



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:04 PM UTC

PDB ID : 4U8V / pdb_00004u8v
Title : Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB
Authors : Pos, K.M.
Deposited on : 2014-08-04
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

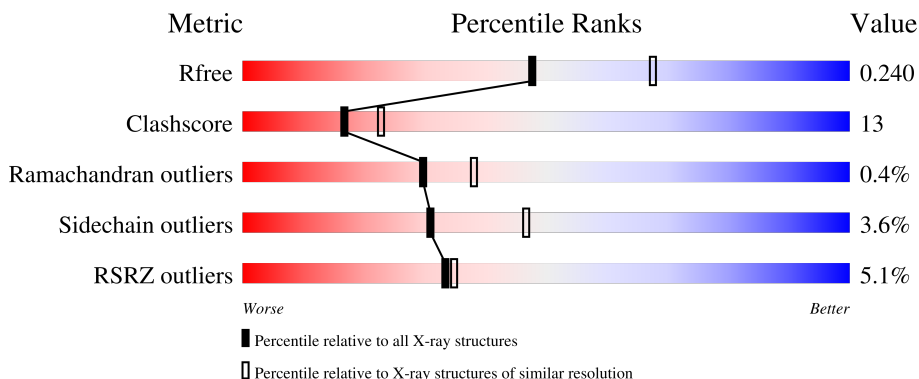
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	10% 69% 27% ..
1	B	1057	3% 76% 20% ..
1	C	1057	2% 78% 18% ..
2	D	169	4% 78% 14% 8%
2	E	169	4% 72% 18% 10%

2 Entry composition

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

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

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

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

There are 27 discrepancies between the modelled and reference sequences:

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

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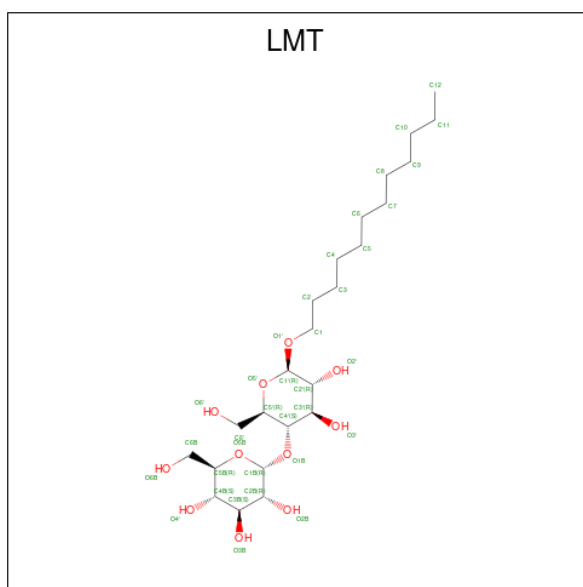
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPin.

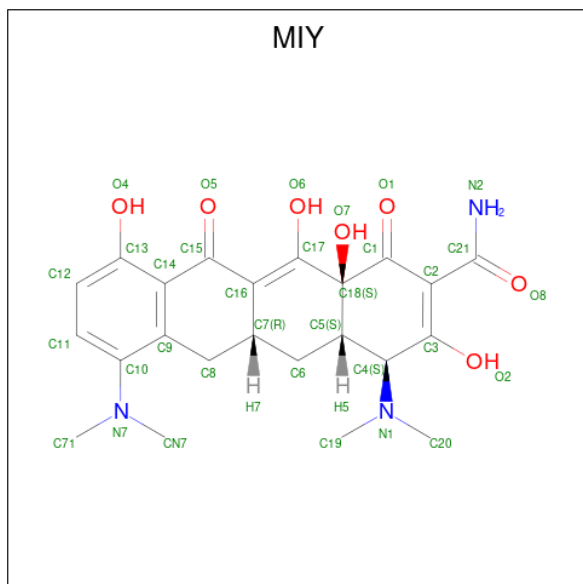
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

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



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	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 (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: MIY) (formula: $C_{23}H_{27}N_3O_7$).

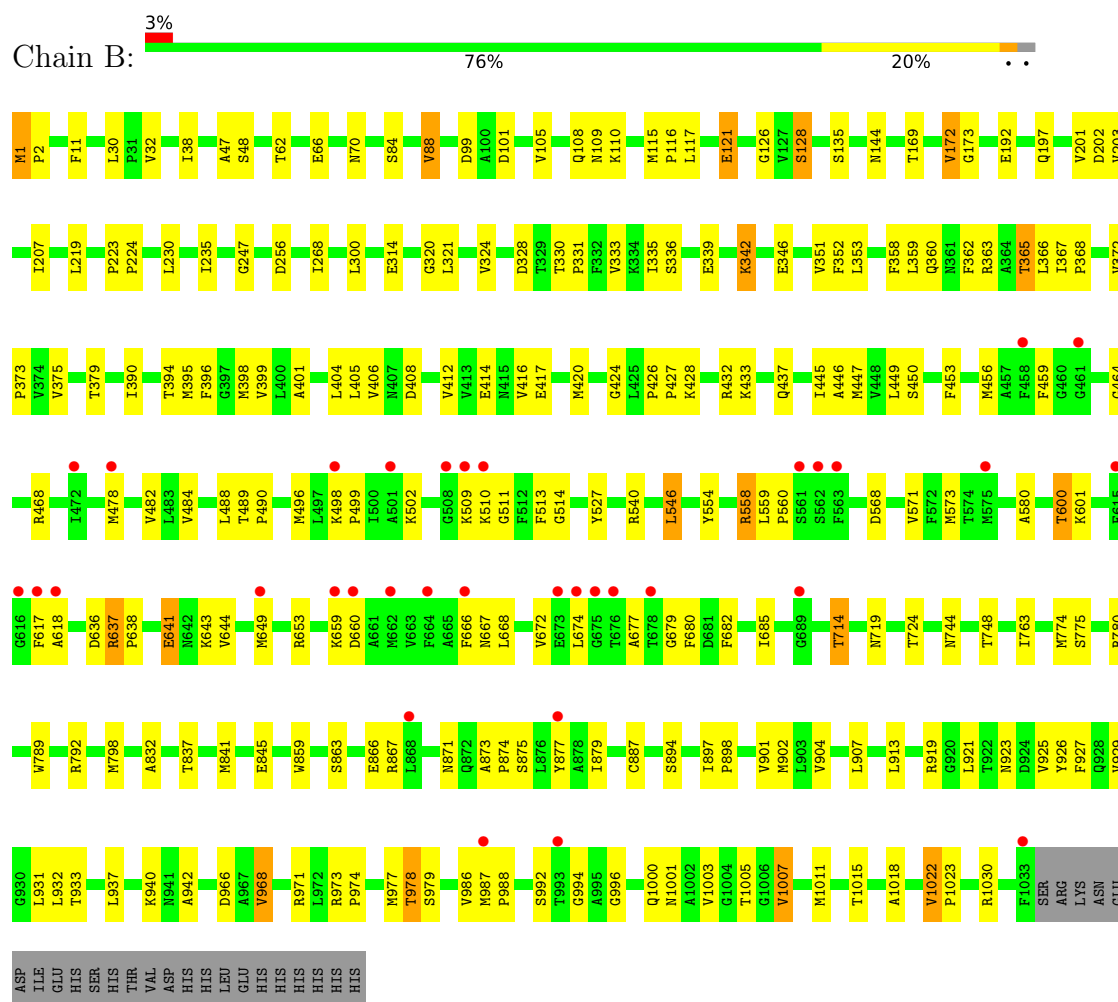


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	
			60	23	27	3	7	

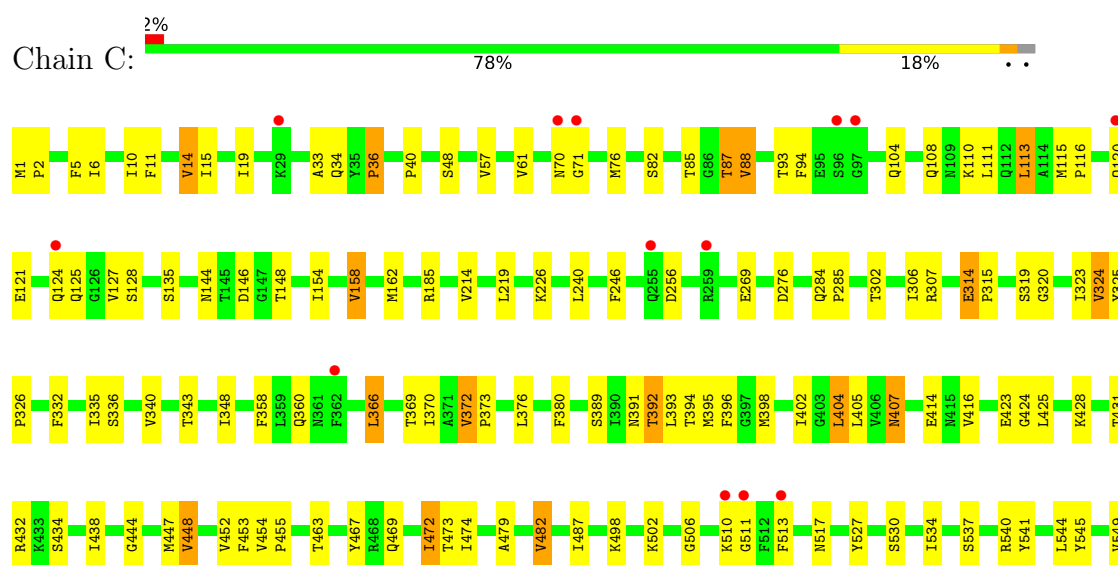
- Molecule 5 is water.

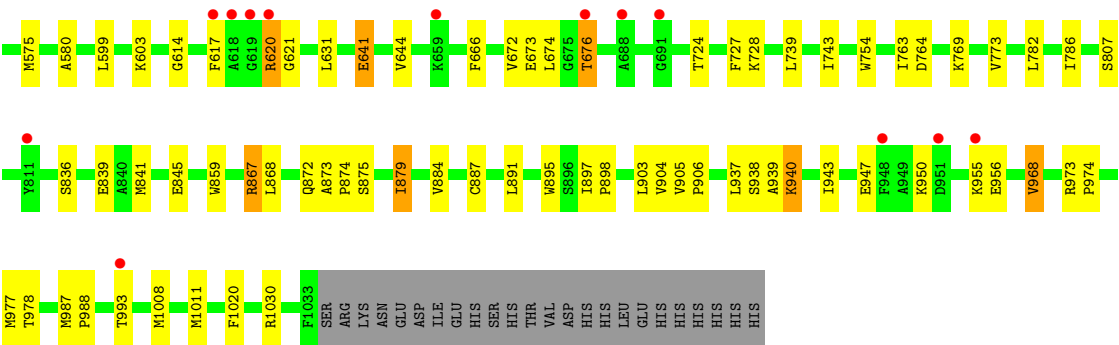
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	391	Total	O		
			391	391	0	0
5	B	376	Total	O		
			376	376	0	0
5	C	469	Total	O		
			469	469	0	0
5	D	61	Total	O		
			61	61	0	0
5	E	46	Total	O		
			46	46	0	0

• Molecule 1: Multidrug efflux pump subunit AcrB

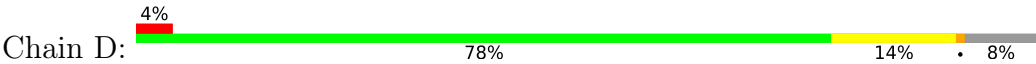


• Molecule 1: Multidrug efflux pump subunit AcrB

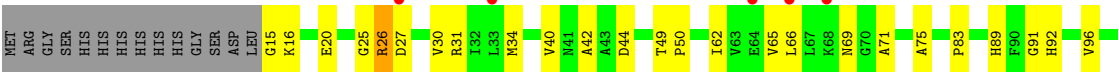




• Molecule 2: DARPin



• Molecule 2: DARPin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.59Å 161.59Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.93 – 2.30 48.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.93-2.30) 99.9 (48.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.191 , 0.238 0.195 , 0.240	Depositor DCC
R_{free} test set	12835 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.0	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	0.95	EDS
Total number of atoms	27546	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, MIY

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	0.48	0/8095	0.84	8/10991 (0.1%)
1	B	0.50	0/7998	0.83	4/10861 (0.0%)
1	C	0.52	0/7999	0.84	4/10863 (0.0%)
2	D	0.44	0/1196	0.73	0/1626
2	E	0.40	0/1170	0.72	0/1591
All	All	0.49	0/26458	0.83	16/35932 (0.0%)

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

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

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	524	THR	N-CA-C	-8.85	101.55	111.82
1	B	426	PRO	O-C-N	6.45	124.18	121.15
1	C	325	TYR	CA-C-N	6.09	125.72	119.56
1	C	325	TYR	C-N-CA	6.09	125.72	119.56
1	B	637	ARG	CA-C-N	5.64	125.92	119.83
1	B	637	ARG	C-N-CA	5.64	125.92	119.83
1	C	782	LEU	CA-C-N	5.63	126.88	119.84
1	C	782	LEU	C-N-CA	5.63	126.88	119.84
1	B	685	ILE	N-CA-C	5.53	115.85	108.11
1	A	605	ASN	CA-C-N	-5.21	116.73	123.19
1	A	605	ASN	C-N-CA	-5.21	116.73	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ARG	CA-C-N	5.21	124.83	119.05
1	A	8	ARG	C-N-CA	5.21	124.83	119.05
1	A	272	GLY	N-CA-C	5.09	117.78	111.93
1	A	325	TYR	CA-C-N	5.05	124.66	119.56
1	A	325	TYR	C-N-CA	5.05	124.66	119.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7943	0	8086	282	0
1	B	7848	0	8003	198	0
1	C	7849	0	8003	167	0
2	D	1177	0	1159	16	0
2	E	1151	0	1136	24	0
3	A	70	0	92	8	0
3	B	70	0	92	8	0
3	C	35	0	46	3	0
4	B	33	27	25	2	0
5	A	391	0	0	12	0
5	B	376	0	0	9	0
5	C	469	0	0	13	0
5	D	61	0	0	0	0
5	E	46	0	0	3	0
All	All	27519	27	26642	674	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 13.

