



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:31 PM UTC

PDB ID : 4DX5 / pdb_00004dx5
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 : 1.90 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

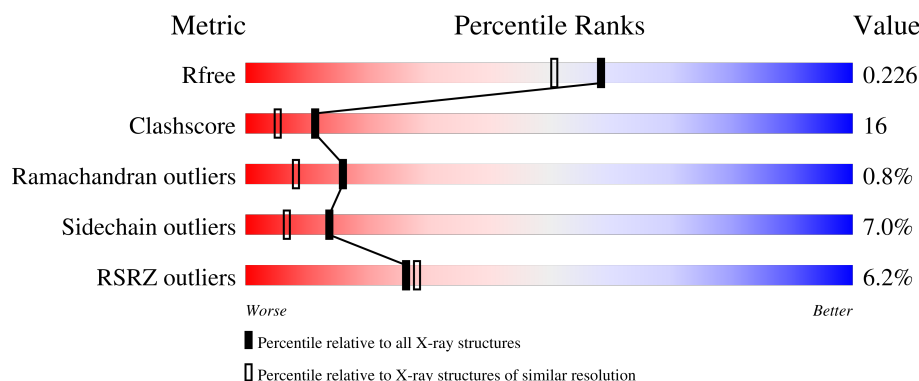
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	8% 70% 23% 5% ..
1	B	1057	5% 77% 17% ..
1	C	1057	5% 78% 17% ..
2	D	169	5% 76% 14% 8%

Continued on next page...

Continued from previous page...

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
3	GOL	B	1116	-	-	X	-
8	D12	A	1111	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 29010 atoms, of which 587 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	1044	Total	C	N	O	S	0	0	0
			7943	5106	1315	1478	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	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

Continued on next page...

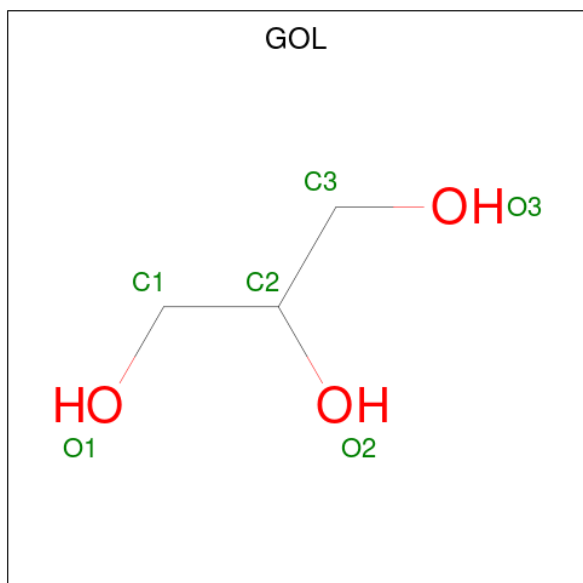
Continued from previous page...

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 GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



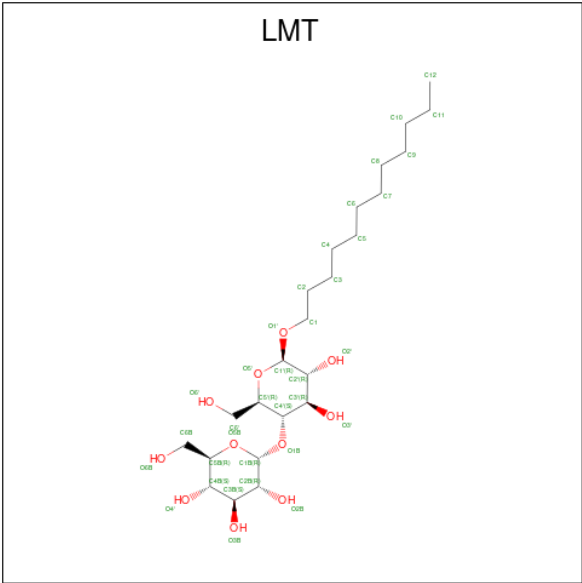
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	0	0	
			6	3	3			
3	C	1	Total	C	O	0	0	
			6	3	3			
3	C	1	Total	C	O	0	0	
			6	3	3			
3	C	1	Total	C	O	0	0	
			6	3	3			
3	C	1	Total	C	O	0	0	
			6	3	3			
3	D	1	Total	C	O	0	0	
			6	3	3			
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	E	1	Total	C	O	0	0	
			6	3	3			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



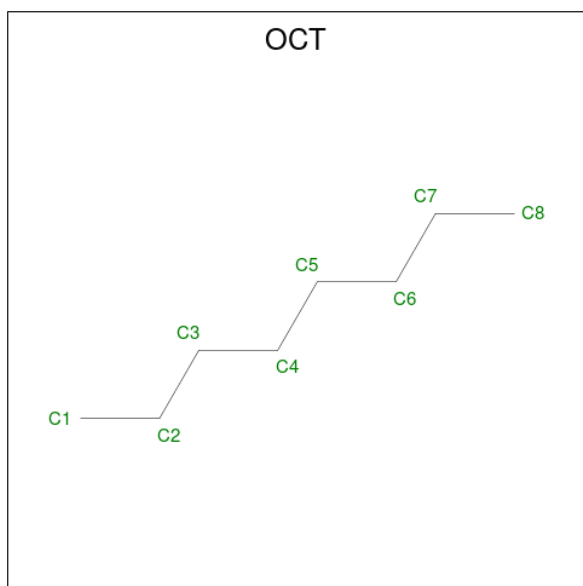
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		
4	A	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

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

- Molecule 5 is N-OCTANE (CCD ID: OCT) (formula: C₈H₁₈).



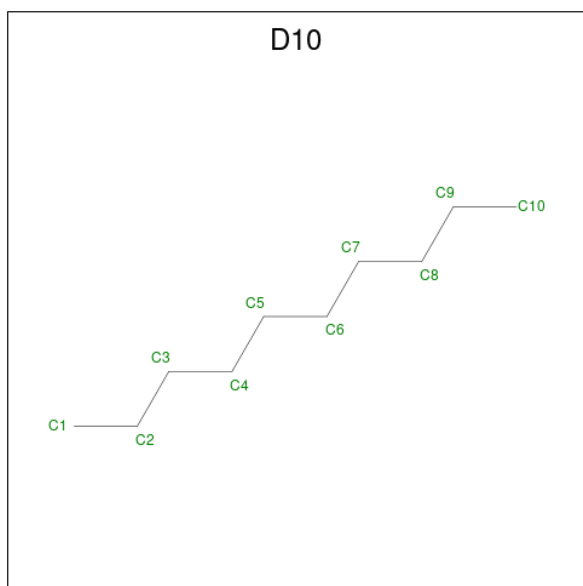
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H 26 8 18	0	0
5	A	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0
5	C	1	Total C H 26 8 18	0	0

Continued on next page...

Continued from previous page...

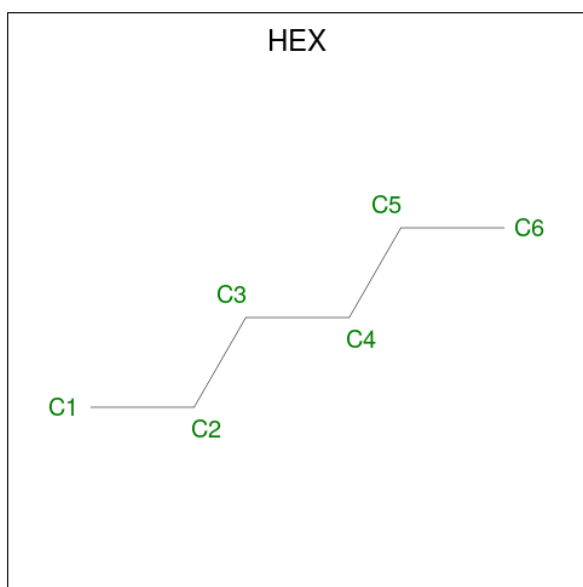
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	H	0	0
			26	8	18		

- Molecule 6 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



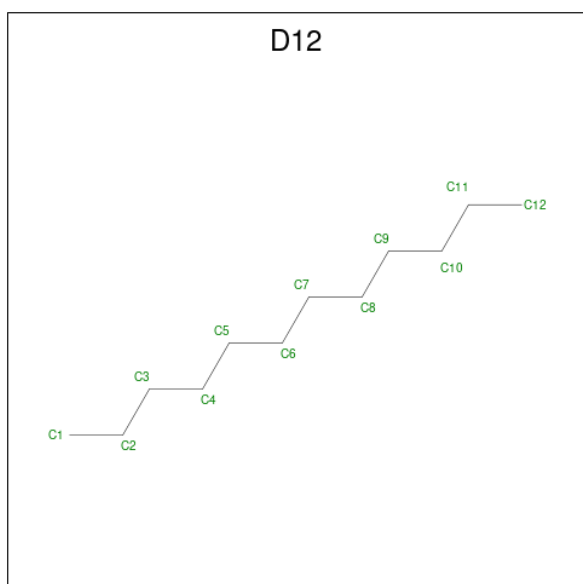
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	H	0	0
			32	10	22		
6	B	1	Total	C	H	0	0
			32	10	22		
6	B	1	Total	C	H	0	0
			32	10	22		
6	C	1	Total	C	H	0	0
			32	10	22		
6	C	1	Total	C	H	0	0
			32	10	22		
6	C	1	Total	C	H	0	0
			32	10	22		

- Molecule 7 is HEXANE (CCD ID: HEX) (formula: C₆H₁₄).



