



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 4DX7 / pdb_00004dx7
Title : Transport of drugs by the multidrug transporter AcrB involves an access and a deep binding pocket that are separated by a switch-loop
Authors : Eicher, T.; Cha, H.; Seeger, M.A.; Brandstaetter, L.; El-Delik, J.; Bohnert, J.A.; Kern, W.V.; Verrey, F.; Gruetter, M.G.; Diederichs, K.; Pos, K.M.
Deposited on : 2012-02-27
Resolution : 2.25 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:

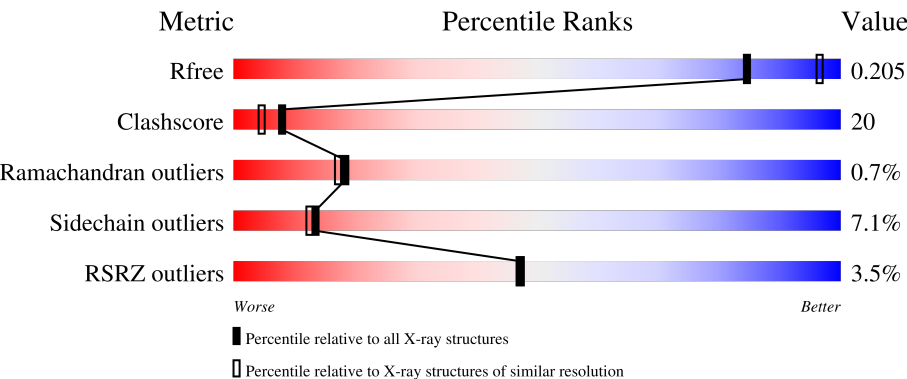
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

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

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	1057	5% 66% 27% 6% .
1	B	1057	3% 73% 20% . .
1	C	1057	3% 76% 19% . .
2	D	169	2% 72% 17% . . 8%

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Mol	Chain	Length	Quality of chain
2	E	169	

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	DM2	A	1105	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28467 atoms, of which 273 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1042	Total	C	N	O	S	0	0	0
			7927	5097	1311	1475	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1036	Total	C	N	O	S	0	0	0
			7875	5067	1302	1462	44			

There are 24 discrepancies between the modelled and reference sequences:

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

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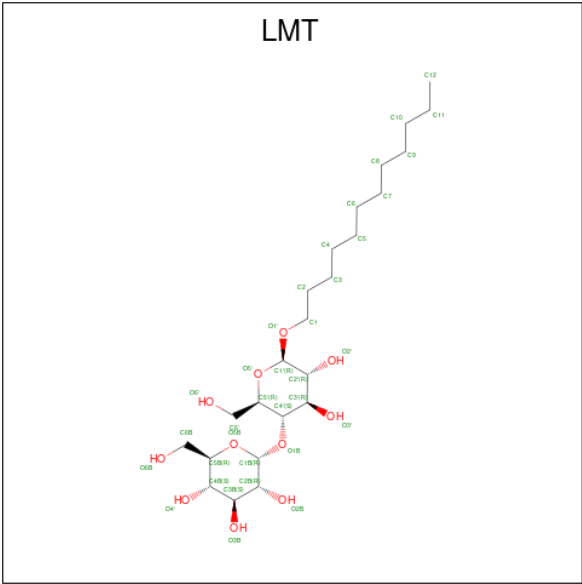
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

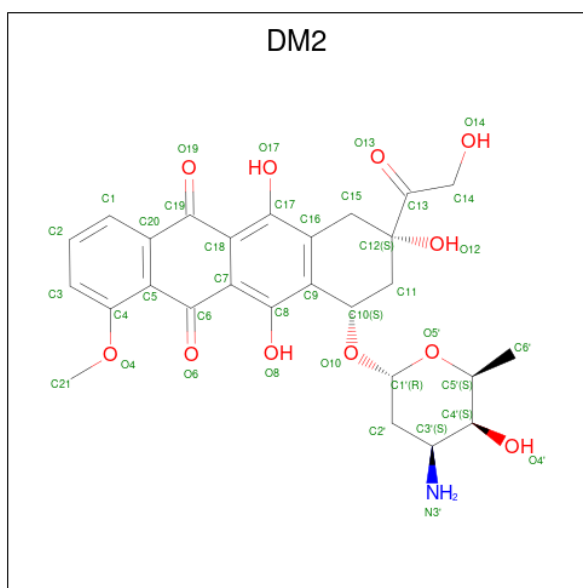
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

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



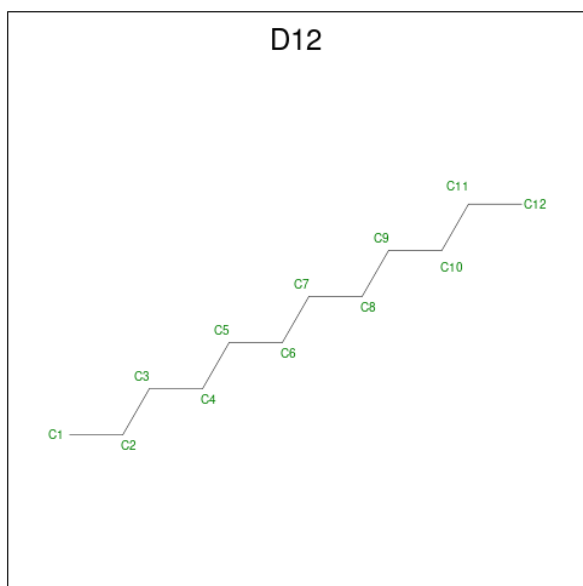
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	B	1	Total	C	O	0	0
			35	24	11		
3	C	1	Total	C	O	0	0
			35	24	11		

- Molecule 4 is DOXORUBICIN (CCD ID: DM2) (formula: $C_{27}H_{29}NO_{11}$).



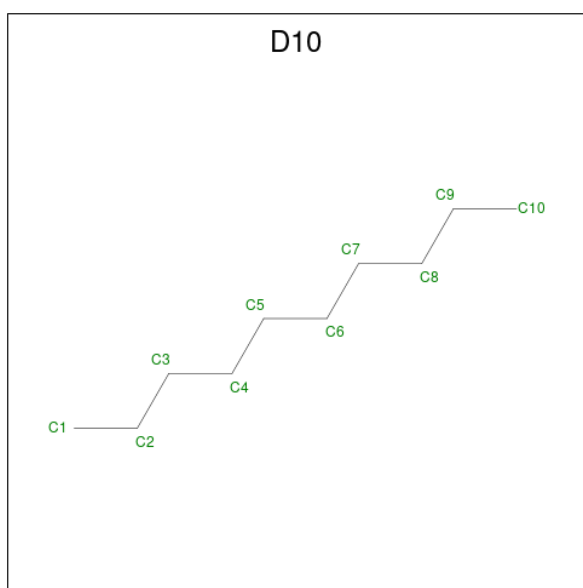
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O		0	0
			39	27	1	11			
4	A	1	Total	C	H	N	O	0	0
			68	27	29	1	11		
4	B	1	Total	C	N	O		0	0
			39	27	1	11			

- Molecule 5 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



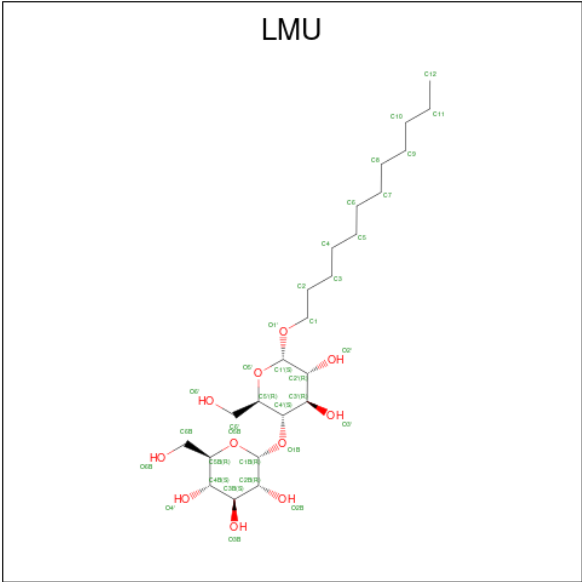
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	H	0	0
			38	12	26		
5	B	1	Total	C	H	0	0
			38	12	26		
5	C	1	Total	C	H	0	0
			38	12	26		
5	C	1	Total	C	H	0	0
			38	12	26		

- Molecule 6 is DECANE (CCD ID: D10) (formula: $C_{10}H_{22}$).



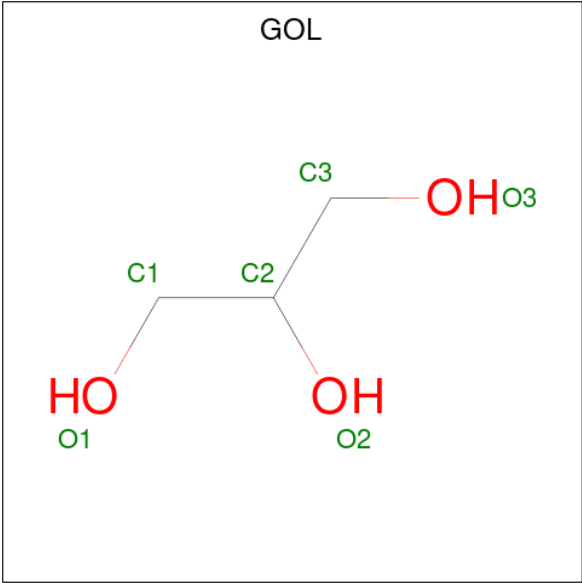
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	0	0
			32	10	22		
6	A	1	Total	C	H	0	0
			32	10	22		
6	B	1	Total	C	H	0	0
			32	10	22		
6	C	1	Total	C	H	0	0
			32	10	22		

- Molecule 7 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



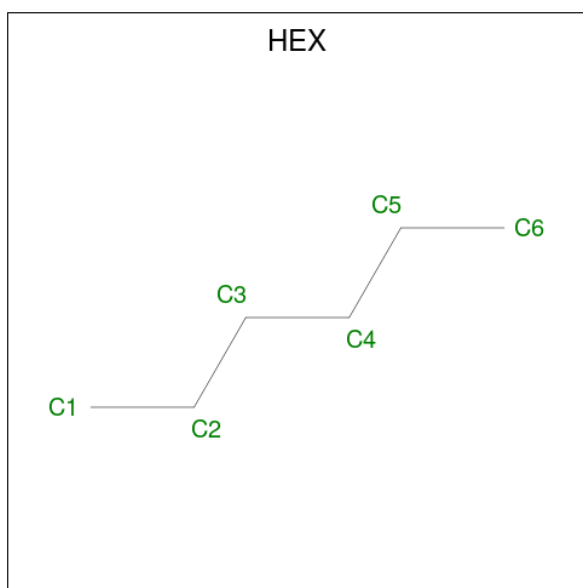
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			35	24	11		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	B	1	Total	C	H	O	0	0
			14	3	8	3		
8	C	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 9 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).

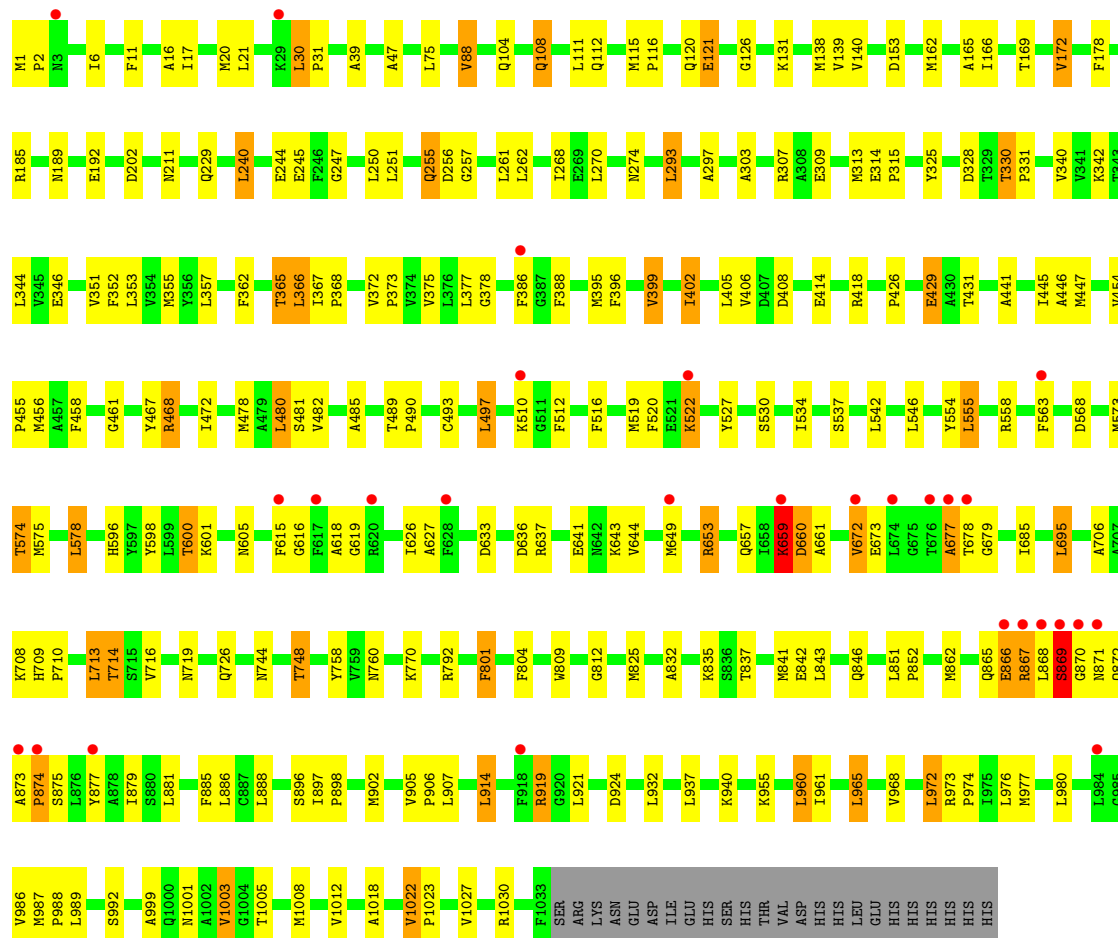
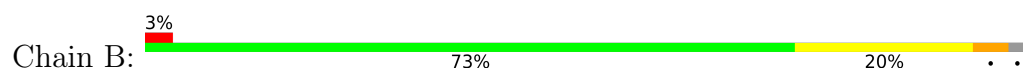


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	H	0	0
			20	6	14		
9	C	1	Total	C	H	0	0
			20	6	14		

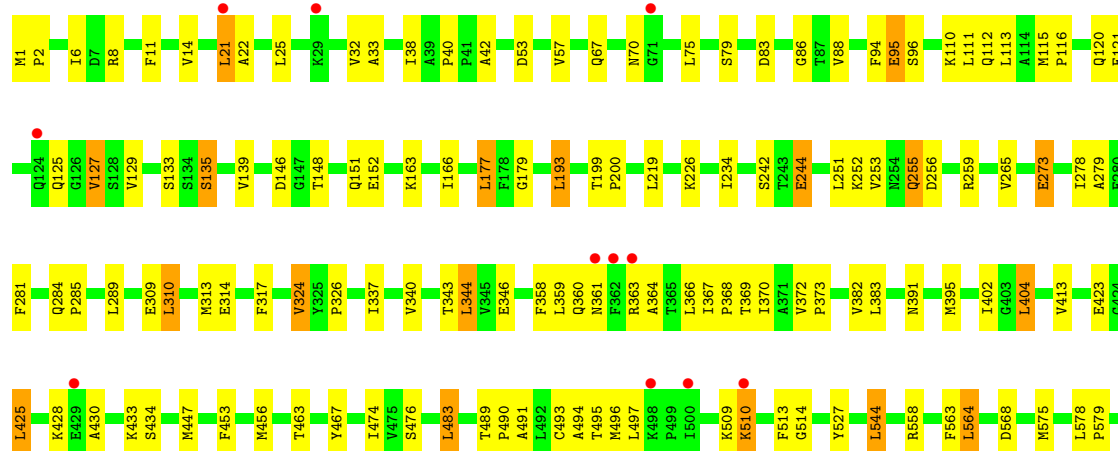
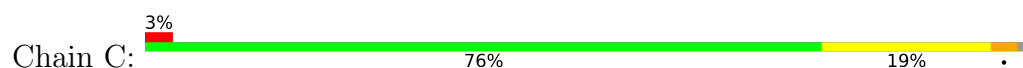
- Molecule 10 is water.

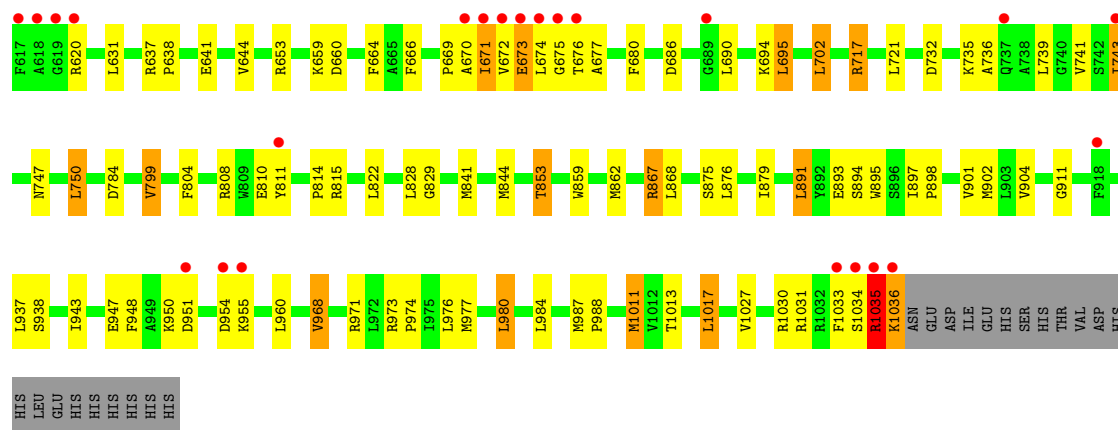
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	497	Total	O	0	0
			497	497		
10	B	494	Total	O	0	0
			494	494		
10	C	572	Total	O	0	0
			572	572		
10	D	81	Total	O	0	0
			81	81		
10	E	56	Total	O	0	0
			56	56		

• Molecule 1: Acriflavine resistance protein B

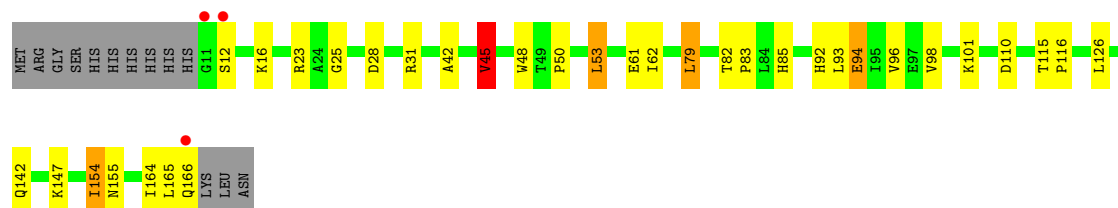
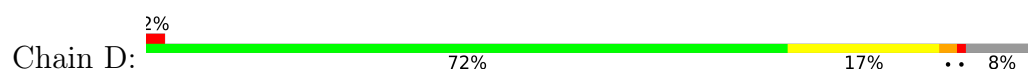


• Molecule 1: Acriflavine resistance protein B

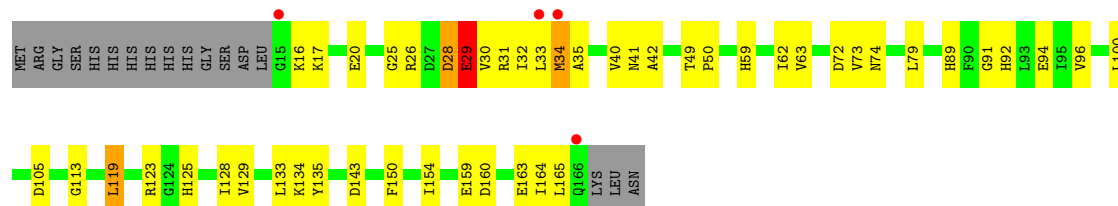




• Molecule 2: DARPIN



• 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	145.94Å 163.28Å 245.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 2.25 49.09 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.09-2.25) 99.6 (49.09-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.185 , 0.227 (Not available) , 0.205	Depositor DCC
R_{free} test set	13724 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28467	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: D10, LMU, LMT, DM2, HEX, D12, GOL

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	0.44	0/8078	0.80	3/10968 (0.0%)
1	B	0.45	0/7999	0.80	2/10863 (0.0%)
1	C	0.47	0/8025	0.80	1/10896 (0.0%)
2	D	0.42	0/1196	0.73	1/1626 (0.1%)
2	E	0.39	0/1170	0.70	0/1591
All	All	0.45	0/26468	0.79	7/35944 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	VAL	CB-CA-C	-5.98	101.29	110.50
1	B	677	ALA	N-CA-C	-5.60	103.13	110.53
1	B	685	ILE	N-CA-C	5.39	115.89	108.12
1	A	426	PRO	CA-C-N	5.34	124.79	119.24
1	A	426	PRO	C-N-CA	5.34	124.79	119.24
1	C	273	GLU	N-CA-C	-5.23	105.58	111.28
2	D	45	VAL	CB-CA-C	-5.16	105.17	112.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7927	0	8072	466	0
1	B	7849	0	8001	247	0
1	C	7875	0	8032	240	0
2	D	1177	0	1159	24	0
2	E	1151	0	1136	49	0
3	A	140	0	184	27	0
3	B	70	0	92	14	0
3	C	35	0	46	1	0
4	A	78	29	58	45	0
4	B	39	0	29	9	0
5	A	12	26	26	3	0
5	B	12	26	26	0	0
5	C	24	52	52	2	0
6	A	20	44	44	2	0
6	B	10	22	22	1	0
6	C	10	22	22	0	0
7	B	35	0	46	4	0
8	B	12	16	16	1	0
8	C	6	8	8	1	0
9	B	6	14	14	0	0
9	C	6	14	14	0	0
10	A	497	0	0	26	0
10	B	494	0	0	21	0
10	C	572	0	0	29	0
10	D	81	0	0	1	0
10	E	56	0	0	4	0
All	All	28194	273	27099	1051	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 20.

