



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 12:32 pm BST

PDB ID : 4U8V
Title : Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB
Authors : Pos, K.M.
Deposited on : 2014-08-04
Resolution : 2.30 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 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 : 2.11
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) : 2.11

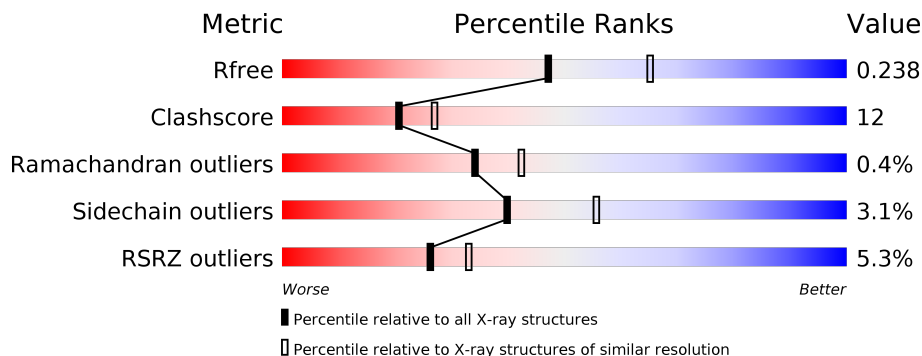
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1057	
1	B	1057	
1	C	1057	
2	D	169	
2	E	169	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27546 atoms, of which 27 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1044	7943	5106	1316	1477	44	0	0	0
1	B	1033	7848	5052	1296	1456	44	0	0	0
1	C	1033	7849	5052	1296	1457	44	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	407	ASN	ASP	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	407	ASN	ASP	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	407	ASN	ASP	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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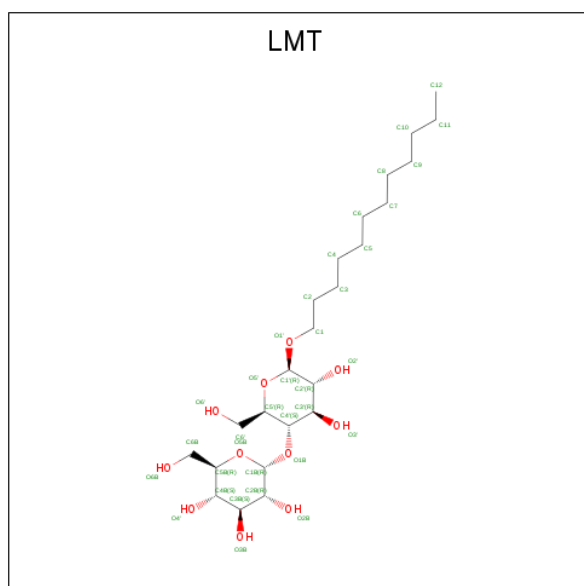
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

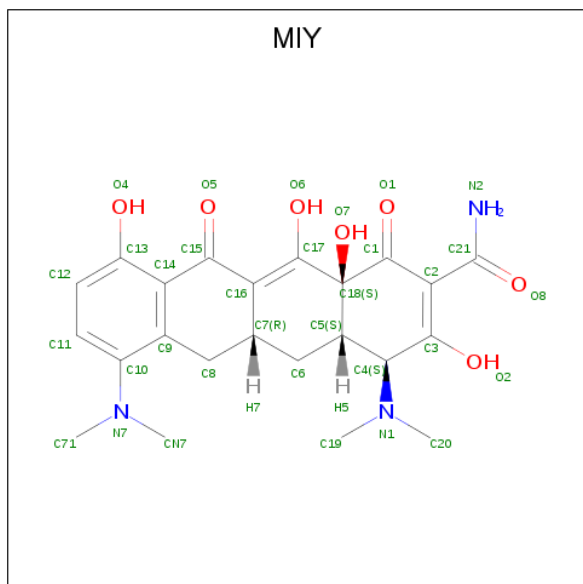
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	156	1177	741	206	229	1	0	0	0
2	E	152	1151	726	202	222	1	0	0	0

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 4 is (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: C₂₃H₂₇N₃O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
4	B	1	60	23	27	3	7	0	0

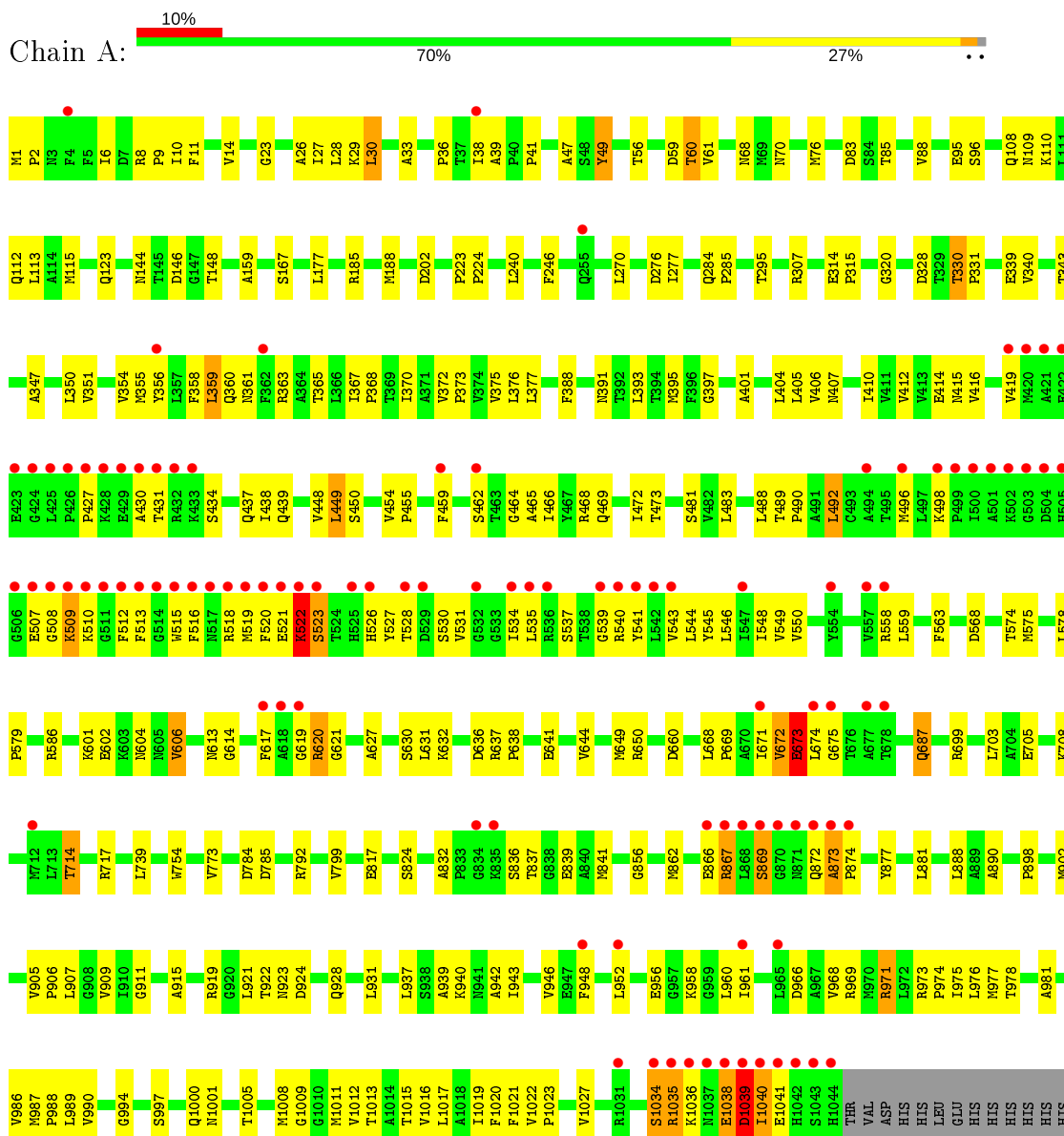
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O	0	0
			391	391		
5	B	376	Total	O	0	0
			376	376		
5	C	469	Total	O	0	0
			469	469		
5	D	61	Total	O	0	0
			61	61		
5	E	46	Total	O	0	0
			46	46		

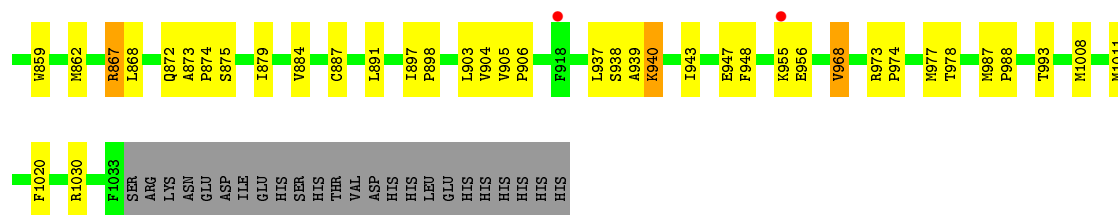
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

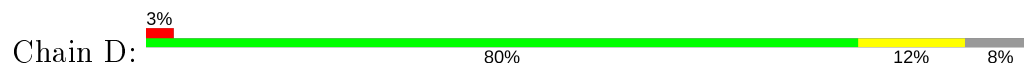
- Molecule 1: Multidrug efflux pump subunit AcrB



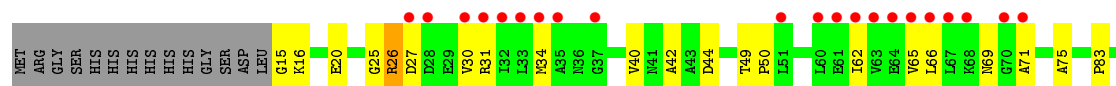
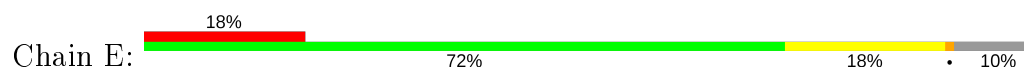
- Molecule 1: Multidrug efflux pump subunit AcrB



• Molecule 2: DARPin



• Molecule 2: DARPin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.59Å 161.59Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.30 48.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.93-2.30) 99.9 (48.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.238 0.194 , 0.238	Depositor DCC
R_{free} test set	12835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.424	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27546	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% 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: MIY, 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	0.38	0/8095	0.53	0/10991
1	B	0.39	0/7998	0.53	0/10861
1	C	0.41	0/7999	0.55	0/10863
2	D	0.34	0/1196	0.48	0/1626
2	E	0.30	0/1170	0.46	0/1591
All	All	0.39	0/26458	0.53	0/35932

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	522	LYS	Peptide

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	7943	0	8086	274	0
1	B	7848	0	8003	185	0
1	C	7849	0	8003	165	0
2	D	1177	0	1159	15	0
2	E	1151	0	1136	24	0
3	A	70	0	92	8	0
3	B	70	0	92	8	0
3	C	35	0	46	3	0
4	B	33	27	25	2	0
5	A	391	0	0	13	0
5	B	376	0	0	9	0
5	C	469	0	0	12	0
5	D	61	0	0	0	0
5	E	46	0	0	3	0
All	All	27519	27	26642	650	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 12.