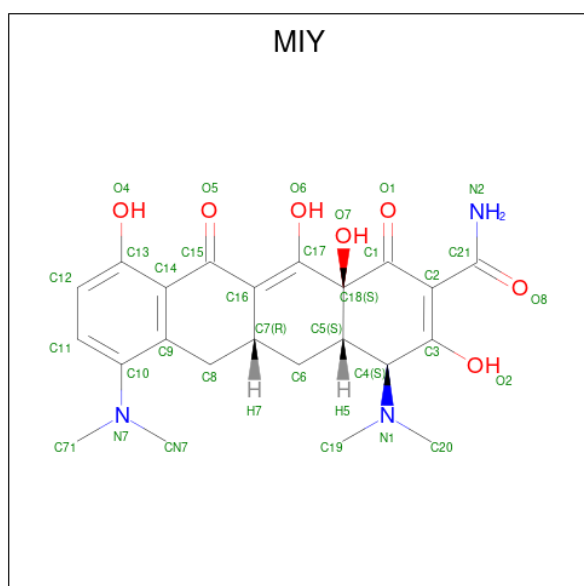
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	H	0	0
			20	6	14		
7	B	1	Total	C	H	0	0
			20	6	14		
7	B	1	Total	C	H	0	0
			20	6	14		
7	C	1	Total	C	H	0	0
			20	6	14		
7	C	1	Total	C	H	0	0
			20	6	14		

- Molecule 8 is DODECANE (CCD ID: D12) (formula: $C_{12}H_{26}$).



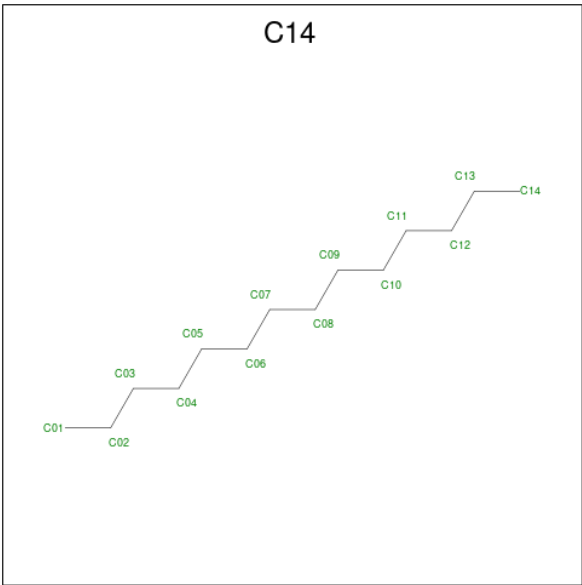
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 38	C 12	H 26	0	0
8	B	1	Total 38	C 12	H 26	0	0
8	C	1	Total 38	C 12	H 26	0	0
8	C	1	Total 38	C 12	H 26	0	0

- Molecule 9 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: $C_{23}H_{27}N_3O_7$).



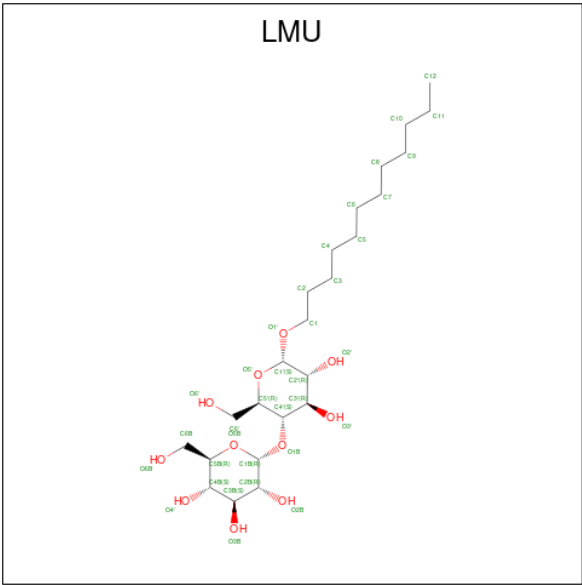
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	0	0
			60	23	27	3	7		

- Molecule 10 is TETRADECANE (CCD ID: C14) (formula: $C_{14}H_{30}$).



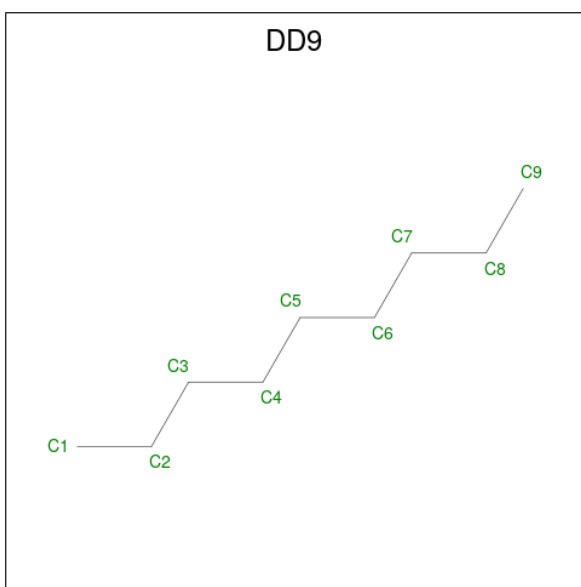
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	H	0	0
			44	14	30		

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



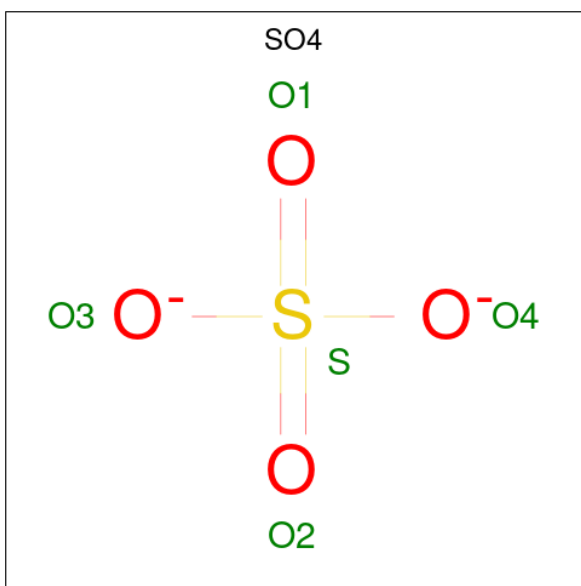
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 12 is nonane (CCD ID: DD9) (formula: C_9H_{20}).



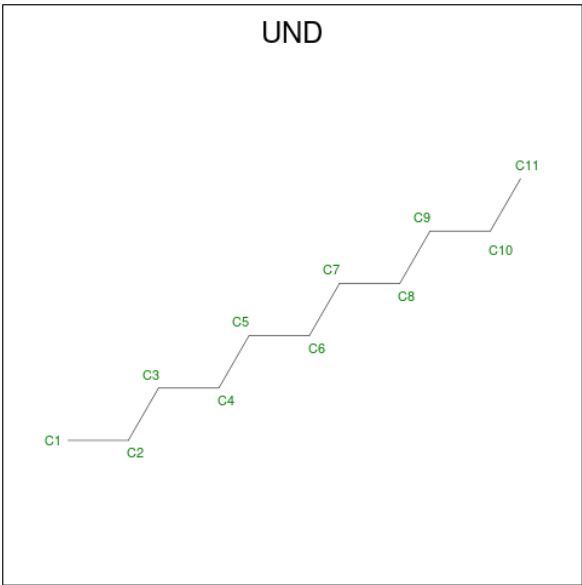
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	H	0	0
			29	9	20		

- Molecule 13 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 14 is UNDECANE (CCD ID: UND) (formula: C₁₁H₂₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	H	0	0
			35	11	24		

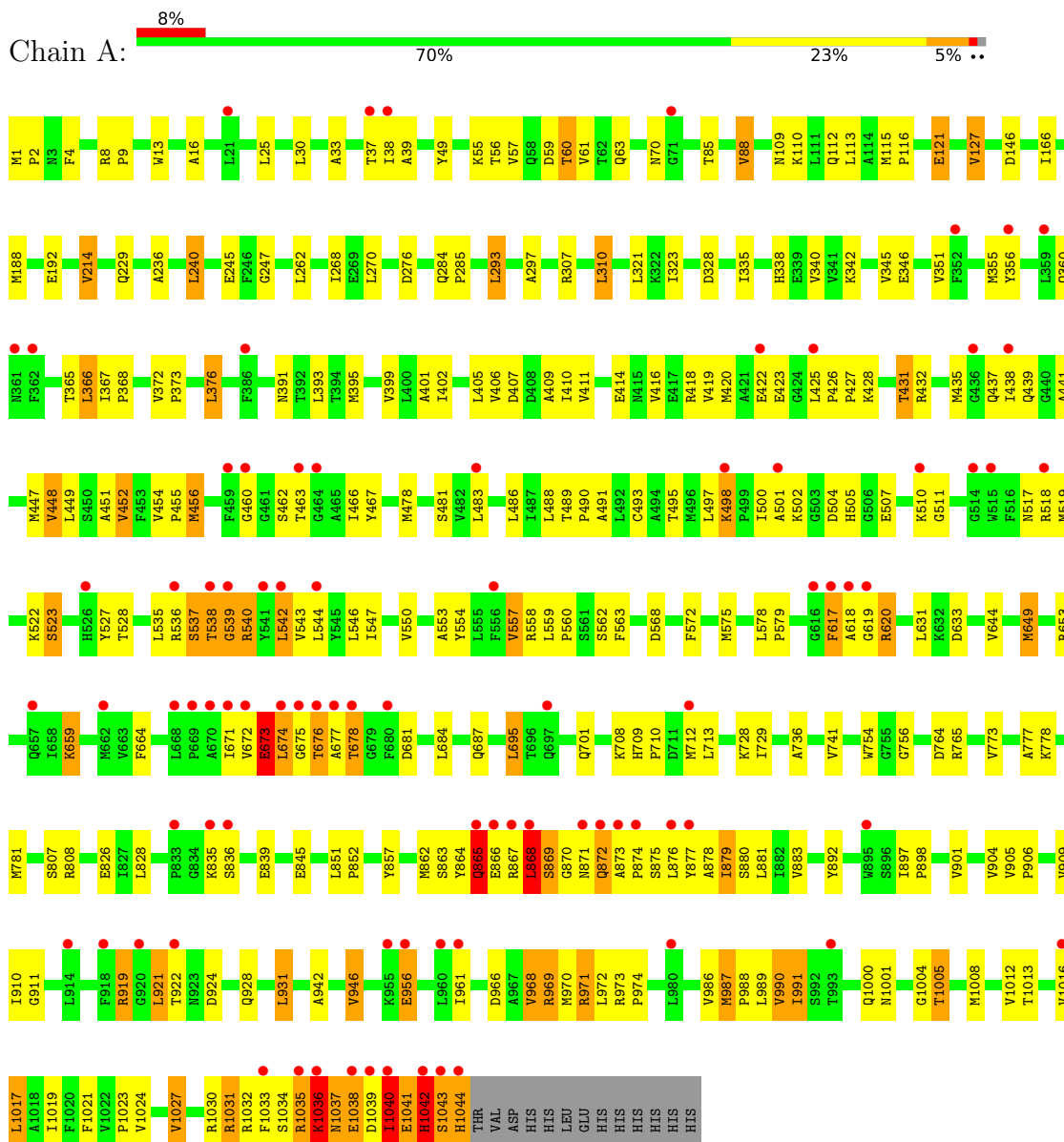
- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	540	Total	O	0	0
			540	540		
15	B	531	Total	O	0	0
			531	531		
15	C	583	Total	O	0	0
			583	583		
15	D	87	Total	O	0	0
			87	87		
15	E	42	Total	O	0	0
			42	42		