All (1051) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ARG:N	1:A:868:LEU:HB2	1.40	1.33
1:A:987:MET:HE1	1:A:1008:MET:SD	1.81	1.21
1:C:509:LYS:CA	1:C:510:LYS:HB2	1.72	1.20
1:A:146:ASP:HB2	10:A:1514:HOH:O	1.45	1.14
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.33	1.11
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.32	1.11
1:A:866:GLU:HG2	1:A:867:ARG:HA	1.21	1.11
1:A:617:PHE:HB2	4:A:1105:DM2:H142	1.15	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:GLU:OE2	1:C:673:GLU:N	1.84	1.09
1:A:671:ILE:O	1:A:674:LEU:HB2	1.54	1.08
1:A:867:ARG:N	1:A:868:LEU:CB	2.16	1.07
1:A:919:ARG:HG3	1:A:919:ARG:HH11	1.18	1.07
1:C:509:LYS:HA	1:C:510:LYS:HB2	1.10	1.07
1:B:414:GLU:HG3	1:B:977:MET:CE	1.87	1.05
1:A:867:ARG:H	1:A:868:LEU:CB	1.68	1.05
1:C:244:GLU:OE1	1:C:244:GLU:N	1.90	1.05
3:A:1103:LMT:O2B	3:A:1103:LMT:H3'	1.55	1.04
1:A:537:SER:HB2	1:A:540:ARG:HD3	1.39	1.03
1:A:866:GLU:OE2	1:A:866:GLU:N	1.90	1.03
1:A:987:MET:CE	1:A:987:MET:HA	1.88	1.03
4:A:1105:DM2:H2'2	4:A:1105:DM2:H6'3	1.41	1.03
1:A:1031:ARG:NH1	1:A:1038:GLU:OE1	1.91	1.02
1:A:866:GLU:C	1:A:868:LEU:HB2	1.83	1.02
1:A:355:MET:HE2	1:A:355:MET:HA	1.40	1.02
1:A:676:THR:HB	4:A:1105:DM2:C21	1.88	1.01
1:A:866:GLU:HG2	1:A:867:ARG:CA	1.89	1.01
1:C:70:ASN:O	1:C:110:LYS:NZ	1.95	1.00
1:B:987:MET:HG3	1:B:1008:MET:HE1	1.38	1.00
1:B:919:ARG:HG2	1:B:919:ARG:HH11	1.22	1.00
2:D:94:GLU:N	2:D:94:GLU:OE1	1.94	0.99
1:A:540:ARG:H	1:A:540:ARG:HD2	1.27	0.99
1:A:919:ARG:HH11	1:A:919:ARG:CG	1.74	0.99
1:C:527:TYR:CE2	1:C:968:VAL:HG13	1.99	0.98
1:B:748:THR:HG21	10:B:1536:HOH:O	1.62	0.98
1:A:672:VAL:HG22	1:A:673:GLU:H	1.28	0.97
1:A:987:MET:HA	1:A:987:MET:HE3	1.46	0.97
1:A:987:MET:HE2	1:A:990:VAL:HG21	1.45	0.97
1:A:1041:GLU:HG3	1:A:1042:HIS:H	1.27	0.96
1:A:507:GLU:HG2	1:A:518:ARG:HD2	1.45	0.96
1:C:671:ILE:HD11	1:C:674:LEU:CD1	1.96	0.95
1:B:447:MET:HE2	1:B:447:MET:HA	1.46	0.95
1:A:671:ILE:H	1:A:674:LEU:HD12	1.29	0.95
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.32	0.94
1:A:866:GLU:CG	1:A:867:ARG:HA	1.98	0.94
1:A:617:PHE:HB2	4:A:1105:DM2:C14	1.98	0.93
1:A:865:GLN:HA	1:A:866:GLU:C	1.92	0.93
1:A:676:THR:HB	4:A:1105:DM2:H211	1.50	0.92
1:C:509:LYS:HA	1:C:510:LYS:CB	1.99	0.92
1:A:1041:GLU:CG	1:A:1042:HIS:H	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.00	0.92
1:C:1011:MET:HE3	1:C:1011:MET:HA	1.48	0.92
2:E:31:ARG:NH2	10:E:204:HOH:O	2.03	0.91
1:A:966:ASP:O	1:A:970:MET:HG3	1.69	0.91
1:A:674:LEU:HB3	1:A:675:GLY:CA	1.99	0.91
1:A:867:ARG:H	1:A:868:LEU:CG	1.83	0.91
1:A:616:GLY:O	1:A:618:ALA:N	2.04	0.91
4:B:1104:DM2:H212	4:B:1104:DM2:O6	1.71	0.90
1:A:659:LYS:HD3	1:A:659:LYS:N	1.87	0.89
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.52	0.89
1:B:414:GLU:CG	1:B:977:MET:HE1	2.02	0.89
1:A:1041:GLU:HG3	1:A:1042:HIS:N	1.88	0.89
1:A:255:GLN:OE1	1:A:255:GLN:N	2.05	0.88
1:A:393:LEU:HD22	1:A:470:PHE:CE1	2.08	0.88
1:B:875:SER:HB3	3:B:1101:LMT:H6'2	1.54	0.88
1:C:671:ILE:HG23	1:C:862:MET:HE1	1.54	0.88
1:A:546:LEU:O	1:A:550:VAL:HG23	1.73	0.87
1:A:674:LEU:HB3	1:A:675:GLY:HA2	1.54	0.87
4:A:1105:DM2:O8	4:A:1105:DM2:H2'1	1.74	0.87
1:B:244:GLU:N	1:B:244:GLU:OE2	2.07	0.87
1:A:537:SER:CB	1:A:540:ARG:HD3	2.04	0.87
4:A:1106:DM2:N3'	10:A:1609:HOH:O	2.06	0.87
3:A:1103:LMT:H6'1	1:C:8:ARG:HH21	1.40	0.86
1:A:534:ILE:HG23	1:A:541:TYR:CZ	2.10	0.86
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.38	0.86
1:C:671:ILE:CD1	1:C:674:LEU:HG	2.06	0.86
1:C:53:ASP:O	1:C:57:VAL:HG23	1.74	0.86
1:B:660:ASP:N	10:B:1560:HOH:O	2.07	0.86
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.36	0.85
1:A:867:ARG:H	1:A:868:LEU:HB2	1.28	0.85
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.06	0.85
1:B:673:GLU:N	1:B:673:GLU:OE2	2.09	0.84
1:C:366:LEU:HD23	1:C:496:MET:HE1	1.55	0.84
1:A:586:ARG:NH2	1:A:660:ASP:HB2	1.91	0.84
1:A:659:LYS:HD3	1:A:659:LYS:H	1.42	0.84
1:A:672:VAL:CG2	1:A:673:GLU:N	2.39	0.84
1:B:527:TYR:OH	1:B:968:VAL:CG1	2.26	0.84
1:C:1:MET:N	10:C:1705:HOH:O	2.08	0.84
1:C:42:ALA:O	10:C:1274:HOH:O	1.96	0.84
1:A:507:GLU:HG2	1:A:518:ARG:CD	2.07	0.84
2:D:94:GLU:CD	2:D:94:GLU:H	1.84	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:672:VAL:CG2	1:A:673:GLU:H	1.91	0.83
3:B:1101:LMT:H22	3:B:1101:LMT:O2'	1.78	0.83
1:C:735:LYS:O	1:C:739:LEU:HD13	1.77	0.83
1:A:987:MET:HE2	1:A:990:VAL:CG2	2.08	0.83
1:A:1:MET:N	10:A:1259:HOH:O	2.08	0.83
1:A:713:LEU:HD22	1:A:843:LEU:HD23	1.60	0.82
2:E:31:ARG:HH11	2:E:31:ARG:HG2	1.44	0.82
1:A:674:LEU:CB	1:A:675:GLY:HA2	2.09	0.82
1:C:309:GLU:HG3	1:C:313:MET:CE	2.10	0.82
1:C:1011:MET:HA	1:C:1011:MET:CE	2.10	0.82
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.60	0.82
1:C:1033:PHE:O	1:C:1034:SER:OG	1.95	0.82
1:C:509:LYS:CB	1:C:510:LYS:HB2	2.09	0.81
1:A:987:MET:HE3	1:A:987:MET:CA	2.10	0.81
1:A:990:VAL:HG11	1:A:1008:MET:HE2	1.61	0.81
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.81	0.81
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.61	0.81
1:C:244:GLU:H	1:C:244:GLU:CD	1.89	0.81
1:C:671:ILE:H	1:C:862:MET:HE1	1.45	0.81
1:A:676:THR:HB	4:A:1105:DM2:H213	1.61	0.81
1:A:356:TYR:HA	1:A:365:THR:HG21	1.60	0.81
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.11	0.81
1:C:423:GLU:OE1	1:C:433:LYS:NZ	2.14	0.81
1:B:919:ARG:HH11	1:B:919:ARG:CG	1.92	0.80
1:C:255:GLN:HE21	1:C:256:ASP:N	1.78	0.80
1:C:702:LEU:HD11	1:C:844:MET:HE1	1.62	0.80
1:A:38:ILE:C	1:A:38:ILE:HD12	2.07	0.80
1:C:671:ILE:HD11	1:C:674:LEU:HG	1.62	0.80
1:A:717:ARG:HH12	4:A:1105:DM2:C1	1.95	0.79
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.13	0.79
1:B:527:TYR:CE2	1:B:968:VAL:HG12	2.18	0.79
1:A:862:MET:HE1	4:A:1105:DM2:C21	2.13	0.78
1:A:866:GLU:N	1:A:867:ARG:HB2	1.98	0.78
1:C:509:LYS:CA	1:C:510:LYS:CB	2.53	0.78
2:E:34:MET:HA	2:E:34:MET:CE	2.13	0.78
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.65	0.78
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.64	0.78
2:E:28:ASP:O	2:E:31:ARG:N	2.14	0.78
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.63	0.78
1:C:163:LYS:HE2	10:C:1769:HOH:O	1.83	0.78
1:A:527:TYR:OH	1:A:1019:ILE:O	2.01	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ASP:OD1	1:A:969:ARG:NH1	2.17	0.78
1:C:395:MET:HE2	1:C:395:MET:HA	1.66	0.78
1:A:815:ARG:NH1	10:A:1658:HOH:O	2.10	0.77
1:B:255:GLN:N	1:B:255:GLN:OE1	2.16	0.77
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.67	0.77
1:C:255:GLN:NE2	1:C:256:ASP:H	1.82	0.77
1:B:987:MET:HG3	1:B:1008:MET:CE	2.15	0.77
1:C:67:GLN:OE1	10:C:1665:HOH:O	2.02	0.77
2:E:16:LYS:NZ	2:E:20:GLU:OE1	2.16	0.77
1:A:57:VAL:CG1	1:A:88:VAL:CG2	2.63	0.77
1:A:866:GLU:HG2	1:A:867:ARG:CB	2.15	0.77
1:A:919:ARG:HG3	1:A:919:ARG:NH1	1.89	0.76
1:B:919:ARG:HD3	1:B:1005:THR:HG21	1.66	0.76
1:C:360:GLN:HG2	1:C:513:PHE:CD2	2.20	0.76
3:B:1102:LMT:H5B	3:B:1102:LMT:H6E	1.67	0.76
1:A:867:ARG:H	1:A:868:LEU:CD2	1.99	0.76
4:B:1104:DM2:H2'2	4:B:1104:DM2:H6'3	1.66	0.76
1:B:744:ASN:O	1:B:748:THR:HG23	1.85	0.75
1:B:16:ALA:O	1:B:20:MET:HG3	1.85	0.75
1:B:869:SER:OG	10:B:1483:HOH:O	2.04	0.75
1:A:867:ARG:O	1:A:867:ARG:HG2	1.84	0.75
1:C:255:GLN:HE21	1:C:256:ASP:H	1.31	0.75
1:A:717:ARG:HH22	4:A:1105:DM2:C2	2.00	0.75
3:A:1101:LMT:O4'	3:B:1101:LMT:H2B	1.87	0.75
1:A:507:GLU:CG	1:A:518:ARG:HD2	2.17	0.74
1:C:259:ARG:NH2	10:C:1499:HOH:O	2.17	0.74
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.68	0.74
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.67	0.74
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.69	0.74
1:A:537:SER:HB2	1:A:540:ARG:CD	2.15	0.74
1:C:146:ASP:OD2	1:C:148:THR:OG1	2.04	0.74
2:E:34:MET:HA	2:E:34:MET:HE3	1.70	0.74
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.70	0.74
4:A:1106:DM2:O4'	10:A:1564:HOH:O	2.05	0.74
1:A:456:MET:HG3	1:A:471:SER:OG	1.88	0.74
1:A:255:GLN:H	1:A:255:GLN:CD	1.94	0.74
1:A:875:SER:O	1:A:879:ILE:HG23	1.88	0.74
1:A:1012:VAL:O	1:A:1016:VAL:HG22	1.88	0.74
2:E:26:ARG:O	2:E:30:VAL:HG23	1.88	0.74
1:C:875:SER:O	1:C:879:ILE:HG22	1.87	0.73
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLN:NE2	1:C:279:ALA:O	2.21	0.73
1:A:862:MET:HE1	4:A:1105:DM2:H211	1.68	0.73
1:B:637:ARG:O	1:B:643:LYS:HE3	1.88	0.73
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.70	0.73
1:A:393:LEU:HD22	1:A:470:PHE:HE1	1.53	0.73
1:A:467:TYR:OH	1:A:928:GLN:OE1	2.06	0.73
1:A:563:PHE:O	1:A:924:ASP:HB2	1.88	0.73
1:A:942:ALA:O	1:A:946:VAL:HG13	1.87	0.73
1:C:259:ARG:NH2	10:C:1489:HOH:O	1.82	0.73
1:A:659:LYS:H	1:A:659:LYS:CD	1.99	0.72
1:C:671:ILE:O	1:C:671:ILE:HG13	1.87	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.89	0.72
1:A:987:MET:HE1	1:A:1008:MET:CE	2.18	0.72
1:B:527:TYR:HE2	1:B:968:VAL:HG12	1.53	0.72
1:A:717:ARG:NH1	4:A:1105:DM2:C1	2.52	0.72
1:C:867:ARG:HG2	1:C:867:ARG:NH1	2.04	0.72
1:B:554:TYR:CE1	1:B:558:ARG:NE	2.55	0.72
3:B:1102:LMT:H5B	3:B:1102:LMT:C6'	2.19	0.72
1:A:1031:ARG:HH12	1:A:1038:GLU:CD	1.97	0.72
1:C:273:GLU:O	8:C:1103:GOL:O2	2.07	0.72
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.90	0.72
1:A:717:ARG:NH1	4:A:1105:DM2:H1	2.04	0.71
1:A:987:MET:HA	1:A:987:MET:HE2	1.71	0.71
1:C:815:ARG:NH2	10:C:1596:HOH:O	2.14	0.71
1:A:1035:ARG:C	1:A:1036:LYS:HD3	2.15	0.71
1:C:671:ILE:N	1:C:862:MET:HE1	2.05	0.71
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.71	0.71
1:C:135:SER:HB3	1:C:672:VAL:O	1.89	0.71
1:A:356:TYR:HA	1:A:365:THR:CG2	2.20	0.71
1:A:797:GLN:OE1	10:A:1570:HOH:O	2.08	0.70
1:C:346:GLU:OE1	10:C:1581:HOH:O	2.09	0.70
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.15	0.70
1:A:709:HIS:N	1:A:710:PRO:HD3	2.06	0.70
2:E:150:PHE:CZ	2:E:154:ILE:HD11	2.27	0.70
1:C:21:LEU:HD12	1:C:22:ALA:N	2.07	0.70
1:A:617:PHE:CB	4:A:1105:DM2:H142	2.09	0.69
1:A:928:GLN:HE21	3:A:1102:LMT:H22	1.57	0.69
1:B:153:ASP:OD1	10:B:1674:HOH:O	2.10	0.69
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.73	0.69
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.73	0.69
1:B:677:ALA:O	1:B:678:THR:OG1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:ALA:O	1:B:1022:VAL:HG13	1.92	0.69
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.23	0.69
1:A:867:ARG:H	1:A:868:LEU:HD23	1.57	0.69
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.74	0.69
1:B:600:THR:HG22	1:B:601:LYS:N	2.06	0.69
4:B:1104:DM2:O19	10:B:1692:HOH:O	2.11	0.69
1:A:355:MET:HE2	1:A:355:MET:CA	2.21	0.69
1:C:867:ARG:NH1	10:C:1700:HOH:O	2.11	0.68
1:A:540:ARG:HG2	1:A:541:TYR:CD1	2.27	0.68
2:D:45:VAL:HG22	10:D:248:HOH:O	1.92	0.68
1:B:672:VAL:CG1	7:B:1103:LMU:H61	2.23	0.68
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.23	0.68
1:C:509:LYS:CB	1:C:510:LYS:CB	2.71	0.68
1:A:259:ARG:NE	10:A:1533:HOH:O	2.24	0.68
3:C:1101:LMT:O3'	10:C:1540:HOH:O	2.11	0.68
1:A:865:GLN:CA	1:A:866:GLU:C	2.66	0.68
1:B:871:ASN:O	3:B:1101:LMT:O6B	2.11	0.68
1:C:808:ARG:NH1	1:C:810:GLU:OE2	2.24	0.68
1:B:352:PHE:CE1	1:B:365:THR:CG2	2.77	0.67
1:C:815:ARG:NE	10:C:1596:HOH:O	2.17	0.67
1:A:534:ILE:HG23	1:A:541:TYR:CE1	2.29	0.67
1:B:672:VAL:HG11	7:B:1103:LMU:H61	1.76	0.67
1:C:430:ALA:O	1:C:434:SER:OG	2.13	0.67
1:A:509:LYS:O	1:A:514:GLY:HA3	1.94	0.67
1:B:636:ASP:O	10:B:1691:HOH:O	2.12	0.67
1:A:444:GLY:CA	3:A:1103:LMT:H12	2.24	0.67
1:A:765:ARG:NH2	10:A:1680:HOH:O	2.26	0.67
1:A:795:ASP:OD1	1:A:797:GLN:HG3	1.94	0.67
1:A:987:MET:O	1:A:990:VAL:HG22	1.95	0.67
1:B:596:HIS:O	1:B:600:THR:HB	1.93	0.67
1:A:585:GLU:OE2	10:A:1654:HOH:O	2.12	0.66
1:A:891:LEU:HD13	3:A:1103:LMT:H11	1.77	0.66
1:B:846:GLN:OE1	10:B:1588:HOH:O	2.13	0.66
1:C:671:ILE:HG23	1:C:862:MET:CE	2.25	0.66
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.77	0.66
1:A:649:MET:HE1	1:A:653:ARG:NH1	2.11	0.66
1:A:539:GLY:O	1:A:543:VAL:HG23	1.96	0.66
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.25	0.66
1:A:360:GLN:HG2	1:A:513:PHE:CD2	2.31	0.66
1:B:527:TYR:OH	1:B:968:VAL:HG11	1.94	0.66
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:HIS:ND1	1:A:1042:HIS:O	2.29	0.66
1:A:674:LEU:HB3	1:A:675:GLY:O	1.95	0.66
4:A:1105:DM2:H6'3	4:A:1105:DM2:C2'	2.22	0.66
1:A:1035:ARG:HG3	1:A:1036:LYS:NZ	2.10	0.66
1:B:138:MET:HE2	1:B:140:VAL:HG22	1.76	0.66
1:B:386:PHE:HB3	1:B:388:PHE:CD2	2.31	0.66
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.78	0.66
1:A:662:MET:HB3	1:A:664:PHE:HE2	1.59	0.66
1:A:112:GLN:HG2	1:B:112:GLN:OE1	1.96	0.65
1:C:309:GLU:HG3	1:C:313:MET:HE3	1.77	0.65
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.78	0.65
1:A:617:PHE:CG	4:A:1106:DM2:H1	2.32	0.65
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.24	0.65
1:C:253:VAL:HG12	1:C:259:ARG:HG2	1.79	0.65
1:A:70:ASN:O	1:A:110:LYS:HE3	1.96	0.65
1:A:507:GLU:HG2	1:A:518:ARG:NE	2.11	0.65
1:B:960:LEU:CD2	1:B:1027:VAL:HG22	2.27	0.65
1:C:344:LEU:HD21	1:C:402:ILE:HD11	1.79	0.65
1:C:671:ILE:HG12	1:C:862:MET:SD	2.37	0.65
2:E:160:ASP:O	2:E:163:GLU:HG2	1.97	0.65
1:B:555:LEU:HD21	1:B:914:LEU:CD1	2.27	0.65
1:B:600:THR:HG22	1:B:601:LYS:HG3	1.79	0.65
1:B:961:ILE:HG22	1:B:965:LEU:CD2	2.27	0.65
1:A:519:MET:O	1:A:523:SER:OG	2.13	0.64
1:A:901:VAL:O	1:A:904:VAL:HG22	1.97	0.64
1:A:891:LEU:CD1	3:A:1103:LMT:H11	2.27	0.64
1:A:562:SER:OG	1:A:922:THR:HG21	1.97	0.64
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.31	0.64
1:C:360:GLN:HG2	1:C:513:PHE:CG	2.32	0.64
1:C:509:LYS:HB3	1:C:510:LYS:HB3	1.79	0.64
1:C:670:ALA:HA	10:C:1332:HOH:O	1.96	0.64
2:E:17:LYS:O	10:E:233:HOH:O	2.14	0.64
1:A:8:ARG:HH12	5:A:1107:D12:H111	1.62	0.64
1:C:867:ARG:NH2	10:C:1700:HOH:O	2.23	0.64
1:C:1035:ARG:HA	1:C:1036:LYS:HG3	1.78	0.64
1:B:138:MET:HE2	1:B:140:VAL:HG23	1.79	0.64
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.28	0.64
1:A:361:ASN:ND2	10:A:1267:HOH:O	2.31	0.64
1:A:881:LEU:HD12	3:A:1102:LMT:H121	1.80	0.64
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.80	0.64
2:E:125:HIS:O	2:E:129:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:GLY:HA3	3:A:1103:LMT:H12	1.80	0.64
1:A:693:GLU:OE1	1:A:693:GLU:N	2.30	0.64
1:A:188:MET:HE2	1:A:773:VAL:HG12	1.79	0.64
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.78	0.64
1:B:229:GLN:O	10:B:1455:HOH:O	2.15	0.63
1:B:309:GLU:OE1	10:B:1337:HOH:O	2.15	0.63
1:B:352:PHE:CE1	1:B:365:THR:HG21	2.33	0.63
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.80	0.63
1:C:1013:THR:O	1:C:1017:LEU:HB2	1.97	0.63
1:B:519:MET:HE3	1:B:520:PHE:N	2.13	0.63
1:C:193:LEU:HD13	1:C:265:VAL:HB	1.80	0.63
1:C:309:GLU:HG3	1:C:313:MET:HE2	1.81	0.63
1:A:674:LEU:HB3	1:A:675:GLY:C	2.23	0.63
1:A:866:GLU:H	1:A:866:GLU:CD	1.95	0.63
1:A:965:LEU:O	1:A:969:ARG:HG2	1.98	0.63
3:A:1102:LMT:H5B	3:A:1102:LMT:H6D	1.80	0.63
4:B:1104:DM2:H6'3	4:B:1104:DM2:C2'	2.29	0.62
1:B:999:ALA:O	1:B:1003:VAL:HG12	1.98	0.62
1:A:115:MET:HB2	1:A:116:PRO:HD3	1.81	0.62
1:C:808:ARG:NH1	10:C:1749:HOH:O	2.20	0.62
2:E:34:MET:CE	2:E:40:VAL:HG12	2.30	0.62
1:B:974:PRO:HA	1:B:977:MET:HE3	1.81	0.62
1:C:360:GLN:HG2	1:C:513:PHE:CE2	2.34	0.62
1:C:671:ILE:O	1:C:671:ILE:CG1	2.48	0.61
1:C:115:MET:N	1:C:116:PRO:HD2	2.14	0.61
2:E:34:MET:HE3	2:E:34:MET:CA	2.30	0.61
1:A:38:ILE:C	1:A:38:ILE:CD1	2.73	0.61
1:A:454:VAL:HB	1:A:455:PRO:HD3	1.83	0.61
1:C:1035:ARG:HA	1:C:1036:LYS:CB	2.31	0.61
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.83	0.61
7:B:1103:LMU:O5'	7:B:1103:LMU:H21	2.01	0.61
1:A:445:ILE:O	1:A:448:VAL:HG22	2.01	0.61
1:A:717:ARG:NH1	4:A:1105:DM2:O19	2.33	0.61
1:C:509:LYS:HB3	1:C:510:LYS:CB	2.30	0.61
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.82	0.60
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.30	0.60
1:A:586:ARG:NH2	1:A:660:ASP:CB	2.64	0.60
1:B:522:LYS:HZ2	1:B:522:LYS:HB2	1.66	0.60
2:E:30:VAL:O	2:E:34:MET:HB2	2.01	0.60
1:A:85:THR:O	1:A:85:THR:HG22	2.00	0.60
4:B:1104:DM2:H112	4:B:1104:DM2:O5'	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.83	0.60
2:D:12:SER:O	2:D:16:LYS:HG2	2.01	0.60
1:A:360:GLN:HG2	1:A:513:PHE:CG	2.37	0.60
1:A:717:ARG:CZ	4:A:1105:DM2:H1	2.32	0.60
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.31	0.60
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.84	0.60
1:A:843:LEU:O	1:A:847:LEU:HG	2.01	0.60
1:B:708:LYS:C	1:B:710:PRO:HD3	2.26	0.60
1:C:314:GLU:HG2	1:C:317:PHE:CE1	2.36	0.60
1:A:971:ARG:HG3	1:A:971:ARG:HH11	1.66	0.60
1:A:1036:LYS:HA	1:A:1037:ASN:HB3	1.83	0.60
1:A:714:THR:HG22	1:A:715:SER:OG	2.01	0.60
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.31	0.60
1:A:1001:ASN:O	1:A:1005:THR:CG2	2.50	0.60
4:A:1105:DM2:H2'2	4:A:1105:DM2:C6'	2.20	0.60
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.84	0.60
1:A:672:VAL:HG23	1:A:673:GLU:N	2.17	0.59
1:A:881:LEU:HD12	3:A:1102:LMT:C12	2.32	0.59
1:B:314:GLU:HB2	1:B:315:PRO:HD3	1.84	0.59
1:B:919:ARG:CD	1:B:1005:THR:HG21	2.32	0.59
1:B:960:LEU:HD21	1:B:1027:VAL:HG22	1.84	0.59
1:A:56:THR:O	1:A:60:THR:HB	2.01	0.59
1:A:971:ARG:HG3	1:A:971:ARG:NH1	2.17	0.59
1:B:352:PHE:CE1	1:B:365:THR:HG23	2.38	0.59
1:B:468:ARG:O	1:B:472:ILE:HD12	2.02	0.59
1:A:420:MET:HE1	1:A:498:LYS:O	2.02	0.59
1:A:716:VAL:O	10:A:1641:HOH:O	2.16	0.59
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.67	0.59
1:C:255:GLN:NE2	1:C:256:ASP:N	2.46	0.59
1:A:1030:ARG:HA	1:A:1030:ARG:NE	2.17	0.59
1:B:919:ARG:CG	1:B:919:ARG:NH1	2.60	0.59
1:A:255:GLN:N	1:A:255:GLN:CD	2.59	0.59
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.18	0.59
1:C:669:PRO:HG3	1:C:675:GLY:O	2.03	0.59
1:A:356:TYR:CA	1:A:365:THR:HG21	2.30	0.59
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.85	0.59
1:C:366:LEU:HD23	1:C:496:MET:CE	2.32	0.59
1:A:958:LYS:HE2	1:A:958:LYS:HA	1.85	0.58
1:B:255:GLN:C	1:B:257:GLY:H	2.10	0.58
1:C:895:TRP:C	1:C:898:PRO:HD2	2.28	0.58
1:A:38:ILE:HD12	1:A:39:ALA:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:PRO:O	1:A:1027:VAL:HG13	2.02	0.58
2:E:74:ASN:HD21	2:E:105:ASP:HB2	1.67	0.58
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.84	0.58
1:A:586:ARG:HD3	10:A:1596:HOH:O	2.02	0.58
1:B:178:PHE:C	4:B:1104:DM2:H213	2.28	0.58
1:C:895:TRP:CD1	5:C:1102:D12:H82	2.38	0.58
3:A:1102:LMT:H5B	3:A:1102:LMT:C6'	2.33	0.58
1:B:960:LEU:HD23	1:B:960:LEU:C	2.28	0.58
1:C:1035:ARG:HA	1:C:1036:LYS:CG	2.34	0.58
1:B:522:LYS:CB	1:B:522:LYS:NZ	2.67	0.58
1:A:616:GLY:C	1:A:618:ALA:H	2.08	0.57
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.34	0.57
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.86	0.57
1:A:865:GLN:HA	1:A:866:GLU:O	2.04	0.57
1:A:866:GLU:CB	1:A:867:ARG:HA	2.34	0.57
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.11	0.57
1:C:671:ILE:CG1	1:C:674:LEU:HG	2.34	0.57
1:C:694:LYS:HG2	10:C:1307:HOH:O	2.05	0.57
1:A:614:GLY:HA2	1:A:621:GLY:O	2.04	0.57
1:C:867:ARG:NH1	10:C:1225:HOH:O	2.36	0.57
1:C:673:GLU:HG3	10:C:1483:HOH:O	2.03	0.57
1:B:2:PRO:O	1:B:6:ILE:HG13	2.03	0.57
2:D:165:LEU:O	2:D:166:GLN:C	2.48	0.57
1:A:717:ARG:HH12	4:A:1105:DM2:C20	2.16	0.57
2:E:74:ASN:ND2	2:E:105:ASP:HB2	2.19	0.57
1:A:408:ASP:OD1	1:A:940:LYS:NZ	2.26	0.57
1:A:717:ARG:HH22	4:A:1105:DM2:C1	2.18	0.56
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.88	0.56
1:A:412:VAL:HG11	1:A:489:THR:CG2	2.35	0.56
1:B:987:MET:CG	1:B:1008:MET:HE1	2.25	0.56
4:A:1105:DM2:H10	4:A:1106:DM2:C1	2.36	0.56
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.88	0.56
1:B:399:VAL:HA	1:B:402:ILE:HD12	1.87	0.56
2:E:92:HIS:O	2:E:96:VAL:HG23	2.04	0.56
1:A:958:LYS:HE2	1:A:958:LYS:CA	2.35	0.56
1:A:1041:GLU:CD	1:A:1042:HIS:H	2.13	0.56
1:B:255:GLN:C	1:B:257:GLY:N	2.64	0.56
2:D:25:GLY:HA2	2:D:62:ILE:HD12	1.87	0.56
1:A:543:VAL:O	1:A:547:ILE:HG12	2.06	0.56
1:A:472:ILE:HD13	1:A:472:ILE:N	2.20	0.56
2:D:48:TRP:HE3	2:D:53:LEU:HD13	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ARG:H	1:A:540:ARG:CD	2.05	0.56
1:B:408:ASP:OD2	1:B:940:LYS:NZ	2.36	0.56
1:B:716:VAL:HG13	10:B:1490:HOH:O	2.05	0.56
1:C:671:ILE:H	1:C:862:MET:CE	2.18	0.56
1:A:438:ILE:HD12	1:A:439:GLN:N	2.20	0.56
2:E:42:ALA:O	2:E:50:PRO:HD3	2.06	0.56
1:A:985:GLY:O	1:A:988:PRO:HD2	2.06	0.56
3:A:1104:LMT:H4B	10:A:1275:HOH:O	2.05	0.56
1:B:865:GLN:O	1:B:868:LEU:N	2.35	0.56
1:C:177:LEU:HD13	1:C:179:GLY:C	2.31	0.56
1:A:376:LEU:HD13	1:A:405:LEU:HD12	1.88	0.55
1:A:504:ASP:C	1:A:505:HIS:ND1	2.64	0.55
1:A:836:SER:O	1:A:839:GLU:HG3	2.06	0.55
4:A:1106:DM2:O14	10:A:1692:HOH:O	2.18	0.55
1:C:659:LYS:HE2	1:C:660:ASP:OD2	2.06	0.55
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.88	0.55
1:B:867:ARG:O	1:B:868:LEU:HD12	2.07	0.55
1:A:677:ALA:O	1:A:678:THR:HG23	2.07	0.55
1:A:867:ARG:N	1:A:868:LEU:HD23	2.22	0.55
1:C:368:PRO:HD3	1:C:413:VAL:HG21	1.86	0.55
1:C:736:ALA:HB1	1:C:741:VAL:HG23	1.87	0.55
1:C:33:ALA:O	1:C:337:ILE:HD11	2.06	0.55
1:B:461:GLY:HA3	1:B:865:GLN:OE1	2.07	0.55
1:B:866:GLU:C	1:B:868:LEU:H	2.14	0.55
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.89	0.55
1:A:836:SER:OG	1:A:839:GLU:HG2	2.06	0.55
1:B:169:THR:OG1	1:B:309:GLU:HG3	2.06	0.55
1:C:1030:ARG:O	1:C:1034:SER:HB2	2.06	0.55
1:A:8:ARG:NH1	5:A:1107:D12:H111	2.21	0.55
1:A:375:VAL:HB	1:A:405:LEU:HD13	1.89	0.55
1:A:276:ASP:O	1:A:614:GLY:HA3	2.07	0.55
1:C:853:THR:HG21	10:C:1723:HOH:O	2.07	0.55
1:B:960:LEU:CD2	1:B:960:LEU:C	2.80	0.55
1:A:152:GLU:OE1	1:A:152:GLU:N	2.31	0.54
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.71	0.54
1:A:252:LYS:NZ	10:A:1450:HOH:O	2.38	0.54
1:A:444:GLY:HA2	3:A:1103:LMT:H12	1.88	0.54
1:A:522:LYS:HG3	1:A:526:HIS:CE1	2.43	0.54
1:A:649:MET:CE	1:A:653:ARG:NH1	2.70	0.54
1:C:808:ARG:HD2	10:C:1749:HOH:O	2.06	0.54
1:A:361:ASN:O	1:A:365:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.88	0.54
1:B:672:VAL:HG23	1:B:673:GLU:CD	2.32	0.54
1:C:139:VAL:O	1:C:326:PRO:HD2	2.07	0.54
1:B:961:ILE:HG22	1:B:965:LEU:HD23	1.89	0.54
1:C:21:LEU:O	1:C:25:LEU:HG	2.07	0.54
1:B:875:SER:CB	3:B:1101:LMT:H6'2	2.33	0.54
1:C:735:LYS:NZ	10:C:1641:HOH:O	2.40	0.54
3:B:1101:LMT:O2'	3:B:1101:LMT:C2	2.52	0.54
1:C:898:PRO:O	1:C:902:MET:HG2	2.07	0.54
2:E:31:ARG:HG2	2:E:31:ARG:NH1	2.18	0.54
1:C:111:LEU:HD21	1:C:127:VAL:HG22	1.88	0.54
1:C:509:LYS:O	1:C:514:GLY:HA3	2.07	0.54
1:A:537:SER:HB2	1:A:540:ARG:NH1	2.22	0.54
1:A:1040:ILE:O	1:A:1041:GLU:HB2	2.07	0.54
1:C:491:ALA:O	1:C:495:THR:HG23	2.08	0.54
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.90	0.53
1:A:836:SER:O	1:A:837:THR:C	2.51	0.53
1:A:896:SER:O	1:A:899:PHE:HD2	1.91	0.53
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.89	0.53
1:B:357:LEU:HD11	1:B:516:PHE:CE2	2.43	0.53
1:C:489:THR:HB	1:C:490:PRO:HD3	1.89	0.53
1:A:449:LEU:HB3	1:A:478:MET:SD	2.48	0.53
1:A:510:LYS:HD2	1:A:511:GLY:N	2.23	0.53
1:A:1035:ARG:HG3	1:A:1036:LYS:HZ2	1.71	0.53
1:B:115:MET:N	1:B:116:PRO:CD	2.71	0.53
1:B:760:ASN:HB2	8:B:1106:GOL:H31	1.90	0.53
1:B:872:GLN:C	1:B:874:PRO:CD	2.82	0.53
1:C:1034:SER:O	1:C:1035:ARG:C	2.51	0.53
1:B:396:PHE:HA	1:B:399:VAL:HG13	1.90	0.53
1:B:414:GLU:CG	1:B:977:MET:CE	2.66	0.53
1:B:530:SER:O	1:B:534:ILE:HG13	2.08	0.53
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.90	0.53
1:B:121:GLU:H	1:B:121:GLU:CD	2.15	0.53
1:A:537:SER:O	1:A:538:THR:CB	2.56	0.53
1:A:717:ARG:NH2	4:A:1105:DM2:C1	2.71	0.53
1:B:605:ASN:OD1	1:B:637:ARG:HG2	2.08	0.53
1:A:881:LEU:CD1	3:A:1102:LMT:H112	2.39	0.53
1:B:447:MET:HE2	1:B:447:MET:CA	2.31	0.53
1:A:777:ALA:O	1:A:781:MET:HG2	2.09	0.53
1:B:211:ASN:HB2	1:B:240:LEU:HD22	1.90	0.53
1:C:120:GLN:HB2	10:C:1522:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:973:ARG:O	1:C:977:MET:HG3	2.09	0.53
2:E:59:HIS:O	2:E:63:VAL:HG23	2.08	0.53
1:A:671:ILE:N	1:A:674:LEU:HD12	2.11	0.53
1:A:866:GLU:O	1:A:868:LEU:HB2	2.06	0.53
1:C:95:GLU:HG3	10:C:1718:HOH:O	2.09	0.53
1:C:563:PHE:CE2	1:C:564:LEU:HD22	2.44	0.53
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.89	0.53
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.24	0.53
1:C:70:ASN:HB2	10:C:1427:HOH:O	2.08	0.53
1:A:708:LYS:C	1:A:710:PRO:HD3	2.34	0.53
1:A:148:THR:HG23	10:A:1514:HOH:O	2.10	0.52
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.91	0.52
1:A:339:GLU:O	1:A:343:THR:HG23	2.08	0.52
1:A:342:LYS:HG3	3:A:1104:LMT:H92	1.92	0.52
1:A:554:TYR:CE1	1:A:558:ARG:CZ	2.92	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.90	0.52
1:A:919:ARG:O	1:A:919:ARG:HD3	2.10	0.52
1:A:989:LEU:HD23	1:A:1000:GLN:OE1	2.10	0.52
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.40	0.52
1:A:676:THR:HG21	4:A:1106:DM2:H1'	1.90	0.52
1:C:671:ILE:HG13	1:C:674:LEU:HG	1.91	0.52
1:C:799:VAL:HG23	1:C:804:PHE:HE1	1.74	0.52
1:C:943:ILE:O	1:C:947:GLU:HB3	2.08	0.52
1:A:1035:ARG:HG3	1:A:1036:LYS:CD	2.40	0.52
1:B:678:THR:HA	1:B:837:THR:HG22	1.91	0.52
4:B:1104:DM2:O5'	4:B:1104:DM2:C11	2.57	0.52
1:A:586:ARG:HH22	1:A:660:ASP:CB	2.23	0.52
