



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 05:27 AM UTC

PDB ID : 6ZOB / pdb_00006zob
Title : 3-Formylrifamycin SV binding to the access pocket of AcrB L protomer
Authors : Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.80 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

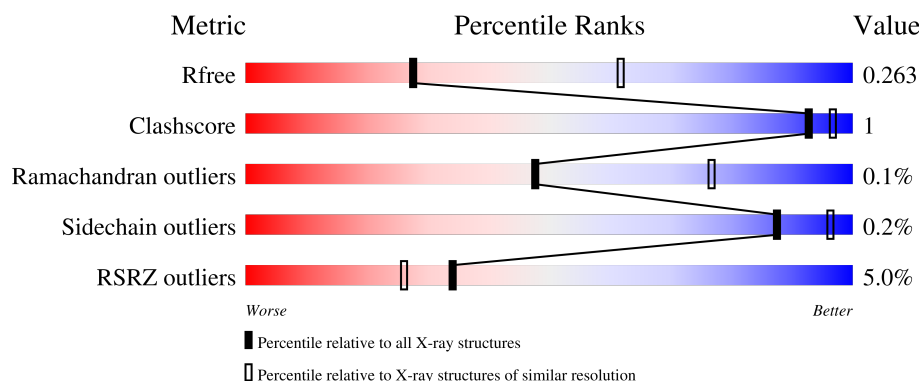
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	5% 93% 5%
1	B	1057	8% 93% 5%
1	C	1057	2% 93% 5%
2	D	169	2% 91% 9%
2	E	169	4% 88% 9%

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26439 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	1035	Total	C	N	O	S	0	0	0
			7866	5061	1300	1461	44			
1	B	1034	Total	C	N	O	S	0	0	0
			7855	5055	1296	1460	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	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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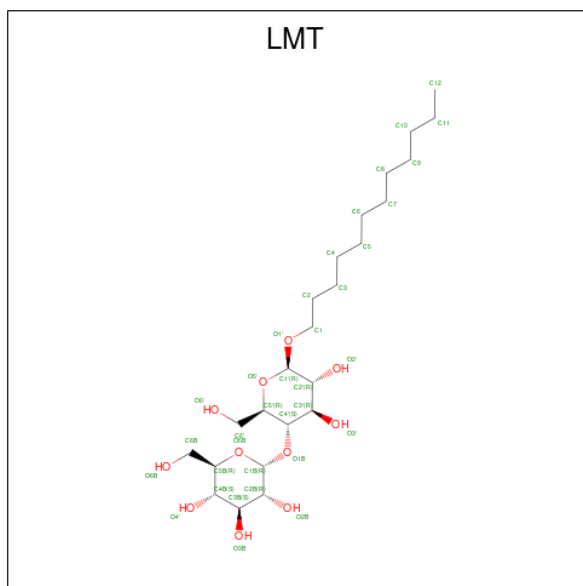
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

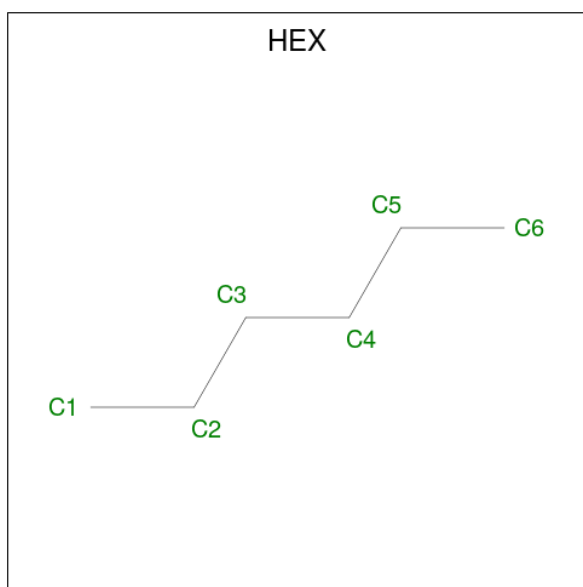
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			
2	E	154	Total	C	N	O	S	0	1	0
			1178	742	208	227	1			

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



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

- Molecule 4 is HEXANE (CCD ID: HEX) (formula: C_6H_{14}).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



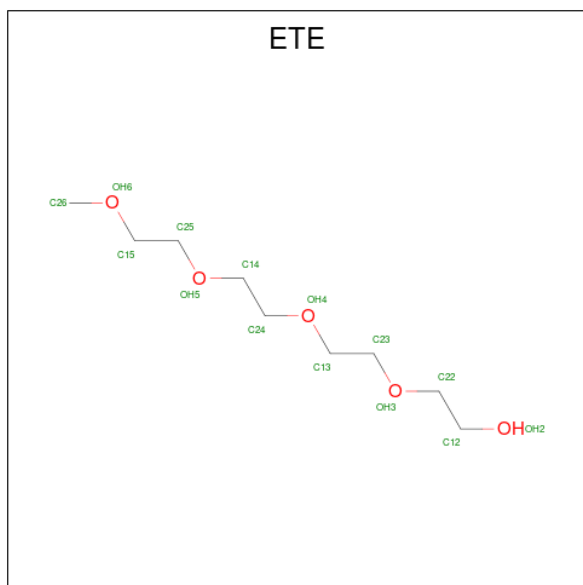
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

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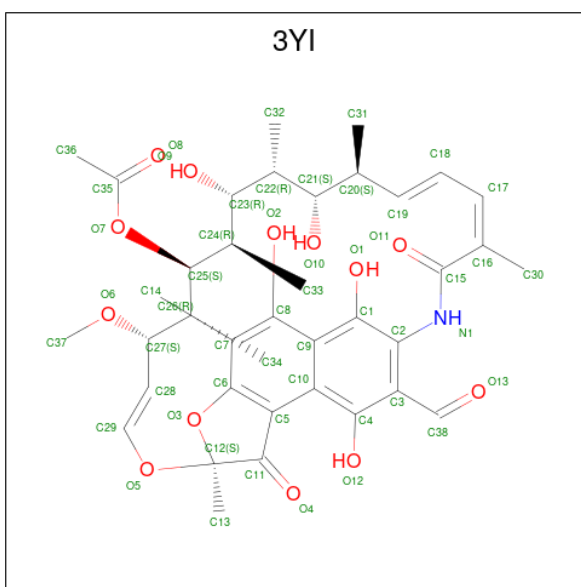
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is 2-{2-[2-2-(METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (CCD ID: ETE) (formula: C₉H₂₀O₅).



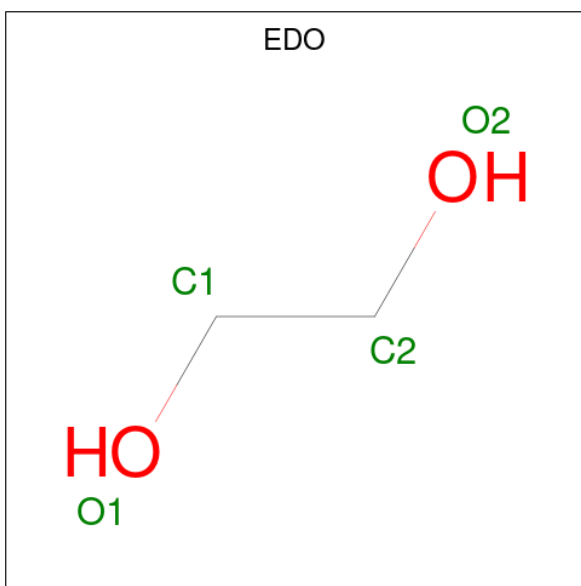
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			14	9	5		

- Molecule 7 is (2S,12Z,14E,16S,17S,18R,19R,20R,21S,22R,23S,24E)-8-formyl-5,6,9,17,19-pentahydroxy-23-methoxy-2,4,12,16,18,20,22-heptamethyl-1,11-dioxo-1,2-dihydro-2,7-(epoxypentadeca[1,11,13]trienoimino)naphtho[2,1-b]furan-21-yl acetate (CCD ID: 3YI) (formula: C₃₈H₄₇NO₁₃) (labeled as "Ligand of Interest" by depositor).



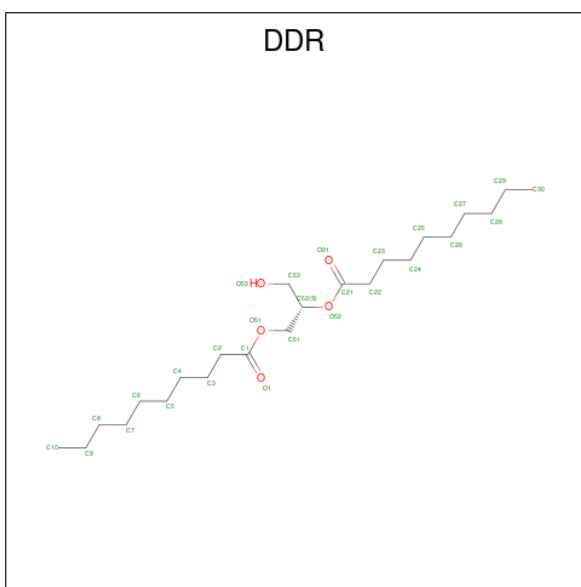
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			52	38	1	13		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



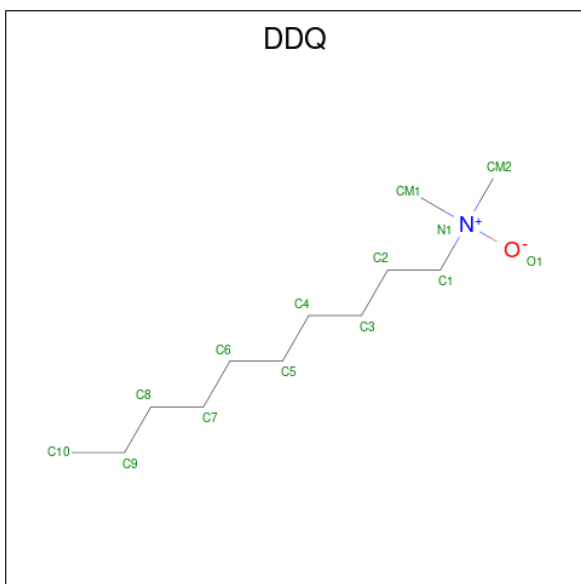
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is (2S)-3-hydroxypropane-1,2-diyl didecanoate (CCD ID: DDR) (formula: $C_{23}H_{44}O_5$).



