



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:18 AM UTC

PDB ID : 4TPJ / pdb_00004tpj
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 : 4-5-2 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

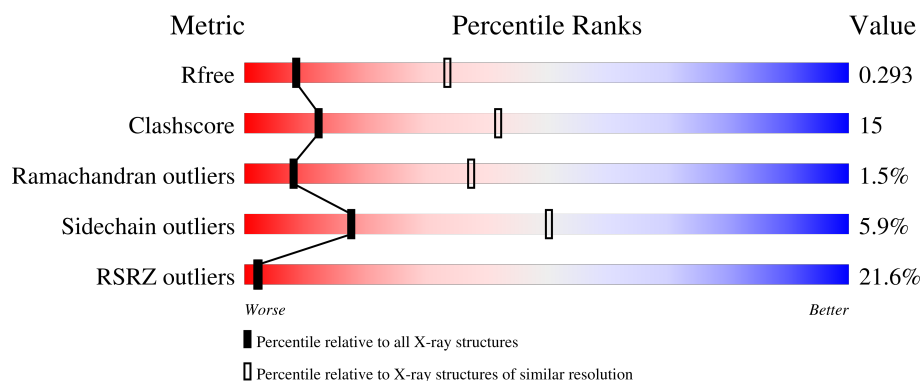
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (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	19% 54% 29% 15%
1	B	523	18% 54% 29% 14%
2	C	3	67% 67% 33%
2	E	3	67% 67% 33%

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			

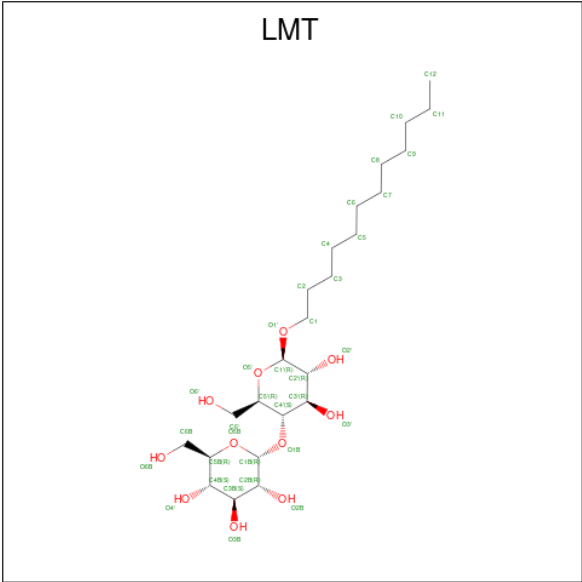
There are 14 discrepancies between the modelled and reference sequences:

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-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



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
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

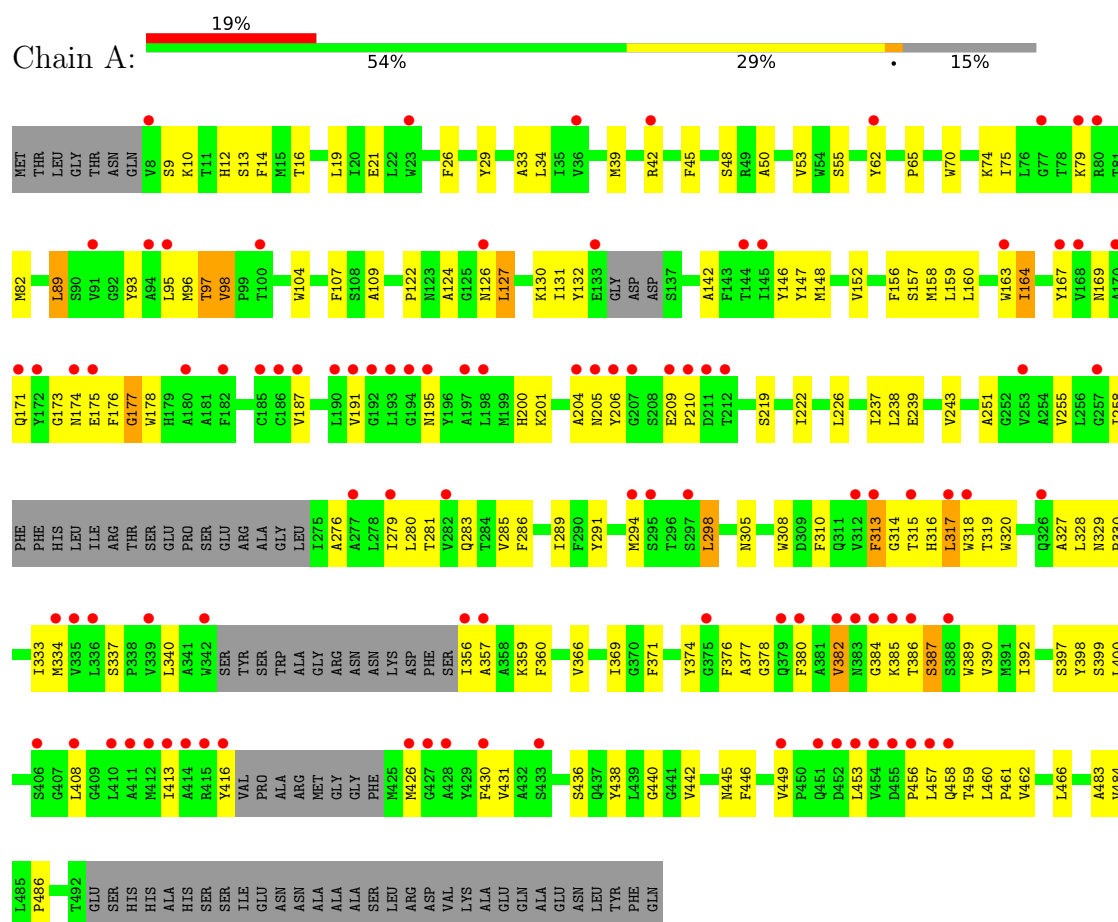
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