1:B:678:THR:HA	1:B:837:THR:CG2	2.39	0.52
1:B:695:LEU:HD13	1:B:825:MET:HG3	1.92	0.52
2:E:29:GLU:O	2:E:33:LEU:HG	2.10	0.52
1:A:418:ARG:NH2	1:A:970:MET:CE	2.72	0.52
1:A:617:PHE:CD2	4:A:1106:DM2:H2	2.45	0.52
1:A:676:THR:CB	4:A:1105:DM2:H213	2.37	0.52
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.88	0.52
1:A:360:GLN:HG2	1:A:513:PHE:CE2	2.44	0.52
1:A:416:VAL:HG22	1:A:431:THR:HA	1.92	0.52
1:A:542:LEU:HD12	1:A:542:LEU:N	2.25	0.52
1:B:522:LYS:HZ2	1:B:522:LYS:CB	2.23	0.52
1:B:837:THR:O	1:B:841:MET:HG3	2.09	0.52
1:A:1036:LYS:HA	1:A:1037:ASN:CB	2.39	0.52
1:B:6:ILE:HD11	1:B:431:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:LEU:HD23	1:B:960:LEU:O	2.10	0.52
1:C:40:PRO:HB2	1:C:94:PHE:O	2.09	0.52
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.40	0.52
1:A:401:ALA:O	1:A:405:LEU:HG	2.10	0.52
1:A:456:MET:C	1:A:458:PHE:H	2.17	0.52
1:B:328:ASP:O	1:B:331:PRO:HD2	2.10	0.52
1:C:33:ALA:O	1:C:391:ASN:HA	2.10	0.52
2:E:26:ARG:HB3	2:E:29:GLU:HB2	1.93	0.52
1:A:489:THR:HB	1:A:490:PRO:HD3	1.92	0.51
1:A:38:ILE:HG22	1:A:465:ALA:HB3	1.93	0.51
1:A:418:ARG:NH2	1:A:970:MET:HE1	2.25	0.51
1:A:427:PRO:O	1:A:431:THR:HG23	2.11	0.51
1:A:990:VAL:HG21	1:A:1008:MET:HE1	1.92	0.51
1:B:138:MET:CE	1:B:140:VAL:HG22	2.40	0.51
1:B:873:ALA:N	1:B:874:PRO:CD	2.73	0.51
1:C:193:LEU:CD1	1:C:265:VAL:HB	2.40	0.51
1:A:712:MET:HG3	1:A:713:LEU:HD13	1.92	0.51
1:A:910:ILE:HG23	1:A:911:GLY:N	2.26	0.51
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.39	0.51
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.45	0.51
1:B:897:ILE:N	1:B:898:PRO:CD	2.74	0.51
2:E:134:LYS:O	2:E:134:LYS:HG2	2.11	0.51
1:A:1035:ARG:HG3	1:A:1036:LYS:HD3	1.93	0.51
1:B:527:TYR:CZ	1:B:968:VAL:CG1	2.93	0.51
1:A:355:MET:HA	1:A:355:MET:CE	2.27	0.51
1:B:255:GLN:OE1	1:B:255:GLN:CA	2.58	0.51
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.93	0.51
2:E:28:ASP:O	2:E:29:GLU:C	2.53	0.51
1:B:527:TYR:CE2	1:B:968:VAL:CG1	2.92	0.51
1:B:955:LYS:HE2	1:B:955:LYS:HA	1.92	0.51
1:B:240:LEU:HG	1:B:245:GLU:HB3	1.91	0.51
1:C:32:VAL:CG1	1:C:337:ILE:HD13	2.40	0.51
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.92	0.51
1:A:343:THR:HG21	1:A:1000:GLN:OE1	2.11	0.51
1:A:538:THR:H	1:A:540:ARG:HD3	1.76	0.51
2:E:40:VAL:HG13	10:E:250:HOH:O	2.11	0.51
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.92	0.50
1:B:386:PHE:HB3	1:B:388:PHE:CE2	2.45	0.50
1:B:868:LEU:C	1:B:870:GLY:H	2.19	0.50
1:B:872:GLN:C	1:B:874:PRO:HD2	2.37	0.50
1:A:344:LEU:HD21	1:A:376:LEU:CD2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:NE	1:A:970:MET:CE	2.75	0.50
4:A:1105:DM2:C2'	4:A:1105:DM2:C6'	2.82	0.50
1:C:868:LEU:C	1:C:868:LEU:HD23	2.36	0.50
1:A:263:ARG:NH2	2:D:155:ASN:O	2.44	0.50
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.93	0.50
1:A:488:LEU:HG	1:A:492:LEU:HD22	1.93	0.50
1:B:138:MET:HE1	1:B:325:TYR:CE2	2.47	0.50
1:C:653:ARG:NH1	10:C:1450:HOH:O	2.44	0.50
1:C:980:LEU:HD12	1:C:984:LEU:CD2	2.42	0.50
2:E:31:ARG:HH11	2:E:31:ARG:CG	2.16	0.50
1:A:617:PHE:CD2	4:A:1106:DM2:C2	2.94	0.50
1:B:447:MET:HA	1:B:447:MET:CE	2.31	0.50
1:C:641:GLU:OE1	1:C:641:GLU:N	2.30	0.50
2:D:93:LEU:HB3	2:D:94:GLU:OE1	2.12	0.50
1:A:418:ARG:NE	1:A:970:MET:HE2	2.27	0.50
1:B:454:VAL:HB	1:B:455:PRO:HD3	1.94	0.50
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.77	0.50
1:C:226:LYS:NZ	10:C:1497:HOH:O	2.45	0.50
1:C:364:ALA:O	1:C:368:PRO:HD2	2.12	0.50
1:B:555:LEU:HD21	1:B:914:LEU:HD12	1.94	0.50
1:B:862:MET:HE2	10:B:1463:HOH:O	2.11	0.50
1:B:873:ALA:O	1:B:877:TYR:CD2	2.65	0.49
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.45	0.49
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.93	0.49
1:A:554:TYR:HE1	1:A:558:ARG:NH2	2.11	0.49
1:A:717:ARG:NH2	4:A:1105:DM2:C2	2.73	0.49
1:A:895:TRP:CG	6:A:1108:D10:H71	2.47	0.49
1:A:662:MET:HB3	1:A:664:PHE:CE2	2.44	0.49
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.09	0.49
1:C:367:ILE:HB	1:C:368:PRO:CD	2.42	0.49
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.94	0.49
1:C:971:ARG:C	1:C:974:PRO:HD2	2.37	0.49
1:A:633:ASP:OD1	3:A:1104:LMT:O4'	2.24	0.49
1:A:676:THR:O	1:A:678:THR:N	2.45	0.49
1:A:729:ILE:CD1	1:C:234:ILE:HG23	2.43	0.49
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.91	0.49
1:A:987:MET:CE	1:A:1008:MET:CE	2.91	0.49
1:B:169:THR:O	1:B:172:VAL:HG13	2.12	0.49
1:B:255:GLN:O	1:B:257:GLY:N	2.45	0.49
1:C:447:MET:HE1	1:C:891:LEU:HG	1.95	0.49
2:D:82:THR:HB	2:D:83:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:41:ASN:HD21	2:E:72:ASP:HB2	1.77	0.49
1:C:666:PHE:CD2	1:C:677:ALA:HB2	2.48	0.49
1:A:879:ILE:HD12	1:A:879:ILE:C	2.37	0.49
1:A:903:LEU:O	1:A:906:PRO:HD2	2.12	0.49
3:B:1102:LMT:H5B	3:B:1102:LMT:H6D	1.92	0.49
1:C:867:ARG:HG2	10:C:1225:HOH:O	2.13	0.49
1:C:951:ASP:O	1:C:955:LYS:HG2	2.12	0.49
1:A:538:THR:H	1:A:540:ARG:CD	2.25	0.49
1:B:189:ASN:CG	1:B:192:GLU:HG2	2.38	0.49
1:B:874:PRO:HD2	1:B:875:SER:H	1.77	0.49
2:D:98:VAL:HA	2:D:101:LYS:HE2	1.94	0.49
1:A:60:THR:CG2	1:A:119:PRO:HG2	2.43	0.48
1:A:254:ASN:HB2	1:A:258:SER:OG	2.13	0.48
1:A:884:VAL:HG12	1:A:902:MET:HE3	1.94	0.48
2:E:34:MET:HA	2:E:34:MET:HE2	1.95	0.48
1:A:695:LEU:HD13	1:A:825:MET:HG3	1.94	0.48
1:B:973:ARG:O	1:B:977:MET:HG3	2.13	0.48
1:C:57:VAL:HG11	1:C:88:VAL:HG23	1.94	0.48
1:C:453:PHE:CE1	1:C:474:ILE:HG21	2.49	0.48
1:A:545:TYR:OH	1:A:906:PRO:HG2	2.13	0.48
1:A:617:PHE:CB	4:A:1105:DM2:C14	2.83	0.48
1:A:910:ILE:CG2	1:A:911:GLY:N	2.76	0.48
1:B:555:LEU:CD2	1:B:914:LEU:HD13	2.43	0.48
1:B:1008:MET:O	1:B:1012:VAL:HG23	2.12	0.48
1:C:151:GLN:OE1	1:C:278:ILE:HG23	2.12	0.48
1:C:370:ILE:O	1:C:373:PRO:HD2	2.14	0.48
1:A:866:GLU:CG	1:A:867:ARG:CB	2.88	0.48
1:A:868:LEU:N	1:A:868:LEU:HD22	2.29	0.48
1:B:303:ALA:O	1:B:307:ARG:HG3	2.13	0.48
1:B:867:ARG:O	1:B:867:ARG:HG2	2.13	0.48
2:E:163:GLU:CG	2:E:164:ILE:N	2.77	0.48
1:A:259:ARG:NH2	10:A:1533:HOH:O	2.46	0.48
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.72	0.48
1:A:729:ILE:HD11	1:C:234:ILE:HG23	1.95	0.48
1:A:867:ARG:HA	1:A:869:SER:H	1.77	0.48
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.12	0.48
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.94	0.48
2:E:31:ARG:O	2:E:35:ALA:N	2.42	0.48
1:A:153:ASP:OD1	1:A:182:TYR:OH	2.26	0.48
1:A:57:VAL:HG11	1:A:88:VAL:CG2	2.44	0.48
1:A:616:GLY:C	1:A:618:ALA:N	2.70	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:THR:HB	2:D:116:PRO:HD2	1.95	0.48
1:A:711:ASP:OD1	1:A:711:ASP:N	2.41	0.48
1:A:845:GLU:HG2	1:A:857:TYR:CZ	2.49	0.48
1:B:139:VAL:HG13	1:B:178:PHE:HE2	1.78	0.48
1:B:649:MET:HB3	1:B:653:ARG:NH2	2.28	0.48
1:A:456:MET:HE3	1:A:932:LEU:HD11	1.96	0.47
1:A:672:VAL:C	1:A:674:LEU:H	2.20	0.47
1:A:836:SER:O	1:A:839:GLU:N	2.46	0.47
3:A:1104:LMT:H2B	3:A:1104:LMT:H5'	1.96	0.47
1:C:750:LEU:HD23	1:C:750:LEU:O	2.14	0.47
1:A:676:THR:CB	4:A:1105:DM2:C21	2.79	0.47
1:A:867:ARG:O	1:A:867:ARG:CG	2.58	0.47
2:E:31:ARG:NH1	2:E:31:ARG:CG	2.73	0.47
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.49	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.96	0.47
1:A:553:ALA:O	1:A:557:VAL:HG13	2.14	0.47
1:A:717:ARG:CZ	4:A:1105:DM2:C1	2.92	0.47
1:A:971:ARG:HH11	1:A:971:ARG:CG	2.27	0.47
1:B:39:ALA:HB2	1:B:673:GLU:HG2	1.96	0.47
1:B:578:LEU:HD22	1:B:661:ALA:HB2	1.95	0.47
1:C:743:ILE:HD12	1:C:743:ILE:O	2.13	0.47
1:C:895:TRP:CD1	5:C:1102:D12:H101	2.49	0.47
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.97	0.47
1:A:11:PHE:HD2	1:A:11:PHE:O	1.98	0.47
1:A:454:VAL:N	1:A:455:PRO:CD	2.78	0.47
1:A:456:MET:N	10:A:1602:HOH:O	2.48	0.47
1:A:532:GLY:O	1:A:536:ARG:HD3	2.13	0.47
1:A:966:ASP:HA	1:A:969:ARG:HG2	1.96	0.47
5:A:1107:D12:H91	10:B:1683:HOH:O	2.14	0.47
1:B:11:PHE:HD2	1:B:11:PHE:O	1.97	0.47
1:B:842:GLU:O	1:B:846:GLN:HG3	2.15	0.47
1:B:986:VAL:HG23	1:B:989:LEU:HD12	1.97	0.47
1:C:2:PRO:O	1:C:6:ILE:HG13	2.15	0.47
1:A:526:HIS:O	1:A:530:SER:OG	2.30	0.47
1:A:537:SER:OG	1:A:540:ARG:HD3	2.14	0.47
1:B:555:LEU:HD12	1:B:555:LEU:HA	1.76	0.47
1:B:713:LEU:HD22	1:B:843:LEU:HD23	1.96	0.47
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.38	0.47
1:A:505:HIS:HD2	1:A:521:GLU:OE1	1.98	0.47
1:A:637:ARG:O	1:A:643:LYS:NZ	2.35	0.47
1:C:363:ARG:O	1:C:367:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:680:PHE:CZ	1:C:829:GLY:HA3	2.50	0.47
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.15	0.47
2:D:154:ILE:HG13	2:D:155:ASN:N	2.28	0.47
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.50	0.47
1:B:104:GLN:OE1	1:B:131:LYS:HG3	2.15	0.47
1:B:972:LEU:HD22	1:B:976:LEU:HD13	1.96	0.47
1:C:340:VAL:HG11	1:C:395:MET:CB	2.44	0.47
1:C:358:PHE:CG	1:C:977:MET:HG2	2.50	0.47
1:C:493:CYS:O	1:C:497:LEU:HB2	2.15	0.47
1:C:732:ASP:OD2	1:C:735:LYS:HE3	2.15	0.47
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.45	0.46
1:A:414:GLU:OE2	1:A:974:PRO:HG3	2.14	0.46
1:A:534:ILE:HG23	1:A:541:TYR:CE2	2.48	0.46
1:A:866:GLU:CD	1:A:867:ARG:HG3	2.40	0.46
1:A:1036:LYS:CA	1:A:1037:ASN:HB3	2.44	0.46
1:B:468:ARG:HG2	1:B:472:ILE:CD1	2.44	0.46
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.97	0.46
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.96	0.46
1:A:351:VAL:O	1:A:355:MET:HG2	2.16	0.46
1:A:676:THR:O	1:A:677:ALA:C	2.59	0.46
1:A:866:GLU:CG	1:A:867:ARG:CA	2.72	0.46
1:A:892:TYR:OH	1:A:946:VAL:HG22	2.15	0.46
4:A:1105:DM2:C1	4:A:1106:DM2:H112	2.45	0.46
1:B:616:GLY:HA3	1:B:619:GLY:O	2.15	0.46
1:C:359:LEU:O	1:C:361:ASN:N	2.36	0.46
1:A:717:ARG:HH12	4:A:1105:DM2:C19	2.29	0.46
1:B:120:GLN:HB3	10:B:1620:HOH:O	2.15	0.46
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.15	0.46
1:C:21:LEU:HD12	1:C:21:LEU:C	2.40	0.46
1:C:255:GLN:HE21	1:C:256:ASP:CB	2.27	0.46
2:E:49:THR:HB	2:E:50:PRO:HD2	1.98	0.46
1:A:420:MET:HG2	1:A:430:ALA:CB	2.45	0.46
1:A:729:ILE:CD1	1:C:234:ILE:CG2	2.93	0.46
1:A:668:LEU:HD23	1:A:668:LEU:HA	1.82	0.46
1:A:842:GLU:O	1:A:846:GLN:HG3	2.16	0.46
1:B:873:ALA:N	1:B:874:PRO:HD3	2.31	0.46
1:A:151:GLN:NE2	10:A:1203:HOH:O	2.18	0.46
1:A:1036:LYS:HD3	1:A:1036:LYS:N	2.31	0.46
1:B:568:ASP:CG	1:B:644:VAL:HG23	2.40	0.46
1:C:83:ASP:OD1	1:C:83:ASP:C	2.59	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:750:LEU:C	1:C:750:LEU:CD2	2.88	0.46
1:A:226:LYS:HD3	1:A:227:GLY:N	2.31	0.46
1:A:554:TYR:OH	1:A:558:ARG:NH1	2.48	0.46
1:A:673:GLU:O	1:A:674:LEU:C	2.59	0.46
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.97	0.46
1:B:178:PHE:CA	4:B:1104:DM2:H213	2.46	0.46
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.68	0.46
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.97	0.46
1:B:709:HIS:N	1:B:710:PRO:HD3	2.30	0.46
1:B:714:THR:CG2	1:B:832:ALA:HA	2.46	0.46
1:B:865:GLN:O	1:B:866:GLU:C	2.59	0.46
1:C:11:PHE:HD1	1:C:11:PHE:O	1.98	0.46
1:B:987:MET:CG	1:B:1008:MET:CE	2.90	0.46
2:D:94:GLU:N	2:D:94:GLU:CD	2.56	0.46
1:B:342:LYS:HD3	1:B:346:GLU:OE2	2.16	0.46
1:C:893:GLU:HG3	1:C:893:GLU:O	2.16	0.46
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.51	0.45
1:A:709:HIS:N	1:A:710:PRO:CD	2.76	0.45
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.47	0.45
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.98	0.45
1:A:921:LEU:HD12	1:A:921:LEU:HA	1.76	0.45
3:A:1104:LMT:H41	3:A:1104:LMT:H12	1.58	0.45
1:B:426:PRO:HD2	1:B:429:GLU:CG	2.46	0.45
1:C:166:ILE:CD1	1:C:313:MET:HE1	2.47	0.45
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.46	0.45
1:A:505:HIS:C	1:A:507:GLU:N	2.71	0.45
1:A:668:LEU:HA	1:A:669:PRO:HD3	1.82	0.45
1:A:708:LYS:CG	1:A:708:LYS:O	2.64	0.45
1:A:919:ARG:CG	1:A:919:ARG:NH1	2.46	0.45
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.97	0.45
1:C:575:MET:SD	1:C:664:PHE:HD2	2.39	0.45
1:A:522:LYS:HE3	1:A:522:LYS:HA	1.99	0.45
1:A:554:TYR:O	1:A:558:ARG:HG2	2.17	0.45
1:A:729:ILE:HD12	1:C:234:ILE:CG2	2.46	0.45
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.46	0.45
1:A:60:THR:HG23	1:A:119:PRO:CG	2.46	0.45
1:A:445:ILE:HD13	1:A:940:LYS:HG3	1.99	0.45
1:A:868:LEU:CD2	1:A:868:LEU:N	2.79	0.45
1:A:925:VAL:O	1:A:929:VAL:HG22	2.17	0.45
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.99	0.45
1:B:408:ASP:CG	1:B:940:LYS:HZ1	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HG2	1:B:977:MET:HE1	1.93	0.45
1:A:373:PRO:HB3	3:A:1101:LMT:H121	1.98	0.45
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.17	0.45
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.47	0.45
1:A:957:GLY:O	1:A:958:LYS:C	2.59	0.45
1:A:1035:ARG:CG	1:A:1036:LYS:NZ	2.78	0.45
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.98	0.45
1:B:418:ARG:HD3	10:B:1229:HOH:O	2.16	0.45
3:A:1104:LMT:H5'	3:A:1104:LMT:H1B	1.61	0.45
1:B:744:ASN:N	10:B:1544:HOH:O	2.19	0.45
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.75	0.45
1:A:462:SER:O	1:A:463:THR:C	2.58	0.45
1:A:866:GLU:HG2	1:A:867:ARG:CG	2.46	0.45
1:A:990:VAL:HG12	1:A:1004:GLY:C	2.41	0.45
3:A:1101:LMT:H4O1	3:B:1101:LMT:H2B	1.80	0.45
1:B:866:GLU:C	1:B:868:LEU:N	2.75	0.45
1:B:968:VAL:HG13	10:B:1377:HOH:O	2.16	0.45
1:C:672:VAL:N	1:C:673:GLU:OE2	2.49	0.45
1:B:386:PHE:HB3	1:B:388:PHE:HD2	1.80	0.45
1:C:177:LEU:HD13	1:C:179:GLY:O	2.16	0.45
1:C:867:ARG:HH11	1:C:867:ARG:CG	2.18	0.45
1:A:897:ILE:N	1:A:898:PRO:CD	2.80	0.45
1:A:421:ALA:HB2	1:A:500:ILE:HG21	1.99	0.44
1:A:462:SER:OG	1:A:463:THR:N	2.49	0.44
1:A:968:VAL:CG2	1:A:1023:PRO:HG3	2.47	0.44
1:B:489:THR:N	1:B:490:PRO:CD	2.80	0.44
1:A:554:TYR:CE1	1:A:558:ARG:NH2	2.85	0.44
3:B:1102:LMT:H6D	3:B:1102:LMT:C5B	2.47	0.44
1:C:664:PHE:CD2	1:C:717:ARG:HD3	2.52	0.44
2:D:82:THR:HB	2:D:83:PRO:CD	2.47	0.44
1:A:418:ARG:CZ	1:A:970:MET:CE	2.95	0.44
1:A:505:HIS:C	1:A:507:GLU:H	2.25	0.44
1:A:670:ALA:HB2	10:A:1623:HOH:O	2.17	0.44
1:B:677:ALA:C	1:B:679:GLY:H	2.25	0.44
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.43	0.44
1:C:620:ARG:NH1	10:C:1579:HOH:O	2.39	0.44
1:A:537:SER:HB2	1:A:540:ARG:CZ	2.46	0.44
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.51	0.44
3:A:1103:LMT:H6'1	1:C:8:ARG:NH2	2.21	0.44
1:C:242:SER:HB2	1:C:244:GLU:OE1	2.18	0.44
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:LEU:HD13	2:E:135:TYR:CD1	2.52	0.44
1:A:148:THR:CG2	10:A:1514:HOH:O	2.64	0.44
1:A:393:LEU:HD13	1:A:466:ILE:HG23	2.00	0.44
1:C:314:GLU:CG	1:C:317:PHE:CE1	3.01	0.44
1:A:355:MET:CA	1:A:355:MET:CE	2.93	0.44
1:A:953:MET:HA	1:A:958:LYS:O	2.17	0.44
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.41	0.44
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.44
1:A:497:LEU:HD23	1:A:497:LEU:HA	1.79	0.44
1:A:679:GLY:HA3	4:A:1105:DM2:H212	2.00	0.44
1:A:879:ILE:HG13	1:A:880:SER:N	2.33	0.44
4:B:1104:DM2:O6	4:B:1104:DM2:C21	2.55	0.44
1:C:199:THR:HB	1:C:200:PRO:HD2	2.00	0.44
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.42	0.44
1:A:865:GLN:C	1:A:867:ARG:HB2	2.42	0.44
1:A:886:LEU:HB3	1:C:14:VAL:HG13	1.99	0.44
1:A:1035:ARG:HD2	1:A:1035:ARG:HA	1.60	0.44
1:B:351:VAL:HG21	1:B:406:VAL:HG22	2.00	0.44
1:C:743:ILE:HD12	1:C:743:ILE:C	2.43	0.44
2:D:110:ASP:C	2:D:110:ASP:OD1	2.60	0.44
1:A:39:ALA:HA	1:A:40:PRO:HD3	1.78	0.43
1:A:307:ARG:HD3	10:A:1357:HOH:O	2.18	0.43
1:A:360:GLN:HG2	1:A:513:PHE:CD1	2.53	0.43
1:B:351:VAL:O	1:B:355:MET:HG2	2.18	0.43
2:E:150:PHE:CE2	2:E:154:ILE:HD11	2.52	0.43
1:A:350:LEU:HD13	1:A:984:LEU:O	2.18	0.43
1:A:449:LEU:HD23	1:A:478:MET:SD	2.58	0.43
1:A:617:PHE:CD2	4:A:1106:DM2:C1	3.01	0.43
1:A:795:ASP:CG	1:A:797:GLN:HG3	2.43	0.43
1:B:104:GLN:OE1	1:B:131:LYS:HE2	2.18	0.43
1:B:575:MET:CE	10:B:1517:HOH:O	2.66	0.43
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.00	0.43
1:A:1:MET:HB2	1:A:2:PRO:HD3	2.00	0.43
1:A:537:SER:O	1:A:538:THR:OG1	2.34	0.43
1:A:1024:VAL:O	1:A:1025:PHE:C	2.61	0.43
2:E:133:LEU:C	2:E:135:TYR:H	2.25	0.43
1:A:57:VAL:CG1	1:A:88:VAL:HG23	2.48	0.43
1:A:618:ALA:HA	1:A:619:GLY:HA2	1.40	0.43
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.43
1:B:578:LEU:N	1:B:578:LEU:HD23	2.34	0.43
1:B:832:ALA:O	1:B:835:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HG	1:A:245:GLU:HB3	2.00	0.43
1:A:456:MET:C	1:A:458:PHE:N	2.76	0.43
1:A:862:MET:HE1	4:A:1105:DM2:H212	1.98	0.43
1:B:615:PHE:CD2	1:B:626:ILE:HD12	2.53	0.43
1:C:79:SER:HB2	10:C:1265:HOH:O	2.17	0.43
1:C:666:PHE:CE2	1:C:677:ALA:HB2	2.53	0.43
2:E:32:ILE:N	2:E:32:ILE:HD13	2.32	0.43
1:A:418:ARG:HE	1:A:970:MET:HE3	1.84	0.43
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.48	0.43
1:A:1030:ARG:HA	1:A:1030:ARG:HE	1.81	0.43
3:B:1101:LMT:H22	3:B:1101:LMT:C2'	2.49	0.43
1:C:695:LEU:HD23	1:C:695:LEU:HA	1.88	0.43
2:E:41:ASN:ND2	2:E:72:ASP:HB2	2.34	0.43
1:A:344:LEU:HD21	1:A:376:LEU:HD21	1.99	0.43
1:A:575:MET:HB2	1:A:617:PHE:HE1	1.83	0.43
1:A:1027:VAL:CG2	1:A:1028:VAL:N	2.81	0.43
3:A:1103:LMT:C2	3:A:1103:LMT:O5'	2.67	0.43
4:A:1106:DM2:H1'	4:A:1106:DM2:O8	2.19	0.43
1:B:328:ASP:OD1	1:B:330:THR:HB	2.19	0.43
1:B:659:LYS:HB3	1:B:660:ASP:H	1.59	0.43
1:C:977:MET:HE2	1:C:977:MET:HB3	1.76	0.43
1:A:1038:GLU:HG3	1:A:1038:GLU:O	2.18	0.43
1:B:456:MET:CG	1:B:467:TYR:HB3	2.44	0.43
1:B:563:PHE:O	1:B:924:ASP:HB2	2.19	0.43
1:C:366:LEU:CD2	1:C:496:MET:HE1	2.39	0.43
2:D:28:ASP:HB3	2:D:31:ARG:NH2	2.34	0.43
1:A:961:ILE:HG22	1:A:962:GLU:N	2.33	0.43
1:B:744:ASN:CG	10:B:1544:HOH:O	2.61	0.43
3:B:1101:LMT:O2'	3:B:1101:LMT:C1	2.67	0.43
1:C:428:LYS:HG3	1:C:494:ALA:HB1	2.00	0.43
1:A:524:THR:O	1:A:527:TYR:HB3	2.19	0.43
1:A:695:LEU:HD23	1:A:695:LEU:HA	1.85	0.43
1:A:717:ARG:NH1	4:A:1105:DM2:C19	2.82	0.43
1:A:961:ILE:HD11	1:A:1031:ARG:NH2	2.34	0.43
1:A:1036:LYS:HA	1:A:1037:ASN:HA	1.83	0.43
1:B:493:CYS:O	1:B:497:LEU:HB2	2.19	0.43
1:B:875:SER:O	1:B:879:ILE:HG13	2.19	0.43
1:C:721:LEU:HB2	1:C:814:PRO:HG2	2.00	0.43
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.54	0.43
1:A:450:SER:O	1:A:454:VAL:HG23	2.18	0.42
1:A:617:PHE:O	4:A:1105:DM2:H141	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:LYS:HE2	1:A:958:LYS:N	2.34	0.42
1:B:441:ALA:O	1:B:445:ILE:HG13	2.19	0.42
1:B:677:ALA:O	1:B:678:THR:CB	2.67	0.42
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.51	0.42
1:A:438:ILE:HD12	1:A:438:ILE:C	2.44	0.42
1:A:456:MET:HB3	10:A:1602:HOH:O	2.19	0.42
1:A:1012:VAL:HG12	1:A:1013:THR:N	2.34	0.42
1:B:378:GLY:C	1:B:480:LEU:HD21	2.44	0.42
1:B:618:ALA:HB1	1:B:719:ASN:O	2.19	0.42
1:B:678:THR:CA	1:B:837:THR:HG22	2.49	0.42
1:B:758:TYR:CE2	1:B:770:LYS:HE2	2.54	0.42
1:C:382:VAL:HG11	1:C:476:SER:OG	2.19	0.42
1:A:418:ARG:O	1:A:419:VAL:C	2.61	0.42
1:A:676:THR:HG21	4:A:1106:DM2:C1'	2.49	0.42
1:A:945:ILE:HG12	1:A:971:ARG:HG2	2.00	0.42
1:B:126:GLY:CA	1:C:116:PRO:HB3	2.46	0.42
1:C:897:ILE:N	1:C:898:PRO:CD	2.82	0.42
1:C:901:VAL:O	1:C:904:VAL:HG12	2.19	0.42
2:E:113:GLY:O	2:E:143:ASP:HA	2.19	0.42
1:A:456:MET:HG3	1:A:471:SER:HG	1.84	0.42
1:A:987:MET:CE	1:A:1008:MET:HE1	2.50	0.42
1:A:987:MET:CE	1:A:1008:MET:SD	2.76	0.42
1:A:176:GLN:HG2	1:A:615:PHE:CE1	2.55	0.42
1:A:881:LEU:HD12	3:A:1102:LMT:C11	2.50	0.42
1:A:898:PRO:O	1:A:902:MET:HG3	2.20	0.42
1:B:17:ILE:HD11	6:B:1105:D10:H42	2.01	0.42
1:B:672:VAL:HG12	7:B:1103:LMU:H61	1.97	0.42
1:B:678:THR:CA	1:B:837:THR:CG2	2.98	0.42
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.55	0.42
1:C:544:LEU:HD12	1:C:544:LEU:HA	1.77	0.42
2:D:82:THR:O	2:D:85:HIS:HB2	2.19	0.42
2:D:142:GLN:HA	2:D:147:LYS:O	2.18	0.42
1:B:874:PRO:CD	1:B:875:SER:H	2.33	0.42
1:C:447:MET:HB2	1:C:447:MET:HE3	1.79	0.42
1:A:987:MET:HB3	1:A:988:PRO:HD3	2.02	0.42
1:B:744:ASN:O	1:B:748:THR:CG2	2.64	0.42
1:C:281:PHE:CE2	1:C:324:VAL:HG21	2.54	0.42
2:E:73:VAL:HG13	2:E:74:ASN:OD1	2.19	0.42
1:A:281:PHE:O	1:A:284:GLN:HG2	2.20	0.42
1:A:418:ARG:HH21	1:A:970:MET:CE	2.33	0.42
1:A:575:MET:HG3	1:A:617:PHE:HD1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:SER:C	1:B:898:PRO:HD2	2.45	0.42
1:C:1011:MET:CE	1:C:1011:MET:CA	2.91	0.42
1:C:1013:THR:HB	1:C:1017:LEU:HD22	2.01	0.42
2:E:94:GLU:HG3	10:E:225:HOH:O	2.19	0.42
1:A:418:ARG:CZ	1:A:970:MET:HE2	2.50	0.42
1:A:895:TRP:CD1	6:A:1108:D10:H71	2.54	0.42
1:B:185:ARG:HD2	10:B:1528:HOH:O	2.20	0.42
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.90	0.42
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.50	0.42
1:C:743:ILE:CD1	1:C:747:ASN:OD1	2.68	0.42
1:C:894:SER:O	1:C:898:PRO:HG2	2.19	0.42
1:C:950:LYS:HE2	1:C:954:ASP:OD1	2.20	0.42
1:A:1035:ARG:HG3	1:A:1036:LYS:CE	2.50	0.42
1:B:454:VAL:N	1:B:455:PRO:CD	2.83	0.42
1:B:573:MET:HE2	1:B:573:MET:HB2	1.83	0.42
1:B:726:GLN:OE1	1:B:812:GLY:HA3	2.20	0.42
1:C:674:LEU:N	1:C:674:LEU:HD23	2.35	0.42
1:C:951:ASP:OD1	1:C:955:LYS:HE3	2.20	0.42
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.19	0.42
1:A:85:THR:O	1:A:85:THR:CG2	2.66	0.41
1:A:284:GLN:HB2	1:A:285:PRO:HD2	2.02	0.41
1:A:412:VAL:CG1	1:A:489:THR:HG22	2.47	0.41
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.38	0.41
1:C:366:LEU:O	1:C:369:THR:HB	2.21	0.41
2:D:126:LEU:HD22	2:D:164:ILE:HD12	2.02	0.41
1:A:1:MET:N	1:A:2:PRO:CD	2.84	0.41
1:A:307:ARG:NH1	10:A:1357:HOH:O	2.07	0.41
1:A:418:ARG:HH21	1:A:970:MET:HE1	1.84	0.41
1:A:448:VAL:O	1:A:451:ALA:HB3	2.21	0.41
1:A:845:GLU:HG2	1:A:857:TYR:OH	2.20	0.41
1:A:867:ARG:N	1:A:868:LEU:CG	2.63	0.41
1:B:960:LEU:HD22	1:B:1027:VAL:HG22	2.01	0.41
1:C:251:LEU:O	1:C:252:LYS:HB3	2.21	0.41
1:C:527:TYR:CE2	1:C:968:VAL:CG1	2.86	0.41
1:A:418:ARG:HE	1:A:970:MET:CE	2.34	0.41
1:A:456:MET:HE3	1:A:932:LEU:CD1	2.50	0.41
2:D:92:HIS:O	2:D:96:VAL:HG23	2.21	0.41
1:A:60:THR:CG2	1:A:119:PRO:CG	2.98	0.41
1:A:372:VAL:HB	1:A:373:PRO:CD	2.50	0.41
1:A:558:ARG:HA	1:A:558:ARG:HD3	1.82	0.41
1:B:478:MET:C	1:B:478:MET:SD	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:PHE:CD1	1:B:512:PHE:C	2.98	0.41
2:D:23:ARG:HB2	2:D:53:LEU:HG	2.01	0.41
1:A:891:LEU:HD12	3:A:1103:LMT:H11	2.00	0.41
1:A:952:LEU:O	1:A:956:GLU:HB2	2.21	0.41
2:E:160:ASP:O	2:E:164:ILE:HG13	2.21	0.41
1:B:307:ARG:NH1	1:B:328:ASP:OD2	2.51	0.41
1:B:542:LEU:O	1:B:546:LEU:HD13	2.20	0.41
1:C:21:LEU:C	1:C:21:LEU:CD1	2.94	0.41
2:E:31:ARG:O	2:E:32:ILE:C	2.63	0.41
1:A:307:ARG:NE	10:A:1366:HOH:O	2.42	0.41
1:A:554:TYR:CZ	1:A:558:ARG:NH1	2.89	0.41
1:A:586:ARG:HH22	1:A:660:ASP:C	2.27	0.41
1:A:867:ARG:N	1:A:868:LEU:CA	2.82	0.41
1:A:881:LEU:HD12	3:A:1102:LMT:H112	2.02	0.41
1:B:162:MET:O	1:B:166:ILE:HG12	2.20	0.41
1:B:165:ALA:HB3	1:B:313:MET:HE2	2.03	0.41
1:B:485:ALA:HA	1:B:489:THR:OG1	2.21	0.41
1:B:851:LEU:HB3	1:B:852:PRO:HD2	2.01	0.41
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.91	0.41
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.55	0.41
1:C:463:THR:CG2	1:C:467:TYR:CZ	3.04	0.41
1:C:670:ALA:HB3	1:C:862:MET:CE	2.51	0.41
1:A:670:ALA:CB	10:A:1623:HOH:O	2.69	0.41
4:A:1105:DM2:O8	4:A:1105:DM2:C2'	2.56	0.41
1:B:458:PHE:CD2	3:B:1101:LMT:H41	2.56	0.41
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.51	0.41
1:B:940:LYS:HG2	10:B:1356:HOH:O	2.21	0.41
2:E:89:HIS:CG	2:E:119:LEU:HG	2.56	0.41
1:A:919:ARG:HH11	1:A:919:ARG:HG2	1.73	0.40
1:B:366:LEU:HD22	1:B:366:LEU:HA	1.89	0.40
1:B:575:MET:HE3	10:B:1517:HOH:O	2.21	0.40
1:C:637:ARG:N	1:C:638:PRO:CD	2.84	0.40
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.21	0.40
1:A:727:PHE:CE2	1:A:729:ILE:HG12	2.56	0.40
1:A:1007:VAL:O	1:A:1011:MET:HG2	2.21	0.40
1:A:1036:LYS:CA	1:A:1037:ASN:CB	2.99	0.40
1:B:657:GLN:OE1	1:B:657:GLN:HA	2.21	0.40
1:B:866:GLU:O	1:B:868:LEU:N	2.54	0.40
1:C:1:MET:N	1:C:2:PRO:CD	2.83	0.40
1:C:483:LEU:HD12	1:C:483:LEU:HA	1.90	0.40
1:C:799:VAL:CG2	1:C:804:PHE:HE1	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:ARG:CZ	10:C:1596:HOH:O	2.49	0.40
2:E:34:MET:SD	2:E:40:VAL:HG12	2.62	0.40
1:A:13:TRP:HH2	1:A:370:ILE:HD13	1.86	0.40
1:A:326:PRO:O	1:A:630:SER:HB2	2.21	0.40
1:A:575:MET:HG3	1:A:617:PHE:CD1	2.56	0.40
1:A:672:VAL:HG22	1:A:673:GLU:N	2.02	0.40
1:C:739:LEU:HD12	1:C:739:LEU:N	2.35	0.40
2:D:42:ALA:O	2:D:50:PRO:HD3	2.21	0.40
2:E:150:PHE:HA	2:E:165:LEU:HD12	2.03	0.40
1:A:510:LYS:HD2	1:A:511:GLY:H	1.84	0.40
1:A:540:ARG:HG2	1:A:541:TYR:CE1	2.57	0.40
1:A:956:GLU:OE2	1:A:956:GLU:CA	2.69	0.40
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.40
1:C:21:LEU:HD12	1:C:22:ALA:H	1.85	0.40
1:C:284:GLN:HG3	1:C:285:PRO:HD2	2.03	0.40
1:C:947:GLU:HG3	1:C:948:PHE:N	2.36	0.40
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.51	0.40
1:B:672:VAL:HG23	1:B:673:GLU:OE2	2.20	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	1040/1057 (98%)	979 (94%)	47 (4%)	14 (1%)	9	6
1	B	1031/1057 (98%)	997 (97%)	29 (3%)	5 (0%)	24	24
1	C	1034/1057 (98%)	997 (96%)	35 (3%)	2 (0%)	43	50
2	D	154/169 (91%)	151 (98%)	3 (2%)	0	100	100
2	E	150/169 (89%)	141 (94%)	7 (5%)	2 (1%)	9	6
All	All	3409/3509 (97%)	3265 (96%)	121 (4%)	23 (1%)	18	17

