligand of Interest" by depositor).



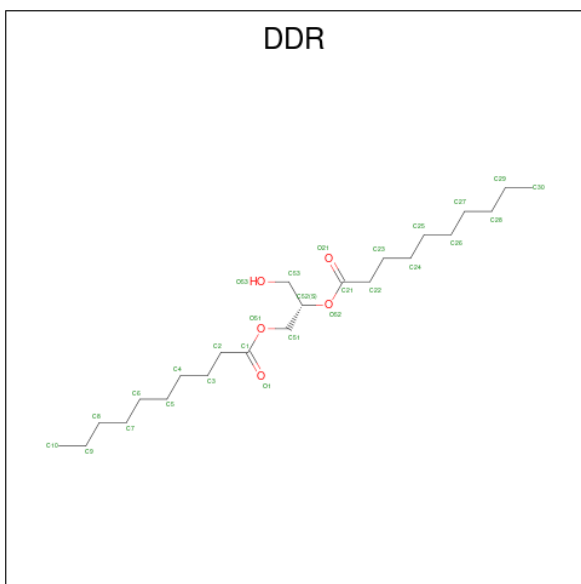
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	Cl	H	N	0
			48	20	1	23	4	0

- Molecule 11 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



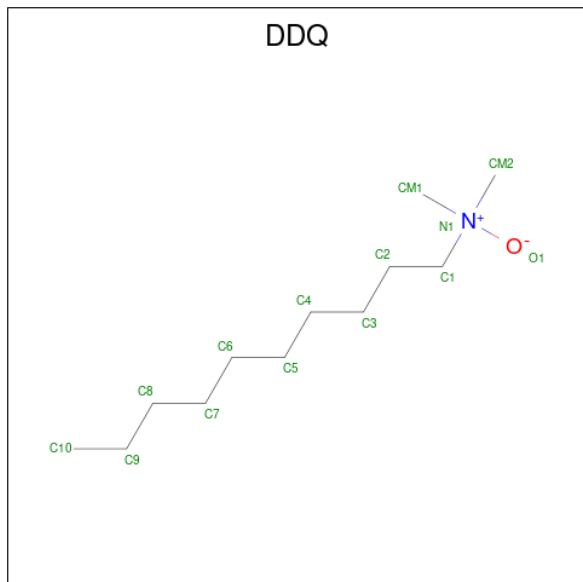
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total 32	C 10	H 22	0	0
11	B	1	Total 32	C 10	H 22	0	0

- Molecule 12 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



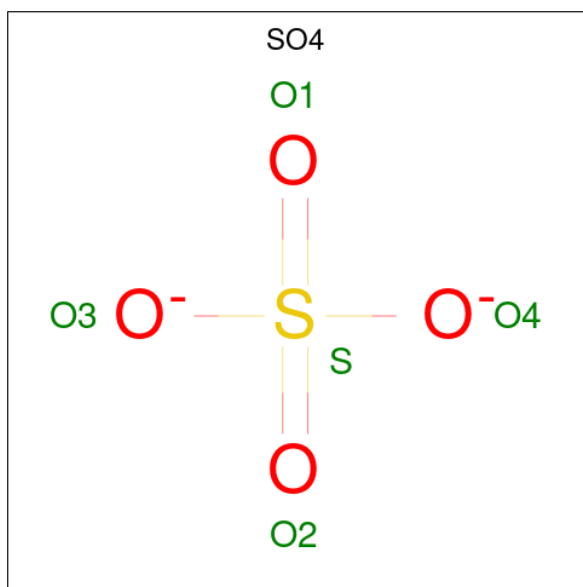
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	C	H	O	0	0
			72	23	44	5		

- Molecule 13 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



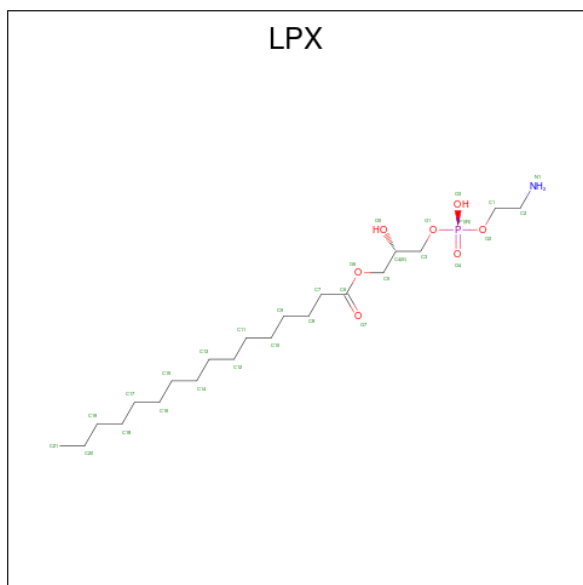
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	H	N	O	0	0
			41	12	27	1	1		
13	C	1	Total	C	H	N	O	0	0
			41	12	27	1	1		

- Molecule 14 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 15 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: C₂₁H₄₄NO₇P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C H N O P 73 21 43 1 7 1	0	0
15	C	1	Total C H N O P 73 21 43 1 7 1	0	0

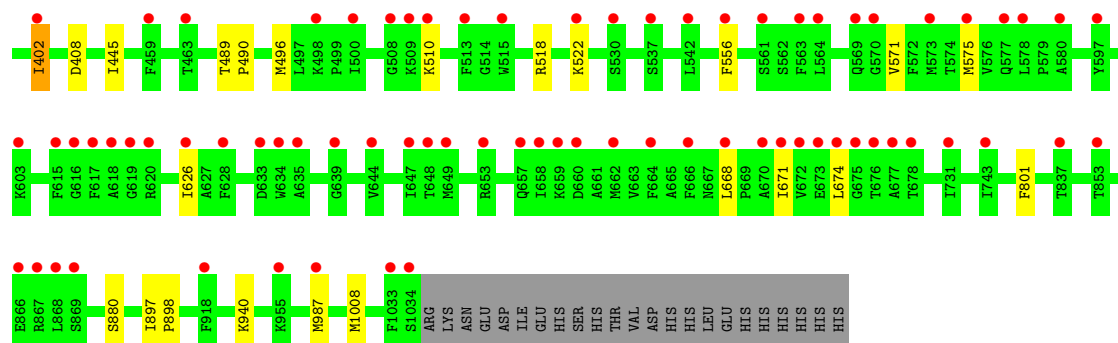
- Molecule 16 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	487	Total O 487 487	0	0
16	B	465	Total O 465 465	0	0
16	C	530	Total O 530 530	0	0
16	D	84	Total O 84 84	0	0

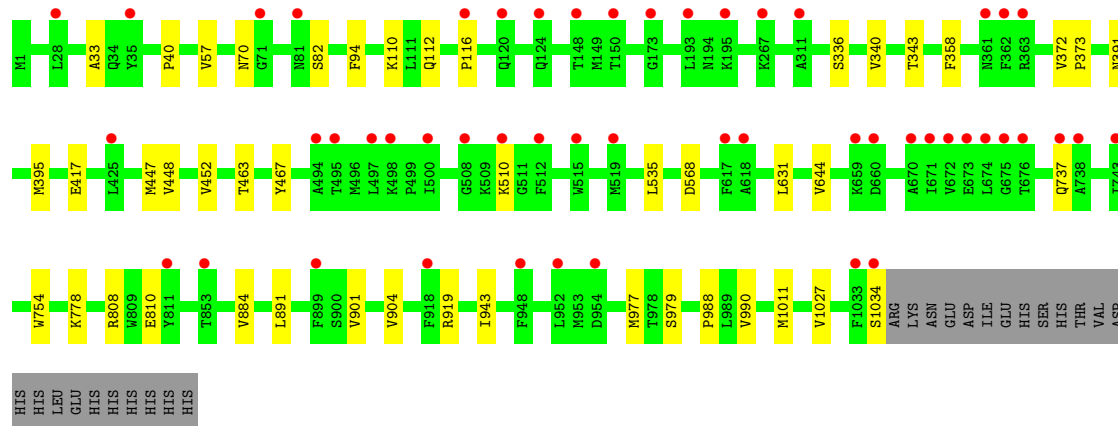
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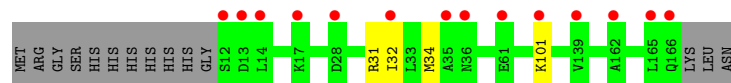
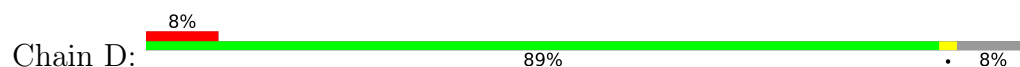
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	E	31	Total	O	0	0
			31	31		



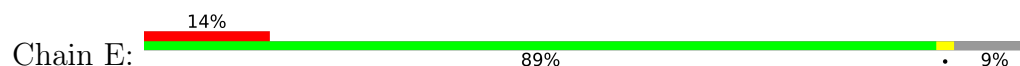
- Molecule 1: Multidrug efflux pump subunit AcrB



- 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	146.18Å 161.14Å 244.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 1.94 49.38 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.38-1.94) 99.1 (49.38-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.202 , 0.225 0.202 , 0.225	Depositor DCC
R_{free} test set	20979 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	56249	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DDQ, XE9, LPX, D12, EDO, HEX, SO4, DDR, LMT, GOL, C14, 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	0.17	0/8013	0.34	0/10880
1	B	0.16	0/8025	0.33	0/10897
1	C	0.18	0/8027	0.36	0/10900
2	D	0.15	0/1192	0.31	0/1621
2	E	0.13	0/1178	0.26	0/1602
All	All	0.17	0/26435	0.34	0/35900

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7854	8012	7997	51	0
1	B	7863	8017	8006	21	0
1	C	7874	8033	8032	27	0
2	D	1173	1156	1156	2	0
2	E	1159	1147	1147	2	0
3	A	105	138	134	0	0
3	B	105	138	136	1	0
3	C	70	92	88	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	16	36	36	0	0
4	B	8	18	18	0	0
4	C	40	90	90	0	0
5	A	14	30	30	0	0
5	C	14	30	30	0	0
6	A	4	6	6	0	0
6	B	36	54	54	0	0
6	C	16	24	24	0	0
7	A	90	118	120	1	0
7	B	48	63	64	0	0
7	C	72	95	96	0	0
7	D	24	31	32	0	0
8	A	24	52	52	0	0
8	B	24	52	52	0	0
9	A	12	28	28	0	0
9	B	18	42	42	0	0
9	C	18	42	42	0	0
10	A	25	23	0	1	0
11	A	10	22	22	0	0
11	B	10	22	22	0	0
12	B	28	44	44	0	0
13	B	14	27	27	0	0
13	C	14	27	27	0	0
14	B	5	0	0	0	0
14	C	10	0	0	0	0
15	C	60	86	86	1	0
16	A	487	0	0	2	0
16	B	465	0	0	1	0
16	C	530	0	0	2	0
16	D	84	0	0	0	0
16	E	31	0	0	0	0
All	All	28454	27795	27740	101	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 (101) 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:A:987:MET:HE3	1:A:1008:MET:HE1	1.66	0.77
1:A:555:LEU:HD22	1:A:917:THR:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:SER:HA	1:C:1011:MET:HE3	1.78	0.65
1:A:81:ASN:ND2	16:A:1204:HOH:O	2.30	0.64
1:A:538:THR:HG23	1:A:1024:VAL:HG13	1.79	0.64
1:A:538:THR:HG21	1:A:1028:VAL:CG2	2.30	0.62
1:A:443:VAL:HG12	1:A:447:MET:HE2	1.81	0.62
1:A:355:MET:HE1	1:A:410:ILE:HD11	1.82	0.60
1:A:492:LEU:HB3	1:A:496:MET:HE2	1.84	0.59
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.85	0.58
1:C:447:MET:HE1	1:C:891:LEU:HD13	1.87	0.56
1:C:901:VAL:O	1:C:904:VAL:HG12	2.05	0.56
1:C:336:SER:O	1:C:340:VAL:HG23	2.07	0.55
1:A:563:PHE:CD2	1:A:674:LEU:HD22	2.42	0.55
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.89	0.54
2:D:34:MET:HA	2:D:34:MET:HE2	1.90	0.54
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.90	0.53
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.91	0.52
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.93	0.50
1:A:703:LEU:O	16:A:1201:HOH:O	2.18	0.50
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.44	0.50
1:A:546:LEU:O	1:A:550:VAL:HG23	2.11	0.50
1:B:489:THR:HG21	16:B:1597:HOH:O	2.11	0.50
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.93	0.50
1:A:1011:MET:HA	1:A:1011:MET:HE2	1.94	0.49
1:C:448:VAL:HG11	1:C:943:ILE:HD11	1.94	0.49
1:A:676:THR:HG22	1:A:678:THR:H	1.77	0.49
1:C:452:VAL:HG12	1:C:884:VAL:HG21	1.94	0.49
2:D:31:ARG:NH2	2:D:32:ILE:HD11	2.27	0.49
1:B:21:LEU:HD21	15:C:1109:LPX:H20	1.94	0.49
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.94	0.48
1:C:395:MET:HA	1:C:395:MET:HE2	1.94	0.48
1:A:366:LEU:O	1:A:370:ILE:HG13	2.13	0.48
1:C:452:VAL:CG1	1:C:884:VAL:HG21	2.44	0.48
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.96	0.48
1:B:575:MET:HA	1:B:575:MET:HE2	1.95	0.47
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.97	0.47
1:A:547:ILE:HD12	1:A:548:ILE:N	2.30	0.47
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.97	0.47
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.49	0.47
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.45	0.47
1:A:563:PHE:CE2	1:A:674:LEU:HD22	2.50	0.47
1:B:518:ARG:O	1:B:522:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:778:LYS:NZ	16:C:1226:HOH:O	2.47	0.46
1:A:868:LEU:HD23	1:A:869:SER:N	2.31	0.46
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	1.98	0.46
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.51	0.46
1:A:873:ALA:N	1:A:874:PRO:HD2	2.31	0.45
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.46	0.45
1:A:343:THR:HG21	1:A:1000:GLN:OE1	2.17	0.45
1:A:956:GLU:N	1:A:956:GLU:OE1	2.50	0.45
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.16	0.45
1:A:50:PRO:HB3	7:A:1115:GOL:H31	1.99	0.45
1:A:559:LEU:HD23	1:A:923:ASN:HB2	1.98	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.17	0.45
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.99	0.44
1:B:344:LEU:CD2	1:B:402:ILE:HD11	2.47	0.44
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.44
1:C:57:VAL:HG13	1:C:82:SER:HB3	2.00	0.44
1:A:580:ALA:HB3	1:A:724:THR:HG21	2.00	0.44
1:A:309:GLU:HG3	1:A:313:MET:HE3	2.00	0.43
1:A:583:THR:OG1	1:A:586:ARG:HG3	2.18	0.43
1:A:408:ASP:OD1	10:A:1122:XE9:N4	2.51	0.43
1:A:468:ARG:O	1:A:472:ILE:HG12	2.18	0.43
1:A:555:LEU:CD1	1:A:914:LEU:HD12	2.48	0.43
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.99	0.43
1:B:575:MET:HE2	1:B:626:ILE:HD13	2.00	0.43
1:B:897:ILE:N	1:B:898:PRO:CD	2.81	0.43
1:B:165:ALA:HB3	1:B:313:MET:CE	2.49	0.43
1:A:284:GLN:HG3	1:A:285:PRO:HD2	1.99	0.43
1:A:547:ILE:HD12	1:A:547:ILE:C	2.43	0.43
1:A:937:LEU:HB3	1:A:1011:MET:HE3	2.00	0.43
1:C:70:ASN:HB2	16:C:1394:HOH:O	2.18	0.43
1:A:667:ASN:OD1	1:A:668:LEU:N	2.51	0.43
1:B:671:ILE:HG22	1:B:674:LEU:H	1.83	0.43
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.43
1:C:40:PRO:HB2	1:C:94:PHE:O	2.19	0.43
1:A:277:ILE:HD11	1:A:620:ARG:HD3	2.01	0.42
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.48	0.42
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.00	0.42
1:B:44:THR:OG1	1:B:132:SER:OG	2.29	0.42
1:A:538:THR:HG21	1:A:1028:VAL:HG21	2.01	0.42
1:A:567:GLU:OE2	1:A:999:ALA:N	2.52	0.42
1:B:363:ARG:HD3	1:B:496:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:919:ARG:NH1	1:C:990:VAL:O	2.51	0.41
1:B:571:VAL:HG23	1:B:668:LEU:HD11	2.03	0.41
1:A:491:ALA:O	1:A:495:THR:HG23	2.20	0.41
1:A:904:VAL:HG21	1:A:942:ALA:HB2	2.02	0.41
3:B:1209:LMT:O1B	3:B:1209:LMT:O6'	2.31	0.41
1:A:442:LEU:HD23	1:A:482:VAL:HG22	2.03	0.41
1:A:987:MET:CE	1:A:1008:MET:HE1	2.43	0.41
2:E:30:VAL:HG12	2:E:34:MET:HE2	2.01	0.41
1:C:70:ASN:O	1:C:110:LYS:CE	2.69	0.41
1:C:358:PHE:CG	1:C:977:MET:HG2	2.57	0.40
2:E:34:MET:HE1	2:E:65:VAL:HG12	2.03	0.40
1:A:135:SER:O	1:A:292:LYS:HD3	2.21	0.40
1:A:845:GLU:OE2	1:A:867:ARG:NH1	2.55	0.40
1:C:70:ASN:O	1:C:110:LYS:HE3	2.21	0.40
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.46	0.40
1:A:1031:ARG:NH1	1:A:1039:ASP:OD1	2.55	0.40
1:B:571:VAL:HG23	1:B:668:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1029/1057 (97%)	1005 (98%)	24 (2%)	0	100	100
1	B	1034/1057 (98%)	1015 (98%)	19 (2%)	0	100	100
1	C	1034/1057 (98%)	1016 (98%)	18 (2%)	0	100	100
2	D	153/169 (90%)	152 (99%)	1 (1%)	0	100	100
2	E	151/169 (89%)	149 (99%)	2 (1%)	0	100	100
All	All	3401/3509 (97%)	3337 (98%)	64 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	843/863 (98%)	835 (99%)	8 (1%)	70	67
1	B	842/863 (98%)	833 (99%)	9 (1%)	65	60
1	C	842/863 (98%)	838 (100%)	4 (0%)	81	82
2	D	120/132 (91%)	119 (99%)	1 (1%)	73	71
2	E	118/132 (89%)	118 (100%)	0	100	100
All	All	2765/2853 (97%)	2743 (99%)	22 (1%)	73	71