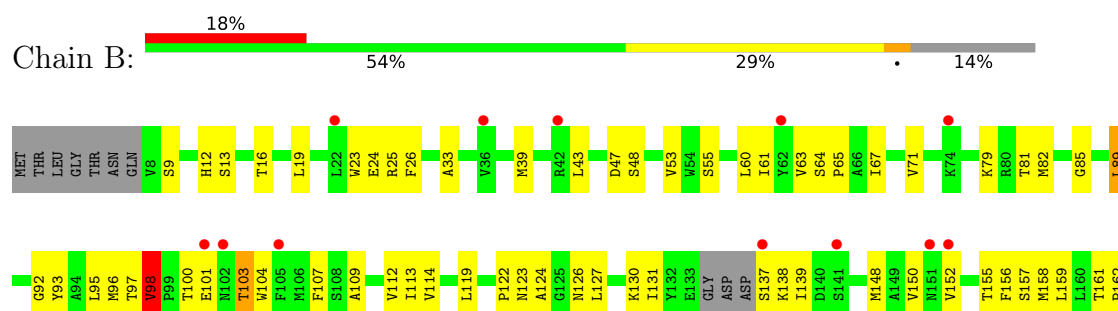
3 Residue-property plots

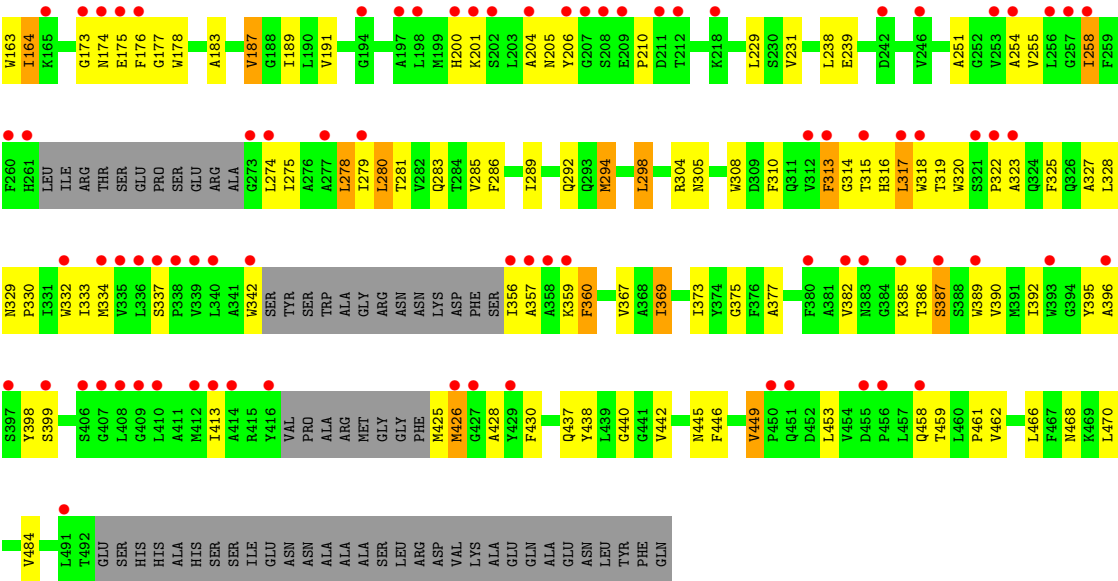
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 0.249 , 0.293	Depositor DCC
R_{free} test set	1299 reflections (4.42%)	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)	0.23 , 52.9	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	0.87	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

