



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:12 AM UTC

PDB ID : 4TPH / pdb_00004tph
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 : 3.15 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

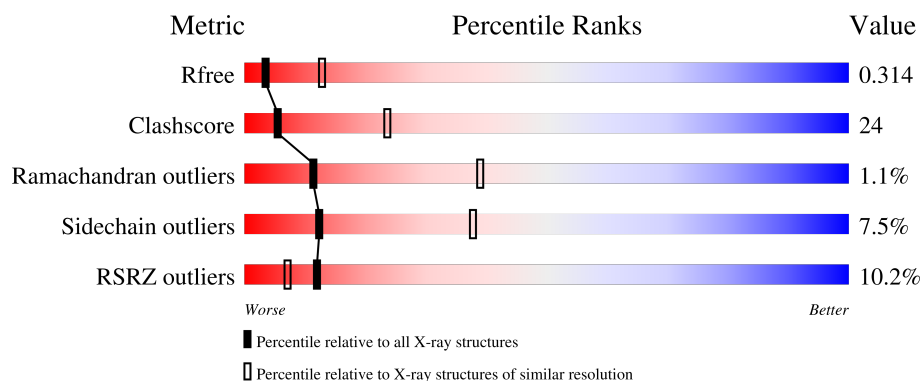
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	9% 43% 36% 7% 13%
1	B	523	9% 46% 36% 5% 13%

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
4	ALA	A	603	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6970 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	453	Total	C	N	O	S	0	0	0
			3422	2277	543	582	20			
1	B	453	Total	C	N	O	S	0	0	0
			3422	2277	543	582	20			

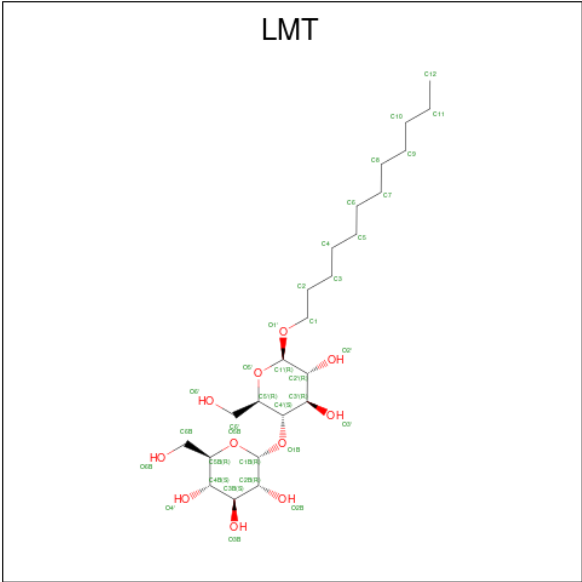
There are 14 discrepancies between the modelled and reference sequences:

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 ZINC ION (CCD ID: ZN) (formula: Zn).

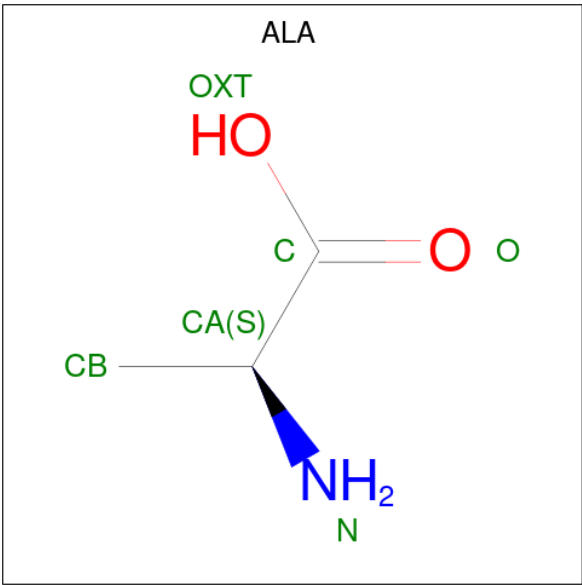
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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



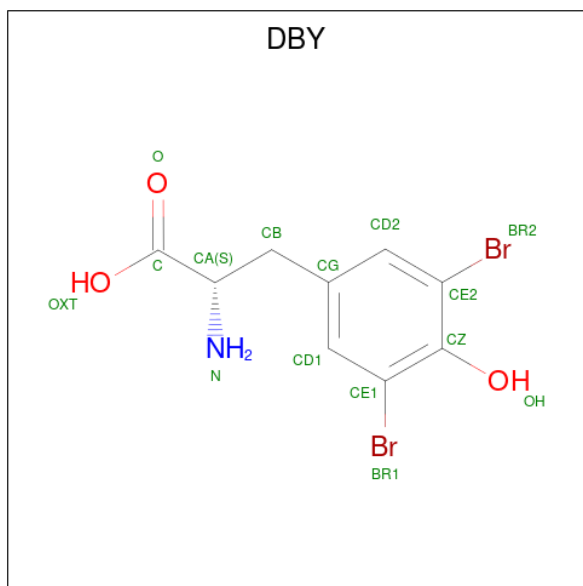
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is ALANINE (CCD ID: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 5 is 3,5 DIBROMOTYROSINE (CCD ID: DBY) (formula: $C_9H_9Br_2NO_3$).

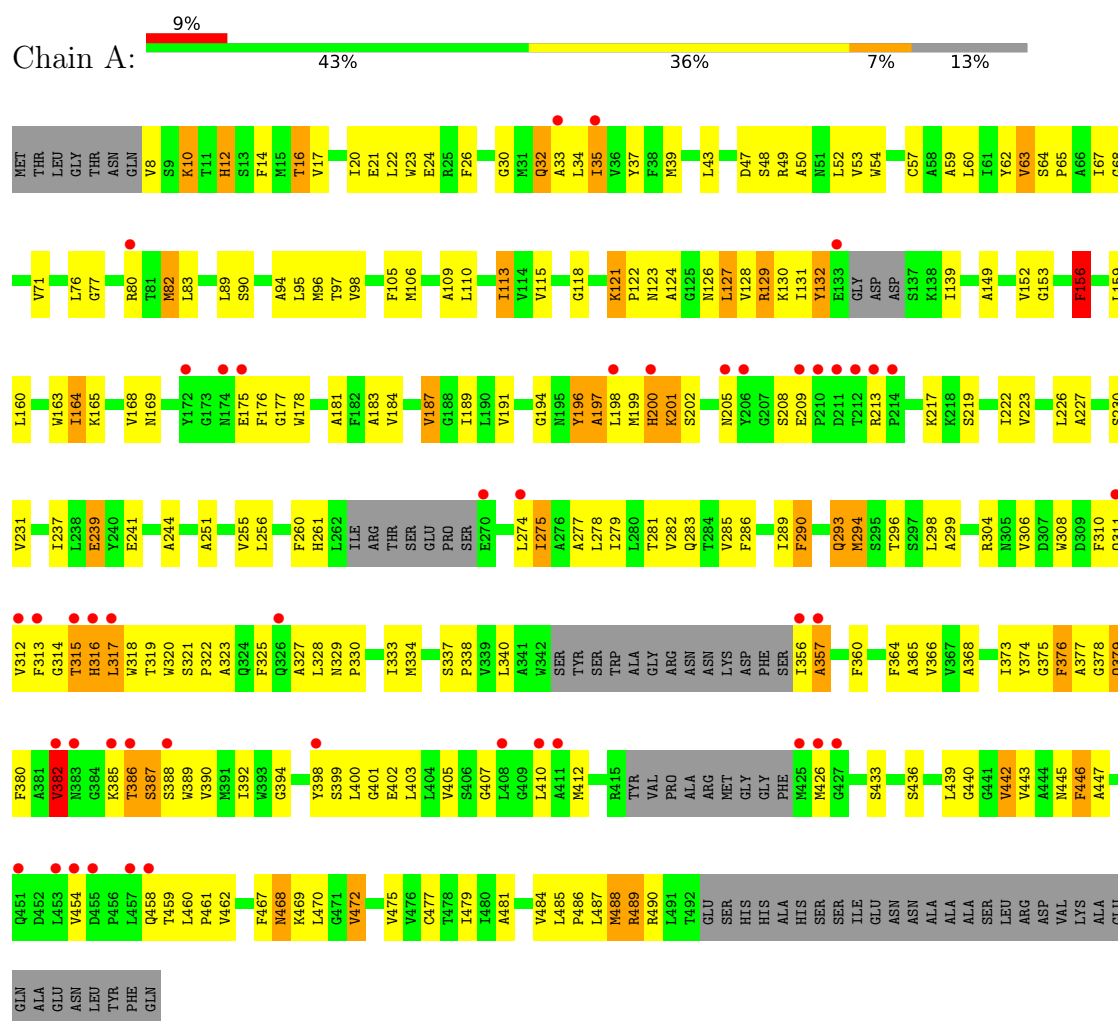


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
5	A	1	15	2	9	1	3	0	0

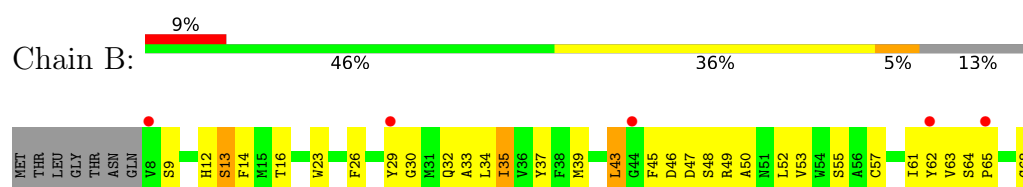
3 Residue-property plots [i](#)

