



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2023 – 05:50 PM EDT

PDB ID : 6NWR
Title : Thioester acyl-intermediate of Apolipoprotein N-acyltransferase (Lnt)
Authors : Wiseman, B.; Hogbom, M.
Deposited on : 2019-02-07
Resolution : 3.50 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

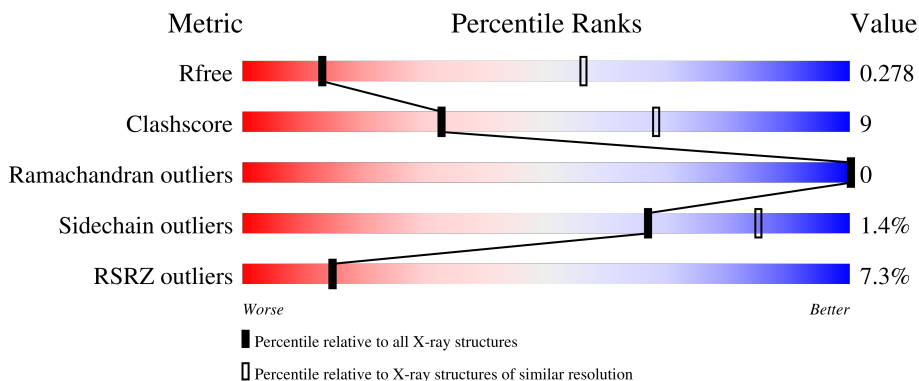
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	527	
2	B	527	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LMT	B	601	-	-	-	X
4	D12	B	603	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7988 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 Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3835	2519	635	667	14	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	513	GLU	-	expression tag	UNP P23930
A	514	PHE	-	expression tag	UNP P23930
A	515	ARG	-	expression tag	UNP P23930
A	516	VAL	-	expression tag	UNP P23930
A	517	PRO	-	expression tag	UNP P23930
A	518	GLY	-	expression tag	UNP P23930
A	519	SER	-	expression tag	UNP P23930
A	520	HIS	-	expression tag	UNP P23930
A	521	HIS	-	expression tag	UNP P23930
A	522	HIS	-	expression tag	UNP P23930
A	523	HIS	-	expression tag	UNP P23930
A	524	HIS	-	expression tag	UNP P23930
A	525	HIS	-	expression tag	UNP P23930
A	526	HIS	-	expression tag	UNP P23930
A	527	HIS	-	expression tag	UNP P23930

- Molecule 2 is a protein called Apolipoprotein N-acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	511	4050	2664	675	696	15	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

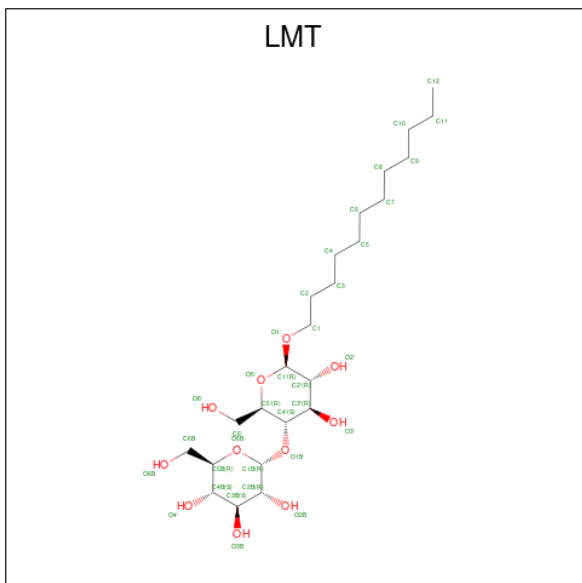
Chain	Residue	Modelled	Actual	Comment	Reference
B	513	GLU	-	expression tag	UNP P23930

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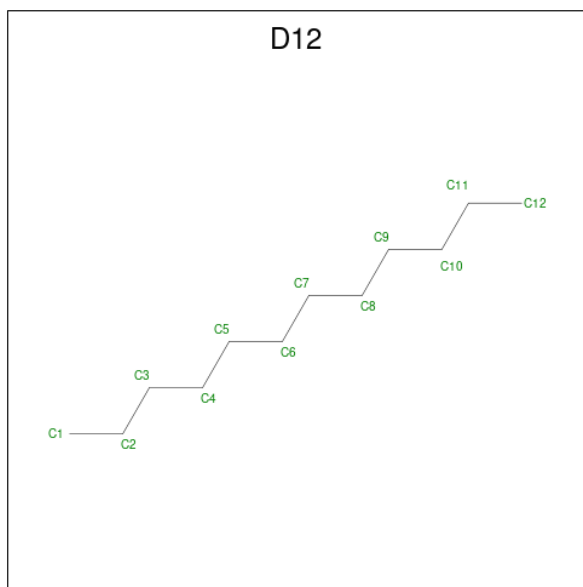
Chain	Residue	Modelled	Actual	Comment	Reference
B	514	PHE	-	expression tag	UNP P23930
B	515	ARG	-	expression tag	UNP P23930
B	516	VAL	-	expression tag	UNP P23930
B	517	PRO	-	expression tag	UNP P23930
B	518	GLY	-	expression tag	UNP P23930
B	519	SER	-	expression tag	UNP P23930
B	520	HIS	-	expression tag	UNP P23930
B	521	HIS	-	expression tag	UNP P23930
B	522	HIS	-	expression tag	UNP P23930
B	523	HIS	-	expression tag	UNP P23930
B	524	HIS	-	expression tag	UNP P23930
B	525	HIS	-	expression tag	UNP P23930
B	526	HIS	-	expression tag	UNP P23930
B	527	HIS	-	expression tag	UNP P23930

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: 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	B	1	Total	C	O	0	0
			28	17	11		
3	B	1	Total	C	O	0	0
			28	17	11		

- Molecule 4 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).