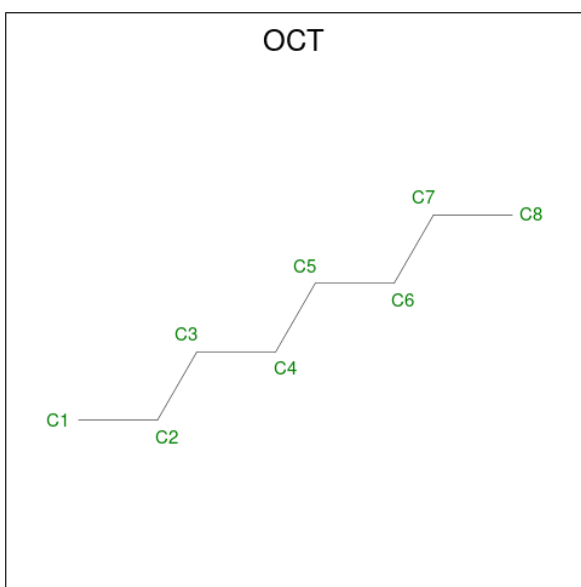
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 10 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (CCD ID: DDQ) (formula: $C_{12}H_{27}NO$).



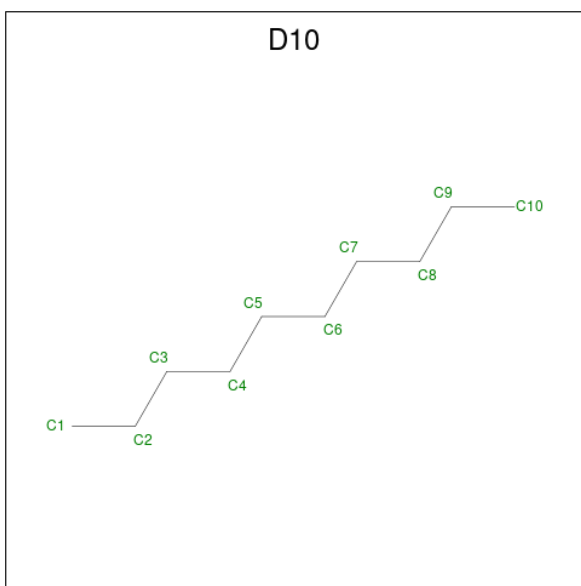
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	N	O	0	0
			14	12	1	1		

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



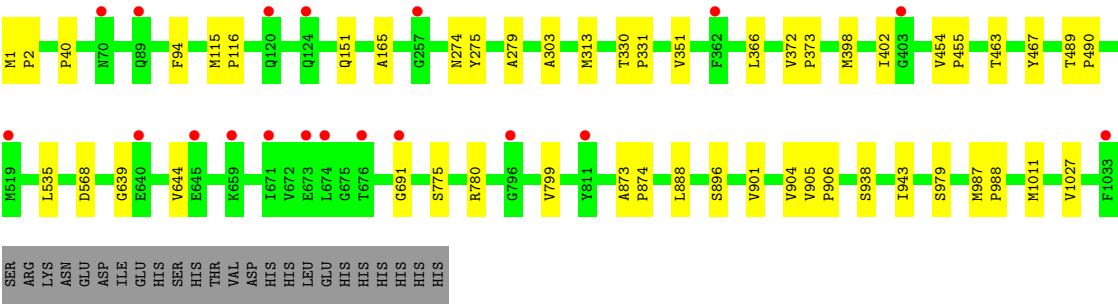
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C 10 10	0	0

- Molecule 13 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

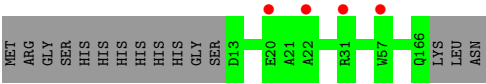
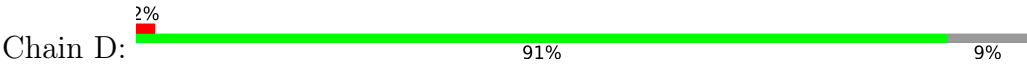
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	C	1	Total	Cl	0	0
			1	1		

- Molecule 14 is water.

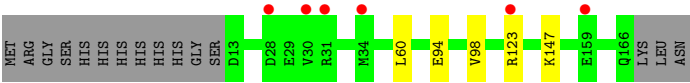
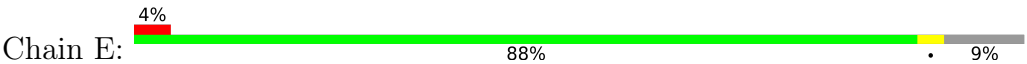
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	62	Total	O	0	0
			62	62		
14	B	30	Total	O	0	0
			30	30		
14	C	51	Total	O	0	0
			51	51		
14	D	2	Total	O	0	0
			2	2		
14	E	8	Total	O	0	0
			8	8		



● 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	145.36Å 160.19Å 244.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.80 49.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.15-2.80) 100.0 (49.15-2.80)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.262 0.240 , 0.263	Depositor DCC
R_{free} test set	6895 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.8	Xtriage
Anisotropy	0.709	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	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	26439	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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: DDQ, D10, 3YI, GOL, OCT, CL, ETE, DDR, LMT, EDO, HEX

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	0/8016	1.57	6/10885 (0.1%)
1	B	1.04	0/8005	1.58	5/10871 (0.0%)
1	C	1.04	1/7999 (0.0%)	1.57	6/10863 (0.1%)
2	D	1.03	0/1186	1.60	0/1613
2	E	1.03	0/1197	1.58	0/1627
All	All	1.04	1/26403 (0.0%)	1.57	17/35859 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	799	VAL	N-CA	5.22	1.50	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	SER	CA-C-N	7.42	124.91	120.24
1	B	896	SER	C-N-CA	7.42	124.91	120.24
1	A	896	SER	CA-C-N	7.17	124.76	120.24
1	A	896	SER	C-N-CA	7.17	124.76	120.24
1	C	366	LEU	CA-C-N	5.83	125.00	120.33
1	C	366	LEU	C-N-CA	5.83	125.00	120.33
1	C	691	GLY	CA-C-O	-5.67	118.23	122.37
1	A	675	GLY	CA-C-O	-5.61	118.27	122.37
1	C	639	GLY	CA-C-O	-5.57	118.39	122.23
1	A	621	GLY	CA-C-O	-5.56	118.31	122.37
1	C	896	SER	CA-C-N	5.52	124.75	120.33
1	C	896	SER	C-N-CA	5.52	124.75	120.33
1	B	984	LEU	CA-C-N	5.12	125.62	119.94
1	B	984	LEU	C-N-CA	5.12	125.62	119.94
1	A	538	THR	CA-C-N	5.04	125.69	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	THR	C-N-CA	5.04	125.69	119.99
1	B	621	GLY	CA-C-O	-5.02	118.26	122.33

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	7866	0	8019	27	0
1	B	7855	0	8006	26	0
1	C	7849	0	8001	25	0
2	D	1167	0	1151	0	0
2	E	1178	0	1163	4	0
3	A	140	0	184	0	0
3	B	35	0	46	0	0
3	C	35	0	46	0	0
4	A	6	0	14	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	14	0	20	0	0
7	A	52	0	0	1	0
8	A	4	0	6	0	0
9	B	28	0	44	0	0
10	B	14	0	27	1	0
11	B	8	0	18	0	0
12	C	10	0	22	0	0
13	C	1	0	0	0	0
14	A	62	0	0	0	0
14	B	30	0	0	0	0
14	C	51	0	0	0	0
14	D	2	0	0	0	0
14	E	8	0	0	0	0
All	All	26439	0	26799	79	0