5.1 Standard geometry

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	0.73	0/3461	1.00	6/4719 (0.1%)
1	B	0.71	0/3508	1.00	11/4782 (0.2%)
2	C	0.45	0/15	1.04	0/18
2	E	0.27	0/15	0.86	0/18
All	All	0.72	0/6999	1.00	17/9537 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	GLU	CA-C-N	6.98	128.57	119.84
1	A	209	GLU	C-N-CA	6.98	128.57	119.84
1	A	98	VAL	N-CA-CB	6.50	116.12	110.08
1	B	357	ALA	N-CA-C	-6.33	105.51	112.72
1	A	357	ALA	N-CA-C	-6.18	105.68	112.72
1	B	138	LYS	N-CA-C	-6.00	106.02	113.15
1	B	449	VAL	N-CA-C	5.74	113.56	107.76
1	B	63	VAL	CA-C-N	5.58	127.73	120.26
1	B	63	VAL	C-N-CA	5.58	127.73	120.26
1	A	316	HIS	N-CA-C	5.44	120.57	113.88
1	B	98	VAL	N-CA-CB	5.41	115.11	110.08
1	B	316	HIS	N-CA-C	5.28	120.38	113.88
1	B	382	VAL	N-CA-C	5.25	115.46	108.27
1	B	426	MET	N-CA-C	5.18	117.59	111.33
1	B	161	THR	CA-C-N	-5.02	113.76	119.28
1	B	161	THR	C-N-CA	-5.02	113.76	119.28
1	A	98	VAL	N-CA-C	-5.01	104.04	108.95

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	3376	0	3382	105	0
1	B	3420	0	3421	106	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	215	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 (215) 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:82:MET:HE1	1:A:127:LEU:HD22	1.62	0.80
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:82:MET:HE2	1:B:124:ALA:HA	1.72	0.70
1:B:39:MET:HE1	1:B:53:VAL:HB	1.74	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
3:A:601:LMT:H1B	3:A:601:LMT:O3'	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:HB2	1:A:158:MET:HG2	1.76	0.66
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:A:148:MET:HE1	1:A:334:MET:HG2	1.80	0.64
1:A:200:HIS:CG	1:A:201:LYS:N	2.64	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:200:HIS:CG	1:B:201:LYS:N	2.66	0.62
1:B:289:ILE:HG23	1:B:440:GLY:HA2	1.81	0.62
1:B:318:TRP:CD1	1:B:319:THR:H	2.18	0.61
1:B:156:PHE:CE1	3:B:602:LMT:H101	2.36	0.61
1:A:453:LEU:HD23	1:A:459:THR:HG22	1.83	0.60
1:A:318:TRP:CD1	1:A:319:THR:H	2.20	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:148:MET:HE1	1:B:334:MET:HA	1.85	0.58
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:B:274:LEU:HD22	1:B:425:MET:HE2	1.86	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:81:THR:HG23	1:B:119:LEU:HD22	1.92	0.50
1:A:39:MET:HE1	1:A:53:VAL:HB	1.93	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: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: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:HA	1:B:159:LEU:HD23	1.68	0.48
1:B:13:SER:O	1:B:16:THR:HG22	2.13	0.48
1:B:426:MET:HE1	1:B:430:PHE:CE2	2.49	0.48
1:A:159:LEU:HB3	3:A:601:LMT:H52	1.96	0.47
1:B:137:SER:C	1:B:139:ILE:H	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:318:TRP:CG	1:B:319:THR:H	2.32	0.47
1:B:342:TRP:CD1	1:B:342:TRP:N	2.82	0.47
1:A:39:MET:HE2	1:A:50:ALA:HA	1.97	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
1:A:426:MET:HE3	1:A:430:PHE:HE2	1.80	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:39:MET:HE1	1:B:53:VAL:CB	2.46	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:HB2	1:B:385:LYS:HE3	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:426:MET:HE3	1:A:430:PHE:CE2	2.53	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
1:A:226:LEU:HA	1:A:226:LEU:HD23	1.78	0.43
1:A:82:MET:HE2	1:A:124:ALA:HA	2.00	0.43
1:B:367:VAL:HG22	1:B:398:TYR:CD1	2.52	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:A:458:GLN:C	1:A:461:PRO:HD2	2.45	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:B:148:MET:CE	1:B:334:MET:HG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H12	3:A:601:LMT:H2'	1.38	0.41
1:B:137:SER:C	1:B:139:ILE:N	2.78	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:HA	1:A:74:LYS:HD3	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: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
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: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:148:MET:HE3	1:A:148:MET:HB3	1.92	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 [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	435/523 (83%)	401 (92%)	28 (6%)	6 (1%)	9	39
1	B	440/523 (84%)	408 (93%)	25 (6%)	7 (2%)	7	36
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%)	8	37