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	617	PHE
1	A	672	VAL
1	A	677	ALA
1	B	659	LYS
1	C	510	LYS
1	A	960	LEU
1	A	1037	ASN
1	B	256	ASP
1	B	867	ARG
1	A	837	THR
1	A	955	LYS
1	A	1040	ILE
1	A	1041	GLU
1	B	869	SER
1	C	1035	ARG
2	E	29	GLU
1	A	958	LYS
1	A	674	LEU
1	A	1025	PHE
2	E	28	ASP
1	B	874	PRO
1	A	419	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/863 (98%)	778 (92%)	70 (8%)	10	8
1	B	839/863 (97%)	777 (93%)	62 (7%)	13	11
1	C	842/863 (98%)	789 (94%)	53 (6%)	16	16
2	D	120/132 (91%)	114 (95%)	6 (5%)	22	24
2	E	117/132 (89%)	111 (95%)	6 (5%)	21	23
All	All	2766/2853 (97%)	2569 (93%)	197 (7%)	13	12

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	30	LEU
1	A	37	THR
1	A	38	ILE
1	A	60	THR
1	A	113	LEU
1	A	121	GLU
1	A	127	VAL
1	A	214	VAL
1	A	229	GLN
1	A	240	LEU
1	A	262	LEU
1	A	263	ARG
1	A	270	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	343	THR
1	A	366	LEU
1	A	376	LEU
1	A	428	LYS
1	A	429	GLU
1	A	431	THR
1	A	449	LEU
1	A	452	VAL
1	A	472	ILE
1	A	483	LEU
1	A	492	LEU
1	A	505	HIS
1	A	522	LYS
1	A	530	SER
1	A	538	THR
1	A	540	ARG
1	A	557	VAL
1	A	577	GLN
1	A	630	SER
1	A	649	MET
1	A	659	LYS
1	A	672	VAL
1	A	673	GLU
1	A	678	THR
1	A	695	LEU