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

All (79) 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:367:ILE:HB	1:A:368:PRO:HD3	1.81	0.62
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.82	0.61
1:C:151:GLN:NE2	1:C:279:ALA:O	2.36	0.58
1:B:344:LEU:HD22	1:B:402:ILE:HD13	1.85	0.56
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.86	0.56
1:C:115:MET:N	1:C:116:PRO:HD2	2.21	0.56
2:E:94:GLU:O	2:E:98:VAL:HG23	2.07	0.55
1:C:901:VAL:O	1:C:904:VAL:HG12	2.08	0.54
1:A:968:VAL:HG11	1:A:1023:PRO:HG3	1.90	0.53
1:B:355:MET:HE1	1:B:413:VAL:HG11	1.91	0.53
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.93	0.50
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.92	0.50
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.11	0.50
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.41	0.50
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.27	0.50
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.95	0.48
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.95	0.48
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.94	0.48
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.94	0.48
1:B:987:MET:N	1:B:988:PRO:CD	2.76	0.48
1:A:247:GLY:HA2	1:A:268:ILE:HD13	1.96	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.94	0.48
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.96	0.47
1:A:777:ALA:O	1:A:781:MET:HG2	2.15	0.47
1:B:399:VAL:O	1:B:402:ILE:HG22	2.15	0.46
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.41	0.46
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.97	0.46
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	1.98	0.45
1:C:165:ALA:HB3	1:C:313:MET:CE	2.47	0.45
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.98	0.45
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.97	0.45
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.99	0.45
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.80	0.45
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.45
2:E:60:LEU:HD11	2:E:98:VAL:HG21	1.98	0.45
1:C:330:THR:N	1:C:331:PRO:CD	2.80	0.44
1:A:8:ARG:HD3	10:B:1103:DDQ:HM11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:TRP:CD2	1:B:995:ALA:HB2	2.51	0.44
1:B:897:ILE:N	1:B:898:PRO:HD2	2.31	0.44
1:A:509:LYS:O	1:A:514:GLY:HA3	2.18	0.44
1:B:573:MET:HE2	1:B:668:LEU:HD23	1.99	0.44
1:A:454:VAL:N	1:A:455:PRO:CD	2.81	0.44
1:C:40:PRO:HB2	1:C:94:PHE:O	2.17	0.44
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.99	0.44
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:B:873:ALA:HB3	1:B:874:PRO:HD3	2.00	0.43
1:A:176:GLN:HG2	1:A:615:PHE:CE2	2.54	0.43
7:A:1208:3YI:O12	7:A:1208:3YI:O4	2.36	0.43
1:C:873:ALA:HB3	1:C:874:PRO:HD3	1.99	0.43
1:A:631:LEU:HD11	1:A:644:VAL:HG22	2.01	0.43
1:A:406:VAL:HG12	1:A:410:ILE:HD12	2.00	0.43
1:B:223:PRO:HD3	1:C:275:TYR:CD1	2.53	0.42
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.54	0.42
1:A:734:GLU:OE2	2:E:147:LYS:NZ	2.42	0.42
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.20	0.42
1:A:178:PHE:HA	1:A:277:ILE:HG21	2.01	0.42
1:B:573:MET:HE2	1:B:668:LEU:CD2	2.49	0.42
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.54	0.42
1:C:775:SER:HB3	1:C:780:ARG:HD3	2.01	0.42
1:C:979:SER:HA	1:C:1011:MET:HE3	2.01	0.42
1:B:489:THR:N	1:B:490:PRO:CD	2.83	0.42
1:B:897:ILE:N	1:B:898:PRO:CD	2.83	0.42
1:A:901:VAL:O	1:A:904:VAL:HG22	2.20	0.41
1:C:303:ALA:HB2	1:C:330:THR:HG21	2.01	0.41
2:E:123[B]:ARG:HD3	2:E:123[B]:ARG:HA	1.81	0.41
1:B:314:GLU:N	1:B:315:PRO:CD	2.83	0.41
1:B:340:VAL:O	1:B:344:LEU:HG	2.21	0.41
1:A:897:ILE:N	1:A:898:PRO:CD	2.84	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.21	0.41
1:C:398:MET:O	1:C:402:ILE:HG12	2.20	0.41
1:C:904:VAL:HG13	1:C:938:SER:HB3	2.01	0.41
1:C:489:THR:HB	1:C:490:PRO:HD3	2.02	0.41
1:A:763:ILE:HD11	1:B:59:ASP:HB3	2.02	0.41
1:C:1:MET:HB3	1:C:2:PRO:HD3	2.02	0.41
1:A:699:ARG:HD2	1:A:718:PRO:HB3	2.03	0.40
1:A:987:MET:N	1:A:988:PRO:CD	2.85	0.40
1:C:888:LEU:HD21	1:C:943:ILE:HD11	2.04	0.40
1:B:973:ARG:N	1:B:974:PRO:HD2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:HA	1:A:987:MET:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1033/1057 (98%)	999 (97%)	32 (3%)	2 (0%)	43	72
1	B	1032/1057 (98%)	1005 (97%)	25 (2%)	2 (0%)	43	72
1	C	1031/1057 (98%)	1004 (97%)	27 (3%)	0	100	100
2	D	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
2	E	153/169 (90%)	149 (97%)	4 (3%)	0	100	100
All	All	3401/3509 (97%)	3304 (97%)	93 (3%)	4 (0%)	48	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	868	LEU
1	A	1034	SER
1	B	134	SER
1	B	216	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	841/863 (98%)	840 (100%)	1 (0%)	88	97
1	B	840/863 (97%)	837 (100%)	3 (0%)	84	94
1	C	839/863 (97%)	838 (100%)	1 (0%)	88	97
2	D	119/132 (90%)	119 (100%)	0	100	100
2	E	120/132 (91%)	120 (100%)	0	100	100
All	All	2759/2853 (97%)	2754 (100%)	5 (0%)	87	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	973	ARG
1	B	84	SER
1	B	321	LEU
1	B	801	PHE
1	C	274	ASN

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	68	ASN
1	A	81	ASN
1	A	161	ASN
1	A	194	ASN
1	A	588	GLN
1	A	737	GLN
1	B	176	GLN
1	B	194	ASN
1	B	231	ASN
1	B	284	GLN
1	B	577	GLN
1	B	923	ASN
1	C	68	ASN
1	C	89	GLN
1	C	194	ASN
1	C	584	GLN
1	C	1001	ASN
2	D	59	HIS
2	D	92	HIS
2	E	59	HIS
2	E	125	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 for Mogul analysis.

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
3	LMT	A	1206	-	36,36,36	0.51	1 (2%)	47,47,47	0.72	0
5	GOL	C	1103	-	5,5,5	0.08	0	5,5,5	0.23	0
7	3YI	A	1208	-	55,55,55	0.99	2 (3%)	82,83,83	1.49	7 (8%)
5	GOL	B	1105	-	5,5,5	0.10	0	5,5,5	0.25	0
6	ETE	A	1207	-	13,13,13	0.18	0	12,12,12	0.10	0
3	LMT	A	1201	-	36,36,36	0.46	0	47,47,47	0.63	0
4	HEX	A	1204	-	5,5,5	0.13	0	4,4,4	0.15	0
5	GOL	D	201	-	5,5,5	0.09	0	5,5,5	0.25	0
8	EDO	A	1209	-	3,3,3	0.07	0	2,2,2	0.12	0
9	DDR	B	1102	-	27,27,27	0.24	0	29,29,29	0.27	0
11	OCT	B	1104	-	7,7,7	0.10	0	6,6,6	0.06	0
3	LMT	B	1101	-	36,36,36	0.48	1 (2%)	47,47,47	0.64	0
5	GOL	A	1205	-	5,5,5	0.09	0	5,5,5	0.31	0
10	DDQ	B	1103	-	11,13,13	0.16	0	12,15,15	0.18	0
3	LMT	A	1203	-	36,36,36	0.48	1 (2%)	47,47,47	0.67	0
12	D10	C	1102	-	9,9,9	0.09	0	8,8,8	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	C	1101	-	36,36,36	0.47	0	47,47,47	0.86	3 (6%)
3	LMT	A	1202	-	36,36,36	0.47	0	47,47,47	0.63	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
3	LMT	A	1206	-	-	14/21/61/61	0/2/2/2
5	GOL	C	1103	-	-	0/4/4/4	-
7	3YI	A	1208	-	-	13/57/72/72	0/4/4/4
5	GOL	B	1105	-	-	0/4/4/4	-
6	ETE	A	1207	-	-	7/11/11/11	-
3	LMT	A	1201	-	-	12/21/61/61	0/2/2/2
4	HEX	A	1204	-	-	1/3/3/3	-
5	GOL	D	201	-	-	2/4/4/4	-
8	EDO	A	1209	-	-	1/1/1/1	-
9	DDR	B	1102	-	-	13/29/29/29	-
11	OCT	B	1104	-	-	4/5/5/5	-
3	LMT	B	1101	-	-	10/21/61/61	0/2/2/2
5	GOL	A	1205	-	-	4/4/4/4	-
10	DDQ	B	1103	-	-	7/11/11/11	-
3	LMT	A	1203	-	-	11/21/61/61	0/2/2/2
12	D10	C	1102	-	-	4/7/7/7	-
3	LMT	C	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1202	-	-	6/21/61/61	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1208	3YI	C15-N1	4.26	1.44	1.35
7	A	1208	3YI	C14-C7	-2.19	1.47	1.51
3	A	1206	LMT	O1'-C1'	2.03	1.43	1.40
3	B	1101	LMT	O1'-C1'	2.02	1.43	1.40
3	A	1203	LMT	O1'-C1'	2.00	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1208	3YI	C2-C3-C4	6.41	123.26	119.19
7	A	1208	3YI	C4-C3-C38	-4.61	113.50	119.83
7	A	1208	3YI	C3-C2-C1	-3.61	118.12	120.68
3	C	1101	LMT	C1B-O5B-C5B	3.41	120.39	113.72
7	A	1208	3YI	O7-C35-C36	2.93	116.31	111.09
7	A	1208	3YI	C3-C4-C10	-2.44	119.21	121.19
7	A	1208	3YI	O4-C11-C12	2.26	125.11	120.56
3	C	1101	LMT	C3B-C4B-C5B	2.25	114.32	110.23
3	C	1101	LMT	O5B-C5B-C4B	2.16	113.59	109.70
7	A	1208	3YI	C2-N1-C15	-2.07	117.76	124.06