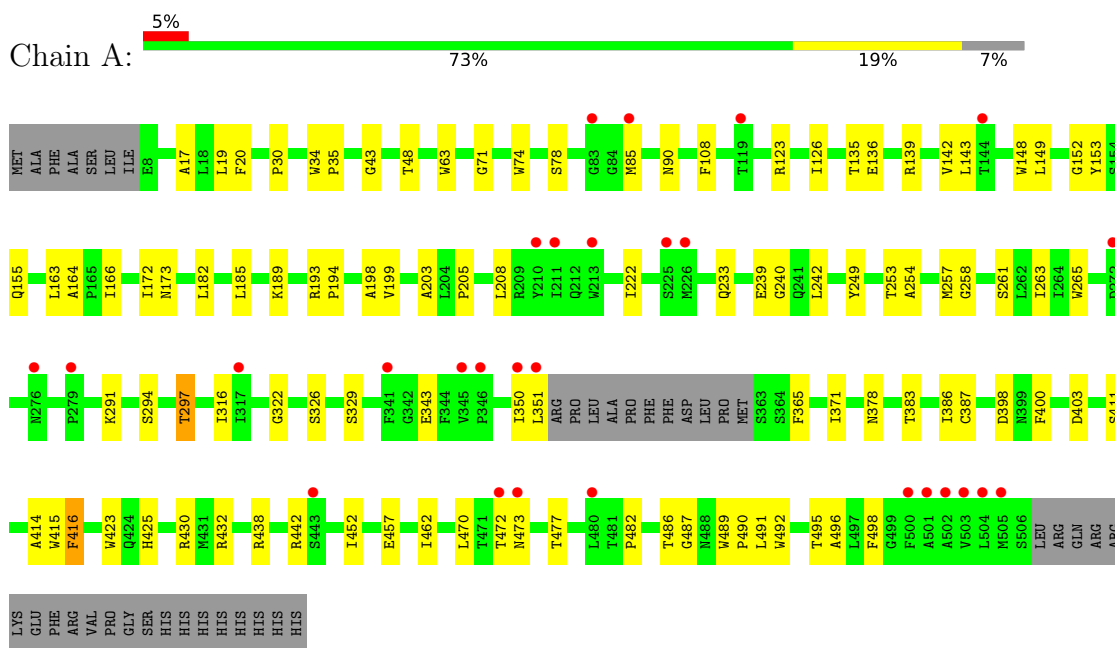


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C 12 12	0	0

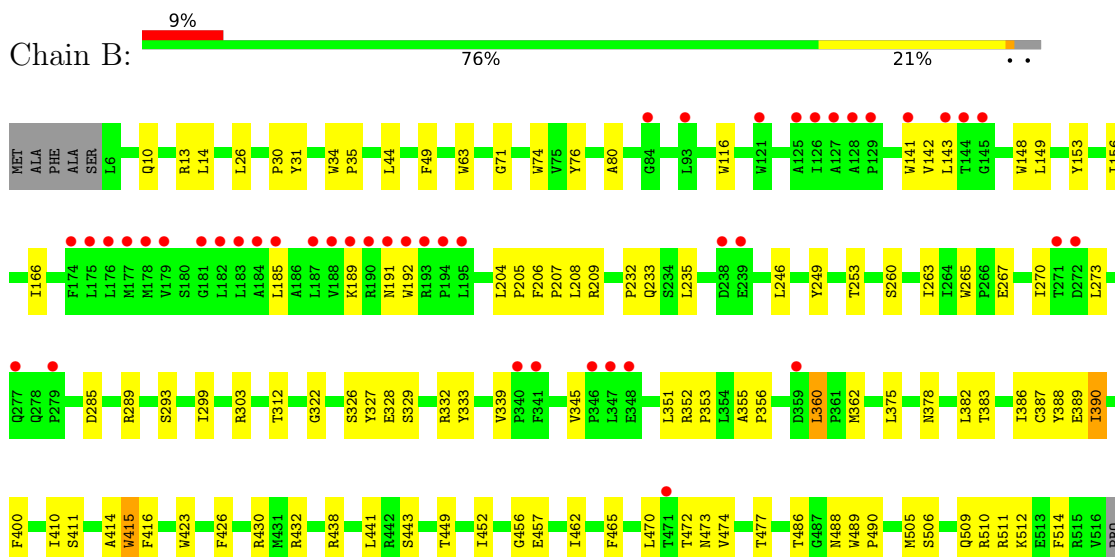
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Apolipoprotein N-acyltransferase



- Molecule 2: Apolipoprotein N-acyltransferase



GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.16Å 136.99Å 220.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.47 – 3.50 48.47 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.47-3.50) 99.9 (48.47-3.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.48Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.259 , 0.275 0.264 , 0.278	Depositor DCC
R_{free} test set	1374 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 25.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	7988	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: D12, LMT, P1L

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	0.25	0/3943	0.42	0/5386
2	B	0.34	0/4147	0.48	0/5660
All	All	0.30	0/8090	0.45	0/11046

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	3835	0	3893	61	0
2	B	4050	0	4130	80	0
3	A	35	0	46	1	0
3	B	56	0	58	0	0
4	B	12	0	26	3	0
All	All	7988	0	8153	141	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 9.