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	387	SER
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%)	318 (94%)	20 (6%)	18	50
1	B	342/417 (82%)	322 (94%)	20 (6%)	18	51
All	All	680/834 (82%)	640 (94%)	40 (6%)	18	50

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	97	THR
1	A	98	VAL
1	A	127	LEU
1	A	152	VAL
1	A	164	ILE
1	A	187	VAL
1	A	191	VAL
1	A	258	ILE
1	A	280	LEU
1	A	281	THR
1	A	298	LEU
1	A	315	THR
1	A	317	LEU
1	A	340	LEU
1	A	360	PHE
1	A	369	ILE
1	A	382	VAL
1	A	413	ILE
1	A	442	VAL
1	B	19	LEU
1	B	43	LEU
1	B	89	LEU
1	B	98	VAL
1	B	101	GLU
1	B	103	THR
1	B	164	ILE
1	B	187	VAL
1	B	191	VAL
1	B	258	ILE
1	B	280	LEU
1	B	281	THR
1	B	285	VAL
1	B	294	MET
1	B	298	LEU
1	B	315	THR
1	B	317	LEU
1	B	360	PHE
1	B	369	ILE
1	B	442	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	51	ASN
1	A	195	ASN
1	A	200	HIS
1	A	216	ASN
1	B	12	HIS
1	B	32	GLN
1	B	41	GLN
1	B	51	ASN
1	B	283	GLN
1	B	329	ASN
1	B	437	GLN
1	B	458	GLN
1	B	468	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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	A	601	-	36,36,36	0.57	0	47,47,47	1.27	7 (14%)

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	1.36	5 (10%)
3	LMT	B	602	-	36,36,36	0.54	0	47,47,47	1.52	10 (21%)

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

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	LMT	C1B-O1B-C4'	-4.11	108.23	117.98
3	B	602	LMT	C1B-O1B-C4'	-3.89	108.75	117.98
3	B	602	LMT	C1'-O5'-C5'	-3.57	106.74	113.72
3	B	603	LMT	C1-O1'-C1'	3.37	119.44	113.68
3	B	603	LMT	O1B-C4'-C3'	3.33	115.68	107.23
3	B	603	LMT	C4B-C3B-C2B	-3.04	105.50	110.83
3	B	602	LMT	C4B-C3B-C2B	-2.89	105.75	110.83
3	A	601	LMT	C1'-O5'-C5'	-2.67	108.51	113.72
3	A	601	LMT	C1'-C2'-C3'	2.62	115.53	110.01
3	B	602	LMT	O5'-C5'-C6'	2.58	112.83	106.44
3	B	602	LMT	C1-O1'-C1'	2.48	117.91	113.68
3	B	602	LMT	C3B-C4B-C5B	-2.47	105.75	110.23
3	B	603	LMT	C3B-C4B-C5B	-2.47	105.75	110.23
3	B	602	LMT	C1'-C2'-C3'	2.36	114.98	110.01
3	A	601	LMT	C1B-O5B-C5B	-2.36	109.11	113.72
3	A	601	LMT	C1-O1'-C1'	2.30	117.61	113.68
3	B	603	LMT	O5'-C1'-C2'	-2.20	105.84	110.37
3	B	602	LMT	O5'-C5'-C4'	-2.07	105.44	109.72
3	B	602	LMT	O1B-C1B-C2B	2.07	113.17	108.09
3	A	601	LMT	C6B-C5B-C4B	-2.05	107.99	113.02
3	B	602	LMT	O1B-C4'-C3'	2.03	112.40	107.23
3	A	601	LMT	C2'-C3'-C4'	2.01	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	603	LMT	C2'-C1'-O1'-C1
3	B	602	LMT	O5'-C5'-C6'-O6'
3	B	602	LMT	C4'-C5'-C6'-O6'
3	B	602	LMT	O5'-C1'-O1'-C1
3	B	603	LMT	O5'-C1'-O1'-C1
3	B	603	LMT	C3'-C4'-O1B-C1B
3	B	603	LMT	C4'-C5'-C6'-O6'
3	A	601	LMT	O1'-C1-C2-C3
3	A	601	LMT	C2-C3-C4-C5
3	B	603	LMT	C5'-C4'-O1B-C1B
3	B	602	LMT	O1'-C1-C2-C3
3	B	603	LMT	C1-C2-C3-C4
3	A	601	LMT	C4-C5-C6-C7
3	B	603	LMT	C5-C6-C7-C8
3	B	603	LMT	O5'-C5'-C6'-O6'
3	B	602	LMT	C4-C5-C6-C7
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	B	603	LMT	O5B-C5B-C6B-O6B
3	A	601	LMT	C5-C6-C7-C8
3	B	602	LMT	C9-C10-C11-C12
3	A	601	LMT	C2-C1-O1'-C1'
3	B	602	LMT	C2-C1-O1'-C1'
3	B	602	LMT	C5'-C4'-O1B-C1B
3	B	602	LMT	C3'-C4'-O1B-C1B
3	B	603	LMT	C3-C4-C5-C6
3	A	601	LMT	O5'-C5'-C6'-O6'
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:

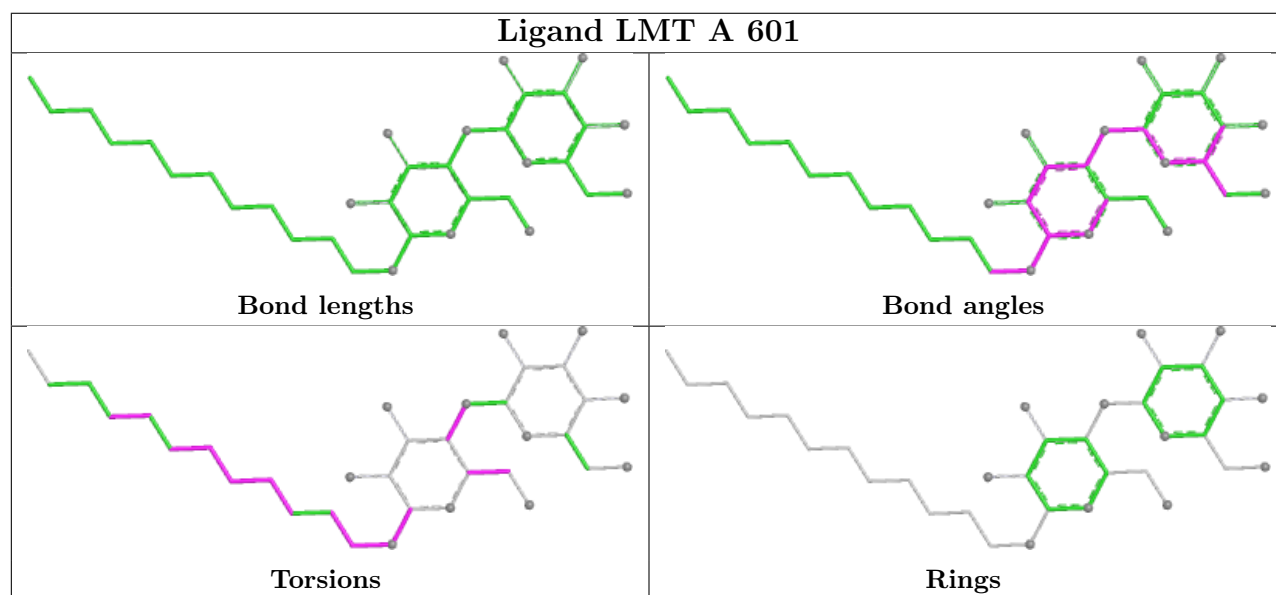
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	LMT	7	0