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	VAL
1	A	355	MET
1	A	393	LEU
1	A	510	LYS
1	A	649[A]	MET
1	A	649[B]	MET
1	A	914	LEU
1	A	1011	MET
1	B	81	ASN
1	B	88	VAL
1	B	314	GLU
1	B	383	LEU
1	B	402	ILE
1	B	510	LYS
1	B	556	PHE
1	B	801	PHE
1	B	880	SER
1	C	417	GLU
1	C	510	LYS
1	C	737	GLN
1	C	1034	SER

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Mol	Chain	Res	Type
2	D	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	89	GLN
1	A	112	GLN
1	A	151	GLN
1	A	194	ASN
1	A	360	GLN
1	A	415	ASN
1	A	437	GLN
1	A	517	ASN
1	A	1001	ASN
1	B	70	ASN
1	B	161	ASN
1	B	469	GLN
1	B	569	GLN
1	B	577	GLN
1	B	584	GLN
1	B	1000	GLN
1	C	81	ASN
1	C	89	GLN
1	C	505	HIS
1	C	596	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

94 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	1108	-	5,5,5	0.98	0	5,5,5	0.97	0
7	GOL	C	1104	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)
7	GOL	C	1127	-	5,5,5	0.85	0	5,5,5	1.15	1 (20%)
7	GOL	A	1116	-	5,5,5	0.80	0	5,5,5	1.01	0
6	EDO	B	1226	-	3,3,3	0.51	0	2,2,2	0.33	0
11	D10	B	1204	-	9,9,9	0.27	0	8,8,8	0.12	0
7	GOL	C	1118	-	5,5,5	0.86	0	5,5,5	1.10	0
3	LMT	B	1202	-	36,36,36	1.06	4 (11%)	47,47,47	0.93	1 (2%)
7	GOL	C	1126	-	5,5,5	0.99	0	5,5,5	1.05	0
8	D12	B	1221	-	11,11,11	0.26	0	10,10,10	0.15	0
7	GOL	A	1125	-	5,5,5	0.83	0	5,5,5	1.13	0
7	GOL	C	1125	-	5,5,5	0.95	0	5,5,5	1.00	0
6	EDO	B	1212	-	3,3,3	0.43	0	2,2,2	0.34	0
7	GOL	B	1219	-	5,5,5	0.94	0	5,5,5	0.95	0
6	EDO	A	1106	-	3,3,3	0.43	0	2,2,2	0.40	0
7	GOL	D	203	-	5,5,5	0.87	0	5,5,5	1.06	0
7	GOL	C	1120	-	5,5,5	0.91	0	5,5,5	1.12	0
7	GOL	A	1111	-	5,5,5	0.91	0	5,5,5	1.04	0
7	GOL	A	1121	-	5,5,5	0.96	0	5,5,5	1.05	0
14	SO4	C	1121	-	4,4,4	0.23	0	6,6,6	0.14	0
8	D12	B	1222	-	11,11,11	0.29	0	10,10,10	0.18	0
6	EDO	C	1112	-	3,3,3	0.38	0	2,2,2	0.52	0
6	EDO	C	1113	-	3,3,3	0.41	0	2,2,2	0.43	0
8	D12	A	1120	-	11,11,11	0.28	0	10,10,10	0.13	0
7	GOL	D	201	-	5,5,5	0.86	0	5,5,5	1.03	0
7	GOL	A	1126	-	5,5,5	0.99	0	5,5,5	0.99	0
4	OCT	C	1116	-	7,7,7	0.26	0	6,6,6	0.20	0
7	GOL	A	1112	-	5,5,5	0.95	0	5,5,5	1.02	0
4	OCT	A	1107	-	7,7,7	0.28	0	6,6,6	0.19	0
7	GOL	C	1124	-	5,5,5	0.92	0	5,5,5	0.99	0
7	GOL	A	1110	-	5,5,5	0.98	0	5,5,5	1.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	B	1217	-	5,5,5	1.13	0	5,5,5	0.69	0
13	DDQ	B	1214	-	11,13,13	0.78	1 (9%)	12,15,15	0.30	0
12	DDR	B	1207	-	27,27,27	0.37	0	29,29,29	0.44	0
6	EDO	C	1101	-	3,3,3	0.44	0	2,2,2	0.35	0
7	GOL	B	1211	-	5,5,5	1.04	0	5,5,5	0.97	0
3	LMT	C	1105	-	36,36,36	1.14	5 (13%)	47,47,47	0.94	2 (4%)
9	HEX	C	1128	-	5,5,5	0.29	0	4,4,4	0.15	0
7	GOL	B	1210	-	5,5,5	0.96	0	5,5,5	1.11	0
4	OCT	C	1132	-	7,7,7	0.29	0	6,6,6	0.10	0
6	EDO	B	1206	-	3,3,3	0.46	0	2,2,2	0.30	0
5	C14	A	1104	-	13,13,13	0.27	0	12,12,12	0.14	0
15	LPX	C	1109	-	29,29,29	0.92	2 (6%)	31,33,33	0.84	1 (3%)
7	GOL	D	202	-	5,5,5	0.84	0	5,5,5	1.14	1 (20%)
9	HEX	C	1129	-	5,5,5	0.29	0	4,4,4	0.14	0
7	GOL	A	1117	-	5,5,5	1.06	0	5,5,5	0.82	0
6	EDO	B	1205	-	3,3,3	0.47	0	2,2,2	0.34	0
6	EDO	B	1225	-	3,3,3	0.39	0	2,2,2	0.39	0
7	GOL	B	1216	-	5,5,5	0.92	0	5,5,5	0.94	0
14	SO4	B	1215	-	4,4,4	0.23	0	6,6,6	0.15	0
7	GOL	A	1109	-	5,5,5	0.97	0	5,5,5	0.96	0
9	HEX	A	1119	-	5,5,5	0.28	0	4,4,4	0.15	0
7	GOL	D	204	-	5,5,5	0.90	0	5,5,5	1.11	0
6	EDO	C	1114	-	3,3,3	0.50	0	2,2,2	0.21	0
15	LPX	C	1107	-	29,29,29	0.91	2 (6%)	31,33,33	0.87	1 (3%)
7	GOL	C	1123	-	5,5,5	0.85	0	5,5,5	0.96	0
7	GOL	C	1131	-	5,5,5	0.95	0	5,5,5	1.07	0
3	LMT	B	1209	-	36,36,36	1.05	4 (11%)	47,47,47	1.13	3 (6%)
3	LMT	A	1101	-	36,36,36	1.13	5 (13%)	47,47,47	0.90	3 (6%)
7	GOL	C	1117	-	5,5,5	0.90	0	5,5,5	1.05	0
4	OCT	C	1102	-	7,7,7	0.26	0	6,6,6	0.18	0
13	DDQ	C	1130	-	11,13,13	0.80	1 (9%)	12,15,15	0.44	0
7	GOL	A	1127	-	5,5,5	1.02	0	5,5,5	0.89	0
7	GOL	A	1114	-	5,5,5	0.91	0	5,5,5	1.02	0
6	EDO	B	1201	-	3,3,3	0.41	0	2,2,2	0.38	0
7	GOL	B	1208	-	5,5,5	0.97	0	5,5,5	1.09	0
10	XE9	A	1122	-	28,28,28	1.23	5 (17%)	37,39,39	0.91	1 (2%)
6	EDO	B	1227	-	3,3,3	0.44	0	2,2,2	0.39	0
6	EDO	B	1213	-	3,3,3	0.45	0	2,2,2	0.33	0
9	HEX	B	1223	-	5,5,5	0.28	0	4,4,4	0.14	0
8	D12	A	1118	-	11,11,11	0.29	0	10,10,10	0.11	0
3	LMT	B	1203	-	36,36,36	1.10	4 (11%)	47,47,47	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	1115	-	5,5,5	0.99	0	5,5,5	1.15	1 (20%)
9	HEX	C	1103	-	5,5,5	0.28	0	4,4,4	0.14	0
9	HEX	B	1229	-	5,5,5	0.28	0	4,4,4	0.14	0
6	EDO	B	1228	-	3,3,3	0.43	0	2,2,2	0.32	0
3	LMT	C	1110	-	36,36,36	1.04	3 (8%)	47,47,47	0.86	0
11	D10	A	1124	-	9,9,9	0.27	0	8,8,8	0.21	0
9	HEX	A	1123	-	5,5,5	0.29	0	4,4,4	0.14	0
5	C14	C	1108	-	13,13,13	0.26	0	12,12,12	0.20	0
14	SO4	C	1115	-	4,4,4	0.25	0	6,6,6	0.11	0
7	GOL	B	1218	-	5,5,5	1.01	0	5,5,5	1.00	0
7	GOL	A	1128	-	5,5,5	0.97	0	5,5,5	1.02	0
4	OCT	C	1106	-	7,7,7	0.25	0	6,6,6	0.23	0
4	OCT	B	1230	-	7,7,7	0.27	0	6,6,6	0.12	0
3	LMT	A	1102	-	36,36,36	1.07	5 (13%)	47,47,47	0.93	1 (2%)
3	LMT	A	1105	-	36,36,36	1.10	4 (11%)	47,47,47	1.00	1 (2%)
9	HEX	B	1224	-	5,5,5	0.30	0	4,4,4	0.15	0
7	GOL	B	1220	-	5,5,5	0.91	0	5,5,5	1.07	0
4	OCT	A	1103	-	7,7,7	0.27	0	6,6,6	0.16	0
4	OCT	C	1122	-	7,7,7	0.25	0	6,6,6	0.16	0
7	GOL	C	1119	-	5,5,5	0.98	0	5,5,5	1.06	0
7	GOL	A	1113	-	5,5,5	1.01	0	5,5,5	0.97	0
7	GOL	C	1111	-	5,5,5	1.04	0	5,5,5	0.78	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1108	-	-	2/4/4/4	-
7	GOL	C	1104	-	-	2/4/4/4	-
7	GOL	C	1127	-	-	2/4/4/4	-
7	GOL	A	1116	-	-	2/4/4/4	-
6	EDO	B	1226	-	-	0/1/1/1	-
11	D10	B	1204	-	-	4/7/7/7	-
7	GOL	C	1118	-	-	4/4/4/4	-
3	LMT	B	1202	-	-	8/21/61/61	0/2/2/2
7	GOL	C	1126	-	-	2/4/4/4	-
8	D12	B	1221	-	-	4/9/9/9	-
7	GOL	A	1125	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	C	1125	-	-	3/4/4/4	-
6	EDO	B	1212	-	-	0/1/1/1	-
7	GOL	B	1219	-	-	0/4/4/4	-
6	EDO	A	1106	-	-	1/1/1/1	-
7	GOL	D	203	-	-	0/4/4/4	-
7	GOL	C	1120	-	-	1/4/4/4	-
7	GOL	A	1111	-	-	0/4/4/4	-
7	GOL	A	1121	-	-	1/4/4/4	-
8	D12	B	1222	-	-	5/9/9/9	-
6	EDO	C	1112	-	-	0/1/1/1	-
6	EDO	C	1113	-	-	0/1/1/1	-
8	D12	A	1120	-	-	3/9/9/9	-
7	GOL	D	201	-	-	0/4/4/4	-
7	GOL	A	1126	-	-	2/4/4/4	-
4	OCT	C	1116	-	-	1/5/5/5	-
7	GOL	A	1112	-	-	2/4/4/4	-
4	OCT	A	1107	-	-	0/5/5/5	-
7	GOL	C	1124	-	-	2/4/4/4	-
7	GOL	A	1110	-	-	0/4/4/4	-
7	GOL	B	1217	-	-	1/4/4/4	-
13	DDQ	B	1214	-	-	3/11/11/11	-
12	DDR	B	1207	-	-	15/29/29/29	-
6	EDO	C	1101	-	-	0/1/1/1	-
7	GOL	B	1211	-	-	2/4/4/4	-
3	LMT	C	1105	-	-	11/21/61/61	0/2/2/2
9	HEX	C	1128	-	-	1/3/3/3	-
7	GOL	B	1210	-	-	2/4/4/4	-
4	OCT	C	1132	-	-	1/5/5/5	-
6	EDO	B	1206	-	-	1/1/1/1	-
5	C14	A	1104	-	-	3/11/11/11	-
15	LPX	C	1109	-	-	17/31/31/31	-
7	GOL	D	202	-	-	2/4/4/4	-
9	HEX	C	1129	-	-	1/3/3/3	-
7	GOL	A	1117	-	-	3/4/4/4	-
6	EDO	B	1205	-	-	0/1/1/1	-
6	EDO	B	1225	-	-	1/1/1/1	-
7	GOL	B	1216	-	-	0/4/4/4	-
7	GOL	A	1109	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	HEX	A	1119	-	-	0/3/3/3	-
7	GOL	D	204	-	-	2/4/4/4	-
6	EDO	C	1114	-	-	1/1/1/1	-
15	LPX	C	1107	-	-	8/31/31/31	-
7	GOL	C	1123	-	-	0/4/4/4	-
7	GOL	C	1131	-	-	0/4/4/4	-
3	LMT	B	1209	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
7	GOL	C	1117	-	-	2/4/4/4	-
4	OCT	C	1102	-	-	0/5/5/5	-
13	DDQ	C	1130	-	-	2/11/11/11	-
7	GOL	A	1127	-	-	0/4/4/4	-
7	GOL	A	1114	-	-	2/4/4/4	-
6	EDO	B	1201	-	-	0/1/1/1	-
7	GOL	B	1208	-	-	2/4/4/4	-
10	XE9	A	1122	-	-	6/10/18/18	0/4/4/4
6	EDO	B	1227	-	-	0/1/1/1	-
6	EDO	B	1213	-	-	0/1/1/1	-
9	HEX	B	1223	-	-	1/3/3/3	-
8	D12	A	1118	-	-	6/9/9/9	-
3	LMT	B	1203	-	-	11/21/61/61	0/2/2/2
7	GOL	A	1115	-	-	2/4/4/4	-
9	HEX	C	1103	-	-	0/3/3/3	-
9	HEX	B	1229	-	-	1/3/3/3	-
6	EDO	B	1228	-	-	0/1/1/1	-
3	LMT	C	1110	-	-	11/21/61/61	0/2/2/2
11	D10	A	1124	-	-	2/7/7/7	-
9	HEX	A	1123	-	-	1/3/3/3	-
5	C14	C	1108	-	-	3/11/11/11	-
7	GOL	B	1218	-	-	1/4/4/4	-
7	GOL	A	1128	-	-	2/4/4/4	-
4	OCT	C	1106	-	-	0/5/5/5	-
4	OCT	B	1230	-	-	3/5/5/5	-
3	LMT	A	1102	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1105	-	-	7/21/61/61	0/2/2/2
9	HEX	B	1224	-	-	2/3/3/3	-
7	GOL	B	1220	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OCT	A	1103	-	-	0/5/5/5	-
4	OCT	C	1122	-	-	3/5/5/5	-
7	GOL	C	1119	-	-	2/4/4/4	-
7	GOL	A	1113	-	-	2/4/4/4	-
7	GOL	C	1111	-	-	2/4/4/4	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1122	XE9	C16-N3	3.00	1.45	1.37
3	A	1101	LMT	O3'-C3'	-2.80	1.36	1.43
3	C	1105	LMT	O3'-C3'	-2.69	1.36	1.43
3	B	1202	LMT	O3'-C3'	-2.63	1.36	1.43
3	A	1105	LMT	O3'-C3'	-2.59	1.36	1.43
3	A	1101	LMT	O2'-C2'	-2.59	1.36	1.43
3	A	1102	LMT	O3'-C3'	-2.53	1.36	1.43
3	C	1110	LMT	O3'-C3'	-2.52	1.36	1.43
13	C	1130	DDQ	O1-N1	-2.51	1.35	1.42
3	B	1209	LMT	O3'-C3'	-2.51	1.36	1.43
15	C	1107	LPX	O6-C6	2.49	1.40	1.33
13	B	1214	DDQ	O1-N1	-2.49	1.36	1.42
3	C	1105	LMT	O2'-C2'	-2.49	1.36	1.43
10	A	1122	XE9	C11-N2	-2.47	1.33	1.37
15	C	1109	LPX	O6-C6	2.47	1.40	1.33
10	A	1122	XE9	C12-C11	-2.42	1.37	1.41
3	B	1203	LMT	O2'-C2'	-2.32	1.37	1.43
3	C	1105	LMT	O3B-C3B	-2.32	1.37	1.43
3	B	1203	LMT	O3'-C3'	-2.30	1.37	1.43
3	A	1101	LMT	O2B-C2B	-2.29	1.37	1.43
3	A	1105	LMT	O3B-C3B	-2.29	1.37	1.43
3	A	1105	LMT	O2B-C2B	-2.27	1.37	1.43
3	C	1105	LMT	O2B-C2B	-2.27	1.37	1.43
3	C	1105	LMT	O4'-C4B	-2.26	1.37	1.43
3	A	1105	LMT	O2'-C2'	-2.24	1.37	1.43
3	B	1202	LMT	O3B-C3B	-2.22	1.37	1.43
3	B	1202	LMT	O2'-C2'	-2.22	1.37	1.43
3	A	1101	LMT	O3B-C3B	-2.21	1.37	1.43
3	A	1102	LMT	O3B-C3B	-2.18	1.37	1.43
3	B	1203	LMT	O2B-C2B	-2.18	1.37	1.43
3	A	1102	LMT	O4'-C4B	-2.16	1.37	1.43
3	B	1209	LMT	O2'-C2'	-2.16	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1122	XE9	C15-CL1	2.16	1.78	1.73
3	B	1209	LMT	O2B-C2B	-2.16	1.37	1.43
15	C	1109	LPX	O6-C5	-2.14	1.40	1.45
3	B	1209	LMT	O3B-C3B	-2.14	1.37	1.43
3	B	1202	LMT	O2B-C2B	-2.14	1.37	1.43
3	B	1203	LMT	O3B-C3B	-2.14	1.37	1.43
10	A	1122	XE9	C14-C10	-2.13	1.37	1.42
3	A	1101	LMT	O4'-C4B	-2.13	1.37	1.43
3	A	1102	LMT	O2'-C2'	-2.10	1.37	1.43
3	C	1110	LMT	O2B-C2B	-2.08	1.37	1.43
3	A	1102	LMT	O2B-C2B	-2.08	1.37	1.43
15	C	1107	LPX	O6-C5	-2.07	1.40	1.45
3	C	1110	LMT	O2'-C2'	-2.03	1.37	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	LMT	C3'-C4'-C5'	-2.93	104.43	110.93
3	B	1203	LMT	O5B-C5B-C4B	2.74	114.64	109.70
15	C	1107	LPX	O6-C6-C7	2.54	119.58	111.83
15	C	1109	LPX	O6-C6-C7	2.43	119.26	111.83
3	A	1101	LMT	C3'-C4'-C5'	-2.36	105.70	110.93
3	B	1209	LMT	O5B-C5B-C6B	2.35	112.26	106.44
10	A	1122	XE9	C17-C18-N4	-2.32	104.98	110.90
3	A	1102	LMT	O1'-C1'-C2'	2.28	111.73	108.27
3	B	1203	LMT	C1'-O5'-C5'	-2.25	109.33	113.72
3	B	1209	LMT	O5B-C5B-C4B	2.23	113.71	109.70
3	B	1209	LMT	C1B-O1B-C4'	2.21	123.21	117.98
3	C	1105	LMT	C3'-C4'-C5'	-2.19	106.07	110.93
3	A	1101	LMT	O5B-C5B-C4B	2.19	113.65	109.70
3	A	1101	LMT	C1'-O5'-C5'	-2.13	109.55	113.72
7	A	1115	GOL	C3-C2-C1	-2.09	104.12	111.80
3	B	1202	LMT	O5'-C1'-O1'	-2.07	105.15	110.04
7	C	1104	GOL	C3-C2-C1	-2.03	104.34	111.80
7	C	1127	GOL	C3-C2-C1	-2.01	104.42	111.80
7	D	202	GOL	C3-C2-C1	-2.01	104.43	111.80
3	C	1105	LMT	C1-O1'-C1'	2.01	117.11	113.68