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Mol	Chain	Res	Type
1	A	708	LYS
1	A	711	ASP
1	A	713	LEU
1	A	715	SER
1	A	717	ARG
1	A	828	LEU
1	A	836	SER
1	A	839	GLU
1	A	866	GLU
1	A	868	LEU
1	A	879	ILE
1	A	881	LEU
1	A	902	MET
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	946	VAL
1	A	968	VAL
1	A	971	ARG
1	A	972	LEU
1	A	984	LEU
1	A	987	MET
1	A	991	ILE
1	A	1005	THR
1	A	1012	VAL
1	A	1027	VAL
1	A	1030	ARG
1	A	1040	ILE
1	B	21	LEU
1	B	30	LEU
1	B	75	LEU
1	B	88	VAL
1	B	108	GLN
1	B	111	LEU
1	B	121	GLU
1	B	172	VAL
1	B	240	LEU
1	B	250	LEU
1	B	255	GLN
1	B	261	LEU
1	B	270	LEU
1	B	274	ASN

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Mol	Chain	Res	Type
1	B	293	LEU
1	B	330	THR
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	377	LEU
1	B	399	VAL
1	B	402	ILE
1	B	429	GLU
1	B	468	ARG
1	B	480	LEU
1	B	497	LEU
1	B	510	LYS
1	B	522	LYS
1	B	537	SER
1	B	555	LEU
1	B	574	THR
1	B	578	LEU
1	B	600	THR
1	B	633	ASP
1	B	641	GLU
1	B	653	ARG
1	B	659	LYS
1	B	660	ASP
1	B	672	VAL
1	B	695	LEU
1	B	713	LEU
1	B	714	THR
1	B	748	THR
1	B	801	PHE
1	B	866	GLU
1	B	869	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	907	LEU
1	B	914	LEU
1	B	919	ARG
1	B	921	LEU
1	B	937	LEU
1	B	960	LEU
1	B	965	LEU

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Mol	Chain	Res	Type
1	B	972	LEU
1	B	980	LEU
1	B	992	SER
1	B	1003	VAL
1	B	1022	VAL
1	B	1030	ARG
1	C	21	LEU
1	C	38	ILE
1	C	75	LEU
1	C	95	GLU
1	C	96	SER
1	C	113	LEU
1	C	121	GLU
1	C	125	GLN
1	C	127	VAL
1	C	133	SER
1	C	135	SER
1	C	152	GLU
1	C	177	LEU
1	C	193	LEU
1	C	244	GLU
1	C	255	GLN
1	C	289	LEU
1	C	310	LEU
1	C	324	VAL
1	C	344	LEU
1	C	383	LEU
1	C	404	LEU
1	C	425	LEU
1	C	483	LEU
1	C	544	LEU
1	C	558	ARG
1	C	564	LEU
1	C	671	ILE
1	C	673	GLU
1	C	676	THR
1	C	690	LEU
1	C	695	LEU
1	C	702	LEU
1	C	717	ARG
1	C	743	ILE
1	C	750	LEU

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Mol	Chain	Res	Type
1	C	784	ASP
1	C	799	VAL
1	C	811	TYR
1	C	822	LEU
1	C	828	LEU
1	C	853	THR
1	C	867	ARG
1	C	876	LEU
1	C	891	LEU
1	C	960	LEU
1	C	968	VAL
1	C	976	LEU
1	C	980	LEU
1	C	1011	MET
1	C	1017	LEU
1	C	1035	ARG
1	C	1036	LYS
2	D	45	VAL
2	D	53	LEU
2	D	61	GLU
2	D	79	LEU
2	D	94	GLU
2	D	154	ILE
2	E	29	GLU
2	E	34	MET
2	E	79	LEU
2	E	119	LEU
2	E	123	ARG
2	E	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	194	ASN
1	A	284	GLN
1	A	569	GLN
1	B	70	ASN
1	B	81	ASN
1	B	197	GLN
1	B	231	ASN
1	B	274	ASN

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Mol	Chain	Res	Type
1	B	469	GLN
1	B	1001	ASN
1	C	63	GLN
1	C	120	GLN
1	C	125	GLN
1	C	231	ASN
1	C	255	GLN
1	C	605	ASN
1	C	642	ASN
1	C	737	GLN
2	D	140	ASN
2	E	69	ASN
2	E	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	$\# Z > 2$
7	LMU	B	1103	-	36,36,36	1.25	4 (11%)	47,47,47	1.22	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	B	1101	-	36,36,36	1.25	4 (11%)	47,47,47	1.33	5 (10%)
4	DM2	A	1105	-	42,43,43	2.54	12 (28%)	56,67,67	1.39	7 (12%)
3	LMT	B	1102	-	36,36,36	1.19	4 (11%)	47,47,47	1.16	4 (8%)
3	LMT	A	1104	-	36,36,36	1.23	4 (11%)	47,47,47	0.99	4 (8%)
9	HEX	C	1105	-	5,5,5	0.27	0	4,4,4	0.61	0
4	DM2	B	1104	-	42,43,43	2.56	12 (28%)	56,67,67	1.46	7 (12%)
5	D12	C	1106	-	11,11,11	0.39	0	10,10,10	0.87	0
6	D10	C	1104	-	9,9,9	0.31	0	8,8,8	0.73	0
3	LMT	A	1101	-	36,36,36	1.22	4 (11%)	47,47,47	1.28	6 (12%)
3	LMT	A	1103	-	36,36,36	1.16	3 (8%)	47,47,47	1.23	5 (10%)
9	HEX	B	1108	-	5,5,5	0.25	0	4,4,4	0.58	0
6	D10	A	1109	-	9,9,9	0.32	0	8,8,8	0.70	0
5	D12	C	1102	-	11,11,11	0.21	0	10,10,10	0.56	0
3	LMT	C	1101	-	36,36,36	1.17	4 (11%)	47,47,47	1.09	3 (6%)
3	LMT	A	1102	-	36,36,36	1.21	4 (11%)	47,47,47	1.15	4 (8%)
8	GOL	B	1107	-	5,5,5	0.38	0	5,5,5	0.14	0
8	GOL	C	1103	-	5,5,5	0.45	0	5,5,5	0.56	0
8	GOL	B	1106	-	5,5,5	0.33	0	5,5,5	0.56	0
5	D12	A	1107	-	11,11,11	0.37	0	10,10,10	0.86	0
6	D10	B	1105	-	9,9,9	0.39	0	8,8,8	0.85	0
5	D12	B	1109	-	11,11,11	0.30	0	10,10,10	0.73	0
6	D10	A	1108	-	9,9,9	0.35	0	8,8,8	0.77	0
4	DM2	A	1106	-	42,43,43	2.55	13 (30%)	56,67,67	1.72	11 (19%)

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
7	LMU	B	1103	-	-	6/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	11/21/61/61	0/2/2/2
4	DM2	A	1105	-	-	6/13/60/60	0/5/5/5
3	LMT	B	1102	-	-	12/21/61/61	0/2/2/2
3	LMT	A	1104	-	-	14/21/61/61	0/2/2/2
9	HEX	C	1105	-	-	0/3/3/3	-
4	DM2	B	1104	-	-	6/13/60/60	0/5/5/5
5	D12	C	1106	-	-	2/9/9/9	-
6	D10	C	1104	-	-	0/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
3	LMT	A	1103	-	-	15/21/61/61	0/2/2/2
9	HEX	B	1108	-	-	0/3/3/3	-
6	D10	A	1109	-	-	0/7/7/7	-
5	D12	C	1102	-	-	1/9/9/9	-
3	LMT	C	1101	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	13/21/61/61	0/2/2/2
8	GOL	B	1107	-	-	3/4/4/4	-
8	GOL	C	1103	-	-	3/4/4/4	-
8	GOL	B	1106	-	-	4/4/4/4	-
5	D12	A	1107	-	-	2/9/9/9	-
6	D10	B	1105	-	-	1/7/7/7	-
5	D12	B	1109	-	-	0/9/9/9	-
6	D10	A	1108	-	-	1/7/7/7	-
4	DM2	A	1106	-	-	2/13/60/60	0/5/5/5