All (141) 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)
2:B:390:ILE:CD1	2:B:432:ARG:HG3	1.34	1.54
2:B:390:ILE:HD11	2:B:432:ARG:CG	1.54	1.36
2:B:390:ILE:HD12	2:B:432:ARG:HG3	1.36	1.02
2:B:390:ILE:CD1	2:B:432:ARG:CG	2.26	0.97
2:B:387:P1L:H141	2:B:387:P1L:H102	1.46	0.95
2:B:390:ILE:HD11	2:B:432:ARG:CB	1.98	0.92
2:B:387:P1L:SG	2:B:388:TYR:N	2.40	0.89
2:B:390:ILE:HD11	2:B:432:ARG:HG3	0.89	0.88
2:B:387:P1L:H141	2:B:387:P1L:C10	2.14	0.77
2:B:352:ARG:HD3	2:B:353:PRO:HD2	1.71	0.71
2:B:326:SER:HB3	2:B:329:SER:HB2	1.77	0.66
2:B:153:TYR:OH	2:B:432:ARG:NH2	2.30	0.65
2:B:232:PRO:HG2	2:B:235:LEU:HB2	1.81	0.62
1:A:71:GLY:O	1:A:74:TRP:NE1	2.33	0.61
1:A:258:GLY:HA2	1:A:291:LYS:HB3	1.84	0.59
1:A:163:LEU:HB2	1:A:205:PRO:HB3	1.85	0.58
1:A:326:SER:HB3	1:A:329:SER:HB2	1.85	0.58
1:A:153:TYR:OH	1:A:432:ARG:NH2	2.36	0.57
1:A:182:LEU:HB2	1:A:198:ALA:HB2	1.85	0.57
1:A:136:GLU:OE1	1:A:139:ARG:NH2	2.35	0.57
2:B:390:ILE:HD12	2:B:390:ILE:O	2.05	0.56
2:B:462:ILE:HD13	2:B:470:LEU:HB2	1.86	0.56
2:B:253:THR:HG23	2:B:263:ILE:HG21	1.88	0.55
2:B:352:ARG:HB3	2:B:360:LEU:HD22	1.89	0.55
1:A:322:GLY:HA3	1:A:378:ASN:H	1.73	0.54
1:A:152:GLY:N	1:A:173:ASN:OD1	2.41	0.54
1:A:233:GLN:HB2	1:A:414:ALA:HB1	1.90	0.54
1:A:350:ILE:HG22	1:A:351:LEU:HG	1.90	0.53
2:B:387:P1L:H4	2:B:411:SER:HB2	1.89	0.53
2:B:387:P1L:N	2:B:410:ILE:O	2.42	0.53
2:B:430:ARG:HG2	2:B:452:ILE:HG12	1.91	0.53
2:B:267:GLU:OE1	2:B:387:P1L:O7	2.26	0.52
2:B:387:P1L:C10	2:B:387:P1L:C14	2.84	0.52
1:A:17:ALA:HB1	1:A:63:TRP:HB2	1.91	0.52
1:A:166:ILE:HA	1:A:482:PRO:HB2	1.92	0.52
2:B:156:ILE:HD11	2:B:456:GLY:HA3	1.90	0.52
1:A:343:GLU:HB3	1:A:365:PHE:HB2	1.92	0.52
2:B:489:TRP:CD1	2:B:490:PRO:HD3	2.45	0.52
2:B:472:THR:OG1	2:B:473:ASN:N	2.42	0.51
1:A:383:THR:HG21	1:A:400:PHE:HA	1.93	0.51
2:B:185:LEU:HD11	2:B:189:LYS:HE2	1.93	0.51
2:B:44:LEU:HB2	2:B:63:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:TRP:NE1	2:B:506:SER:HB3	2.26	0.50
1:A:199:VAL:O	1:A:203:ALA:N	2.42	0.50
2:B:312:THR:HG21	2:B:345:VAL:HG12	1.94	0.50
1:A:400:PHE:HE1	1:A:438:ARG:HG3	1.77	0.50
1:A:492:TRP:O	1:A:496:ALA:N	2.41	0.50
2:B:76:TYR:O	2:B:80:ALA:N	2.42	0.50
2:B:355:ALA:HB3	2:B:356:PRO:HD3	1.94	0.49
1:A:185:LEU:HD22	1:A:194:PRO:HG2	1.95	0.49
2:B:443:SER:HA	2:B:449:THR:HG23	1.94	0.49
1:A:239:GLU:N	2:B:510:ARG:O	2.34	0.49
1:A:489:TRP:CG	1:A:490:PRO:HD3	2.47	0.49
2:B:390:ILE:HD11	2:B:432:ARG:HB2	1.89	0.48
1:A:193:ARG:HB2	1:A:194:PRO:HD3	1.95	0.48
2:B:400:PHE:HE1	2:B:438:ARG:HG3	1.80	0.47
2:B:505:MET:O	2:B:509:GLN:HG2	2.14	0.47
1:A:148:TRP:HD1	1:A:149:LEU:HG	1.79	0.47
2:B:270:ILE:HB	2:B:299:ILE:HG13	1.96	0.47
2:B:489:TRP:CG	2:B:490:PRO:HD3	2.49	0.47
1:A:222:ILE:HB	1:A:261:SER:HB2	1.97	0.46
2:B:387:P1L:SG	2:B:388:TYR:HB2	2.55	0.46
1:A:30:PRO:HG3	1:A:423:TRP:CG	2.50	0.46
2:B:13:ARG:NH1	2:B:49:PHE:O	2.43	0.46
2:B:206:PHE:O	2:B:209:ARG:HG2	2.16	0.46
2:B:339:VAL:HG11	2:B:387:P1L:H142	1.98	0.46
1:A:371:ILE:HD11	1:A:398:ASP:HB3	1.97	0.46
1:A:240:GLY:C	1:A:242:LEU:H	2.19	0.46
1:A:430:ARG:HG2	1:A:452:ILE:HG12	1.98	0.46
2:B:333:TYR:HE2	2:B:386:ILE:HG12	1.81	0.46
1:A:253:THR:HG23	1:A:263:ILE:HG21	1.99	0.45
4:B:603:D12:H62	4:B:603:D12:H31	1.75	0.45
2:B:71:GLY:O	2:B:74:TRP:NE1	2.49	0.45
2:B:383:THR:HG21	2:B:400:PHE:HA	1.99	0.45