There are no chirality outliers.

All (234) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	O5'-C1'-O1'-C1
3	B	1202	LMT	O5'-C1'-O1'-C1
3	B	1202	LMT	C2-C1-O1'-C1'
7	A	1113	GOL	C1-C2-C3-O3
7	A	1114	GOL	C1-C2-C3-O3
7	A	1115	GOL	C1-C2-C3-O3
7	A	1115	GOL	O2-C2-C3-O3
7	B	1210	GOL	C1-C2-C3-O3
7	B	1211	GOL	C1-C2-C3-O3
7	B	1220	GOL	C1-C2-C3-O3
7	C	1111	GOL	O1-C1-C2-C3
7	C	1124	GOL	C1-C2-C3-O3
7	C	1125	GOL	C1-C2-C3-O3
7	C	1126	GOL	O1-C1-C2-C3
7	D	204	GOL	C1-C2-C3-O3
15	C	1107	LPX	C3-O1-P1-O3
15	C	1107	LPX	C3-O1-P1-O2
15	C	1107	LPX	O2-C1-C2-N1
15	C	1109	LPX	O5-C4-C5-O6
15	C	1109	LPX	C3-C4-C5-O6
15	C	1109	LPX	C3-O1-P1-O4
3	B	1209	LMT	C3'-C4'-O1B-C1B
3	A	1105	LMT	C3'-C4'-O1B-C1B
3	B	1203	LMT	O5B-C1B-O1B-C4'
3	C	1110	LMT	C3'-C4'-O1B-C1B
3	C	1110	LMT	O5'-C5'-C6'-O6'
3	B	1203	LMT	C4B-C5B-C6B-O6B
3	B	1203	LMT	O5B-C5B-C6B-O6B
3	C	1110	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	C	1110	LMT	C4B-C5B-C6B-O6B
15	C	1107	LPX	C7-C6-O6-C5
15	C	1109	LPX	C7-C6-O6-C5
3	B	1202	LMT	C2'-C1'-O1'-C1
15	C	1107	LPX	O7-C6-O6-C5
3	A	1102	LMT	O5'-C5'-C6'-O6'
12	B	1207	DDR	C2-C1-O51-C51
7	B	1210	GOL	O2-C2-C3-O3
7	B	1220	GOL	O2-C2-C3-O3
7	C	1126	GOL	O1-C1-C2-O2
7	D	202	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1105	LMT	O5'-C5'-C6'-O6'
3	C	1110	LMT	O5B-C5B-C6B-O6B
15	C	1109	LPX	O7-C6-O6-C5
3	C	1105	LMT	C4B-C5B-C6B-O6B
10	A	1122	XE9	C5-C4-C8-C9
3	C	1105	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C4B-C5B-C6B-O6B
10	A	1122	XE9	C3-C4-C8-C9
12	B	1207	DDR	O1-C1-O51-C51
7	A	1109	GOL	C1-C2-C3-O3
7	A	1112	GOL	C1-C2-C3-O3
7	A	1116	GOL	O1-C1-C2-C3
7	A	1117	GOL	O1-C1-C2-C3
7	A	1121	GOL	C1-C2-C3-O3
7	A	1126	GOL	C1-C2-C3-O3
7	A	1128	GOL	C1-C2-C3-O3
7	B	1208	GOL	C1-C2-C3-O3
7	C	1117	GOL	C1-C2-C3-O3
7	C	1118	GOL	C1-C2-C3-O3
7	C	1119	GOL	O1-C1-C2-C3
7	D	202	GOL	C1-C2-C3-O3
3	C	1105	LMT	O5'-C1'-O1'-C1
3	B	1202	LMT	C4B-C5B-C6B-O6B
12	B	1207	DDR	C24-C25-C26-C27
13	B	1214	DDQ	C6-C7-C8-C9
15	C	1107	LPX	C17-C18-C19-C20
3	C	1105	LMT	O5B-C5B-C6B-O6B
8	B	1221	D12	C6-C7-C8-C9
3	B	1203	LMT	C2-C1-O1'-C1'
3	B	1209	LMT	C2-C1-O1'-C1'
3	C	1105	LMT	C2-C1-O1'-C1'
7	A	1113	GOL	O2-C2-C3-O3
7	A	1114	GOL	O2-C2-C3-O3
7	B	1211	GOL	O2-C2-C3-O3
7	C	1111	GOL	O1-C1-C2-O2
7	C	1118	GOL	O2-C2-C3-O3
7	C	1125	GOL	O2-C2-C3-O3
7	D	204	GOL	O2-C2-C3-O3
3	B	1209	LMT	C6-C7-C8-C9
4	C	1132	OCT	C4-C5-C6-C7
4	C	1116	OCT	C3-C4-C5-C6
3	A	1102	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
3	B	1209	LMT	C7-C8-C9-C10
3	A	1105	LMT	C11-C10-C9-C8
3	B	1202	LMT	C4-C5-C6-C7
8	B	1221	D12	C3-C4-C5-C6
15	C	1107	LPX	C11-C10-C9-C8
12	B	1207	DDR	C26-C27-C28-C29
15	C	1109	LPX	C10-C11-C12-C13
15	C	1109	LPX	C17-C18-C19-C20
3	C	1105	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	C1-C2-C3-C4
11	A	1124	D10	C5-C6-C7-C8
5	A	1104	C14	C02-C03-C04-C05
15	C	1109	LPX	C11-C12-C13-C14
3	B	1209	LMT	C1-C2-C3-C4
8	A	1118	D12	C5-C6-C7-C8
3	C	1105	LMT	C3-C4-C5-C6
11	B	1204	D10	C4-C5-C6-C7
8	B	1222	D12	C4-C5-C6-C7
15	C	1109	LPX	C15-C16-C17-C18
3	A	1101	LMT	C3-C4-C5-C6
3	A	1105	LMT	C6-C7-C8-C9
7	A	1109	GOL	O2-C2-C3-O3
7	B	1208	GOL	O2-C2-C3-O3
10	A	1122	XE9	C5-C4-C8-C13
3	B	1209	LMT	C4-C5-C6-C7
12	B	1207	DDR	C25-C26-C27-C28
15	C	1109	LPX	C13-C14-C15-C16
9	C	1129	HEX	C2-C3-C4-C5
3	C	1110	LMT	C5'-C4'-O1B-C1B
3	A	1105	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C2'-C1'-O1'-C1
3	B	1203	LMT	C2B-C1B-O1B-C4'
12	B	1207	DDR	C22-C23-C24-C25
6	B	1225	EDO	O1-C1-C2-O2
3	B	1202	LMT	C6-C7-C8-C9