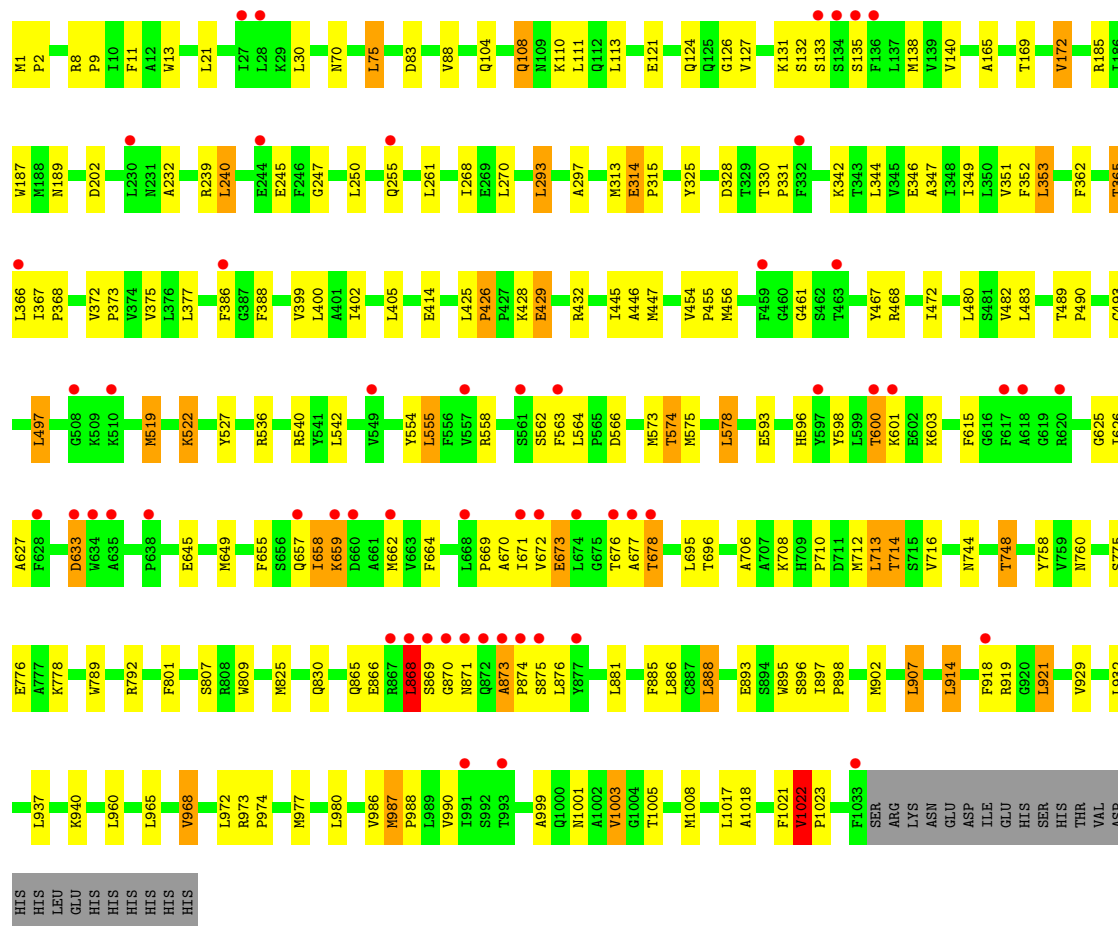
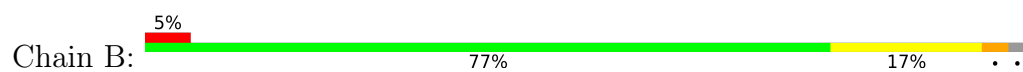
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

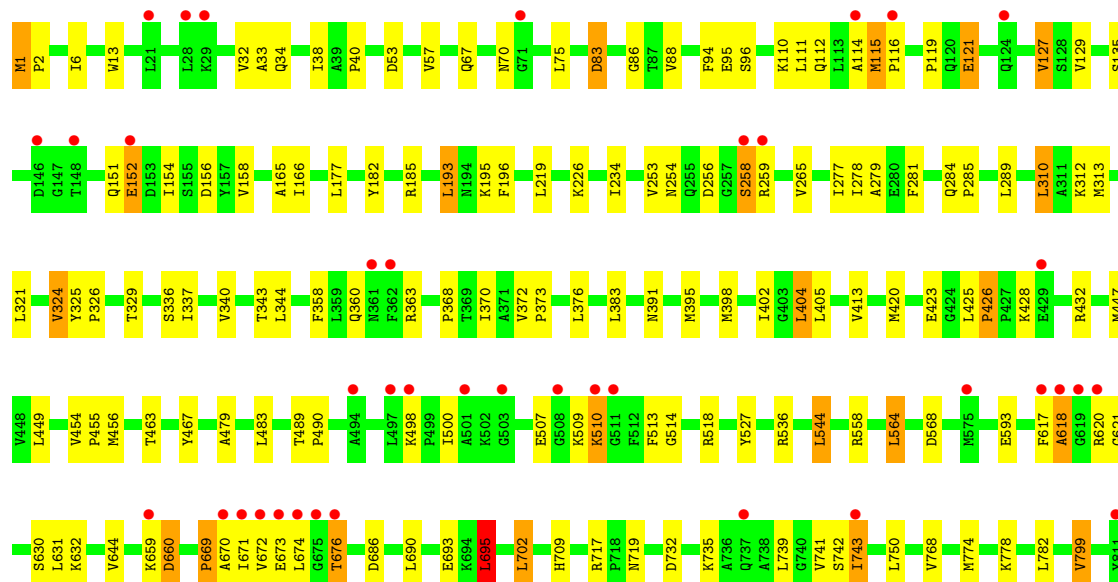
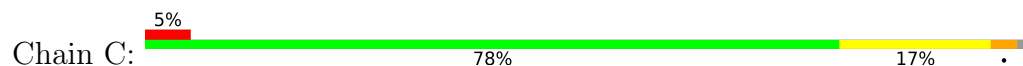
• Molecule 1: Acriflavine resistance protein B

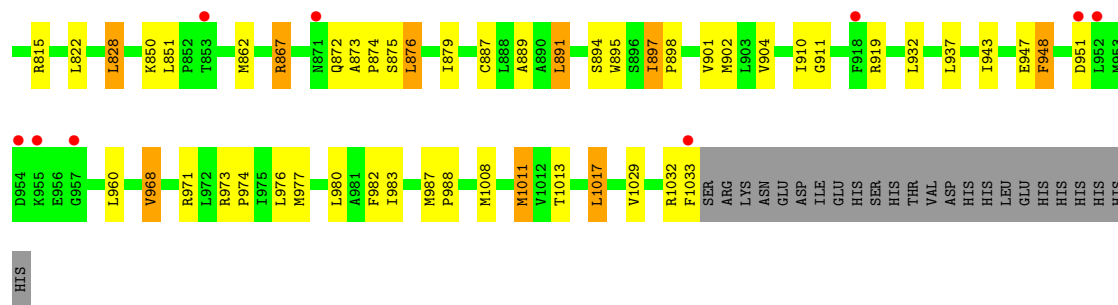


• Molecule 1: Acriflavine resistance protein B

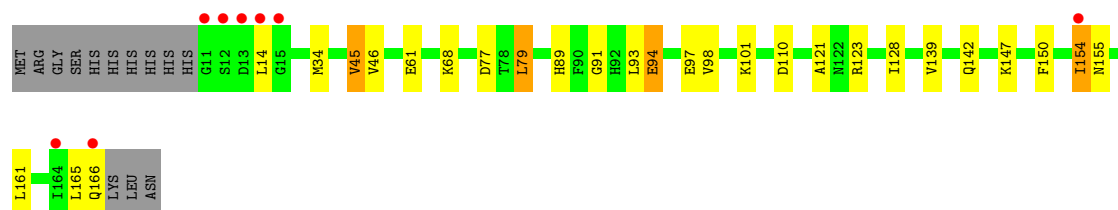
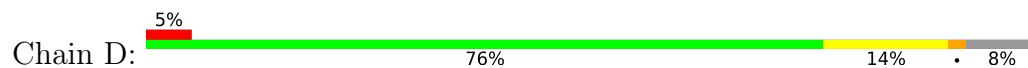