All (674) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.36	1.06
1:B:363:ARG:HD2	1:B:498:LYS:HE2	1.39	1.03
1:A:528:THR:HG21	1:A:969:ARG:HG3	1.37	1.03
1:A:38:ILE:HG12	1:A:671:ILE:HD13	1.36	1.02
2:E:34:MET:HE2	2:E:40:VAL:HG12	1.46	0.98
1:C:447:MET:HE1	1:C:891:LEU:HD13	1.43	0.97
1:A:356:TYR:HA	1:A:365:THR:HG21	1.52	0.91
1:A:641:GLU:O	1:A:650:ARG:NH2	2.04	0.89
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.53	0.89
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.55	0.88
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.52	0.88
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.55	0.88
1:A:528:THR:HG21	1:A:969:ARG:CG	2.04	0.87
1:C:867:ARG:NH1	5:C:1315:HOH:O	2.08	0.87
1:A:459:PHE:HD2	1:A:464:GLY:HA2	1.40	0.86
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.58	0.86
1:C:391:ASN:H	1:C:394:THR:HG22	1.40	0.85
1:A:907:LEU:HD22	1:A:1017:LEU:HD23	1.59	0.84
1:A:523:SER:CB	1:A:526:HIS:HB2	2.06	0.84
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.60	0.83
1:A:188:MET:HE2	1:A:773:VAL:HG12	1.60	0.83
1:B:449:LEU:HB3	1:B:478:MET:CE	2.09	0.82
1:A:523:SER:HA	1:A:526:HIS:H	1.46	0.81
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.63	0.80
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.81	0.80
1:C:70:ASN:O	1:C:110:LYS:NZ	2.15	0.80
1:B:420:MET:HE1	1:B:499:PRO:HA	1.64	0.79
1:A:672:VAL:O	1:A:675:GLY:N	2.13	0.79
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.15	0.78
1:C:395:MET:HE2	1:C:395:MET:HA	1.65	0.78
1:B:414:GLU:CG	1:B:977:MET:HE1	2.13	0.78
1:B:363:ARG:HD2	1:B:498:LYS:CE	2.14	0.77
1:A:519:MET:O	1:A:522:LYS:HE3	1.85	0.77
1:A:523:SER:HA	1:A:526:HIS:HB2	1.67	0.76
1:A:36:PRO:CG	1:A:469:GLN:HG3	2.17	0.75
1:B:974:PRO:O	1:B:978:THR:HB	1.87	0.75
1:B:618:ALA:HB1	1:B:719:ASN:O	1.86	0.75
1:A:416:VAL:HG11	1:A:431:THR:HG22	1.69	0.75
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.69	0.75
1:B:573:MET:HE1	1:B:617:PHE:HE2	1.52	0.75
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.69	0.74
1:A:459:PHE:CD2	1:A:464:GLY:HA2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:VAL:HG23	1:B:668:LEU:HD11	1.68	0.74
1:B:974:PRO:HA	1:B:977:MET:CE	2.18	0.74
2:E:34:MET:HE2	2:E:40:VAL:CG1	2.15	0.73
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.69	0.73
1:C:307:ARG:NH1	5:C:1561:HOH:O	2.18	0.73
1:B:456:MET:HE1	1:B:877:TYR:CE1	2.24	0.73
1:B:994:GLY:N	5:B:1489:HOH:O	2.22	0.73
1:A:527:TYR:OH	1:A:1019:ILE:O	2.07	0.72
1:B:363:ARG:HD2	1:B:498:LYS:HG3	1.72	0.72
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.21	0.72
1:B:919:ARG:HD3	1:B:1005:THR:HG21	1.72	0.71
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.70	0.71
1:A:568:ASP:CG	1:A:637:ARG:HH22	1.97	0.71
1:A:516:PHE:HA	1:A:519:MET:HG2	1.70	0.71
1:B:871:ASN:HB3	3:B:1102:LMT:H6'1	1.71	0.71
1:B:573:MET:HE1	1:B:617:PHE:CE2	2.25	0.71
1:A:958:LYS:NZ	1:A:966:ASP:OD2	2.23	0.70
1:C:34:GLN:O	1:C:392:THR:HB	1.91	0.70
1:C:575:MET:HG2	1:C:666:PHE:HE2	1.56	0.70
1:B:414:GLU:HG3	1:B:977:MET:CE	2.17	0.70
1:C:336:SER:O	1:C:340:VAL:HG23	1.92	0.70
1:A:393:LEU:CD1	1:A:466:ILE:HG23	2.22	0.70
1:A:669:PRO:HG2	1:A:672:VAL:HA	1.74	0.70
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.74	0.69
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.56	0.69
1:B:363:ARG:CD	1:B:498:LYS:HE2	2.19	0.69
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.74	0.69
1:C:85:THR:O	5:C:1246:HOH:O	2.10	0.69
1:C:987:MET:SD	1:C:1008:MET:HE1	2.31	0.69
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.93	0.69
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.73	0.69
1:A:902:MET:O	1:A:905:VAL:HG23	1.93	0.69
1:A:877:TYR:CE2	3:A:1102:LMT:H31	2.29	0.68
1:A:427:PRO:O	1:A:431:THR:HG23	1.94	0.68
1:A:523:SER:O	1:A:527:TYR:HB3	1.94	0.68
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.29	0.68
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.28	0.68
1:B:449:LEU:HD13	1:B:478:MET:SD	2.35	0.67
1:C:391:ASN:H	1:C:394:THR:CG2	2.07	0.67
1:A:407:ASN:HD22	1:A:978:THR:HG21	1.58	0.67
1:A:563:PHE:O	1:A:924:ASP:HB2	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:MET:HA	1:B:395:MET:HE2	1.76	0.67
1:C:452:VAL:HG13	1:C:884:VAL:HG21	1.77	0.67
1:A:619:GLY:O	1:A:621:GLY:N	2.29	0.66
1:A:355:MET:HE1	1:A:410:ILE:HD11	1.77	0.66
1:B:456:MET:HE1	1:B:877:TYR:HE1	1.60	0.66
1:A:523:SER:HA	1:A:526:HIS:N	2.10	0.66
1:B:450:SER:HB2	3:B:1102:LMT:H121	1.77	0.66
1:A:343:THR:HG21	1:A:1000:GLN:OE1	1.96	0.66
1:A:523:SER:CA	1:A:526:HIS:HB2	2.26	0.66
1:A:347:ALA:O	1:A:351:VAL:HG23	1.95	0.65
2:D:121:ALA:HB1	2:D:161:LEU:HD21	1.79	0.65
1:C:580:ALA:CB	1:C:724:THR:HG22	2.26	0.65
1:B:335:ILE:O	1:B:339:GLU:HG2	1.96	0.65
1:C:872:GLN:HG3	5:C:1543:HOH:O	1.97	0.65
1:A:465:ALA:O	1:A:469:GLN:HG2	1.97	0.65
1:A:905:VAL:O	1:A:909:VAL:HG23	1.97	0.64
1:B:744:ASN:O	1:B:748:THR:HG22	1.96	0.64
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.29	0.64
1:B:342:LYS:HE3	1:B:346:GLU:OE2	1.98	0.64
1:C:85:THR:OG1	1:C:87:THR:HG23	1.97	0.64
1:C:993:THR:HG22	5:C:1298:HOH:O	1.97	0.64
2:E:34:MET:CE	2:E:40:VAL:HG12	2.25	0.64
1:A:459:PHE:CE1	1:A:872:GLN:HG3	2.33	0.63
1:A:602:GLU:HB3	1:A:606:VAL:HG13	1.81	0.63
1:A:188:MET:HE2	1:A:773:VAL:CG1	2.27	0.63
1:A:558:ARG:NH1	1:A:558:ARG:HB2	2.13	0.63
1:B:201:VAL:HG22	1:B:748:THR:CG2	2.28	0.63
1:A:70:ASN:O	1:A:110:LYS:HE3	1.98	0.63
1:B:428:LYS:HZ1	1:B:432:ARG:HH22	1.47	0.63
1:A:911:GLY:HA2	1:A:1013:THR:HG21	1.81	0.63
1:B:875:SER:O	1:B:879:ILE:HG13	1.99	0.63
1:B:636:ASP:C	1:B:638:PRO:HD3	2.23	0.63
1:A:355:MET:HE2	1:A:355:MET:HA	1.81	0.62
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.33	0.62
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.26	0.62
1:A:509:LYS:HG3	1:A:510:LYS:N	2.14	0.62
1:B:509:LYS:HG3	1:B:510:LYS:N	2.13	0.62
1:C:447:MET:SD	1:C:887:CYS:HB3	2.39	0.62
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.64	0.62
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	1.80	0.62
1:A:468:ARG:O	1:A:472:ILE:HG12	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:HD3	1:B:496:MET:O	1.99	0.62
1:A:38:ILE:HG12	1:A:671:ILE:CD1	2.21	0.62
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.65	0.62
1:B:600:THR:HG22	1:B:601:LYS:HG2	1.81	0.62
1:A:407:ASN:ND2	1:A:978:THR:HG21	2.14	0.62
1:B:351:VAL:CG2	1:B:406:VAL:HG13	2.30	0.62
2:E:15:GLY:N	5:E:202:HOH:O	2.32	0.62
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.63	0.61
1:A:393:LEU:HD13	1:A:466:ILE:HG23	1.83	0.61
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.30	0.61
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.80	0.61
2:E:44:ASP:HB2	5:E:242:HOH:O	2.00	0.61
1:C:575:MET:HG2	1:C:666:PHE:CE2	2.34	0.61
1:B:47:ALA:HB3	1:B:88:VAL:HG13	1.82	0.61
1:C:428:LYS:HE3	1:C:432:ARG:NH2	2.16	0.61
1:A:328:ASP:OD1	1:A:330:THR:HB	2.00	0.61
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.83	0.61
1:B:904:VAL:HG11	1:B:942:ALA:HB2	1.82	0.61
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.82	0.60
1:B:979:SER:HA	1:B:1011:MET:HE2	1.83	0.60
1:A:575:MET:HE2	1:A:617:PHE:CE2	2.36	0.60
1:B:637:ARG:O	1:B:643:LYS:HE3	2.01	0.60
1:C:620:ARG:NH1	5:C:1606:HOH:O	2.30	0.60
1:A:355:MET:HE1	1:A:410:ILE:CD1	2.31	0.60
2:D:34:MET:HE2	2:D:34:MET:HA	1.84	0.60
1:A:492:LEU:O	1:A:496:MET:HB2	2.01	0.60
1:B:573:MET:CE	1:B:617:PHE:HE2	2.14	0.60
1:B:714:THR:CG2	1:B:832:ALA:HA	2.32	0.59
2:D:12:SER:HB2	2:D:15:GLY:H	1.66	0.59
1:C:392:THR:HG22	1:C:393:LEU:HD23	1.85	0.59
1:A:416:VAL:CG1	1:A:431:THR:HG22	2.31	0.59
1:B:837:THR:HG22	5:B:1469:HOH:O	2.02	0.59
1:A:784:ASP:OD1	5:A:1484:HOH:O	2.17	0.59
1:B:201:VAL:HG22	1:B:748:THR:HG21	1.85	0.59
1:B:450:SER:CB	3:B:1102:LMT:H121	2.33	0.59
1:C:452:VAL:HG13	1:C:884:VAL:CG2	2.32	0.59
1:B:352:PHE:CD2	1:B:365:THR:HG21	2.38	0.59
1:C:87:THR:HG22	5:C:1246:HOH:O	2.00	0.59
1:A:370:ILE:O	1:A:373:PRO:HD2	2.03	0.59
1:A:351:VAL:O	1:A:355:MET:HG2	2.03	0.58
1:A:559:LEU:HD23	1:A:923:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PHE:O	1:B:365:THR:HB	2.03	0.58
1:B:919:ARG:HG2	1:B:921:LEU:CD1	2.33	0.58
1:B:979:SER:OG	1:B:1015:THR:HG21	2.03	0.58
1:B:1011:MET:O	1:B:1015:THR:HG23	2.03	0.58
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.85	0.58
1:C:575:MET:HE3	1:C:666:PHE:HZ	1.68	0.58
1:C:575:MET:HE1	1:C:617:PHE:HD2	1.69	0.58
2:E:65:VAL:O	2:E:69:ASN:ND2	2.34	0.58
1:A:785:ASP:OD1	5:A:1201:HOH:O	2.17	0.58
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.34	0.58
1:C:111:LEU:HD21	1:C:127:VAL:CG1	2.33	0.58
1:C:395:MET:CE	1:C:398:MET:HG3	2.33	0.58
1:A:202:ASP:CG	1:A:792:ARG:HH22	2.12	0.58
1:B:395:MET:HE2	1:B:395:MET:CA	2.33	0.58
2:E:106:VAL:HG12	5:E:234:HOH:O	2.03	0.58
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.29	0.58
1:A:987:MET:N	1:A:988:PRO:HD2	2.19	0.58
1:B:396:PHE:O	1:B:399:VAL:HG22	2.03	0.58
1:B:919:ARG:HG2	1:B:921:LEU:HD13	1.85	0.58
1:B:1011:MET:HE3	1:B:1015:THR:CG2	2.34	0.58
1:A:38:ILE:CG1	1:A:671:ILE:HD13	2.25	0.57
1:C:115:MET:N	1:C:116:PRO:HD2	2.20	0.57
1:C:452:VAL:CG1	1:C:884:VAL:HG21	2.34	0.57
1:A:507:GLU:HB3	1:A:518:ARG:HG3	1.85	0.57
1:B:459:PHE:O	1:B:464:GLY:HA3	2.03	0.57
1:C:575:MET:CE	1:C:666:PHE:HZ	2.17	0.57
1:A:38:ILE:HD12	1:A:39:ALA:N	2.19	0.57
1:A:672:VAL:O	1:A:674:LEU:N	2.38	0.57
1:B:359:LEU:HD13	1:B:417:GLU:HG3	1.85	0.57
1:B:987:MET:N	1:B:988:PRO:HD2	2.18	0.57
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.34	0.57
2:E:16:LYS:NZ	2:E:20:GLU:OE1	2.36	0.57
1:A:862:MET:O	1:A:866:GLU:HG2	2.05	0.57
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.87	0.57
1:C:369:THR:O	1:C:372:VAL:HG13	2.05	0.57
1:C:530:SER:OG	3:C:1101:LMT:H11	2.04	0.57
1:A:645:GLU:HG2	1:A:649:MET:HE2	1.86	0.57
1:A:705:GLU:OE2	1:A:708:LYS:HE3	2.03	0.57
1:A:393:LEU:HD11	1:A:466:ILE:HG23	1.86	0.57
1:A:523:SER:HA	1:A:526:HIS:CB	2.34	0.57
1:A:952:LEU:O	1:A:956:GLU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ILE:O	1:C:373:PRO:HD2	2.05	0.57
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.40	0.56
1:B:974:PRO:HA	1:B:977:MET:HE2	1.86	0.56
1:B:1018:ALA:O	1:B:1022:VAL:HG13	2.05	0.56
1:A:575:MET:HE2	1:A:617:PHE:CD2	2.40	0.56
1:A:714:THR:HG23	1:A:832:ALA:HA	1.87	0.56
1:C:372:VAL:HG22	1:C:373:PRO:CD	2.33	0.56
1:C:395:MET:HE2	1:C:398:MET:HG3	1.87	0.56
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.86	0.56
1:B:416:VAL:O	1:B:420:MET:HG3	2.06	0.56
1:A:604:ASN:O	1:A:632:LYS:HD2	2.06	0.56
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.88	0.56
1:C:226:LYS:NZ	5:C:1203:HOH:O	2.39	0.56
1:A:960:LEU:HB2	1:A:1038:GLU:OE2	2.06	0.55