3	B	1209	LMT	O5B-C5B-C6B-O6B
3	B	1209	LMT	O5'-C5'-C6'-O6'
3	B	1203	LMT	C11-C10-C9-C8
4	C	1122	OCT	C4-C5-C6-C7
8	B	1221	D12	C5-C6-C7-C8
3	C	1105	LMT	C7-C8-C9-C10
3	B	1202	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
8	B	1222	D12	C1-C2-C3-C4
5	A	1104	C14	C01-C02-C03-C04
3	B	1209	LMT	C11-C10-C9-C8
4	B	1230	OCT	C4-C5-C6-C7
3	B	1202	LMT	O5B-C5B-C6B-O6B
8	A	1120	D12	C2-C3-C4-C5
9	C	1128	HEX	C2-C3-C4-C5
3	A	1102	LMT	C2-C1-O1'-C1'
7	A	1112	GOL	O2-C2-C3-O3
7	A	1117	GOL	O1-C1-C2-O2
7	A	1126	GOL	O2-C2-C3-O3
7	C	1117	GOL	O2-C2-C3-O3
7	C	1124	GOL	O2-C2-C3-O3
3	C	1110	LMT	C2'-C1'-O1'-C1
12	B	1207	DDR	C27-C28-C29-C30
15	C	1107	LPX	C14-C15-C16-C17
3	B	1203	LMT	C6-C7-C8-C9
12	B	1207	DDR	C51-C52-C53-O53
8	B	1222	D12	C7-C8-C9-C10
9	B	1229	HEX	C2-C3-C4-C5
3	C	1110	LMT	C4-C5-C6-C7
10	A	1122	XE9	C3-C4-C8-C13
4	C	1122	OCT	C1-C2-C3-C4
3	C	1105	LMT	C4-C5-C6-C7
9	B	1224	HEX	C2-C3-C4-C5
4	C	1122	OCT	C3-C4-C5-C6
13	B	1214	DDQ	C5-C6-C7-C8
8	A	1118	D12	C1-C2-C3-C4
7	A	1108	GOL	O2-C2-C3-O3
7	A	1116	GOL	O1-C1-C2-O2
7	A	1128	GOL	O2-C2-C3-O3
7	B	1218	GOL	O1-C1-C2-O2
7	C	1119	GOL	O2-C2-C3-O3
3	B	1203	LMT	C4-C5-C6-C7
3	B	1209	LMT	C3-C4-C5-C6
7	C	1104	GOL	O1-C1-C2-C3
3	B	1203	LMT	C2-C3-C4-C5
3	C	1110	LMT	O5'-C1'-O1'-C1
8	A	1118	D12	C4-C5-C6-C7
3	C	1105	LMT	C6-C7-C8-C9
3	A	1101	LMT	C2-C3-C4-C5
11	B	1204	D10	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
8	B	1222	D12	C2-C3-C4-C5
3	C	1110	LMT	C1-C2-C3-C4
15	C	1109	LPX	C11-C10-C9-C8
3	C	1105	LMT	C2-C3-C4-C5
8	A	1120	D12	C11-C10-C9-C8
3	A	1105	LMT	C5'-C4'-O1B-C1B
8	B	1221	D12	C7-C8-C9-C10
8	A	1118	D12	C3-C4-C5-C6
3	B	1209	LMT	O1'-C1-C2-C3
5	C	1108	C14	C10-C11-C12-C13
4	B	1230	OCT	C3-C4-C5-C6
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	B	1203	LMT	C1-C2-C3-C4
15	C	1109	LPX	C7-C8-C9-C10
7	C	1127	GOL	O1-C1-C2-C3
5	C	1108	C14	C09-C10-C11-C12
8	A	1118	D12	C7-C8-C9-C10
3	A	1101	LMT	C5'-C4'-O1B-C1B
3	A	1102	LMT	C1-C2-C3-C4
6	A	1106	EDO	O1-C1-C2-O2
6	B	1206	EDO	O1-C1-C2-O2
6	C	1114	EDO	O1-C1-C2-O2
8	A	1118	D12	C2-C3-C4-C5
12	B	1207	DDR	C23-C24-C25-C26
4	B	1230	OCT	C2-C3-C4-C5
9	B	1223	HEX	C3-C4-C5-C6
5	A	1104	C14	C08-C09-C10-C11
8	B	1222	D12	C11-C10-C9-C8
15	C	1109	LPX	C14-C15-C16-C17
7	B	1217	GOL	O1-C1-C2-C3
7	C	1118	GOL	O1-C1-C2-C3
12	B	1207	DDR	C53-C52-O52-C21
7	C	1104	GOL	O1-C1-C2-O2
9	B	1224	HEX	C1-C2-C3-C4
9	A	1123	HEX	C1-C2-C3-C4
12	B	1207	DDR	C2-C3-C4-C5
8	A	1120	D12	C3-C4-C5-C6
12	B	1207	DDR	O52-C52-C53-O53
7	C	1118	GOL	O1-C1-C2-O2
7	C	1127	GOL	O1-C1-C2-O2
13	C	1130	DDQ	C1-C2-C3-C4
15	C	1109	LPX	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	C9-C10-C11-C12
7	A	1108	GOL	C1-C2-C3-O3
7	C	1125	GOL	O1-C1-C2-C3
3	A	1105	LMT	C4'-C5'-C6'-O6'
10	A	1122	XE9	N2-C16-N3-C20
7	C	1120	GOL	O2-C2-C3-O3
5	C	1108	C14	C07-C08-C09-C10
3	C	1110	LMT	C9-C10-C11-C12
12	B	1207	DDR	C21-C22-C23-C24
13	B	1214	DDQ	C2-C3-C4-C5
7	A	1117	GOL	O2-C2-C3-O3
3	A	1102	LMT	C11-C10-C9-C8
15	C	1109	LPX	O6-C6-C7-C8
11	B	1204	D10	C3-C4-C5-C6
15	C	1109	LPX	O1-C3-C4-C5
13	C	1130	DDQ	C6-C7-C8-C9
3	B	1203	LMT	C5-C6-C7-C8
12	B	1207	DDR	O51-C1-C2-C3
11	A	1124	D10	C4-C5-C6-C7
10	A	1122	XE9	C1-C6-C7-N1
11	B	1204	D10	C2-C3-C4-C5
15	C	1109	LPX	O7-C6-C7-C8
12	B	1207	DDR	O1-C1-C2-C3

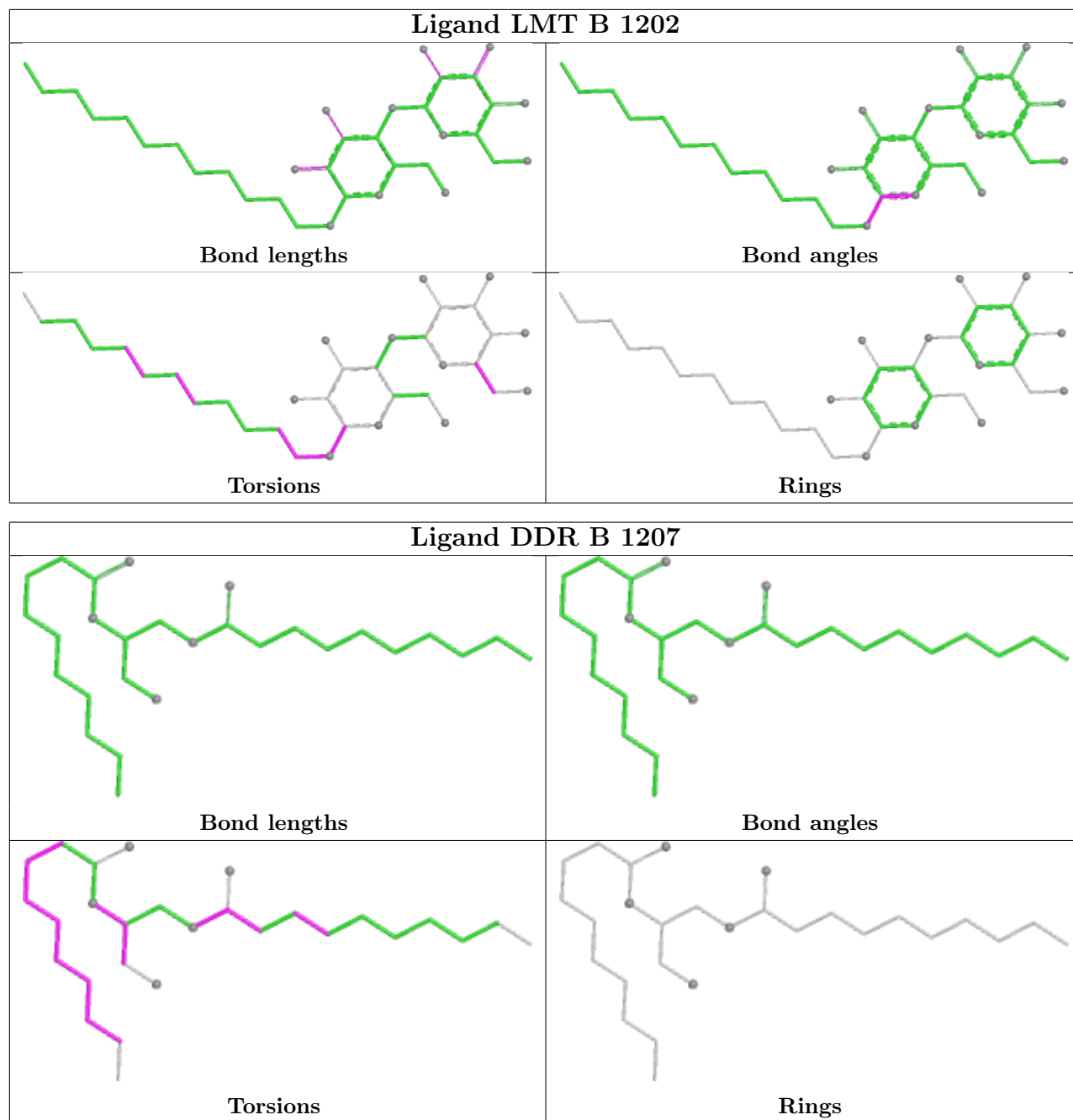
There are no ring outliers.

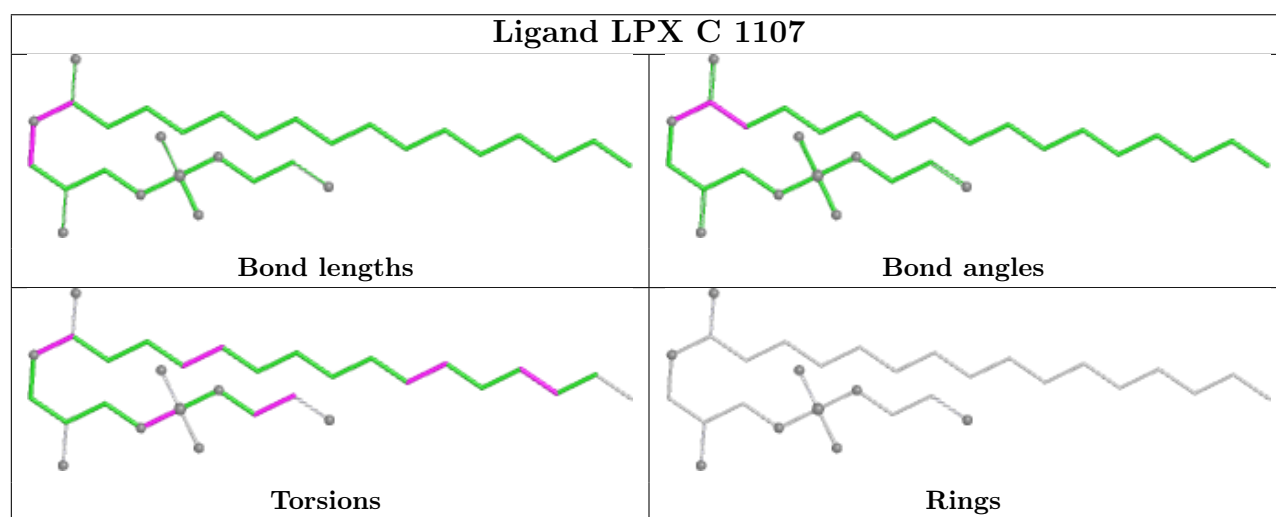
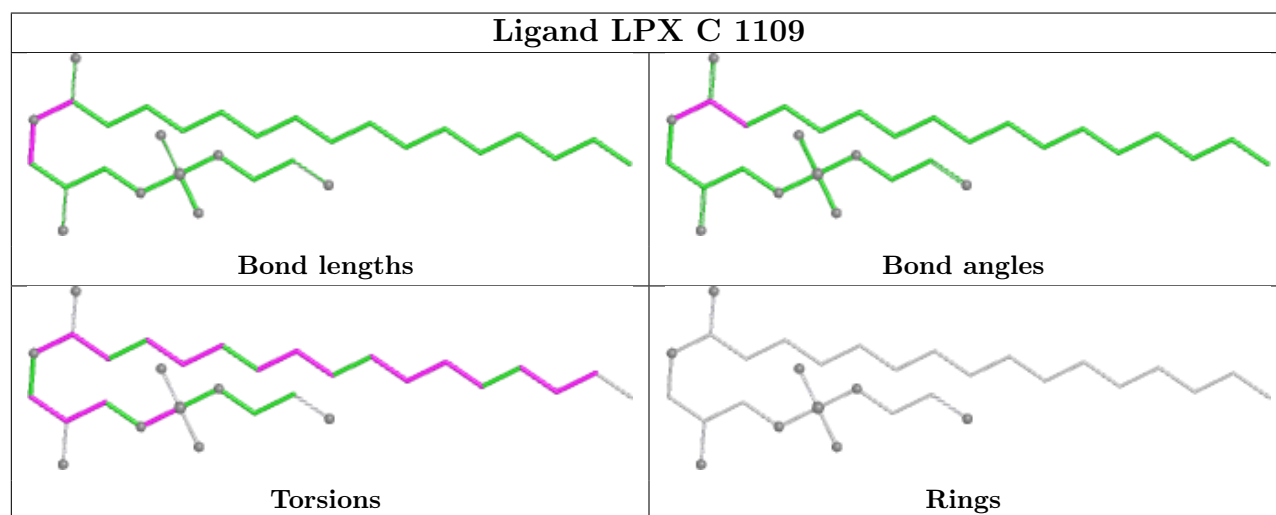
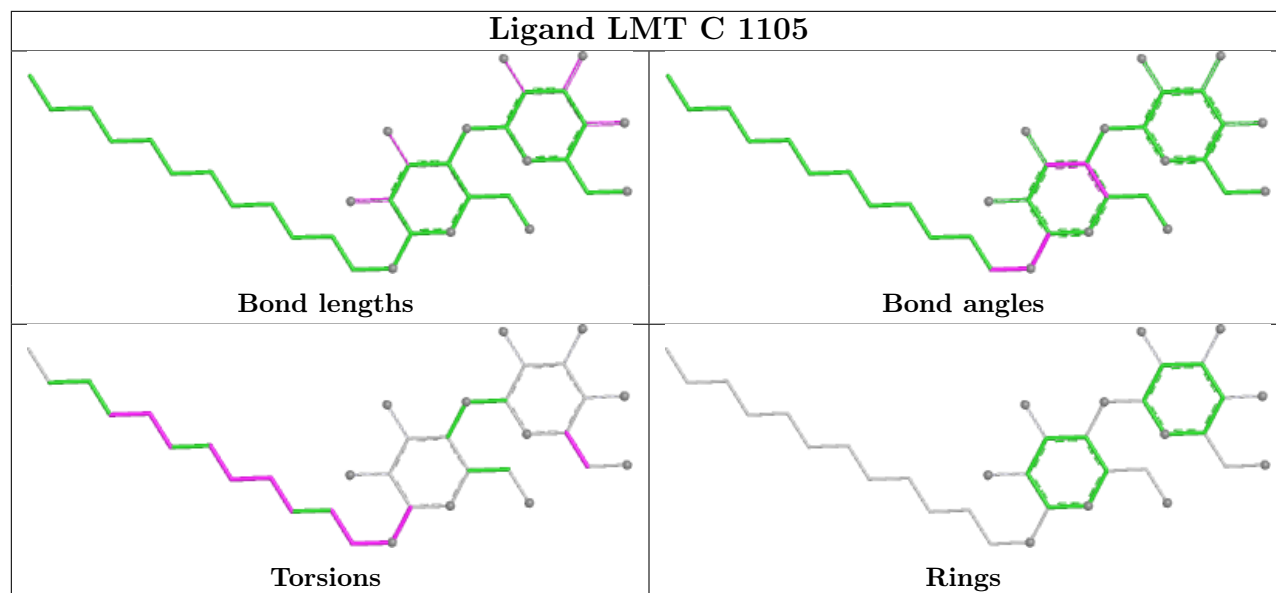
4 monomers are involved in 4 short contacts:

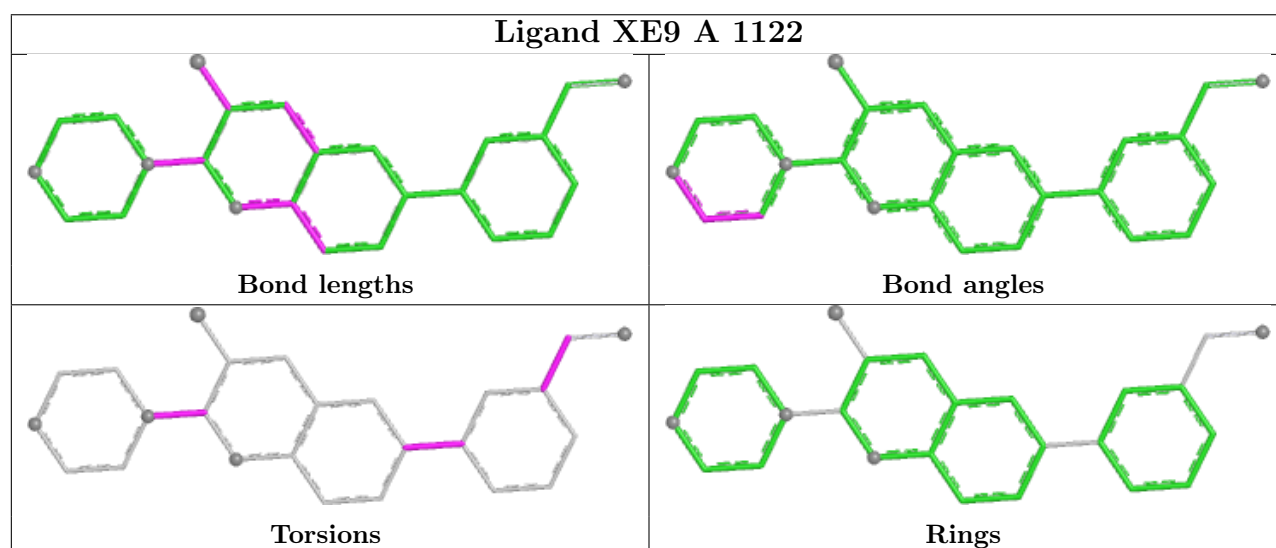
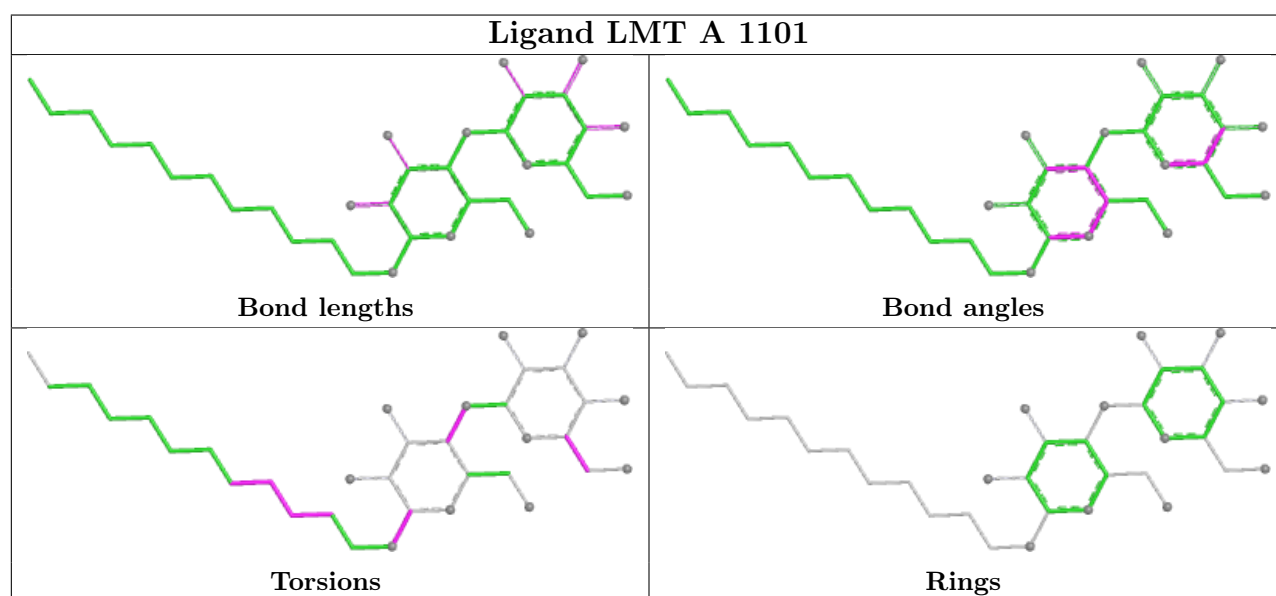
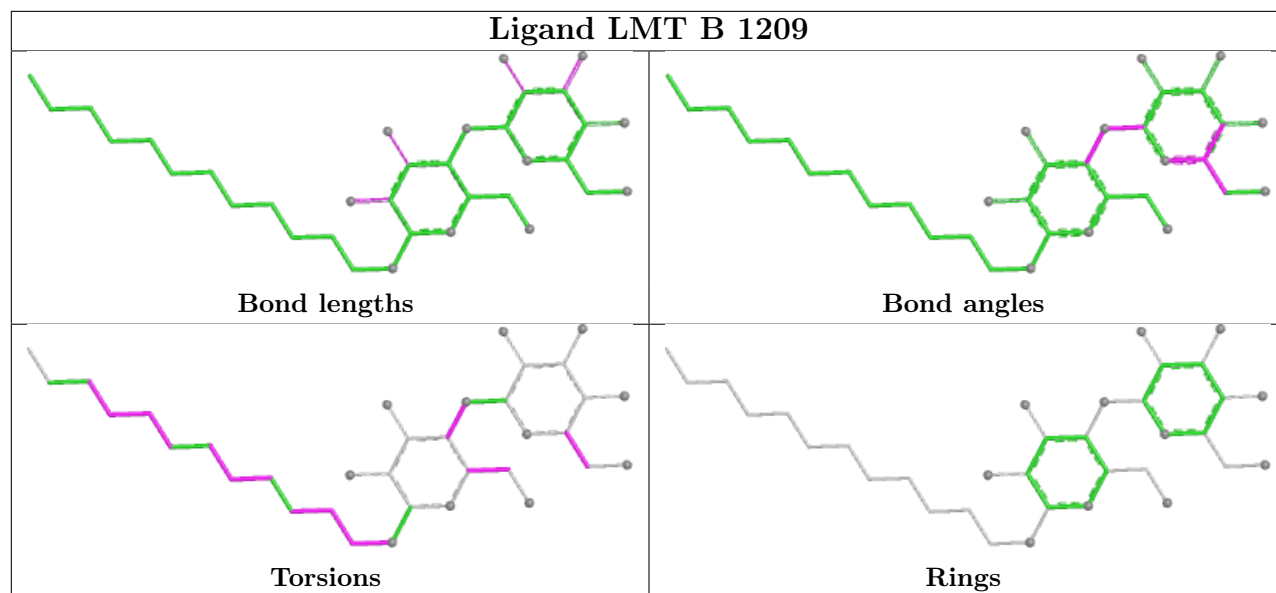
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1109	LPX	1	0
3	B	1209	LMT	1	0
10	A	1122	XE9	1	0
7	A	1115	GOL	1	0

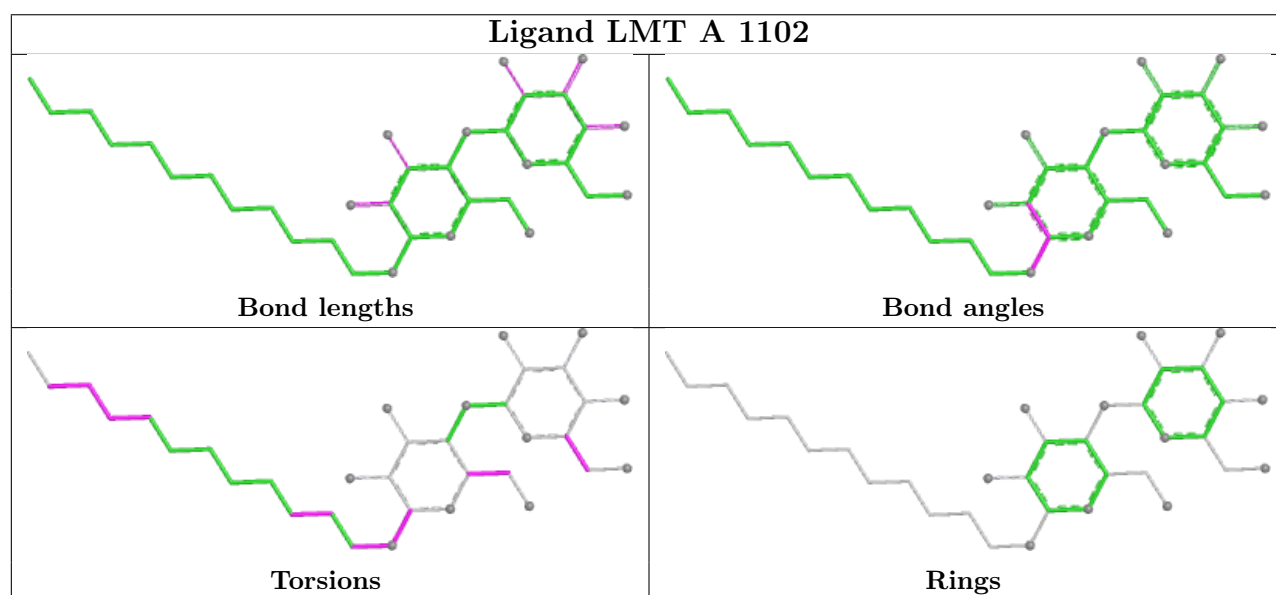
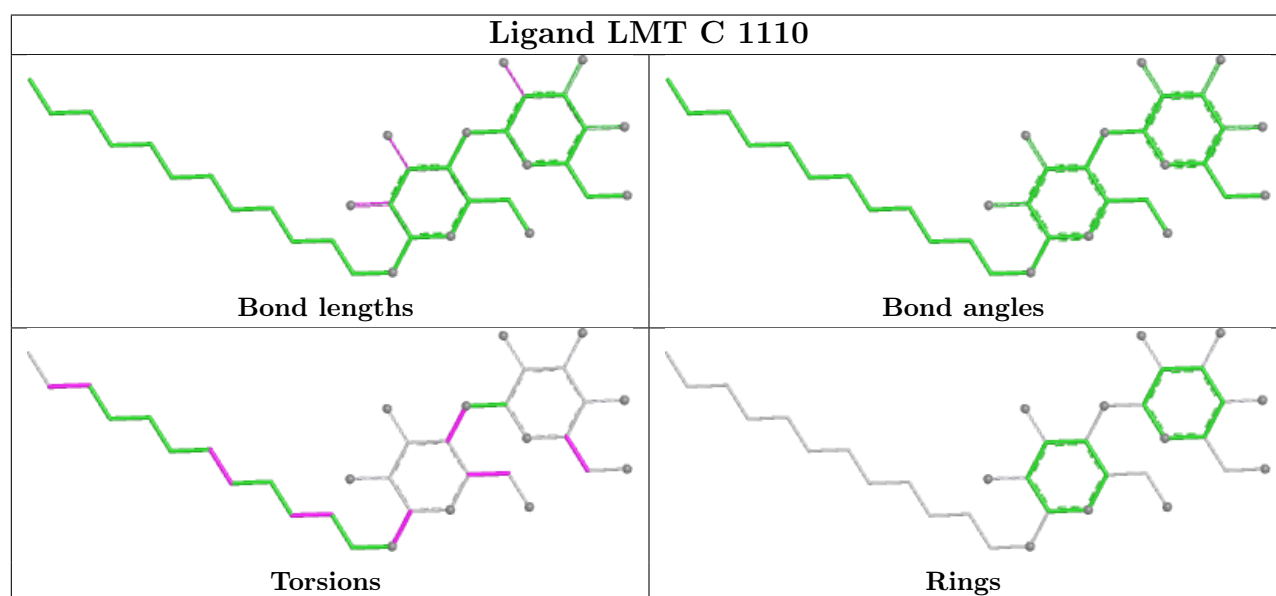
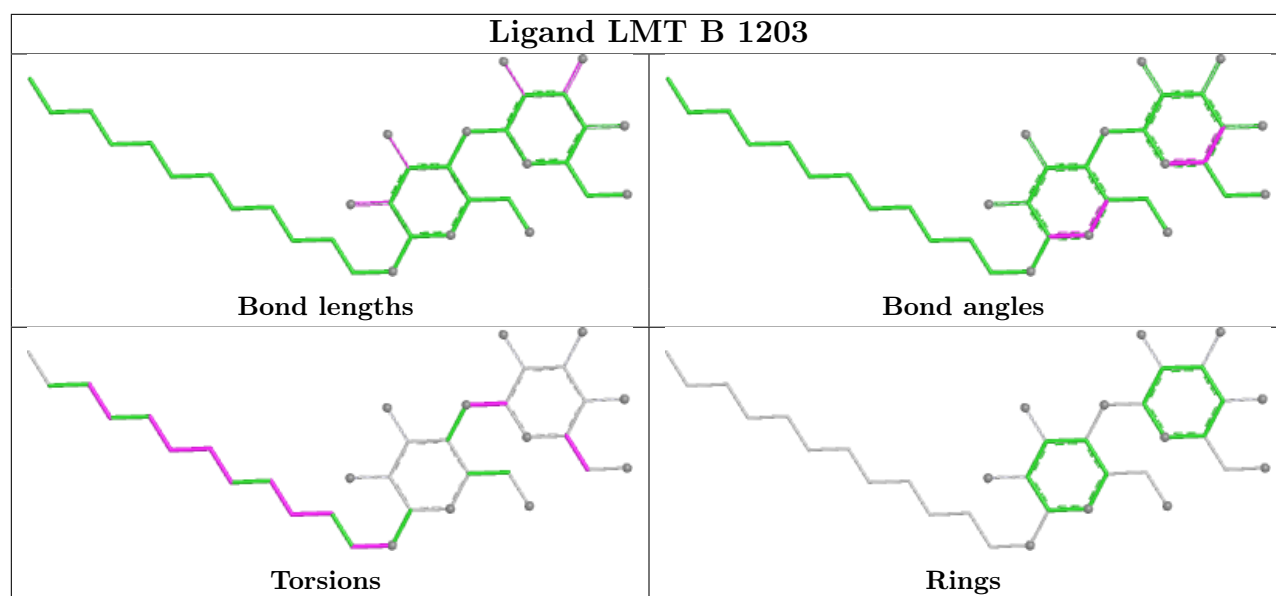
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