• Molecule 1: Acriflavine resistance protein B

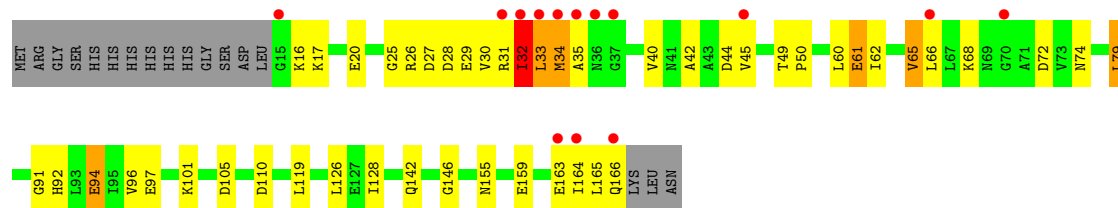




• Molecule 2: DARPIN



• 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	145.99Å 161.72Å 245.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.47 – 1.90 39.47 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.47-1.90) 99.3 (39.47-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.200 , 0.231 0.197 , 0.226	Depositor DCC
R_{free} test set	22550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.8	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	29010	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% 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: OCT, GOL, HEX, LMT, D12, LMU, D10, SO4, DD9, C14, MIY, UND

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	0.46	0/8095	0.81	6/10991 (0.1%)
1	B	0.46	1/7999 (0.0%)	0.79	5/10863 (0.0%)
1	C	0.49	0/7999	0.80	9/10863 (0.1%)
2	D	0.44	0/1196	0.72	0/1626
2	E	0.39	0/1170	0.71	0/1591
All	All	0.46	1/26459 (0.0%)	0.79	20/35934 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1022	VAL	CA-CB	8.00	1.59	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1022	VAL	N-CA-CB	10.46	117.09	110.50
1	A	1040	ILE	N-CA-C	-9.53	99.44	110.21
1	B	1021	PHE	CA-C-N	-7.13	115.75	120.24
1	B	1021	PHE	C-N-CA	-7.13	115.75	120.24
1	A	426	PRO	CA-C-N	6.63	126.14	119.24
1	A	426	PRO	C-N-CA	6.63	126.14	119.24
1	A	88	VAL	CB-CA-C	-6.62	100.75	110.62
1	C	695	LEU	N-CA-C	-5.57	105.21	111.28
1	C	782	LEU	CA-C-N	5.52	125.61	119.32
1	C	782	LEU	C-N-CA	5.52	125.61	119.32
1	C	115	MET	CA-C-N	5.51	125.03	119.19
1	C	115	MET	C-N-CA	5.51	125.03	119.19
1	C	426	PRO	O-C-N	5.39	123.69	121.15
1	A	872	GLN	N-CA-C	-5.25	107.04	113.50
1	B	426	PRO	O-C-N	5.23	123.72	121.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	865	GLN	N-CA-C	5.21	118.65	108.18
1	B	868	LEU	CB-CA-C	-5.16	108.95	116.53
1	C	83	ASP	N-CA-C	5.13	116.47	109.18
1	C	325	TYR	CA-C-N	5.02	125.46	120.04
1	C	325	TYR	C-N-CA	5.02	125.46	120.04

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7943	0	8084	373	0
1	B	7849	0	8001	210	0
1	C	7849	0	8001	202	0
2	D	1177	0	1159	25	0
2	E	1151	0	1136	49	0
3	A	12	0	16	1	0
3	B	36	0	48	11	0
3	C	24	0	32	5	0
3	D	12	8	16	1	0
3	E	6	0	8	1	0
4	A	140	0	184	33	0
4	B	105	0	138	17	0
4	C	35	0	46	1	0
5	A	16	36	36	0	0
5	C	40	90	90	1	0
6	A	10	22	22	1	0
6	B	20	44	44	1	0
6	C	30	66	66	0	0
7	A	6	14	14	0	0
7	B	12	28	28	0	0
7	C	12	28	28	0	0
8	A	12	26	26	8	0
8	B	12	26	26	1	0
8	C	24	52	52	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	33	27	26	2	0
10	B	14	30	30	2	0
11	B	35	46	45	3	0
12	C	9	20	20	0	0
13	C	5	0	0	0	0
14	C	11	24	24	0	0
15	A	540	0	0	15	0
15	B	531	0	0	16	0
15	C	583	0	0	20	0
15	D	87	0	0	4	0
15	E	42	0	0	1	0
All	All	28423	587	27446	871	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 16.