1:A:34:TRP:CG	1:A:35:PRO:HD3	2.52	0.45
2:B:260:SER:O	2:B:293:SER:OG	2.35	0.45
2:B:273:LEU:HD21	2:B:351:LEU:HD12	1.99	0.45
2:B:488:ASN:HD21	4:B:603:D12:H51	1.81	0.45
1:A:164:ALA:HB2	1:A:172:ILE:HD11	1.99	0.44
2:B:34:TRP:CG	2:B:35:PRO:HD3	2.52	0.44
2:B:390:ILE:HD12	2:B:432:ARG:CG	2.25	0.44
2:B:204:LEU:O	2:B:207:PRO:HD2	2.17	0.44
2:B:426:PHE:CE1	2:B:452:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:GLY:HA3	2:B:378:ASN:H	1.82	0.44
1:A:34:TRP:CD1	1:A:35:PRO:HD3	2.52	0.44
1:A:249:TYR:O	1:A:253:THR:N	2.50	0.43
1:A:126:ILE:HA	1:A:498:PHE:CD2	2.53	0.43
1:A:489:TRP:CD1	1:A:490:PRO:HD3	2.54	0.43
2:B:510:ARG:HG3	2:B:511:ARG:H	1.84	0.43
1:A:438:ARG:HD3	1:A:477:THR:OG1	2.19	0.43
2:B:387:P1L:H112	2:B:415:TRP:CZ2	2.53	0.43
2:B:438:ARG:HD3	2:B:477:THR:OG1	2.19	0.42
2:B:441:LEU:HD21	2:B:474:VAL:HG11	2.00	0.42
1:A:166:ILE:HD12	1:A:208:LEU:HD13	2.00	0.42
1:A:486:THR:OG1	1:A:487:GLY:N	2.50	0.42
1:A:472:THR:OG1	1:A:473:ASN:N	2.52	0.42
2:B:10:GLN:O	2:B:14:LEU:HG	2.19	0.42
2:B:387:P1L:HB2	2:B:388:TYR:H	1.34	0.42
1:A:387:CYS:HA	1:A:411:SER:HB2	2.01	0.42
2:B:285:ASP:OD2	2:B:289:ARG:NH2	2.52	0.42
1:A:155:GLN:HG3	1:A:172:ILE:HG21	2.02	0.42
1:A:78:SER:HB2	1:A:416:PHE:CE1	2.55	0.42
1:A:254:ALA:HA	1:A:257:MET:SD	2.60	0.42
1:A:240:GLY:O	1:A:242:LEU:N	2.52	0.42
1:A:294:SER:OG	1:A:378:ASN:HB2	2.20	0.42
2:B:191:ASN:OD1	2:B:192:TRP:N	2.53	0.42
1:A:462:ILE:HD13	1:A:470:LEU:HB2	2.02	0.41
2:B:387:P1L:O	2:B:390:ILE:HG22	2.20	0.41
2:B:486:THR:HB	2:B:489:TRP:NE1	2.35	0.41
2:B:148:TRP:HD1	2:B:149:LEU:HG	1.85	0.41
2:B:432:ARG:HA	2:B:432:ARG:HD3	1.91	0.41
1:A:182:LEU:HD22	1:A:194:PRO:HB3	2.02	0.41
1:A:189:LYS:HE2	1:A:189:LYS:HB3	1.90	0.41
1:A:316:ILE:HD11	1:A:386:ILE:HG12	2.01	0.41
1:A:265:TRP:HB2	1:A:297:THR:HB	2.03	0.41
1:A:403:ASP:OD1	1:A:403:ASP:N	2.48	0.41
1:A:48:THR:O	1:A:123:ARG:NH2	2.53	0.41
1:A:108:PHE:HB2	1:A:135:THR:HG21	2.01	0.41
2:B:166:ILE:HD12	2:B:208:LEU:HD13	2.03	0.41
2:B:233:GLN:HB2	2:B:414:ALA:HB1	2.02	0.41
2:B:328:GLU:OE1	2:B:328:GLU:N	2.54	0.41
1:A:239:GLU:HG2	2:B:512:LYS:HE3	2.02	0.41
1:A:491:LEU:O	1:A:495:THR:N	2.46	0.41
3:A:601:LMT:H82	3:A:601:LMT:H52	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:TRP:HD1	4:B:603:D12:H111	1.86	0.41
2:B:246:LEU:HD21	2:B:270:ILE:HG23	2.03	0.41
2:B:332:ARG:HH11	2:B:332:ARG:HD3	1.66	0.41
2:B:142:VAL:HG12	2:B:143:LEU:HG	2.03	0.41
2:B:249:TYR:HB3	2:B:265:TRP:CZ2	2.56	0.41
2:B:375:LEU:N	2:B:382:LEU:O	2.50	0.41
1:A:142:VAL:HG12	1:A:143:LEU:HG	2.01	0.40
1:A:85:MET:HB2	1:A:90:ASN:HD21	1.85	0.40
1:A:425:HIS:CE1	1:A:442:ARG:HH22	2.39	0.40
2:B:30:PRO:HG3	2:B:423:TRP:CD1	2.56	0.40
2:B:303:ARG:NH2	2:B:327:TYR:O	2.47	0.40
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.97	0.40
1:A:20:PHE:CD1	1:A:43:GLY:HA3	2.57	0.40
1:A:205:PRO:HA	1:A:208:LEU:HD12	2.04	0.40
2:B:26:LEU:HA	2:B:31:TYR:HD2	1.87	0.40
2:B:204:LEU:HB3	2:B:205:PRO:HD3	2.03	0.40
2:B:387:P1L:C	2:B:389:GLU:H	2.34	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	484/527 (92%)	455 (94%)	29 (6%)	0	100	100
2	B	508/527 (96%)	477 (94%)	31 (6%)	0	100	100
All	All	992/1054 (94%)	932 (94%)	60 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/441 (92%)	402 (99%)	4 (1%)	76	88
2	B	427/440 (97%)	419 (98%)	8 (2%)	57	80
All	All	833/881 (95%)	821 (99%)	12 (1%)	67	85