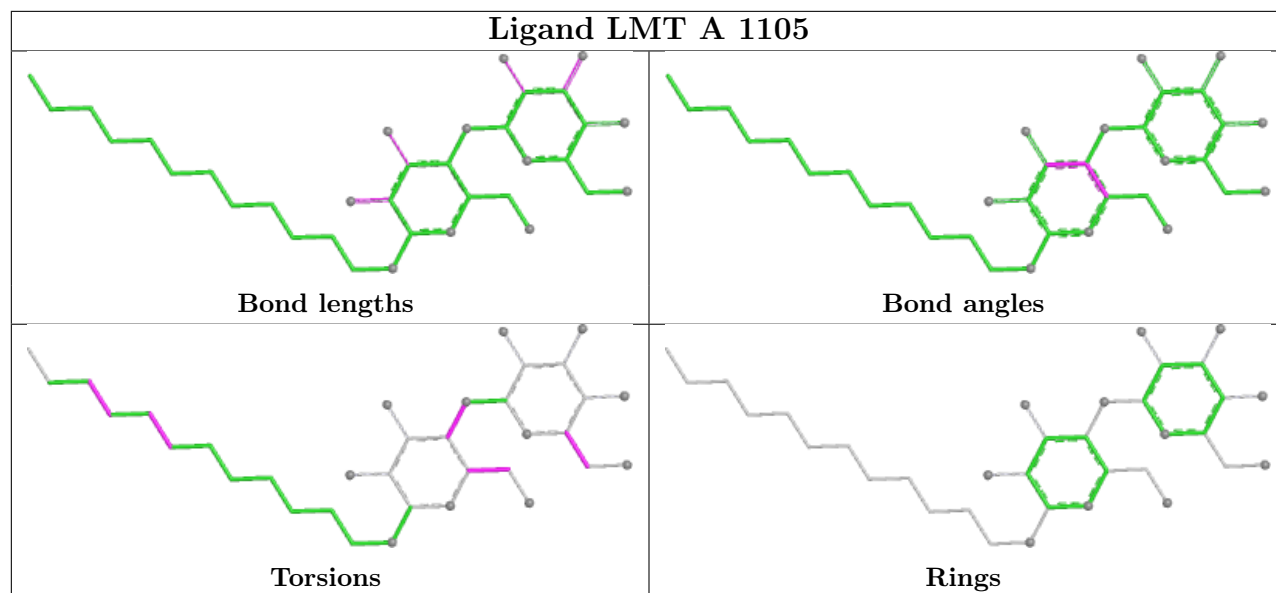
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	1031/1057 (97%)	0.97	229 (22%) 2 2	27, 54, 112, 136	1 (0%)
1	B	1034/1057 (97%)	0.65	93 (8%) 15 17	23, 51, 78, 100	1 (0%)
1	C	1034/1057 (97%)	0.34	51 (4%) 35 39	27, 46, 69, 100	2 (0%)
2	D	155/169 (91%)	0.60	14 (9%) 15 17	42, 51, 74, 100	0
2	E	153/169 (90%)	1.27	24 (15%) 5 5	46, 65, 88, 100	0
All	All	3407/3509 (97%)	0.68	411 (12%) 8 10	23, 51, 89, 136	4 (0%)