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	DM2	O6-C6	8.62	1.38	1.22
4	A	1105	DM2	O6-C6	8.54	1.38	1.22
4	A	1106	DM2	O6-C6	8.49	1.38	1.22
4	B	1104	DM2	O19-C19	7.70	1.36	1.22
4	A	1105	DM2	O19-C19	7.64	1.36	1.22
4	A	1106	DM2	O19-C19	7.61	1.36	1.22
4	A	1105	DM2	C8-C9	6.98	1.51	1.40
4	A	1106	DM2	C8-C9	6.97	1.51	1.40
4	B	1104	DM2	C8-C9	6.78	1.51	1.40
3	A	1101	LMT	O5B-C1B	3.96	1.52	1.41
3	A	1102	LMT	O5B-C1B	3.91	1.51	1.41
3	B	1101	LMT	O5B-C1B	3.90	1.51	1.41
3	A	1104	LMT	O5B-C1B	3.84	1.51	1.41
3	B	1102	LMT	O5B-C1B	3.72	1.51	1.41
7	B	1103	LMU	O5B-C1B	3.69	1.51	1.41
3	C	1101	LMT	O5B-C1B	3.68	1.51	1.41
3	A	1103	LMT	O5B-C1B	3.67	1.51	1.41
4	A	1105	DM2	C17-C16	3.58	1.45	1.40
7	B	1103	LMU	C3'-C4'	-3.58	1.42	1.52
4	B	1104	DM2	C17-C16	3.56	1.45	1.40
4	A	1105	DM2	C5-C6	3.25	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1104	DM2	C5-C6	3.25	1.55	1.47
4	A	1106	DM2	C4'-C5'	-3.24	1.45	1.52
4	A	1106	DM2	C5-C6	3.23	1.55	1.47
4	A	1106	DM2	C9-C16	-3.15	1.34	1.39
3	B	1102	LMT	C3'-C4'	-3.14	1.43	1.52
3	B	1101	LMT	C3'-C4'	-3.11	1.43	1.52
3	C	1101	LMT	C3'-C4'	-3.07	1.43	1.52
4	B	1104	DM2	C4'-C5'	-3.01	1.45	1.52
3	A	1104	LMT	C3'-C4'	-3.00	1.44	1.52
3	A	1102	LMT	C3'-C4'	-3.00	1.44	1.52
4	A	1105	DM2	C9-C16	-2.88	1.35	1.39
3	A	1101	LMT	C3'-C4'	-2.87	1.44	1.52
4	B	1104	DM2	C9-C16	-2.85	1.35	1.39
3	A	1103	LMT	C3'-C4'	-2.79	1.44	1.52
4	A	1106	DM2	C17-C16	2.76	1.44	1.40
4	A	1106	DM2	O10-C10	-2.60	1.40	1.44
4	B	1104	DM2	C2'-C1'	2.57	1.57	1.50
4	A	1105	DM2	C4'-C5'	-2.51	1.47	1.52
3	B	1101	LMT	C3B-C2B	-2.46	1.45	1.52
3	A	1101	LMT	C3B-C2B	-2.46	1.46	1.52
4	B	1104	DM2	O4-C4	2.45	1.41	1.37
3	A	1102	LMT	C3B-C2B	-2.44	1.46	1.52
4	A	1106	DM2	C15-C16	2.43	1.55	1.51
4	B	1104	DM2	C15-C16	2.43	1.55	1.51
4	A	1106	DM2	C2'-C1'	2.38	1.56	1.50
3	A	1104	LMT	C3B-C2B	-2.34	1.46	1.52
3	A	1103	LMT	C3B-C2B	-2.33	1.46	1.52
4	A	1106	DM2	C7-C6	2.29	1.53	1.47
3	B	1102	LMT	O5'-C5'	2.27	1.49	1.44
7	B	1103	LMU	O3'-C3'	2.26	1.48	1.43
3	A	1104	LMT	O5'-C5'	2.25	1.49	1.44
4	A	1106	DM2	O8-C8	2.24	1.42	1.36
3	A	1101	LMT	O5'-C5'	2.22	1.49	1.44
3	B	1101	LMT	O5'-C5'	2.20	1.49	1.44
4	A	1105	DM2	O4-C4	2.20	1.40	1.37
3	C	1101	LMT	O5'-C5'	2.19	1.49	1.44
4	A	1106	DM2	O4-C4	2.18	1.40	1.37
7	B	1103	LMU	C3'-C2'	-2.18	1.46	1.52
4	A	1105	DM2	C15-C16	2.16	1.54	1.51
3	B	1102	LMT	C3B-C2B	-2.15	1.46	1.52
3	C	1101	LMT	C3B-C2B	-2.14	1.46	1.52
4	A	1105	DM2	C7-C6	2.14	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1105	DM2	O10-C10	-2.14	1.41	1.44
4	B	1104	DM2	O8-C8	2.10	1.41	1.36
4	B	1104	DM2	C7-C6	2.04	1.52	1.47
3	A	1102	LMT	O5'-C5'	2.02	1.49	1.44
4	A	1105	DM2	C2'-C1'	2.01	1.56	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1106	DM2	O4-C4-C5	4.82	122.67	115.84
3	B	1101	LMT	C1-O1'-C1'	4.50	121.36	113.68
4	A	1106	DM2	C4-C5-C6	4.19	127.83	122.22
4	A	1106	DM2	O4-C4-C3	-4.13	117.33	124.30
3	B	1101	LMT	C1B-O1B-C4'	-4.03	108.43	117.98
4	B	1104	DM2	O4-C4-C5	3.95	121.44	115.84
4	A	1106	DM2	C1-C20-C19	-3.90	113.18	119.26
4	A	1105	DM2	O4-C4-C5	3.86	121.31	115.84
3	A	1103	LMT	C2'-C3'-C4'	3.84	118.39	109.68
3	A	1101	LMT	O5B-C5B-C4B	3.76	116.48	109.70
3	B	1102	LMT	C1-O1'-C1'	3.69	119.98	113.68
4	B	1104	DM2	C21-O4-C4	3.68	122.91	117.51
3	A	1101	LMT	C1-O1'-C1'	3.45	119.57	113.68
3	A	1102	LMT	O5B-C5B-C4B	3.45	115.91	109.70
4	A	1105	DM2	O4-C4-C3	-3.43	118.51	124.30
4	A	1105	DM2	C4-C5-C6	3.32	126.67	122.22
3	A	1104	LMT	C1-O1'-C1'	3.29	119.29	113.68
3	A	1103	LMT	C1B-O1B-C4'	-3.28	110.21	117.98
4	B	1104	DM2	O4-C4-C3	-3.27	118.78	124.30
3	C	1101	LMT	C1-O1'-C1'	3.26	119.25	113.68
3	A	1103	LMT	C1'-C2'-C3'	3.17	116.67	110.01
4	B	1104	DM2	C4-C5-C6	3.06	126.32	122.22
3	A	1101	LMT	C3B-C4B-C5B	3.02	115.71	110.23
4	B	1104	DM2	C1-C20-C19	-2.67	115.09	119.26
3	C	1101	LMT	O1'-C1-C2	2.67	118.41	109.37
4	A	1106	DM2	C7-C18-C17	2.65	123.45	119.65
4	A	1106	DM2	C5-C20-C19	2.64	124.09	120.69
3	B	1102	LMT	O1'-C1-C2	2.64	118.31	109.37
7	B	1103	LMU	O5'-C1'-C2'	2.62	115.75	110.37
4	A	1106	DM2	C20-C5-C6	-2.62	115.87	119.87
3	A	1102	LMT	C3B-C4B-C5B	2.61	114.97	110.23
4	A	1106	DM2	C15-C16-C17	-2.59	114.48	119.22
4	A	1105	DM2	C20-C5-C6	-2.58	115.92	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1101	LMT	C1B-O1B-C4'	-2.53	111.98	117.98
3	A	1104	LMT	O1'-C1-C2	2.51	117.88	109.37
4	A	1106	DM2	O10-C1'-C2'	2.48	113.05	108.28
3	B	1102	LMT	O6B-C6B-C5B	2.44	119.63	111.33
3	A	1103	LMT	O5'-C1'-C2'	2.43	115.37	110.37
3	A	1101	LMT	C1B-O5B-C5B	2.41	118.42	113.72
3	B	1102	LMT	C1B-O1B-C4'	-2.39	112.30	117.98
7	B	1103	LMU	C3B-C4B-C5B	2.38	114.55	110.23
3	B	1101	LMT	O1'-C1-C2	2.35	117.34	109.37
7	B	1103	LMU	C1-O1'-C1'	2.29	117.60	113.68
3	B	1101	LMT	O1'-C1'-C2'	2.29	111.76	108.27
4	B	1104	DM2	C20-C5-C6	-2.25	116.42	119.87
3	A	1102	LMT	O1'-C1-C2	2.22	116.91	109.37
3	A	1102	LMT	O6B-C6B-C5B	2.21	118.84	111.33
4	A	1105	DM2	C1-C20-C19	-2.19	115.85	119.26
7	B	1103	LMU	O1'-C1-C2	2.14	116.64	109.37
3	A	1101	LMT	C1B-O1B-C4'	-2.14	112.91	117.98
7	B	1103	LMU	C4B-C3B-C2B	2.14	114.58	110.83
3	A	1104	LMT	O6'-C6'-C5'	2.13	118.60	111.33
3	A	1104	LMT	O1B-C4'-C5'	2.12	115.04	109.48
7	B	1103	LMU	C1B-O5B-C5B	-2.11	109.60	113.72
3	B	1101	LMT	O5B-C5B-C4B	2.08	113.45	109.70
4	A	1105	DM2	C15-C16-C17	-2.08	115.42	119.22
4	A	1106	DM2	O6-C6-C5	-2.05	118.02	121.44
3	A	1101	LMT	O6B-C6B-C5B	2.04	118.29	111.33
7	B	1103	LMU	O6'-C6'-C5'	2.02	118.20	111.33
4	B	1104	DM2	C15-C16-C17	-2.02	115.53	119.22
4	A	1105	DM2	O5'-C5'-C4'	2.01	113.18	109.55
3	A	1103	LMT	O1'-C1-C2	2.01	116.19	109.37
4	A	1106	DM2	C17-C18-C19	-2.01	117.22	120.46
7	B	1103	LMU	O5'-C5'-C6'	2.01	111.41	106.44

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	O5'-C1'-O1'-C1
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1104	LMT	O5'-C1'-O1'-C1
3	B	1101	LMT	O5'-C1'-O1'-C1
4	A	1105	DM2	C2'-C1'-O10-C10

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Mol	Chain	Res	Type	Atoms
4	A	1105	DM2	O5'-C1'-O10-C10
4	A	1105	DM2	C11-C12-C13-O13
4	A	1105	DM2	C11-C12-C13-C14
4	A	1105	DM2	O12-C12-C13-O13
4	B	1104	DM2	O5'-C1'-O10-C10
7	B	1103	LMU	C2-C1-O1'-C1'
8	B	1106	GOL	O1-C1-C2-O2
8	B	1106	GOL	C1-C2-C3-O3
8	B	1107	GOL	O1-C1-C2-C3
8	C	1103	GOL	O1-C1-C2-C3
3	A	1104	LMT	C5'-C4'-O1B-C1B
4	B	1104	DM2	C5-C4-O4-C21
3	B	1101	LMT	O5B-C1B-O1B-C4'
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	B	1102	LMT	O5B-C5B-C6B-O6B
3	C	1101	LMT	O5B-C5B-C6B-O6B
3	A	1104	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	O5B-C5B-C6B-O6B
3	A	1104	LMT	C4-C5-C6-C7
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	B	1101	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	C4B-C5B-C6B-O6B
3	A	1104	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	O5'-C1'-O1'-C1
3	A	1104	LMT	O5'-C5'-C6'-O6'
3	A	1104	LMT	C1-C2-C3-C4
3	A	1104	LMT	C4'-C5'-C6'-O6'
3	B	1102	LMT	C2'-C1'-O1'-C1
3	A	1104	LMT	C11-C10-C9-C8
3	A	1103	LMT	C4'-C5'-C6'-O6'
4	B	1104	DM2	C3-C4-O4-C21
3	C	1101	LMT	C4B-C5B-C6B-O6B
3	B	1102	LMT	O1'-C1-C2-C3
3	C	1101	LMT	O1'-C1-C2-C3
3	A	1101	LMT	O1'-C1-C2-C3
3	B	1102	LMT	O5'-C5'-C6'-O6'
3	A	1103	LMT	O1'-C1-C2-C3
3	A	1102	LMT	O5B-C5B-C6B-O6B
3	A	1103	LMT	C2'-C1'-O1'-C1
8	B	1106	GOL	O1-C1-C2-C3
3	A	1104	LMT	C2B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
3	B	1101	LMT	C2-C1-O1'-C1'
8	B	1107	GOL	O1-C1-C2-O2
8	C	1103	GOL	O1-C1-C2-O2
3	A	1104	LMT	O5B-C1B-O1B-C4'
3	A	1103	LMT	C1-C2-C3-C4
3	A	1102	LMT	C4-C5-C6-C7
3	B	1102	LMT	C5-C6-C7-C8
3	A	1103	LMT	C3'-C4'-O1B-C1B
7	B	1103	LMU	C4-C5-C6-C7
3	A	1102	LMT	C5-C6-C7-C8
5	C	1102	D12	C11-C10-C9-C8
3	B	1102	LMT	C3-C4-C5-C6
3	B	1102	LMT	C11-C10-C9-C8
3	B	1102	LMT	C4-C5-C6-C7
3	A	1103	LMT	C6-C7-C8-C9
7	B	1103	LMU	C3-C4-C5-C6
3	A	1101	LMT	C11-C10-C9-C8
3	A	1102	LMT	C6-C7-C8-C9
3	A	1103	LMT	C5'-C4'-O1B-C1B
4	B	1104	DM2	C12-C13-C14-O14
3	A	1103	LMT	C5-C6-C7-C8
7	B	1103	LMU	C11-C10-C9-C8
3	C	1101	LMT	C1-C2-C3-C4
3	A	1102	LMT	O5'-C5'-C6'-O6'
3	B	1101	LMT	C2'-C1'-O1'-C1
3	A	1103	LMT	C11-C10-C9-C8
3	A	1102	LMT	O5B-C1B-O1B-C4'
7	B	1103	LMU	C1-C2-C3-C4
3	C	1101	LMT	C3-C4-C5-C6
3	A	1102	LMT	C2-C1-O1'-C1'
3	C	1101	LMT	C2-C1-O1'-C1'
8	B	1106	GOL	O2-C2-C3-O3
4	A	1105	DM2	C15-C12-C13-C14
3	A	1101	LMT	C1-C2-C3-C4
3	A	1101	LMT	O5'-C1'-O1'-C1
3	A	1102	LMT	C4B-C5B-C6B-O6B
3	C	1101	LMT	C4-C5-C6-C7
3	B	1101	LMT	C3-C4-C5-C6
3	C	1101	LMT	O5'-C5'-C6'-O6'
7	B	1103	LMU	C5-C6-C7-C8
4	B	1104	DM2	O13-C13-C14-O14
3	A	1104	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
4	B	1104	DM2	C11-C10-O10-C1'
3	A	1103	LMT	C9-C10-C11-C12
3	A	1103	LMT	C4-C5-C6-C7
3	A	1103	LMT	C3-C4-C5-C6
3	C	1101	LMT	C6-C7-C8-C9
3	A	1104	LMT	C2-C3-C4-C5
3	A	1104	LMT	C6-C7-C8-C9
3	B	1101	LMT	C4-C5-C6-C7
6	B	1105	D10	C2-C3-C4-C5
6	A	1108	D10	C7-C8-C9-C10
3	A	1102	LMT	C3-C4-C5-C6
5	A	1107	D12	C2-C3-C4-C5
3	A	1101	LMT	C7-C8-C9-C10
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	C2'-C1'-O1'-C1
3	B	1101	LMT	C1-C2-C3-C4
3	B	1102	LMT	O5B-C1B-O1B-C4'
8	C	1103	GOL	O2-C2-C3-O3
3	B	1102	LMT	C2B-C1B-O1B-C4'
8	B	1107	GOL	C1-C2-C3-O3
5	C	1106	D12	C11-C10-C9-C8
3	A	1102	LMT	C2B-C1B-O1B-C4'
3	C	1101	LMT	C7-C8-C9-C10
3	B	1101	LMT	C6-C7-C8-C9
3	C	1101	LMT	C2-C3-C4-C5
3	A	1102	LMT	C1-C2-C3-C4
5	C	1106	D12	C7-C8-C9-C10
5	A	1107	D12	C11-C10-C9-C8
4	A	1106	DM2	C15-C12-C13-C14
4	A	1106	DM2	C11-C10-O10-C1'
3	B	1101	LMT	C9-C10-C11-C12

There are no ring outliers.

17 monomers are involved in 108 short contacts:

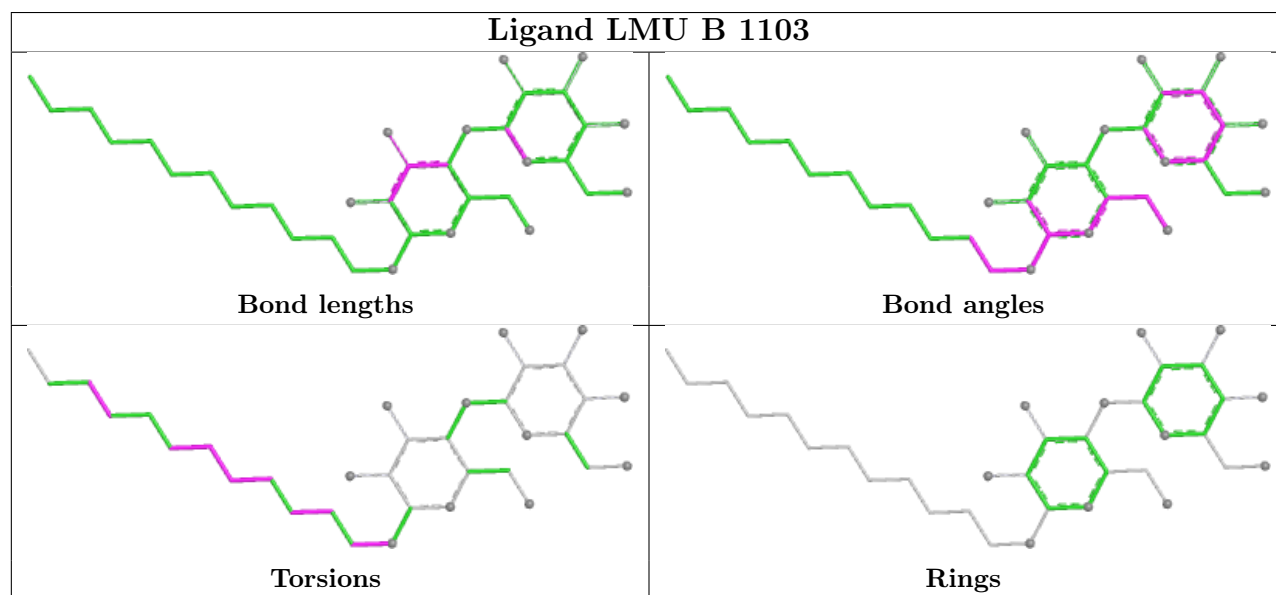
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1103	LMU	4	0
3	B	1101	LMT	10	0
4	A	1105	DM2	35	0
3	B	1102	LMT	4	0
3	A	1104	LMT	6	0
4	B	1104	DM2	9	0