1:C:940:LYS:NZ	5:C:1371:HOH:O	2.39	0.55
1:A:202:ASP:OD2	1:A:792:ARG:NH2	2.38	0.55
1:A:649:MET:HB3	5:A:1514:HOH:O	2.06	0.55
1:B:714:THR:HG22	1:B:832:ALA:HA	1.89	0.55
1:A:412:VAL:O	1:A:416:VAL:HG23	2.06	0.55
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.41	0.55
1:B:571:VAL:CG2	1:B:668:LEU:HD11	2.35	0.55
1:C:154:ILE:O	1:C:158:VAL:HG13	2.07	0.55
1:A:1008:MET:O	1:A:1012:VAL:HG23	2.07	0.55
1:C:479:ALA:O	1:C:482:VAL:HG23	2.07	0.55
1:A:687:GLN:OE1	1:A:856:GLY:HA3	2.07	0.55
1:C:502:LYS:NZ	5:C:1202:HOH:O	2.37	0.55
1:A:56:THR:O	1:A:60:THR:HB	2.06	0.54
1:C:448:VAL:HG22	1:C:884:VAL:HG13	1.89	0.54
1:A:531:VAL:O	1:A:535:LEU:HG	2.08	0.54
1:B:540:ARG:NH2	3:B:1101:LMT:H6'1	2.22	0.54
1:B:974:PRO:HA	1:B:977:MET:HE3	1.88	0.54
1:C:120:GLN:O	1:C:124:GLN:HG2	2.07	0.54
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.90	0.54
2:E:42:ALA:O	2:E:50:PRO:HD3	2.06	0.54
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.88	0.54
1:A:223:PRO:HD2	1:B:780:ARG:NH1	2.22	0.54
1:C:40:PRO:HB2	1:C:94:PHE:O	2.08	0.54
1:C:534:ILE:HG12	1:C:541:TYR:CZ	2.43	0.54
1:C:1020:PHE:CZ	3:C:1101:LMT:H51	2.42	0.54
1:A:546:LEU:O	1:A:550:VAL:HG23	2.07	0.54
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG22	1:A:462:SER:O	2.08	0.54
1:A:363:ARG:HH11	1:A:498:LYS:HG3	1.73	0.54
1:A:523:SER:HB2	1:A:526:HIS:HB2	1.88	0.54
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.90	0.54
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.88	0.54
1:B:331:PRO:O	1:B:335:ILE:HG12	2.08	0.54
1:A:948:PHE:CZ	1:A:970:MET:HE1	2.43	0.54
1:B:32:VAL:HG12	1:B:333:VAL:HG11	1.89	0.54
1:B:926:TYR:O	1:B:1003:VAL:HG12	2.08	0.54
1:B:412:VAL:O	1:B:416:VAL:HG23	2.08	0.53
1:A:415:ASN:O	1:A:419:VAL:HG23	2.08	0.53
1:C:392:THR:HG23	1:C:396:PHE:CE2	2.44	0.53
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.91	0.53
1:A:430:ALA:O	1:A:434:SER:HB2	2.08	0.53
1:B:449:LEU:HB3	1:B:478:MET:HE1	1.90	0.53
1:B:898:PRO:O	1:B:902:MET:HG3	2.08	0.53
1:A:109:ASN:O	1:A:112:GLN:HG3	2.09	0.53
1:A:898:PRO:O	1:A:902:MET:HG3	2.09	0.53
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.39	0.53
1:C:836:SER:OG	1:C:839:GLU:HG3	2.09	0.53
1:A:414:GLU:OE2	1:A:973:ARG:NH1	2.41	0.53
1:A:948:PHE:CE1	1:A:970:MET:HE1	2.44	0.53
3:B:1101:LMT:H5B	3:B:1101:LMT:H6E	1.91	0.53
1:C:1011:MET:HE3	1:C:1011:MET:HA	1.90	0.53
1:A:1:MET:N	5:A:1331:HOH:O	2.35	0.53
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.91	0.53
1:A:586:ARG:HB3	5:A:1487:HOH:O	2.09	0.53
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.39	0.53
1:A:520:PHE:CZ	1:A:973:ARG:HB2	2.44	0.53
1:B:901:VAL:O	1:B:904:VAL:HG22	2.09	0.53
1:C:447:MET:HE1	1:C:891:LEU:CD1	2.29	0.53
1:A:867:ARG:NH1	5:A:1522:HOH:O	2.09	0.52
1:B:395:MET:HE2	1:B:395:MET:N	2.25	0.52
1:C:447:MET:CE	1:C:891:LEU:HD13	2.30	0.52
1:C:764:ASP:HB3	1:C:769:LYS:HD2	1.90	0.52
2:D:25:GLY:HA2	2:D:62:ILE:HD12	1.91	0.52
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.90	0.52
1:C:57:VAL:O	1:C:61:VAL:HB	2.09	0.52
1:C:380:PHE:CZ	1:C:395:MET:HE1	2.44	0.52
1:A:507:GLU:HB3	1:A:518:ARG:CG	2.40	0.52
1:A:649:MET:HG2	5:A:1533:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HA	1:A:613:ASN:O	2.08	0.52
1:A:351:VAL:HG11	1:A:406:VAL:HG21	1.92	0.52
1:B:363:ARG:CD	1:B:498:LYS:HG3	2.39	0.52
1:C:57:VAL:HG13	1:C:82:SER:HB3	1.92	0.52
1:C:641:GLU:CD	1:C:641:GLU:H	2.18	0.52
1:B:841:MET:O	1:B:845:GLU:HG3	2.10	0.52
1:C:424:GLY:HA3	1:C:502:LYS:HB2	1.92	0.52
1:C:506:GLY:C	1:C:517:ASN:HD22	2.18	0.52
2:D:94:GLU:CD	2:D:94:GLU:H	2.17	0.52
1:A:29:LYS:HE3	3:B:1102:LMT:O6'	2.09	0.52
1:A:489:THR:HB	1:A:490:PRO:HD3	1.92	0.52
1:B:108:GLN:HG3	1:B:109:ASN:N	2.22	0.52
1:B:375:VAL:HG11	1:B:405:LEU:CD2	2.36	0.51
1:A:890:ALA:HB2	1:C:14:VAL:HG21	1.92	0.51
1:B:379:THR:HG22	1:B:398:MET:HE1	1.93	0.51
1:B:401:ALA:O	1:B:405:LEU:HG	2.09	0.51
2:D:92:HIS:O	2:D:96:VAL:HG23	2.09	0.51
2:E:34:MET:CE	2:E:66:LEU:HD23	2.40	0.51
1:A:545:TYR:O	1:A:549:VAL:HG23	2.09	0.51
1:A:837:THR:O	1:A:841:MET:HG3	2.10	0.51
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.92	0.51
1:B:447:MET:HB3	1:B:887:CYS:SG	2.51	0.51
2:E:26:ARG:O	2:E:30:VAL:HG23	2.10	0.51
1:A:621:GLY:HA3	5:A:1352:HOH:O	2.11	0.51
1:A:881:LEU:HG	3:A:1102:LMT:C12	2.41	0.51
1:A:1016:VAL:HG23	1:A:1017:LEU:HD13	1.92	0.51
1:B:11:PHE:O	1:B:11:PHE:HD1	1.92	0.51
1:A:961:ILE:HD12	1:A:961:ILE:H	1.75	0.51
1:B:128:SER:HB3	1:C:113:LEU:CD1	2.41	0.51
1:C:6:ILE:HD11	1:C:431:THR:HG22	1.93	0.51
1:C:599:LEU:O	1:C:603:LYS:HB3	2.10	0.51
2:D:43:ALA:HA	2:D:48:TRP:O	2.11	0.51
1:A:928:GLN:HG2	3:A:1102:LMT:H21	1.92	0.51
1:C:904:VAL:HG13	1:C:938:SER:HB3	1.91	0.51
1:B:390:ILE:HG23	1:B:395:MET:SD	2.51	0.51
1:B:449:LEU:HB3	1:B:478:MET:HE3	1.90	0.51
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.18	0.50
1:B:554:TYR:CZ	1:B:558:ARG:HD3	2.46	0.50
1:C:376:LEU:HD11	1:C:402:ILE:HD11	1.93	0.50
1:A:276:ASP:O	1:A:614:GLY:HA3	2.12	0.50
1:A:523:SER:O	1:A:527:TYR:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:GLU:CD	1:A:1039:ASP:N	2.69	0.50
1:B:62:THR:O	1:B:66:GLU:HG3	2.11	0.50
1:A:2:PRO:HG2	1:A:439:GLN:OE1	2.11	0.50
1:B:580:ALA:CB	1:B:724:THR:HG22	2.41	0.50
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.92	0.50
1:C:453:PHE:CE2	1:C:474:ILE:HG21	2.46	0.50
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.41	0.50
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.93	0.50
1:A:714:THR:CG2	1:A:832:ALA:HA	2.42	0.50
1:A:971:ARG:O	1:A:975:ILE:HG13	2.12	0.50
1:A:60:THR:CG2	1:A:61:VAL:HG23	2.39	0.49
1:A:523:SER:HB3	1:A:526:HIS:HB2	1.91	0.49
1:A:614:GLY:O	1:A:620:ARG:HA	2.12	0.49
1:C:57:VAL:HG22	1:C:88:VAL:CG1	2.42	0.49
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	1.93	0.49
1:B:1022:VAL:HG22	1:B:1023:PRO:CD	2.42	0.49
1:C:15:ILE:O	1:C:19:ILE:HG13	2.13	0.49
1:A:343:THR:HG22	5:A:1580:HOH:O	2.13	0.49
1:A:372:VAL:CB	1:A:373:PRO:HD3	2.43	0.49
1:A:512:PHE:O	1:A:515:TRP:HB3	2.13	0.49
1:B:328:ASP:O	1:B:331:PRO:HD2	2.12	0.49
1:B:420:MET:CE	1:B:499:PRO:HA	2.39	0.49
2:D:91:GLY:HA2	2:D:128:ILE:HD12	1.92	0.49
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.94	0.49
1:B:363:ARG:HD2	1:B:498:LYS:CG	2.42	0.49
1:C:111:LEU:HD21	1:C:127:VAL:HG12	1.93	0.49
1:A:358:PHE:CG	1:A:977:MET:HG2	2.48	0.49
1:A:540:ARG:HA	1:A:543:VAL:HG23	1.95	0.49
1:A:544:LEU:HD22	1:A:1021:PHE:HZ	1.77	0.49
1:A:919:ARG:NE	1:A:1005:THR:HG21	2.28	0.49
1:C:545:TYR:O	1:C:549:VAL:HG23	2.13	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.48	0.48
1:B:456:MET:HE1	1:B:877:TYR:CD1	2.48	0.48
1:B:926:TYR:HB3	1:B:1003:VAL:HG13	1.94	0.48
1:B:926:TYR:HB3	1:B:1003:VAL:CG1	2.42	0.48
1:A:534:ILE:HG22	1:A:541:TYR:OH	2.13	0.48
1:A:942:ALA:O	1:A:946:VAL:HG23	2.13	0.48
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.95	0.48
1:B:433:LYS:O	1:B:437:GLN:HG3	2.12	0.48
1:A:454:VAL:HB	1:A:455:PRO:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:THR:HB	1:A:627:ALA:HB3	1.95	0.48
1:A:866:GLU:O	1:A:869:SER:N	2.47	0.48
1:C:939:ALA:O	1:C:943:ILE:HG12	2.14	0.48
1:A:223:PRO:HD2	1:B:780:ARG:HH12	1.79	0.48
1:A:531:VAL:O	1:A:534:ILE:HG12	2.13	0.48
1:C:414:GLU:OE1	1:C:973:ARG:HD3	2.13	0.48
1:C:498:LYS:HA	1:C:498:LYS:HD3	1.65	0.48
1:C:867:ARG:NH1	1:C:867:ARG:HG2	2.26	0.48
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.49	0.48
1:B:105:VAL:HA	1:B:108:GLN:HG2	1.94	0.48
1:B:201:VAL:HG22	1:B:748:THR:HG23	1.95	0.48
1:C:11:PHE:HD1	1:C:11:PHE:O	1.97	0.48
1:C:540:ARG:O	1:C:544:LEU:HD23	2.13	0.48
1:C:111:LEU:HD21	1:C:127:VAL:HG11	1.96	0.48
1:A:350:LEU:O	1:A:354:VAL:HG23	2.14	0.48
1:A:958:LYS:HA	1:A:1041:GLU:HB2	1.96	0.48
1:B:641:GLU:H	1:B:641:GLU:HG3	1.41	0.48
1:C:5:PHE:CD2	1:C:487:ILE:HG23	2.49	0.48
1:A:185:ARG:HD2	5:A:1561:HOH:O	2.13	0.47
1:A:361:ASN:O	1:A:365:THR:HG23	2.14	0.47
1:B:424:GLY:HA3	1:B:502:LYS:HB2	1.95	0.47
1:B:679:GLY:HA2	5:B:1469:HOH:O	2.14	0.47
1:C:10:ILE:O	1:C:14:VAL:HG13	2.14	0.47
1:C:314:GLU:N	1:C:315:PRO:CD	2.77	0.47
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.49	0.47
1:B:1011:MET:HE3	1:B:1015:THR:HG21	1.95	0.47
1:C:36:PRO:HG3	1:C:469:GLN:CD	2.39	0.47
1:C:875:SER:O	1:C:879:ILE:HG22	2.15	0.47
1:A:437:GLN:HG3	1:A:438:ILE:HG23	1.97	0.47
1:B:559:LEU:HD23	1:B:923:ASN:HB2	1.96	0.47
1:B:580:ALA:HB1	1:B:724:THR:CG2	2.44	0.47
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.97	0.47
1:A:188:MET:CE	1:A:773:VAL:HG12	2.38	0.47
1:B:360:GLN:HG2	1:B:513:PHE:CD1	2.48	0.47
1:B:672:VAL:HG21	5:B:1359:HOH:O	2.14	0.47
1:A:223:PRO:HA	1:A:224:PRO:HD3	1.82	0.47
1:A:339:GLU:O	1:A:343:THR:HG23	2.14	0.47
1:A:527:TYR:O	1:A:530:SER:HB2	2.14	0.47
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.47
1:C:575:MET:HE1	1:C:617:PHE:CD2	2.49	0.47
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:OD1	1:A:85:THR:HB	2.14	0.47
1:C:162:MET:HE1	1:C:323:ILE:HD11	1.97	0.47
1:A:26:ALA:O	1:A:30:LEU:HB2	2.14	0.46
1:A:537:SER:C	1:A:539:GLY:H	2.22	0.46
1:B:351:VAL:HG22	1:B:406:VAL:HG13	1.97	0.46
1:B:904:VAL:O	1:B:907:LEU:HB2	2.15	0.46
1:C:146:ASP:OD1	1:C:148:THR:HG23	2.14	0.46
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.98	0.46
1:B:925:VAL:O	1:B:929:VAL:HG23	2.15	0.46
2:D:12:SER:O	2:D:16:LYS:HG2	2.16	0.46
2:E:89:HIS:HD2	2:E:123:ARG:HG3	1.80	0.46
1:A:330:THR:HG22	1:A:331:PRO:N	2.29	0.46
1:C:617:PHE:CD2	1:C:676:THR:HG21	2.49	0.46
1:B:674:LEU:HD23	1:B:674:LEU:O	2.15	0.46
2:D:25:GLY:HA2	2:D:62:ILE:CD1	2.46	0.46
1:B:169:THR:O	1:B:172:VAL:HG13	2.15	0.46
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.97	0.46
1:C:370:ILE:C	1:C:373:PRO:HD2	2.40	0.46
1:A:85:THR:O	1:A:85:THR:HG22	2.15	0.46
1:A:602:GLU:CB	1:A:606:VAL:HG13	2.45	0.46
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.37	0.46
1:B:256:ASP:OD1	1:B:256:ASP:N	2.49	0.46
1:B:449:LEU:HB3	1:B:478:MET:SD	2.56	0.46
1:C:407:ASN:ND2	1:C:978:THR:HG21	2.30	0.46
1:C:841:MET:O	1:C:845:GLU:HG3	2.16	0.46
1:C:867:ARG:HG2	5:C:1315:HOH:O	2.15	0.46
1:A:8:ARG:N	1:A:9:PRO:HD3	2.30	0.46
1:C:2:PRO:O	1:C:6:ILE:HG13	2.16	0.46
1:A:1038:GLU:O	1:A:1039:ASP:HB2	2.15	0.46
1:B:540:ARG:HH22	3:B:1101:LMT:H6'1	1.80	0.46
1:A:527:TYR:HE2	1:A:968:VAL:CG1	2.28	0.46
1:A:961:ILE:HD12	1:A:961:ILE:N	2.31	0.46
1:C:104:GLN:NE2	1:C:108:GLN:OE1	2.33	0.46
1:C:376:LEU:HD11	1:C:402:ILE:CD1	2.46	0.46
1:C:943:ILE:O	1:C:947:GLU:HB3	2.16	0.46
1:A:987:MET:O	1:A:990:VAL:HG22	2.16	0.45
1:B:682:PHE:HB2	1:B:859:TRP:CZ3	2.51	0.45
1:C:868:LEU:O	1:C:872:GLN:HG2	2.15	0.45
1:A:836:SER:OG	1:A:839:GLU:HG3	2.15	0.45
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.97	0.45