All (650) 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:363:ARG:HD2	1:B:498:LYS:HE2	1.39	1.03
1:A:528:THR:HG21	1:A:969:ARG:HG3	1.37	1.03
1:A:38:ILE:HG12	1:A:671:ILE:HD13	1.36	1.02
1:C:447:MET:HE1	1:C:891:LEU:HD13	1.44	0.96
1:A:356:TYR:HA	1:A:365:THR:HG21	1.52	0.91
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.52	0.90
1:A:641:GLU:O	1:A:650:ARG:NH2	2.04	0.89
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.53	0.89
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.55	0.88
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.52	0.88
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.55	0.88
1:C:395:MET:HE1	1:C:398:MET:HG3	1.54	0.88
1:A:528:THR:HG21	1:A:969:ARG:CG	2.04	0.87
1:C:867:ARG:NH1	5:C:1315:HOH:O	2.08	0.87
1:A:459:PHE:HD2	1:A:464:GLY:HA2	1.40	0.86
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.58	0.86
1:C:391:ASN:H	1:C:394:THR:HG22	1.40	0.85
1:B:974:PRO:HA	1:B:977:MET:HE2	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:LEU:HD22	1:A:1017:LEU:HD23	1.59	0.84
1:A:523:SER:CB	1:A:526:HIS:HB2	2.06	0.84
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.60	0.83
1:B:449:LEU:HB3	1:B:478:MET:CE	2.09	0.82
1:A:523:SER:HA	1:A:526:HIS:H	1.46	0.81
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.63	0.80
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.81	0.80
1:C:70:ASN:O	1:C:110:LYS:NZ	2.15	0.80
1:A:672:VAL:O	1:A:675:GLY:N	2.13	0.79
2:E:34:MET:HE2	2:E:40:VAL:HG12	1.63	0.78
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.15	0.78
1:B:363:ARG:HD2	1:B:498:LYS:CE	2.14	0.77
1:A:519:MET:O	1:A:522:LYS:HE3	1.85	0.77
1:A:523:SER:HA	1:A:526:HIS:HB2	1.67	0.76
1:A:36:PRO:CG	1:A:469:GLN:HG3	2.17	0.75
1:B:974:PRO:O	1:B:978:THR:HB	1.87	0.75
1:B:618:ALA:HB1	1:B:719:ASN:O	1.86	0.75
1:A:416:VAL:HG11	1:A:431:THR:HG22	1.69	0.75
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.69	0.75
1:B:414:GLU:HG3	1:B:977:MET:CE	2.17	0.74
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.69	0.74
1:A:459:PHE:CD2	1:A:464:GLY:HA2	2.22	0.74
1:B:571:VAL:HG23	1:B:668:LEU:HD11	1.68	0.74
1:B:974:PRO:HA	1:B:977:MET:CE	2.18	0.74
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.69	0.73
1:C:307:ARG:NH1	5:C:1561:HOH:O	2.18	0.73
1:B:994:GLY:N	5:B:1489:HOH:O	2.22	0.73
1:A:527:TYR:OH	1:A:1019:ILE:O	2.07	0.72
1:B:363:ARG:HD2	1:B:498:LYS:HG3	1.72	0.72
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.21	0.72
1:B:919:ARG:HD3	1:B:1005:THR:HG21	1.72	0.71
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.70	0.71
1:A:516:PHE:HA	1:A:519:MET:HG2	1.70	0.71
1:B:871:ASN:HB3	3:B:1102:LMT:H6'1	1.71	0.71
1:A:958:LYS:NZ	1:A:966:ASP:OD2	2.23	0.70
1:C:34:GLN:O	1:C:392:THR:HB	1.91	0.70
1:C:575:MET:HG2	1:C:666:PHE:HE2	1.56	0.70
1:B:420:MET:HE1	1:B:499:PRO:HA	1.73	0.70
1:C:336:SER:O	1:C:340:VAL:HG23	1.92	0.70
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.22	0.70
1:A:669:PRO:HG2	1:A:672:VAL:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.74	0.69
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.56	0.69
1:B:363:ARG:CD	1:B:498:LYS:HE2	2.19	0.69
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.74	0.69
1:C:85:THR:O	5:C:1246:HOH:O	2.10	0.69
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.93	0.69
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.73	0.69
2:E:34:MET:HE2	2:E:40:VAL:CG1	2.23	0.69
1:A:902:MET:O	1:A:905:VAL:HG23	1.93	0.69
1:A:877:TYR:CE2	3:A:1102:LMT:H31	2.29	0.68
1:A:427:PRO:O	1:A:431:THR:HG23	1.94	0.68
1:A:523:SER:O	1:A:527:TYR:HB3	1.94	0.68
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.29	0.68
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.28	0.68
1:B:449:LEU:HB3	1:B:478:MET:HE3	1.75	0.68
1:B:449:LEU:HD13	1:B:478:MET:SD	2.35	0.67
1:C:391:ASN:H	1:C:394:THR:CG2	2.07	0.67
1:A:407:ASN:HD22	1:A:978:THR:HG21	1.58	0.67
1:A:563:PHE:O	1:A:924:ASP:HB2	1.95	0.67
1:A:568:ASP:CG	1:A:637:ARG:HH22	1.97	0.67
1:C:452:VAL:HG13	1:C:884:VAL:HG21	1.77	0.67
1:A:619:GLY:O	1:A:621:GLY:N	2.29	0.66
1:A:523:SER:HA	1:A:526:HIS:N	2.10	0.66
1:B:450:SER:HB2	3:B:1102:LMT:H121	1.77	0.66
1:A:343:THR:HG21	1:A:1000:GLN:OE1	1.96	0.66
1:A:523:SER:CA	1:A:526:HIS:HB2	2.26	0.66
1:A:347:ALA:O	1:A:351:VAL:HG23	1.95	0.65
2:D:121:ALA:HB1	2:D:161:LEU:HD21	1.79	0.65
1:C:580:ALA:CB	1:C:724:THR:HG22	2.26	0.65
1:B:335:ILE:O	1:B:339:GLU:HG2	1.96	0.65
1:C:872:GLN:HG3	5:C:1543:HOH:O	1.97	0.65
2:E:34:MET:CE	2:E:40:VAL:HG12	2.25	0.65
1:A:465:ALA:O	1:A:469:GLN:HG2	1.97	0.65
1:A:905:VAL:O	1:A:909:VAL:HG23	1.97	0.64
1:B:744:ASN:O	1:B:748:THR:HG22	1.96	0.64
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.29	0.64
2:E:34:MET:HE1	2:E:66:LEU:HD23	1.78	0.64
1:B:342:LYS:HE3	1:B:346:GLU:OE2	1.98	0.64
1:C:85:THR:OG1	1:C:87:THR:HG23	1.97	0.64
1:C:993:THR:HG22	5:C:1298:HOH:O	1.97	0.64
1:A:459:PHE:CE1	1:A:872:GLN:HG3	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:GLU:HB3	1:A:606:VAL:HG13	1.81	0.63
1:A:558:ARG:NH1	1:A:558:ARG:HB2	2.13	0.63
1:B:201:VAL:HG22	1:B:748:THR:CG2	2.28	0.63
1:A:70:ASN:O	1:A:110:LYS:HE3	1.98	0.63
1:A:911:GLY:HA2	1:A:1013:THR:HG21	1.81	0.63
1:B:875:SER:O	1:B:879:ILE:HG13	1.99	0.63
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.33	0.62
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.26	0.62
1:A:509:LYS:HG3	1:A:510:LYS:N	2.14	0.62
1:B:509:LYS:HG3	1:B:510:LYS:N	2.13	0.62
1:C:447:MET:SD	1:C:887:CYS:HB3	2.39	0.62
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	1.80	0.62
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.64	0.62
1:A:468:ARG:O	1:A:472:ILE:HG12	1.98	0.62
1:B:363:ARG:HD3	1:B:496:MET:O	1.99	0.62
1:A:38:ILE:HG12	1:A:671:ILE:CD1	2.21	0.62
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.65	0.62
1:B:600:THR:HG22	1:B:601:LYS:HG2	1.81	0.62
1:A:407:ASN:ND2	1:A:978:THR:HG21	2.14	0.62
1:B:351:VAL:CG2	1:B:406:VAL:HG13	2.30	0.62
2:E:15:GLY:N	5:E:202:HOH:O	2.32	0.62
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.63	0.61
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.30	0.61
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.83	0.61
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.80	0.61
2:E:44:ASP:HB2	5:E:242:HOH:O	2.00	0.61
1:C:575:MET:HG2	1:C:666:PHE:CE2	2.34	0.61
1:B:47:ALA:HB3	1:B:88:VAL:HG13	1.82	0.61
1:C:428:LYS:HE3	1:C:432:ARG:NH2	2.16	0.61
1:C:395:MET:HA	1:C:395:MET:HE2	1.82	0.61
1:A:328:ASP:OD1	1:A:330:THR:HB	2.00	0.61
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.83	0.61
1:B:904:VAL:HG11	1:B:942:ALA:HB2	1.82	0.61
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.82	0.60
1:B:637:ARG:O	1:B:643:LYS:HE3	2.01	0.60
1:C:620:ARG:NH1	5:C:1606:HOH:O	2.30	0.60
1:A:492:LEU:O	1:A:496:MET:HB2	2.01	0.60
1:B:573:MET:CE	1:B:617:PHE:HE2	2.14	0.60
1:B:714:THR:CG2	1:B:832:ALA:HA	2.32	0.59
2:D:12:SER:HB2	2:D:15:GLY:H	1.66	0.59
1:C:392:THR:HG22	1:C:393:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:CG1	1:A:431:THR:HG22	2.31	0.59
1:B:837:THR:HG22	5:B:1469:HOH:O	2.02	0.59
1:A:784:ASP:OD1	5:A:1484:HOH:O	2.17	0.59
1:B:450:SER:CB	3:B:1102:LMT:H121	2.33	0.59
1:B:201:VAL:HG22	1:B:748:THR:HG21	1.85	0.59
1:C:452:VAL:HG13	1:C:884:VAL:CG2	2.32	0.59
1:B:352:PHE:CD2	1:B:365:THR:HG21	2.38	0.59
1:C:87:THR:HG22	5:C:1246:HOH:O	2.00	0.59
1:A:370:ILE:O	1:A:373:PRO:HD2	2.03	0.59
1:A:355:MET:HA	1:A:355:MET:HE2	1.83	0.58
1:A:351:VAL:O	1:A:355:MET:HG2	2.03	0.58
1:A:559:LEU:HD23	1:A:923:ASN:HB2	1.85	0.58
1:B:1011:MET:O	1:B:1015:THR:HG23	2.03	0.58
1:B:362:PHE:O	1:B:365:THR:HB	2.03	0.58
1:B:919:ARG:HG2	1:B:921:LEU:CD1	2.33	0.58
1:B:979:SER:OG	1:B:1015:THR:HG21	2.03	0.58
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.85	0.58
2:E:65:VAL:O	2:E:69:ASN:ND2	2.34	0.58
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.34	0.58
1:A:785:ASP:OD1	5:A:1201:HOH:O	2.17	0.58
1:C:111:LEU:HD21	1:C:127:VAL:CG1	2.33	0.58
1:B:636:ASP:C	1:B:638:PRO:HD3	2.23	0.58
2:E:106:VAL:HG12	5:E:234:HOH:O	2.03	0.58
1:A:987:MET:N	1:A:988:PRO:HD2	2.19	0.58
1:B:396:PHE:O	1:B:399:VAL:HG22	2.03	0.58
1:B:919:ARG:HG2	1:B:921:LEU:HD13	1.85	0.58
1:A:38:ILE:CG1	1:A:671:ILE:HD13	2.25	0.57
1:C:395:MET:CE	1:C:398:MET:HG3	2.33	0.57
1:C:115:MET:N	1:C:116:PRO:HD2	2.20	0.57
1:C:452:VAL:CG1	1:C:884:VAL:HG21	2.34	0.57
1:A:507:GLU:HB3	1:A:518:ARG:HG3	1.85	0.57
1:B:459:PHE:O	1:B:464:GLY:HA3	2.03	0.57
1:C:575:MET:CE	1:C:666:PHE:HZ	2.17	0.57
1:A:38:ILE:HD12	1:A:39:ALA:N	2.19	0.57
1:A:672:VAL:O	1:A:674:LEU:N	2.38	0.57
1:B:359:LEU:HD13	1:B:417:GLU:HG3	1.85	0.57
1:B:987:MET:N	1:B:988:PRO:HD2	2.18	0.57
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.34	0.57
2:E:16:LYS:NZ	2:E:20:GLU:OE1	2.36	0.57
1:A:862:MET:O	1:A:866:GLU:HG2	2.05	0.57
1:C:530:SER:OG	3:C:1101:LMT:H11	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.87	0.57
1:C:369:THR:O	1:C:372:VAL:HG13	2.05	0.57
1:A:705:GLU:OE2	1:A:708:LYS:HE3	2.03	0.57
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.86	0.57
1:A:523:SER:HA	1:A:526:HIS:CB	2.34	0.57
1:A:952:LEU:O	1:A:956:GLU:HB2	2.05	0.57
1:C:370:ILE:O	1:C:373:PRO:HD2	2.05	0.57
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.40	0.56
1:B:1018:ALA:O	1:B:1022:VAL:HG13	2.05	0.56
1:C:372:VAL:HG22	1:C:373:PRO:CD	2.33	0.56
1:A:714:THR:HG23	1:A:832:ALA:HA	1.87	0.56
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.86	0.56
1:B:416:VAL:O	1:B:420:MET:HG3	2.06	0.56
1:B:428:LYS:HZ1	1:B:432:ARG:HH22	1.53	0.56
1:A:604:ASN:O	1:A:632:LYS:HD2	2.06	0.56
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.88	0.56
1:C:226:LYS:NZ	5:C:1203:HOH:O	2.39	0.56
1:A:960:LEU:HB2	1:A:1038:GLU:OE2	2.06	0.55
1:A:202:ASP:OD2	1:A:792:ARG:NH2	2.38	0.55
1:A:649:MET:HB3	5:A:1514:HOH:O	2.06	0.55
1:B:714:THR:HG22	1:B:832:ALA:HA	1.89	0.55
1:A:412:VAL:O	1:A:416:VAL:HG23	2.06	0.55
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.41	0.55
1:B:571:VAL:CG2	1:B:668:LEU:HD11	2.35	0.55
1:C:154:ILE:O	1:C:158:VAL:HG13	2.07	0.55
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.07	0.55
1:C:479:ALA:O	1:C:482:VAL:HG23	2.07	0.55
1:A:687:GLN:OE1	1:A:856:GLY:HA3	2.07	0.55
1:A:56:THR:O	1:A:60:THR:HB	2.06	0.54
1:C:448:VAL:HG22	1:C:884:VAL:HG13	1.89	0.54
1:A:531:VAL:O	1:A:535:LEU:HG	2.08	0.54
