



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 08:03 PM EDT

PDB ID : 4TPJ
Title : Selectivity mechanism of a bacterial homologue of the human drug peptide transporters PepT1 and PepT2
Authors : Guettou, F.; Quistgaard, E.; Raba, M.; Moberg, P.; Low, C.; Nordlund, P.
Deposited on : 2014-06-07
Resolution : 3.20 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:

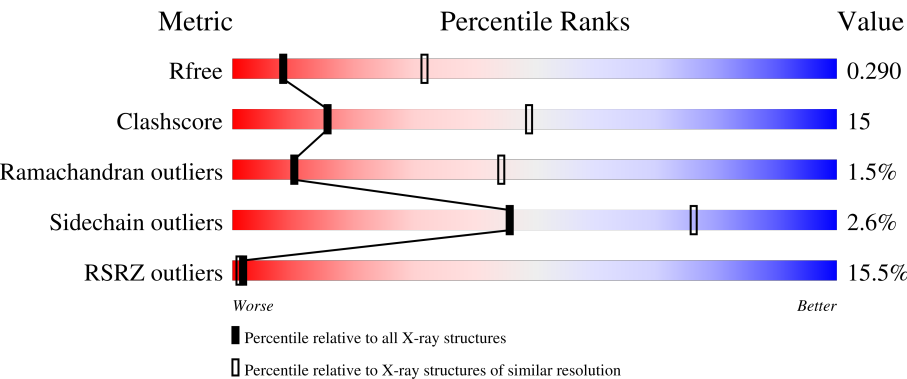
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	523	<div><div>12%</div><div>57%</div><div>27%</div><div>•</div><div>15%</div></div>
1	B	523	<div><div>15%</div><div>57%</div><div>27%</div><div>•</div><div>14%</div></div>
2	C	3	<div><div>33%</div><div>67%</div><div>33%</div></div>
2	E	3	<div><div>33%</div><div>67%</div><div>33%</div></div>

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	603	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6934 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 Proton:oligopeptide symporter POT family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3376	2245	536	575	20			
1	B	450	Total	C	N	O	S	0	0	0
			3420	2277	543	580	20			

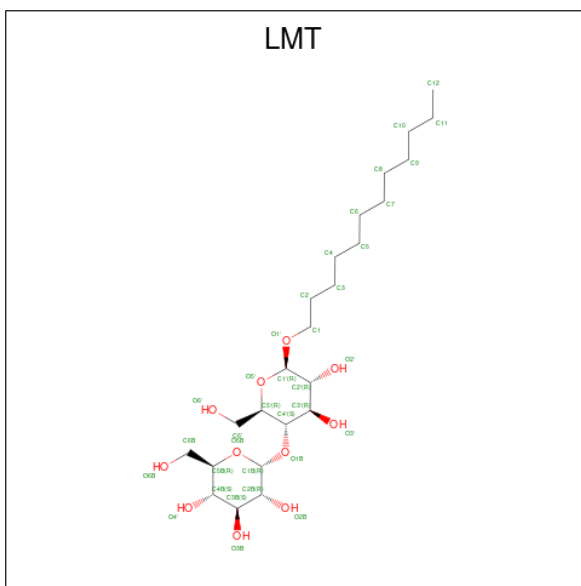
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	517	ALA	-	expression tag	UNP Q8EHE6
A	518	GLU	-	expression tag	UNP Q8EHE6
A	519	ASN	-	expression tag	UNP Q8EHE6
A	520	LEU	-	expression tag	UNP Q8EHE6
A	521	TYR	-	expression tag	UNP Q8EHE6
A	522	PHE	-	expression tag	UNP Q8EHE6
A	523	GLN	-	expression tag	UNP Q8EHE6
B	517	ALA	-	expression tag	UNP Q8EHE6
B	518	GLU	-	expression tag	UNP Q8EHE6
B	519	ASN	-	expression tag	UNP Q8EHE6
B	520	LEU	-	expression tag	UNP Q8EHE6
B	521	TYR	-	expression tag	UNP Q8EHE6
B	522	PHE	-	expression tag	UNP Q8EHE6
B	523	GLN	-	expression tag	UNP Q8EHE6

- Molecule 2 is a protein called ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			16	9	3	4			
2	E	3	Total	C	N	O	0	0	0
			16	9	3	4			

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:

$\text{C}_{24}\text{H}_{46}\text{O}_{11}).$ 

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

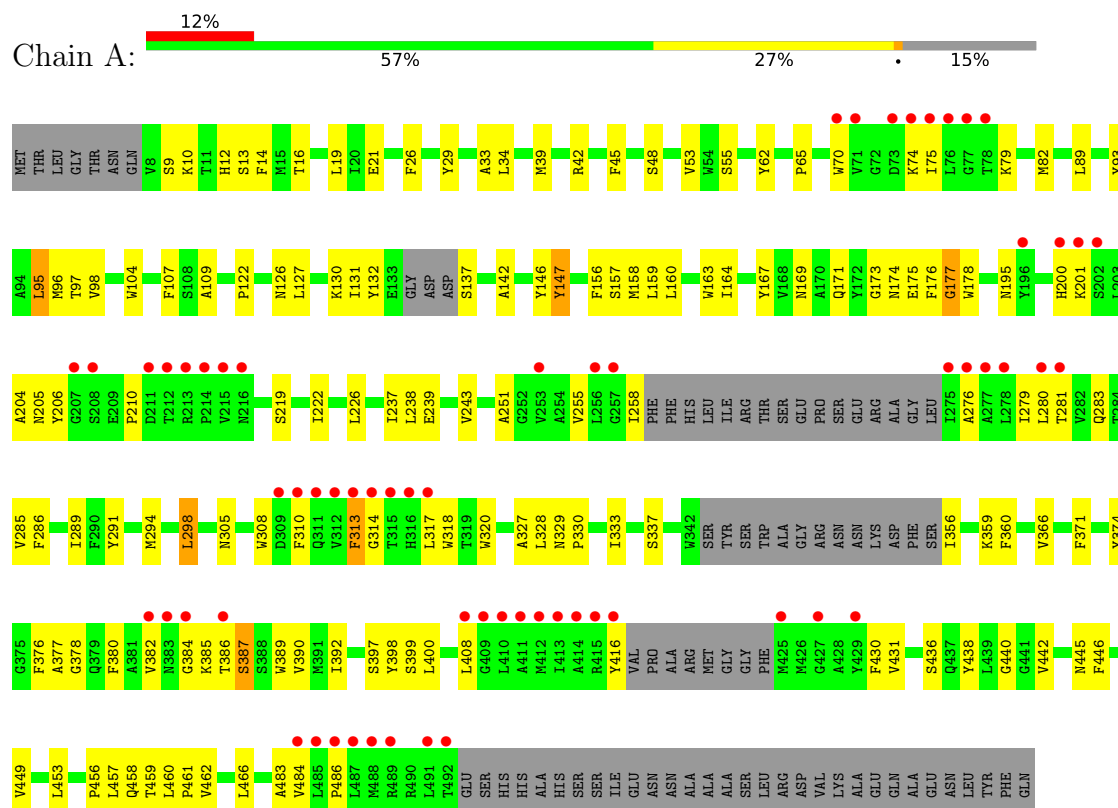
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0