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	THR
1	A	415	TRP
1	A	416	PHE
1	A	457	GLU
2	B	360	LEU
2	B	362	MET
2	B	390	ILE
2	B	415	TRP
2	B	416	PHE
2	B	457	GLU
2	B	465	PHE
2	B	514	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	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](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	P1L	B	387	2	15,16,23	0.68	0	12,17,25	0.35	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
2	P1L	B	387	2	-	5/14/16/24	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	387	P1L	CA-CB-SG-C7
2	B	387	P1L	C10-C11-C12-C13
2	B	387	P1L	O7-C7-SG-CB
2	B	387	P1L	C8-C7-SG-CB
2	B	387	P1L	C12-C13-C14-C15

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	387	P1L	13	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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
4	D12	B	603	-	11,11,11	0.31	0	10,10,10	0.81	0
3	LMT	B	602	-	29,29,36	1.27	5 (17%)	40,40,47	1.05	1 (2%)
3	LMT	B	601	-	29,29,36	1.26	5 (17%)	40,40,47	1.00	1 (2%)
3	LMT	A	601	-	36,36,36	1.14	5 (13%)	47,47,47	0.98	1 (2%)

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
4	D12	B	603	-	-	3/9/9/9	-
3	LMT	B	602	-	-	4/14/54/61	0/2/2/2
3	LMT	B	601	-	-	4/14/54/61	0/2/2/2
3	LMT	A	601	-	-	5/21/61/61	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	601	LMT	O3'-C3'	-2.55	1.37	1.43
3	A	601	LMT	O3'-C3'	-2.55	1.37	1.43
3	B	602	LMT	O3'-C3'	-2.55	1.37	1.43
3	B	602	LMT	O3B-C3B	-2.34	1.37	1.43
3	B	602	LMT	O2B-C2B	-2.32	1.37	1.43
3	B	601	LMT	O3B-C3B	-2.30	1.37	1.43
3	B	601	LMT	O2B-C2B	-2.27	1.37	1.43
3	A	601	LMT	O2B-C2B	-2.24	1.37	1.43
3	A	601	LMT	O3B-C3B	-2.24	1.37	1.43
3	B	601	LMT	O4'-C4B	-2.20	1.37	1.43
3	B	601	LMT	O2'-C2'	-2.14	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	LMT	O2'-C2'	-2.11	1.38	1.43
3	A	601	LMT	O4'-C4B	-2.08	1.38	1.43
3	B	602	LMT	O4'-C4B	-2.06	1.38	1.43
3	A	601	LMT	O2'-C2'	-2.02	1.38	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	LMT	C3'-C4'-C5'	-3.02	104.00	110.93
3	B	602	LMT	C1'-O5'-C5'	-2.87	108.05	113.69
3	A	601	LMT	C1'-O5'-C5'	-2.40	108.97	113.69

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	601	LMT	C2'-C1'-O1'-C1
3	B	601	LMT	O5'-C1'-O1'-C1
3	B	602	LMT	O5'-C1'-O1'-C1
3	B	602	LMT	C3'-C4'-O1B-C1B
3	B	602	LMT	C2'-C1'-O1'-C1
3	B	601	LMT	O5'-C5'-C6'-O6'
3	B	602	LMT	O1'-C1-C2-C3
4	B	603	D12	C6-C7-C8-C9
3	A	601	LMT	C4-C5-C6-C7
4	B	603	D12	C1-C2-C3-C4
4	B	603	D12	C7-C8-C9-C10
3	A	601	LMT	O5'-C1'-O1'-C1
3	B	601	LMT	C4'-C5'-C6'-O6'
3	A	601	LMT	C2'-C1'-O1'-C1
3	A	601	LMT	C2-C3-C4-C5
3	A	601	LMT	O5B-C1B-O1B-C4'