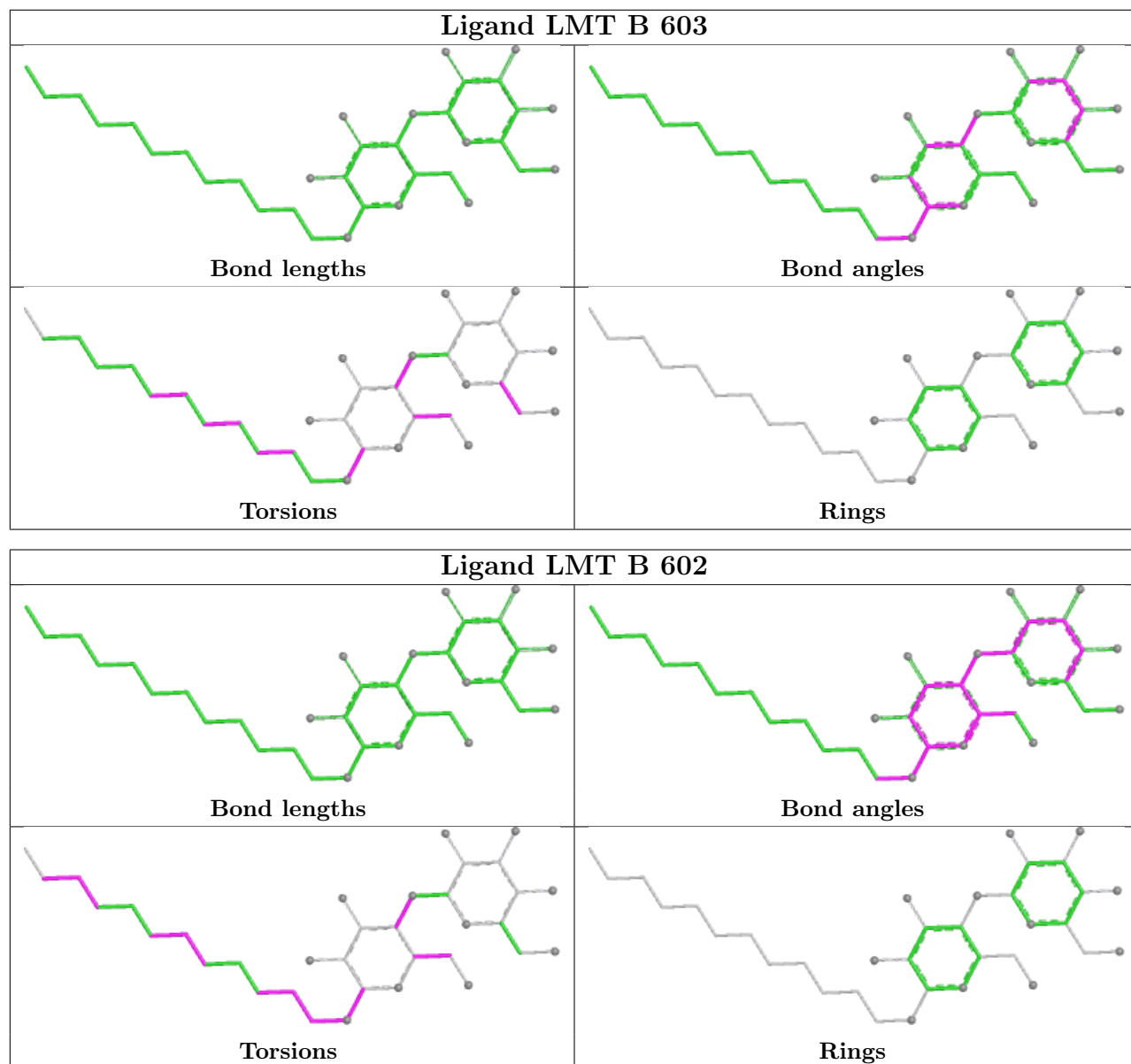
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	603	LMT	1	0
3	B	602	LMT	3	0