1:B:913:LEU:HD23	1:B:927:PHE:CZ	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.45
1:C:185:ARG:HB2	1:C:269:GLU:O	2.16	0.45
1:C:841:MET:HE3	1:C:859:TRP:CD2	2.52	0.45
1:B:489:THR:N	1:B:490:PRO:CD	2.79	0.45
1:B:714:THR:HG21	1:B:832:ALA:HA	1.98	0.45
1:C:358:PHE:CG	1:C:977:MET:HG2	2.52	0.45
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.98	0.45
1:A:509:LYS:CG	1:A:510:LYS:N	2.78	0.45
1:A:636:ASP:C	1:A:638:PRO:HD3	2.41	0.45
1:A:714:THR:HG22	5:A:1530:HOH:O	2.17	0.45
1:B:394:THR:C	1:B:395:MET:HE2	2.42	0.45
1:B:986:VAL:HG21	1:B:1007:VAL:CG1	2.47	0.45
1:A:415:ASN:ND2	1:A:438:ILE:HG21	2.32	0.45
1:A:450:SER:O	1:A:454:VAL:HG23	2.16	0.45
1:A:937:LEU:HD23	1:A:1011:MET:CE	2.47	0.45
1:B:197:GLN:HA	1:B:798:MET:SD	2.57	0.45
1:B:527:TYR:CZ	1:B:968:VAL:HG13	2.52	0.45
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.51	0.45
3:A:1101:LMT:H121	3:A:1101:LMT:H91	1.86	0.45
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.98	0.45
2:E:49:THR:HB	2:E:50:PRO:HD2	1.99	0.45
1:A:10:ILE:O	1:A:14:VAL:HG23	2.17	0.45
1:C:48:SER:HB3	1:C:125:GLN:HG2	1.99	0.45
1:C:276:ASP:O	1:C:614:GLY:HA3	2.17	0.45
1:A:406:VAL:O	1:A:410:ILE:HG13	2.17	0.44
1:B:600:THR:HG22	1:B:601:LYS:N	2.32	0.44
1:A:522:LYS:O	1:A:526:HIS:ND1	2.48	0.44
1:A:909:VAL:HG13	1:A:931:LEU:HD21	1.98	0.44
2:D:58:GLY:HA2	2:D:95:ILE:HD12	1.99	0.44
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.47	0.44
1:A:76:MET:HG2	1:A:95:GLU:OE1	2.18	0.44
1:B:121:GLU:CD	1:B:121:GLU:H	2.25	0.44
1:C:743:ILE:HD12	1:C:743:ILE:N	2.31	0.44
1:A:699:ARG:O	1:A:703:LEU:HG	2.18	0.44
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.99	0.44
1:B:99:ASP:OD1	1:B:101:ASP:HB2	2.18	0.44
1:B:358:PHE:CD1	1:B:977:MET:HG2	2.53	0.44
1:C:76:MET:HE2	1:C:93:THR:HG22	1.99	0.44
1:A:10:ILE:HD12	1:B:894:SER:HA	1.99	0.44
1:A:672:VAL:HB	1:A:673:GLU:H	1.65	0.44
1:A:673:GLU:CD	1:A:673:GLU:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.17	0.44
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.18	0.44
1:B:973:ARG:HG2	1:B:977:MET:HE2	2.00	0.44
1:A:284:GLN:HB2	1:A:285:PRO:HD2	2.00	0.44
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.99	0.44
1:A:739:LEU:HD13	1:A:799:VAL:HG11	2.00	0.44
1:B:395:MET:O	1:B:398:MET:HB2	2.17	0.44
1:B:714:THR:HG22	1:B:832:ALA:CA	2.47	0.44
1:C:621:GLY:N	5:C:1581:HOH:O	2.12	0.44
1:A:636:ASP:O	1:A:638:PRO:HD3	2.18	0.44
1:A:972:LEU:HD13	1:A:972:LEU:C	2.42	0.44
1:A:1009:GLY:O	1:A:1013:THR:HG23	2.17	0.44
1:C:360:GLN:HB3	1:C:513:PHE:CD2	2.53	0.44
1:C:955:LYS:HG3	1:C:956:GLU:HG3	1.99	0.44
1:A:397:GLY:HA3	1:A:473:THR:HG21	2.00	0.44
1:B:70:ASN:O	1:B:110:LYS:HE3	2.18	0.44
1:B:144:ASN:HA	1:B:320:GLY:O	2.17	0.44
1:B:509:LYS:HG3	1:B:510:LYS:H	1.83	0.44
1:A:59:ASP:HB3	1:C:763:ILE:HD11	2.00	0.43
1:A:375:VAL:HB	1:A:405:LEU:HD13	2.00	0.43
1:A:544:LEU:O	1:A:548:ILE:HG13	2.18	0.43
1:A:881:LEU:HG	3:A:1102:LMT:H122	2.00	0.43
1:B:115:MET:N	1:B:116:PRO:CD	2.81	0.43
1:B:300:LEU:CD2	1:B:330:THR:HG23	2.48	0.43
1:B:464:GLY:O	1:B:468:ARG:HB2	2.18	0.43
1:C:185:ARG:HD3	1:C:185:ARG:HA	1.84	0.43
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.48	0.43
1:A:356:TYR:CA	1:A:365:THR:HG21	2.37	0.43
1:A:817:GLU:HB2	1:A:824:SER:O	2.18	0.43
1:A:960:LEU:HG	1:A:1027:VAL:HG12	2.00	0.43
1:A:888:LEU:HB2	1:A:898:PRO:HB3	2.00	0.43
1:A:919:ARG:O	1:A:919:ARG:HG2	2.18	0.43
1:A:1034:SER:O	1:A:1035:ARG:HB2	2.18	0.43
1:B:38:ILE:HG21	1:B:674:LEU:HD12	1.99	0.43
1:B:680:PHE:HA	5:B:1240:HOH:O	2.17	0.43
1:B:973:ARG:N	1:B:974:PRO:HD2	2.32	0.43
1:C:620:ARG:HE	1:C:620:ARG:HB3	1.44	0.43
1:A:2:PRO:O	1:A:6:ILE:HG13	2.18	0.43
1:A:1039:ASP:O	1:A:1040:ILE:HD13	2.17	0.43
1:B:527:TYR:CE2	1:B:968:VAL:CG1	3.00	0.43
2:E:25:GLY:O	2:E:27:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:THR:HG21	1:A:969:ARG:HG2	1.96	0.43
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.18	0.43
1:A:1012:VAL:HA	1:A:1015:THR:HG22	2.00	0.43
1:A:1038:GLU:CG	1:A:1039:ASP:N	2.81	0.43
1:A:68:ASN:O	1:A:110:LYS:HB3	2.19	0.43
1:A:483:LEU:HD12	1:A:483:LEU:HA	1.90	0.43
1:B:192:GLU:OE2	1:B:192:GLU:HA	2.18	0.43
4:B:1103:MIY:H81	4:B:1103:MIY:HN72	2.01	0.43
1:A:881:LEU:CD2	3:A:1102:LMT:H121	2.49	0.43
1:B:235:ILE:O	1:C:728:LYS:HD2	2.18	0.43
1:C:937:LEU:HD13	1:C:1011:MET:SD	2.59	0.43
1:A:144:ASN:HA	1:A:320:GLY:O	2.19	0.43
1:A:375:VAL:HG11	1:A:405:LEU:CD2	2.48	0.43
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.81	0.43
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.01	0.43
1:B:456:MET:HG3	1:B:932:LEU:HD11	2.00	0.43
1:B:573:MET:HE2	1:B:666:PHE:CZ	2.54	0.43
2:D:121:ALA:CB	2:D:161:LEU:HD21	2.47	0.43
1:A:8:ARG:HG2	5:B:1223:HOH:O	2.19	0.43
1:A:167:SER:HB3	1:B:70:ASN:HB3	2.01	0.42
1:A:614:GLY:HA2	1:A:621:GLY:O	2.18	0.42
1:A:907:LEU:CD2	1:A:1017:LEU:HD23	2.41	0.42
1:C:33:ALA:O	1:C:391:ASN:HA	2.19	0.42
1:A:27:ILE:HD13	3:A:1101:LMT:H51	2.00	0.42
1:C:348:ILE:HG12	1:C:402:ILE:HD12	2.00	0.42
1:A:994:GLY:O	1:A:997:SER:HB2	2.19	0.42
1:A:1036:LYS:HE3	1:A:1036:LYS:HB2	1.86	0.42
1:C:434:SER:O	1:C:438:ILE:HG12	2.19	0.42
1:A:401:ALA:O	1:A:405:LEU:HG	2.19	0.42
1:A:520:PHE:HZ	1:A:973:ARG:HB2	1.81	0.42
1:B:173:GLY:HA2	1:C:71:GLY:HA3	2.01	0.42
1:C:144:ASN:HA	1:C:320:GLY:O	2.20	0.42
1:C:444:GLY:HA2	1:C:891:LEU:CD2	2.49	0.42
1:A:28:LEU:HD22	3:A:1101:LMT:H5B	2.01	0.42
1:A:108:GLN:NE2	1:B:109:ASN:O	2.51	0.42
1:A:330:THR:HG22	1:A:331:PRO:HD3	2.01	0.42
1:A:358:PHE:HB2	1:A:977:MET:HE3	2.01	0.42
1:C:135:SER:OG	1:C:672:VAL:HB	2.19	0.42
1:C:510:LYS:HD2	1:C:511:GLY:N	2.35	0.42
1:C:673:GLU:OE2	1:C:673:GLU:N	2.51	0.42
1:A:188:MET:CE	1:A:773:VAL:CG1	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:GLU:N	1:A:315:PRO:CD	2.82	0.42
1:A:376:LEU:CD1	1:A:405:LEU:HD11	2.49	0.42
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.42
1:C:895:TRP:C	1:C:898:PRO:HD2	2.45	0.42
1:A:33:ALA:O	1:A:391:ASN:HA	2.20	0.42
1:A:330:THR:HG22	1:A:331:PRO:CD	2.50	0.42
1:A:367:ILE:HB	1:A:368:PRO:CD	2.50	0.42
1:A:519:MET:O	1:A:522:LYS:HG3	2.19	0.42
1:B:546:LEU:HA	1:B:546:LEU:HD12	1.81	0.42
1:C:360:GLN:HB3	1:C:513:PHE:CE2	2.55	0.42
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.79	0.42
1:A:23:GLY:HA3	1:A:377:LEU:O	2.19	0.42
1:A:1019:ILE:HG22	1:A:1020:PHE:CD2	2.55	0.42
1:C:240:LEU:HB2	1:C:246:PHE:CE2	2.55	0.42
1:C:366:LEU:HD12	1:C:366:LEU:HA	1.79	0.42
1:C:544:LEU:HD13	1:C:544:LEU:HA	1.75	0.42
1:C:754:TRP:CE2	1:C:786:ILE:HD13	2.54	0.42
1:A:146:ASP:O	1:A:148:THR:HG23	2.20	0.42
1:A:668:LEU:HD12	1:A:668:LEU:HA	1.89	0.42
1:B:919:ARG:HH11	1:B:1005:THR:CG2	2.32	0.42
1:B:927:PHE:CE2	1:B:931:LEU:HD11	2.55	0.42
1:C:537:SER:HB3	3:C:1101:LMT:O6B	2.20	0.42
2:E:92:HIS:O	2:E:96:VAL:HG23	2.19	0.42
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.35	0.41
1:C:319:SER:HA	5:C:1385:HOH:O	2.18	0.41
1:C:404:LEU:CD1	1:C:937:LEU:HD21	2.50	0.41
1:B:509:LYS:O	1:B:514:GLY:HA3	2.20	0.41
4:B:1103:MIY:HN72	4:B:1103:MIY:C8	2.50	0.41
2:D:58:GLY:HA2	2:D:95:ILE:CD1	2.51	0.41
2:E:105:ASP:HB3	2:E:108:ALA:HB2	2.02	0.41
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.21	0.41
1:B:559:LEU:HD12	1:B:560:PRO:HD2	2.01	0.41
1:B:971:ARG:HD3	5:B:1473:HOH:O	2.19	0.41
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.56	0.41
1:A:488:LEU:HG	1:A:492:LEU:HD22	2.02	0.41
1:A:976:LEU:HD23	1:A:976:LEU:HA	1.85	0.41
1:B:420:MET:HE1	1:B:427:PRO:HD3	2.01	0.41
1:B:863:SER:O	1:B:867:ARG:HG3	2.20	0.41
2:D:117:LEU:HD11	2:D:129:VAL:HG13	2.02	0.41
1:A:520:PHE:C	1:A:522:LYS:N	2.78	0.41
1:A:1038:GLU:OE2	1:A:1039:ASP:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:PHE:CE2	1:C:676:THR:HG21	2.55	0.41
1:A:38:ILE:HD12	1:A:39:ALA:H	1.83	0.41
1:A:388:PHE:HE2	1:A:472:ILE:HB	1.86	0.41
1:B:84:SER:HB2	5:B:1404:HOH:O	2.21	0.41
1:B:203:VAL:O	1:B:207:ILE:HG13	2.20	0.41
1:B:453:PHE:HZ	1:B:933:THR:HG22	1.86	0.41
2:E:34:MET:HE1	2:E:66:LEU:HD23	2.03	0.41
2:E:75:ALA:O	2:E:83:PRO:HD3	2.21	0.41
1:A:307:ARG:NH2	1:A:330:THR:HG21	2.36	0.41
1:A:939:ALA:O	1:A:943:ILE:HG13	2.21	0.41
1:A:1012:VAL:O	1:A:1016:VAL:HG22	2.20	0.41
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.90	0.41
1:B:637:ARG:N	1:B:638:PRO:HD3	2.36	0.41
1:A:10:ILE:HD12	1:B:894:SER:CA	2.51	0.41
1:A:360:GLN:HB3	1:A:513:PHE:CE2	2.55	0.41
1:A:404:LEU:HD23	1:A:937:LEU:HD13	2.02	0.41
1:A:405:LEU:CD2	1:A:481:SER:HB2	2.46	0.41
1:A:434:SER:O	1:A:438:ILE:HG12	2.20	0.41
1:A:516:PHE:CA	1:A:519:MET:HG2	2.46	0.41
1:A:907:LEU:HD13	1:A:1017:LEU:HB3	2.02	0.41
1:B:1:MET:HB3	1:B:2:PRO:CD	2.51	0.41
1:B:484:VAL:HG13	1:B:488:LEU:HB3	2.03	0.41
1:B:667:ASN:OD1	1:B:668:LEU:N	2.54	0.41
1:C:405:LEU:C	1:C:405:LEU:HD12	2.46	0.41
1:C:879:ILE:HD12	1:C:879:ILE:O	2.20	0.41
1:A:449:LEU:HD21	1:A:940:LYS:HB2	2.02	0.41
1:A:953:MET:HE3	1:A:1038:GLU:OE1	2.21	0.41
1:B:897:ILE:N	1:B:898:PRO:CD	2.84	0.41
3:B:1102:LMT:H6D	3:B:1102:LMT:O2B	2.21	0.41
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.56	0.41
1:C:873:ALA:HB3	1:C:874:PRO:HD3	2.02	0.41
1:C:973:ARG:HB3	1:C:974:PRO:HD3	2.02	0.41
1:A:509:LYS:HG3	1:A:510:LYS:H	1.85	0.40
1:A:1034:SER:O	1:A:1035:ARG:CB	2.69	0.40
1:C:302:THR:O	1:C:306:ILE:HG13	2.21	0.40
1:C:416:VAL:HG22	1:C:431:THR:HA	2.02	0.40
1:A:185:ARG:HD3	1:A:185:ARG:HA	1.77	0.40
1:A:284:GLN:HB2	1:A:285:PRO:CD	2.51	0.40
1:A:360:GLN:HB3	1:A:513:PHE:CD2	2.57	0.40
1:A:986:VAL:O	1:A:989:LEU:HB2	2.21	0.40
1:C:332:PHE:HA	1:C:335:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:903:LEU:O	1:C:906:PRO:HD2	2.21	0.40
1:A:449:LEU:HD12	1:A:449:LEU:HA	1.87	0.40
1:A:530:SER:O	1:A:534:ILE:HG23	2.20	0.40
1:B:996:GLY:O	1:B:1000:GLN:HG3	2.21	0.40
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.51	0.40
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	2.04	0.40
1:A:1016:VAL:O	1:A:1019:ILE:HG22	2.22	0.40
1:B:404:LEU:HD23	1:B:937:LEU:HD21	2.03	0.40
1:B:510:LYS:CD	1:B:511:GLY:H	2.34	0.40
1:B:674:LEU:CD2	1:B:677:ALA:HB2	2.51	0.40
1:B:774:MET:HE2	1:B:780:ARG:CZ	2.51	0.40
1:B:966:ASP:HB2	5:B:1207:HOH:O	2.21	0.40
1:C:472:ILE:HG23	1:C:473:THR:N	2.36	0.40
2:E:40:VAL:HG23	2:E:71:ALA:HA	2.03	0.40
2:E:89:HIS:CE1	2:E:119:LEU:HD22	2.56	0.40
5:A:1375:HOH:O	1:C:214:VAL:HG21	2.21	0.40
1:C:395:MET:HE1	1:C:398:MET:HG3	2.01	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1042/1057 (99%)	992 (95%)	38 (4%)	12 (1%)	10	12
1	B	1031/1057 (98%)	1007 (98%)	23 (2%)	1 (0%)	48	60
1	C	1031/1057 (98%)	1004 (97%)	26 (2%)	1 (0%)	48	60
2	D	154/169 (91%)	150 (97%)	4 (3%)	0	100	100
2	E	150/169 (89%)	145 (97%)	4 (3%)	1 (1%)	18	23
All	All	3408/3509 (97%)	3298 (97%)	95 (3%)	15 (0%)	30	38