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1205	GOL	C1-C2-C3-O3
5	D	201	GOL	C1-C2-C3-O3
7	A	1208	3YI	C26-C27-O6-C37
7	A	1208	3YI	C28-C27-O6-C37
7	A	1208	3YI	C25-C26-C27-O6
7	A	1208	3YI	C25-C26-C27-C28
7	A	1208	3YI	C34-C26-C27-O6
7	A	1208	3YI	C34-C26-C27-C28
10	B	1103	DDQ	C2-C1-N1-CM1
10	B	1103	DDQ	N1-C1-C2-C3
7	A	1208	3YI	C36-C35-O7-C25
3	A	1206	LMT	O5B-C1B-O1B-C4'
9	B	1102	DDR	O21-C21-O52-C52
9	B	1102	DDR	O1-C1-O51-C51
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	A	1202	LMT	O5'-C5'-C6'-O6'
9	B	1102	DDR	C2-C1-O51-C51
3	A	1203	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C5'-C6'-O6'
9	B	1102	DDR	C22-C21-O52-C52
3	A	1206	LMT	C2B-C1B-O1B-C4'
3	A	1202	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	A	1203	LMT	C4B-C5B-C6B-O6B
3	A	1202	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
6	A	1207	ETE	OH6-C15-C25-OH5
6	A	1207	ETE	OH5-C14-C24-OH4

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Mol	Chain	Res	Type	Atoms
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	C	1101	LMT	C4B-C5B-C6B-O6B
7	A	1208	3YI	O8-C35-O7-C25
3	A	1202	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	C2'-C1'-O1'-C1
3	A	1206	LMT	C2'-C1'-O1'-C1
5	A	1205	GOL	O1-C1-C2-C3
3	A	1206	LMT	O5'-C1'-O1'-C1
7	A	1208	3YI	C18-C19-C20-C31
3	A	1206	LMT	C4-C5-C6-C7
5	A	1205	GOL	O1-C1-C2-O2
5	D	201	GOL	O2-C2-C3-O3
3	A	1206	LMT	C2-C3-C4-C5
11	B	1104	OCT	C3-C4-C5-C6
9	B	1102	DDR	C2-C3-C4-C5
3	A	1206	LMT	C1-C2-C3-C4
7	A	1208	3YI	C4-C3-C38-O13
3	A	1203	LMT	C5-C6-C7-C8
10	B	1103	DDQ	C3-C4-C5-C6
3	C	1101	LMT	C5-C6-C7-C8
8	A	1209	EDO	O1-C1-C2-O2
3	A	1203	LMT	C7-C8-C9-C10
3	C	1101	LMT	C2-C3-C4-C5
10	B	1103	DDQ	C2-C3-C4-C5
12	C	1102	D10	C2-C3-C4-C5
3	A	1201	LMT	O1'-C1-C2-C3
10	B	1103	DDQ	C1-C2-C3-C4
12	C	1102	D10	C3-C4-C5-C6
7	A	1208	3YI	C16-C17-C18-C19
3	C	1101	LMT	C11-C10-C9-C8
3	A	1201	LMT	C5-C6-C7-C8
3	A	1206	LMT	O5'-C5'-C6'-O6'
11	B	1104	OCT	C4-C5-C6-C7
3	C	1101	LMT	O1'-C1-C2-C3
3	A	1203	LMT	O5'-C5'-C6'-O6'
3	C	1101	LMT	C9-C10-C11-C12
9	B	1102	DDR	C27-C28-C29-C30
11	B	1104	OCT	C2-C3-C4-C5
3	B	1101	LMT	O1'-C1-C2-C3
3	A	1206	LMT	C7-C8-C9-C10
3	A	1202	LMT	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
4	A	1204	HEX	C3-C4-C5-C6
3	A	1201	LMT	C2-C1-O1'-C1'
3	A	1203	LMT	C2-C1-O1'-C1'
3	A	1206	LMT	C2-C1-O1'-C1'
9	B	1102	DDR	C3-C4-C5-C6
3	C	1101	LMT	C3-C4-C5-C6
9	B	1102	DDR	C26-C27-C28-C29
3	A	1202	LMT	C7-C8-C9-C10
3	B	1101	LMT	C11-C10-C9-C8
6	A	1207	ETE	C14-C24-OH4-C13
9	B	1102	DDR	C6-C7-C8-C9
9	B	1102	DDR	C24-C25-C26-C27
12	C	1102	D10	C1-C2-C3-C4
10	B	1103	DDQ	C5-C6-C7-C8
3	B	1101	LMT	C5-C6-C7-C8
6	A	1207	ETE	C15-C25-OH5-C14
3	A	1201	LMT	C3'-C4'-O1B-C1B
3	A	1203	LMT	C9-C10-C11-C12
3	A	1201	LMT	C5'-C4'-O1B-C1B
3	A	1201	LMT	O5B-C1B-O1B-C4'
6	A	1207	ETE	C13-C23-OH3-C22
5	A	1205	GOL	O2-C2-C3-O3
3	A	1203	LMT	C2-C3-C4-C5
3	C	1101	LMT	C1-C2-C3-C4
9	B	1102	DDR	C1-C2-C3-C4
3	A	1201	LMT	C2B-C1B-O1B-C4'
6	A	1207	ETE	OH4-C13-C23-OH3
11	B	1104	OCT	C1-C2-C3-C4
3	A	1201	LMT	C3-C4-C5-C6
3	B	1101	LMT	C6-C7-C8-C9
3	A	1201	LMT	C7-C8-C9-C10
3	A	1203	LMT	O5'-C1'-O1'-C1
7	A	1208	3YI	C18-C19-C20-C21
3	A	1201	LMT	C11-C10-C9-C8
3	A	1203	LMT	C6-C7-C8-C9
6	A	1207	ETE	OH2-C12-C22-OH3
3	A	1201	LMT	C9-C10-C11-C12
3	A	1206	LMT	O1'-C1-C2-C3
3	A	1206	LMT	C9-C10-C11-C12
3	A	1206	LMT	C5'-C4'-O1B-C1B
12	C	1102	D10	C6-C7-C8-C9
10	B	1103	DDQ	C2-C1-N1-CM2

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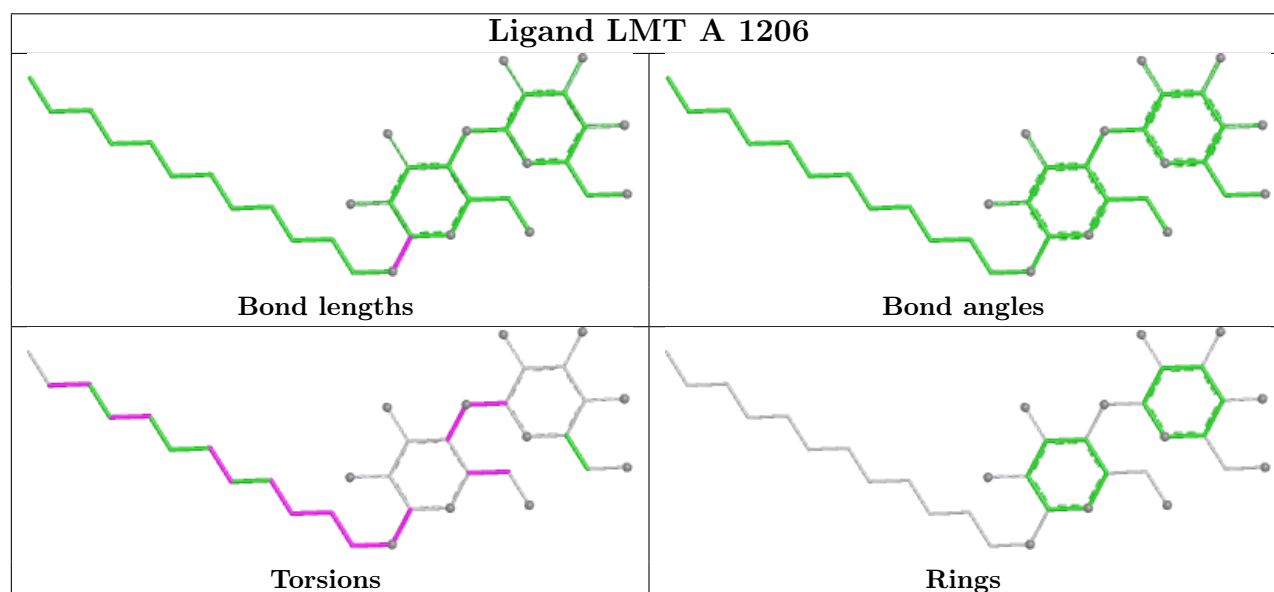
Mol	Chain	Res	Type	Atoms
3	A	1206	LMT	C3'-C4'-O1B-C1B
9	B	1102	DDR	O51-C1-C2-C3
7	A	1208	3YI	O6-C27-C28-C29
3	A	1203	LMT	C4'-C5'-C6'-O6'
9	B	1102	DDR	O1-C1-C2-C3
3	A	1201	LMT	C2-C3-C4-C5

There are no ring outliers.