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: Proton:oligopeptide symporter POT family



• Molecule 1: Proton:oligopeptide symporter POT family





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.65Å 107.68Å 204.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.54 – 3.15 29.54 – 3.15	Depositor EDS
% Data completeness (in resolution range)	78.2 (29.54-3.15) 78.2 (29.54-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.251 , 0.307 0.256 , 0.314	Depositor DCC
R_{free} test set	1256 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	101.4	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 54.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6970	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: DBY, ZN, LMT

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	0.84	9/3509 (0.3%)	1.24	26/4785 (0.5%)
1	B	0.83	6/3509 (0.2%)	1.21	16/4785 (0.3%)
All	All	0.83	15/7018 (0.2%)	1.22	42/9570 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ALA	C-O	8.67	1.34	1.24
1	A	200	HIS	CA-C	-8.53	1.42	1.52
1	B	33	ALA	C-O	8.06	1.33	1.24
1	B	290	PHE	C-O	6.81	1.31	1.24
1	B	200	HIS	CA-C	-6.52	1.44	1.52
1	A	32	GLN	C-O	5.81	1.30	1.24
1	A	196	TYR	C-O	-5.75	1.17	1.24
1	A	30	GLY	C-O	5.67	1.30	1.23
1	B	197	ALA	C-O	5.59	1.30	1.24
1	B	30	GLY	C-O	5.56	1.30	1.23
1	A	290	PHE	C-O	5.53	1.30	1.24
1	B	196	TYR	C-O	-5.26	1.18	1.24
1	A	197	ALA	C-O	5.07	1.30	1.24
1	A	296	THR	CA-C	5.07	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	HIS	N-CA	5.02	1.52	1.46

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	HIS	N-CA-C	-8.84	101.34	110.97
1	B	449	VAL	N-CA-C	8.66	117.33	107.89
1	B	200	HIS	N-CA-C	-7.66	102.62	110.97
1	B	316	HIS	CB-CA-C	-7.48	100.87	112.31
1	B	98	VAL	N-CA-C	7.30	114.91	108.63
1	A	35	ILE	CA-C-N	-7.29	110.07	120.42
1	A	35	ILE	C-N-CA	-7.29	110.07	120.42
1	B	293	GLN	CA-C-N	-6.88	109.11	121.14
1	B	293	GLN	C-N-CA	-6.88	109.11	121.14
1	A	382	VAL	N-CA-C	6.79	118.08	108.17
1	A	139	ILE	N-CA-C	-6.55	102.86	112.04
1	A	201	LYS	N-CA-C	-6.44	104.46	112.90
1	B	357	ALA	N-CA-C	-6.24	105.60	112.72
1	A	446	PHE	CA-C-N	-6.24	112.71	123.25
1	A	446	PHE	C-N-CA	-6.24	112.71	123.25
1	B	201	LYS	N-CA-C	-6.15	104.84	112.90
1	A	213	ARG	CA-C-N	-6.04	113.75	119.85
1	A	213	ARG	C-N-CA	-6.04	113.75	119.85
1	B	35	ILE	CA-C-N	-5.94	112.96	120.56
1	B	35	ILE	C-N-CA	-5.94	112.96	120.56
1	A	200	HIS	N-CA-CB	5.88	118.50	109.91
1	A	316	HIS	N-CA-C	5.86	120.81	113.43
1	A	293	GLN	CA-C-N	-5.77	111.05	121.14
1	A	293	GLN	C-N-CA	-5.77	111.05	121.14
1	A	321	SER	CA-C-N	5.74	127.01	119.84
1	A	321	SER	C-N-CA	5.74	127.01	119.84
1	A	488	MET	CA-C-N	-5.66	113.20	122.54
1	A	488	MET	C-N-CA	-5.66	113.20	122.54
1	B	43	LEU	N-CA-C	-5.58	103.17	110.53
1	A	357	ALA	N-CA-C	-5.53	106.74	112.93
1	A	468	ASN	CA-C-N	-5.52	111.47	121.14
1	A	468	ASN	C-N-CA	-5.52	111.47	121.14
1	A	317	LEU	N-CA-C	5.50	118.42	110.28
1	A	275	ILE	N-CA-C	-5.46	104.13	111.44
1	B	488	MET	CA-C-N	-5.38	114.21	122.60
1	B	488	MET	C-N-CA	-5.38	114.21	122.60
1	B	446	PHE	CA-C-N	-5.28	114.33	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	PHE	C-N-CA	-5.28	114.33	123.25
1	A	386	THR	N-CA-C	5.10	117.66	108.48
1	B	275	ILE	N-CA-C	-5.04	104.69	111.44
1	A	156	PHE	CB-CA-C	-5.03	102.98	110.88
1	A	294	MET	N-CA-C	5.02	119.12	112.89

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	TYR	Peptide
1	B	274	LEU	Peptide

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	3422	0	3412	180	0
1	B	3422	0	3412	150	0
2	A	1	0	0	0	0
3	A	35	0	46	9	0
3	B	70	0	92	6	0
4	A	5	0	4	0	0
5	A	15	0	6	1	0
All	All	6970	0	6972	332	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 24.