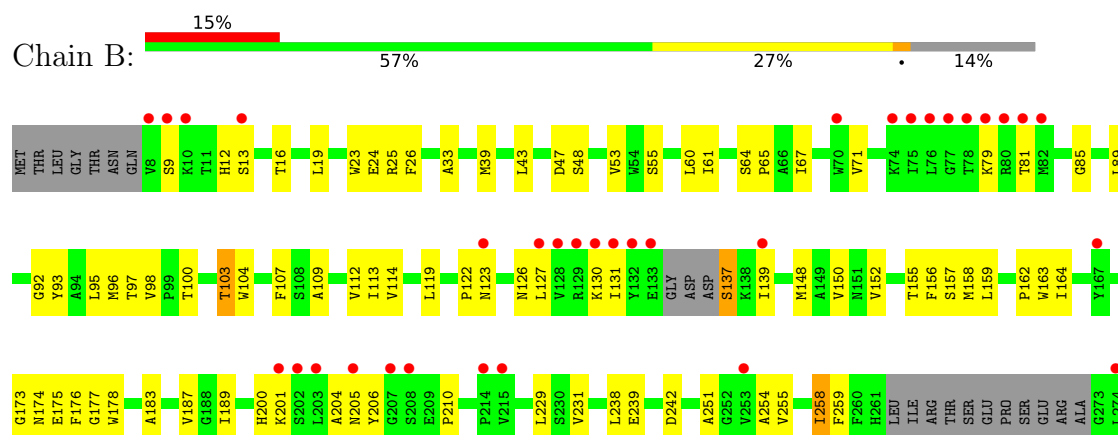
3 Residue-property plots

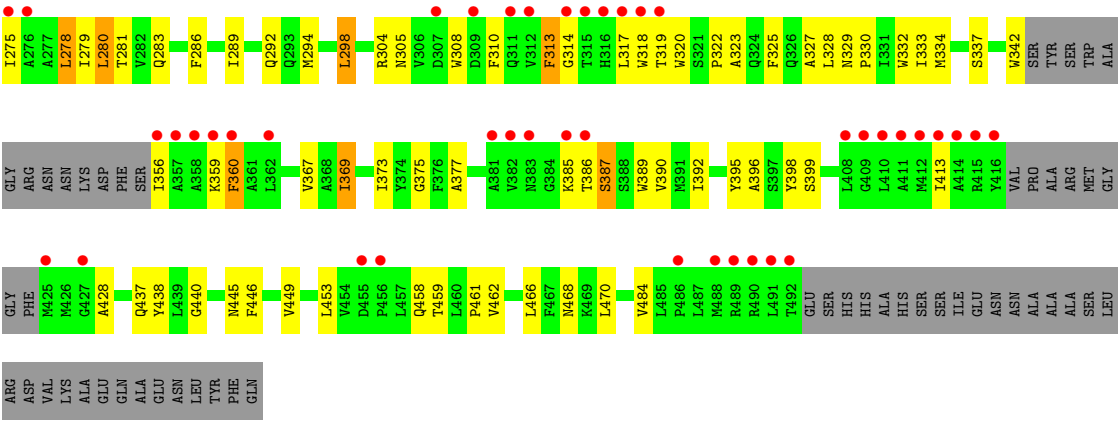
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Proton:oligopeptide symporter POT family



• Molecule 1: Proton:oligopeptide symporter POT family





• Molecule 2: ALA-ALA-ALA



• Molecule 2: ALA-ALA-ALA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.99Å 107.56Å 203.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 3.20 47.56 – 3.20	Depositor EDS
% Data completeness (in resolution range)	86.8 (47.56-3.20) 86.9 (47.56-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.243 , 0.290 0.243 , 0.290	Depositor DCC
R_{free} test set	1299 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: LMT, ZN

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	0.58	2/3461 (0.1%)	0.67	1/4719 (0.0%)
1	B	0.54	1/3508 (0.0%)	0.66	0/4782
2	C	0.30	0/15	0.75	0/18
2	E	0.29	0/15	0.70	0/18
All	All	0.56	3/6999 (0.0%)	0.66	1/9537 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	137	SER	CB-OG	5.77	1.49	1.42
1	B	137	SER	CB-OG	5.39	1.49	1.42
1	A	147	TYR	CE2-CZ	5.05	1.45	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	LEU	CB-CG-CD2	-5.18	102.19	111.00

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	3376	0	3382	99	0
1	B	3420	0	3421	101	0
2	C	16	0	14	1	0
2	E	16	0	14	1	0
3	A	35	0	46	7	0
3	B	70	0	92	4	0
4	B	1	0	0	0	0
All	All	6934	0	6969	204	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 15.