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	676	THR	8.0
1	A	1040	ILE	7.8
1	B	674	LEU	7.7
2	E	14	LEU	7.6
1	A	421	ALA	6.8
1	B	617	PHE	6.7
1	B	618	ALA	6.5
1	A	678	THR	6.4
1	A	500	ILE	6.4
1	A	674	LEU	6.3
1	A	369	THR	6.1
1	A	38	ILE	6.1
1	B	677	ALA	6.0
1	A	672	VAL	6.0
1	C	1034	SER	6.0
1	A	671	ILE	5.9
1	B	332	PHE	5.8
1	A	535	LEU	5.6
1	B	563	PHE	5.6
1	A	675	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	616	GLY	5.5
1	B	634	TRP	5.4
1	B	868	LEU	5.4
1	A	716	VAL	5.4
1	A	677	ALA	5.4
1	B	675	GLY	5.3
1	B	615	PHE	5.3
1	A	424	GLY	5.2
1	C	671	ILE	5.2
1	A	425	LEU	5.2
1	A	868	LEU	5.1
1	A	513	PHE	5.1
1	A	542	LEU	5.1
1	C	672	VAL	5.0
1	A	952	LEU	4.9
1	C	811	TYR	4.9
1	A	533	GLY	4.9
1	B	672	VAL	4.9
1	A	676	THR	4.8
1	A	918	PHE	4.8
1	A	1039	ASP	4.7
1	C	675	GLY	4.7
1	A	965	LEU	4.7
1	A	368	PRO	4.6
1	B	561	SER	4.6
1	A	961	ILE	4.6
1	A	668	LEU	4.5
1	B	619	GLY	4.5
1	A	984	LEU	4.5
1	A	37	THR	4.5
1	A	618	ALA	4.5
1	A	516	PHE	4.5
1	A	359	LEU	4.4
1	C	674	LEU	4.4
1	A	869	SER	4.3
1	A	362	PHE	4.3
1	A	980	LEU	4.3
1	A	827	ILE	4.2
1	B	575	MET	4.2
1	A	462	SER	4.1
1	B	386	PHE	4.1
1	A	497	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	957	GLY	4.1
2	D	14	LEU	4.1
1	A	617	PHE	4.0
1	A	1026	PHE	4.0
1	A	1029	VAL	4.0
1	A	512	PHE	4.0
1	C	670	ALA	4.0
1	A	649[A]	MET	4.0
1	A	39	ALA	4.0
1	A	459	PHE	4.0
1	A	515	TRP	3.9
1	A	367	ILE	3.9
1	C	362	PHE	3.9
1	C	659	LYS	3.9
1	C	1033	PHE	3.9
1	A	970	MET	3.9
1	C	116	PRO	3.9
1	A	556	PHE	3.9
1	A	422	GLU	3.8
1	A	531	VAL	3.8
1	A	538	THR	3.8
1	A	514	GLY	3.8
1	A	3	ASN	3.7
1	B	635	ALA	3.7
1	A	990	VAL	3.7
1	A	527	TYR	3.7
1	A	1033	PHE	3.7
1	B	666	PHE	3.7
1	A	430	ALA	3.7
1	A	1020	PHE	3.7
1	B	134	SER	3.6
1	A	712	MET	3.6
1	B	508	GLY	3.6
1	B	1033	PHE	3.6
1	A	534	ILE	3.6
1	B	678	THR	3.6
1	A	520	PHE	3.6
1	C	494	ALA	3.6
1	A	541	TYR	3.6
2	D	166	GLN	3.6
1	A	1024	VAL	3.6
1	C	676	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	358	PHE	3.6
1	A	463	THR	3.5
1	A	555	LEU	3.5
1	A	539	GLY	3.5
1	A	963	ALA	3.5
1	B	133	SER	3.5
1	A	1027	VAL	3.5
1	B	178	PHE	3.5
1	A	679	GLY	3.5
1	C	124	GLN	3.4
1	A	543	VAL	3.4
1	A	563	PHE	3.4
1	A	707	ALA	3.4
1	B	869	SER	3.4
2	E	166	GLN	3.4
1	A	544	LEU	3.4
1	A	713	LEU	3.4
2	D	13	ASP	3.3
1	A	419	VAL	3.3
1	B	620	ARG	3.3
1	A	499	PRO	3.3
1	A	619	GLY	3.3
1	A	835	LYS	3.3
1	A	526	HIS	3.3
1	B	628	PHE	3.3
1	A	1032	ARG	3.3
1	A	956	GLU	3.3
1	A	917	THR	3.3
1	A	972	LEU	3.3
2	D	12	SER	3.3
1	A	496	MET	3.2
1	A	510	LYS	3.2
1	B	662	MET	3.2
1	A	364	ALA	3.2
1	A	866	GLU	3.2
1	A	1019	ILE	3.2
1	A	1016	VAL	3.2
2	E	106	VAL	3.2
1	B	522	LYS	3.2
1	C	71	GLY	3.2
1	A	580	ALA	3.1
1	B	837	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1034	SER	3.1
1	A	351	VAL	3.1
2	D	165	LEU	3.1
1	A	493	CYS	3.1
1	A	352	PHE	3.1
1	A	355	MET	3.1
1	A	528	THR	3.1
1	B	135	SER	3.1
1	A	669	PRO	3.1
1	A	353	LEU	3.0
1	A	702	LEU	3.0
1	B	395[A]	MET	3.0
1	A	948	PHE	3.0
1	A	1021	PHE	3.0
1	B	918	PHE	3.0
1	C	495	THR	3.0
1	B	660	ASP	3.0
1	A	548	ILE	3.0
2	E	40	VAL	3.0
1	A	993	THR	3.0
1	C	673	GLU	3.0
1	A	357	LEU	2.9
1	A	456	MET	2.9
1	B	556	PHE	2.9
1	C	918	PHE	2.9
1	A	536	ARG	2.9
1	A	1022	VAL	2.9
1	A	524	THR	2.9
1	A	616	GLY	2.9
1	A	662	MET	2.9
1	B	670	ALA	2.9
1	C	618	ALA	2.9
1	B	626	ILE	2.9
1	C	743	ILE	2.9
1	B	564	LEU	2.9
1	A	420	MET	2.9
1	A	904	VAL	2.9
1	A	467	TYR	2.9
1	A	427	PRO	2.9
1	B	603	LYS	2.9
1	A	1028	VAL	2.8
1	B	510	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	664	PHE	2.8
1	C	519	MET	2.8
1	A	964	THR	2.8
1	C	120	GLN	2.8
1	A	557	VAL	2.8
1	A	433	LYS	2.8
1	A	833	PRO	2.8
2	E	76	TYR	2.8
1	A	673	GLU	2.8
1	A	875	SER	2.8
1	A	871	ASN	2.8
1	A	1017	LEU	2.8
2	E	33	LEU	2.8
1	A	416	VAL	2.8
1	A	554	TYR	2.8
1	A	1025	PHE	2.8
1	A	854	GLY	2.8
1	A	960	LEU	2.8
1	B	649	MET	2.8
1	C	738	ALA	2.7
1	B	498	LYS	2.7
1	A	703	LEU	2.7
1	C	35	TYR	2.7
1	A	1015	THR	2.7
1	C	853	THR	2.7
1	B	28	LEU	2.7
1	B	671	ILE	2.7
1	A	518	ARG	2.7
1	A	955	LYS	2.7
1	A	709	HIS	2.7
1	A	981	ALA	2.7
1	B	515	TRP	2.7
1	A	356	TYR	2.7
1	A	532	GLY	2.7
1	B	577	GLN	2.7
1	C	361	ASN	2.7
1	A	525	HIS	2.7
1	C	660	ASP	2.6
1	A	540	ARG	2.6
1	B	648	THR	2.6
1	C	512	PHE	2.6
1	B	866	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	522	LYS	2.6
2	D	101	LYS	2.6
1	A	547	ILE	2.6
1	A	831	ALA	2.6
1	A	498	LYS	2.6
1	B	463	THR	2.6
1	C	150	THR	2.6
1	B	542	LEU	2.6
1	A	413	VAL	2.6
1	A	670	ALA	2.6
2	D	139	VAL	2.6
2	E	137	ALA	2.6
1	B	653	ARG	2.6
1	C	954	ASP	2.6
2	E	146	GLY	2.6
1	C	497	LEU	2.5
1	A	410	ILE	2.5
1	A	706	ALA	2.5
1	B	580	ALA	2.5
1	A	986	VAL	2.5
1	A	867	ARG	2.5
1	B	509	LYS	2.5
1	A	907	LEU	2.5
1	B	366	LEU	2.5
1	A	257	GLY	2.5
1	A	575	MET	2.5
1	C	498	LYS	2.5
1	A	959	GLY	2.5
1	B	570	GLY	2.5
1	B	668	LEU	2.5
1	C	617	PHE	2.5
1	A	423	GLU	2.5
1	B	573	MET	2.5
1	A	978	THR	2.5
1	A	354	VAL	2.5
1	A	923	ASN	2.4
2	E	135	TYR	2.4
1	A	862	MET	2.4
1	A	987	MET	2.4
1	A	951	ASP	2.4
1	A	895	TRP	2.4
1	A	426	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1007	VAL	2.4
1	B	644	VAL	2.4
1	A	953	MET	2.4
1	B	597	TYR	2.4
1	C	952	LEU	2.4
1	B	136	PHE	2.4
1	A	966	ASP	2.4
1	A	991	ILE	2.4
1	A	714	THR	2.4
1	A	360	GLN	2.4
1	B	229	GLN	2.4
1	A	828	LEU	2.4
1	A	711	ASP	2.4
1	A	717	ARG	2.4
1	A	969	ARG	2.4
1	A	872	GLN	2.4
1	B	633	ASP	2.3
1	A	432	ARG	2.3
2	E	165	LEU	2.3
1	A	949	ALA	2.3
1	B	647	ILE	2.3
2	E	107	ASN	2.3
1	B	639	GLY	2.3
1	A	537	SER	2.3
1	A	836	SER	2.3
1	B	867	ARG	2.3
1	A	1038	GLU	2.3
1	A	932	LEU	2.3
1	B	380	PHE	2.3
1	B	513	PHE	2.3
2	E	38	ALA	2.3
1	B	658	ILE	2.3
2	E	32	ILE	2.3
2	E	164	ILE	2.3
1	A	461	GLY	2.3
1	A	1031	ARG	2.3
1	A	947	GLU	2.3
1	A	697	GLN	2.3
1	A	361	ASN	2.3
1	C	148	THR	2.3
1	A	428	LYS	2.3
1	A	718	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	2.3
1	B	500	ILE	2.3
2	D	32	ILE	2.3
2	E	65	VAL	2.3
1	A	442	LEU	2.3
1	A	922	THR	2.3
1	B	659	LYS	2.3
1	B	853	THR	2.3
1	C	193	LEU	2.3
2	E	133	LEU	2.3
1	A	620	ARG	2.2
1	A	859	TRP	2.2
1	A	429	GLU	2.2
1	A	834	GLY	2.2
1	C	173	GLY	2.2
1	C	508	GLY	2.2
2	E	35	ALA	2.2
1	B	731	ILE	2.2
1	A	968	VAL	2.2
1	B	253	VAL	2.2
1	A	517	ASN	2.2
1	A	659	LYS	2.2
1	B	955	LYS	2.2
1	C	267	LYS	2.2
1	A	546	LEU	2.2
1	B	230	LEU	2.2
1	B	578	LEU	2.2
1	C	28	LEU	2.2
1	A	511	GLY	2.2
1	A	985	GLY	2.2
1	A	832	ALA	2.2
2	D	35	ALA	2.2
1	C	948	PHE	2.2
1	A	1030	ARG	2.2
1	A	684	LEU	2.2
1	A	494	ALA	2.2
2	D	162	ALA	2.2
1	A	545	TYR	2.2
1	C	515	TRP	2.2
1	C	81	ASN	2.2
1	B	673	GLU	2.2
1	A	901	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	495	THR	2.2
1	A	639	GLY	2.2
2	E	60	LEU	2.2
1	A	704	ALA	2.2
1	C	195	LYS	2.2
2	D	61	GLU	2.1
2	E	159	GLU	2.1
1	B	743	ILE	2.1
1	A	657	GLN	2.1
1	B	569	GLN	2.1
1	C	737	GLN	2.1
1	B	530	SER	2.1
1	A	559	LEU	2.1
1	A	1035	ARG	2.1
1	C	425	LEU	2.1
2	E	101	LYS	2.1
1	A	873	ALA	2.1
1	A	967	ALA	2.1
1	C	311	ALA	2.1
1	B	657	GLN	2.1
1	A	900	SER	2.1
1	B	132	SER	2.1
1	B	147	GLY	2.1
1	A	1014	ALA	2.1
1	B	388	PHE	2.1
1	C	500	ILE	2.1
2	E	81	SER	2.1
1	A	962	GLU	2.1
1	A	519	MET	2.1
2	E	131	VAL	2.1
1	A	865	GLN	2.1
1	A	944	LEU	2.1
1	C	363	ARG	2.1
1	A	899	PHE	2.0
1	C	510	LYS	2.0
1	C	899	PHE	2.0
1	B	537	SER	2.0
1	A	343	THR	2.0
1	B	987	MET	2.0
2	D	36	ASN	2.0
1	A	1023	PRO	2.0
1	A	876	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	100	LEU	2.0
1	A	418	ARG	2.0
2	D	28	ASP	2.0
1	A	1036	LYS	2.0
2	D	17	LYS	2.0
1	A	910	ILE	2.0
1	A	982	PHE	2.0
1	B	402	ILE	2.0
1	B	459	PHE	2.0
1	A	928	GLN	2.0
1	B	176	GLN	2.0
1	B	284	GLN	2.0
2	E	140	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($\text{\AA}^2$)	Q<0.9
3	LMT	C	1110	35/35	0.62	0.23	66,96,119,124	0
14	SO4	C	1121	5/5	0.66	0.18	70,75,91,98	0
7	GOL	C	1119	6/6	0.68	0.21	56,81,96,97	0
7	GOL	A	1113	6/6	0.72	0.17	57,75,83,90	0
3	LMT	B	1203	35/35	0.72	0.22	68,95,119,128	0
7	GOL	C	1131	6/6	0.72	0.19	71,85,94,97	0
6	EDO	B	1226	4/4	0.72	0.23	55,66,76,89	0
7	GOL	B	1220	6/6	0.73	0.18	71,86,100,102	0
8	D12	B	1221	12/12	0.74	0.25	55,75,101,101	0
9	HEX	B	1224	6/6	0.74	0.28	65,79,86,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	C14	A	1104	14/14	0.74	0.26	61,86,103,105	0
7	GOL	A	1110	6/6	0.75	0.22	70,84,96,99	0
7	GOL	C	1118	6/6	0.76	0.22	53,69,79,83	0
4	OCT	B	1230	8/8	0.76	0.24	57,78,93,93	0
7	GOL	A	1126	6/6	0.77	0.22	57,69,81,83	0
7	GOL	A	1114	6/6	0.77	0.22	41,65,79,80	0
9	HEX	A	1123	6/6	0.78	0.27	68,84,88,88	0
4	OCT	A	1107	8/8	0.78	0.21	61,76,86,86	0
9	HEX	C	1128	6/6	0.78	0.24	60,73,82,82	0
7	GOL	C	1125	6/6	0.78	0.18	56,69,78,82	0
15	LPX	C	1107	30/30	0.78	0.20	61,78,90,98	0
3	LMT	A	1102	35/35	0.79	0.17	69,94,113,118	0
7	GOL	B	1218	6/6	0.79	0.17	59,73,86,90	0
9	HEX	C	1129	6/6	0.79	0.21	58,79,88,88	0
13	DDQ	C	1130	14/14	0.79	0.21	52,79,101,107	0
7	GOL	B	1219	6/6	0.79	0.17	66,82,98,102	0
7	GOL	C	1120	6/6	0.79	0.14	64,77,90,99	0
5	C14	C	1108	14/14	0.80	0.24	48,65,103,104	0
7	GOL	B	1217	6/6	0.80	0.22	47,62,83,86	0
7	GOL	D	204	6/6	0.80	0.18	48,69,83,83	0
8	D12	A	1120	12/12	0.80	0.23	61,75,88,88	0
9	HEX	C	1103	6/6	0.81	0.22	68,83,87,87	0
7	GOL	B	1208	6/6	0.81	0.19	61,78,97,100	0
4	OCT	C	1106	8/8	0.81	0.27	53,69,80,86	0
11	D10	A	1124	10/10	0.81	0.22	56,73,93,93	0
13	DDQ	B	1214	14/14	0.81	0.21	50,69,99,109	0
4	OCT	C	1102	8/8	0.81	0.23	57,78,93,93	0
6	EDO	B	1227	4/4	0.81	0.18	52,63,72,72	0
7	GOL	A	1108	6/6	0.81	0.21	68,81,91,91	0
4	OCT	C	1132	8/8	0.82	0.26	57,70,80,80	0
7	GOL	B	1211	6/6	0.82	0.17	54,67,81,83	0
3	LMT	B	1209	35/35	0.82	0.15	54,88,126,131	0
6	EDO	C	1101	4/4	0.82	0.18	48,58,75,75	0
11	D10	B	1204	10/10	0.82	0.22	56,73,93,93	0
8	D12	B	1222	12/12	0.82	0.21	52,73,84,86	0
9	HEX	A	1119	6/6	0.82	0.21	68,84,88,88	0
3	LMT	A	1105	35/35	0.82	0.16	54,82,123,142	0
7	GOL	C	1127	6/6	0.82	0.17	59,70,81,89	0
15	LPX	C	1109	30/30	0.82	0.19	54,76,95,99	0
4	OCT	A	1103	8/8	0.83	0.23	68,82,94,94	0
6	EDO	B	1205	4/4	0.83	0.18	46,55,71,71	0
7	GOL	A	1109	6/6	0.83	0.19	51,66,79,83	0

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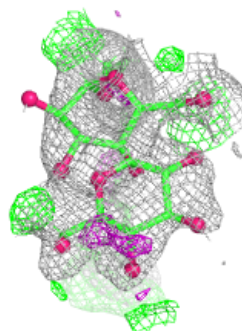
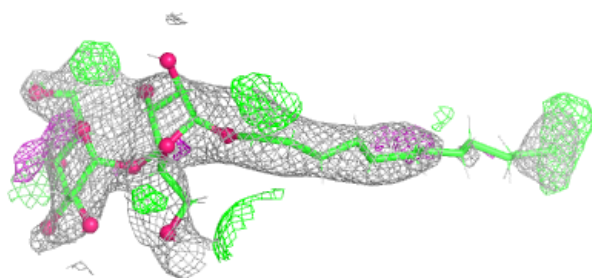
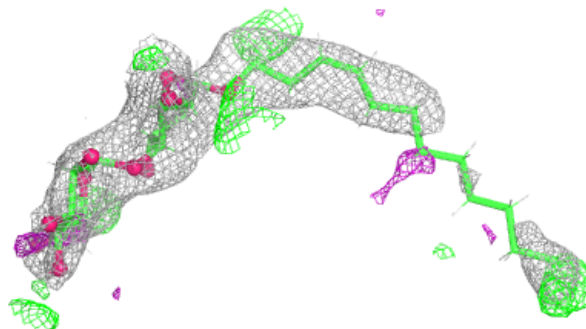
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	EDO	B	1212	4/4	0.84	0.15	66,79,89,89	0
7	GOL	C	1123	6/6	0.84	0.18	57,68,77,85	0
3	LMT	B	1202	35/35	0.84	0.16	49,73,113,113	0
8	D12	A	1118	12/12	0.84	0.20	61,78,88,93	0
4	OCT	C	1116	8/8	0.85	0.19	64,80,82,86	0
3	LMT	A	1101	35/35	0.85	0.14	48,77,115,125	0
6	EDO	B	1225	4/4	0.85	0.17	57,69,74,77	0
9	HEX	B	1229	6/6	0.85	0.25	63,81,89,89	0
7	GOL	C	1124	6/6	0.85	0.17	47,60,75,84	0
6	EDO	C	1114	4/4	0.85	0.21	47,63,75,78	0
7	GOL	B	1216	6/6	0.85	0.13	63,76,87,94	0
7	GOL	A	1117	6/6	0.86	0.16	40,61,71,79	0
7	GOL	D	201	6/6	0.86	0.20	53,64,77,92	0
7	GOL	C	1104	6/6	0.86	0.18	61,73,84,86	0
7	GOL	A	1128	6/6	0.86	0.16	63,75,86,87	0
12	DDR	B	1207	28/28	0.86	0.20	58,74,84,86	0
6	EDO	C	1113	4/4	0.87	0.19	60,72,84,84	0
9	HEX	B	1223	6/6	0.87	0.18	63,81,89,89	0
7	GOL	A	1112	6/6	0.87	0.16	53,69,81,83	0
7	GOL	A	1121	6/6	0.87	0.13	52,67,81,84	0
6	EDO	B	1201	4/4	0.87	0.21	46,60,81,81	0
7	GOL	C	1126	6/6	0.88	0.14	54,64,72,77	0
6	EDO	A	1106	4/4	0.88	0.17	51,64,75,76	0
14	SO4	B	1215	5/5	0.88	0.11	51,63,83,89	0
3	LMT	C	1105	35/35	0.88	0.15	55,73,94,98	0
7	GOL	B	1210	6/6	0.88	0.16	42,51,70,75	0
7	GOL	A	1116	6/6	0.88	0.17	46,56,69,79	0
4	OCT	C	1122	8/8	0.89	0.19	57,70,80,80	0
7	GOL	D	202	6/6	0.90	0.14	61,73,79,82	0
7	GOL	D	203	6/6	0.90	0.17	50,68,81,82	0
6	EDO	B	1228	4/4	0.90	0.13	55,66,75,83	0
14	SO4	C	1115	5/5	0.90	0.10	66,67,77,78	0
7	GOL	C	1117	6/6	0.90	0.14	39,57,68,72	0
7	GOL	A	1111	6/6	0.90	0.13	43,70,83,84	0
6	EDO	B	1206	4/4	0.90	0.17	35,70,77,85	0
6	EDO	C	1112	4/4	0.91	0.18	48,57,70,70	0
6	EDO	B	1213	4/4	0.91	0.18	68,82,88,93	0
7	GOL	A	1115	6/6	0.93	0.12	34,45,62,65	0
7	GOL	A	1127	6/6	0.93	0.11	38,51,66,68	0
7	GOL	A	1125	6/6	0.93	0.12	35,52,63,69	0
10	XE9	A	1122	25/25	0.94	0.13	50,67,91,94	0
7	GOL	C	1111	6/6	0.95	0.09	38,51,63,63	0