All (332) 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:B:364:PHE:CD2	1:B:477:CYS:HB3	2.03	0.93
1:A:152:VAL:HG22	1:A:156:PHE:CE1	2.08	0.89
1:A:94:ALA:O	1:A:97:THR:HG22	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HA	1:A:446:PHE:HD2	1.42	0.84
1:B:200:HIS:CG	1:B:201:LYS:N	2.51	0.77
1:A:32:GLN:O	1:A:35:ILE:HG22	1.86	0.76
1:B:366:VAL:HG11	1:B:400:LEU:HD23	1.66	0.75
1:A:200:HIS:CG	1:A:201:LYS:N	2.55	0.75
1:A:76:LEU:HD11	1:A:223:VAL:HG21	1.68	0.74
1:A:219:SER:HA	1:A:222:ILE:HG22	1.69	0.74
1:A:20:ILE:HD12	1:A:196:TYR:HB2	1.70	0.74
1:A:382:VAL:HA	1:A:386:THR:HB	1.69	0.74
1:B:410:LEU:HD21	1:B:429:TYR:CD2	2.24	0.73
1:B:317:LEU:HD12	1:B:318:TRP:HA	1.73	0.71
1:A:156:PHE:HD1	3:A:602:LMT:H101	1.57	0.70
1:A:376:PHE:HA	1:A:379:GLN:OE1	1.91	0.70
1:A:374:TYR:HE2	1:A:398:TYR:CE2	2.10	0.69
1:B:197:ALA:O	1:B:200:HIS:ND1	2.24	0.69
1:B:39:MET:HE1	1:B:53:VAL:HB	1.75	0.69
1:B:477:CYS:HA	1:B:480:ILE:HD12	1.73	0.69
1:A:22:LEU:HD21	1:A:156:PHE:HE2	1.59	0.68
1:B:32:GLN:O	1:B:35:ILE:HG22	1.94	0.68
1:A:159:LEU:HB3	3:A:602:LMT:H52	1.74	0.68
1:B:13:SER:HA	1:B:16:THR:HG22	1.75	0.68
1:B:85:GLY:O	1:B:89:LEU:HD12	1.94	0.68
1:B:289:ILE:HG23	1:B:440:GLY:HA2	1.73	0.68
1:A:286:PHE:HA	1:A:289:ILE:HD12	1.76	0.68
1:B:382:VAL:HA	1:B:386:THR:HB	1.77	0.67
1:A:310:PHE:HB2	1:A:320:TRP:NE1	2.10	0.67
1:A:76:LEU:HB3	1:A:80:ARG:NH1	2.10	0.66
1:B:377:ALA:HB2	1:B:390:VAL:HG11	1.77	0.66
1:B:449:VAL:HG13	1:B:453:LEU:HD23	1.78	0.66
1:A:199:MET:HA	1:A:202:SER:CB	2.26	0.66
1:A:16:THR:HG22	1:A:199:MET:SD	2.36	0.66
1:B:488:MET:O	1:B:489:ARG:HD3	1.97	0.65
1:B:364:PHE:CE2	1:B:477:CYS:HB3	2.31	0.65
1:A:163:TRP:HE3	1:A:164:ILE:HD12	1.61	0.65
1:B:443:VAL:HA	1:B:446:PHE:HD2	1.62	0.65
1:A:315:THR:OG1	1:A:316:HIS:N	2.30	0.64
1:A:49:ARG:NH2	1:A:239:GLU:OE1	2.30	0.64
1:A:329:ASN:HB3	1:A:330:PRO:HD3	1.80	0.64
1:A:152:VAL:HG22	1:A:156:PHE:HE1	1.59	0.64
1:B:200:HIS:CG	1:B:201:LYS:H	2.14	0.64
1:A:156:PHE:CD1	3:A:602:LMT:H101	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:HG23	1:A:440:GLY:HA2	1.79	0.63
1:B:283:GLN:CD	1:B:360:PHE:HD2	2.06	0.63
1:A:327:ALA:O	1:A:330:PRO:HD2	1.99	0.62
1:A:95:LEU:O	1:A:98:VAL:HG12	1.99	0.62
1:B:291:TYR:HA	1:B:398:TYR:OH	1.98	0.62
1:A:83:LEU:HD21	1:A:196:TYR:CD2	2.35	0.62
1:A:82:MET:HE2	1:A:124:ALA:HA	1.81	0.61
1:A:364:PHE:CD1	1:A:477:CYS:HB3	2.35	0.61
1:B:55:SER:HB3	1:B:438:TYR:HA	1.82	0.61
1:B:219:SER:HA	1:B:222:ILE:HG22	1.83	0.60
1:A:377:ALA:HB2	1:A:390:VAL:HG11	1.83	0.60
1:A:283:GLN:NE2	1:A:481:ALA:HB2	2.16	0.60
1:A:14:PHE:HB2	1:A:132:TYR:HE2	1.66	0.60
1:A:306:VAL:HG13	1:A:388:SER:H	1.66	0.60
1:B:308:TRP:O	1:B:320:TRP:N	2.35	0.60
1:B:306:VAL:HG13	1:B:388:SER:H	1.65	0.60
1:A:443:VAL:HA	1:A:446:PHE:CD2	2.30	0.59
1:A:197:ALA:O	1:A:200:HIS:N	2.32	0.59
1:B:316:HIS:C	1:B:316:HIS:HD1	2.09	0.59
1:A:365:ALA:O	1:A:368:ALA:HB3	2.02	0.59
1:A:373:ILE:HG22	1:A:390:VAL:HG13	1.83	0.59
1:B:34:LEU:HD11	1:B:162:PRO:HA	1.83	0.59
1:B:107:PHE:CD2	1:B:239:GLU:HG2	2.37	0.59
1:A:310:PHE:HB2	1:A:320:TRP:HE1	1.67	0.59
1:A:333:ILE:HG12	1:A:403:LEU:HD13	1.85	0.59
1:B:83:LEU:HD11	1:B:196:TYR:CE2	2.37	0.59
1:A:152:VAL:HG22	1:A:156:PHE:CZ	2.37	0.59
1:B:327:ALA:O	1:B:330:PRO:HD2	2.03	0.59
1:B:68:GLY:HA3	1:B:118:GLY:O	2.03	0.58
1:B:187:VAL:HA	1:B:190:LEU:HD12	1.83	0.58
1:A:96:MET:HG2	1:A:109:ALA:HB1	1.85	0.58
1:B:147:TYR:O	1:B:150:VAL:HB	2.04	0.58
1:A:153:GLY:HA2	1:A:156:PHE:CE2	2.38	0.58
1:A:197:ALA:O	1:A:200:HIS:ND1	2.37	0.58
1:A:375:GLY:HA3	1:A:468:ASN:OD1	2.04	0.57
1:A:65:PRO:HB3	1:A:122:PRO:HD3	1.86	0.57
1:A:39:MET:HE1	1:A:53:VAL:HB	1.85	0.57
1:B:328:LEU:HD13	1:B:392:ILE:HA	1.86	0.57
1:A:68:GLY:HA3	1:A:118:GLY:O	2.05	0.57
1:A:278:LEU:O	1:A:282:VAL:HG13	2.05	0.57
1:B:315:THR:CG2	1:B:316:HIS:H	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HA	1:A:445:ASN:OD1	2.04	0.57
1:A:67:ILE:O	1:A:71:VAL:HG23	2.04	0.57
1:B:316:HIS:C	1:B:316:HIS:ND1	2.63	0.56
1:B:48:SER:HA	1:B:445:ASN:OD1	2.05	0.56
1:B:274:LEU:HA	1:B:277:ALA:H	1.70	0.56
1:A:379:GLN:H	1:A:379:GLN:CD	2.14	0.56
1:B:458:GLN:O	1:B:461:PRO:HD2	2.05	0.56
1:A:298:LEU:HD23	1:A:467:PHE:CZ	2.41	0.55
1:A:311:GLN:NE2	1:A:315:THR:H	2.04	0.55
1:A:378:GLY:C	1:A:380:PHE:H	2.13	0.55
1:A:357:ALA:HB3	1:A:488:MET:HE1	1.89	0.55
1:B:29:TYR:HB3	1:B:158:MET:HE3	1.87	0.55
1:A:311:GLN:NE2	1:A:315:THR:N	2.54	0.55
1:B:46:ASP:HB3	1:B:451:GLN:HE21	1.72	0.55
1:B:334:MET:O	1:B:338:PRO:HD3	2.06	0.55
1:A:479:ILE:HD12	1:B:369:ILE:HD12	1.88	0.55
1:B:37:TYR:OH	1:B:299:ALA:O	2.20	0.55
1:B:298:LEU:HD23	1:B:467:PHE:CZ	2.42	0.55
1:A:181:ALA:O	1:A:184:VAL:HB	2.07	0.55
1:A:387:SER:HB3	1:A:390:VAL:HB	1.89	0.55
1:A:200:HIS:CG	1:A:201:LYS:H	2.25	0.55
1:B:82:MET:HE2	1:B:124:ALA:HA	1.88	0.54
1:A:256:LEU:HD22	1:A:260:PHE:HE2	1.72	0.54
1:B:138:LYS:HD2	1:B:141:SER:HB3	1.88	0.54
1:A:128:VAL:HA	1:A:131:ILE:HD12	1.90	0.54
1:A:340:LEU:HD22	1:A:403:LEU:HD23	1.90	0.54
1:B:197:ALA:O	1:B:200:HIS:N	2.33	0.54
1:A:374:TYR:CE2	1:A:398:TYR:CE2	2.93	0.53