All (204) 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:156:PHE:CD1	3:A:601:LMT:H101	2.19	0.77
1:A:200:HIS:CG	1:A:201:LYS:H	2.04	0.76
1:B:292:GLN:OE1	1:B:437:GLN:NE2	2.18	0.76
1:B:279:ILE:HG12	1:B:484:VAL:HG21	1.68	0.75
1:B:377:ALA:HB2	1:B:390:VAL:HG11	1.68	0.74
1:A:387:SER:HB3	1:A:390:VAL:HB	1.68	0.74
1:B:200:HIS:CG	1:B:201:LYS:H	2.07	0.73
1:A:163:TRP:HE3	1:A:164:ILE:HD12	1.55	0.71
1:A:156:PHE:HD1	3:A:601:LMT:H101	1.53	0.70
1:B:387:SER:HB3	1:B:390:VAL:HB	1.75	0.69
1:B:65:PRO:HB3	1:B:122:PRO:HD3	1.72	0.69
1:B:93:TYR:O	1:B:97:THR:HG23	1.92	0.69
1:B:449:VAL:HG13	1:B:453:LEU:HD23	1.75	0.68
1:A:65:PRO:HB3	1:A:122:PRO:HD3	1.77	0.67
1:A:107:PHE:CD2	1:A:239:GLU:HG2	2.30	0.67
1:A:308:TRP:O	1:A:320:TRP:N	2.26	0.67
1:B:39:MET:HE1	1:B:53:VAL:HB	1.76	0.66
3:A:601:LMT:H1B	3:A:601:LMT:O3'	1.96	0.66
1:A:33:ALA:HB2	1:A:158:MET:HG2	1.76	0.66
1:A:200:HIS:CG	1:A:201:LYS:N	2.64	0.65
1:A:359:LYS:HB2	1:A:408:LEU:HD11	1.77	0.65
1:B:328:LEU:HD13	1:B:392:ILE:HA	1.80	0.64
1:B:200:HIS:CG	1:B:201:LYS:N	2.66	0.64
1:A:333:ILE:O	1:A:337:SER:HB2	1.98	0.63
1:A:26:PHE:CD1	1:A:157:SER:HB3	2.33	0.63
1:B:289:ILE:HG23	1:B:440:GLY:HA2	1.81	0.62
1:B:156:PHE:CE1	3:B:602:LMT:H101	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD23	1:A:459:THR:HG22	1.83	0.60
1:B:255:VAL:HG23	1:B:428:ALA:HA	1.84	0.59
1:B:294:MET:HA	1:B:298:LEU:HB2	1.84	0.59
1:B:333:ILE:O	1:B:337:SER:HB2	2.03	0.59
1:B:104:TRP:CZ2	1:B:239:GLU:HG3	2.38	0.58
1:A:294:MET:HA	1:A:298:LEU:HB2	1.86	0.58
1:B:33:ALA:HB2	1:B:158:MET:HG2	1.84	0.58
3:B:603:LMT:O3'	3:B:603:LMT:H1B	2.04	0.57
1:A:163:TRP:CE3	1:A:164:ILE:HD12	2.37	0.57
1:A:96:MET:HG2	1:A:109:ALA:HB1	1.86	0.57
1:A:147:TYR:OH	1:A:333:ILE:HD13	2.04	0.57
1:B:327:ALA:O	1:B:330:PRO:HD2	2.03	0.57
1:A:283:GLN:HA	1:A:286:PHE:HD2	1.70	0.56
1:A:382:VAL:HA	1:A:386:THR:HB	1.87	0.56
1:B:329:ASN:HB3	1:B:330:PRO:HD3	1.88	0.56
1:B:148:MET:HE3	1:B:334:MET:HG2	1.87	0.55
1:B:126:ASN:O	1:B:130:LYS:HG2	2.07	0.55
1:B:107:PHE:CD2	1:B:239:GLU:HG2	2.42	0.55
1:A:378:GLY:HA2	1:A:382:VAL:HG21	1.89	0.54
1:B:98:VAL:HG22	1:B:100:THR:HG22	1.89	0.54
1:A:386:THR:O	1:A:387:SER:OG	2.16	0.54
1:A:104:TRP:CZ2	1:A:239:GLU:HG3	2.42	0.54
1:B:329:ASN:OD1	2:C:10:ALA:N	2.41	0.54
1:B:308:TRP:O	1:B:320:TRP:N	2.37	0.54
1:B:173:GLY:O	1:B:175:GLU:N	2.38	0.53
1:A:70:TRP:CH2	1:A:75:ILE:HD11	2.43	0.53
1:B:26:PHE:CD1	1:B:157:SER:HB3	2.43	0.53
1:A:377:ALA:HB2	1:A:390:VAL:HG11	1.90	0.53
1:B:332:TRP:CE2	1:B:396:ALA:HB2	2.44	0.53
1:A:13:SER:O	1:A:16:THR:HG22	2.09	0.53
1:B:163:TRP:HE3	1:B:164:ILE:HD12	1.73	0.53
1:B:458:GLN:O	1:B:461:PRO:HD2	2.09	0.52
1:B:95:LEU:O	1:B:98:VAL:HG13	2.08	0.52
1:B:367:VAL:HG22	1:B:398:TYR:HD1	1.73	0.52
1:A:79:LYS:HD3	1:A:204:ALA:HB1	1.91	0.52
1:A:384:GLY:HA2	1:A:457:LEU:HD12	1.91	0.51
1:A:93:TYR:O	1:A:97:THR:HG23	2.10	0.51
1:A:446:PHE:HB2	1:A:466:LEU:HD13	1.92	0.51
1:B:319:THR:OG1	3:B:602:LMT:H3B	2.10	0.51
1:A:10:LYS:HD2	1:A:131:ILE:O	2.11	0.51
1:B:395:TYR:O	1:B:399:SER:OG	2.17	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:THR:HG23	1:B:119:LEU:HD22	1.92	0.50
1:B:148:MET:HE1	1:B:334:MET:HA	1.94	0.50
1:A:458:GLN:O	1:A:461:PRO:HD2	2.11	0.50
1:B:61:ILE:HG13	1:B:114:VAL:HG22	1.94	0.50
1:B:356:ILE:HG22	1:B:359:LYS:HG2	1.92	0.50
1:B:39:MET:HE1	1:B:53:VAL:CB	2.43	0.49
1:A:173:GLY:O	1:A:175:GLU:N	2.41	0.49
1:B:375:GLY:HA3	1:B:468:ASN:ND2	2.28	0.49
1:B:24:GLU:HA	1:B:189:ILE:HD13	1.94	0.49
1:B:162:PRO:HB3	1:B:323:ALA:HB3	1.94	0.49
1:A:169:ASN:OD1	1:A:177:GLY:HA3	2.12	0.49
1:A:329:ASN:ND2	1:A:399:SER:HB3	2.27	0.49
1:A:107:PHE:HD2	1:A:239:GLU:HG2	1.77	0.49
1:A:82:MET:CE	1:A:127:LEU:HD22	2.43	0.49
1:A:329:ASN:HD22	1:A:399:SER:HB3	1.77	0.49
1:A:126:ASN:O	1:A:130:LYS:HG2	2.12	0.49
1:B:183:ALA:O	1:B:187:VAL:HG13	2.13	0.49
1:A:204:ALA:O	1:A:206:TYR:N	2.46	0.48
1:A:21:GLU:OE1	1:A:146:TYR:OH	2.29	0.48
1:B:283:GLN:HB3	1:B:360:PHE:CE1	2.48	0.48
1:A:459:THR:O	1:A:462:VAL:HG22	2.13	0.48
1:A:156:PHE:HB2	3:A:601:LMT:H121	1.95	0.48
1:A:276:ALA:HB3	1:A:416:TYR:CZ	2.49	0.48
1:A:294:MET:SD	1:A:398:TYR:HE2	2.37	0.48
1:B:104:TRP:CE2	1:B:239:GLU:HG3	2.48	0.48
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.68	0.48
1:B:13:SER:O	1:B:16:THR:HG22	2.13	0.48
1:A:159:LEU:HB3	3:A:601:LMT:H52	1.96	0.47
1:B:275:ILE:O	1:B:278:LEU:HB2	2.14	0.47
1:B:310:PHE:HB2	1:B:320:TRP:CD1	2.50	0.47
1:B:386:THR:O	1:B:387:SER:OG	2.17	0.47
1:A:39:MET:HE1	1:A:53:VAL:HB	1.96	0.47
1:B:342:TRP:N	1:B:342:TRP:CD1	2.82	0.47
1:B:329:ASN:ND2	1:B:399:SER:HB3	2.29	0.47
1:A:95:LEU:HB3	1:A:109:ALA:HB2	1.97	0.47
1:A:107:PHE:CE2	1:A:239:GLU:HG2	2.50	0.47
1:A:310:PHE:HE1	1:A:389:TRP:CZ2	2.32	0.47
1:A:366:VAL:HG11	1:A:400:LEU:HD23	1.97	0.47