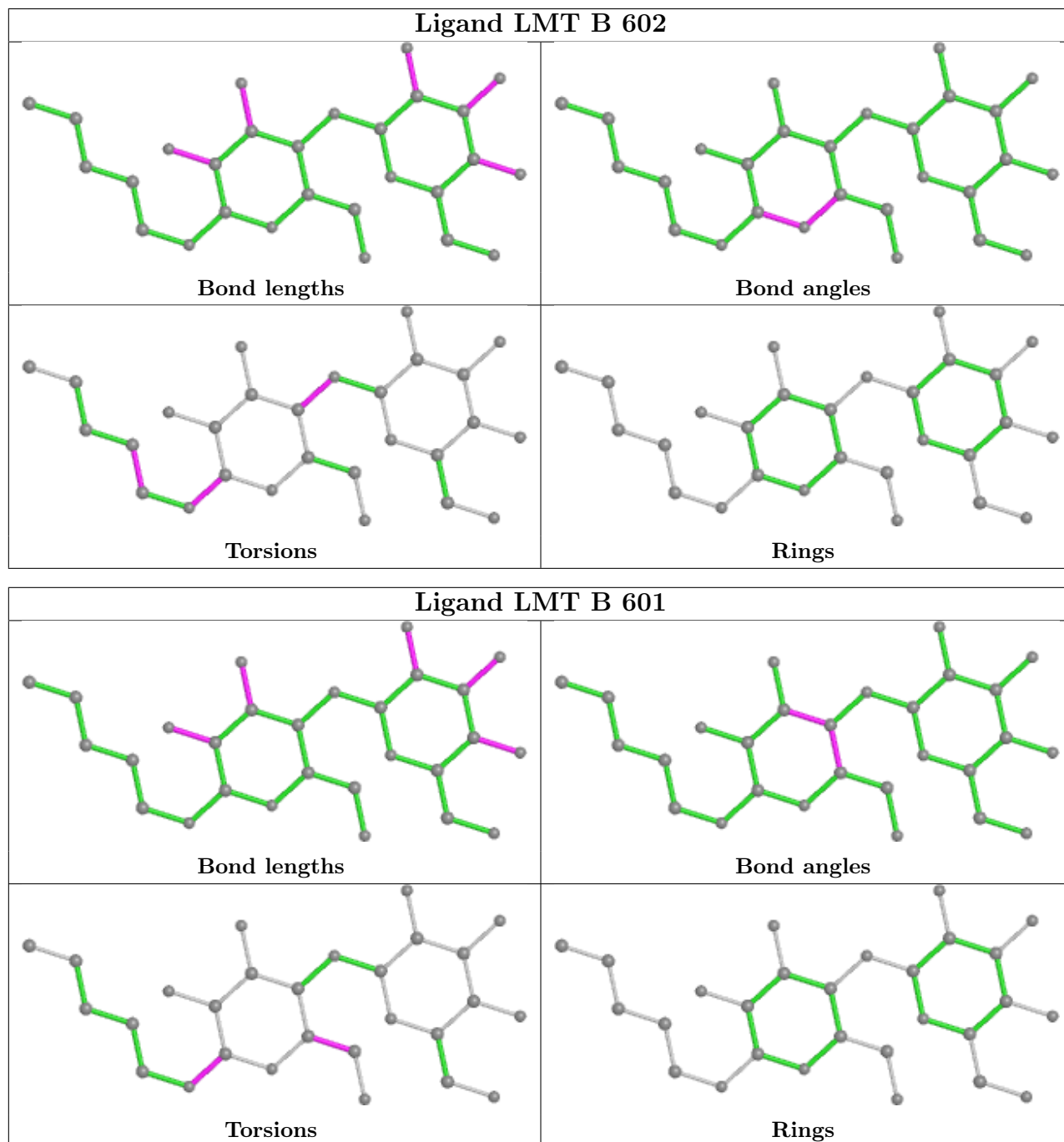
There are no ring outliers.