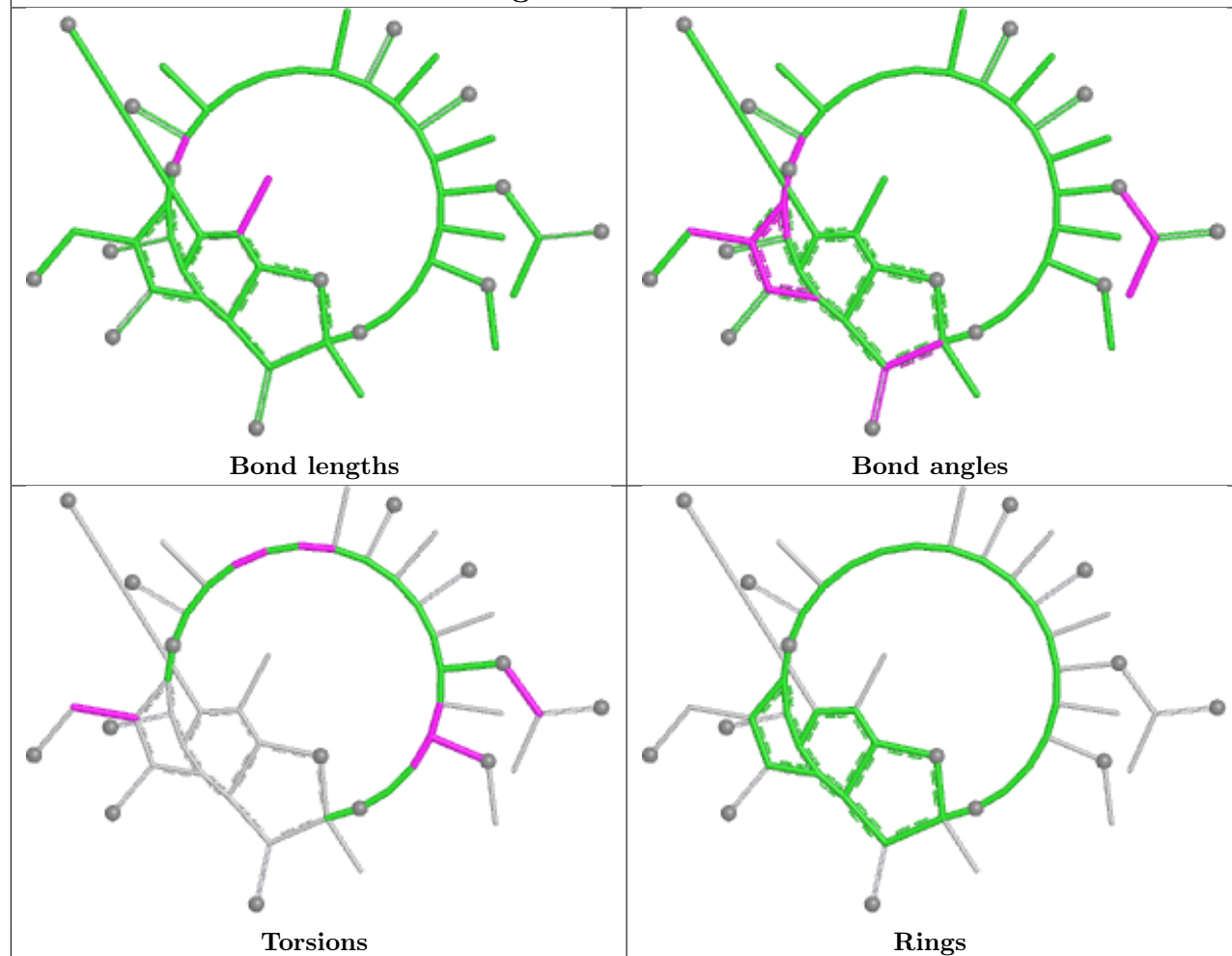
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1208	3YI	1	0
10	B	1103	DDQ	1	0

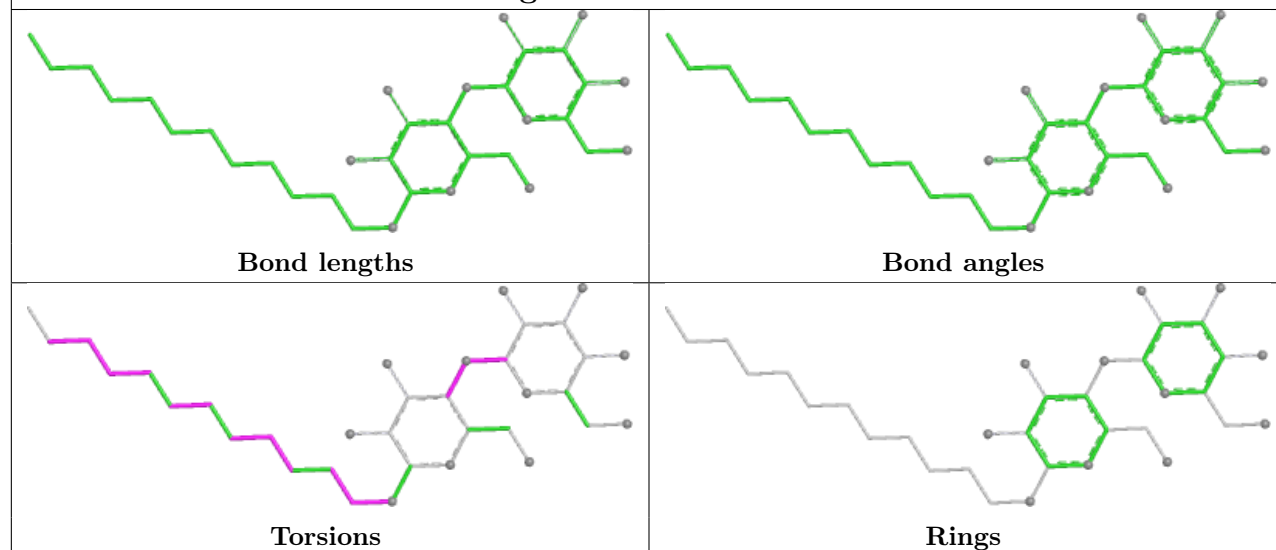
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

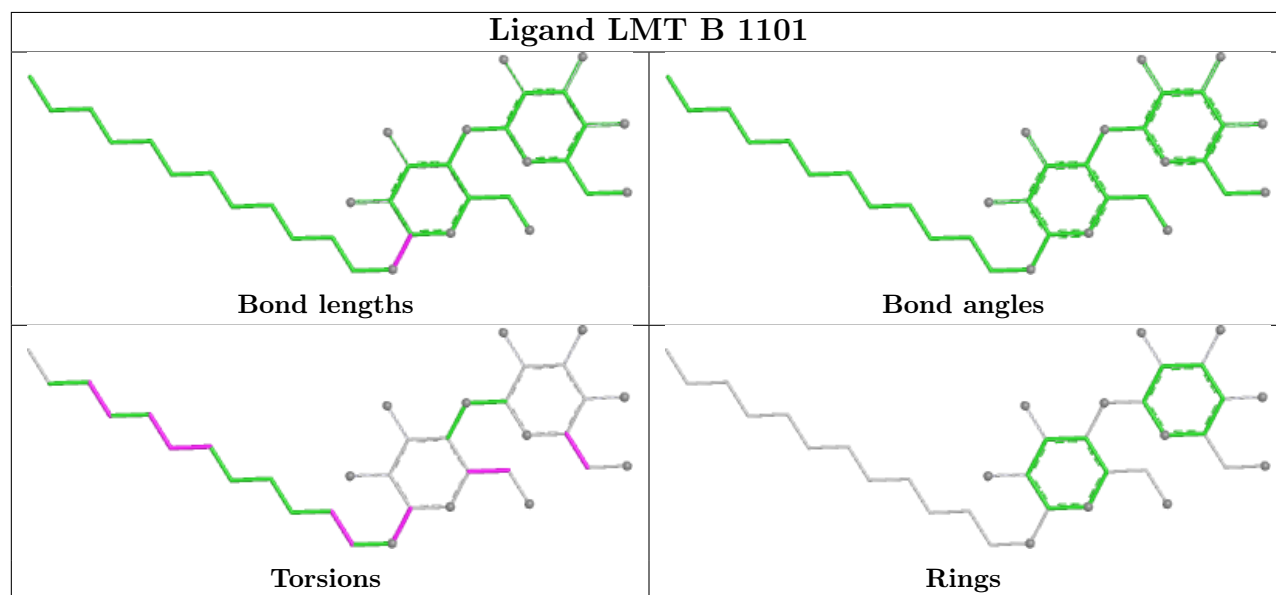
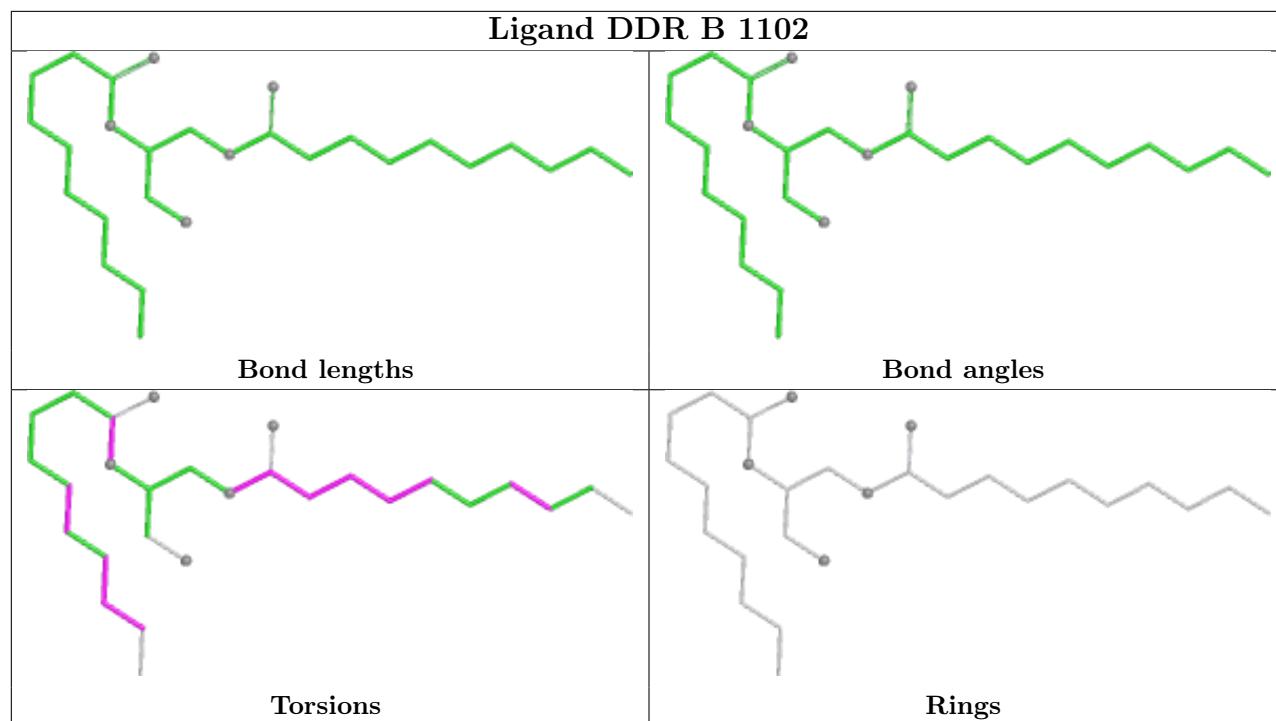