All (15) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/863 (98%)	818 (96%)	32 (4%)	29	44
1	B	839/863 (97%)	805 (96%)	34 (4%)	27	41
1	C	839/863 (97%)	811 (97%)	28 (3%)	33	50
2	D	120/132 (91%)	116 (97%)	4 (3%)	33	50
2	E	117/132 (89%)	116 (99%)	1 (1%)	70	84
All	All	2765/2853 (97%)	2666 (96%)	99 (4%)	31	47

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	30	LEU
1	A	37	THR

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	60	THR
1	A	96	SER
1	A	121	GLU
1	A	270	LEU
1	A	330	THR
1	A	359	LEU
1	A	448	VAL
1	A	449	LEU
1	A	492	LEU
1	A	522	LYS
1	A	606	VAL
1	A	630	SER
1	A	660	ASP
1	A	672	VAL
1	A	673	GLU
1	A	687	GLN
1	A	714	THR
1	A	717	ARG
1	A	768	VAL
1	A	867	ARG
1	A	921	LEU
1	A	922	THR
1	A	932	LEU
1	A	987	MET
1	A	1019	ILE
1	A	1038	GLU
1	A	1039	ASP
1	A	1040	ILE
1	B	1	MET
1	B	30	LEU
1	B	48	SER
1	B	88	VAL
1	B	117	LEU
1	B	121	GLU
1	B	128	SER
1	B	135	SER
1	B	172	VAL
1	B	230	LEU
1	B	314	GLU
1	B	321	LEU
1	B	324	VAL