1:A:308:TRP:O	1:A:320:TRP:N	2.36	0.53
1:B:329:ASN:HB3	1:B:330:PRO:HD3	1.91	0.53
1:B:237:ILE:O	1:B:244:ALA:HB2	2.07	0.53
1:A:160:LEU:HG	1:A:164:ILE:HD13	1.90	0.53
1:A:366:VAL:HG11	1:A:400:LEU:HD23	1.91	0.53
1:A:183:ALA:O	1:A:187:VAL:HG13	2.08	0.53
1:B:447:ALA:HB2	1:B:466:LEU:HB2	1.91	0.53
1:B:137:SER:OG	1:B:138:LYS:N	2.39	0.53
1:B:148:MET:HE1	1:B:334:MET:HA	1.92	0.52
1:B:132:TYR:HB2	1:B:139:ILE:HG22	1.90	0.52
1:B:279:ILE:O	1:B:282:VAL:HG22	2.09	0.52
1:A:475:VAL:HG21	1:B:475:VAL:HG21	1.90	0.52
1:B:199:MET:HA	1:B:202:SER:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLN:NE2	1:B:360:PHE:HD2	2.08	0.52
1:B:458:GLN:C	1:B:461:PRO:HD2	2.35	0.52
3:B:602:LMT:H1B	3:B:602:LMT:O3'	2.08	0.52
1:B:101:GLU:OE1	1:B:101:GLU:N	2.42	0.52
1:B:286:PHE:HA	1:B:289:ILE:HD12	1.91	0.52
1:A:109:ALA:O	1:A:113:ILE:HD12	2.11	0.51
1:A:442:VAL:O	1:A:445:ASN:HB2	2.11	0.51
1:A:386:THR:O	1:A:387:SER:OG	2.20	0.51
1:A:489:ARG:O	1:A:489:ARG:HG3	2.10	0.51
1:B:315:THR:HG23	1:B:316:HIS:H	1.74	0.51
1:A:39:MET:HE2	1:A:50:ALA:HA	1.93	0.51
1:A:310:PHE:HB2	1:A:320:TRP:CD1	2.45	0.51
1:B:65:PRO:HB3	1:B:122:PRO:HD3	1.92	0.51
1:A:328:LEU:HD13	1:A:392:ILE:HA	1.92	0.51
1:A:98:VAL:HG11	1:A:105:PHE:CZ	2.46	0.50
1:A:115:VAL:HG21	1:A:231:VAL:HG23	1.93	0.50
1:B:79:LYS:HD3	1:B:204:ALA:HB1	1.93	0.50
1:B:143:PHE:O	1:B:146:TYR:HB3	2.10	0.50
1:A:459:THR:O	1:A:462:VAL:HG22	2.11	0.50
1:B:315:THR:CG2	1:B:316:HIS:N	2.73	0.50
1:A:129:ARG:NH1	1:A:130:LYS:HZ1	2.09	0.50
1:B:9:SER:HB2	1:B:12:HIS:CD2	2.46	0.50
1:B:62:TYR:CE2	1:B:433:SER:HB2	2.47	0.49
1:A:460:LEU:HB3	1:A:461:PRO:HD3	1.94	0.49
1:B:16:THR:OG1	1:B:199:MET:HB3	2.12	0.49
1:B:410:LEU:HD21	1:B:429:TYR:CE2	2.47	0.49
1:B:481:ALA:O	1:B:484:VAL:HG12	2.12	0.49
1:B:410:LEU:N	1:B:410:LEU:HD23	2.27	0.49
1:B:485:LEU:N	1:B:486:PRO:HD2	2.27	0.49
1:A:76:LEU:HA	1:A:80:ARG:NH2	2.27	0.49
1:A:274:LEU:HA	1:A:277:ALA:H	1.77	0.49
1:A:379:GLN:OE1	1:A:379:GLN:N	2.34	0.49
1:B:39:MET:HE2	1:B:50:ALA:HA	1.93	0.49
1:A:127:LEU:O	1:A:131:ILE:HG13	2.13	0.49
1:B:290:PHE:O	1:B:293:GLN:HB2	2.12	0.49
1:A:21:GLU:OE2	1:A:121:LYS:HE2	2.12	0.49
1:A:237:ILE:HG23	1:A:244:ALA:HA	1.94	0.49
1:A:12:HIS:O	1:A:16:THR:HG23	2.13	0.49
1:A:251:ALA:O	1:A:255:VAL:HG13	2.13	0.48
1:B:412:MET:SD	1:B:412:MET:N	2.86	0.48
1:A:98:VAL:HG11	1:A:105:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG11	1:A:227:ALA:HB1	1.96	0.48
1:B:64:SER:HB3	1:B:65:PRO:HD3	1.95	0.48
1:B:47:ASP:OD2	1:B:304:ARG:NH1	2.47	0.48
1:A:319:THR:OG1	3:A:602:LMT:H3B	2.13	0.48
1:B:55:SER:OG	1:B:441:GLY:HA3	2.14	0.47
1:B:57:CYS:SG	1:B:110:LEU:HD22	2.54	0.47
1:B:197:ALA:HA	1:B:200:HIS:HB3	1.96	0.47
1:A:458:GLN:C	1:A:461:PRO:HD2	2.40	0.47
1:B:128:VAL:HA	1:B:131:ILE:HD12	1.96	0.47
1:A:469:LYS:HE2	1:A:469:LYS:HB3	1.44	0.47
1:B:319:THR:OG1	3:B:601:LMT:H3B	2.14	0.47
1:A:60:LEU:HD23	1:A:60:LEU:HA	1.52	0.47
1:A:285:VAL:HG13	1:A:436:SER:HB3	1.97	0.47
1:A:394:GLY:O	1:A:398:TYR:HD2	1.97	0.47
1:B:127:LEU:O	1:B:131:ILE:HG13	2.15	0.47
1:B:387:SER:HB3	1:B:390:VAL:HB	1.97	0.47
1:A:334:MET:O	1:A:338:PRO:HD3	2.15	0.47
1:A:374:TYR:HE2	1:A:398:TYR:CZ	2.31	0.47
1:B:201:LYS:O	1:B:202:SER:C	2.57	0.47
1:B:374:TYR:CZ	1:B:394:GLY:HA3	2.50	0.47
1:A:163:TRP:CE3	1:A:164:ILE:HD12	2.47	0.46
1:A:277:ALA:O	1:A:281:THR:HG23	2.15	0.46
1:B:283:GLN:NE2	1:B:360:PHE:CD2	2.83	0.46
1:B:370:GLY:O	1:B:373:ILE:HB	2.15	0.46
1:A:23:TRP:O	1:A:26:PHE:HB3	2.16	0.46
1:A:153:GLY:HA2	1:A:156:PHE:CD2	2.51	0.46
1:A:165:LYS:O	1:A:169:ASN:HB2	2.16	0.46
1:B:102:ASN:HD21	3:B:602:LMT:H3'	1.79	0.46
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.65	0.46
1:A:194:GLY:O	1:A:198:LEU:HG	2.15	0.46
1:B:104:TRP:CE2	1:B:239:GLU:HG3	2.50	0.46
1:B:14:PHE:HB2	1:B:132:TYR:HE2	1.81	0.46
1:B:313:PHE:HA	1:B:314:GLY:HA2	1.50	0.46
1:B:386:THR:O	1:B:387:SER:OG	2.21	0.46
1:A:311:GLN:HE21	1:A:314:GLY:HA2	1.81	0.46
1:A:458:GLN:O	1:A:461:PRO:HD2	2.15	0.46
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.78	0.46
1:A:62:TYR:HE2	1:A:433:SER:HB2	1.81	0.46
1:A:64:SER:OG	1:A:118:GLY:HA3	2.16	0.46
1:A:410:LEU:HD22	1:A:426:MET:HA	1.98	0.46
1:B:233:ALA:O	1:B:237:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:PHE:HB2	1:B:320:TRP:CD1	2.51	0.46
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.74	0.45
1:A:39:MET:CE	1:A:50:ALA:HA	2.46	0.45
1:A:52:LEU:HG	1:A:445:ASN:HD21	1.80	0.45
1:B:194:GLY:O	1:B:198:LEU:HG	2.17	0.45
1:B:83:LEU:HD21	1:B:196:TYR:CD2	2.51	0.45
1:B:216:ASN:HD21	1:B:218:LYS:NZ	2.14	0.45
1:B:279:ILE:HG21	1:B:484:VAL:HG21	1.97	0.45
1:B:476:VAL:HG12	1:B:480:ILE:HD11	1.98	0.45
1:A:126:ASN:OD1	1:A:130:LYS:NZ	2.49	0.45
1:A:196:TYR:O	1:A:196:TYR:CG	2.69	0.45
1:A:378:GLY:C	1:A:380:PHE:N	2.75	0.45
1:B:183:ALA:O	1:B:187:VAL:HG13	2.17	0.45
1:B:278:LEU:O	1:B:282:VAL:HG13	2.15	0.45
1:A:168:VAL:HB	1:A:177:GLY:HA2	1.99	0.45
1:A:311:GLN:NE2	1:A:312:VAL:C	2.75	0.45
1:A:47:ASP:OD2	1:A:304:ARG:NH1	2.50	0.45
1:A:389:TRP:CE3	1:A:392:ILE:HD12	2.51	0.45
1:A:394:GLY:O	1:A:398:TYR:CD2	2.70	0.45