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

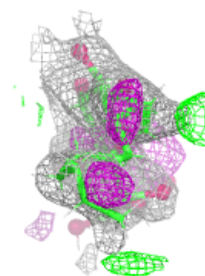
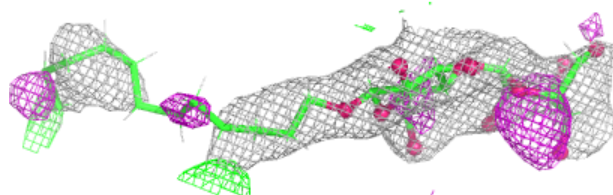
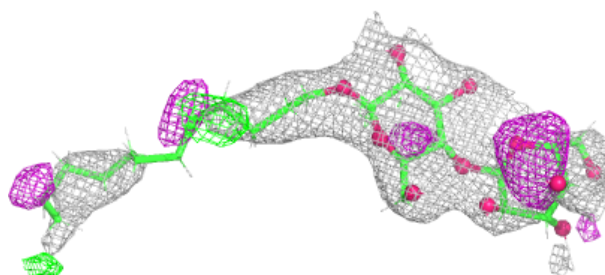
Electron density around LMT C 1110:

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

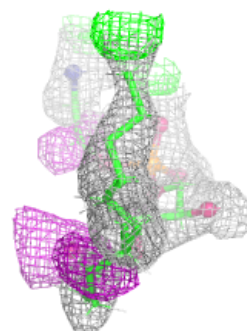
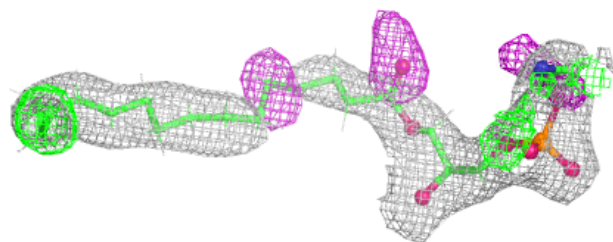
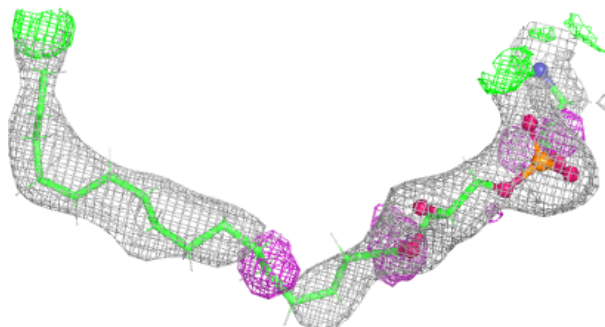


Electron density around LMT B 1203:

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

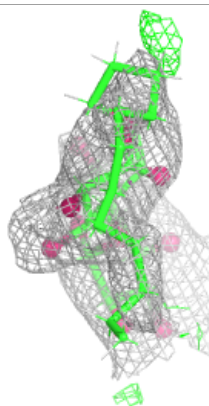
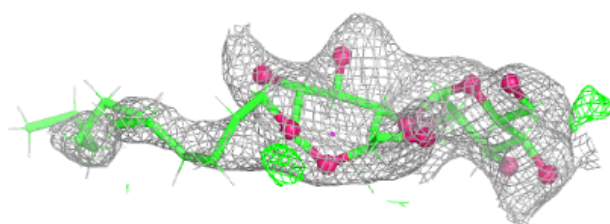
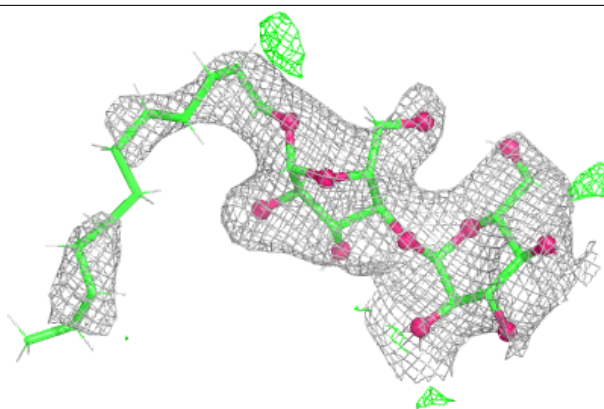
**Electron density around LPX C 1107:**

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

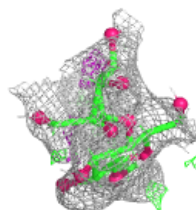
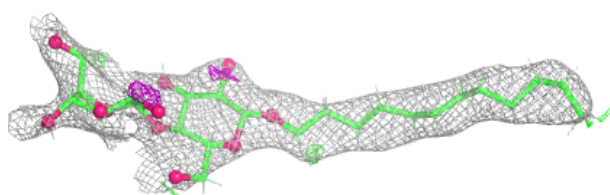
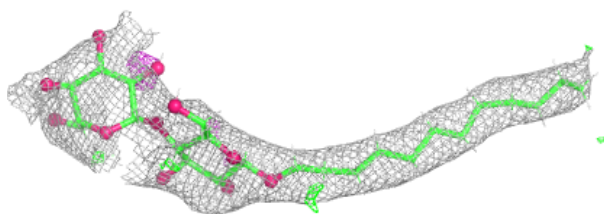


Electron density around LMT A 1102:

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

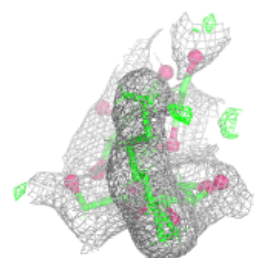
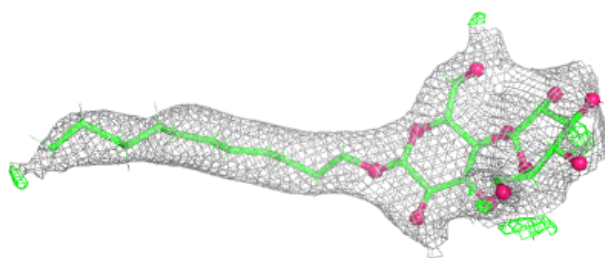
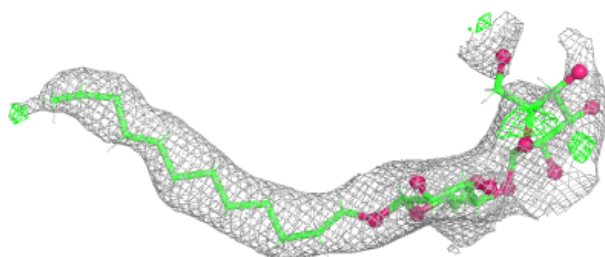
**Electron density around LMT B 1209:**

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

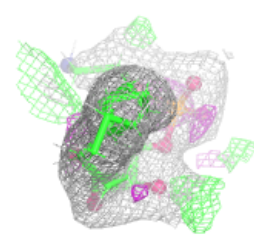
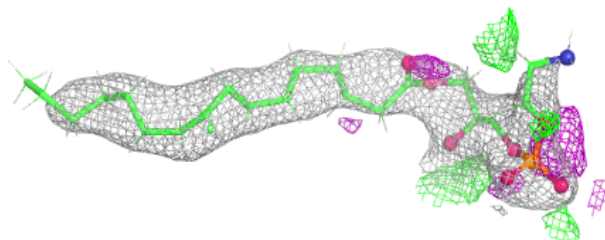
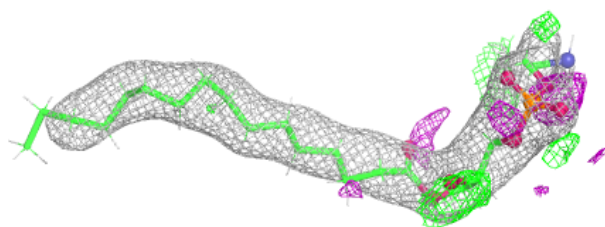


Electron density around LMT A 1105:

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

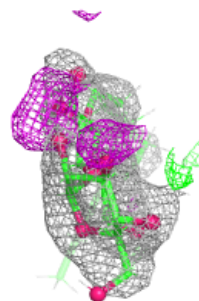
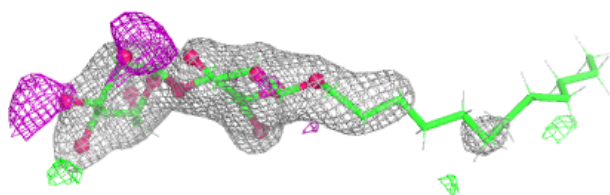
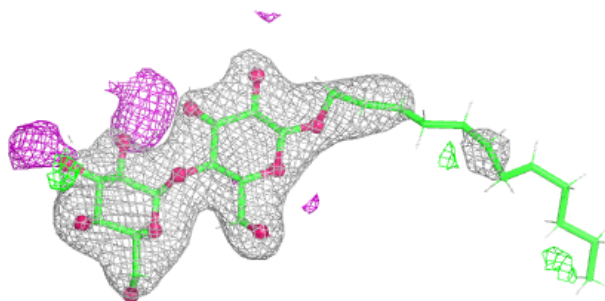
**Electron density around LPX C 1109:**

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

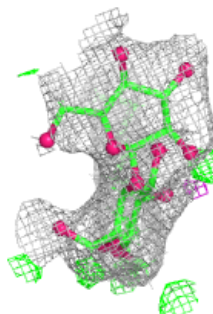
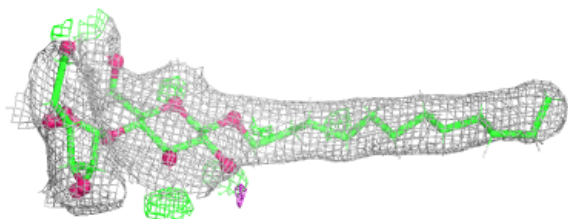
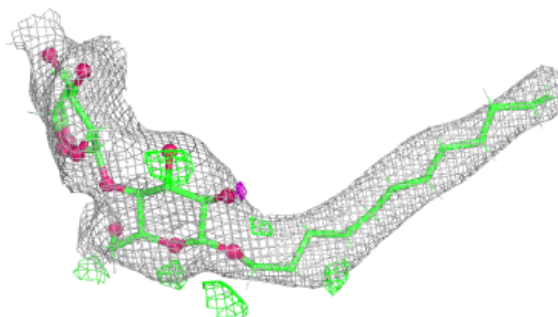


Electron density around LMT B 1202:

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

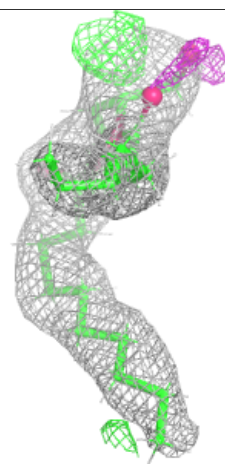
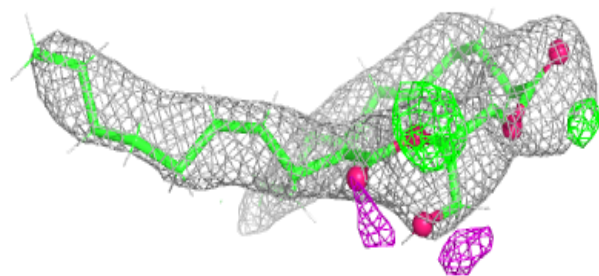
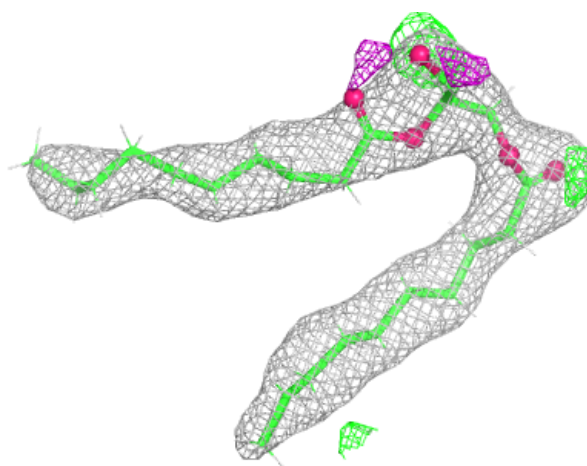
**Electron density around LMT A 1101:**

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



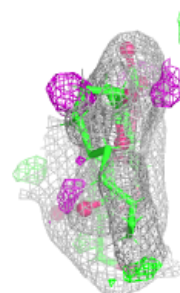
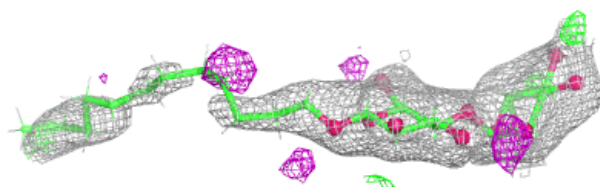
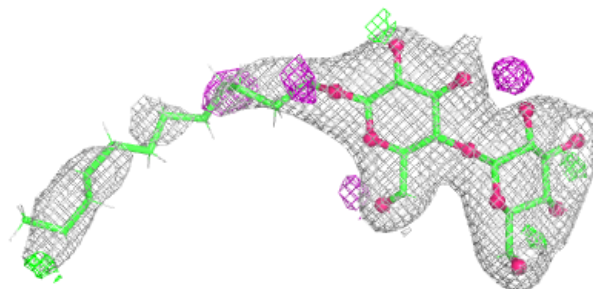
Electron density around DDR B 1207:

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

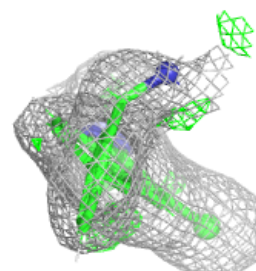
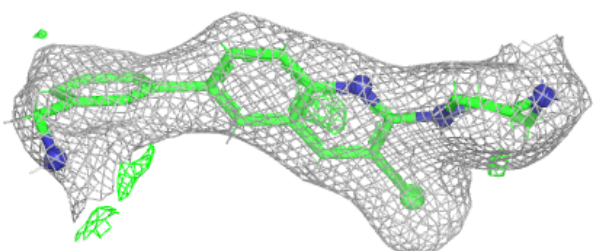
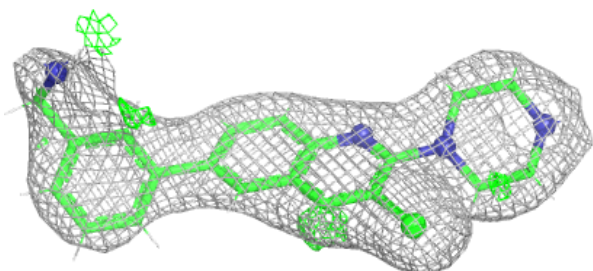


Electron density around LMT C 1105:

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

**Electron density around XE9 A 1122:**

$2mF_o-DF_c$ (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.