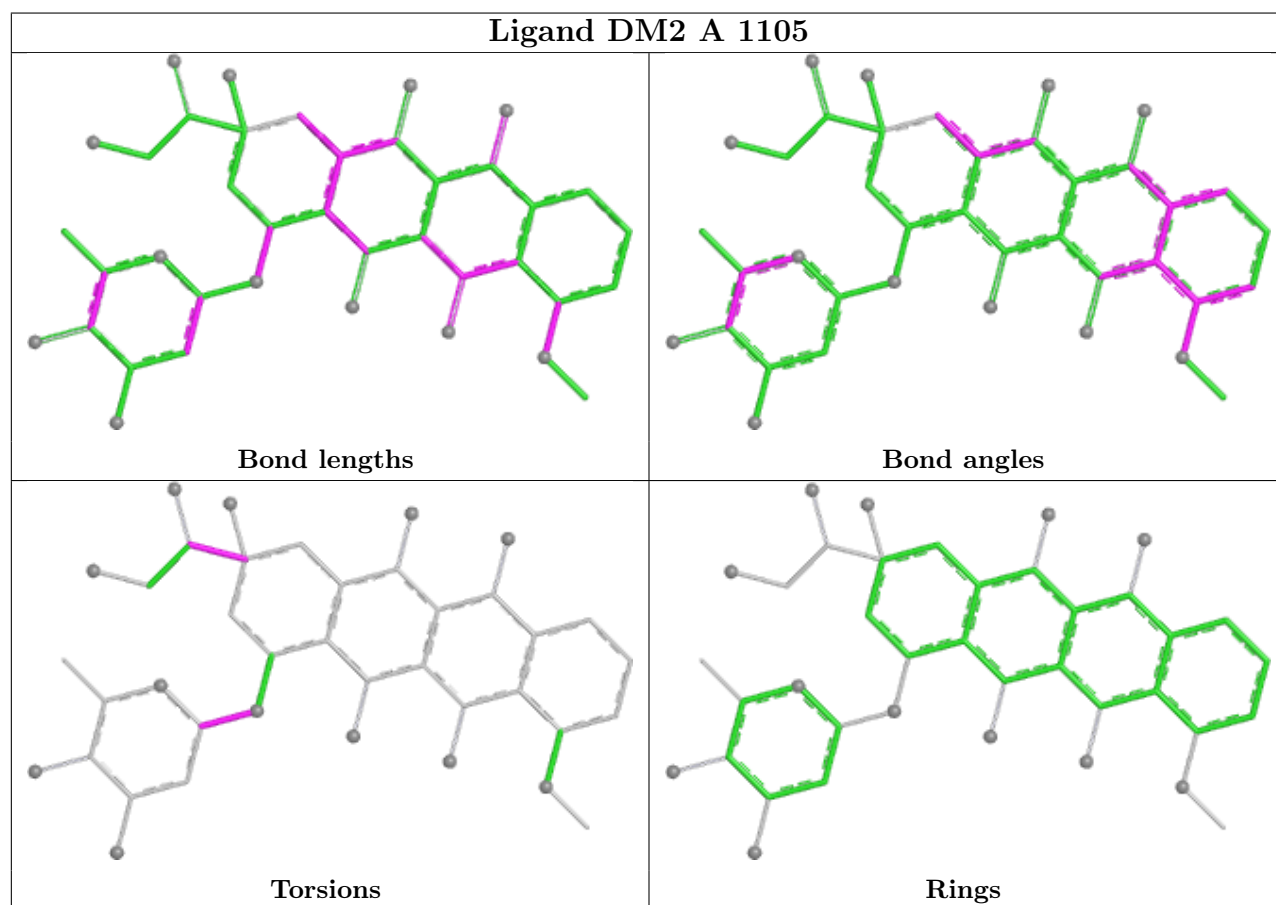
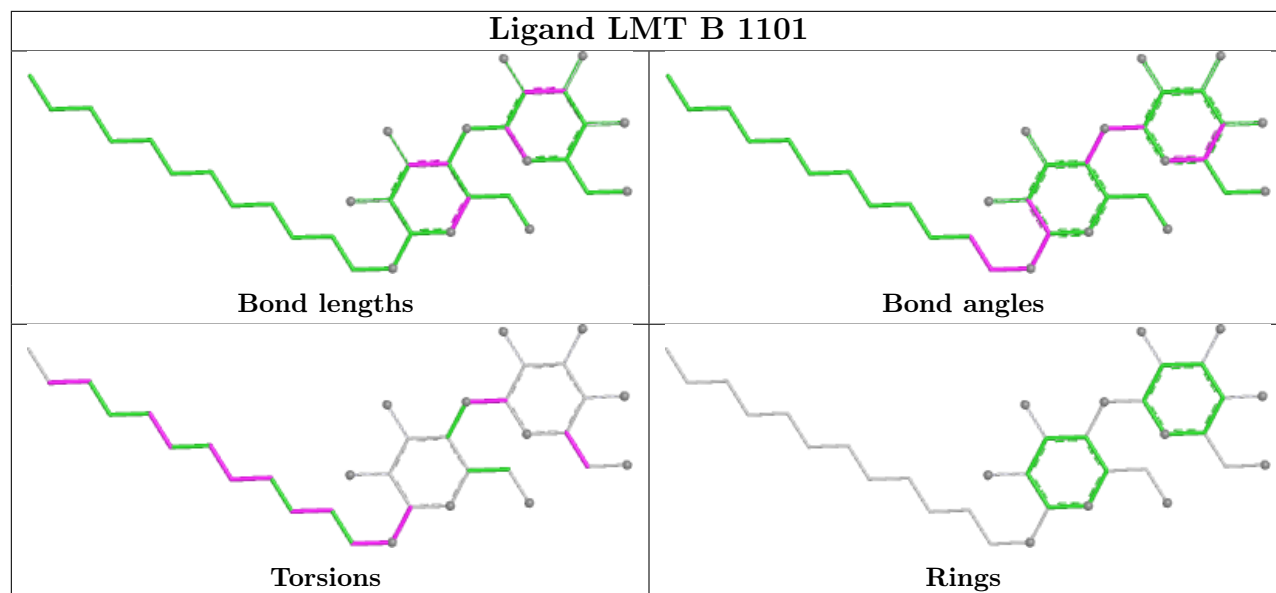
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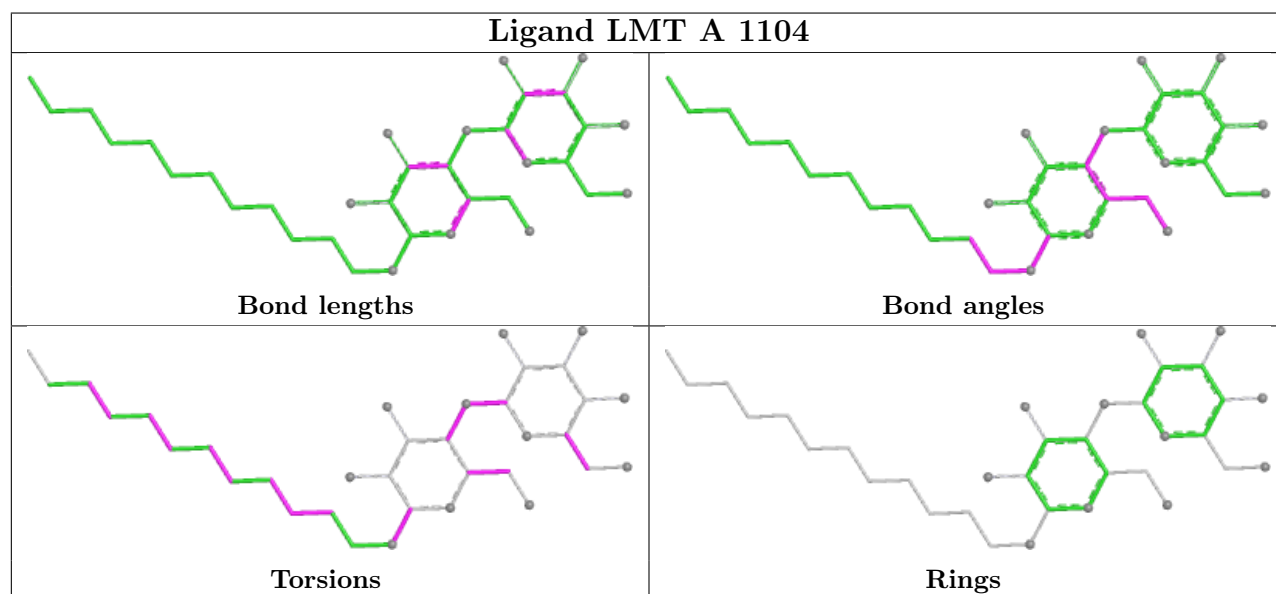
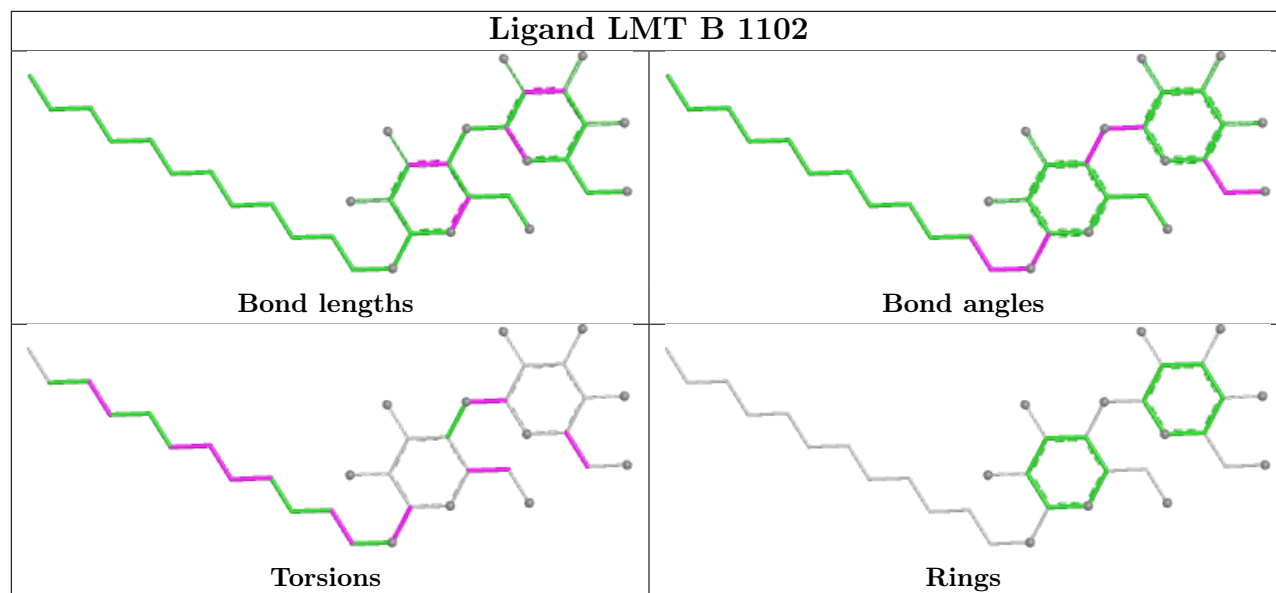
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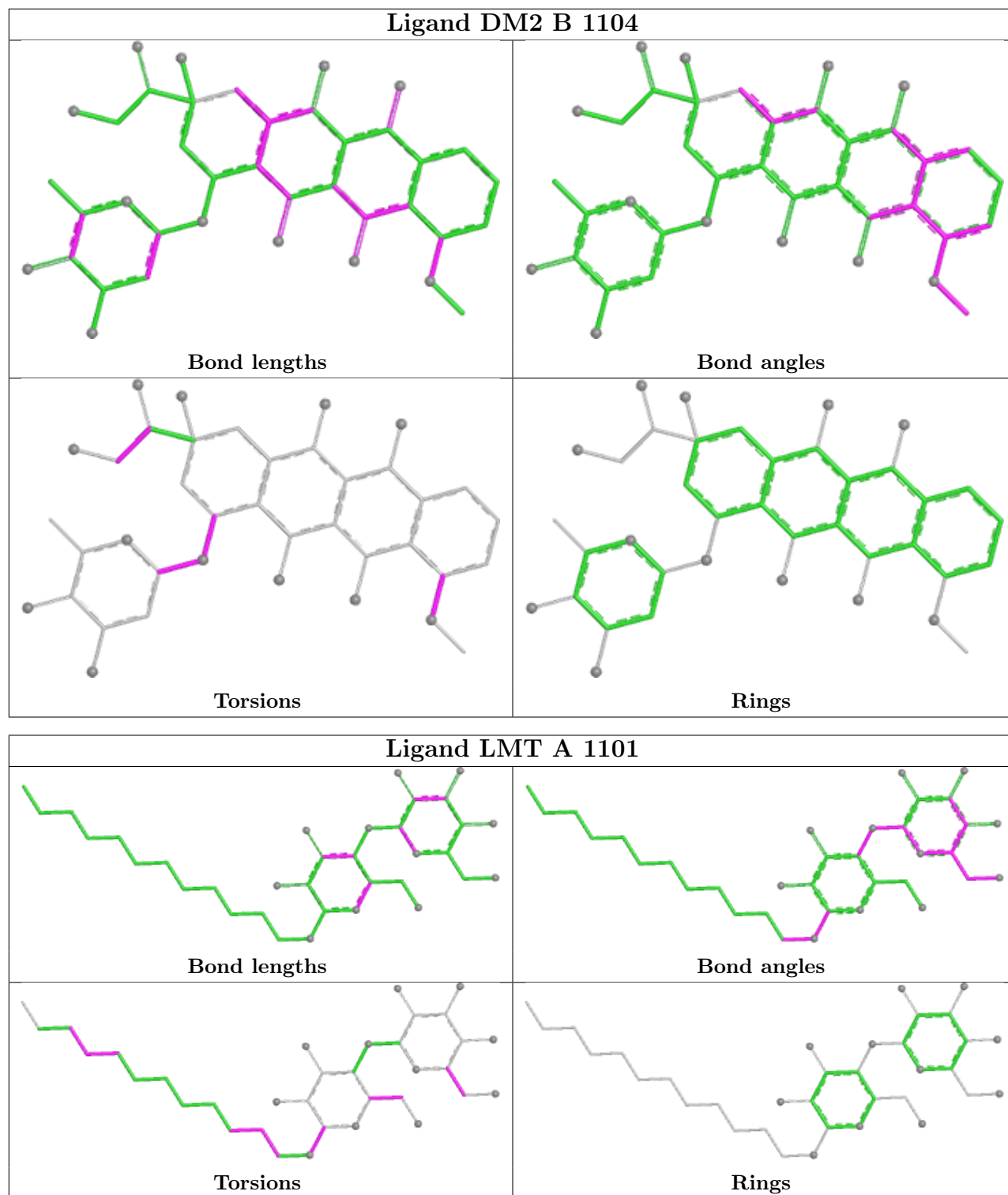
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	LMT	3	0
3	A	1103	LMT	10	0
5	C	1102	D12	2	0
3	C	1101	LMT	1	0
3	A	1102	LMT	8	0
8	C	1103	GOL	1	0
8	B	1106	GOL	1	0
5	A	1107	D12	3	0
6	B	1105	D10	1	0
6	A	1108	D10	2	0
4	A	1106	DM2	12	0

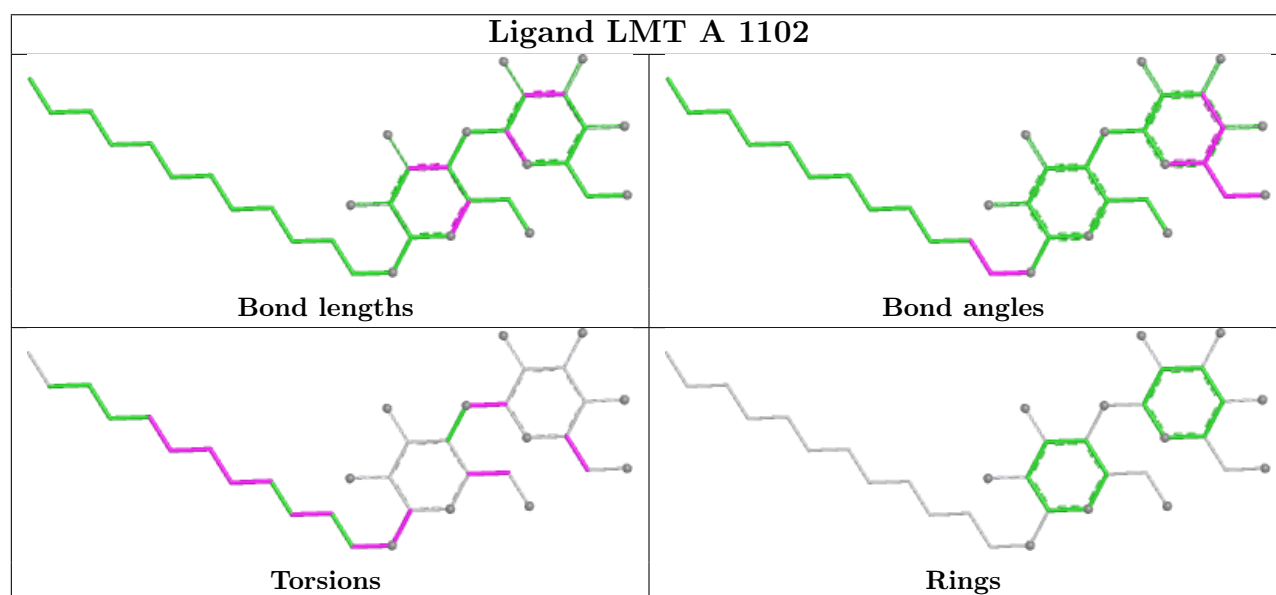
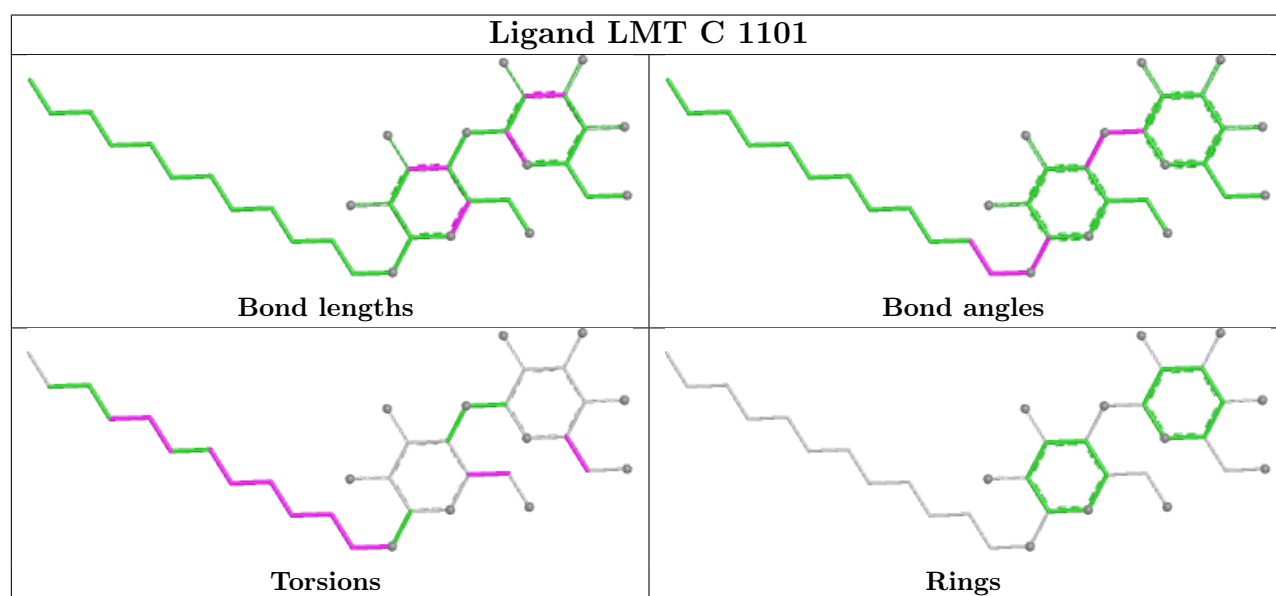
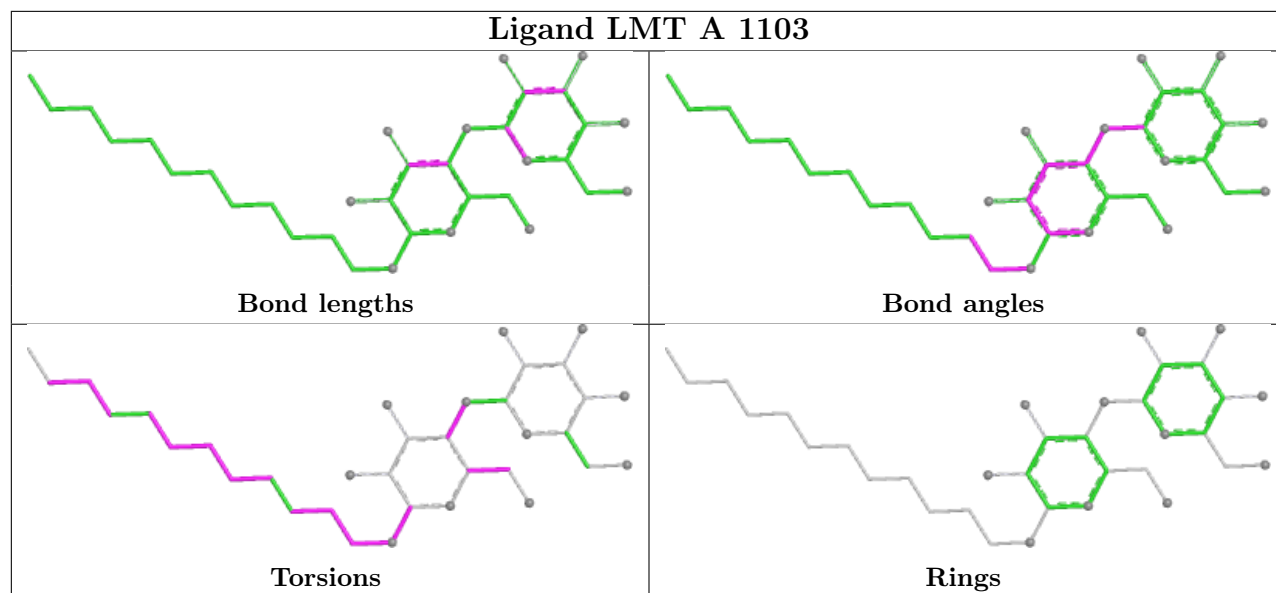
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