1:B:39:MET:HE2	1:B:39:MET:HB3	1.74	0.45
1:B:317:LEU:HA	1:B:318:TRP:HA	1.57	0.45
1:A:294:MET:HE1	1:A:329:ASN:ND2	2.31	0.45
3:B:601:LMT:H2'	3:B:601:LMT:H12	1.53	0.45
1:A:275:ILE:O	1:A:279:ILE:HG12	2.17	0.45
1:B:294:MET:SD	1:B:398:TYR:CE2	3.10	0.45
1:B:311:GLN:HB2	1:B:315:THR:O	2.17	0.45
1:A:37:TYR:OH	1:A:299:ALA:O	2.28	0.44
1:B:62:TYR:HE2	1:B:433:SER:HB2	1.81	0.44
1:A:126:ASN:O	1:A:130:LYS:HD3	2.17	0.44
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.43	0.44
1:A:8:VAL:CG1	1:A:12:HIS:CD2	3.00	0.44
1:A:156:PHE:CD1	3:A:602:LMT:H121	2.53	0.44
1:A:311:GLN:CD	1:A:312:VAL:N	2.76	0.44
1:A:77:GLY:H	1:A:80:ARG:CG	2.30	0.44
1:A:89:LEU:CD2	1:A:113:ILE:HA	2.48	0.44
1:B:310:PHE:HB2	1:B:320:TRP:NE1	2.32	0.44
1:A:124:ALA:O	1:A:128:VAL:HG23	2.17	0.44
1:B:340:LEU:HD22	1:B:403:LEU:HD23	1.99	0.44
1:A:57:CYS:SG	1:A:110:LEU:HD22	2.58	0.44
1:A:115:VAL:HG22	1:A:230:SER:HB2	1.99	0.44
1:A:322:PRO:HA	1:A:325:PHE:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:GLU:HG3	5:A:604:DBY:BR2	2.73	0.43
1:A:35:ILE:HG21	1:A:54:TRP:CE3	2.53	0.43
1:B:487:LEU:HD23	1:B:487:LEU:HA	1.92	0.43
1:A:281:THR:O	1:A:285:VAL:HG23	2.18	0.43
1:B:39:MET:O	1:B:45:PHE:HB2	2.18	0.43
1:B:160:LEU:HG	1:B:164:ILE:HD13	1.99	0.43
1:B:109:ALA:O	1:B:113:ILE:HD12	2.17	0.43
1:B:342:TRP:CD1	1:B:342:TRP:N	2.83	0.43
1:B:398:TYR:CD2	1:B:398:TYR:C	2.95	0.43
1:A:197:ALA:O	1:A:198:LEU:C	2.61	0.43
1:B:280:LEU:HD13	1:B:413:ILE:HG22	2.01	0.43
1:B:285:VAL:HG22	1:B:436:SER:HB3	2.01	0.43
1:B:439:LEU:HA	1:B:442:VAL:HG13	2.00	0.43
1:B:72:GLY:HA3	1:B:123:ASN:OD1	2.18	0.43
1:B:156:PHE:CD1	3:B:601:LMT:H72	2.54	0.43
1:B:197:ALA:O	1:B:198:LEU:C	2.61	0.43
1:B:371:PHE:CE1	1:B:470:LEU:HB3	2.54	0.43
1:A:401:GLY:O	1:A:405:VAL:HG22	2.18	0.42
1:A:487:LEU:HD23	1:A:487:LEU:HA	1.86	0.42
1:B:61:ILE:HG13	1:B:114:VAL:HG22	2.01	0.42
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.92	0.42
1:A:226:LEU:HD23	1:A:226:LEU:HA	1.70	0.42
1:A:197:ALA:O	1:A:200:HIS:CB	2.67	0.42
1:B:115:VAL:HG22	1:B:230:SER:HB2	2.02	0.42
1:A:10:LYS:HB3	1:A:10:LYS:HE2	1.64	0.42
1:A:49:ARG:HA	1:A:241:GLU:OE2	2.20	0.42
1:A:95:LEU:HA	1:A:95:LEU:HD12	1.64	0.42
1:A:16:THR:O	1:A:20:ILE:HG22	2.19	0.42
1:A:123:ASN:HA	1:A:126:ASN:HB2	2.01	0.42
1:B:96:MET:HG2	1:B:109:ALA:HB1	2.02	0.42
1:A:374:TYR:CD1	1:A:390:VAL:HG12	2.55	0.42
1:A:472:VAL:HG22	1:B:372:PHE:CD1	2.54	0.42
1:B:34:LEU:HD22	1:B:165:LYS:HD3	2.01	0.42
1:A:378:GLY:O	1:A:380:PHE:N	2.53	0.42
1:A:407:GLY:O	1:A:412:MET:HG3	2.20	0.42
1:A:175:GLU:HA	1:A:176:PHE:O	2.20	0.41
1:A:317:LEU:HA	1:A:318:TRP:HA	1.74	0.41
1:A:156:PHE:CE1	3:A:602:LMT:H121	2.55	0.41
1:A:290:PHE:O	1:A:293:GLN:HB2	2.20	0.41
1:B:102:ASN:HD21	3:B:602:LMT:C3'	2.33	0.41
1:B:115:VAL:HG21	1:B:231:VAL:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:TRP:CE2	1:B:322:PRO:HD3	2.55	0.41
1:A:149:ALA:O	1:A:152:VAL:HG12	2.20	0.41
1:A:96:MET:SD	1:A:106:MET:HG3	2.60	0.41
1:A:376:PHE:O	1:A:376:PHE:CD1	2.74	0.41
1:A:439:LEU:HA	1:A:442:VAL:HG13	2.01	0.41
1:A:481:ALA:O	1:A:484:VAL:HG12	2.21	0.41
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.78	0.41
1:B:126:ASN:O	1:B:130:LYS:HG2	2.21	0.41
1:A:37:TYR:HE2	1:A:323:ALA:N	2.18	0.41
3:A:602:LMT:H72	3:A:602:LMT:H102	1.61	0.41
1:B:197:ALA:O	1:B:200:HIS:CB	2.69	0.41
1:A:176:PHE:O	1:A:178:TRP:N	2.54	0.41
1:B:366:VAL:O	1:B:397:SER:OG	2.38	0.41
1:A:165:LYS:HA	1:A:177:GLY:O	2.20	0.41
1:A:256:LEU:O	1:A:260:PHE:CD2	2.74	0.41
1:A:356:ILE:HG12	1:A:356:ILE:O	2.21	0.41
1:A:445:ASN:C	1:A:447:ALA:N	2.78	0.41
1:B:95:LEU:HB3	1:B:109:ALA:HB2	2.02	0.41
1:A:294:MET:HE1	1:A:329:ASN:CG	2.46	0.41
1:B:140:ASP:O	1:B:144:THR:HG23	2.21	0.41
1:B:144:THR:O	1:B:147:TYR:HB3	2.21	0.41
1:B:163:TRP:HA	1:B:166:ASP:HB2	2.03	0.41
1:A:59:ALA:O	1:A:63:VAL:HG13	2.20	0.41
1:A:169:ASN:HD21	1:A:178:TRP:NE1	2.19	0.41
1:B:70:TRP:HE1	1:B:74:LYS:HD3	1.86	0.41
1:B:317:LEU:CD1	1:B:318:TRP:HA	2.48	0.41
3:A:602:LMT:O3'	3:A:602:LMT:H1B	2.21	0.40
1:B:49:ARG:HA	1:B:241:GLU:OE2	2.21	0.40
1:A:279:ILE:HG21	1:A:484:VAL:HG21	2.03	0.40
1:A:333:ILE:HG13	1:A:399:SER:HB2	2.04	0.40
1:A:485:LEU:N	1:A:486:PRO:HD2	2.36	0.40
1:B:378:GLY:HA2	1:B:382:VAL:HG21	2.02	0.40
1:A:410:LEU:H	1:A:410:LEU:HD12	1.87	0.40
1:B:332:TRP:CZ3	1:B:335:VAL:HG11	2.57	0.40
1:A:17:VAL:HG11	1:A:128:VAL:HG22	2.04	0.40
1:A:24:GLU:HA	1:A:189:ILE:HD13	2.03	0.40
1:A:293:GLN:HG3	1:A:470:LEU:CD1	2.51	0.40
1:B:488:MET:HE3	1:B:488:MET:HB3	1.82	0.40
1:A:8:VAL:HG11	1:A:12:HIS:CD2	2.57	0.40
3:A:602:LMT:H2'	3:A:602:LMT:H12	1.49	0.40
1:B:23:TRP:O	1:B:26:PHE:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ALA:HB1	1:B:413:ILE:HD12	2.04	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	443/523 (85%)	403 (91%)	35 (8%)	5 (1%)	11	39
1	B	443/523 (85%)	403 (91%)	35 (8%)	5 (1%)	11	39
All	All	886/1046 (85%)	806 (91%)	70 (8%)	10 (1%)	11	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	208	SER
1	A	313	PHE
1	B	205	ASN
1	B	208	SER
1	A	387	SER
1	B	313	PHE
1	B	387	SER
1	B	209	GLU
1	A	209	GLU