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%)	1.06	98 (22%) 2 2	50, 86, 148, 181	0
1	B	450/523 (86%)	0.94	93 (20%) 2 2	52, 86, 153, 204	0
2	C	3/3 (100%)	2.33	2 (66%) 0 0	116, 116, 119, 138	0
2	E	3/3 (100%)	1.81	2 (66%) 0 0	114, 114, 118, 136	0
All	All	901/1052 (85%)	1.01	195 (21%) 2 2	50, 86, 152, 204	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	LYS	8.4
1	B	202	SER	7.8
1	A	412	MET	7.7
1	B	198	LEU	7.7
1	A	458	GLN	7.6
1	A	415	ARG	7.6
1	A	167	TYR	7.2
1	A	414	ALA	6.6
1	A	172	TYR	6.4
1	B	334	MET	6.4
1	A	342	TRP	6.3
1	A	326	GLN	6.1
1	A	198	LEU	5.8
1	A	168	VAL	5.7
1	B	342	TRP	5.5
1	B	101	GLU	5.2
1	A	187	VAL	5.1
1	A	279	ILE	5.0
1	B	253	VAL	5.0
1	A	454	VAL	4.9
1	B	408	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	4.8
1	A	339	VAL	4.7
1	A	455	ASP	4.6
1	B	312	VAL	4.6
1	A	197	ALA	4.6
1	B	455	ASP	4.5
1	A	356	ILE	4.5
1	A	174	ASN	4.5
1	A	411	ALA	4.4
1	A	408	LEU	4.3
2	C	12	ALA	4.2
1	B	175	GLU	4.2
1	B	406	SER	4.2
1	A	334	MET	4.2
1	B	410	LEU	4.2
1	B	356	ILE	4.1
1	A	312	VAL	4.1
1	B	257	GLY	4.1
1	B	338	PRO	3.9
1	A	385	LYS	3.9
1	B	242	ASP	3.9
1	A	206	TYR	3.8
1	B	396	ALA	3.8
1	A	335	VAL	3.8
1	A	195	ASN	3.8
1	A	357	ALA	3.7
1	B	399	SER	3.7
1	A	451	GLN	3.7
1	B	451	GLN	3.6
1	A	456	PRO	3.6
1	A	191	VAL	3.6
1	B	339	VAL	3.6
1	A	317	LEU	3.5
1	B	335	VAL	3.5
1	B	317	LEU	3.4
1	A	163	TRP	3.4
1	A	382	VAL	3.4
1	A	204	ALA	3.4
1	B	174	ASN	3.3
1	B	413	ILE	3.3
1	A	205	ASN	3.3
1	A	212	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	152	VAL	3.2
1	B	407	GLY	3.2
1	B	137	SER	3.2
1	A	336	LEU	3.2
1	A	193	LEU	3.2
1	A	457	LEU	3.2
1	A	453	LEU	3.1
1	B	273	GLY	3.1
1	B	393	TRP	3.1
1	B	22	LEU	3.1
1	A	190	LEU	3.1
1	A	94	ALA	3.0
1	A	192	GLY	3.0
1	A	79	LYS	3.0
1	B	173	GLY	3.0
1	B	208	SER	2.9
1	B	207	GLY	2.9
1	A	126	ASN	2.9
1	B	397	SER	2.9
1	B	323	ALA	2.9
1	B	206	TYR	2.9
1	B	256	LEU	2.9
1	A	170	ALA	2.9
1	B	389	TRP	2.9
1	B	42	ARG	2.9
1	A	426	MET	2.9
1	A	211	ASP	2.9
1	A	100	THR	2.9
1	A	171	GLN	2.8
1	B	340	LEU	2.8
1	B	211	ASP	2.8
1	A	277	ALA	2.8
1	A	175	GLU	2.8
1	A	23	TRP	2.8
1	B	426	MET	2.7
1	B	277	ALA	2.7
1	B	279	ILE	2.7
1	B	385	LYS	2.7
2	E	12	ALA	2.7
1	B	380	PHE	2.7
1	A	295	SER	2.7
1	B	337	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	180	ALA	2.7
1	A	145	ILE	2.6
1	B	102	ASN	2.6
1	A	388	SER	2.6
1	B	336	LEU	2.6
1	B	313	PHE	2.6
1	A	144	THR	2.6
1	A	194	GLY	2.6
1	A	209	GLU	2.6
1	B	209	GLU	2.6
1	A	36	VAL	2.6
1	A	449	VAL	2.6
1	A	182	PHE	2.5
1	A	8	VAL	2.5
1	B	204	ALA	2.5
1	A	315	THR	2.5
1	B	258	ILE	2.5
1	A	210	PRO	2.5
1	A	384	GLY	2.5
1	B	141	SER	2.5
1	B	274	LEU	2.5
1	A	416	TYR	2.5
1	B	62	TYR	2.5
1	B	315	THR	2.5
1	B	416	TYR	2.5
1	B	194	GLY	2.5
1	B	412	MET	2.5
1	B	151	ASN	2.5
1	B	332	TRP	2.5
1	A	375	GLY	2.5
1	B	383	ASN	2.4
1	B	254	ALA	2.4
1	A	430	PHE	2.4
1	A	42	ARG	2.4
1	A	80	ARG	2.4
1	B	456	PRO	2.4
1	A	413	ILE	2.4
1	A	386	THR	2.4
1	B	414	ALA	2.4
1	A	380	PHE	2.4
1	A	406	SER	2.4
1	B	382	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	218	LYS	2.3
1	A	95	LEU	2.3
1	B	165	LYS	2.3
1	A	452	ASP	2.3
1	B	212	THR	2.3
1	B	450	PRO	2.3
1	B	358	ALA	2.3
1	A	186	CYS	2.3
1	A	383	ASN	2.3
1	B	36	VAL	2.3
1	B	321	SER	2.2
1	B	491	LEU	2.2
1	A	253	VAL	2.2
1	B	427	GLY	2.2
1	A	318	TRP	2.2
1	B	200	HIS	2.2
1	A	91	VAL	2.2
1	A	297	SER	2.2
1	A	185	CYS	2.2
1	A	428	ALA	2.2
1	A	433	SER	2.2
1	B	359	LYS	2.2
2	C	10	ALA	2.2
2	E	10	ALA	2.2
1	A	313	PHE	2.2
1	B	246	VAL	2.1
1	A	62	TYR	2.1
1	A	133	GLU	2.1
1	A	427	GLY	2.1
1	B	322	PRO	2.1
1	B	429	TYR	2.1
1	B	74	LYS	2.1
1	A	294	MET	2.1
1	A	77	GLY	2.1
1	A	207	GLY	2.1
1	A	257	GLY	2.1
1	A	282	VAL	2.1
1	B	387	SER	2.1
1	B	261	HIS	2.1
1	B	409	GLY	2.1
1	B	458	GLN	2.1
1	B	105	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	176	PHE	2.1
1	B	260	PHE	2.1
1	B	318	TRP	2.0
1	B	197	ALA	2.0
1	B	357	ALA	2.0
1	A	379	GLN	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](#)