1:B:103:THR:HG23	1:B:107:PHE:CE2	2.50	0.46
1:A:176:PHE:O	1:A:178:TRP:N	2.48	0.46
1:A:291:TYR:HA	1:A:398:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASN:ND2	1:A:456:PRO:O	2.46	0.46
1:A:310:PHE:HB2	1:A:320:TRP:NE1	2.30	0.46
1:A:147:TYR:CG	1:A:147:TYR:O	2.68	0.46
1:A:55:SER:HB3	1:A:438:TYR:HA	1.98	0.46
1:B:369:ILE:O	1:B:373:ILE:HG13	2.16	0.46
1:A:329:ASN:HB3	1:A:330:PRO:HD3	1.98	0.46
1:A:376:PHE:HD2	1:A:380:PHE:HD2	1.63	0.45
1:B:85:GLY:O	1:B:89:LEU:HB2	2.15	0.45
1:B:317:LEU:HA	1:B:318:TRP:HA	1.69	0.45
1:B:55:SER:HB3	1:B:438:TYR:HA	1.98	0.45
1:B:310:PHE:HE1	1:B:389:TRP:CE2	2.34	0.45
1:B:329:ASN:HD22	1:B:399:SER:HB3	1.82	0.45
1:B:155:THR:OG1	1:B:330:PRO:HB2	2.15	0.45
1:A:29:TYR:CZ	2:E:10:ALA:HB1	2.52	0.45
1:B:96:MET:HG2	1:B:109:ALA:HB1	1.99	0.45
1:A:378:GLY:HA2	1:A:460:LEU:HD21	1.99	0.45
1:B:112:VAL:HA	1:B:231:VAL:HG22	1.98	0.45
1:B:275:ILE:HA	1:B:278:LEU:HD12	1.97	0.45
1:B:204:ALA:O	1:B:206:TYR:N	2.50	0.45
1:B:251:ALA:O	1:B:255:VAL:HG12	2.17	0.45
1:A:328:LEU:HD13	1:A:392:ILE:HA	1.98	0.44
1:B:60:LEU:O	1:B:64:SER:HB2	2.17	0.44
1:B:64:SER:HB3	1:B:65:PRO:HD3	1.99	0.44
1:A:279:ILE:HG21	1:A:484:VAL:HG21	1.99	0.44
1:B:254:ALA:O	1:B:258:ILE:HG23	2.16	0.44
1:B:127:LEU:O	1:B:131:ILE:N	2.43	0.44
1:B:310:PHE:HB2	1:B:320:TRP:NE1	2.32	0.44
1:A:251:ALA:O	1:A:255:VAL:HG12	2.18	0.44
1:A:14:PHE:CE1	1:A:142:ALA:HB1	2.53	0.44
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.84	0.44
1:A:89:LEU:HD12	1:A:89:LEU:HA	1.78	0.44
1:A:356:ILE:HG22	1:A:359:LYS:HG2	1.99	0.44
1:B:109:ALA:O	1:B:113:ILE:HD12	2.17	0.44
1:B:385:LYS:HE3	1:B:385:LYS:HB2	1.81	0.44
3:B:602:LMT:O2'	3:B:602:LMT:H12	2.10	0.44
1:A:289:ILE:HG23	1:A:440:GLY:HA2	1.99	0.44
1:A:366:VAL:O	1:A:397:SER:OG	2.36	0.44
1:A:62:TYR:O	1:A:430:PHE:HD1	2.01	0.44
1:A:449:VAL:HG13	1:A:453:LEU:HD23	1.99	0.43
1:A:317:LEU:HA	1:A:318:TRP:HA	1.81	0.43
1:A:310:PHE:HB2	1:A:320:TRP:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.78	0.43
1:B:367:VAL:HG22	1:B:398:TYR:CD1	2.52	0.43
1:B:137:SER:C	1:B:139:ILE:H	2.21	0.43
1:A:19:LEU:HD13	1:A:195:ASN:HD21	1.84	0.43
1:A:48:SER:HA	1:A:445:ASN:OD1	2.19	0.43
1:A:313:PHE:HA	1:A:314:GLY:HA2	1.61	0.43
1:B:280:LEU:HB3	1:B:413:ILE:HD11	2.00	0.43
1:B:9:SER:HB2	1:B:12:HIS:HB2	2.00	0.43
1:B:176:PHE:O	1:B:178:TRP:N	2.52	0.43
1:B:446:PHE:HB2	1:B:466:LEU:HD13	1.99	0.43
1:B:229:LEU:HD12	1:B:229:LEU:HA	1.81	0.42
1:A:483:ALA:O	1:A:486:PRO:HD2	2.19	0.42
1:B:25:ARG:HG3	1:B:150:VAL:HG22	2.01	0.42
1:B:47:ASP:OD2	1:B:304:ARG:NH1	2.37	0.42
1:B:92:GLY:HA3	1:B:113:ILE:HG13	2.01	0.42
1:B:283:GLN:HA	1:B:286:PHE:HD2	1.84	0.42
1:A:255:VAL:HB	1:A:431:VAL:HG11	2.02	0.42
1:A:285:VAL:HG13	1:A:436:SER:HB3	2.01	0.42
1:A:237:ILE:HG12	1:A:243:VAL:HG12	2.01	0.42
1:B:148:MET:O	1:B:152:VAL:HG12	2.19	0.42
1:A:310:PHE:CE1	1:A:389:TRP:CZ2	3.07	0.42
1:A:327:ALA:O	1:A:330:PRO:HD2	2.19	0.42
1:A:219:SER:HA	1:A:222:ILE:HG22	2.01	0.42
1:A:385:LYS:HE3	1:A:385:LYS:HB2	1.83	0.42
1:B:332:TRP:CZ2	1:B:396:ALA:HB2	2.54	0.42
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.85	0.41
3:A:601:LMT:H2'	3:A:601:LMT:H12	1.38	0.41
1:B:148:MET:CE	1:B:334:MET:HG2	2.50	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.84	0.41
1:B:308:TRP:CE2	1:B:322:PRO:HD3	2.54	0.41
1:B:313:PHE:HA	1:B:314:GLY:HA2	1.53	0.41
1:B:470:LEU:HD23	1:B:470:LEU:HA	1.79	0.41
1:A:74:LYS:HD3	1:A:74:LYS:HA	1.78	0.41
1:B:48:SER:HA	1:B:445:ASN:OD1	2.20	0.41
1:B:79:LYS:HD3	1:B:204:ALA:HB1	2.03	0.41
1:A:39:MET:O	1:A:45:PHE:HB2	2.20	0.41
1:B:23:TRP:O	1:B:26:PHE:HB3	2.20	0.41
1:B:67:ILE:O	1:B:71:VAL:HG23	2.20	0.41
1:A:39:MET:HB3	1:A:39:MET:HE2	1.86	0.41
1:A:9:SER:HB2	1:A:12:HIS:HB2	2.02	0.41
1:A:14:PHE:HB2	1:A:132:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:PHE:O	1:B:328:LEU:HB2	2.21	0.41
1:A:42:ARG:HB2	1:A:178:TRP:CE2	2.55	0.41
1:A:160:LEU:HG	1:A:164:ILE:HD13	2.03	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.83	0.41
1:B:89:LEU:HD12	1:B:89:LEU:HA	1.75	0.41
1:B:305:ASN:OD1	1:B:459:THR:OG1	2.35	0.41
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.85	0.41
1:A:82:MET:HE1	1:A:127:LEU:HD22	2.03	0.41
1:A:167:TYR:CE1	1:A:171:GLN:HG3	2.56	0.41
1:A:371:PHE:HA	1:A:374:TYR:HD2	1.86	0.41
1:B:459:THR:O	1:B:462:VAL:HG22	2.21	0.41
1:A:156:PHE:CG	3:A:601:LMT:H121	2.57	0.40
1:B:119:LEU:O	1:B:123:ASN:ND2	2.51	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	435/523 (83%)	401 (92%)	28 (6%)	6 (1%)	11	46
1	B	440/523 (84%)	408 (93%)	25 (6%)	7 (2%)	9	43
2	C	1/3 (33%)	1 (100%)	0	0	100	100
2	E	1/3 (33%)	1 (100%)	0	0	100	100
All	All	877/1052 (83%)	811 (92%)	53 (6%)	13 (2%)	10	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	387	SER