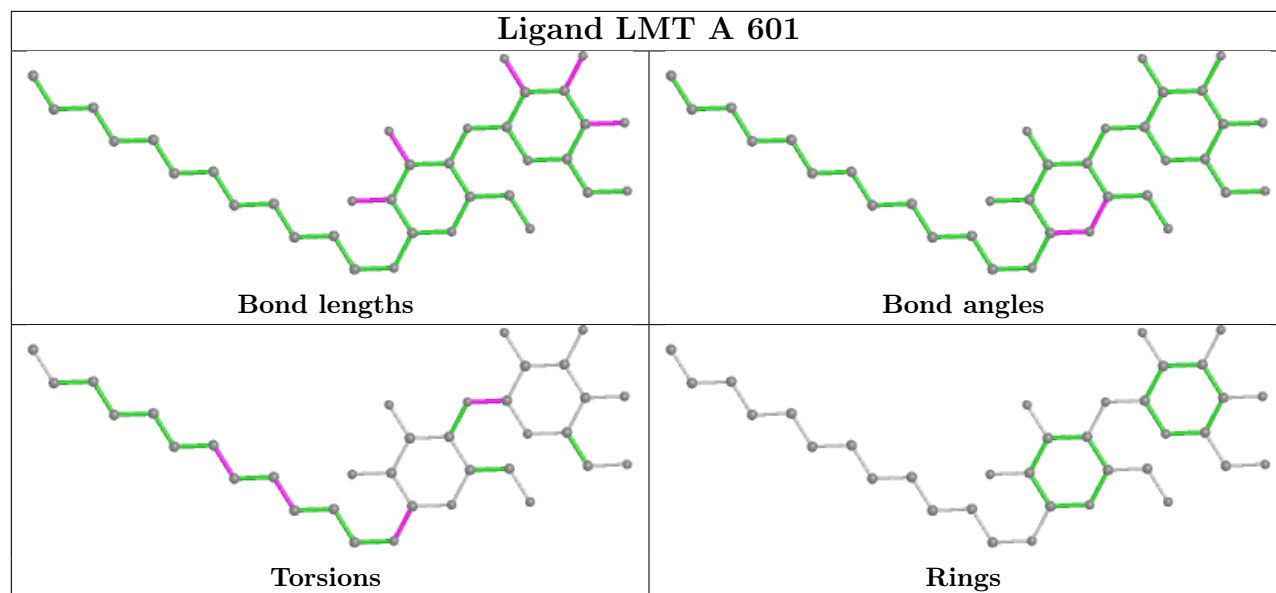
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	D12	3	0
3	A	601	LMT	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	488/527 (92%)	-0.02	28 (5%) 23 21	55, 109, 172, 208	0
2	B	510/527 (96%)	0.07	45 (8%) 10 10	52, 97, 162, 188	0
All	All	998/1054 (94%)	0.03	73 (7%) 15 15	52, 103, 169, 208	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	ARG	6.1
2	B	191	ASN	5.8
2	B	348	GLU	5.5
2	B	239	GLU	5.4
1	A	504	LEU	5.0
2	B	192	TRP	5.0
2	B	121	TRP	4.7
2	B	194	PRO	4.1
2	B	178	MET	4.0
2	B	341	PHE	4.0
1	A	119	THR	3.7
2	B	177	MET	3.6
2	B	144	THR	3.6
1	A	503	VAL	3.6
2	B	145	GLY	3.6
1	A	225	SER	3.6
2	B	125	ALA	3.6
2	B	129	PRO	3.5
1	A	500	PHE	3.4
2	B	347	LEU	3.3
2	B	175	LEU	3.2
2	B	346	PRO	3.2
2	B	193	ARG	3.2
2	B	189	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	238	ASP	3.1
2	B	272	ASP	3.1
2	B	179	VAL	3.0
2	B	143	LEU	3.0
2	B	271	THR	3.0
2	B	277	GLN	3.0
1	A	345	VAL	2.9
2	B	84	GLY	2.9
2	B	126	ILE	2.9
2	B	128	ALA	2.9
1	A	226	MET	2.8
1	A	272	ASP	2.8
1	A	443	SER	2.8
2	B	182	LEU	2.8
1	A	502	ALA	2.8
2	B	181	GLY	2.8
2	B	340	PRO	2.7
1	A	83	GLY	2.7
1	A	210	TYR	2.7
2	B	183	LEU	2.6
2	B	187	LEU	2.6
2	B	127	ALA	2.6
1	A	341	PHE	2.6
1	A	211	ILE	2.5
1	A	501	ALA	2.5
1	A	351	LEU	2.4
1	A	480	LEU	2.4
1	A	213	TRP	2.4
1	A	85	MET	2.4
1	A	276	ASN	2.4
2	B	471	THR	2.4
2	B	184	ALA	2.3
2	B	279	PRO	2.3
2	B	195	LEU	2.3
1	A	472	THR	2.2
2	B	359	ASP	2.2
1	A	350	ILE	2.2
2	B	176	LEU	2.2
2	B	141	TRP	2.2
2	B	185	LEU	2.2
2	B	174	PHE	2.1
1	A	346	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	279	PRO	2.1
1	A	144	THR	2.1
1	A	473	ASN	2.1
1	A	317	ILE	2.0
2	B	188	VAL	2.0
2	B	93	LEU	2.0
1	A	505	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	P1L	B	387	17/24	0.93	0.30	103,122,143,148	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

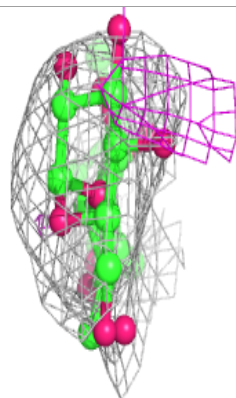
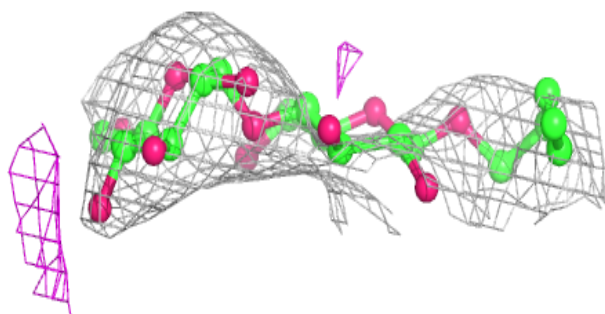
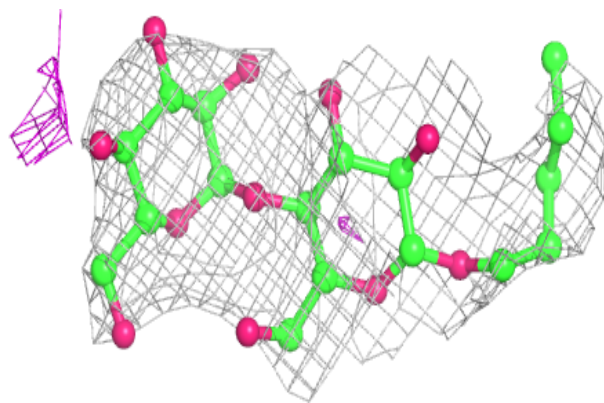
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LMT	B	601	28/35	0.61	0.45	129,167,195,200	0
3	LMT	B	602	28/35	0.63	0.26	124,188,207,211	0
4	D12	B	603	12/12	0.69	0.51	81,108,130,134	0
3	LMT	A	601	35/35	0.74	0.24	108,161,188,195	0