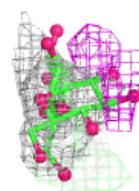
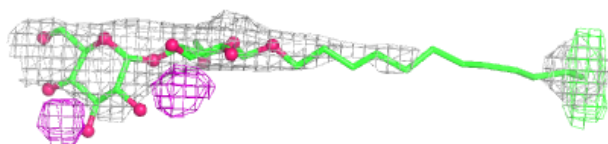
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	603	35/35	0.58	0.23	77,114,128,129	0
3	LMT	A	601	35/35	0.70	0.22	73,106,137,140	0
3	LMT	B	602	35/35	0.78	0.20	89,123,142,146	0
4	ZN	B	601	1/1	0.90	0.16	131,131,131,131	0

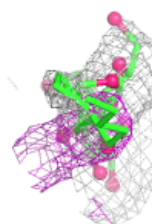
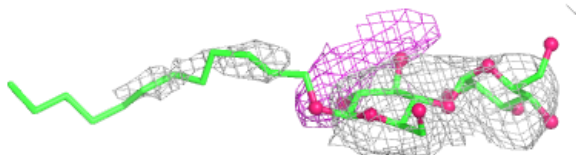
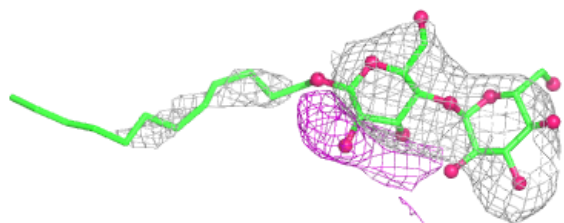
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 603:

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

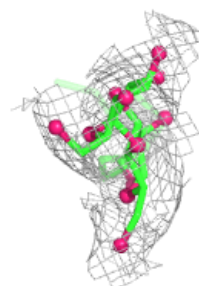
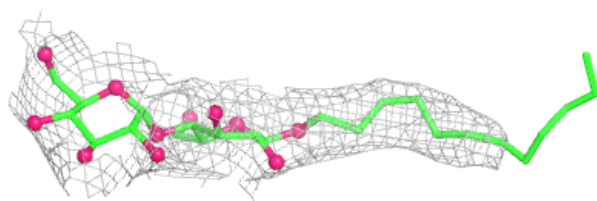
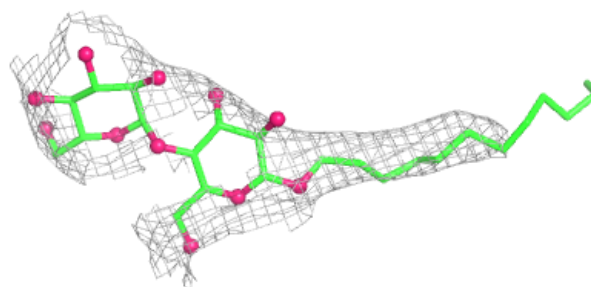
**Electron density around LMT A 601:**

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



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.