1:B:540:ARG:NH2	3:B:1101:LMT:H6'1	2.22	0.54
1:C:120:GLN:O	1:C:124:GLN:HG2	2.07	0.54
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.90	0.54
2:E:42:ALA:O	2:E:50:PRO:HD3	2.06	0.54
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.88	0.54
1:A:223:PRO:HD2	1:B:780:ARG:NH1	2.22	0.54
1:C:1020:PHE:CZ	3:C:1101:LMT:H51	2.42	0.54
1:C:40:PRO:HB2	1:C:94:PHE:O	2.08	0.54
1:C:534:ILE:HG12	1:C:541:TYR:CZ	2.43	0.54
1:A:546:LEU:O	1:A:550:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.43	0.54
1:A:363:ARG:HH11	1:A:498:LYS:HG3	1.73	0.54
1:A:38:ILE:HG22	1:A:462:SER:O	2.08	0.54
1:A:523:SER:HB2	1:A:526:HIS:HB2	1.88	0.54
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.90	0.54
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.88	0.54
1:B:331:PRO:O	1:B:335:ILE:HG12	2.08	0.54
1:B:32:VAL:HG12	1:B:333:VAL:HG11	1.89	0.54
1:B:926:TYR:O	1:B:1003:VAL:HG12	2.08	0.54
1:B:412:VAL:O	1:B:416:VAL:HG23	2.08	0.53
1:A:415:ASN:O	1:A:419:VAL:HG23	2.08	0.53
1:A:202:ASP:CG	1:A:792:ARG:HH22	2.12	0.53
1:C:392:THR:HG23	1:C:396:PHE:CE2	2.44	0.53
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.91	0.53
1:A:430:ALA:O	1:A:434:SER:HB2	2.08	0.53
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.29	0.53
1:A:188:MET:CE	1:A:773:VAL:HG12	2.38	0.53
1:B:898:PRO:O	1:B:902:MET:HG3	2.08	0.53
1:A:109:ASN:O	1:A:112:GLN:HG3	2.09	0.53
1:A:898:PRO:O	1:A:902:MET:HG3	2.09	0.53
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.39	0.53
1:C:670:ALA:HB3	1:C:862:MET:HE1	1.90	0.53
1:C:836:SER:OG	1:C:839:GLU:HG3	2.09	0.53
1:A:414:GLU:OE2	1:A:973:ARG:NH1	2.41	0.53
3:B:1101:LMT:H6E	3:B:1101:LMT:H5B	1.91	0.53
1:A:1:MET:N	5:A:1331:HOH:O	2.35	0.53
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.91	0.53
1:A:586:ARG:HB3	5:A:1487:HOH:O	2.09	0.53
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.39	0.53
1:A:520:PHE:CZ	1:A:973:ARG:HB2	2.44	0.53
1:B:108:GLN:HG3	1:B:109:ASN:N	2.22	0.53
1:B:901:VAL:O	1:B:904:VAL:HG22	2.09	0.53
1:A:867:ARG:NH1	5:A:1522:HOH:O	2.09	0.52
1:C:764:ASP:HB3	1:C:769:LYS:HD2	1.90	0.52
2:D:25:GLY:HA2	2:D:62:ILE:HD12	1.91	0.52
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.90	0.52
1:C:575:MET:HE1	1:C:617:PHE:HD2	1.74	0.52
1:C:57:VAL:O	1:C:61:VAL:HB	2.09	0.52
1:A:507:GLU:HB3	1:A:518:ARG:CG	2.40	0.52
1:A:649:MET:HG2	5:A:1533:HOH:O	2.09	0.52
1:A:277:ILE:HA	1:A:613:ASN:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:VAL:HG11	1:A:406:VAL:HG21	1.92	0.52
1:B:363:ARG:CD	1:B:498:LYS:HG3	2.39	0.52
1:C:57:VAL:HG13	1:C:82:SER:HB3	1.92	0.52
1:B:841:MET:O	1:B:845:GLU:HG3	2.10	0.52
1:C:424:GLY:HA3	1:C:502:LYS:HB2	1.92	0.52
1:A:489:THR:HB	1:A:490:PRO:HD3	1.92	0.52
1:A:29:LYS:HE3	3:B:1102:LMT:O6'	2.09	0.52
1:B:375:VAL:HG11	1:B:405:LEU:CD2	2.36	0.51
1:B:401:ALA:O	1:B:405:LEU:HG	2.09	0.51
1:A:890:ALA:HB2	1:C:14:VAL:HG21	1.92	0.51
2:D:92:HIS:O	2:D:96:VAL:HG23	2.09	0.51
2:E:34:MET:CE	2:E:66:LEU:HD23	2.40	0.51
1:A:545:TYR:O	1:A:549:VAL:HG23	2.09	0.51
1:A:837:THR:O	1:A:841:MET:HG3	2.10	0.51
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.92	0.51
1:B:447:MET:HB3	1:B:887:CYS:SG	2.51	0.51
2:E:26:ARG:O	2:E:30:VAL:HG23	2.10	0.51
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.92	0.51
1:A:881:LEU:HG	3:A:1102:LMT:C12	2.41	0.51
1:A:621:GLY:HA3	5:A:1352:HOH:O	2.11	0.51
1:B:11:PHE:O	1:B:11:PHE:HD1	1.92	0.51
1:B:573:MET:HE3	1:B:617:PHE:HE2	1.75	0.51
1:A:961:ILE:HD12	1:A:961:ILE:H	1.75	0.51
1:B:128:SER:HB3	1:C:113:LEU:CD1	2.41	0.51
1:C:6:ILE:HD11	1:C:431:THR:HG22	1.93	0.51
1:C:599:LEU:O	1:C:603:LYS:HB3	2.10	0.51
2:D:43:ALA:HA	2:D:48:TRP:O	2.11	0.51
1:A:928:GLN:HG2	3:A:1102:LMT:H21	1.92	0.51
1:B:395:MET:HA	1:B:395:MET:HE2	1.92	0.51
1:C:575:MET:HE3	1:C:666:PHE:HZ	1.75	0.51
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.91	0.51
1:B:390:ILE:HG23	1:B:395:MET:SD	2.51	0.51
1:B:554:TYR:CZ	1:B:558:ARG:HD3	2.46	0.50
1:C:376:LEU:HD11	1:C:402:ILE:HD11	1.93	0.50
1:A:276:ASP:O	1:A:614:GLY:HA3	2.12	0.50
1:A:523:SER:O	1:A:527:TYR:CB	2.60	0.50
1:B:62:THR:O	1:B:66:GLU:HG3	2.11	0.50
1:A:2:PRO:HG2	1:A:439:GLN:OE1	2.11	0.50
1:B:580:ALA:CB	1:B:724:THR:HG22	2.41	0.50
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.92	0.50
1:C:453:PHE:CE2	1:C:474:ILE:HG21	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.41	0.50
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.93	0.50
1:A:714:THR:CG2	1:A:832:ALA:HA	2.42	0.50
1:A:971:ARG:O	1:A:975:ILE:HG13	2.12	0.50
1:A:523:SER:HB3	1:A:526:HIS:HB2	1.91	0.49
1:A:60:THR:CG2	1:A:61:VAL:HG23	2.39	0.49
1:A:614:GLY:O	1:A:620:ARG:HA	2.12	0.49
1:C:57:VAL:HG22	1:C:88:VAL:CG1	2.42	0.49
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.93	0.49
1:B:395:MET:CE	1:B:395:MET:HA	2.42	0.49
1:B:1022:VAL:HG22	1:B:1023:PRO:CD	2.42	0.49
1:C:15:ILE:O	1:C:19:ILE:HG13	2.13	0.49
1:A:343:THR:HG22	5:A:1580:HOH:O	2.13	0.49
1:A:372:VAL:CB	1:A:373:PRO:HD3	2.43	0.49
1:A:512:PHE:O	1:A:515:TRP:HB3	2.13	0.49
1:B:328:ASP:O	1:B:331:PRO:HD2	2.12	0.49
1:B:420:MET:CE	1:B:499:PRO:HA	2.39	0.49
2:D:91:GLY:HA2	2:D:128:ILE:HD12	1.92	0.49
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.94	0.49
1:B:363:ARG:HD2	1:B:498:LYS:CG	2.42	0.49
1:C:111:LEU:HD21	1:C:127:VAL:HG12	1.93	0.49
1:A:540:ARG:HA	1:A:543:VAL:HG23	1.95	0.49
1:A:544:LEU:HD22	1:A:1021:PHE:HZ	1.77	0.49
1:A:919:ARG:NE	1:A:1005:THR:HG21	2.28	0.49
1:A:358:PHE:CG	1:A:977:MET:HG2	2.48	0.49
1:C:545:TYR:O	1:C:549:VAL:HG23	2.13	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:B:926:TYR:HB3	1:B:1003:VAL:CG1	2.42	0.48
1:B:926:TYR:HB3	1:B:1003:VAL:HG13	1.94	0.48
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.48	0.48
1:A:359:LEU:HG	1:A:977:MET:HE3	1.95	0.48
1:A:534:ILE:HG22	1:A:541:TYR:OH	2.13	0.48
1:A:942:ALA:O	1:A:946:VAL:HG23	2.13	0.48
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.95	0.48
1:B:433:LYS:O	1:B:437:GLN:HG3	2.12	0.48
1:A:454:VAL:HB	1:A:455:PRO:HD3	1.96	0.48
1:A:574:THR:HB	1:A:627:ALA:HB3	1.95	0.48
1:A:866:GLU:O	1:A:869:SER:N	2.47	0.48
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.48	0.48
1:C:939:ALA:O	1:C:943:ILE:HG12	2.14	0.48
1:A:531:VAL:O	1:A:534:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HD2	1:B:780:ARG:HH12	1.79	0.48
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.13	0.48
1:C:498:LYS:HA	1:C:498:LYS:HD3	1.65	0.48
1:C:867:ARG:NH1	1:C:867:ARG:HG2	2.26	0.48
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.49	0.48
1:B:105:VAL:HA	1:B:108:GLN:HG2	1.94	0.48
1:B:201:VAL:HG22	1:B:748:THR:HG23	1.95	0.48
1:C:987:MET:HA	1:C:1008:MET:HE1	1.94	0.48
1:C:11:PHE:O	1:C:11:PHE:HD1	1.97	0.48
1:C:540:ARG:O	1:C:544:LEU:HD23	2.13	0.48
1:C:111:LEU:HD21	1:C:127:VAL:HG11	1.96	0.48
1:A:958:LYS:HA	1:A:1041:GLU:HB2	1.96	0.48
1:A:350:LEU:O	1:A:354:VAL:HG23	2.14	0.48
1:B:641:GLU:H	1:B:641:GLU:HG3	1.41	0.48
1:C:5:PHE:CD2	1:C:487:ILE:HG23	2.49	0.48
1:A:185:ARG:HD2	5:A:1561:HOH:O	2.13	0.47
1:A:361:ASN:O	1:A:365:THR:HG23	2.14	0.47
1:A:601:LYS:NZ	5:A:1521:HOH:O	2.46	0.47
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.95	0.47
1:B:679:GLY:HA2	5:B:1469:HOH:O	2.14	0.47
1:C:10:ILE:O	1:C:14:VAL:HG13	2.14	0.47
1:C:314:GLU:N	1:C:315:PRO:CD	2.77	0.47
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.49	0.47
1:B:420:MET:HE1	1:B:427:PRO:HD3	1.96	0.47
1:C:875:SER:O	1:C:879:ILE:HG22	2.15	0.47
1:A:437:GLN:HG3	1:A:438:ILE:HG23	1.97	0.47
1:B:580:ALA:HB1	1:B:724:THR:CG2	2.44	0.47
1:B:559:LEU:HD23	1:B:923:ASN:HB2	1.96	0.47
1:C:641:GLU:H	1:C:641:GLU:CD	2.18	0.47
1:B:672:VAL:HG21	5:B:1359:HOH:O	2.14	0.47
1:C:506:GLY:C	1:C:517:ASN:HD22	2.18	0.47
2:D:94:GLU:CD	2:D:94:GLU:H	2.17	0.47
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.97	0.47
1:B:360:GLN:HG2	1:B:513:PHE:CD1	2.48	0.47
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.47
1:A:339:GLU:O	1:A:343:THR:HG23	2.14	0.47
1:A:527:TYR:O	1:A:530:SER:HB2	2.14	0.47
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.47
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.97	0.47
1:A:83:ASP:OD1	1:A:85:THR:HB	2.14	0.47
1:A:26:ALA:O	1:A:30:LEU:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:VAL:HG22	1:B:406:VAL:HG13	1.97	0.46
1:B:904:VAL:O	1:B:907:LEU:HB2	2.15	0.46
1:C:146:ASP:OD1	1:C:148:THR:HG23	2.14	0.46
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.98	0.46
1:B:925:VAL:O	1:B:929:VAL:HG23	2.15	0.46
2:D:12:SER:O	2:D:16:LYS:HG2	2.16	0.46
2:E:89:HIS:HD2	2:E:123:ARG:HG3	1.80	0.46
1:A:330:THR:HG22	1:A:331:PRO:N	2.29	0.46
1:C:617:PHE:CD2	1:C:676:THR:HG21	2.49	0.46
1:B:674:LEU:HD23	1:B:674:LEU:O	2.15	0.46
2:D:25:GLY:HA2	2:D:62:ILE:CD1	2.46	0.46
1:B:169:THR:O	1:B:172:VAL:HG13	2.15	0.46
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.97	0.46
1:A:602:GLU:CB	1:A:606:VAL:HG13	2.45	0.46
1:A:85:THR:O	1:A:85:THR:HG22	2.15	0.46
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.37	0.46
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.18	0.46
1:B:256:ASP:OD1	1:B:256:ASP:N	2.49	0.46
1:B:449:LEU:HB3	1:B:478:MET:SD	2.56	0.46
1:C:407:ASN:ND2	1:C:978:THR:HG21	2.30	0.46
1:C:841:MET:O	1:C:845:GLU:HG3	2.16	0.46
1:C:867:ARG:HG2	5:C:1315:HOH:O	2.15	0.46
1:C:940:LYS:NZ	5:C:1371:HOH:O	2.39	0.46
1:A:8:ARG:N	1:A:9:PRO:HD3	2.30	0.46
1:C:2:PRO:O	1:C:6:ILE:HG13	2.16	0.46
1:A:1038:GLU:O	1:A:1039:ASP:HB2	2.15	0.46
1:B:540:ARG:HH22	3:B:1101:LMT:HG1	1.80	0.46
1:A:527:TYR:HE2	1:A:968:VAL:CG1	2.28	0.46
1:A:961:ILE:N	1:A:961:ILE:HD12	2.31	0.46
1:C:104:GLN:NE2	1:C:108:GLN:OE1	2.33	0.46
1:C:376:LEU:HD11	1:C:402:ILE:CD1	2.46	0.46
1:C:76:MET:HE2	1:C:93:THR:HG22	1.97	0.46
1:C:943:ILE:O	1:C:947:GLU:HB3	2.16	0.46
1:A:1038:GLU:CD	1:A:1039:ASP:N	2.69	0.45
1:A:987:MET:O	1:A:990:VAL:HG22	2.16	0.45
1:B:682:PHE:HB2	1:B:859:TRP:CZ3	2.51	0.45
1:C:868:LEU:O	1:C:872:GLN:HG2	2.15	0.45
1:A:836:SER:OG	1:A:839:GLU:HG3	2.15	0.45
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.97	0.45
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.45
1:B:913:LEU:HD23	1:B:927:PHE:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HB2	1:C:269:GLU:O	2.16	0.45
1:B:489:THR:N	1:B:490:PRO:CD	2.79	0.45
1:B:714:THR:HG21	1:B:832:ALA:HA	1.98	0.45
1:C:987:MET:SD	1:C:1008:MET:HE1	2.57	0.45
1:C:358:PHE:CG	1:C:977:MET:HG2	2.52	0.45