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Mol	Chain	Res	Type
1	B	336	SER
1	B	342	LYS
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	546	LEU
1	B	558	ARG
1	B	600	THR
1	B	641	GLU
1	B	649	MET
1	B	653	ARG
1	B	660	ASP
1	B	714	THR
1	B	763	ILE
1	B	866	GLU
1	B	968	VAL
1	B	978	THR
1	B	992	SER
1	B	1007	VAL
1	B	1022	VAL
1	B	1030	ARG
1	C	14	VAL
1	C	87	THR
1	C	88	VAL
1	C	113	LEU
1	C	121	GLU
1	C	158	VAL
1	C	256	ASP
1	C	314	GLU
1	C	324	VAL
1	C	366	LEU
1	C	372	VAL
1	C	392	THR
1	C	404	LEU
1	C	407	ASN
1	C	448	VAL
1	C	472	ILE
1	C	482	VAL
1	C	620	ARG
1	C	641	GLU
1	C	676	THR
1	C	739	LEU

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Mol	Chain	Res	Type
1	C	773	VAL
1	C	867	ARG
1	C	879	ILE
1	C	940	LYS
1	C	950	LYS
1	C	968	VAL
1	C	1030	ARG
2	D	45	VAL
2	D	61	GLU
2	D	94	GLU
2	D	154	ILE
2	E	31	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	361	ASN
1	A	437	GLN
1	A	469	GLN
1	A	737	GLN
1	B	108	GLN
1	B	194	ASN
1	B	284	GLN
1	B	604	ASN
1	B	1001	ASN
1	C	58	GLN
1	C	89	GLN
1	C	360	GLN
1	C	517	ASN
1	C	526	HIS
1	C	657	GLN
1	C	797	GLN
2	D	166	GLN
2	E	59	HIS

5.3.3 RNA ⓘ

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](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	LMT	A	1101	-	36,36,36	0.46	1 (2%)	47,47,47	0.86	1 (2%)
3	LMT	B	1101	-	36,36,36	0.44	0	47,47,47	0.97	2 (4%)
3	LMT	B	1102	-	36,36,36	0.48	1 (2%)	47,47,47	1.23	5 (10%)
3	LMT	A	1102	-	36,36,36	0.47	0	47,47,47	0.85	1 (2%)
3	LMT	C	1101	-	36,36,36	0.46	0	47,47,47	1.00	1 (2%)
4	MIY	B	1103	-	36,36,36	1.98	14 (38%)	42,58,58	2.71	17 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	B	1101	-	-	9/21/61/61	0/2/2/2
3	LMT	B	1102	-	-	10/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	7/21/61/61	0/2/2/2
3	LMT	C	1101	-	-	5/21/61/61	0/2/2/2
4	MIY	B	1103	-	-	3/12/70/70	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1103	MIY	C11-C10	4.03	1.45	1.39
4	B	1103	MIY	C71-N7	3.76	1.53	1.45
4	B	1103	MIY	C4-N1	3.21	1.54	1.47
4	B	1103	MIY	CN7-N7	3.15	1.52	1.45
4	B	1103	MIY	C14-C13	-3.06	1.36	1.41
4	B	1103	MIY	C7-C16	-2.74	1.48	1.51
4	B	1103	MIY	O4-C13	2.67	1.41	1.36
4	B	1103	MIY	C18-C17	2.58	1.54	1.52
4	B	1103	MIY	C21-N2	2.48	1.40	1.33
4	B	1103	MIY	C6-C5	2.45	1.57	1.53
4	B	1103	MIY	O7-C18	2.45	1.45	1.42
4	B	1103	MIY	C18-C1	-2.31	1.52	1.55
4	B	1103	MIY	C10-C9	2.13	1.42	1.40
3	A	1101	LMT	O1'-C1'	2.07	1.43	1.40
3	B	1102	LMT	O1'-C1'	2.06	1.43	1.40
4	B	1103	MIY	C20-N1	2.03	1.53	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	MIY	C1-C18-C17	7.59	118.78	109.88
4	B	1103	MIY	C11-C12-C13	-6.68	113.82	120.50
4	B	1103	MIY	C15-C16-C17	6.00	123.55	118.80
4	B	1103	MIY	C12-C13-C14	5.35	126.98	120.15
4	B	1103	MIY	O5-C15-C14	-3.85	115.10	122.06
4	B	1103	MIY	O7-C18-C17	-3.83	104.02	110.14
4	B	1103	MIY	C11-C10-N7	-3.69	116.57	121.65
3	B	1102	LMT	O5B-C1B-C2B	3.47	117.49	110.37
3	C	1101	LMT	C4B-C3B-C2B	-3.41	104.85	110.83
3	B	1102	LMT	C1B-C2B-C3B	3.28	116.91	110.01
4	B	1103	MIY	C9-C10-N7	3.27	122.77	118.87
3	B	1102	LMT	C1B-O5B-C5B	3.12	119.81	113.72
4	B	1103	MIY	O2-C3-C2	-2.96	117.97	122.93
3	A	1101	LMT	O1'-C1'-C2'	2.84	112.58	108.27
4	B	1103	MIY	C19-N1-C4	2.64	120.13	114.10
3	B	1102	LMT	O1B-C4'-C3'	2.64	113.94	107.23
3	B	1102	LMT	O1'-C1'-C2'	2.59	112.20	108.27
4	B	1103	MIY	C18-C17-C16	2.58	125.69	123.06
4	B	1103	MIY	C71-N7-CN7	2.57	124.46	116.18
4	B	1103	MIY	O8-C21-N2	-2.54	117.20	122.89
3	B	1101	LMT	C4B-C3B-C2B	-2.48	106.48	110.83
3	A	1102	LMT	O1B-C4'-C3'	2.44	113.44	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	MIY	O6-C17-C16	-2.39	118.89	123.52
4	B	1103	MIY	C18-C1-C2	2.23	119.30	115.75
4	B	1103	MIY	CN7-N7-C10	2.10	121.68	115.16
4	B	1103	MIY	O4-C13-C12	-2.10	113.74	119.36
3	B	1101	LMT	O1B-C1B-C2B	2.02	113.05	108.09

There are no chirality outliers.

All (46) torsion outliers are listed below:

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

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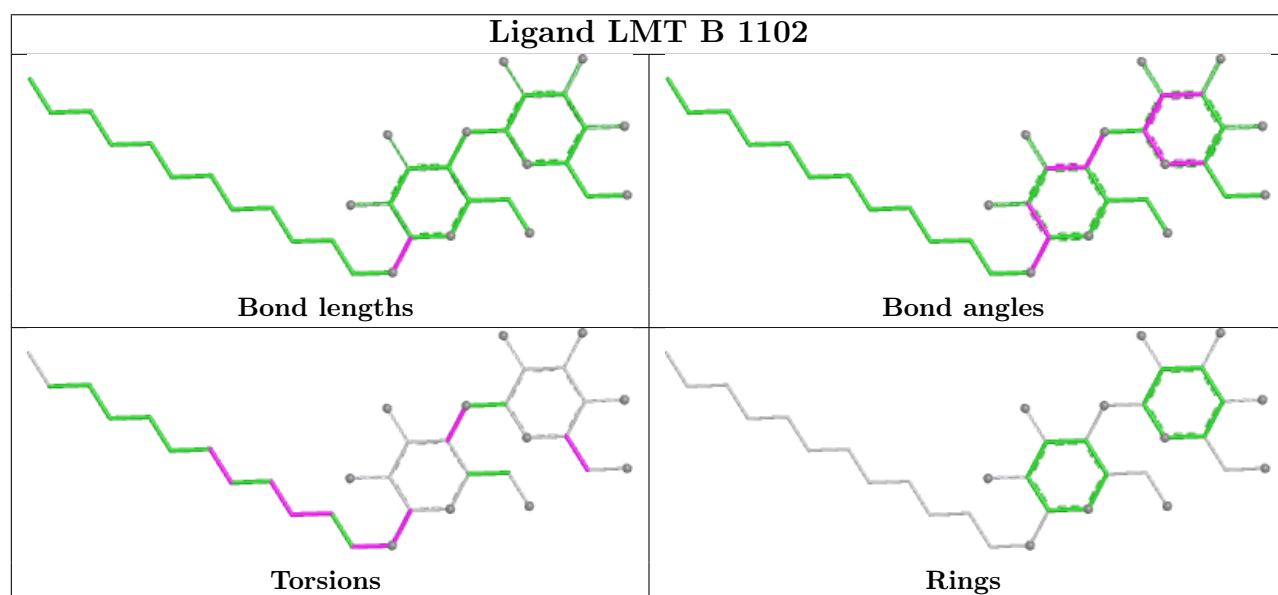
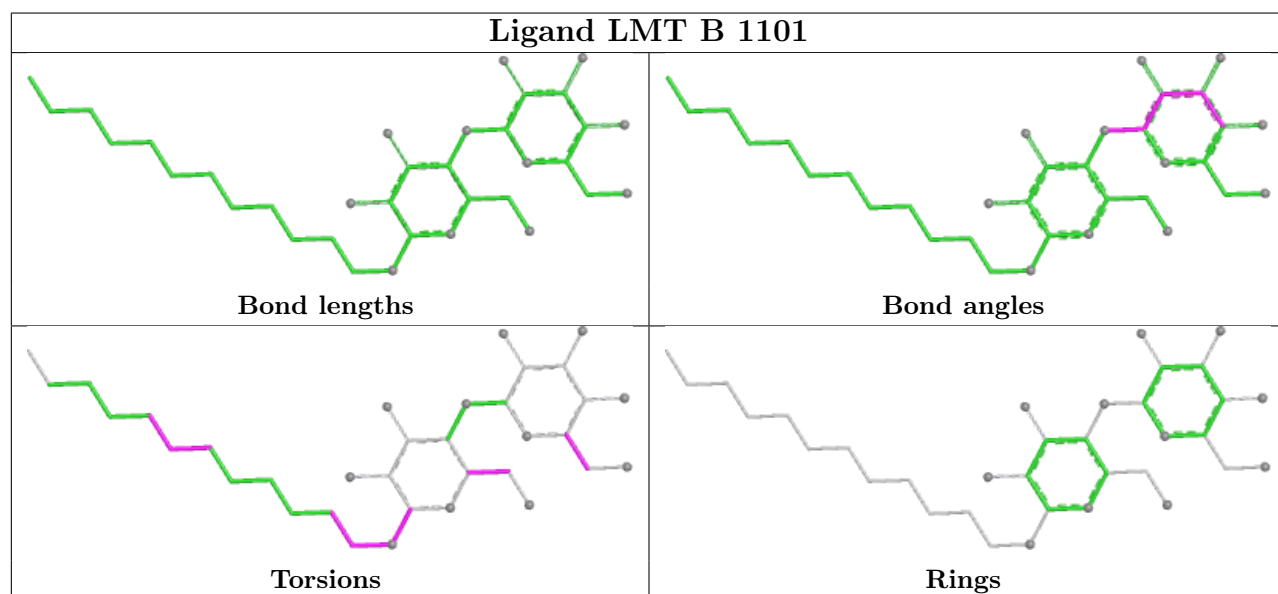
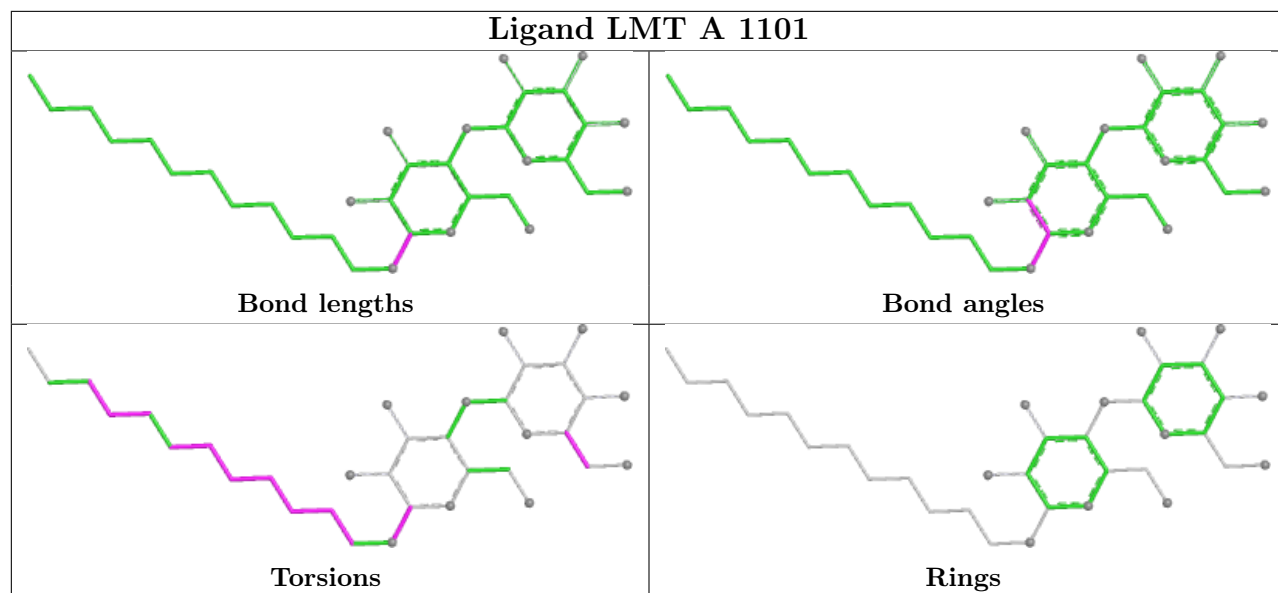
Mol	Chain	Res	Type	Atoms
3	B	1102	LMT	C4-C5-C6-C7
3	A	1102	LMT	C1-C2-C3-C4
4	B	1103	MIY	C3-C2-C21-N2
4	B	1103	MIY	C3-C2-C21-O8
4	B	1103	MIY	C1-C2-C21-N2
3	A	1102	LMT	C5'-C4'-O1B-C1B
3	A	1102	LMT	C3'-C4'-O1B-C1B
3	B	1101	LMT	C2-C1-O1'-C1'
3	B	1102	LMT	C1-C2-C3-C4
3	B	1102	LMT	C4B-C5B-C6B-O6B
3	A	1101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