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	340/417 (82%)	310 (91%)	30 (9%)	9	31
1	B	340/417 (82%)	319 (94%)	21 (6%)	16	44
All	All	680/834 (82%)	629 (92%)	51 (8%)	12	38

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	12	HIS
1	A	16	THR
1	A	43	LEU
1	A	63	VAL
1	A	82	MET
1	A	90	SER
1	A	113	ILE
1	A	121	LYS
1	A	127	LEU
1	A	129	ARG
1	A	156	PHE
1	A	164	ILE
1	A	187	VAL
1	A	191	VAL
1	A	217	LYS
1	A	239	GLU
1	A	261	HIS
1	A	315	THR
1	A	337	SER
1	A	360	PHE
1	A	376	PHE
1	A	379	GLN
1	A	382	VAL
1	A	385	LYS
1	A	442	VAL
1	A	454	VAL
1	A	472	VAL
1	A	489	ARG
1	A	490	ARG
1	B	13	SER
1	B	43	LEU
1	B	63	VAL

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Mol	Chain	Res	Type
1	B	74	LYS
1	B	80	ARG
1	B	113	ILE
1	B	133	GLU
1	B	152	VAL
1	B	164	ILE
1	B	187	VAL
1	B	253	VAL
1	B	283	GLN
1	B	315	THR
1	B	317	LEU
1	B	369	ILE
1	B	382	VAL
1	B	403	LEU
1	B	442	VAL
1	B	462	VAL
1	B	472	VAL
1	B	490	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	32	GLN
1	A	169	ASN
1	A	311	GLN
1	A	451	GLN
1	B	32	GLN
1	B	102	ASN
1	B	283	GLN
1	B	305	ASN
1	B	379	GLN
1	B	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	1.24	4 (11%)	47,47,47	1.41	7 (14%)
3	LMT	B	601	-	36,36,36	1.17	2 (5%)	47,47,47	1.52	8 (17%)
5	DBY	A	604	4	14,15,15	1.10	1 (7%)	17,21,21	1.37	3 (17%)
3	LMT	A	602	-	36,36,36	1.28	4 (11%)	47,47,47	1.72	8 (17%)
4	ALA	A	603	5	3,4,5	1.08	0	2,4,6	1.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	B	602	-	-	11/21/61/61	0/2/2/2
3	LMT	B	601	-	-	14/21/61/61	0/2/2/2
5	DBY	A	604	4	-	4/8/8/8	0/1/1/1
3	LMT	A	602	-	-	12/21/61/61	0/2/2/2
4	ALA	A	603	5	-	1/1/2/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	LMT	O5B-C1B	3.49	1.50	1.41
3	B	601	LMT	O5B-C1B	3.45	1.50	1.41
3	A	602	LMT	O5'-C1'	3.32	1.50	1.41
3	A	602	LMT	O5B-C1B	2.90	1.49	1.41
3	B	601	LMT	O5'-C1'	2.87	1.49	1.41
3	B	602	LMT	O5'-C1'	2.62	1.48	1.41
5	A	604	DBY	BR1-CE1	2.41	1.95	1.89
3	A	602	LMT	O5'-C5'	2.23	1.49	1.44
3	B	602	LMT	O1B-C4'	2.19	1.49	1.43
3	B	602	LMT	O5'-C5'	2.18	1.49	1.44
3	A	602	LMT	O1'-C1'	2.02	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	LMT	C1-O1'-C1'	4.94	122.11	113.68
3	A	602	LMT	C1'-C2'-C3'	4.36	119.18	110.01
3	B	601	LMT	C1'-C2'-C3'	4.35	119.15	110.01
3	A	602	LMT	C2'-C3'-C4'	4.08	118.94	109.68
3	B	602	LMT	C1-O1'-C1'	3.81	120.19	113.68
3	B	601	LMT	O5'-C5'-C6'	3.41	114.90	106.44
3	A	602	LMT	C1B-O1B-C4'	-3.39	109.95	117.98
3	B	602	LMT	O1B-C4'-C3'	3.33	115.69	107.23
3	A	602	LMT	O5'-C5'-C6'	3.04	113.97	106.44
3	B	602	LMT	O1'-C1'-C2'	2.92	112.72	108.27
3	B	601	LMT	O5B-C1B-C2B	2.91	116.36	110.37
3	B	601	LMT	C1B-O1B-C4'	-2.86	111.20	117.98
3	A	602	LMT	O5'-C1'-C2'	2.85	116.23	110.37
3	B	601	LMT	C2'-C3'-C4'	2.82	116.07	109.68
3	B	601	LMT	C1-O1'-C1'	2.79	118.45	113.68
3	B	602	LMT	O5B-C1B-C2B	2.73	115.97	110.37
3	B	601	LMT	O5'-C1'-C2'	2.66	115.84	110.37
5	A	604	DBY	CE2-CZ-CE1	2.51	119.94	116.67
3	A	602	LMT	O5B-C5B-C4B	2.41	114.05	109.70
5	A	604	DBY	CD1-CE1-CZ	-2.38	119.36	121.92
3	B	602	LMT	O5'-C5'-C6'	2.35	112.26	106.44
5	A	604	DBY	BR2-CE2-CZ	2.25	121.31	118.80
3	B	601	LMT	C6'-C5'-C4'	-2.10	107.48	113.38
3	B	602	LMT	O5'-C5'-C4'	2.08	114.03	109.72
3	A	602	LMT	O3'-C3'-C2'	-2.07	105.49	110.38
3	B	602	LMT	O4'-C4B-C3B	2.06	115.23	110.38

There are no chirality outliers.

All (42) torsion outliers are listed below:

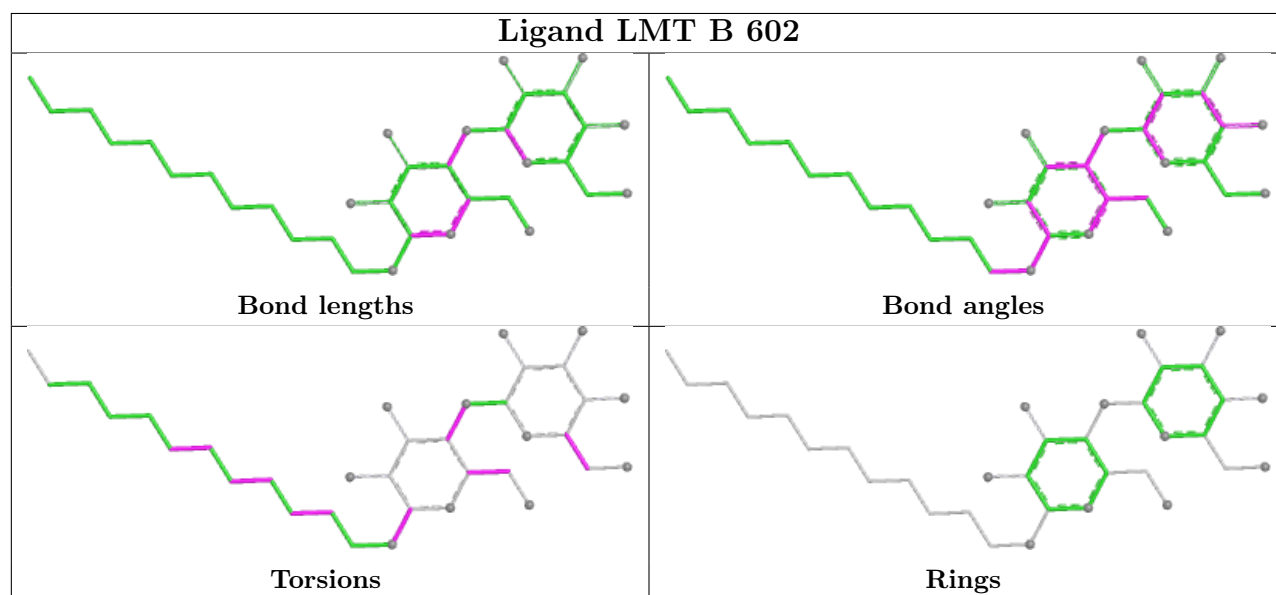
Mol	Chain	Res	Type	Atoms
3	A	602	LMT	C2'-C1'-O1'-C1
3	B	601	LMT	C2'-C1'-O1'-C1
3	B	601	LMT	O5'-C1'-O1'-C1
3	B	602	LMT	C2'-C1'-O1'-C1
4	A	603	ALA	O-C-CA-CB
3	B	601	LMT	O5'-C5'-C6'-O6'
3	A	602	LMT	C2-C3-C4-C5
3	B	602	LMT	C3'-C4'-O1B-C1B
3	B	602	LMT	C4'-C5'-C6'-O6'
3	B	601	LMT	C4'-C5'-C6'-O6'
3	B	602	LMT	O5B-C5B-C6B-O6B
3	B	602	LMT	O5'-C1'-O1'-C1
3	B	602	LMT	C5'-C4'-O1B-C1B
3	A	602	LMT	O1'-C1-C2-C3
3	B	601	LMT	C2-C3-C4-C5
3	A	602	LMT	C11-C10-C9-C8
3	B	601	LMT	C2-C1-O1'-C1'
3	B	602	LMT	C5-C6-C7-C8
3	B	602	LMT	O5'-C5'-C6'-O6'
3	A	602	LMT	C5-C6-C7-C8
3	B	602	LMT	C1-C2-C3-C4
3	B	601	LMT	C4-C5-C6-C7
3	B	601	LMT	O1'-C1-C2-C3
3	A	602	LMT	C4-C5-C6-C7
3	A	602	LMT	C3'-C4'-O1B-C1B
3	A	602	LMT	C7-C8-C9-C10
3	A	602	LMT	C3-C4-C5-C6
3	B	601	LMT	C1-C2-C3-C4
3	A	602	LMT	C2-C1-O1'-C1'
3	B	601	LMT	C9-C10-C11-C12
3	B	601	LMT	C5-C6-C7-C8
3	A	602	LMT	C5'-C4'-O1B-C1B
3	B	602	LMT	C4B-C5B-C6B-O6B
3	B	602	LMT	C3-C4-C5-C6
3	B	601	LMT	O5B-C5B-C6B-O6B
3	B	601	LMT	C5'-C4'-O1B-C1B
3	B	601	LMT	C3'-C4'-O1B-C1B
5	A	604	DBY	OXT-C-CA-N
5	A	604	DBY	O-C-CA-CB
5	A	604	DBY	OXT-C-CA-CB
3	A	602	LMT	O5'-C1'-O1'-C1
5	A	604	DBY	O-C-CA-N