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.98	0.45
1:A:509:LYS:CG	1:A:510:LYS:N	2.78	0.45
1:A:714:THR:HG22	5:A:1530:HOH:O	2.17	0.45
1:B:986:VAL:HG21	1:B:1007:VAL:CG1	2.47	0.45
1:C:395:MET:CE	1:C:395:MET:HA	2.44	0.45
1:A:415:ASN:ND2	1:A:438:ILE:HG21	2.32	0.45
1:A:450:SER:O	1:A:454:VAL:HG23	2.16	0.45
1:A:937:LEU:HD23	1:A:1011:MET:CE	2.47	0.45
1:B:197:GLN:HA	1:B:798:MET:SD	2.57	0.45
1:B:527:TYR:CZ	1:B:968:VAL:HG13	2.52	0.45
3:A:1101:LMT:H121	3:A:1101:LMT:H91	1.86	0.45
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.51	0.45
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.98	0.45
2:E:49:THR:HB	2:E:50:PRO:HD2	1.99	0.45
1:A:115:MET:HE3	1:A:123:GLN:HG2	1.99	0.45
1:A:10:ILE:O	1:A:14:VAL:HG23	2.17	0.45
1:C:276:ASP:O	1:C:614:GLY:HA3	2.17	0.45
1:C:48:SER:HB3	1:C:125:GLN:HG2	1.99	0.45
1:A:406:VAL:O	1:A:410:ILE:HG13	2.17	0.44
1:B:600:THR:HG22	1:B:601:LYS:N	2.32	0.44
1:A:522:LYS:O	1:A:526:HIS:ND1	2.48	0.44
1:A:909:VAL:HG13	1:A:931:LEU:HD21	1.98	0.44
2:D:58:GLY:HA2	2:D:95:ILE:HD12	1.99	0.44
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.47	0.44
1:A:76:MET:HG2	1:A:95:GLU:OE1	2.18	0.44
1:C:743:ILE:N	1:C:743:ILE:HD12	2.31	0.44
1:A:699:ARG:O	1:A:703:LEU:HG	2.18	0.44
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.99	0.44
1:B:99:ASP:OD1	1:B:101:ASP:HB2	2.18	0.44
1:B:358:PHE:CD1	1:B:977:MET:HG2	2.53	0.44
1:A:10:ILE:HD12	1:B:894:SER:HA	1.99	0.44
1:C:447:MET:CE	1:C:891:LEU:HD13	2.30	0.44
1:A:672:VAL:HB	1:A:673:GLU:H	1.65	0.44
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.17	0.44
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.18	0.44
1:A:284:GLN:HB2	1:A:285:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.99	0.44
1:A:739:LEU:HD13	1:A:799:VAL:HG11	2.00	0.44
1:B:395:MET:O	1:B:398:MET:HB2	2.17	0.44
1:B:714:THR:HG22	1:B:832:ALA:CA	2.47	0.44
1:C:621:GLY:N	5:C:1581:HOH:O	2.12	0.44
1:A:1009:GLY:O	1:A:1013:THR:HG23	2.17	0.44
1:A:1034:SER:O	1:A:1035:ARG:HB2	2.18	0.44
1:A:636:ASP:O	1:A:638:PRO:HD3	2.18	0.44
1:C:360:GLN:HB3	1:C:513:PHE:CD2	2.53	0.44
1:C:955:LYS:HG3	1:C:956:GLU:HG3	1.99	0.44
1:A:397:GLY:HA3	1:A:473:THR:HG21	2.00	0.44
1:B:70:ASN:O	1:B:110:LYS:HE3	2.18	0.44
1:B:144:ASN:HA	1:B:320:GLY:O	2.17	0.44
1:B:509:LYS:HG3	1:B:510:LYS:H	1.83	0.44
1:A:881:LEU:HG	3:A:1102:LMT:H122	2.00	0.43
1:A:375:VAL:HB	1:A:405:LEU:HD13	2.00	0.43
1:A:544:LEU:O	1:A:548:ILE:HG13	2.18	0.43
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:B:300:LEU:CD2	1:B:330:THR:HG23	2.48	0.43
1:B:464:GLY:O	1:B:468:ARG:HB2	2.18	0.43
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.84	0.43
1:A:59:ASP:HB3	1:C:763:ILE:HD11	2.00	0.43
1:A:356:TYR:CA	1:A:365:THR:HG21	2.37	0.43
1:A:817:GLU:HB2	1:A:824:SER:O	2.18	0.43
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.48	0.43
1:A:960:LEU:HG	1:A:1027:VAL:HG12	2.00	0.43
1:A:888:LEU:HB2	1:A:898:PRO:HB3	2.00	0.43
1:A:919:ARG:O	1:A:919:ARG:HG2	2.18	0.43
1:B:192:GLU:OE2	1:B:192:GLU:HA	2.18	0.43
1:B:38:ILE:HG21	1:B:674:LEU:HD12	1.99	0.43
1:B:680:PHE:HA	5:B:1240:HOH:O	2.17	0.43
1:B:973:ARG:N	1:B:974:PRO:HD2	2.32	0.43
1:C:620:ARG:HE	1:C:620:ARG:HB3	1.44	0.43
1:A:1039:ASP:O	1:A:1040:ILE:HD13	2.17	0.43
1:A:2:PRO:O	1:A:6:ILE:HG13	2.18	0.43
1:B:527:TYR:CE2	1:B:968:VAL:CG1	3.00	0.43
2:E:25:GLY:O	2:E:27:ASP:N	2.51	0.43
1:A:1012:VAL:HA	1:A:1015:THR:HG22	2.00	0.43
1:A:1038:GLU:CG	1:A:1039:ASP:N	2.81	0.43
1:A:528:THR:HG21	1:A:969:ARG:HG2	1.96	0.43
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:CG	1:B:977:MET:HE1	2.38	0.43
1:A:68:ASN:O	1:A:110:LYS:HB3	2.19	0.43
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.90	0.43
4:B:1103:MIY:H81	4:B:1103:MIY:HN72	2.01	0.43
1:B:573:MET:CE	1:B:617:PHE:CE2	3.00	0.43
1:C:36:PRO:HG3	1:C:469:GLN:CD	2.39	0.43
1:A:881:LEU:CD2	3:A:1102:LMT:H121	2.49	0.43
1:B:235:ILE:O	1:C:728:LYS:HD2	2.18	0.43
1:C:937:LEU:HD13	1:C:1011:MET:SD	2.59	0.43
1:A:144:ASN:HA	1:A:320:GLY:O	2.19	0.43
1:A:375:VAL:HG11	1:A:405:LEU:CD2	2.48	0.43
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.81	0.43
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.01	0.43
1:B:456:MET:HG3	1:B:932:LEU:HD11	2.00	0.43
2:D:121:ALA:CB	2:D:161:LEU:HD21	2.47	0.43
1:A:8:ARG:HG2	5:B:1223:HOH:O	2.19	0.43
1:A:907:LEU:CD2	1:A:1017:LEU:HD23	2.41	0.42
1:A:167:SER:HB3	1:B:70:ASN:HB3	2.01	0.42
1:A:355:MET:HE2	1:A:355:MET:CA	2.49	0.42
1:A:575:MET:HE2	1:A:617:PHE:HE2	1.84	0.42
1:A:614:GLY:HA2	1:A:621:GLY:O	2.18	0.42
1:C:33:ALA:O	1:C:391:ASN:HA	2.19	0.42
1:A:27:ILE:HD13	3:A:1101:LMT:H51	2.00	0.42
1:C:348:ILE:HG12	1:C:402:ILE:HD12	2.00	0.42
1:A:994:GLY:O	1:A:997:SER:HB2	2.19	0.42
1:A:1036:LYS:HE3	1:A:1036:LYS:HB2	1.86	0.42
1:C:434:SER:O	1:C:438:ILE:HG12	2.19	0.42
1:C:575:MET:HE2	1:C:666:PHE:HZ	1.84	0.42
1:A:401:ALA:O	1:A:405:LEU:HG	2.19	0.42
1:A:520:PHE:HZ	1:A:973:ARG:HB2	1.81	0.42
1:B:173:GLY:HA2	1:C:71:GLY:HA3	2.01	0.42
1:C:144:ASN:HA	1:C:320:GLY:O	2.20	0.42
1:C:444:GLY:HA2	1:C:891:LEU:CD2	2.49	0.42
1:A:28:LEU:HD22	3:A:1101:LMT:H5B	2.01	0.42
1:A:330:THR:HG22	1:A:331:PRO:HD3	2.01	0.42
1:A:188:MET:CE	1:A:773:VAL:CG1	2.97	0.42
1:A:108:GLN:NE2	1:B:109:ASN:O	2.51	0.42
1:C:510:LYS:HD2	1:C:511:GLY:N	2.35	0.42
1:C:135:SER:OG	1:C:672:VAL:HB	2.19	0.42
1:C:673:GLU:N	1:C:673:GLU:OE2	2.51	0.42
1:A:314:GLU:N	1:A:315:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:CD1	1:A:405:LEU:HD11	2.49	0.42
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.42
1:A:330:THR:HG22	1:A:331:PRO:CD	2.50	0.42
1:A:33:ALA:O	1:A:391:ASN:HA	2.20	0.42
1:A:367:ILE:HB	1:A:368:PRO:CD	2.50	0.42
1:A:519:MET:O	1:A:522:LYS:HG3	2.19	0.42
1:B:546:LEU:HA	1:B:546:LEU:HD12	1.81	0.42
1:C:360:GLN:HB3	1:C:513:PHE:CE2	2.55	0.42
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.79	0.42
1:A:1019:ILE:HG22	1:A:1020:PHE:CD2	2.55	0.42
1:A:23:GLY:HA3	1:A:377:LEU:O	2.19	0.42
1:A:537:SER:C	1:A:539:GLY:H	2.22	0.42
1:C:240:LEU:HB2	1:C:246:PHE:CE2	2.55	0.42
1:C:366:LEU:HA	1:C:366:LEU:HD12	1.79	0.42
1:C:544:LEU:HD13	1:C:544:LEU:HA	1.75	0.42
1:C:754:TRP:CE2	1:C:786:ILE:HD13	2.54	0.42
1:A:146:ASP:O	1:A:148:THR:HG23	2.20	0.42
1:A:668:LEU:HD12	1:A:668:LEU:HA	1.89	0.42
1:B:919:ARG:HH11	1:B:1005:THR:CG2	2.32	0.42
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.55	0.42
1:C:447:MET:HE3	1:C:891:LEU:HD22	2.01	0.42
1:C:537:SER:HB3	3:C:1101:LMT:O6B	2.20	0.42
1:C:575:MET:HE1	1:C:617:PHE:CD2	2.54	0.42
2:E:92:HIS:O	2:E:96:VAL:HG23	2.19	0.42
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.35	0.41
1:C:319:SER:HA	5:C:1385:HOH:O	2.18	0.41
1:C:404:LEU:CD1	1:C:937:LEU:HD21	2.50	0.41
4:B:1103:MIY:C8	4:B:1103:MIY:HN72	2.50	0.41
1:B:509:LYS:O	1:B:514:GLY:HA3	2.20	0.41
1:B:573:MET:HB3	1:B:573:MET:HE2	1.74	0.41
2:D:58:GLY:HA2	2:D:95:ILE:CD1	2.51	0.41
2:E:105:ASP:HB3	2:E:108:ALA:HB2	2.02	0.41
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.21	0.41
1:C:370:ILE:C	1:C:373:PRO:HD2	2.40	0.41
1:B:559:LEU:HD12	1:B:560:PRO:HD2	2.01	0.41
1:B:971:ARG:HD3	5:B:1473:HOH:O	2.19	0.41
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.56	0.41
1:A:488:LEU:HG	1:A:492:LEU:HD22	2.02	0.41
1:A:575:MET:HE2	1:A:575:MET:HB2	1.89	0.41
1:A:976:LEU:HD23	1:A:976:LEU:HA	1.85	0.41
1:B:863:SER:O	1:B:867:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:117:LEU:HD11	2:D:129:VAL:HG13	2.02	0.41
1:A:1038:GLU:OE2	1:A:1039:ASP:HA	2.19	0.41
1:C:617:PHE:CE2	1:C:676:THR:HG21	2.55	0.41
1:A:388:PHE:HE2	1:A:472:ILE:HB	1.86	0.41
1:A:38:ILE:HD12	1:A:39:ALA:H	1.83	0.41
1:B:203:VAL:O	1:B:207:ILE:HG13	2.20	0.41
1:B:453:PHE:HZ	1:B:933:THR:HG22	1.86	0.41
1:B:84:SER:HB2	5:B:1404:HOH:O	2.21	0.41
2:E:75:ALA:O	2:E:83:PRO:HD3	2.21	0.41
1:A:1012:VAL:O	1:A:1016:VAL:HG22	2.20	0.41
1:A:307:ARG:NH2	1:A:330:THR:HG21	2.36	0.41
1:A:939:ALA:O	1:A:943:ILE:HG13	2.21	0.41
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.90	0.41
1:B:637:ARG:N	1:B:638:PRO:HD3	2.36	0.41
1:A:360:GLN:HB3	1:A:513:PHE:CE2	2.55	0.41
1:A:405:LEU:CD2	1:A:481:SER:HB2	2.46	0.41
1:A:516:PHE:CA	1:A:519:MET:HG2	2.46	0.41
1:A:404:LEU:HD23	1:A:937:LEU:HD13	2.02	0.41
1:C:879:ILE:O	1:C:879:ILE:HD12	2.20	0.41
1:A:10:ILE:HD12	1:B:894:SER:CA	2.51	0.41
1:A:434:SER:O	1:A:438:ILE:HG12	2.20	0.41
1:A:907:LEU:HD13	1:A:1017:LEU:HB3	2.02	0.41
1:B:1:MET:HB3	1:B:2:PRO:CD	2.51	0.41
1:B:484:VAL:HG13	1:B:488:LEU:HB3	2.03	0.41
1:B:667:ASN:OD1	1:B:668:LEU:N	2.54	0.41
1:A:449:LEU:HD21	1:A:940:LYS:HB2	2.02	0.41
3:B:1102:LMT:H6D	3:B:1102:LMT:O2B	2.21	0.41
1:B:897:ILE:N	1:B:898:PRO:CD	2.84	0.41
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.56	0.41
1:C:873:ALA:HB3	1:C:874:PRO:HD3	2.02	0.41
1:C:973:ARG:HB3	1:C:974:PRO:HD3	2.02	0.41
1:A:1034:SER:O	1:A:1035:ARG:CB	2.69	0.40
1:A:509:LYS:HG3	1:A:510:LYS:H	1.85	0.40
1:C:302:THR:O	1:C:306:ILE:HG13	2.21	0.40
1:C:416:VAL:HG22	1:C:431:THR:HA	2.02	0.40
1:A:185:ARG:HD3	1:A:185:ARG:HA	1.77	0.40
1:A:284:GLN:HB2	1:A:285:PRO:CD	2.51	0.40
1:A:360:GLN:HB3	1:A:513:PHE:CD2	2.57	0.40
1:A:986:VAL:O	1:A:989:LEU:HB2	2.21	0.40
1:C:332:PHE:HA	1:C:335:ILE:HG22	2.02	0.40
1:C:903:LEU:O	1:C:906:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.87	0.40
1:A:530:SER:O	1:A:534:ILE:HG23	2.20	0.40
1:A:636:ASP:C	1:A:638:PRO:HD3	2.41	0.40
1:B:121:GLU:CD	1:B:121:GLU:H	2.25	0.40
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.21	0.40
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	2.04	0.40
1:A:1016:VAL:O	1:A:1019:ILE:HG22	2.22	0.40
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.51	0.40
1:B:510:LYS:CD	1:B:511:GLY:H	2.34	0.40
1:B:674:LEU:CD2	1:B:677:ALA:HB2	2.51	0.40
1:B:404:LEU:HD23	1:B:937:LEU:HD21	2.03	0.40
1:B:966:ASP:HB2	5:B:1207:HOH:O	2.21	0.40
1:C:395:MET:CA	1:C:395:MET:HE2	2.48	0.40
1:C:472:ILE:HG23	1:C:473:THR:N	2.36	0.40
2:E:89:HIS:CE1	2:E:119:LEU:HD22	2.56	0.40
2:E:40:VAL:HG23	2:E:71:ALA:HA	2.03	0.40
5:A:1375:HOH:O	1:C:214:VAL:HG21	2.21	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	1042/1057 (99%)	992 (95%)	38 (4%)	12 (1%)	13	14
1	B	1031/1057 (98%)	1007 (98%)	23 (2%)	1 (0%)	51	64
1	C	1031/1057 (98%)	1004 (97%)	26 (2%)	1 (0%)	51	64
2	D	154/169 (91%)	150 (97%)	4 (3%)	0	100	100
2	E	150/169 (89%)	145 (97%)	4 (3%)	1 (1%)	22	26
All	All	3408/3509 (97%)	3298 (97%)	95 (3%)	15 (0%)	34	42