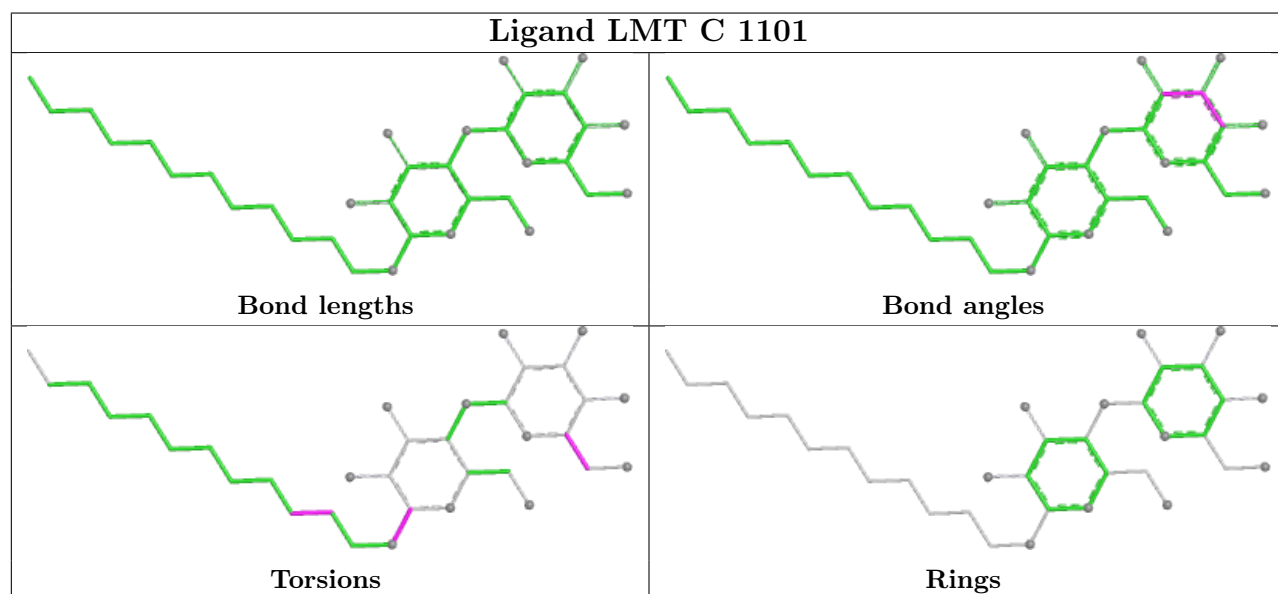
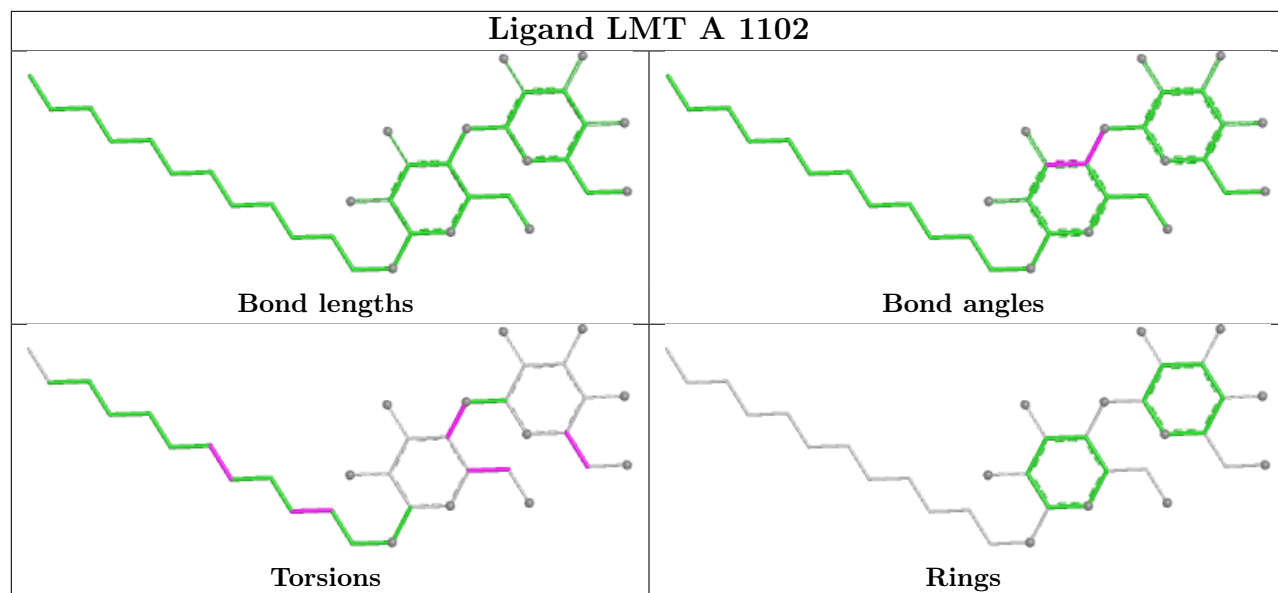
There are no ring outliers.

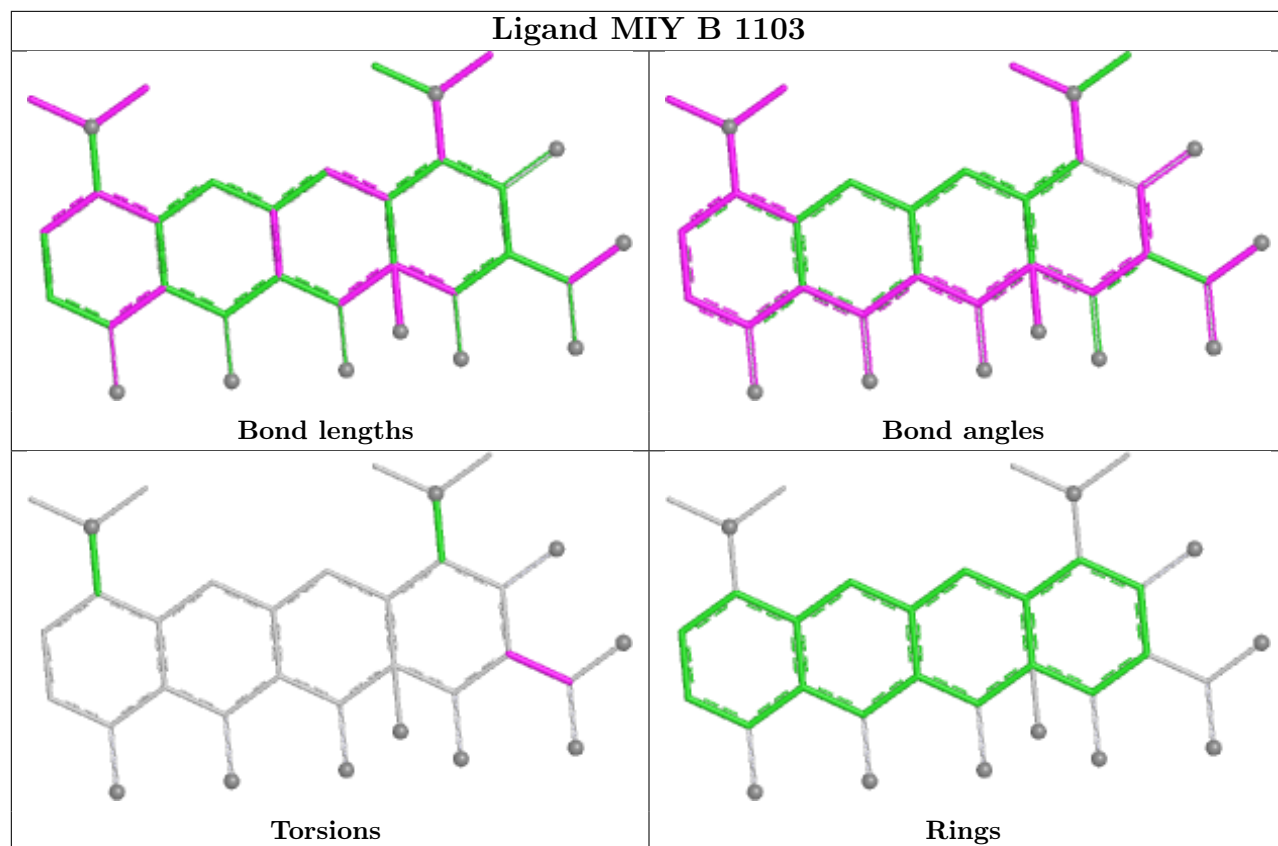
6 monomers are involved in 21 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1044/1057 (98%)	0.40	104 (9%) 12 14	23, 51, 115, 155	0
1	B	1033/1057 (97%)	0.09	34 (3%) 49 51	24, 48, 71, 109	0
1	C	1033/1057 (97%)	-0.08	26 (2%) 58 60	24, 43, 71, 111	0
2	D	156/169 (92%)	0.04	6 (3%) 44 46	40, 48, 74, 110	0
2	E	152/169 (89%)	0.34	6 (3%) 43 45	49, 66, 95, 120	0
All	All	3418/3509 (97%)	0.14	176 (5%) 33 35	23, 48, 92, 155	0