All (871) 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:1040:ILE:CA	1:A:1041:GLU:HB2	1.68	1.18
1:B:414:GLU:HG3	1:B:977:MET:CE	1.76	1.16
1:A:1038:GLU:CB	1:A:1039:ASP:HA	1.74	1.14
2:D:94:GLU:OE2	2:D:94:GLU:N	1.82	1.12
1:A:971:ARG:HG3	1:A:971:ARG:HH11	0.99	1.11
1:A:1038:GLU:HB2	1:A:1039:ASP:HA	1.14	1.10
1:B:414:GLU:CG	1:B:977:MET:HE1	1.82	1.10
1:C:509:LYS:CA	1:C:510:LYS:HB2	1.80	1.09
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.29	1.09
1:A:1040:ILE:HG22	1:A:1041:GLU:CB	1.81	1.09
1:A:866:GLU:C	1:A:868:LEU:HB2	1.79	1.08
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.29	1.08
1:C:671:ILE:HD11	1:C:674:LEU:HD12	1.26	1.08
1:A:865:GLN:N	1:A:866:GLU:HB2	1.68	1.07
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.13	1.06
1:A:987:MET:HE1	1:A:1008:MET:SD	1.95	1.06
1:A:542:LEU:HD12	1:A:542:LEU:H	1.18	1.06
1:C:509:LYS:HA	1:C:510:LYS:HB2	1.06	1.05
1:A:1040:ILE:HA	1:A:1041:GLU:HB2	1.27	1.05
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.38	1.04
1:C:527:TYR:CE2	1:C:968:VAL:HG13	1.92	1.03
1:A:538:THR:HG22	1:A:539:GLY:H	1.19	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ASN:O	1:C:110:LYS:NZ	1.90	1.03
1:A:618:ALA:H	1:A:619:GLY:HA2	1.23	1.03
1:A:672:VAL:HG23	1:A:673:GLU:H	1.20	1.03
1:A:538:THR:O	1:A:540:ARG:N	1.92	1.02
1:A:617:PHE:N	1:A:617:PHE:HD1	1.53	1.02
1:C:671:ILE:HD11	1:C:674:LEU:CD1	1.90	1.02
1:A:865:GLN:HA	1:A:868:LEU:HG	1.41	1.01
1:A:865:GLN:CA	1:A:868:LEU:HG	1.90	1.01
1:C:185:ARG:HH12	3:C:1115:GOL:H31	1.24	1.01
1:A:1040:ILE:CB	1:A:1041:GLU:HB2	1.90	1.01
4:B:1104:LMT:H5B	4:B:1104:LMT:H6E	1.44	1.00
1:A:1035:ARG:HD2	1:A:1035:ARG:N	1.80	0.95
1:B:885:PHE:HB2	1:B:902:MET:HE1	1.47	0.95
1:A:659:LYS:HD3	1:A:659:LYS:H	1.33	0.94
1:A:971:ARG:HG3	1:A:971:ARG:NH1	1.72	0.94
1:A:618:ALA:HB3	1:A:619:GLY:O	1.67	0.93
1:A:865:GLN:N	1:A:865:GLN:OE1	2.01	0.93
1:A:538:THR:HG22	1:A:539:GLY:N	1.80	0.93
1:C:423:GLU:HB2	1:C:425:LEU:HD13	1.50	0.92
2:E:34:MET:HA	2:E:34:MET:HE3	1.47	0.92
1:A:1027:VAL:O	1:A:1031:ARG:HG2	1.66	0.92
1:C:867:ARG:HG2	1:C:867:ARG:HH11	1.34	0.92
1:A:867:ARG:N	1:A:868:LEU:HB2	1.84	0.91
1:A:1035:ARG:HD2	1:A:1035:ARG:H	1.32	0.91
1:A:1038:GLU:HB2	1:A:1039:ASP:CA	2.00	0.91
1:A:1040:ILE:CG2	1:A:1041:GLU:HB2	2.00	0.90
1:C:509:LYS:HA	1:C:510:LYS:CB	1.97	0.90
2:E:32:ILE:O	2:E:34:MET:N	2.05	0.89
2:E:32:ILE:O	2:E:35:ALA:N	2.04	0.89
1:B:919:ARG:NE	15:B:1353:HOH:O	2.04	0.89
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.06	0.89
1:A:868:LEU:O	1:A:869:SER:HB2	1.73	0.89
1:A:659:LYS:H	1:A:659:LYS:CD	1.82	0.88
1:B:625:GLY:C	1:B:626:ILE:HD12	1.98	0.88
1:A:649:MET:HE1	1:A:653:ARG:NH1	1.88	0.88
1:A:1040:ILE:HG22	1:A:1041:GLU:HB2	1.55	0.87
2:D:123:ARG:NH1	15:D:338:HOH:O	2.06	0.87
1:A:971:ARG:HH11	1:A:971:ARG:CG	1.86	0.87
1:A:617:PHE:N	1:A:617:PHE:CD1	2.29	0.86
1:A:672:VAL:O	1:A:675:GLY:N	2.09	0.86
1:B:677:ALA:O	1:B:678:THR:HB	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:PHE:HD1	1:A:617:PHE:H	0.85	0.85
1:C:259:ARG:NH1	2:E:155:ASN:OD1	2.10	0.85
1:A:919:ARG:NH2	1:A:990:VAL:O	2.10	0.85
2:E:60:LEU:HD22	2:E:94:GLU:HG2	1.58	0.85
1:B:131:LYS:NZ	15:B:1633:HOH:O	2.09	0.84
1:C:527:TYR:HE2	1:C:968:VAL:HG13	1.35	0.84
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.06	0.84
1:B:1:MET:N	15:B:1286:HOH:O	2.10	0.84
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.57	0.84
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.07	0.84
1:A:676:THR:H	1:A:862:MET:HE1	1.43	0.83
1:A:1040:ILE:CG2	1:A:1041:GLU:CB	2.54	0.83
1:B:75:LEU:HD13	3:B:1101:GOL:H32	1.57	0.83
1:A:342:LYS:HD2	4:A:1109:LMT:H1'	1.59	0.83
1:A:672:VAL:HG23	1:A:673:GLU:N	1.92	0.83
1:C:447:MET:HE1	1:C:891:LEU:HG	1.60	0.83
1:A:881:LEU:HD22	4:A:1103:LMT:H122	1.61	0.83
1:A:1042:HIS:CD2	1:A:1043:SER:N	2.47	0.83
1:A:542:LEU:H	1:A:542:LEU:CD1	1.91	0.83
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.60	0.83
1:A:676:THR:HG23	1:A:862:MET:HE1	1.60	0.82
1:A:542:LEU:HD12	1:A:542:LEU:N	1.95	0.82
1:B:645:GLU:HG2	1:B:649:MET:HE3	1.60	0.82
1:B:352:PHE:CE2	1:B:365:THR:HG21	2.13	0.82
1:B:748:THR:HG21	15:B:1499:HOH:O	1.79	0.82
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.60	0.81
1:A:987:MET:CE	1:A:987:MET:HA	2.11	0.81
1:A:1:MET:N	15:A:1630:HOH:O	2.13	0.81
1:C:509:LYS:CA	1:C:510:LYS:CB	2.56	0.81
2:E:34:MET:CE	2:E:40:VAL:HG12	2.10	0.81
1:C:1011:MET:HE3	1:C:1011:MET:HA	1.63	0.80
2:E:25:GLY:HA2	2:E:62:ILE:HD12	1.62	0.80
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.62	0.80
1:A:836:SER:OG	1:A:839:GLU:HG3	1.80	0.80
1:A:1042:HIS:HD2	1:A:1043:SER:N	1.79	0.80
2:D:94:GLU:H	2:D:94:GLU:CD	1.85	0.80
1:A:672:VAL:CG2	1:A:673:GLU:H	1.94	0.80
1:A:1012:VAL:O	1:A:1016:VAL:HG22	1.80	0.80
1:C:370:ILE:O	1:C:373:PRO:HD2	1.81	0.80
1:A:38:ILE:HD11	1:A:674:LEU:HD21	1.64	0.80
1:B:885:PHE:CB	1:B:902:MET:HE1	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:30:VAL:O	2:E:34:MET:HB2	1.82	0.79
1:A:1040:ILE:HG22	1:A:1041:GLU:CG	2.12	0.79
4:B:1110:LMT:O2'	4:B:1110:LMT:H21	1.83	0.79
1:A:729:ILE:HD11	1:C:234:ILE:CG2	2.13	0.79
1:B:873:ALA:CB	1:B:874:PRO:HD3	2.13	0.79
1:B:974:PRO:HA	1:B:977:MET:HE3	1.64	0.79
1:A:708:LYS:C	1:A:710:PRO:HD3	2.08	0.78
1:B:868:LEU:O	1:B:870:GLY:N	2.16	0.78
1:A:618:ALA:N	1:A:619:GLY:HA2	1.94	0.78
1:B:447:MET:HE2	1:B:447:MET:HA	1.64	0.78
1:A:649:MET:HE1	1:A:653:ARG:CZ	2.14	0.78
1:C:363:ARG:HH11	1:C:498:LYS:HE3	1.49	0.78
1:A:1001:ASN:O	1:A:1005:THR:HG23	1.84	0.78
1:A:1038:GLU:CG	1:A:1039:ASP:HA	2.13	0.77
2:D:68:LYS:NZ	15:D:350:HOH:O	2.11	0.77
1:A:146:ASP:OD1	15:A:1501:HOH:O	2.01	0.77
1:A:538:THR:CG2	1:A:542:LEU:HD11	2.14	0.77
1:A:676:THR:O	1:A:678:THR:N	2.17	0.77
1:B:876:LEU:HD21	4:B:1110:LMT:H11	1.65	0.77
1:C:593:GLU:OE1	15:C:1684:HOH:O	2.02	0.76
1:A:659:LYS:HD3	1:A:659:LYS:N	1.99	0.76
2:E:34:MET:HA	2:E:34:MET:CE	2.16	0.75
1:B:600:THR:HG22	1:B:601:LYS:N	2.00	0.75
1:B:990:VAL:O	15:B:1353:HOH:O	2.04	0.75
1:A:866:GLU:C	1:A:867:ARG:HG3	2.12	0.75
1:C:659:LYS:NZ	1:C:660:ASP:OD2	2.19	0.75
1:A:4:PHE:O	1:A:8:ARG:HD2	1.85	0.75
1:A:1040:ILE:CB	1:A:1041:GLU:CB	2.64	0.75
4:A:1102:LMT:H6'1	4:B:1110:LMT:O3B	1.85	0.75
2:D:45:VAL:HG22	15:D:351:HOH:O	1.86	0.74
1:A:38:ILE:CD1	1:A:674:LEU:HD21	2.18	0.74
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.20	0.74
1:A:535:LEU:HD22	1:A:1027:VAL:HG11	1.69	0.74
1:A:672:VAL:O	1:A:674:LEU:N	2.20	0.74
1:A:676:THR:H	1:A:862:MET:CE	2.00	0.74
1:B:428:LYS:CE	1:B:432:ARG:HH22	2.00	0.74
1:B:625:GLY:O	1:B:626:ILE:HD12	1.86	0.74