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	522	LYS
1	A	523	SER
1	A	620	ARG
1	A	672	VAL
1	A	673	GLU
1	A	869	SER
1	A	1034	SER
1	B	659	LYS
1	A	1035	ARG
1	A	508	GLY
2	E	26	ARG
1	A	509	LYS
1	A	1039	ASP
1	C	36	PRO
1	A	873	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/863 (98%)	823 (97%)	27 (3%)	39	54
1	B	839/863 (97%)	807 (96%)	32 (4%)	33	47
1	C	839/863 (97%)	813 (97%)	26 (3%)	40	55
2	D	120/132 (91%)	119 (99%)	1 (1%)	81	91
2	E	117/132 (89%)	116 (99%)	1 (1%)	78	89
All	All	2765/2853 (97%)	2678 (97%)	87 (3%)	40	55

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	30	LEU
1	A	49	TYR

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Mol	Chain	Res	Type
1	A	60	THR
1	A	96	SER
1	A	270	LEU
1	A	330	THR
1	A	359	LEU
1	A	448	VAL
1	A	449	LEU
1	A	492	LEU
1	A	522	LYS
1	A	606	VAL
1	A	630	SER
1	A	660	ASP
1	A	673	GLU
1	A	687	GLN
1	A	714	THR
1	A	717	ARG
1	A	867	ARG
1	A	921	LEU
1	A	922	THR
1	A	948	PHE
1	A	971	ARG
1	A	1038	GLU
1	A	1039	ASP
1	A	1040	ILE
1	B	1	MET
1	B	11	PHE
1	B	30	LEU
1	B	48	SER
1	B	49	TYR
1	B	88	VAL
1	B	117	LEU
1	B	128	SER
1	B	172	VAL
1	B	230	LEU
1	B	274	ASN
1	B	324	VAL
1	B	336	SER
1	B	353	LEU
1	B	365	THR
1	B	396	PHE
1	B	546	LEU
1	B	558	ARG

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Mol	Chain	Res	Type
1	B	610	PHE
1	B	641	GLU
1	B	649	MET
1	B	653	ARG
1	B	660	ASP
1	B	714	THR
1	B	763	ILE
1	B	801	PHE
1	B	968	VAL
1	B	978	THR
1	B	992	SER
1	B	1007	VAL
1	B	1022	VAL
1	B	1030	ARG
1	C	11	PHE
1	C	14	VAL
1	C	49	TYR
1	C	87	THR
1	C	88	VAL
1	C	256	ASP
1	C	366	LEU
1	C	372	VAL
1	C	392	THR
1	C	404	LEU
1	C	407	ASN
1	C	448	VAL
1	C	472	ILE
1	C	482	VAL
1	C	540	ARG
1	C	620	ARG
1	C	641	GLU
1	C	676	THR
1	C	739	LEU
1	C	758	TYR
1	C	773	VAL
1	C	867	ARG
1	C	940	LYS
1	C	948	PHE
1	C	968	VAL
1	C	1030	ARG
2	D	61	GLU
2	E	31	ARG

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

Mol	Chain	Res	Type
1	A	415	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LMT	B	1102	-	36,36,36	0.48	1 (2%)	47,47,47	1.21	5 (10%)
3	LMT	A	1102	-	36,36,36	0.47	0	47,47,47	0.83	1 (2%)
3	LMT	C	1101	-	36,36,36	0.45	0	47,47,47	0.99	1 (2%)
3	LMT	A	1101	-	36,36,36	0.46	1 (2%)	47,47,47	0.84	1 (2%)
3	LMT	B	1101	-	36,36,36	0.44	0	47,47,47	0.96	1 (2%)
4	MIY	B	1103	-	35,36,36	1.93	12 (34%)	41,58,58	2.72	17 (41%)