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Mol	Chain	Res	Type
1	B	387	SER
1	A	177	GLY
1	B	205	ASN
1	A	174	ASN
1	A	313	PHE
1	B	174	ASN
1	B	313	PHE
1	B	177	GLY
1	A	210	PRO
1	B	278	LEU
1	B	210	PRO

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	338/417 (81%)	331 (98%)	7 (2%)	53	79
1	B	342/417 (82%)	331 (97%)	11 (3%)	39	71
All	All	680/834 (82%)	662 (97%)	18 (3%)	46	76

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

Mol	Chain	Res	Type
1	A	98	VAL
1	A	258	ILE
1	A	280	LEU
1	A	281	THR
1	A	298	LEU
1	A	360	PHE
1	A	442	VAL
1	B	19	LEU
1	B	43	LEU
1	B	103	THR
1	B	242	ASP
1	B	258	ILE

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Mol	Chain	Res	Type
1	B	259	PHE
1	B	280	LEU
1	B	281	THR
1	B	298	LEU
1	B	360	PHE
1	B	369	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	292	GLN
1	B	437	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	B	602	-	36,36,36	0.55	0	47,47,47	1.50	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	B	603	-	36,36,36	0.45	0	47,47,47	1.34	5 (10%)
3	LMT	A	601	-	36,36,36	0.58	0	47,47,47	1.26	7 (14%)

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	B	602	-	-	13/21/61/61	0/2/2/2
3	LMT	B	603	-	-	10/21/61/61	0/2/2/2
3	LMT	A	601	-	-	12/21/61/61	0/2/2/2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	LMT	C1B-O1B-C4'	-3.93	108.23	117.96
3	B	602	LMT	C1B-O1B-C4'	-3.72	108.75	117.96
3	B	602	LMT	C1'-O5'-C5'	-3.54	106.74	113.69
3	B	603	LMT	C1-O1'-C1'	3.38	119.44	113.84
3	B	603	LMT	O1B-C4'-C3'	3.16	115.68	107.28
3	B	603	LMT	C4B-C3B-C2B	-3.05	105.50	110.82
3	B	602	LMT	C4B-C3B-C2B	-2.90	105.75	110.82
3	A	601	LMT	C1'-C2'-C3'	2.66	115.53	110.00
3	A	601	LMT	C1'-O5'-C5'	-2.64	108.51	113.69
3	B	602	LMT	O5'-C5'-C6'	2.57	112.83	106.44
3	B	602	LMT	C3B-C4B-C5B	-2.52	105.75	110.24
3	B	603	LMT	C3B-C4B-C5B	-2.52	105.75	110.24
3	B	602	LMT	C1-O1'-C1'	2.46	117.91	113.84
3	B	602	LMT	C1'-C2'-C3'	2.40	114.98	110.00
3	A	601	LMT	C1B-O5B-C5B	-2.33	109.11	113.69
3	A	601	LMT	C1-O1'-C1'	2.28	117.61	113.84
3	A	601	LMT	C6B-C5B-C4B	-2.14	107.99	113.00
3	B	603	LMT	O5'-C1'-C2'	-2.13	105.84	110.35
3	B	602	LMT	O5'-C5'-C4'	-2.05	105.44	109.75
3	A	601	LMT	C2'-C3'-C4'	2.00	114.25	109.68

There are no chirality outliers.