1:A:675:GLY:HA3	1:A:862:MET:HE2	1.67	0.74
9:B:1103:MIY:H81	9:B:1103:MIY:HN72	1.69	0.74
1:A:538:THR:O	1:A:540:ARG:HG2	1.88	0.74
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASP:OD1	1:B:633:ASP:N	2.20	0.73
1:A:537:SER:O	1:A:538:THR:HB	1.86	0.73
1:B:744:ASN:O	1:B:748:THR:HG23	1.86	0.73
1:B:873:ALA:HB3	1:B:874:PRO:CD	2.14	0.73
1:B:645:GLU:CG	1:B:649:MET:HE3	2.18	0.73
1:B:555:LEU:HD21	1:B:914:LEU:CD1	2.19	0.73
1:A:504:ASP:O	1:A:505:HIS:ND1	2.14	0.72
1:A:507:GLU:HG2	1:A:518:ARG:HD3	1.70	0.72
1:A:865:GLN:HA	1:A:868:LEU:CG	2.19	0.72
1:C:321:LEU:O	15:C:1513:HOH:O	2.07	0.72
8:A:1111:D12:H111	1:B:447:MET:HG3	1.69	0.72
2:E:28:ASP:O	2:E:31:ARG:HB3	1.89	0.72
2:E:164:ILE:O	2:E:166:GLN:N	2.19	0.72
1:B:1001:ASN:O	1:B:1005:THR:HG23	1.90	0.72
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.71	0.72
1:A:527:TYR:CE2	1:A:968:VAL:HG13	2.25	0.72
1:B:352:PHE:CE2	1:B:365:THR:CG2	2.72	0.72
1:A:546:LEU:O	1:A:550:VAL:HG23	1.88	0.72
2:E:164:ILE:C	2:E:166:GLN:H	1.97	0.72
1:A:866:GLU:OE1	1:A:866:GLU:HA	1.88	0.72
1:A:1040:ILE:CA	1:A:1041:GLU:CB	2.58	0.72
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.72	0.72
1:A:1035:ARG:HA	1:A:1036:LYS:HE2	1.70	0.71
1:A:539:GLY:CA	1:A:542:LEU:HD13	2.20	0.71
1:C:115:MET:N	1:C:116:PRO:HD2	2.05	0.71
1:C:867:ARG:HG2	1:C:867:ARG:NH1	2.05	0.71
1:A:342:LYS:CD	4:A:1109:LMT:H1'	2.20	0.71
1:C:135:SER:HB3	1:C:672:VAL:O	1.89	0.71
1:C:259:ARG:NH1	15:C:1437:HOH:O	2.19	0.71
1:A:504:ASP:C	1:A:505:HIS:HD1	1.98	0.71
1:A:866:GLU:C	1:A:867:ARG:CG	2.63	0.71
1:A:881:LEU:HD21	4:A:1103:LMT:H92	1.73	0.71
1:A:867:ARG:H	1:A:869:SER:H	1.39	0.71
1:A:987:MET:CE	1:A:1008:MET:SD	2.76	0.70
1:A:729:ILE:HD11	1:C:234:ILE:HG21	1.72	0.70
1:B:386:PHE:HB3	1:B:388:PHE:CE1	2.26	0.70
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.71	0.70
1:A:338:HIS:HB3	4:A:1109:LMT:H11	1.74	0.70
1:B:386:PHE:HB3	1:B:388:PHE:CD1	2.26	0.70
1:C:673:GLU:OE2	1:C:673:GLU:N	2.25	0.70
1:C:32:VAL:CG1	1:C:337:ILE:HD13	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.22	0.69
1:B:1018:ALA:O	1:B:1022:VAL:HG13	1.93	0.69
1:A:866:GLU:O	1:A:867:ARG:HG3	1.93	0.69
1:C:617:PHE:O	1:C:618:ALA:CB	2.40	0.69
1:A:881:LEU:CD2	4:A:1103:LMT:H122	2.21	0.69
1:A:942:ALA:O	1:A:946:VAL:HG13	1.92	0.69
1:B:522:LYS:HA	1:B:522:LYS:HE3	1.73	0.69
1:B:138:MET:HE2	1:B:140:VAL:HG22	1.73	0.69
1:A:671:ILE:HG22	1:A:674:LEU:HD23	1.74	0.69
4:B:1111:LMT:O6'	4:B:1111:LMT:H6'1	1.92	0.69
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.29	0.68
1:C:57:VAL:CG1	1:C:88:VAL:CG2	2.71	0.68
1:A:968:VAL:CG2	1:A:1023:PRO:HG3	2.23	0.68
1:C:151:GLN:HG2	3:C:1117:GOL:O3	1.94	0.68
1:B:232:ALA:HA	3:B:1115:GOL:H31	1.75	0.68
1:B:706:ALA:HB3	1:B:716:VAL:HG11	1.76	0.68
1:A:519:MET:O	1:A:523:SER:OG	2.11	0.68
1:A:987:MET:HA	1:A:987:MET:HE2	1.76	0.67
1:C:151:GLN:NE2	1:C:279:ALA:O	2.27	0.67
1:A:866:GLU:O	1:A:868:LEU:HD23	1.93	0.67
1:A:537:SER:HB3	1:A:540:ARG:HH11	1.60	0.67
4:B:1104:LMT:H6E	4:B:1104:LMT:C5B	2.21	0.67
1:C:57:VAL:CG1	1:C:88:VAL:HG23	2.24	0.67
2:E:60:LEU:CD2	2:E:94:GLU:HG2	2.25	0.67
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.78	0.66
1:A:553:ALA:O	1:A:557:VAL:HG12	1.95	0.66
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.77	0.66
1:A:456:MET:HE2	1:A:467:TYR:CD1	2.30	0.66
1:C:185:ARG:NH1	3:C:1115:GOL:H31	2.06	0.66
4:B:1111:LMT:H5'	4:B:1111:LMT:O5B	1.95	0.66
1:C:872:GLN:OE1	15:C:1449:HOH:O	2.12	0.66
1:A:538:THR:HG23	1:A:542:LEU:HD11	1.77	0.66
1:A:491:ALA:O	1:A:495:THR:HG23	1.95	0.66
1:B:776:GLU:OE1	15:B:1321:HOH:O	2.13	0.66
2:E:25:GLY:HA2	2:E:62:ILE:CD1	2.25	0.66
2:E:44:ASP:OD2	3:E:201:GOL:O3	2.14	0.66
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.78	0.66
1:B:885:PHE:HA	1:B:902:MET:HE2	1.77	0.66
1:A:192:GLU:OE1	15:A:1390:HOH:O	2.13	0.66
1:A:538:THR:HG22	1:A:542:LEU:HD11	1.78	0.66
1:A:276:ASP:OD2	1:A:620:ARG:NH1	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:HIS:CD2	1:A:1042:HIS:C	2.73	0.65
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.77	0.65
1:C:671:ILE:CD1	1:C:674:LEU:CD1	2.73	0.65
1:C:57:VAL:HG11	1:C:88:VAL:HG23	1.78	0.65
1:C:95:GLU:OE2	15:C:1567:HOH:O	2.15	0.65
1:A:966:ASP:O	1:A:970:MET:HG3	1.96	0.65
1:A:865:GLN:H	1:A:866:GLU:HB2	1.61	0.65
1:C:671:ILE:HG13	1:C:674:LEU:HG	1.78	0.65
1:B:885:PHE:CD1	1:B:902:MET:HE1	2.32	0.65
1:C:671:ILE:HG23	1:C:862:MET:HE1	1.79	0.65
1:A:671:ILE:CG2	1:A:674:LEU:HD23	2.27	0.64
1:A:1040:ILE:HG22	1:A:1041:GLU:HG3	1.80	0.64
1:B:104:GLN:OE1	1:B:131:LYS:HD2	1.97	0.64
1:A:709:HIS:N	1:A:710:PRO:HD3	2.13	0.64
1:B:575:MET:HE1	1:B:626:ILE:HD11	1.79	0.64
1:A:346:GLU:HG3	4:A:1109:LMT:H102	1.79	0.64
1:A:1040:ILE:HG22	1:A:1041:GLU:HB3	1.73	0.64
1:A:8:ARG:HH12	8:A:1111:D12:H13	1.62	0.63
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.80	0.63
1:C:669:PRO:HD2	15:C:1773:HOH:O	1.99	0.63
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.79	0.63
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.23	0.63
1:B:596:HIS:O	1:B:600:THR:HB	1.98	0.63
15:B:1438:HOH:O	1:C:743:ILE:HD11	1.99	0.63
1:A:307:ARG:NE	15:A:1662:HOH:O	2.30	0.62
1:A:360:GLN:HE22	1:A:517:ASN:CG	2.06	0.62
1:B:456:MET:CG	1:B:467:TYR:HB3	2.29	0.62
1:A:527:TYR:OH	1:A:1019:ILE:O	2.09	0.62
2:D:154:ILE:HG13	2:D:155:ASN:N	2.12	0.62
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.24	0.62
1:A:865:GLN:HA	1:A:866:GLU:O	1.99	0.62
1:A:346:GLU:CG	4:A:1109:LMT:H102	2.30	0.62
1:A:365:THR:O	1:A:368:PRO:HD2	1.99	0.62
1:A:510:LYS:HD2	1:A:511:GLY:H	1.65	0.62
1:B:468:ARG:O	1:B:472:ILE:HD13	2.00	0.62
11:B:1114:LMU:O5'	11:B:1114:LMU:H21	1.98	0.62
1:C:509:LYS:HB3	1:C:510:LYS:HB3	1.82	0.62
1:A:423:GLU:OE2	1:A:425:LEU:HD11	2.00	0.62
1:A:427:PRO:O	1:A:431:THR:HG23	2.00	0.61
1:C:509:LYS:CB	1:C:510:LYS:HB2	2.30	0.61
1:A:507:GLU:HG2	1:A:518:ARG:CD	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.82	0.61
1:A:8:ARG:NH1	8:A:1111:D12:H13	2.15	0.61
1:A:70:ASN:O	1:A:110:LYS:HE3	2.00	0.61
1:A:865:GLN:CB	1:A:868:LEU:HG	2.30	0.61
1:A:881:LEU:HD13	4:A:1103:LMT:H122	1.82	0.61
1:A:1040:ILE:HA	1:A:1041:GLU:CB	2.17	0.61
1:B:108:GLN:CG	1:C:112:GLN:HG3	2.19	0.61
1:C:671:ILE:HG13	1:C:671:ILE:O	2.01	0.61
1:A:57:VAL:HG12	1:A:88:VAL:HG22	1.81	0.61
1:A:563:PHE:O	1:A:924:ASP:HB2	2.00	0.61
1:A:672:VAL:HG23	1:A:673:GLU:CD	2.26	0.61
4:A:1102:LMT:O6'	4:A:1102:LMT:O5B	2.18	0.61
1:A:987:MET:HA	1:A:987:MET:HE3	1.82	0.61
1:B:987:MET:SD	1:B:1008:MET:HE1	2.41	0.61
1:C:312:LYS:NZ	15:C:1752:HOH:O	2.34	0.61
2:E:32:ILE:O	2:E:33:LEU:C	2.43	0.61