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	1102	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	7/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	5/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	9/21/61/61	0/2/2/2
4	MIY	B	1103	-	-	3/12/70/70	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	MIY	C11-C10	3.74	1.45	1.39
4	B	1103	MIY	C71-N7	3.60	1.53	1.45
4	B	1103	MIY	CN7-N7	3.01	1.52	1.45
4	B	1103	MIY	C4-N1	3.01	1.54	1.47
4	B	1103	MIY	C14-C13	-2.99	1.36	1.41
4	B	1103	MIY	C21-N2	2.70	1.40	1.33
4	B	1103	MIY	C7-C16	-2.69	1.48	1.51
4	B	1103	MIY	O4-C13	2.61	1.41	1.36
4	B	1103	MIY	C18-C17	2.58	1.54	1.52
4	B	1103	MIY	O7-C18	2.50	1.45	1.42
4	B	1103	MIY	C6-C5	2.40	1.57	1.53
4	B	1103	MIY	C18-C1	-2.34	1.52	1.55
3	A	1101	LMT	O1'-C1'	2.03	1.43	1.40
3	B	1102	LMT	O1'-C1'	2.01	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	MIY	C1-C18-C17	7.59	118.78	109.88
4	B	1103	MIY	C11-C12-C13	-6.50	113.82	120.50
4	B	1103	MIY	C15-C16-C17	6.00	123.55	118.80
4	B	1103	MIY	C12-C13-C14	5.30	126.98	120.17
4	B	1103	MIY	O7-C18-C17	-3.83	104.02	110.14
4	B	1103	MIY	O6-C17-C16	-3.66	118.89	123.90
4	B	1103	MIY	O5-C15-C14	-3.64	115.10	121.99
4	B	1103	MIY	C11-C10-N7	-3.55	116.57	121.59
3	C	1101	LMT	C4B-C3B-C2B	-3.42	104.85	110.82
3	B	1102	LMT	O5B-C1B-C2B	3.37	117.49	110.35
3	B	1102	LMT	C1B-C2B-C3B	3.32	116.91	110.00
4	B	1103	MIY	C9-C10-N7	3.16	122.77	118.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	LMT	C1B-O5B-C5B	3.12	119.81	113.69
4	B	1103	MIY	O2-C3-C2	-2.84	117.97	122.96
3	A	1101	LMT	O1'-C1'-C2'	2.74	112.58	108.30
4	B	1103	MIY	C71-N7-CN7	2.59	124.46	116.12
4	B	1103	MIY	C18-C17-C16	2.58	125.69	123.06
4	B	1103	MIY	C19-N1-C4	2.57	120.13	114.09
3	B	1102	LMT	O1B-C4'-C3'	2.51	113.94	107.28
3	B	1102	LMT	O1'-C1'-C2'	2.50	112.20	108.30
3	B	1101	LMT	C4B-C3B-C2B	-2.49	106.48	110.82
4	B	1103	MIY	O8-C21-N2	-2.43	117.20	122.88
3	A	1102	LMT	O1B-C4'-C3'	2.32	113.44	107.28
4	B	1103	MIY	C18-C1-C2	2.23	119.30	115.75
4	B	1103	MIY	CN7-N7-C10	2.10	121.68	115.17
4	B	1103	MIY	O4-C13-C12	-2.06	113.74	119.33

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	LMT	C2'-C1'-O1'-C1
3	B	1102	LMT	O5'-C1'-O1'-C1
3	B	1102	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C2'-C1'-O1'-C1
3	C	1101	LMT	O5'-C1'-O1'-C1
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	O5'-C1'-O1'-C1
3	B	1102	LMT	C3'-C4'-O1B-C1B
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	B	1101	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	B	1101	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C6-C7-C8-C9
3	B	1101	LMT	O1'-C1-C2-C3
3	B	1101	LMT	C2'-C1'-O1'-C1
3	A	1101	LMT	C3-C4-C5-C6
3	A	1101	LMT	C4-C5-C6-C7
3	B	1101	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	C1-C2-C3-C4
3	A	1101	LMT	C7-C8-C9-C10
3	C	1101	LMT	C1-C2-C3-C4
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	C5-C6-C7-C8
3	B	1102	LMT	C2-C3-C4-C5
3	A	1101	LMT	O1'-C1-C2-C3
3	B	1101	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	C4-C5-C6-C7
3	B	1101	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C1-C2-C3-C4
4	B	1103	MIY	C3-C2-C21-N2
4	B	1103	MIY	C3-C2-C21-O8
4	B	1103	MIY	C1-C2-C21-N2
3	A	1102	LMT	C5'-C4'-O1B-C1B
3	A	1102	LMT	C3'-C4'-O1B-C1B
3	B	1102	LMT	C1-C2-C3-C4
3	B	1102	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C2-C3-C4-C5
3	A	1102	LMT	C4-C5-C6-C7
3	A	1101	LMT	C11-C10-C9-C8

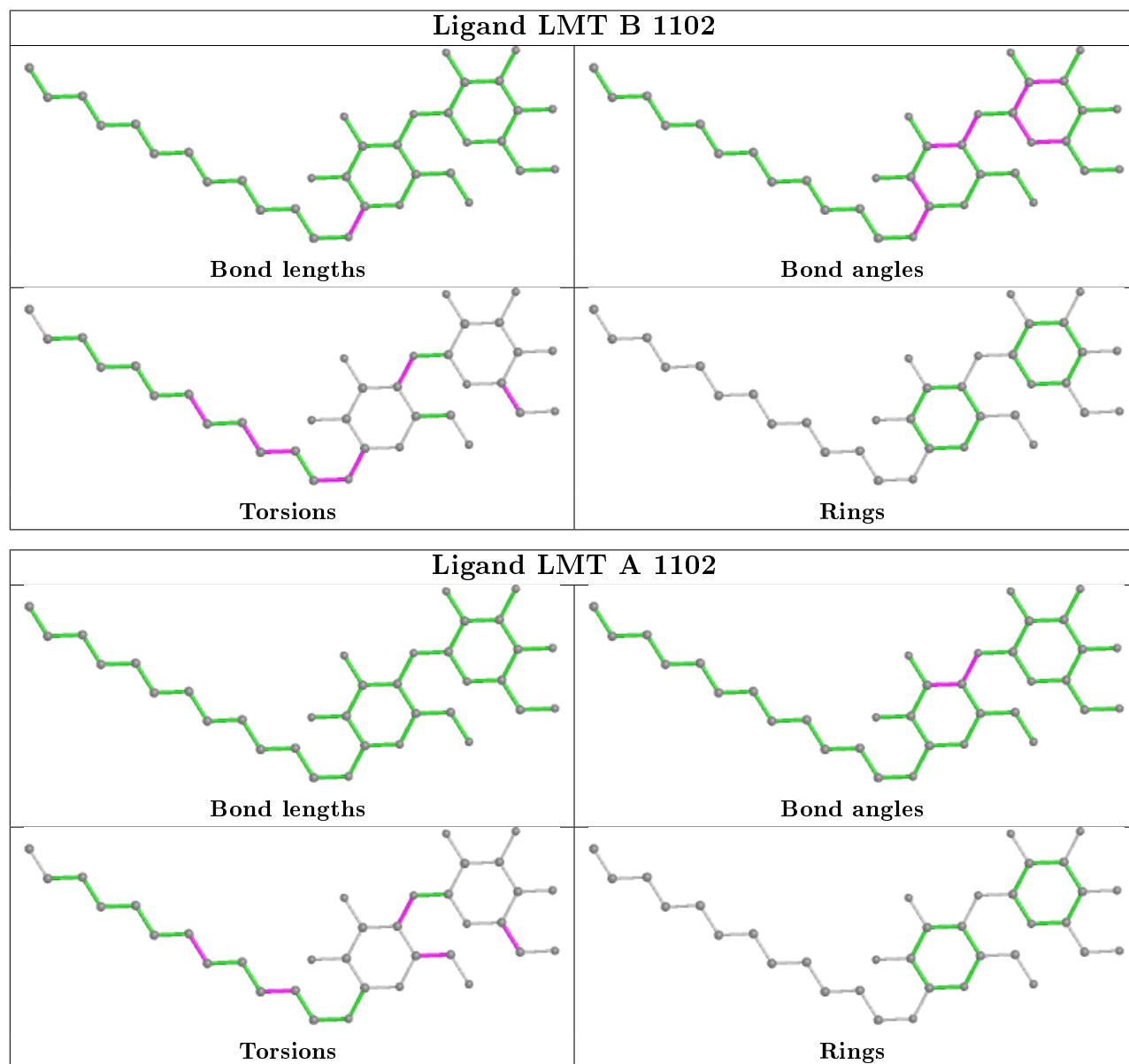
There are no ring outliers.

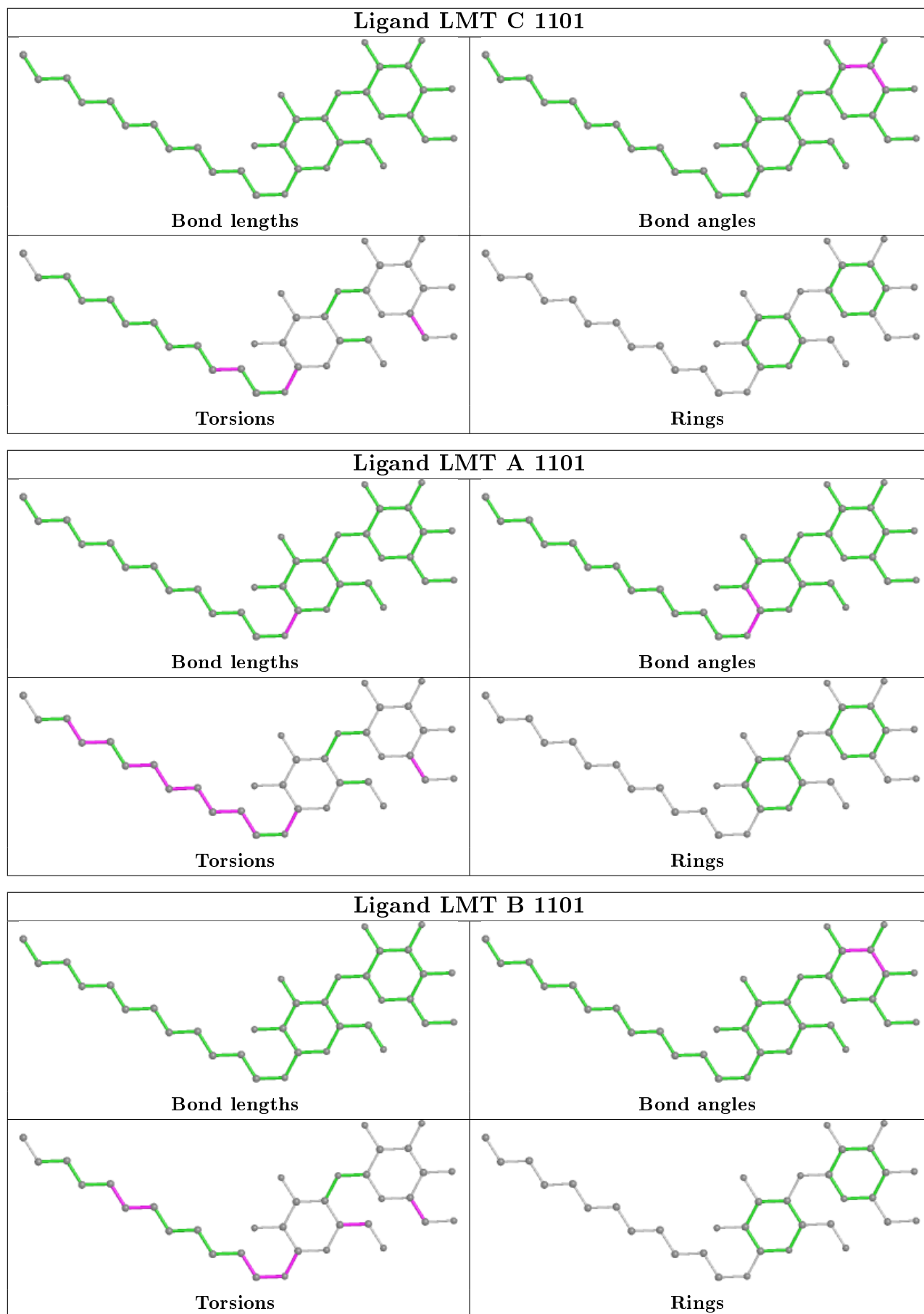
6 monomers are involved in 21 short contacts:

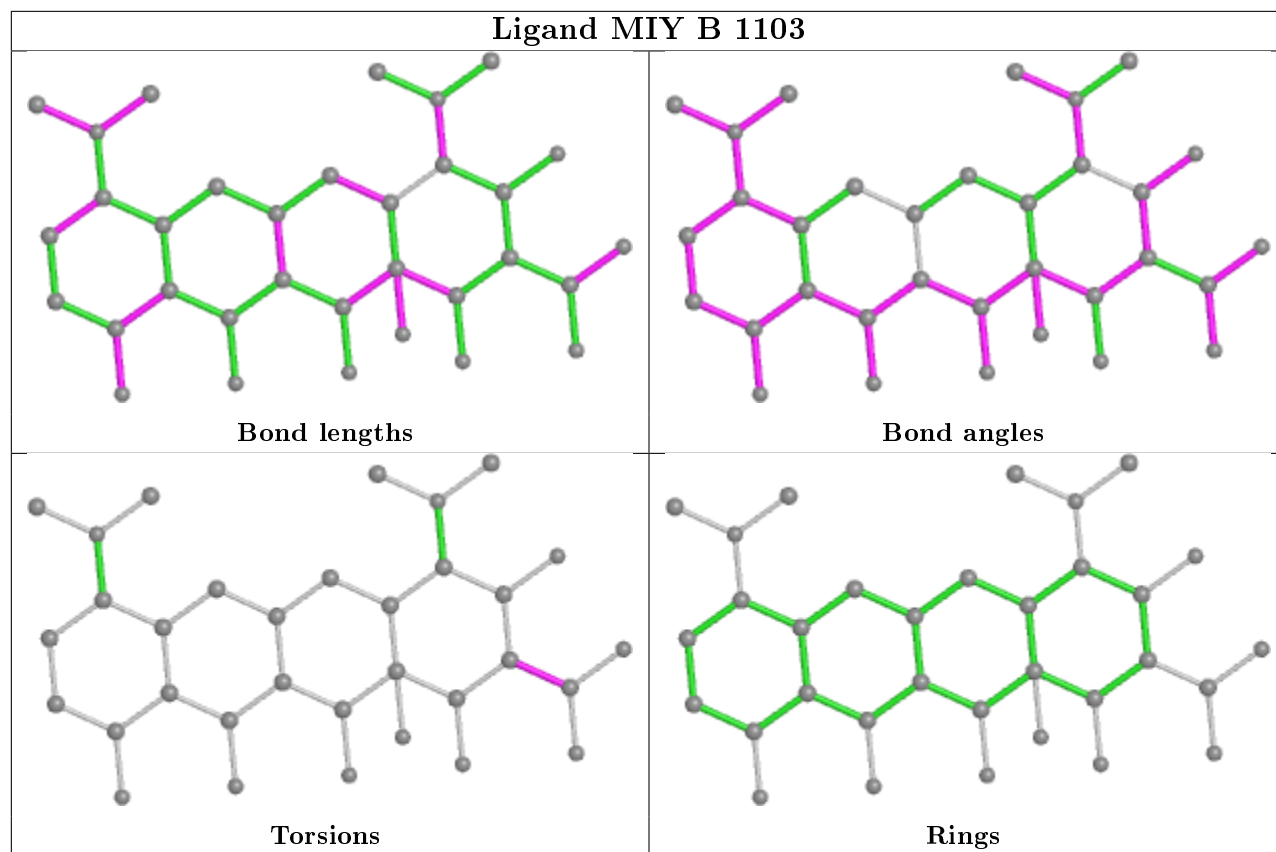
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1102	LMT	5	0
3	A	1102	LMT	5	0
3	C	1101	LMT	3	0
3	A	1101	LMT	3	0
3	B	1101	LMT	3	0
4	B	1103	MIY	2	0

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	1044/1057 (98%)	0.25	103 (9%) 7 10	23, 51, 115, 155	0
1	B	1033/1057 (97%)	-0.11	28 (2%) 54 62	24, 48, 71, 109	0
1	C	1033/1057 (97%)	-0.15	16 (1%) 73 79	24, 43, 71, 111	0
2	D	156/169 (92%)	-0.19	5 (3%) 47 54	40, 48, 74, 110	0
2	E	152/169 (89%)	0.94	30 (19%) 1 1	49, 66, 95, 120	0
All	All	3418/3509 (97%)	0.03	182 (5%) 26 33	23, 48, 92, 155	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	678	THR	10.6
1	A	870	GLY	7.9
1	A	511	GLY	7.7
1	A	677	ALA	7.7
1	A	421	ALA	6.6
2	E	66	LEU	6.6
1	A	510	LYS	6.5
1	A	501	ALA	6.3
1	A	618	ALA	6.2
1	A	512	PHE	6.0
1	A	514	GLY	6.0
1	A	518	ARG	5.9
1	A	515	TRP	5.9
1	A	869	SER	5.8
1	A	540	ARG	5.8
1	A	459	PHE	5.7
2	E	31	ARG	5.6
2	E	68	LYS	5.6
2	D	11	GLY	5.5
1	C	362	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	506	GLY	5.4
1	A	1034	SER	5.4
2	E	33	LEU	5.4
1	A	1037	ASN	5.1
1	A	871	ASN	4.9
1	A	1035	ARG	4.9
1	A	513	PHE	4.8
1	A	508	GLY	4.8
1	A	503	GLY	4.8
1	B	509	LYS	4.7
1	A	505	HIS	4.7
1	A	509	LYS	4.7
1	A	500	ILE	4.7
1	C	513	PHE	4.7
1	A	536	ARG	4.6
1	A	422	GLU	4.6
2	E	63	VAL	4.6
1	A	425	LEU	4.6
1	A	558	ARG	4.5
1	A	1036	LYS	4.5
2	E	67	LEU	4.5
1	A	1038	GLU	4.5
1	A	424	GLY	4.3
1	A	433	LYS	4.3
1	A	517	ASN	4.1
1	A	519	MET	4.1
1	C	510	LYS	4.1
1	A	541	TYR	4.1
1	A	543	VAL	4.0
2	E	62	ILE	4.0
1	A	674	LEU	4.0
1	A	554	TYR	4.0
1	A	529	ASP	3.9
2	E	65	VAL	3.8
1	A	507	GLU	3.8
1	A	462	SER	3.8
2	E	64	GLU	3.8
1	A	1042	HIS	3.7
1	A	521	GLU	3.7
1	A	520	PHE	3.7
1	A	38	ILE	3.7
1	B	603	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	547	ILE	3.6
1	A	362	PHE	3.6
1	A	1041	GLU	3.6
2	E	35	ALA	3.6
1	A	502	LYS	3.6
1	A	498	LYS	3.6
1	A	504	ASP	3.5
2	E	27	ASP	3.5
1	B	501	ALA	3.5
1	C	955	LYS	3.5
2	E	32	ILE	3.4
2	E	100	LEU	3.4
1	A	675	GLY	3.3
1	A	868	LEU	3.3
1	A	619	GLY	3.3
1	A	617	PHE	3.2
1	A	952	LEU	3.2
2	E	34	MET	3.2
1	B	641	GLU	3.2
2	E	99	LEU	3.2
1	B	510	LYS	3.2
1	A	430	ALA	3.2
1	C	512	PHE	3.2
2	E	61	GLU	3.1
1	B	513	PHE	3.1
1	C	811	TYR	3.1
1	A	867	ARG	3.1
1	A	4	PHE	3.1
2	E	97	GLU	3.1
2	E	60	LEU	3.1
1	A	539	GLY	3.1
1	B	511	GLY	3.1
1	A	526	HIS	3.1
1	A	499	PRO	3.1
1	A	961	ILE	3.1
1	B	558	ARG	3.0
1	B	255	GLN	3.0
1	A	1044	HIS	3.0
1	A	948	PHE	3.0
2	D	12	SER	3.0
1	A	428	LYS	3.0
2	E	28	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	523	SER	3.0
1	C	503	GLY	3.0
1	B	674	LEU	3.0
1	A	525	HIS	2.9
1	A	423	GLU	2.9
1	A	432	ARG	2.9
1	A	496	MET	2.9
1	C	501	ALA	2.8
1	A	1043	SER	2.8
2	E	30	VAL	2.8
1	A	834	GLY	2.8
1	B	557	VAL	2.7
2	E	70	GLY	2.7
1	A	532	GLY	2.7
2	E	101	LYS	2.7
1	A	872	GLN	2.7
1	B	257	GLY	2.7
1	B	508	GLY	2.7
2	E	71	ALA	2.6
1	A	494	ALA	2.6
1	B	600	THR	2.6
1	A	426	PRO	2.6
1	B	458	PHE	2.6
2	E	139	VAL	2.6
1	B	653	ARG	2.6
1	B	554	TYR	2.6
1	A	522	LYS	2.6
1	A	965	LEU	2.5
1	B	601	LYS	2.5
1	B	834	GLY	2.5
1	A	873	ALA	2.5
1	A	835	LYS	2.5
2	E	165	LEU	2.5
1	C	511	GLY	2.4
1	A	712	MET	2.4
1	A	1040	ILE	2.4
1	C	500	ILE	2.4
1	B	515	TRP	2.4
1	B	640	GLU	2.4
1	A	516	PHE	2.4
1	C	255	GLN	2.4
2	E	51	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	427	PRO	2.4
1	A	528	THR	2.3
1	A	535	LEU	2.3
1	A	429	GLU	2.3
1	A	874	PRO	2.2
1	A	671	ILE	2.2
1	C	425	LEU	2.2
1	A	255	GLN	2.2
2	E	37	GLY	2.2
1	B	599	LEU	2.2
2	E	93	LEU	2.2
1	A	420	MET	2.2
1	A	419	VAL	2.2
1	A	542	LEU	2.2
1	A	1039	ASP	2.2
1	B	561	SER	2.2
1	B	635	ALA	2.1
2	D	141	ALA	2.1
2	D	150	PHE	2.1
1	C	659	LYS	2.1
2	E	95	ILE	2.1
1	C	496	MET	2.1
1	A	431	THR	2.1
1	A	356	TYR	2.1
1	A	534	ILE	2.1
2	E	126	LEU	2.1
1	A	1031	ARG	2.1
1	B	604	ASN	2.1
1	C	363	ARG	2.1
1	B	560	PRO	2.1
1	B	642	ASN	2.0
1	A	866	GLU	2.0
1	B	461	GLY	2.0
1	A	557	VAL	2.0
2	D	139	VAL	2.0
1	C	918	PHE	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](#)

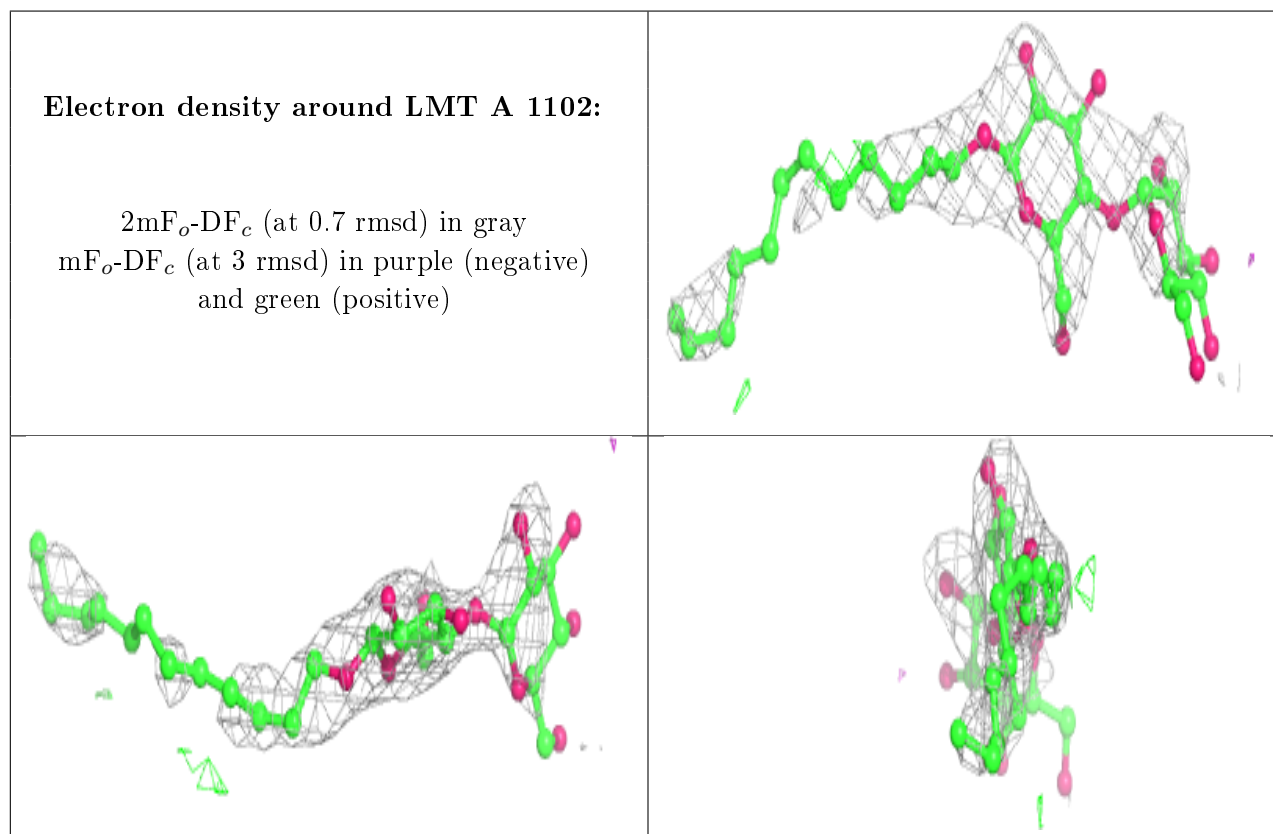
There are no carbohydrates in this entry.