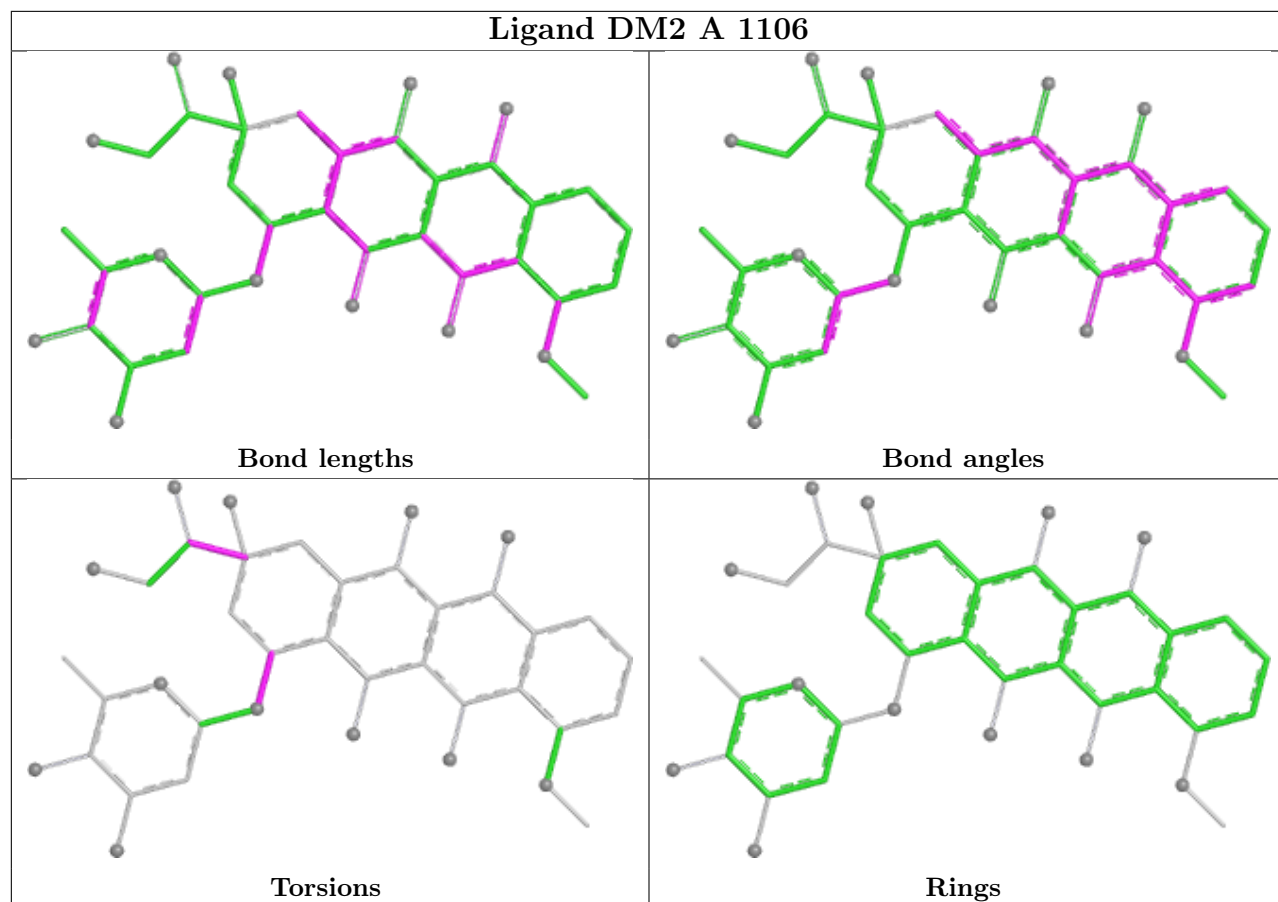












5.7 Other polymers [i](#)

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	1042/1057 (98%)	0.10	52 (4%)	34	33	23, 48, 95, 151	0
1	B	1033/1057 (97%)	-0.09	28 (2%)	56	57	23, 46, 75, 131	0
1	C	1036/1057 (98%)	-0.14	34 (3%)	49	49	25, 43, 74, 151	0
2	D	156/169 (92%)	-0.13	3 (1%)	66	67	33, 45, 74, 110	0
2	E	152/169 (89%)	0.26	4 (2%)	57	58	38, 56, 87, 104	0
All	All	3419/3509 (97%)	-0.03	121 (3%)	47	47	23, 46, 83, 151	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	THR	6.6
1	A	672	VAL	6.2
1	A	1040	ILE	6.1
2	D	11	GLY	6.0
1	A	674	LEU	5.9
1	C	29	LYS	5.1
1	B	677	ALA	5.1
1	A	618	ALA	4.5
1	A	677	ALA	4.2
1	A	498	LYS	4.2
2	D	166	GLN	4.0
1	B	674	LEU	4.0
1	C	620	ARG	4.0
1	A	836	SER	4.0
1	A	617	PHE	3.9
1	A	865	GLN	3.9
1	A	510	LYS	3.9
1	A	678	THR	3.8
1	A	673	GLU	3.7
2	D	12	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	868	LEU	3.7
1	C	811	TYR	3.7
1	B	877	TYR	3.5
1	B	510	LYS	3.5
1	C	617	PHE	3.5
1	A	1036	LYS	3.4
1	A	362	PHE	3.3
1	B	386	PHE	3.3
2	E	34	MET	3.3
1	C	618	ALA	3.3
1	C	1035	ARG	3.2
1	A	955	LYS	3.2
1	C	1036	LYS	3.2
1	C	672	VAL	3.2
1	A	1042	HIS	3.2
1	A	37	THR	3.2
2	E	15	GLY	3.1
1	C	954	ASP	3.1
1	A	38	ILE	3.1
1	C	362	PHE	3.1
1	A	668	LEU	3.0
1	B	984	LEU	3.0
1	C	1033	PHE	3.0
1	A	833	PRO	3.0
1	B	870	GLY	2.9
1	A	662	MET	2.9
1	B	874	PRO	2.8
1	B	867	ARG	2.8
2	E	166	GLN	2.8
1	A	956	GLU	2.8
1	A	918	PHE	2.8
1	B	869	SER	2.7
1	C	670	ALA	2.7
1	C	675	GLY	2.7
1	C	955	LYS	2.6
1	A	670	ALA	2.6
1	A	462	SER	2.6
1	C	498	LYS	2.5
1	A	877	TYR	2.5
1	C	673	GLU	2.5
1	C	21	LEU	2.5
1	A	993	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	620	ARG	2.5
1	B	563	PHE	2.5
2	E	33	LEU	2.5
1	B	868	LEU	2.4
1	B	871	ASN	2.4
1	A	506	GLY	2.4
1	C	510	LYS	2.4
1	C	951	ASP	2.4
1	A	873	ALA	2.4
1	A	518	ARG	2.4
1	A	657	GLN	2.4
1	C	619	GLY	2.3
1	C	918	PHE	2.3
1	A	676	THR	2.3
1	C	500	ILE	2.3
1	C	743	ILE	2.3
1	B	3	ASN	2.3
1	C	429	GLU	2.3
1	A	512	PHE	2.2
1	A	461	GLY	2.2
1	B	866	GLU	2.2
1	A	500	ILE	2.2
1	C	671	ILE	2.2
1	B	615	PHE	2.2
1	A	1037	ASN	2.2
1	C	363	ARG	2.2
1	A	255	GLN	2.2
1	B	29	LYS	2.2
1	C	124	GLN	2.2
1	A	442	LEU	2.2
1	B	628	PHE	2.2
1	C	361	ASN	2.2
1	A	834	GLY	2.2
1	B	659	LYS	2.2
1	C	1034	SER	2.2
1	C	674	LEU	2.2
1	B	672	VAL	2.2
1	A	835	LYS	2.2
1	A	501	ALA	2.2
1	A	1035	ARG	2.1
1	A	448	VAL	2.1
1	B	617	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	918	PHE	2.1
1	A	870	GLY	2.1
1	C	676	THR	2.1
1	A	869	SER	2.1
1	B	873	ALA	2.1
1	B	649	MET	2.1
1	A	526	HIS	2.1
1	A	669	PRO	2.1
1	A	874	PRO	2.1
1	C	71	GLY	2.1
1	C	689	GLY	2.1
1	A	922	THR	2.0
1	A	1041	GLU	2.0
1	B	676	THR	2.0
1	C	737	GLN	2.0
1	A	540	ARG	2.0
1	B	522	LYS	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
6	D10	A	1109	10/10	0.63	0.27	83,107,121,121	0
5	D12	C	1106	12/12	0.65	0.27	81,98,109,109	0
4	DM2	A	1106	39/39	0.67	0.20	81,141,174,176	0
5	D12	C	1102	12/12	0.67	0.24	58,91,99,100	0
5	D12	B	1109	12/12	0.69	0.20	52,73,88,91	0
5	D12	A	1107	12/12	0.71	0.25	58,82,125,125	0

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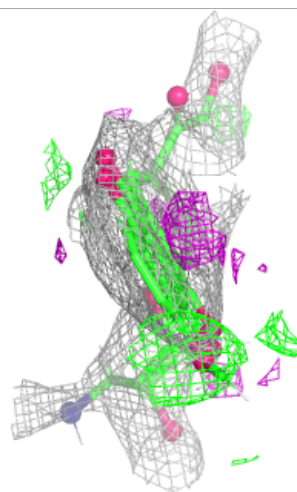
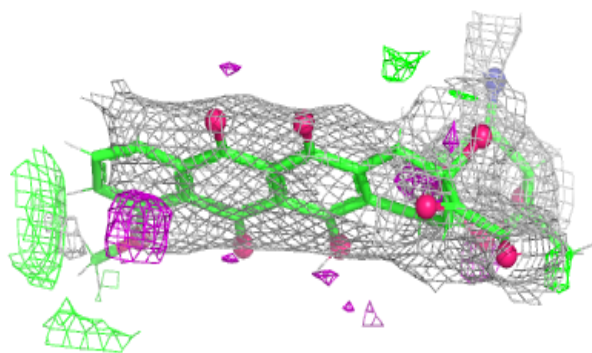
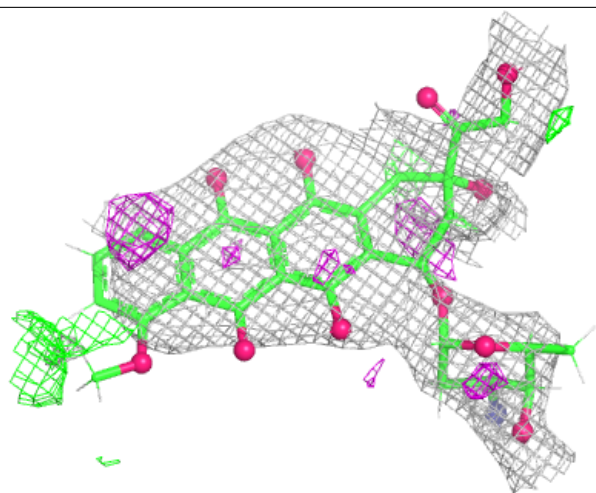
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	D10	B	1105	10/10	0.71	0.22	75,97,109,110	0
9	HEX	B	1108	6/6	0.72	0.35	84,101,109,109	0
4	DM2	B	1104	39/39	0.73	0.22	93,121,139,142	0
6	D10	C	1104	10/10	0.74	0.28	80,97,104,107	0
6	D10	A	1108	10/10	0.77	0.20	85,103,113,113	0
4	DM2	A	1105	39/39	0.79	0.15	75,91,110,115	0
7	LMU	B	1103	35/35	0.81	0.19	65,84,96,105	0
3	LMT	B	1101	35/35	0.82	0.18	73,114,134,136	0
8	GOL	B	1107	6/6	0.84	0.26	95,119,134,143	0
3	LMT	A	1103	35/35	0.85	0.17	59,95,115,119	0
3	LMT	A	1104	35/35	0.86	0.19	74,94,100,104	0
9	HEX	C	1105	6/6	0.86	0.20	84,101,105,105	0
3	LMT	A	1102	35/35	0.87	0.15	73,105,119,120	0
8	GOL	C	1103	6/6	0.89	0.18	37,48,59,68	0
3	LMT	B	1102	35/35	0.91	0.16	63,77,111,112	0
8	GOL	B	1106	6/6	0.91	0.18	73,88,107,114	0
3	LMT	A	1101	35/35	0.92	0.12	49,74,107,108	0
3	LMT	C	1101	35/35	0.94	0.13	62,74,93,97	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.

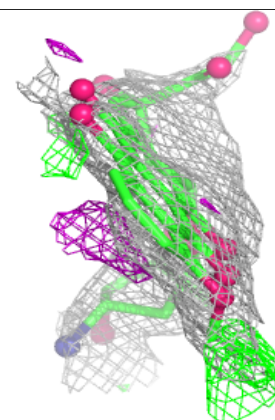
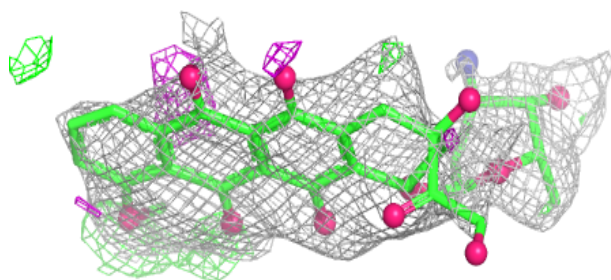
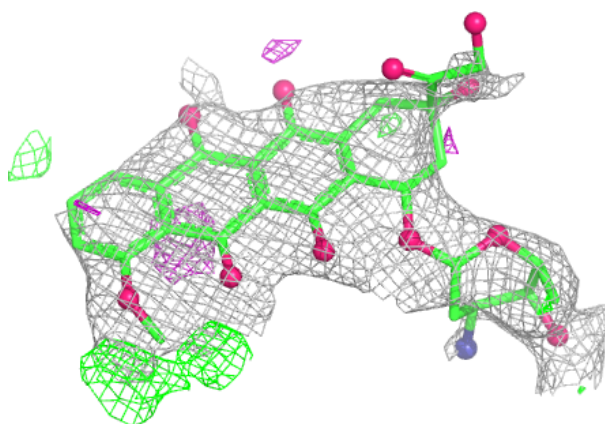
Electron density around DM2 A 1106:

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

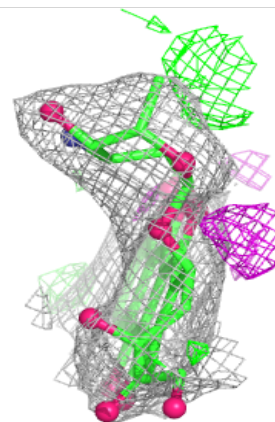
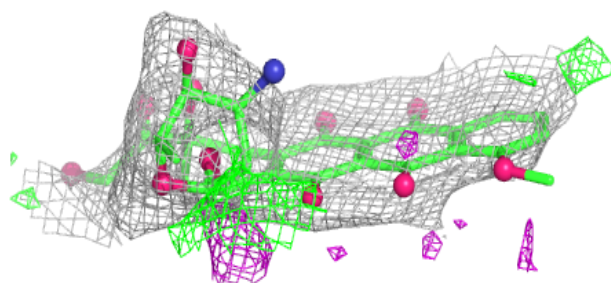
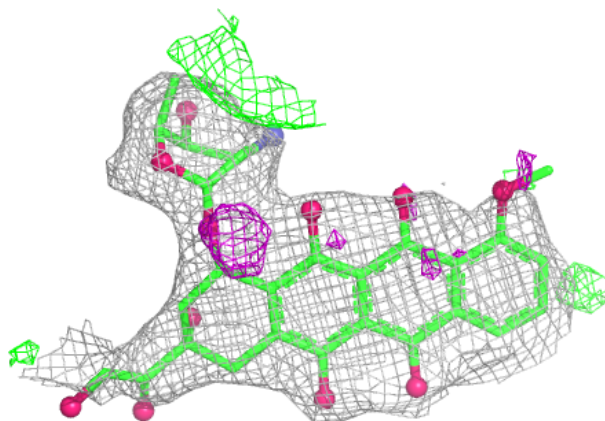


Electron density around DM2 B 1104:

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

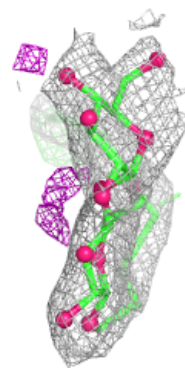
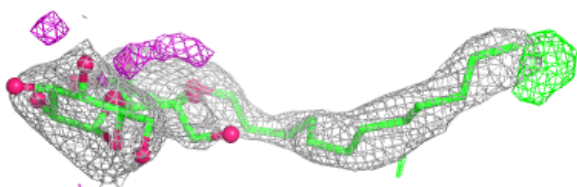
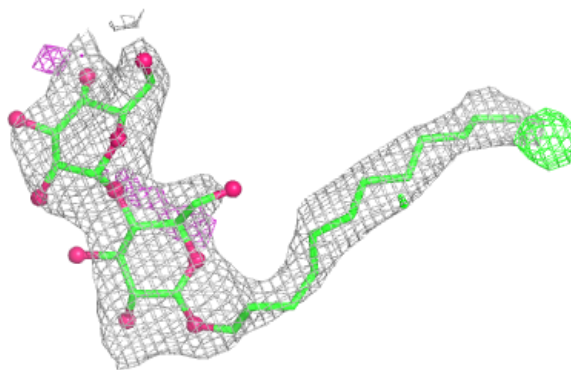
**Electron density around DM2 A 1105:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

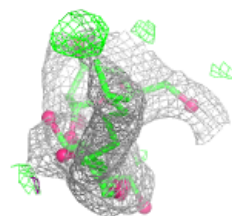
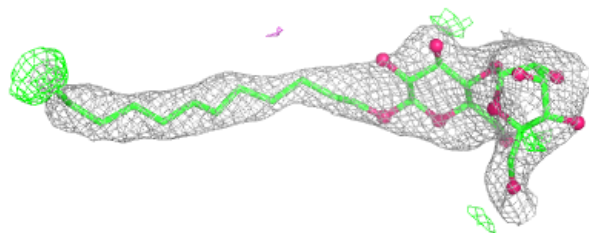
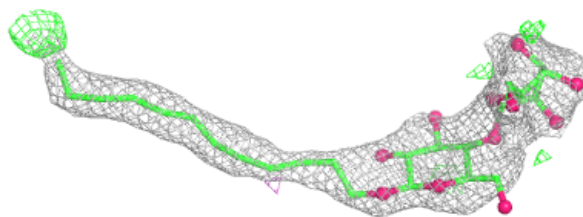


Electron density around LMU B 1103:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

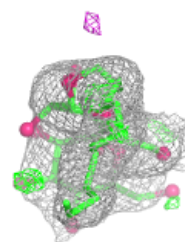
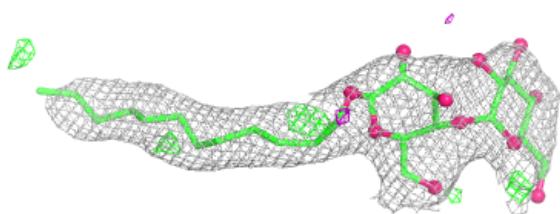
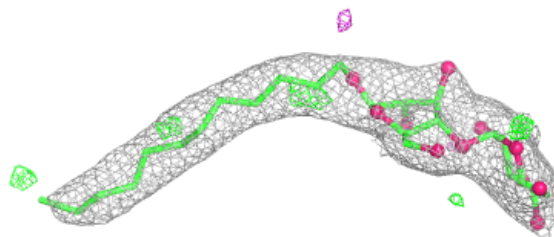
**Electron density around LMT B 1101:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

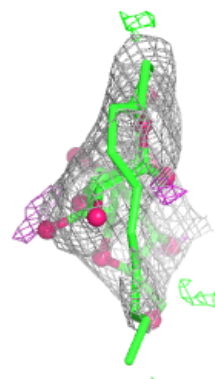
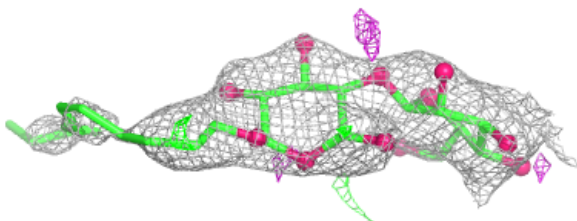
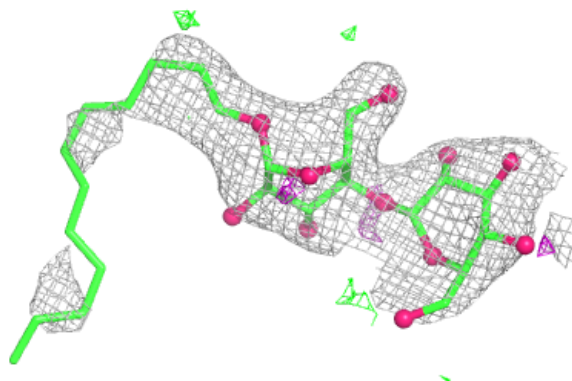


Electron density around LMT A 1103:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

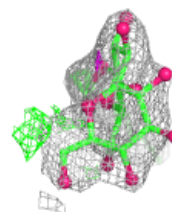
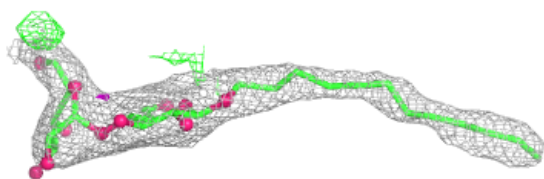
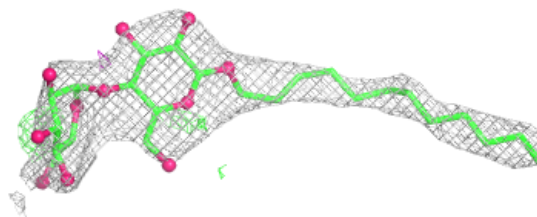
**Electron density around LMT A 1104:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

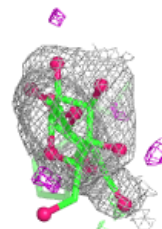
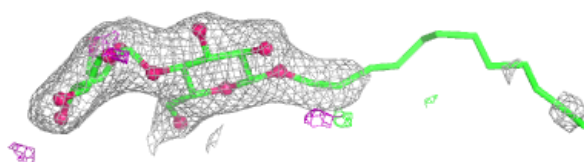
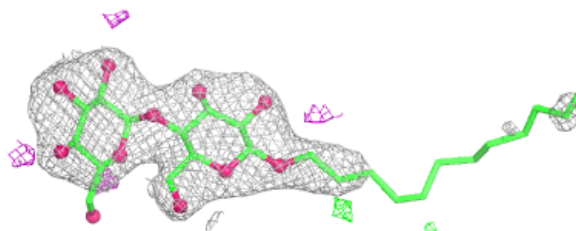


Electron density around LMT A 1102:

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

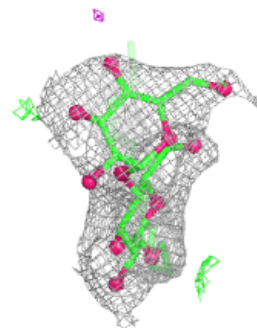
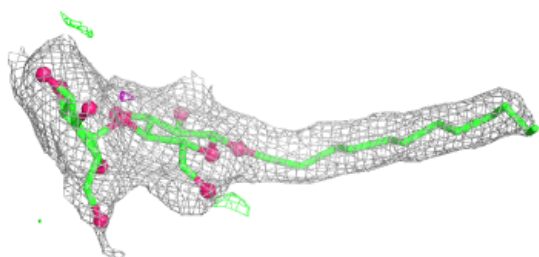
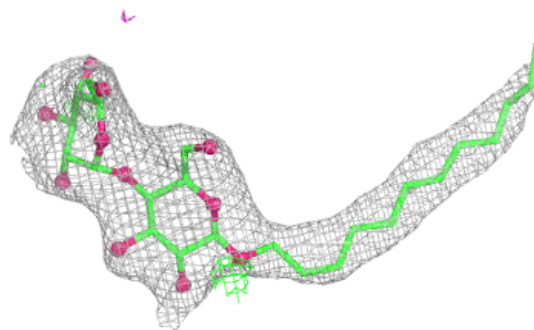
**Electron density around LMT B 1102:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

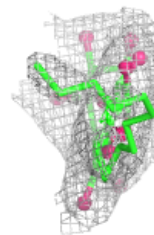
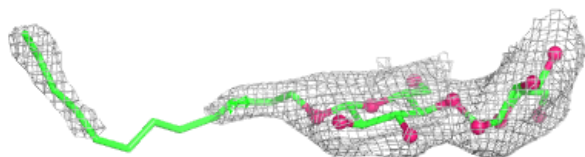
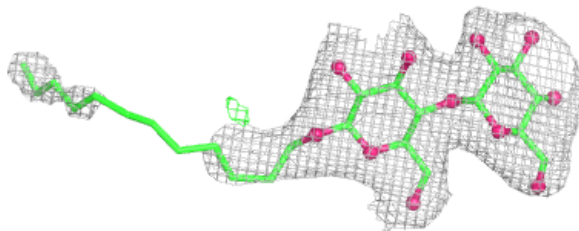


Electron density around LMT A 1101:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.