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.33	0.61
1:A:342:LYS:HE3	4:A:1109:LMT:H92	1.83	0.61
1:A:867:ARG:N	1:A:869:SER:H	1.97	0.61
1:B:540:ARG:NH2	4:B:1104:LMT:H6'1	2.16	0.61
1:A:537:SER:HB3	1:A:540:ARG:HD2	1.83	0.60
1:C:447:MET:CE	1:C:891:LEU:HG	2.29	0.60
1:B:600:THR:CG2	1:B:601:LYS:N	2.64	0.60
1:B:973:ARG:O	1:B:977:MET:HG3	2.01	0.60
1:A:701:GLN:OE1	15:A:1598:HOH:O	2.16	0.60
1:A:956:GLU:CA	1:A:956:GLU:OE2	2.48	0.60
1:B:247:GLY:HA2	1:B:268:ILE:HD12	1.83	0.60
1:C:815:ARG:NH2	15:C:1329:HOH:O	2.34	0.60
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.36	0.60
1:A:868:LEU:N	1:A:868:LEU:HD22	2.17	0.60
1:B:428:LYS:CE	1:B:432:ARG:NH2	2.65	0.60
1:B:809:TRP:NE1	2:D:79:LEU:HD22	2.16	0.60
2:D:34:MET:HE2	2:D:34:MET:HA	1.84	0.60
1:B:428:LYS:HE3	1:B:432:ARG:HH22	1.65	0.60
1:B:974:PRO:HA	1:B:977:MET:CE	2.30	0.60
1:C:617:PHE:O	1:C:618:ALA:HB2	2.01	0.60
2:D:165:LEU:C	2:D:166:GLN:HG2	2.27	0.60
1:A:463:THR:HG23	1:A:467:TYR:HE2	1.67	0.59
2:E:68:LYS:HG2	2:E:68:LYS:O	2.00	0.59
2:E:163:GLU:O	2:E:166:GLN:HB2	2.02	0.59
1:A:971:ARG:NH1	15:A:1735:HOH:O	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:ASN:O	1:A:1038:GLU:HB3	2.02	0.59
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.32	0.59
1:A:49:TYR:HE2	1:A:60:THR:HG21	1.67	0.59
1:A:987:MET:HE3	1:A:987:MET:CA	2.32	0.59
1:A:342:LYS:HD2	4:A:1109:LMT:C1'	2.32	0.59
1:B:677:ALA:O	1:B:678:THR:CB	2.49	0.59
1:C:336:SER:O	1:C:340:VAL:HG23	2.03	0.59
1:A:575:MET:SD	1:A:664:PHE:CE1	2.96	0.59
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.10	0.59
1:A:538:THR:O	1:A:539:GLY:C	2.46	0.58
1:A:538:THR:CG2	1:A:539:GLY:N	2.54	0.58
1:A:863:SER:HA	1:A:866:GLU:HG3	1.84	0.58
4:B:1110:LMT:O2'	4:B:1110:LMT:C2	2.51	0.58
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.85	0.58
1:C:971:ARG:C	1:C:974:PRO:HD2	2.27	0.58
1:C:671:ILE:HG12	1:C:862:MET:SD	2.44	0.58
1:C:815:ARG:NE	15:C:1329:HOH:O	2.04	0.58
1:A:676:THR:HG23	1:A:862:MET:CE	2.33	0.58
1:C:509:LYS:O	1:C:514:GLY:HA3	2.03	0.58
1:A:500:ILE:O	15:A:1731:HOH:O	2.17	0.58
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.86	0.58
1:C:111:LEU:HD21	1:C:127:VAL:HG22	1.84	0.58
1:B:429:GLU:OE1	15:B:1581:HOH:O	2.16	0.58
1:A:989:LEU:HD23	1:A:1000:GLN:OE1	2.03	0.58
1:B:352:PHE:HE2	1:B:365:THR:HG21	1.67	0.58
1:A:868:LEU:N	1:A:868:LEU:CD2	2.66	0.58
1:A:987:MET:CE	1:A:987:MET:CA	2.82	0.58
2:E:34:MET:HE3	2:E:34:MET:CA	2.28	0.58
1:A:562:SER:OG	1:A:922:THR:HG21	2.04	0.57
1:A:971:ARG:HG3	15:A:1735:HOH:O	2.03	0.57
1:B:555:LEU:HD21	1:B:914:LEU:HD13	1.85	0.57
1:A:8:ARG:HH12	8:A:1111:D12:C1	2.18	0.57
1:A:510:LYS:HD2	1:A:511:GLY:N	2.19	0.57
1:B:428:LYS:HE2	1:B:432:ARG:NH1	2.19	0.57
1:B:873:ALA:O	1:B:876:LEU:N	2.37	0.57
1:A:877:TYR:O	1:A:881:LEU:HD23	2.05	0.57
4:A:1102:LMT:H6'1	4:B:1110:LMT:C3B	2.35	0.57
1:B:536:ARG:NH2	15:B:1522:HOH:O	2.37	0.57
1:B:676:THR:HB	1:B:678:THR:HG22	1.86	0.57
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.35	0.57
1:C:875:SER:O	1:C:879:ILE:HG22	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:ARG:O	1:C:974:PRO:HD2	2.05	0.57
1:A:1035:ARG:O	1:A:1036:LYS:C	2.47	0.56
1:A:456:MET:HG3	1:A:467:TYR:HB3	1.88	0.56
1:A:539:GLY:HA2	1:A:542:LEU:HD13	1.88	0.56
1:A:435:MET:O	1:A:439:GLN:HB3	2.06	0.56
1:A:672:VAL:C	1:A:674:LEU:N	2.64	0.56
1:A:862:MET:HG2	15:A:1417:HOH:O	2.04	0.56
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.68	0.56
1:C:527:TYR:CE2	1:C:968:VAL:CG1	2.79	0.56
1:A:870:GLY:HA3	4:A:1103:LMT:O3B	2.06	0.56
1:A:901:VAL:O	1:A:904:VAL:HG22	2.05	0.56
1:C:358:PHE:CG	1:C:977:MET:HG2	2.41	0.56
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.87	0.56
1:C:111:LEU:CD2	1:C:129:VAL:CG2	2.84	0.56
1:C:509:LYS:CB	1:C:510:LYS:CB	2.85	0.55
1:A:868:LEU:O	1:A:869:SER:CB	2.51	0.55
1:B:461:GLY:HA3	1:B:865:GLN:OE1	2.06	0.55
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.88	0.55
2:E:27:ASP:OD2	2:E:61:GLU:HB3	2.06	0.55
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.88	0.55
1:A:1035:ARG:N	1:A:1035:ARG:CD	2.53	0.55
1:C:671:ILE:CD1	1:C:674:LEU:HG	2.36	0.55
1:A:956:GLU:OE2	1:A:956:GLU:N	2.40	0.55
1:A:402:ILE:O	1:A:406:VAL:HG12	2.05	0.55
1:A:422:GLU:C	1:A:423:GLU:HG3	2.32	0.55
1:A:527:TYR:HE2	1:A:968:VAL:HG13	1.68	0.55
4:A:1102:LMT:O4'	4:B:1110:LMT:H3B	2.05	0.55
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.86	0.55
1:B:428:LYS:HE2	1:B:432:ARG:HH12	1.69	0.55
1:C:67:GLN:OE1	15:C:1673:HOH:O	2.18	0.55
1:C:620:ARG:NH1	15:C:1722:HOH:O	2.25	0.55
1:A:928:GLN:HG2	4:A:1103:LMT:H22	1.88	0.55
1:C:670:ALA:HB3	1:C:862:MET:CE	2.37	0.55
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.06	0.55
1:C:152:GLU:CD	1:C:152:GLU:H	2.15	0.55
1:B:885:PHE:HD1	1:B:902:MET:CE	2.20	0.55
1:A:401:ALA:O	1:A:405:LEU:HG	2.06	0.54
4:A:1103:LMT:O3'	4:A:1103:LMT:H1B	2.06	0.54
1:A:405:LEU:HD22	1:A:481:SER:HB2	1.87	0.54
2:E:72:ASP:OD2	15:E:339:HOH:O	2.18	0.54
2:E:91:GLY:HA2	2:E:128:ILE:HD12	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:LYS:HE2	1:B:432:ARG:NH2	2.22	0.54
4:B:1111:LMT:O2B	4:B:1111:LMT:H3'	2.06	0.54
1:C:659:LYS:HZ2	1:C:660:ASP:HB2	1.73	0.54
1:A:729:ILE:CD1	1:C:234:ILE:CG2	2.84	0.54
1:B:240:LEU:HG	1:B:245:GLU:HB3	1.90	0.54
2:D:98:VAL:HA	2:D:101:LYS:HE2	1.90	0.54
1:A:865:GLN:C	1:A:868:LEU:HG	2.32	0.54
3:B:1116:GOL:H2	1:C:119:PRO:HA	1.89	0.54
1:C:33:ALA:O	1:C:391:ASN:HA	2.08	0.54
1:C:702:LEU:HG	1:C:851:LEU:HD11	1.89	0.54
1:B:671:ILE:HG22	1:B:673:GLU:HG2	1.88	0.54
1:C:284:GLN:HG3	1:C:285:PRO:HD2	1.88	0.54
1:C:898:PRO:O	1:C:902:MET:HG2	2.07	0.54
2:E:91:GLY:HA2	2:E:128:ILE:CD1	2.38	0.54
1:A:971:ARG:NH2	15:A:1736:HOH:O	2.36	0.54
1:A:881:LEU:CD1	4:A:1103:LMT:H122	2.37	0.54
1:B:428:LYS:HE2	1:B:432:ARG:HH22	1.73	0.54
1:B:472:ILE:N	1:B:472:ILE:HD12	2.23	0.54
1:C:226:LYS:NZ	15:C:1560:HOH:O	2.41	0.54
1:C:360:GLN:HG2	1:C:513:PHE:CD1	2.43	0.54
2:E:49:THR:HB	2:E:50:PRO:HD2	1.90	0.54
1:A:676:THR:C	1:A:678:THR:H	2.15	0.53
1:A:881:LEU:HD13	4:A:1103:LMT:C12	2.38	0.53
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.74	0.53
1:B:239:ARG:HH21	3:B:1116:GOL:H11	1.73	0.53
1:A:1038:GLU:OE1	1:A:1039:ASP:HA	2.08	0.53
1:C:423:GLU:HB3	1:C:425:LEU:HD13	1.87	0.53
1:A:968:VAL:HG21	1:A:1023:PRO:CG	2.34	0.53
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.90	0.53
1:A:539:GLY:C	1:A:542:LEU:HD13	2.34	0.53
1:A:865:GLN:N	1:A:865:GLN:CD	2.67	0.53
2:E:16:LYS:O	2:E:20:GLU:HG3	2.08	0.53
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.91	0.53
1:B:615:PHE:O	1:B:626:ILE:HD13	2.08	0.53