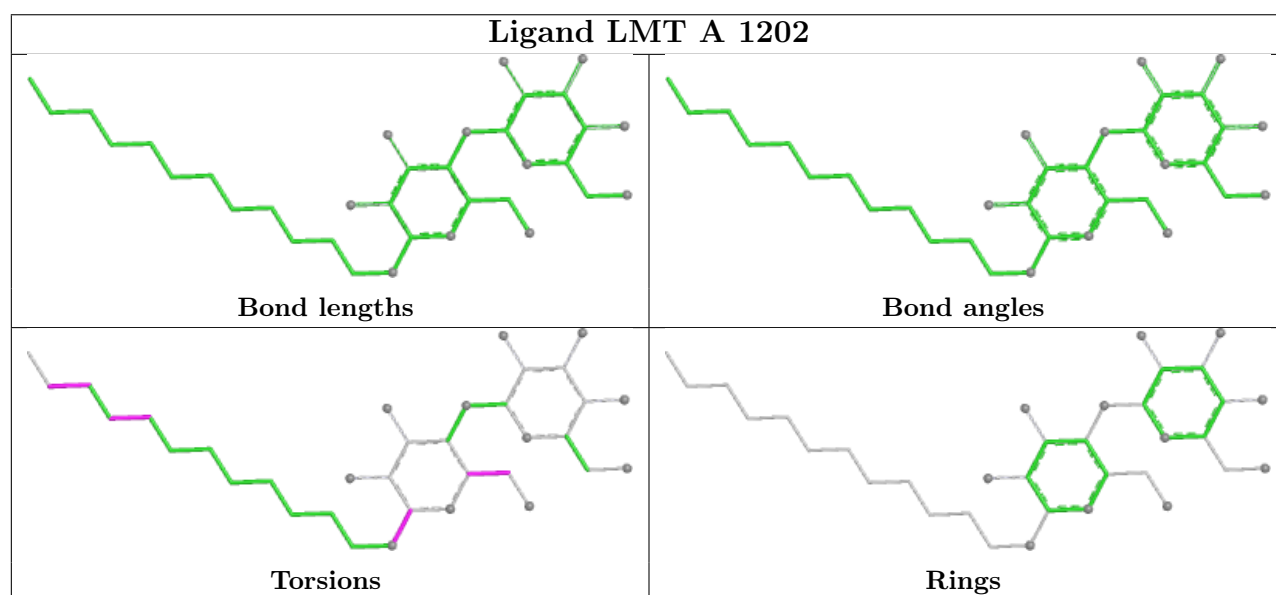
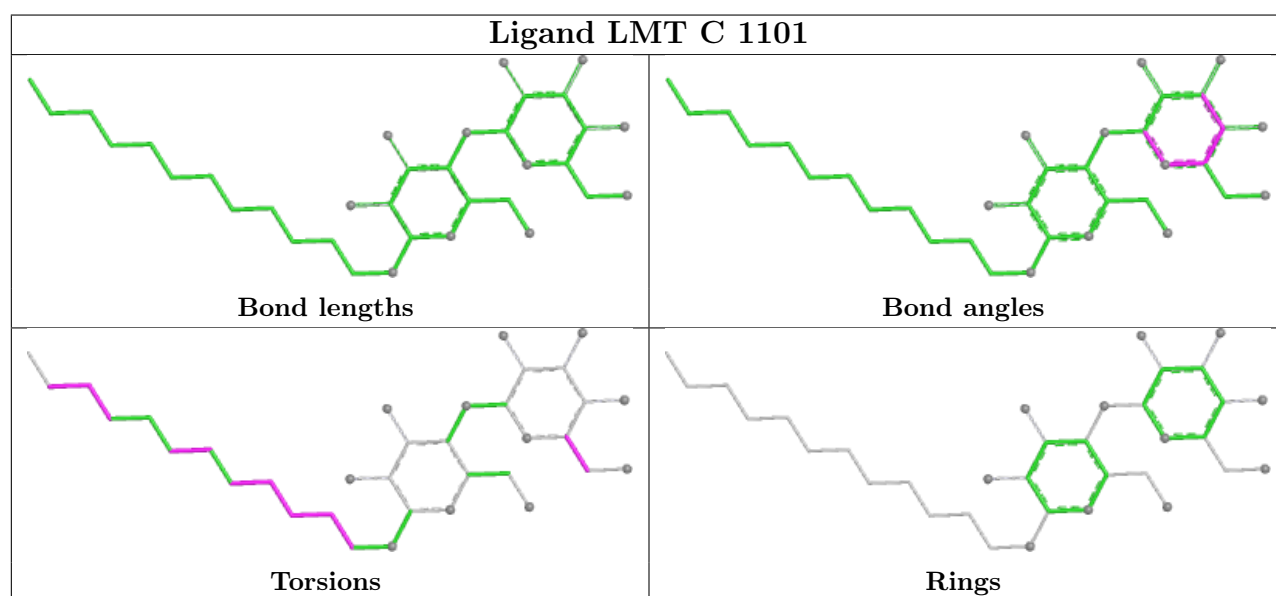
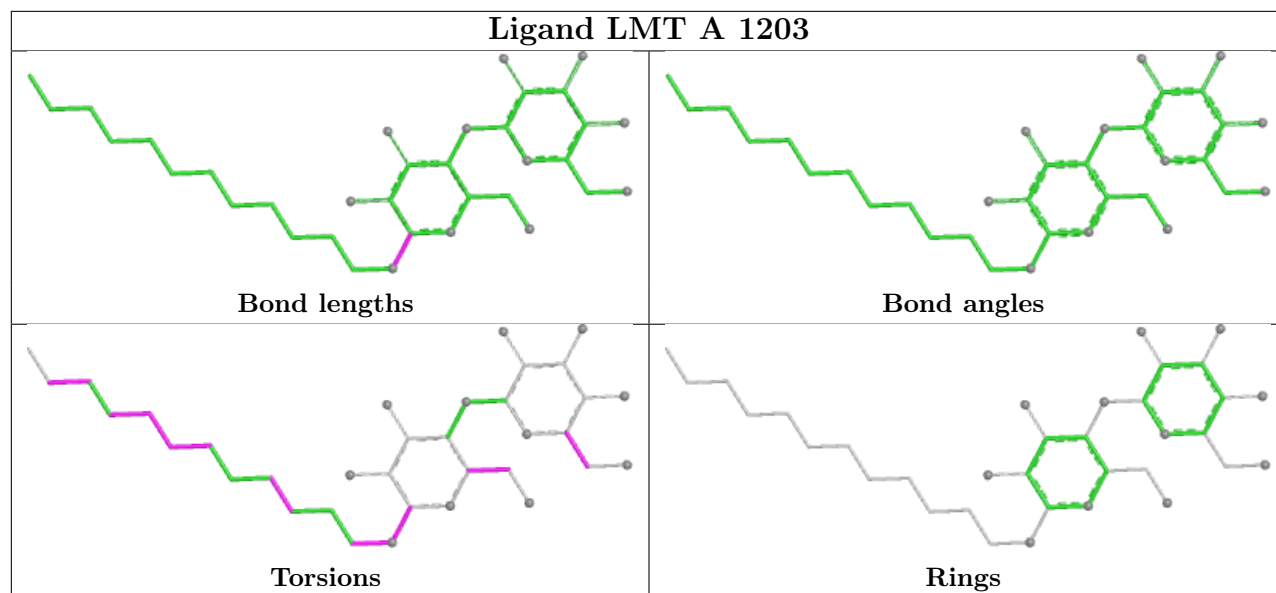
Ligand 3YI A 1208