All (35) torsion outliers are listed below:

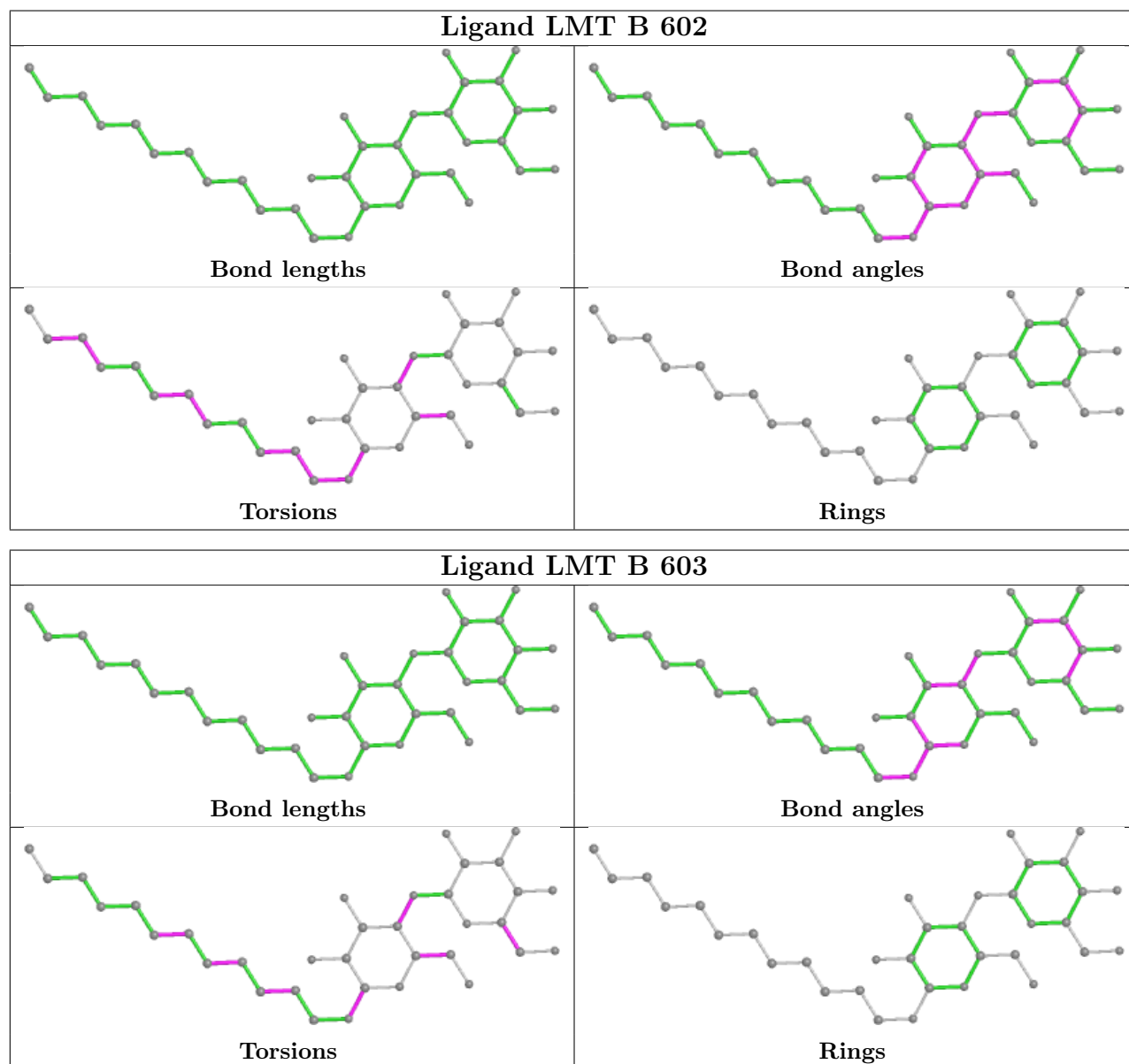
Mol	Chain	Res	Type	Atoms
3	A	601	LMT	C2'-C1'-O1'-C1
3	B	602	LMT	C2'-C1'-O1'-C1
3	B	602	LMT	O5'-C1'-O1'-C1
3	B	603	LMT	C2'-C1'-O1'-C1
3	B	603	LMT	O5'-C1'-O1'-C1
3	B	602	LMT	O5'-C5'-C6'-O6'
3	B	602	LMT	C4'-C5'-C6'-O6'
3	B	603	LMT	C3'-C4'-O1B-C1B
3	A	601	LMT	C2-C3-C4-C5
3	B	603	LMT	C4'-C5'-C6'-O6'
3	A	601	LMT	O1'-C1-C2-C3
3	B	603	LMT	C5'-C4'-O1B-C1B
3	B	602	LMT	O1'-C1-C2-C3
3	B	603	LMT	C5-C6-C7-C8
3	B	602	LMT	C4-C5-C6-C7
3	A	601	LMT	C4-C5-C6-C7
3	A	601	LMT	C2-C1-O1'-C1'
3	B	602	LMT	C2-C1-O1'-C1'
3	B	603	LMT	C1-C2-C3-C4
3	B	603	LMT	O5'-C5'-C6'-O6'
3	A	601	LMT	C5'-C4'-O1B-C1B
3	B	602	LMT	C1-C2-C3-C4
3	A	601	LMT	C3'-C4'-O1B-C1B
3	A	601	LMT	C5-C6-C7-C8
3	B	603	LMT	O5B-C5B-C6B-O6B
3	B	602	LMT	C9-C10-C11-C12
3	B	603	LMT	C3-C4-C5-C6
3	B	602	LMT	C5'-C4'-O1B-C1B
3	A	601	LMT	O5'-C5'-C6'-O6'
3	B	602	LMT	C3'-C4'-O1B-C1B
3	B	602	LMT	C5-C6-C7-C8
3	A	601	LMT	C4'-C5'-C6'-O6'
3	B	602	LMT	C11-C10-C9-C8
3	A	601	LMT	C7-C8-C9-C10
3	A	601	LMT	C3-C4-C5-C6