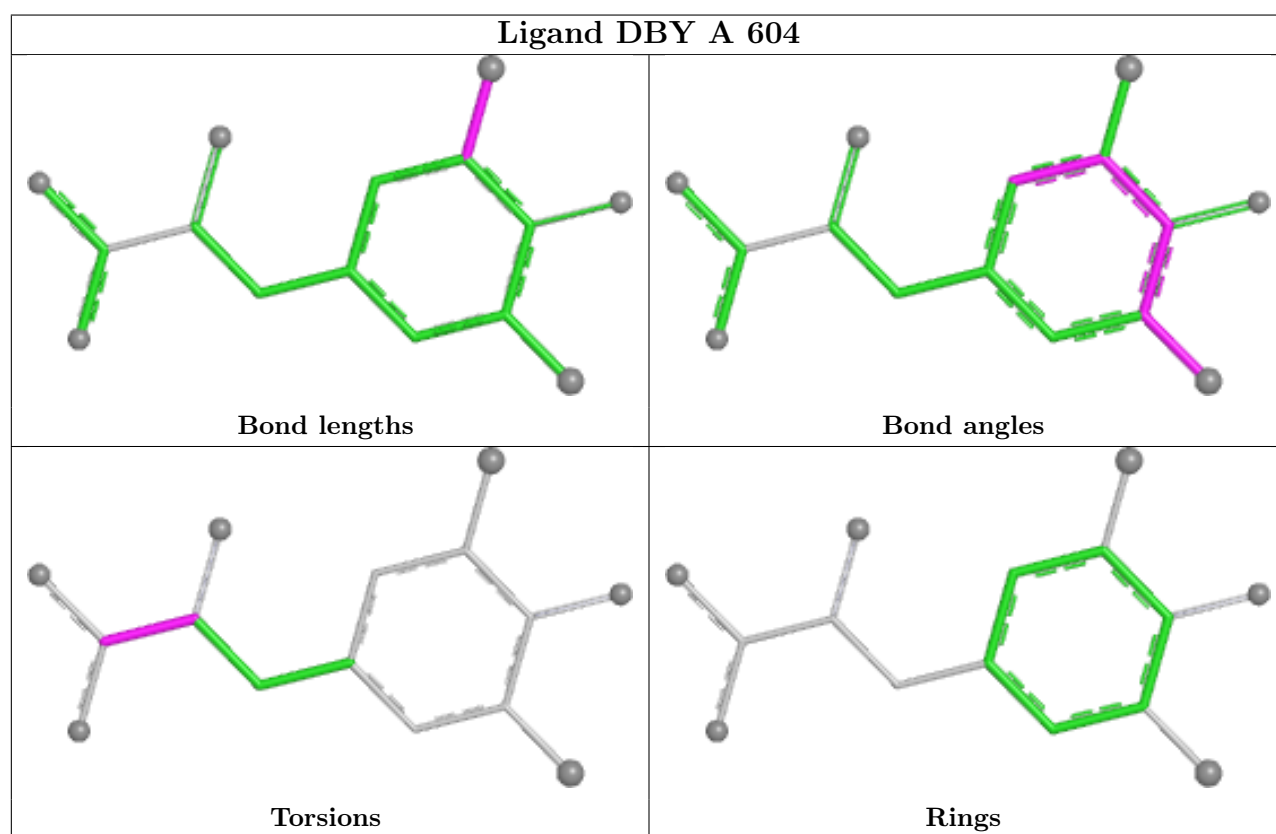
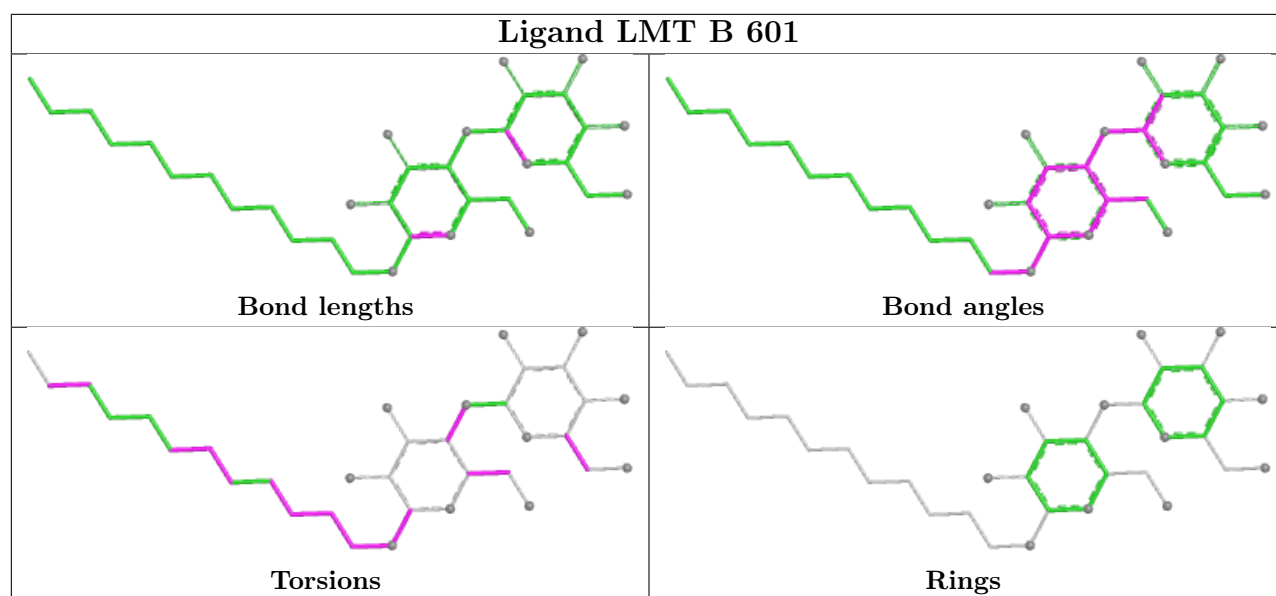
There are no ring outliers.

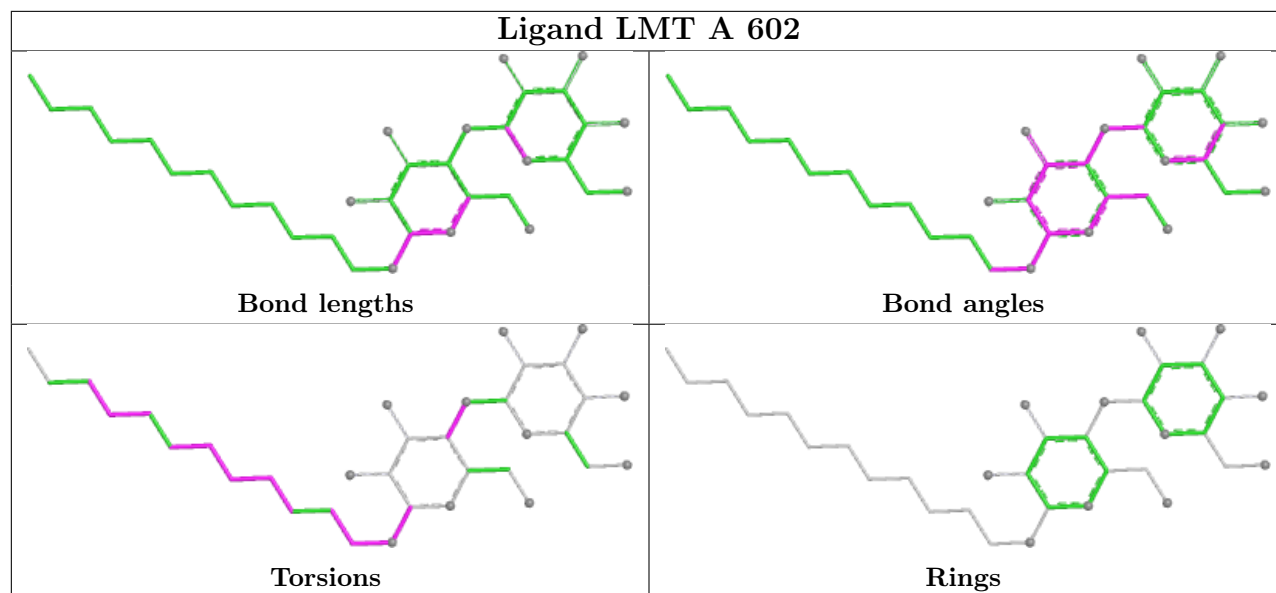
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	LMT	3	0
3	B	601	LMT	3	0
5	A	604	DBY	1	0
3	A	602	LMT	9	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	453/523 (86%)	0.53	46 (10%)	12 7	61, 93, 141, 159	0
1	B	453/523 (86%)	0.56	46 (10%)	12 7	56, 91, 143, 165	0
All	All	906/1046 (86%)	0.54	92 (10%)	12 7	56, 93, 142, 165	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	THR	7.2
1	A	385	LYS	6.2
1	A	312	VAL	5.7
1	B	315	THR	5.1
1	A	315	THR	5.0
1	A	454	VAL	5.0
1	A	455	ASP	4.9
1	B	175	GLU	4.8
1	B	398	TYR	4.6
1	B	385	LYS	4.5
1	B	202	SER	4.4
1	A	388	SER	4.3
1	B	270	GLU	4.3
1	B	425	MET	4.3
1	A	211	ASP	4.3
1	A	451	GLN	3.9
1	A	411	ALA	3.9
1	B	316	HIS	3.8
1	B	383	ASN	3.7
1	B	451	GLN	3.7
1	B	117	ASN	3.6
1	A	386	THR	3.6
1	A	458	GLN	3.5
1	B	380	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	383	ASN	3.4
1	B	412	MET	3.3
1	B	428	ALA	3.3
1	A	317	LEU	3.2
1	A	175	GLU	3.2
1	B	62	TYR	3.2
1	A	274	LEU	3.2
1	A	426	MET	3.2
1	A	210	PRO	3.1
1	A	200	HIS	3.1
1	B	426	MET	3.1
1	A	214	PRO	3.0
1	A	410	LEU	3.0
1	A	408	LEU	3.0
1	A	174	ASN	3.0
1	B	411	ALA	2.9
1	A	316	HIS	2.9
1	B	455	ASP	2.9
1	A	356	ILE	2.8
1	A	313	PHE	2.8
1	A	457	LEU	2.8
1	B	74	LYS	2.8
1	B	291	TYR	2.8
1	B	283	GLN	2.7
1	A	198	LEU	2.7
1	B	410	LEU	2.7
1	B	408	LEU	2.7
1	A	326	GLN	2.7
1	A	425	MET	2.7
1	B	121	LYS	2.6
1	A	33	ALA	2.6
1	B	342	TRP	2.6
1	A	311	GLN	2.6
1	B	211	ASP	2.6
1	A	213	ARG	2.6
1	B	201	LYS	2.5
1	A	133	GLU	2.5
1	A	270	GLU	2.5
1	B	376	PHE	2.5
1	A	398	TYR	2.4
1	B	173	GLY	2.4
1	B	272	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	313	PHE	2.4
1	B	8	VAL	2.4
1	A	453	LEU	2.4
1	A	382	VAL	2.4
1	A	172	TYR	2.4
1	B	456	PRO	2.4
1	B	200	HIS	2.3
1	B	29	TYR	2.3
1	B	415	ARG	2.3
1	A	427	GLY	2.3
1	B	206	TYR	2.3
1	A	35	ILE	2.3
1	B	65	PRO	2.3
1	B	317	LEU	2.3
1	B	295	SER	2.3
1	B	409	GLY	2.2
1	A	209	GLU	2.2
1	B	44	GLY	2.2
1	B	172	TYR	2.2
1	B	199	MET	2.1
1	A	206	TYR	2.1
1	A	80	ARG	2.1
1	A	357	ALA	2.1
1	B	384	GLY	2.1
1	A	205	ASN	2.1
1	B	386	THR	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 [\(i\)](#)