Ligand LMT A 1201







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	1035/1057 (97%)	0.52	53 (5%)	33	25	40, 60, 97, 122	6 (0%)
1	B	1034/1057 (97%)	0.74	89 (8%)	16	12	41, 65, 95, 124	0
1	C	1033/1057 (97%)	0.29	19 (1%)	67	58	41, 56, 75, 86	0
2	D	154/169 (91%)	0.47	4 (2%)	57	47	57, 65, 84, 90	0
2	E	154/169 (91%)	0.68	6 (3%)	43	34	34, 70, 87, 93	1 (0%)
All	All	3410/3509 (97%)	0.52	171 (5%)	34	26	34, 61, 92, 124	7 (0%)

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	989	LEU	7.6
1	B	986	VAL	7.1
1	B	134	SER	6.7
1	B	1009	GLY	6.6
1	B	672	VAL	6.2
1	B	984	LEU	6.2
1	B	991	ILE	6.0
1	B	675	GLY	5.8
1	A	674	LEU	5.8
1	B	987	MET	5.5
1	A	868	LEU	5.3
2	E	123[A]	ARG	5.2
1	B	1003	VAL	5.1
1	B	676	THR	5.1
1	B	566	ASP	4.9
1	B	563	PHE	4.9
1	A	677	ALA	4.9
1	B	983	ILE	4.9
1	A	672	VAL	4.8
1	B	575	MET	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	615	PHE	4.4
1	B	662	MET	4.4
1	B	990	VAL	4.2
1	B	617	PHE	4.1
1	B	1007	VAL	4.1
1	B	1010	GLY	4.1
1	B	1008	MET	4.1
1	B	670	ALA	4.1
1	B	1011	MET	4.0
1	B	569	GLN	4.0
1	B	1004	GLY	3.9
1	A	429	GLU	3.9
1	B	628	PHE	3.9
1	A	918	PHE	3.8
1	C	674	LEU	3.7
1	A	873	ALA	3.6
1	B	673	GLU	3.6
1	B	133	SER	3.6
1	B	999	ALA	3.6
1	B	677	ALA	3.6
1	A	1035	ARG	3.6
1	A	870	GLY	3.6
1	A	676	THR	3.6
1	B	674	LEU	3.5
1	B	635	ALA	3.5
1	B	366	LEU	3.4
1	B	985	GLY	3.3
1	A	229	GLN	3.3
1	B	624	THR	3.2
1	A	956	GLU	3.2
1	B	396	PHE	3.1
1	B	988	PRO	3.1
1	B	664	PHE	3.1
1	B	634	TRP	3.0
1	B	576	VAL	3.0
1	B	1006	GLY	3.0
1	A	423	GLU	3.0
1	A	37	THR	3.0
1	A	678	THR	3.0
1	B	993	THR	3.0
1	B	1002	ALA	3.0
1	A	675	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	627	ALA	2.9
1	B	666	PHE	2.9
1	C	120	GLN	2.9
1	B	1034	SER	2.9
1	B	616	GLY	2.9
1	B	618	ALA	2.9
1	B	982	PHE	2.9
1	A	994	GLY	2.9
1	A	877	TYR	2.9
1	B	660	ASP	2.8
1	A	432	ARG	2.8
1	C	673	GLU	2.8
1	A	406	VAL	2.8
1	A	510	LYS	2.8
1	B	671	ILE	2.7
1	A	866	GLU	2.7
1	C	691	GLY	2.7
1	C	1033	PHE	2.7
1	A	538	THR	2.7
1	A	867	ARG	2.7
1	A	192	GLU	2.7
1	B	258	SER	2.7
1	C	671	ILE	2.6
1	C	811	TYR	2.6
1	A	874	PRO	2.6
1	B	868	LEU	2.6
1	A	865	GLN	2.6
2	D	31	ARG	2.6
1	B	659	LYS	2.6
1	A	38	ILE	2.6
1	A	543	VAL	2.6
1	B	918	PHE	2.6
1	C	124	GLN	2.5
1	B	407	ASP	2.5
1	B	620	ARG	2.5
1	C	403	GLY	2.5
1	A	503	GLY	2.5
1	B	574	THR	2.5
1	B	363	ARG	2.5
1	B	338	HIS	2.5
1	B	1012	VAL	2.5
1	A	430	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	132	SER	2.4
1	A	501	ALA	2.4
1	C	89	GLN	2.4
1	B	669	PRO	2.4
1	B	332	PHE	2.4
2	D	22	ALA	2.4
1	A	436	GLY	2.4
1	A	1006	GLY	2.4
1	B	998	GLY	2.4
2	E	31	ARG	2.4
1	C	640	GLU	2.4
1	A	255	GLN	2.4
1	B	478	MET	2.4
1	A	669	PRO	2.4
1	A	511	GLY	2.3
1	B	629	VAL	2.3
1	C	362	PHE	2.3
2	E	159	GLU	2.3
1	B	573	MET	2.3
1	B	663	VAL	2.3
1	B	178	PHE	2.3
1	B	256	ASP	2.3
1	A	123	GLN	2.3
1	A	29	LYS	2.3
1	A	869	SER	2.3
1	B	508	GLY	2.3
1	A	871	ASN	2.3
1	B	135	SER	2.3
1	C	659	LYS	2.2
1	B	938	SER	2.2
1	B	625	GLY	2.2
1	A	955	LYS	2.2
1	B	1000	GLN	2.2
1	A	403	GLY	2.2
1	A	982	PHE	2.2
1	B	136	PHE	2.2
2	D	20	GLU	2.2
1	B	623	ASN	2.2
1	A	540	ARG	2.2
1	C	70	ASN	2.2
1	B	408	ASP	2.2
1	B	996	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	257	GLY	2.2
1	B	336	SER	2.2
1	A	995	ALA	2.2
2	E	30	VAL	2.1
2	E	28	ASP	2.1
1	B	344	LEU	2.1
1	C	645	GLU	2.1
1	A	660	ASP	2.1
1	A	957	GLY	2.1
1	C	796	GLY	2.1
1	B	837	THR	2.1
1	C	676	THR	2.1
1	A	96	SER	2.1
1	B	994	GLY	2.1
2	D	57	TRP	2.1
2	E	34	MET	2.0
1	A	565	PRO	2.0
1	B	579	PRO	2.0
1	B	405	LEU	2.0
1	A	459	PHE	2.0
1	A	620	ARG	2.0
1	A	461	GLY	2.0
1	B	339	GLU	2.0
1	B	641	GLU	2.0
1	C	519	MET	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](#)

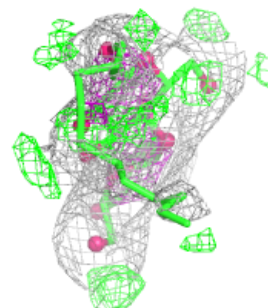
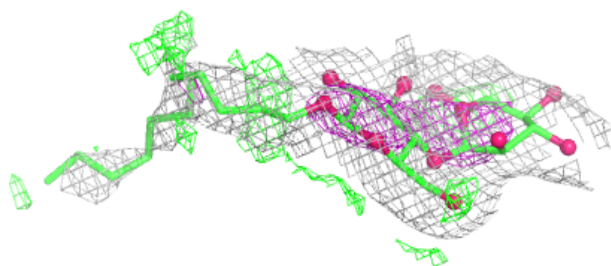
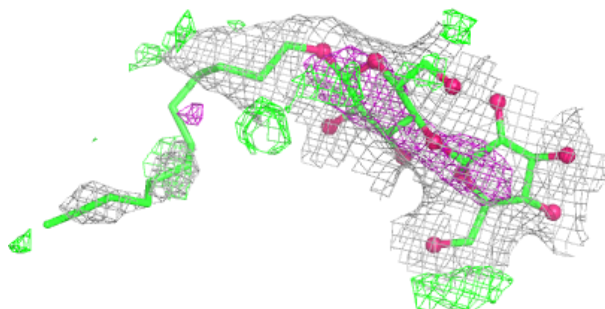
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	1206	35/35	0.42	0.24	66,78,79,79	0
10	DDQ	B	1103	14/14	0.65	0.25	53,55,57,58	0
4	HEX	A	1204	6/6	0.68	0.30	48,48,48,48	0
6	ETE	A	1207	14/14	0.69	0.26	91,93,93,93	0
5	GOL	B	1105	6/6	0.69	0.22	75,75,75,76	0
11	OCT	B	1104	8/8	0.69	0.34	53,53,53,53	0
3	LMT	A	1203	35/35	0.77	0.19	100,105,106,106	0
3	LMT	A	1202	35/35	0.79	0.21	81,96,102,102	0
8	EDO	A	1209	4/4	0.80	0.18	58,58,58,58	0
5	GOL	D	201	6/6	0.82	0.21	74,74,74,74	0
3	LMT	C	1101	35/35	0.83	0.19	78,79,80,80	0
12	D10	C	1102	10/10	0.84	0.27	61,62,62,62	0
3	LMT	B	1101	35/35	0.86	0.18	94,95,99,99	0
5	GOL	A	1205	6/6	0.86	0.23	52,53,53,53	0
3	LMT	A	1201	35/35	0.86	0.17	82,88,92,93	0
5	GOL	C	1103	6/6	0.90	0.13	58,58,58,58	0
7	3YI	A	1208	52/52	0.91	0.13	47,49,50,50	0
9	DDR	B	1102	28/28	0.92	0.18	85,87,89,89	0
13	CL	C	1104	1/1	0.97	0.10	51,51,51,51	0