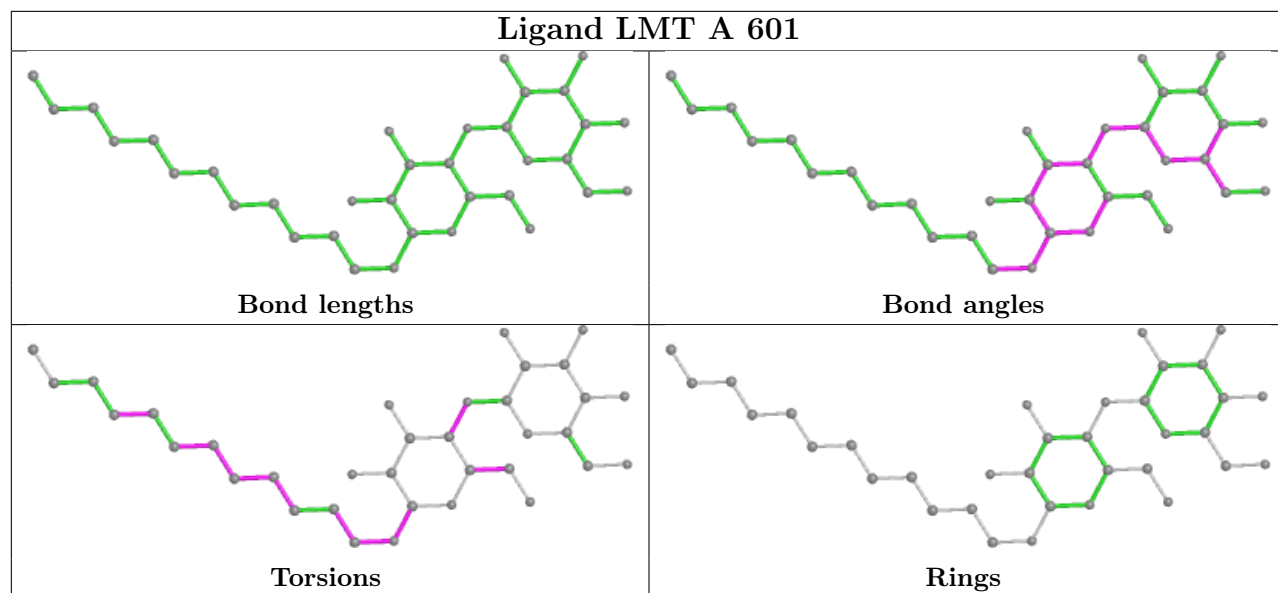
There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	LMT	3	0
3	B	603	LMT	1	0
3	A	601	LMT	7	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	445/523 (85%)	0.45	62 (13%) 2 1	50, 86, 148, 181	0
1	B	450/523 (86%)	0.61	76 (16%) 1 1	52, 86, 153, 204	0
2	C	3/3 (100%)	0.96	1 (33%) 0 0	116, 116, 119, 138	0
2	E	3/3 (100%)	1.65	1 (33%) 0 0	114, 114, 118, 136	0
All	All	901/1052 (85%)	0.54	140 (15%) 2 1	50, 86, 152, 204	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	10.6
1	A	412	MET	9.9
1	A	315	THR	9.1
1	B	208	SER	8.5
1	A	311	GLN	8.3
1	B	412	MET	8.3
1	B	133	GLU	8.2
1	B	415	ARG	8.1
1	A	312	VAL	7.4
1	B	414	ALA	7.1
1	B	131	ILE	7.1
1	B	202	SER	6.9
1	B	316	HIS	6.8
1	B	315	THR	6.5
1	A	313	PHE	6.5
1	B	490	ARG	6.3
1	B	382	VAL	6.2
1	A	488	MET	6.0
1	A	212	THR	6.0
1	A	275	ILE	5.7
1	A	213	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	276	ALA	5.6
1	B	201	LYS	5.5
1	A	214	PRO	5.5
1	A	411	ALA	5.5
1	B	491	LEU	5.4
1	A	317	LEU	5.3
1	A	76	LEU	5.3
1	A	414	ALA	5.3
1	A	75	ILE	5.2
1	B	9	SER	5.2
1	B	383	ASN	5.1
1	B	416	TYR	5.0
1	B	413	ILE	4.9
1	B	312	VAL	4.9
1	B	10	LYS	4.8
1	B	408	LEU	4.7
1	A	425	MET	4.7
1	B	132	TYR	4.7
1	A	78	THR	4.7
1	A	208	SER	4.6
1	A	278	LEU	4.6
1	A	316	HIS	4.5
1	A	410	LEU	4.4
1	A	415	ARG	4.3
1	B	79	LYS	4.2
1	B	381	ALA	4.2
1	B	386	THR	4.2
1	B	427	GLY	4.2
1	A	489	ARG	4.2
1	A	314	GLY	4.1
1	A	310	PHE	4.1
1	B	130	LYS	4.1
1	B	410	LEU	3.9
1	A	309	ASP	3.9
1	B	207	GLY	3.9
1	B	409	GLY	3.8
1	B	80	ARG	3.8
1	B	8	VAL	3.8
1	B	274	LEU	3.7
1	B	311	GLN	3.7
1	A	427	GLY	3.7
1	B	76	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	413	ILE	3.6
1	A	277	ALA	3.6
1	A	382	VAL	3.6
1	A	216	ASN	3.5
1	B	75	ILE	3.5
1	B	74	LYS	3.5
1	A	211	ASP	3.5
1	A	485	LEU	3.4
1	A	257	GLY	3.4
1	B	214	PRO	3.4
1	A	77	GLY	3.3
1	B	314	GLY	3.3
1	A	486	PRO	3.3
1	B	488	MET	3.3
1	A	215	VAL	3.3
1	B	13	SER	3.2
1	B	356	ILE	3.2
1	B	425	MET	3.2
1	A	202	SER	3.1
2	E	10	ALA	3.1
1	B	123	ASN	3.1
1	A	487	LEU	3.1
1	B	385	LYS	3.0
1	B	319	THR	3.0
1	A	281	THR	3.0
1	B	492	THR	3.0
1	B	309	ASP	3.0
1	B	78	THR	3.0
1	B	128	VAL	2.9
1	A	74	LYS	2.9
1	B	129	ARG	2.8
1	A	409	GLY	2.8
1	A	408	LEU	2.8
1	A	484	VAL	2.8
1	B	318	TRP	2.8
1	A	386	THR	2.8
1	A	196	TYR	2.7
1	B	77	GLY	2.7
1	B	139	ILE	2.7
1	B	275	ILE	2.7
1	B	205	ASN	2.7
1	B	411	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	489	ARG	2.6
1	A	73	ASP	2.6
1	A	207	GLY	2.6
1	A	200	HIS	2.5
1	A	491	LEU	2.5
1	B	486	PRO	2.5
2	C	10	ALA	2.5
1	B	455	ASP	2.4
1	B	70	TRP	2.4
1	A	383	ASN	2.4
1	B	203	LEU	2.4
1	B	82	MET	2.4
1	B	456	PRO	2.4
1	A	256	LEU	2.3
1	B	81	THR	2.3
1	A	416	TYR	2.3
1	A	280	LEU	2.3
1	B	357	ALA	2.3
1	A	71	VAL	2.2
1	B	276	ALA	2.2
1	B	127	LEU	2.2
1	A	492	THR	2.2
1	B	360	PHE	2.2
1	B	167	TYR	2.2
1	A	201	LYS	2.2
1	B	307	ASP	2.2
1	B	215	VAL	2.1
1	A	70	TRP	2.1
1	B	253	VAL	2.1
1	A	429	TYR	2.1
1	B	362	LEU	2.1
1	A	253	VAL	2.1
1	A	384	GLY	2.0
1	B	359	LYS	2.0
1	B	358	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