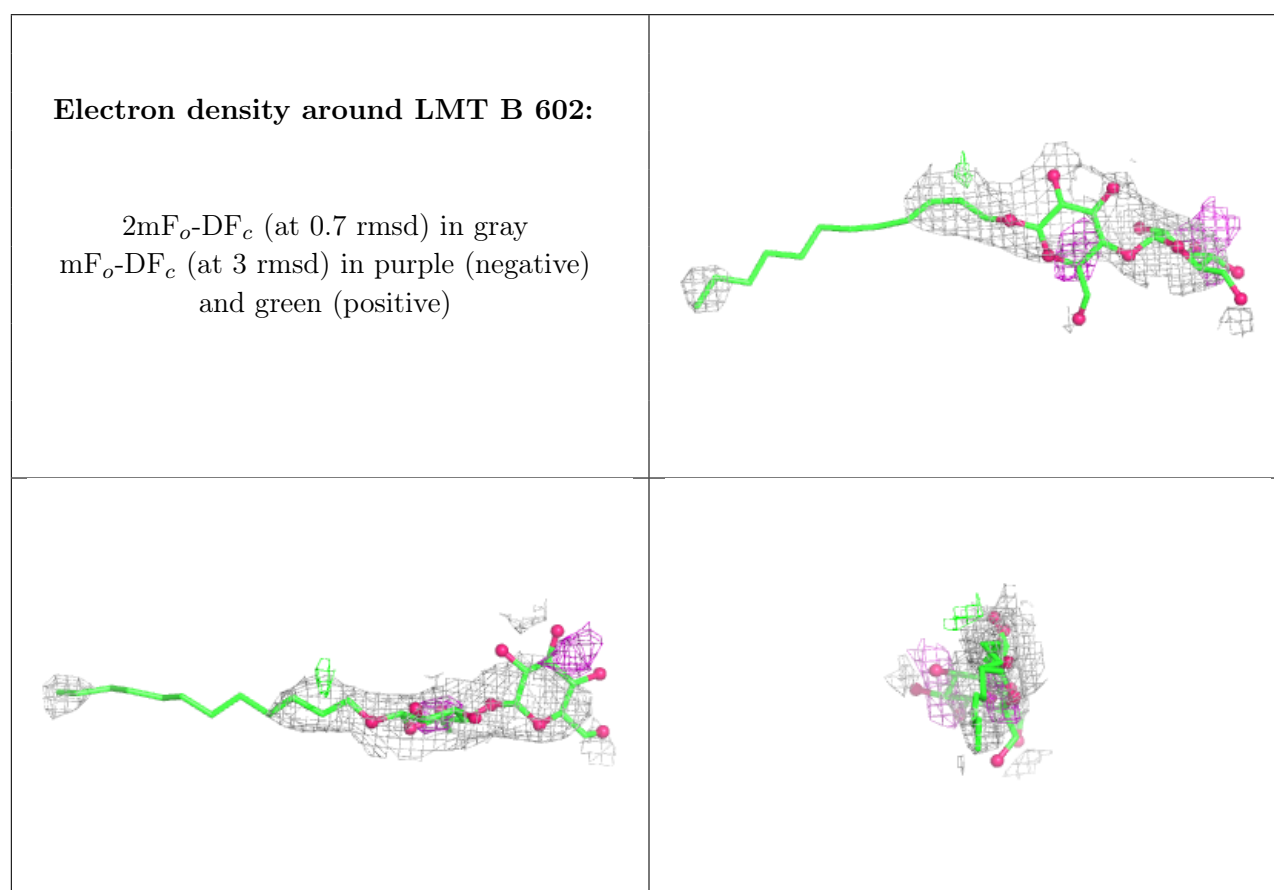
There are no oligosaccharides in this entry.

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.

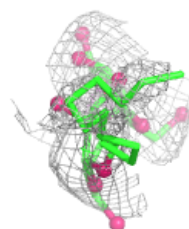
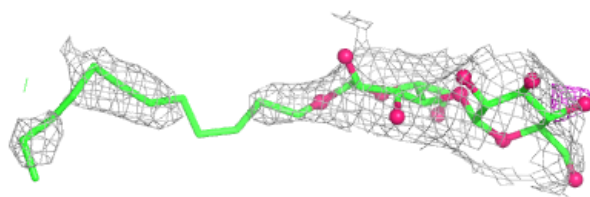
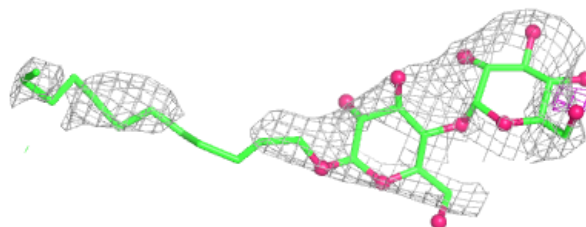
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	LMT	B	602	35/35	0.62	0.19	64,117,125,128	0
3	LMT	B	601	35/35	0.64	0.20	85,115,126,134	0
3	LMT	A	602	35/35	0.65	0.18	57,114,125,135	0
4	ALA	A	603	5/6	0.75	0.43	115,116,136,137	0
5	DBY	A	604	15/15	0.77	0.20	140,168,246,276	0
2	ZN	A	601	1/1	0.89	0.23	150,150,150,150	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.

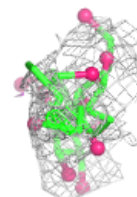
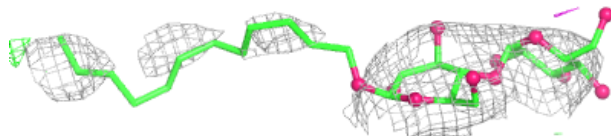
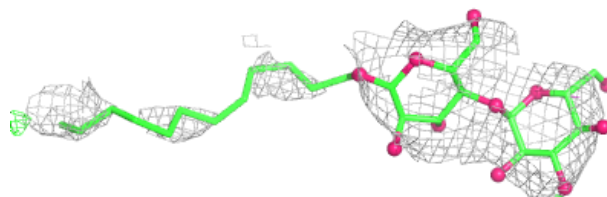


Electron density around LMT B 601:

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

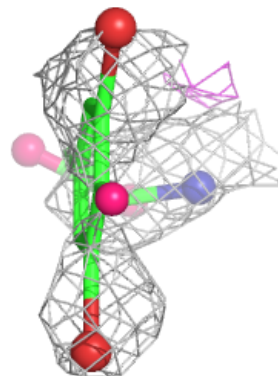
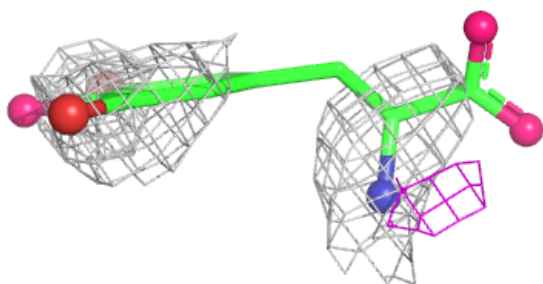
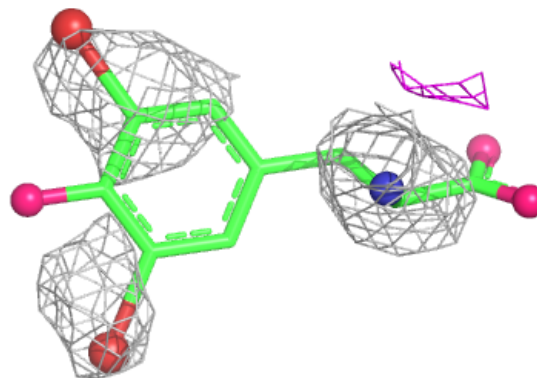
**Electron density around LMT A 602:**

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



Electron density around DBY A 604:

$2mF_o-DF_c$ (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.