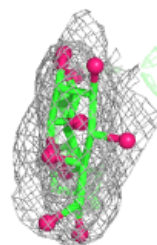
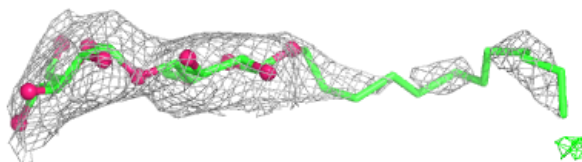
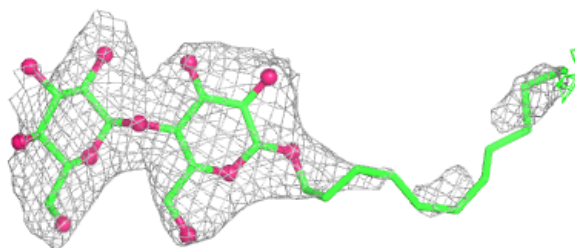
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT A 1206:

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

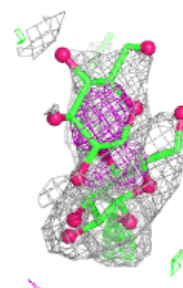
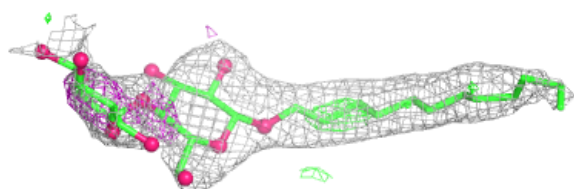
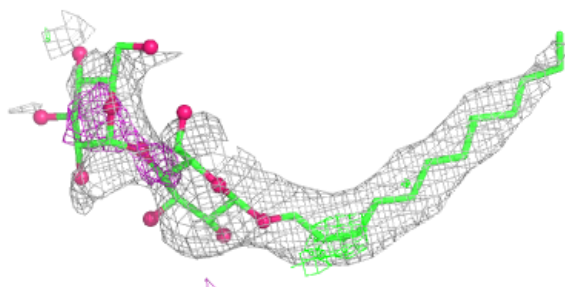
**Electron density around LMT A 1203:**

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

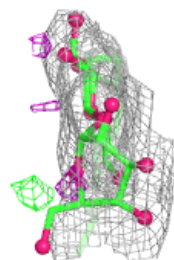
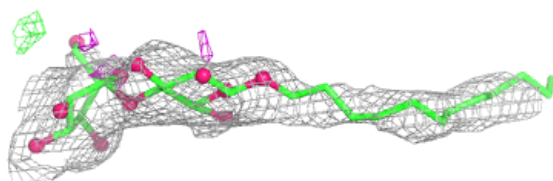
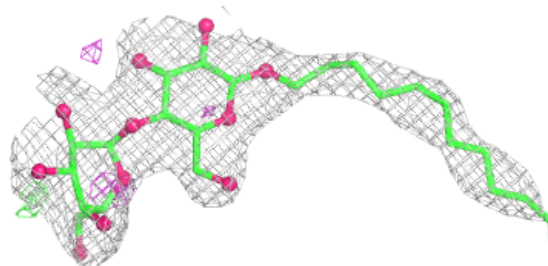


Electron density around LMT A 1202:

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

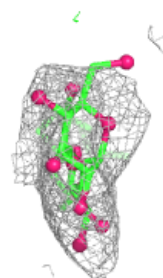
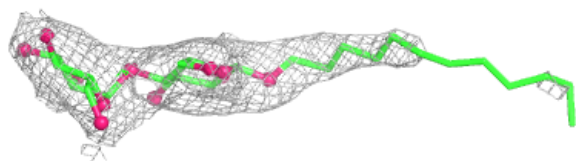
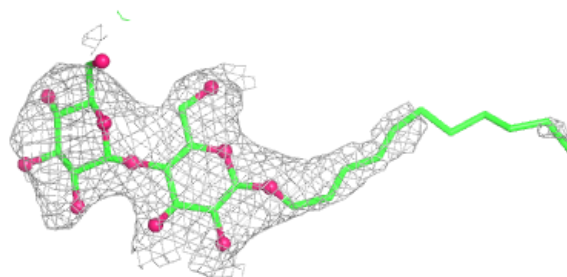
**Electron density around LMT C 1101:**

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

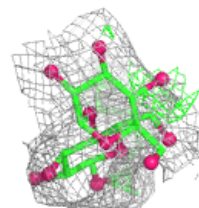
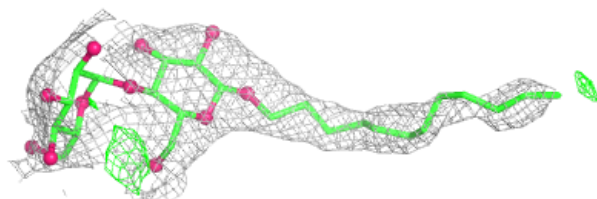
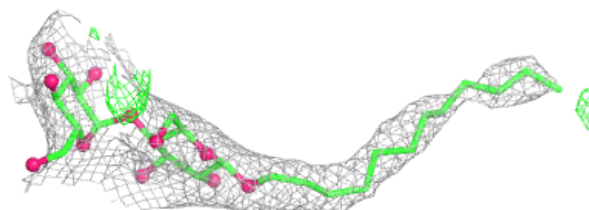


Electron density around LMT B 1101:

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

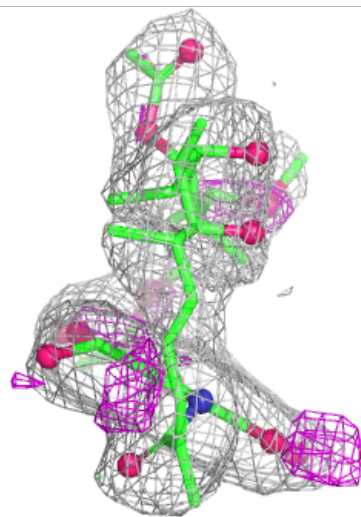
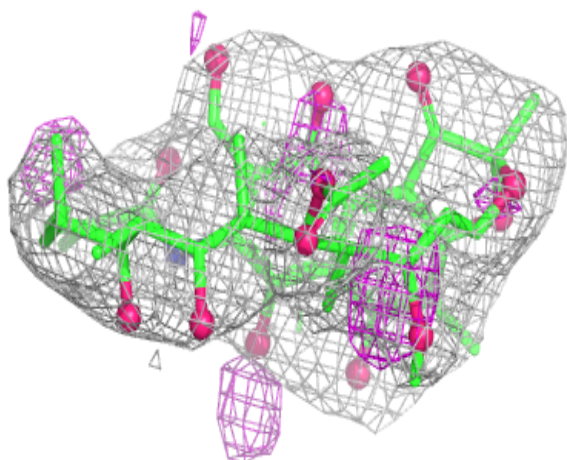
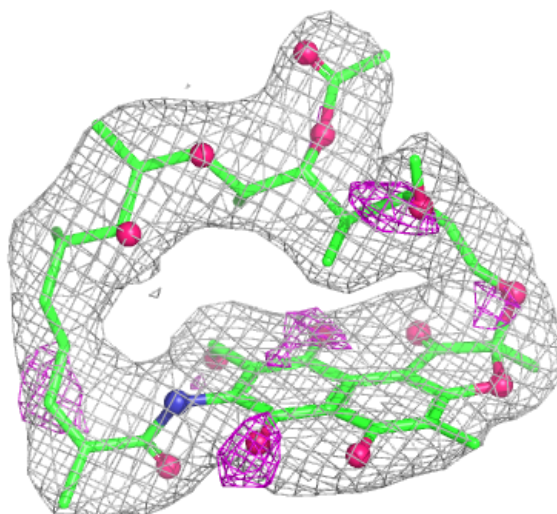
**Electron density around LMT A 1201:**

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



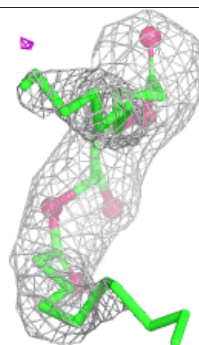
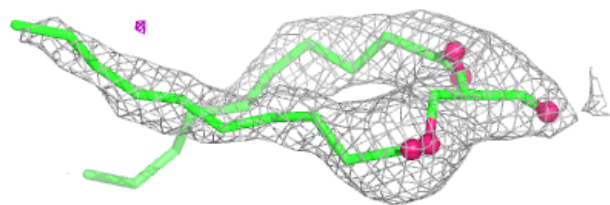
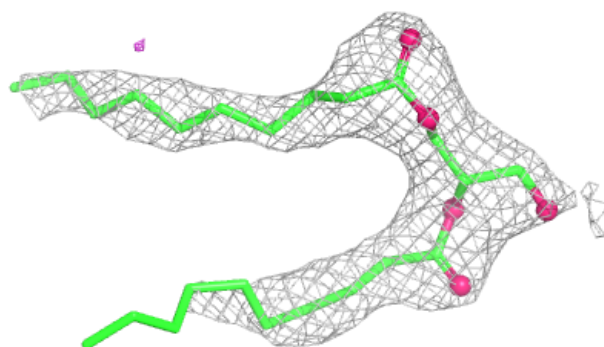
Electron density around 3YI A 1208:

$2mF_o-DF_c$ (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)



6.5 Other polymers ⓘ

There are no such residues in this entry.