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	678	THR	7.9
1	A	618	ALA	7.5
1	A	672	VAL	7.1
1	A	617	PHE	6.7
1	B	617	PHE	6.6
1	A	677	ALA	6.4
1	A	674	LEU	6.4
1	A	1040	ILE	6.3
1	A	619	GLY	5.8
2	D	11	GLY	5.4
1	A	38	ILE	5.3
1	A	540	ARG	5.1
1	A	1042	HIS	4.9
1	A	1044	HIS	4.9
1	A	918	PHE	4.7
1	B	674	LEU	4.7
1	B	563	PHE	4.7
1	B	561	SER	4.6
1	A	520	PHE	4.5
1	A	948	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	501	ALA	4.4
1	A	509	LYS	4.4
1	A	1034	SER	4.4
1	A	459	PHE	4.2
1	A	868	LEU	4.2
1	A	547	ILE	4.1
1	B	993	THR	4.0
1	C	659	LYS	3.9
1	B	868	LEU	3.9
1	C	948	PHE	3.9
1	A	362	PHE	3.9
1	A	675	GLY	3.8
1	B	666	PHE	3.8
1	A	539	GLY	3.7
1	B	659	LYS	3.7
1	C	618	ALA	3.7
1	C	70	ASN	3.7
2	E	166	GLN	3.6
1	B	676	THR	3.6
1	B	662	MET	3.5
1	A	536	ARG	3.5
2	D	12	SER	3.4
1	B	616	GLY	3.4
1	B	673	GLU	3.4
1	B	461	GLY	3.4
2	D	166	GLN	3.4
1	A	467	TYR	3.4
1	A	364	ALA	3.4
1	A	961	ILE	3.3
1	B	575	MET	3.3
1	A	676	THR	3.3
1	B	509	LYS	3.3
1	A	869	SER	3.2
1	C	96	SER	3.2
1	A	1038	GLU	3.2
1	A	671	ILE	3.2
1	C	362	PHE	3.2
1	A	522	LYS	3.2
1	C	255	GLN	3.2
1	A	1036	LYS	3.1
1	A	421	ALA	3.1
1	B	987	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	510	LYS	3.1
1	C	511	GLY	3.0
1	C	811	TYR	3.0
1	A	361	ASN	3.0
1	A	673	GLU	3.0
1	A	462	SER	3.0
1	B	615	PHE	2.9
1	A	1035	ARG	2.9
1	A	511	GLY	2.9
1	A	965	LEU	2.9
1	B	498	LYS	2.9
1	A	711	ASP	2.8
1	A	525	HIS	2.8
1	A	866	GLU	2.8
1	C	71	GLY	2.8
1	A	541	TYR	2.8
1	A	417	GLU	2.8
1	C	510	LYS	2.8
1	A	833	PRO	2.8
1	C	688	ALA	2.8
1	A	510	LYS	2.7
1	C	955	LYS	2.7
1	A	867	ARG	2.7
1	B	689	GLY	2.7
1	A	1039	ASP	2.6
1	A	463	THR	2.6
1	B	649	MET	2.6
1	A	1043	SER	2.6
1	A	519	MET	2.6
1	C	617	PHE	2.6
1	B	877	TYR	2.6
1	A	544	LEU	2.5
1	C	124	GLN	2.5
1	A	433	LYS	2.5
1	A	561	SER	2.5
1	A	526	HIS	2.5
1	B	508	GLY	2.5
1	A	37	THR	2.5
1	A	518	ARG	2.5
2	E	66	LEU	2.5
1	A	1031	ARG	2.4
1	A	563	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	1033	PHE	2.4
1	A	991	ILE	2.4
1	C	951	ASP	2.4
1	B	678	THR	2.4
2	D	101	LYS	2.4
1	B	478	MET	2.4
1	A	449	LEU	2.4
1	A	554	TYR	2.4
1	C	120	GLN	2.4
1	A	660	ASP	2.4
1	A	1037	ASN	2.4
1	A	359	LEU	2.3
1	A	498	LYS	2.3
1	C	691	GLY	2.3
1	C	620	ARG	2.3
2	E	27	ASP	2.3
1	A	873	ALA	2.3
1	B	501	ALA	2.3
1	A	363	ARG	2.3
1	A	1030	ARG	2.3
1	A	870	GLY	2.3
1	C	619	GLY	2.3
1	B	562	SER	2.3
1	A	952	LEU	2.2
1	A	1027	VAL	2.3
1	C	97	GLY	2.2
1	A	515	TRP	2.2
1	A	21	LEU	2.2
1	A	447	MET	2.2
1	A	662	MET	2.2
1	A	834	GLY	2.2
2	D	16	LYS	2.2
1	A	527	TYR	2.2
1	A	944	LEU	2.2
1	A	448	VAL	2.2
1	A	557	VAL	2.2
1	A	871	ASN	2.2
1	A	422	GLU	2.2
1	A	538	THR	2.2
1	B	618	ALA	2.2
1	B	472	ILE	2.2
1	A	1032	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	2.2
1	A	1033	PHE	2.2
1	B	458	PHE	2.2
1	C	513	PHE	2.2
1	C	676	THR	2.2
1	A	466	ILE	2.1
2	D	13	ASP	2.1
1	A	922	THR	2.1
2	E	64	GLU	2.1
1	B	675	GLY	2.1
1	C	259	ARG	2.1
1	C	993	THR	2.1
1	A	835	LYS	2.1
1	C	29	LYS	2.1
1	A	386	PHE	2.1
1	B	664	PHE	2.1
1	A	494	ALA	2.1
2	E	68	LYS	2.1
2	E	33	LEU	2.1
1	A	71	GLY	2.1
1	A	506	GLY	2.1
1	A	35	TYR	2.0
1	A	424	GLY	2.0
1	A	514	GLY	2.0
1	A	513	PHE	2.0
1	A	516	PHE	2.0
1	A	837	THR	2.0
1	A	580	ALA	2.0
1	B	660	ASP	2.0
1	A	955	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

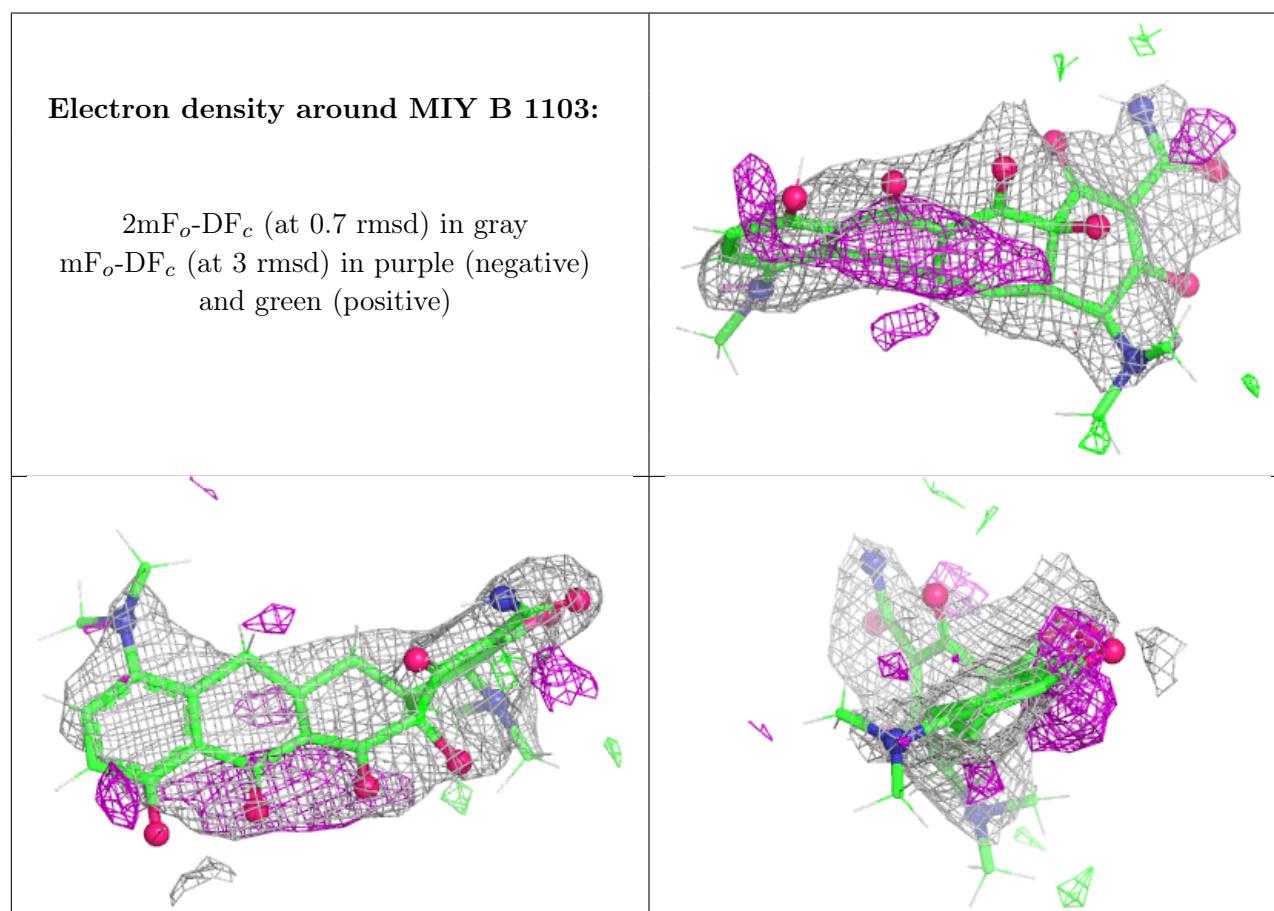
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

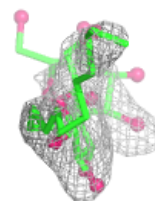
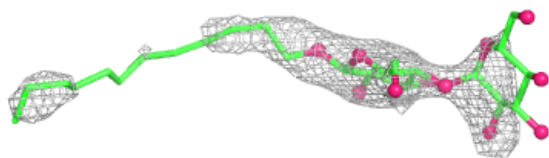
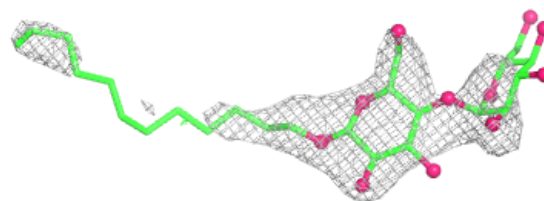
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MIY	B	1103	33/33	0.77	0.18	64,89,104,135	0
3	LMT	A	1102	35/35	0.85	0.18	83,104,125,130	0
3	LMT	B	1102	35/35	0.89	0.13	56,93,106,106	0
3	LMT	B	1101	35/35	0.90	0.14	49,70,86,88	0
3	LMT	C	1101	35/35	0.92	0.13	52,64,80,81	0
3	LMT	A	1101	35/35	0.92	0.11	45,65,90,96	0

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

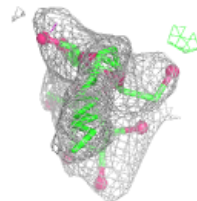
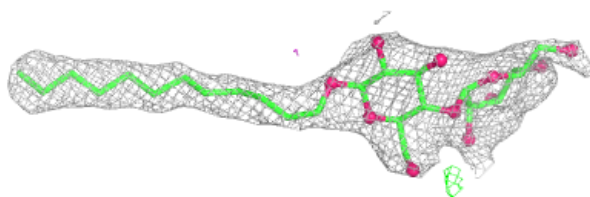
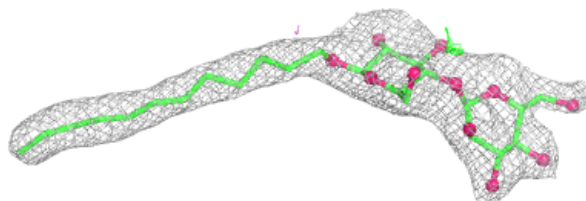


Electron density around LMT A 1102:

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

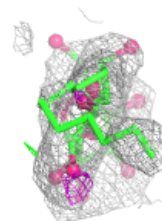
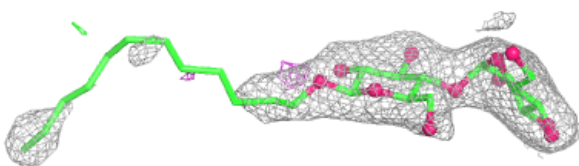
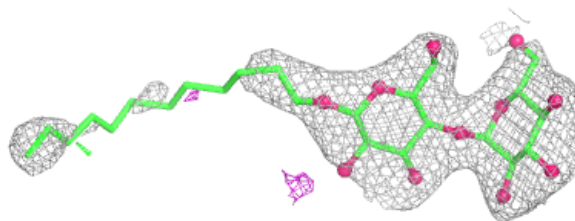
**Electron density around LMT B 1102:**

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

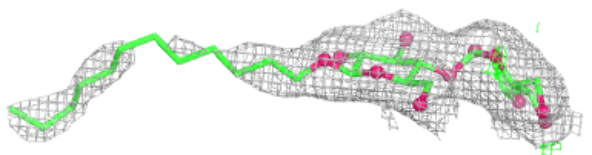
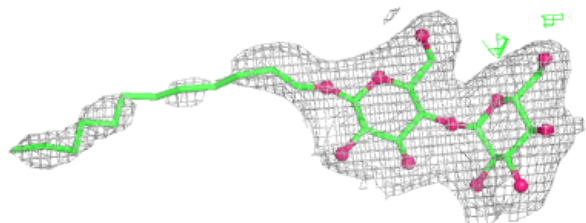


Electron density around LMT B 1101:

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

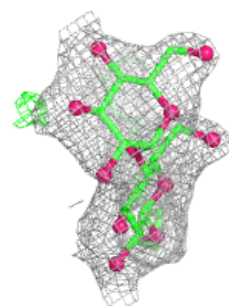
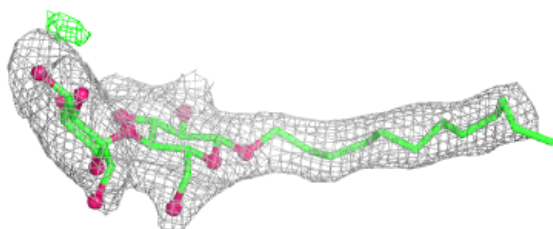
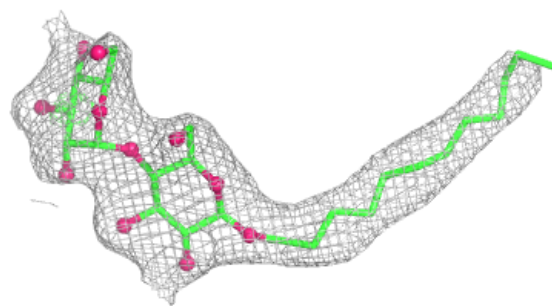
**Electron density around LMT C 1101:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.