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.

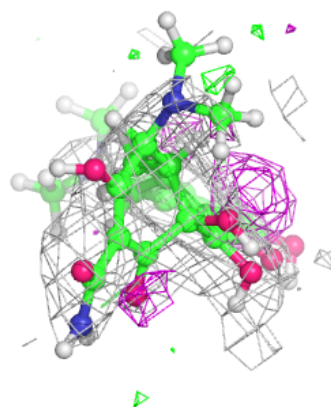
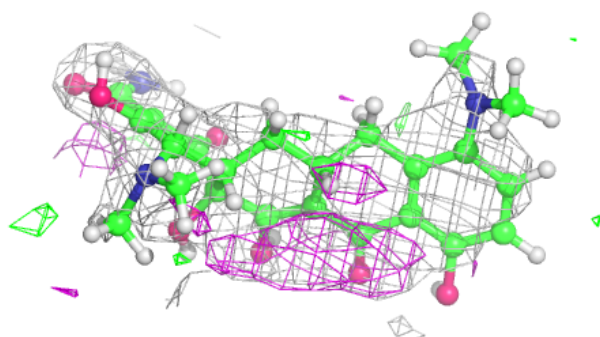
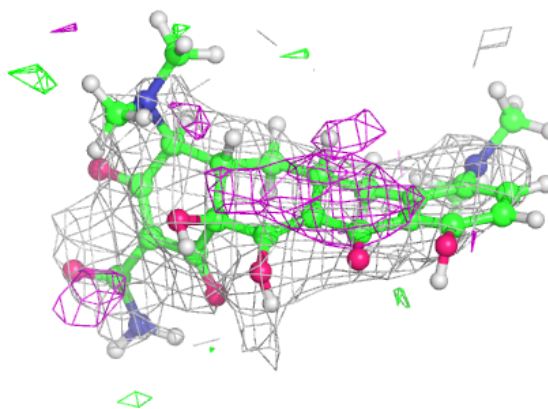
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	LMT	A	1102	35/35	0.77	0.38	83,104,125,130	0
4	MIY	B	1103	33/33	0.84	0.21	64,89,104,135	0
3	LMT	B	1102	35/35	0.89	0.24	56,93,106,106	0
3	LMT	B	1101	35/35	0.91	0.20	49,70,86,88	0
3	LMT	C	1101	35/35	0.94	0.14	52,64,80,81	0
3	LMT	A	1101	35/35	0.94	0.16	45,65,90,96	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.

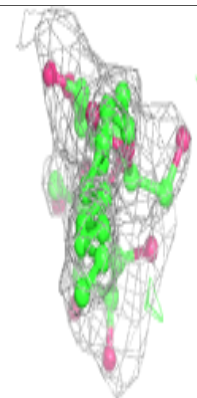
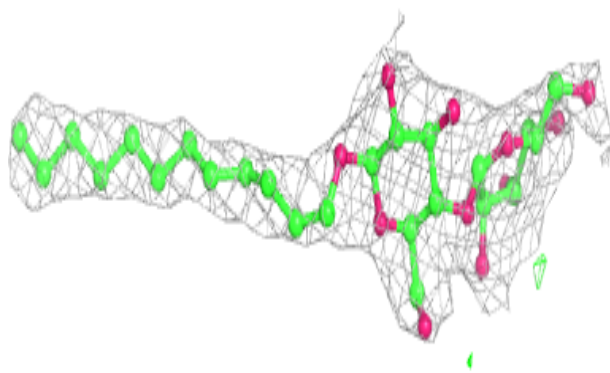
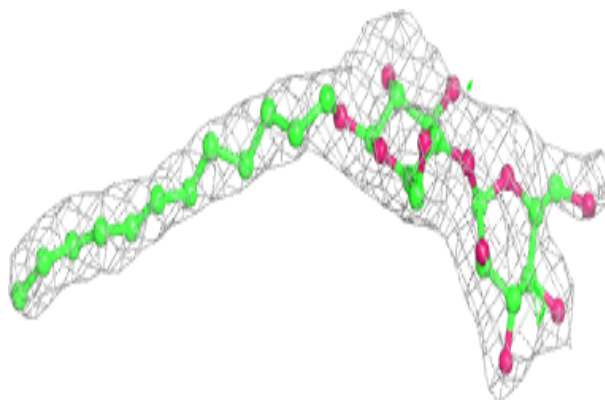


Electron density around MIY B 1103:

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

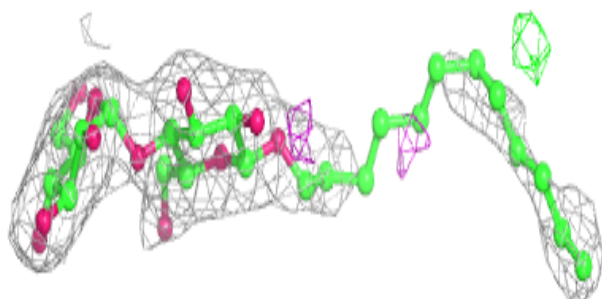
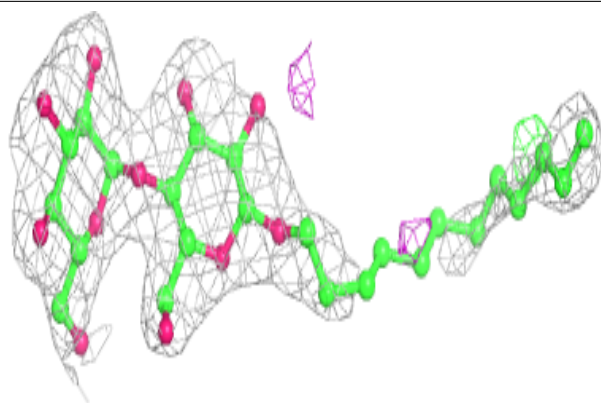
**Electron density around LMT B 1102:**

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

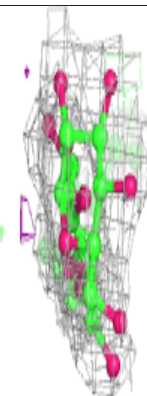
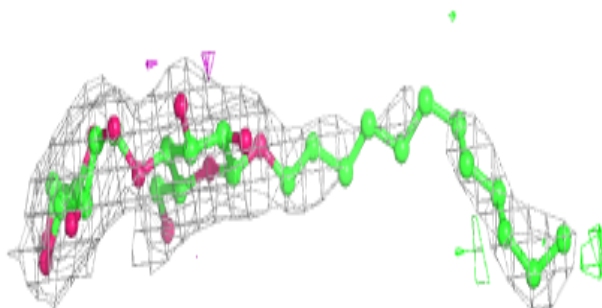
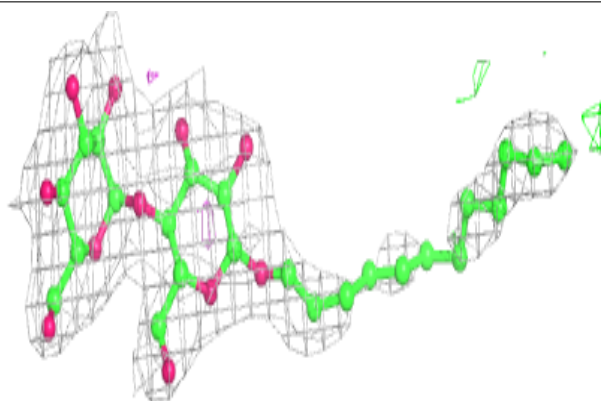


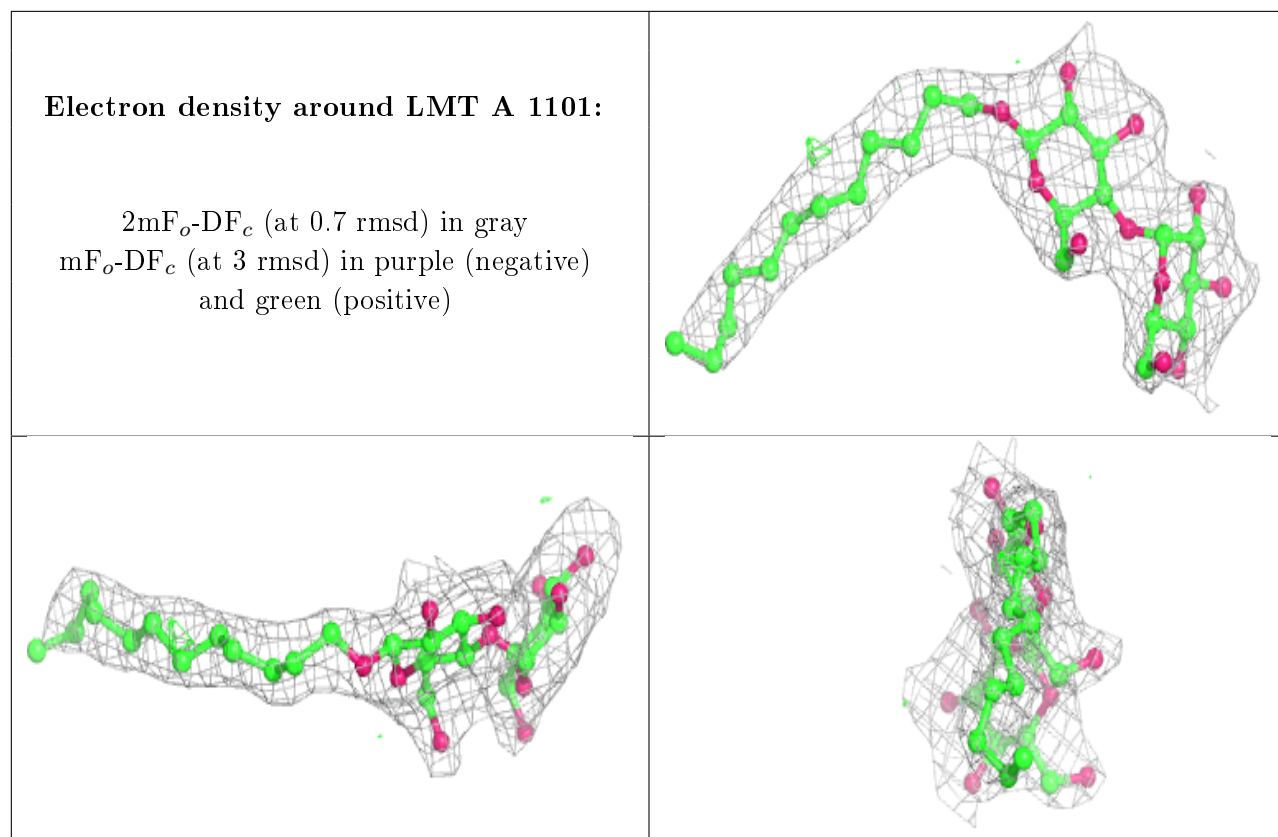
Electron density around LMT B 1101:

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

**Electron density around LMT C 1101:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.