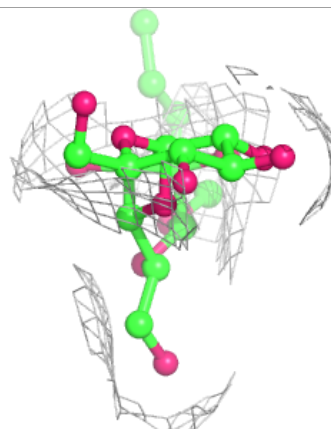
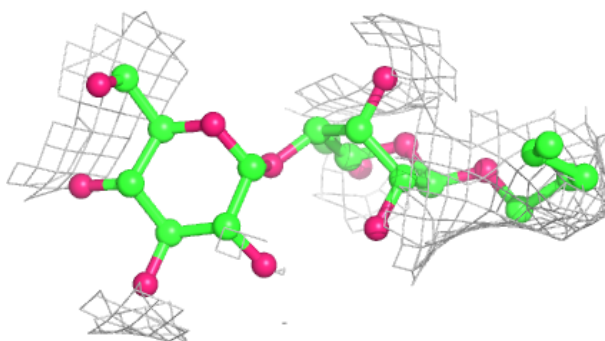
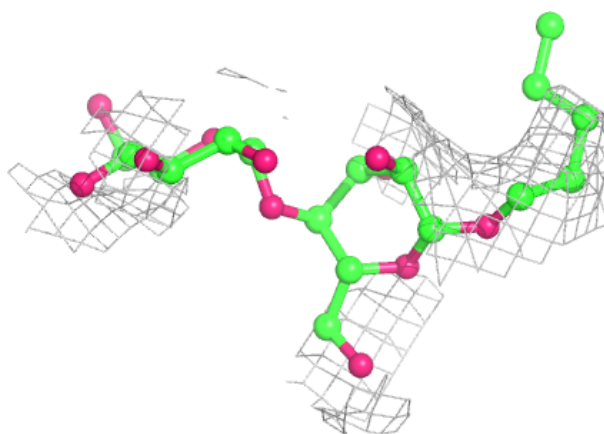
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

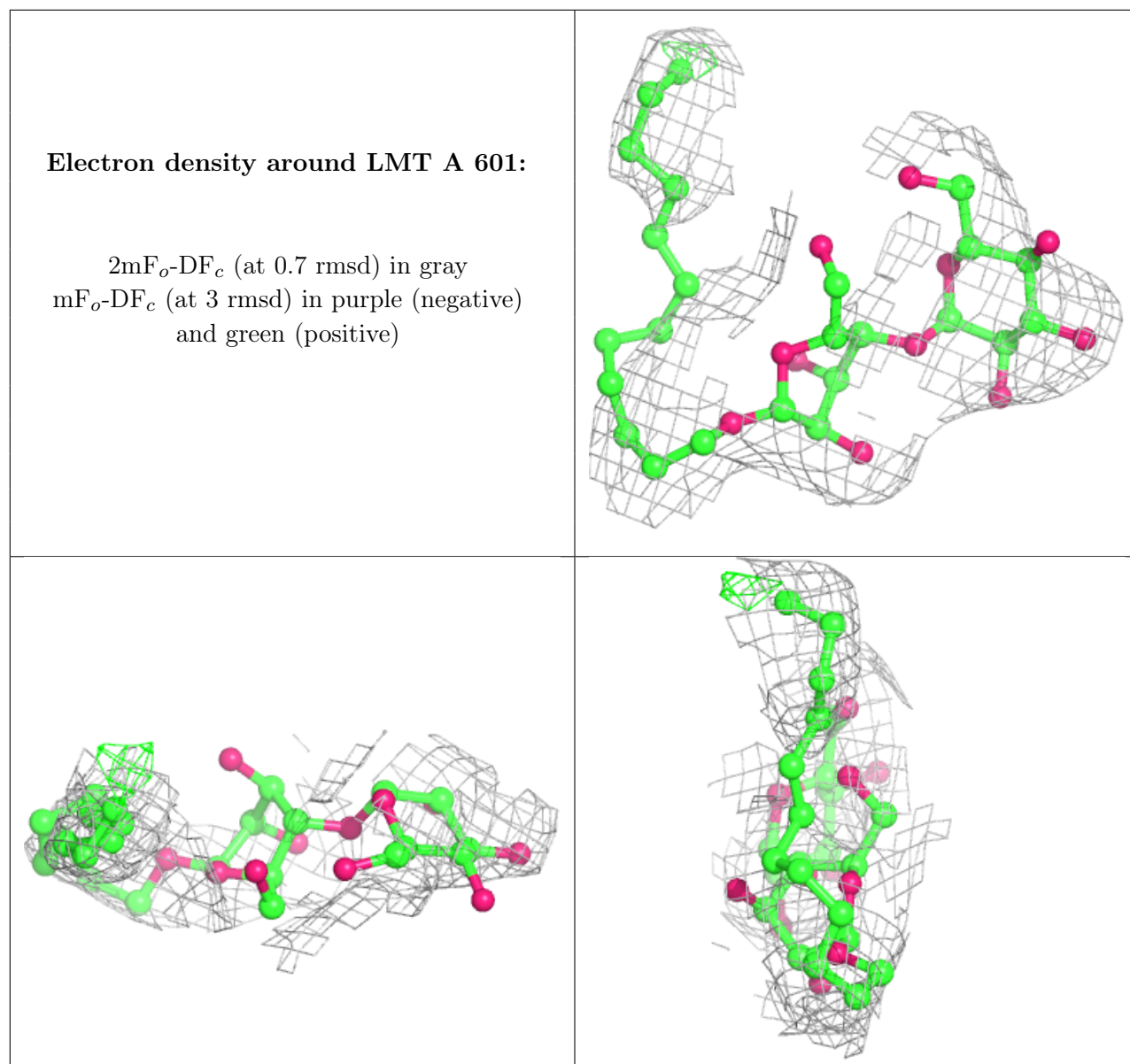
Electron density around LMT B 601:

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

**Electron density around LMT B 602:**

$2mF_o-DF_c$ (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.