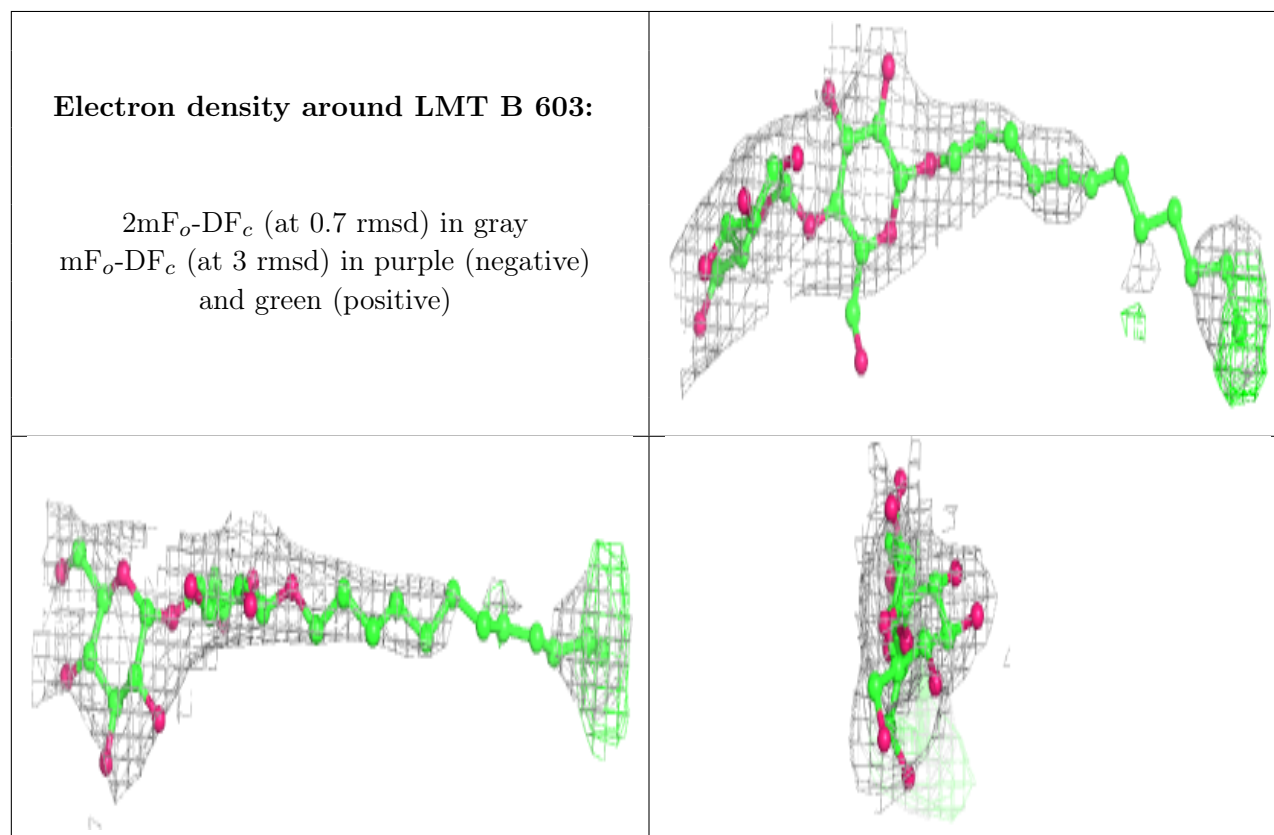
There are no monosaccharides in this entry.

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.

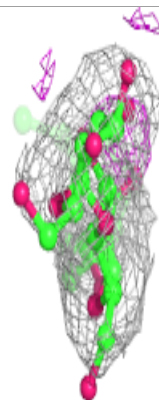
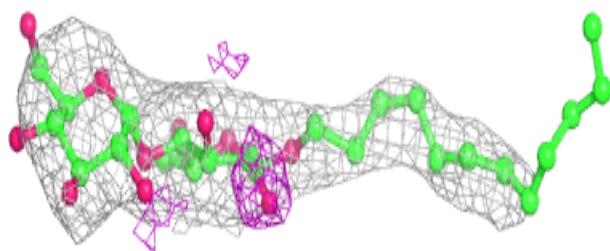
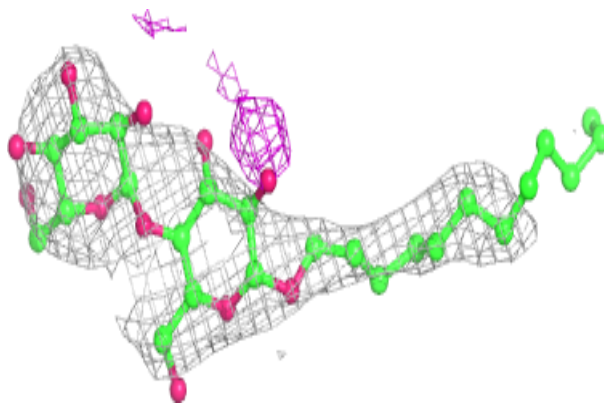
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	LMT	B	603	35/35	0.76	0.44	77,114,128,129	0
3	LMT	B	602	35/35	0.84	0.47	89,123,142,146	0
3	LMT	A	601	35/35	0.88	0.24	73,106,137,140	0
4	ZN	B	601	1/1	0.88	0.19	131,131,131,131	0

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.

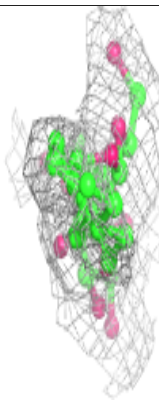
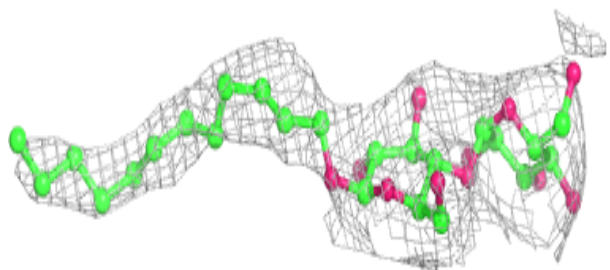
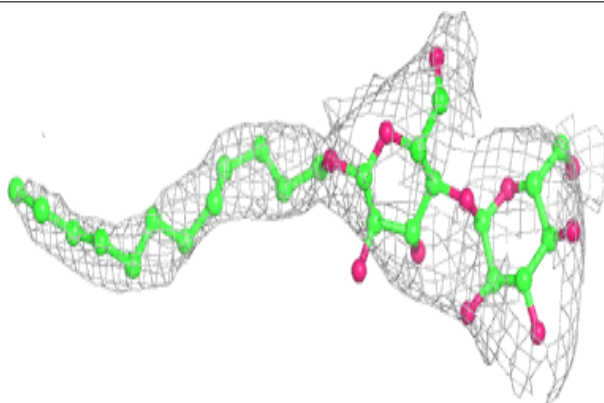


Electron density around LMT B 602:

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

**Electron density around LMT A 601:**

$2mF_o-DF_c$ (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.