1:B:645:GLU:O	1:B:649:MET:HG3	2.09	0.53
1:A:240:LEU:HG	1:A:245:GLU:HB3	1.91	0.53
1:B:562:SER:HA	1:B:677:ALA:HB3	1.91	0.53
1:C:151:GLN:OE1	1:C:278:ILE:HG23	2.09	0.53
2:E:42:ALA:O	2:E:50:PRO:HD3	2.09	0.53
2:D:165:LEU:O	2:D:166:GLN:HG2	2.08	0.53
1:A:729:ILE:HD11	1:C:234:ILE:HG23	1.87	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1110:LMT:H21	4:B:1110:LMT:H2O2	1.74	0.52
1:C:671:ILE:H	1:C:862:MET:HE1	1.73	0.52
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.91	0.52
1:A:345:VAL:HG21	4:A:1109:LMT:H61	1.89	0.52
1:B:807:SER:OG	3:B:1113:GOL:H31	2.09	0.52
3:B:1116:GOL:O3	3:B:1116:GOL:O1	2.27	0.52
1:A:57:VAL:CG1	1:A:88:VAL:CG2	2.83	0.52
1:A:85:THR:O	1:A:85:THR:HG22	2.08	0.52
1:A:633:ASP:OD2	4:A:1109:LMT:O4'	2.26	0.52
1:B:352:PHE:CD2	1:B:365:THR:HG23	2.44	0.52
1:A:423:GLU:HB2	1:A:425:LEU:HG	1.92	0.52
1:A:865:GLN:CA	1:A:866:GLU:HB2	2.38	0.52
4:B:1111:LMT:O5B	4:B:1111:LMT:C5'	2.57	0.52
2:D:150:PHE:O	2:D:154:ILE:HG23	2.08	0.52
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.90	0.52
1:A:674:LEU:N	1:A:674:LEU:CD2	2.72	0.52
1:A:1037:ASN:O	1:A:1038:GLU:CB	2.58	0.52
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.39	0.52
1:C:428:LYS:NZ	1:C:432:ARG:HH21	2.08	0.52
1:A:568:ASP:OD2	1:A:644:VAL:HG23	2.09	0.52
1:B:885:PHE:HB2	1:B:902:MET:CE	2.31	0.52
1:A:543:VAL:O	1:A:547:ILE:HG12	2.10	0.52
1:A:1044:HIS:C	1:A:1044:HIS:ND1	2.67	0.52
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.93	0.52
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.36	0.52
1:C:405:LEU:C	1:C:405:LEU:HD12	2.34	0.52
1:A:247:GLY:HA2	1:A:268:ILE:CD1	2.39	0.51
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.92	0.51
1:B:428:LYS:HE3	1:B:432:ARG:NH2	2.23	0.51
1:C:617:PHE:CD2	1:C:676:THR:HG21	2.46	0.51
1:A:188:MET:HE2	1:A:773:VAL:HG12	1.91	0.51
9:B:1103:MIY:HN72	9:B:1103:MIY:C8	2.40	0.51
1:C:40:PRO:HB2	1:C:94:PHE:O	2.11	0.51
1:C:193:LEU:HD13	1:C:265:VAL:HB	1.92	0.51
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.92	0.51
2:E:92:HIS:O	2:E:96:VAL:HG23	2.10	0.51
1:A:1038:GLU:CD	1:A:1039:ASP:HA	2.33	0.51
1:A:1042:HIS:O	1:A:1043:SER:CB	2.58	0.51
1:C:34:GLN:NE2	15:C:1648:HOH:O	2.44	0.51
1:C:57:VAL:HG12	1:C:88:VAL:CG2	2.41	0.51
1:C:115:MET:N	1:C:116:PRO:CD	2.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:VAL:HG12	1:C:326:PRO:HD3	1.91	0.51
1:A:672:VAL:CG2	1:A:673:GLU:N	2.61	0.51
1:C:671:ILE:O	1:C:671:ILE:CG1	2.58	0.51
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.10	0.51
2:D:46:VAL:O	2:D:77:ASP:HB2	2.10	0.51
1:B:13:TRP:CD1	10:B:1109:C14:H051	2.46	0.51
1:A:537:SER:O	1:A:538:THR:CB	2.54	0.51
1:B:328:ASP:O	1:B:331:PRO:HD2	2.10	0.51
1:B:400:LEU:HD13	1:B:929:VAL:HG12	1.93	0.51
1:B:493:CYS:HA	1:B:497:LEU:HD22	1.92	0.51
1:B:542:LEU:N	1:B:542:LEU:HD23	2.26	0.51
1:C:423:GLU:HB3	1:C:425:LEU:CD1	2.41	0.51
2:E:26:ARG:O	2:E:30:VAL:HG23	2.11	0.51
1:C:428:LYS:HZ3	1:C:432:ARG:HH21	1.58	0.51
1:C:509:LYS:HB3	1:C:510:LYS:CB	2.40	0.51
1:C:943:ILE:O	1:C:947:GLU:HB3	2.11	0.51
1:B:555:LEU:CD2	1:B:914:LEU:HD13	2.41	0.51
1:C:741:VAL:CG1	1:C:799:VAL:HG11	2.41	0.51
1:C:895:TRP:C	1:C:898:PRO:HD2	2.36	0.51
1:B:672:VAL:HG22	1:B:673:GLU:OE2	2.11	0.50
1:B:673:GLU:CD	1:B:673:GLU:H	2.17	0.50
1:A:864:TYR:C	1:A:866:GLU:HB2	2.33	0.50
1:A:376:LEU:HD13	1:A:405:LEU:CD1	2.41	0.50
1:A:672:VAL:CG2	1:A:673:GLU:CD	2.84	0.50
1:A:881:LEU:CD2	4:A:1103:LMT:H92	2.41	0.50
2:D:94:GLU:HG2	15:D:347:HOH:O	2.11	0.50
1:A:862:MET:O	1:A:866:GLU:HG2	2.10	0.50
2:E:31:ARG:HH12	2:E:65:VAL:HG22	1.76	0.50
2:E:34:MET:CE	2:E:40:VAL:CG1	2.88	0.50
1:A:13:TRP:NE1	6:A:1107:D10:H32	2.27	0.50
1:B:885:PHE:HA	1:B:902:MET:CE	2.40	0.50
1:C:671:ILE:CG1	1:C:674:LEU:HG	2.41	0.50
2:D:121:ALA:HB1	2:D:161:LEU:HD21	1.94	0.50
2:E:28:ASP:O	2:E:31:ARG:CB	2.57	0.50
1:B:362:PHE:O	1:B:365:THR:HG22	2.12	0.50
1:C:111:LEU:HD22	1:C:129:VAL:CG2	2.42	0.50
1:C:709:HIS:HE1	15:C:1731:HOH:O	1.94	0.50
1:A:8:ARG:HH22	8:A:1111:D12:C1	2.24	0.50
1:B:871:ASN:O	1:B:871:ASN:ND2	2.41	0.50
1:C:428:LYS:NZ	1:C:432:ARG:NH2	2.59	0.50
15:A:1655:HOH:O	2:D:154:ILE:HD11	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:LYS:NZ	1:C:660:ASP:CG	2.69	0.50
1:B:655:PHE:C	1:B:657:GLN:H	2.20	0.49
1:C:1032:ARG:HG3	1:C:1032:ARG:O	2.11	0.49
2:E:74:ASN:HD21	2:E:105:ASP:HB2	1.77	0.49
1:A:39:ALA:HB2	1:A:673:GLU:HG3	1.93	0.49
1:A:49:TYR:CE2	1:A:60:THR:HG21	2.46	0.49
1:C:671:ILE:HD11	1:C:674:LEU:CG	2.41	0.49
1:A:284:GLN:HB2	1:A:285:PRO:HD2	1.94	0.49
1:C:536:ARG:HH21	4:C:1102:LMT:C3B	2.25	0.49
1:A:431:THR:O	1:A:435:MET:HG2	2.13	0.49
1:A:897:ILE:N	1:A:898:PRO:CD	2.76	0.49
1:B:897:ILE:N	1:B:898:PRO:CD	2.75	0.49
1:C:114:ALA:C	1:C:116:PRO:HD2	2.38	0.49
1:C:463:THR:HG22	1:C:467:TYR:CZ	2.47	0.49
1:A:376:LEU:HD13	1:A:405:LEU:HD12	1.94	0.49
1:A:712:MET:SD	1:A:835:LYS:HD2	2.53	0.49
1:C:40:PRO:HD2	1:C:674:LEU:HD21	1.94	0.49
3:C:1101:GOL:O1	3:C:1101:GOL:O3	2.14	0.49
2:E:32:ILE:C	2:E:34:MET:N	2.69	0.49
2:E:163:GLU:HG3	2:E:164:ILE:N	2.28	0.49
1:A:428:LYS:O	1:A:432:ARG:HG3	2.13	0.49
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.95	0.49
2:E:97:GLU:O	2:E:101:LYS:HG3	2.13	0.49
1:A:454:VAL:N	1:A:455:PRO:CD	2.76	0.49
1:A:1001:ASN:O	1:A:1005:THR:CG2	2.59	0.49
1:C:420:MET:HE3	1:C:500:ILE:HD12	1.95	0.49
1:B:708:LYS:C	1:B:710:PRO:HD3	2.38	0.48
1:C:281:PHE:CE1	1:C:324:VAL:HG11	2.47	0.48
2:E:164:ILE:C	2:E:166:GLN:N	2.62	0.48
1:B:519:MET:SD	1:B:519:MET:C	2.97	0.48
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.95	0.48
1:B:165:ALA:HB3	1:B:313:MET:HE2	1.94	0.48
15:B:1683:HOH:O	1:C:70:ASN:HB2	2.12	0.48
1:B:133:SER:HA	15:B:1724:HOH:O	2.13	0.48
1:B:352:PHE:CE2	1:B:365:THR:HG23	2.48	0.48
1:B:400:LEU:HD13	1:B:929:VAL:CG1	2.43	0.48
1:A:1:MET:CA	15:A:1630:HOH:O	2.60	0.48
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.43	0.48
10:B:1109:C14:H052	1:C:895:TRP:HE1	1.79	0.48
1:C:617:PHE:CE2	1:C:676:THR:HG21	2.48	0.48
1:C:621:GLY:N	15:C:1227:HOH:O	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:THR:HG22	1:B:601:LYS:H	1.77	0.48
1:A:355:MET:CE	1:A:410:ILE:HD11	2.44	0.48
1:A:33:ALA:O	1:A:391:ASN:HA	2.14	0.48
1:B:573:MET:HE2	1:B:573:MET:HB2	1.72	0.48
1:C:987:MET:CG	1:C:1008:MET:HE1	2.44	0.48
1:A:672:VAL:C	1:A:674:LEU:H	2.21	0.48
1:C:732:ASP:OD2	1:C:735:LYS:HG3	2.14	0.48
1:B:716:VAL:HG13	1:B:716:VAL:O	2.14	0.47
1:B:775:SER:HB2	1:B:789:TRP:CZ2	2.49	0.47
1:C:983:ILE:HG13	1:C:1011:MET:HG2	1.96	0.47
1:A:493:CYS:O	1:A:497:LEU:HB2	2.13	0.47
4:A:1104:LMT:H1B	4:A:1104:LMT:O3'	2.13	0.47
1:B:375:VAL:CG1	1:B:405:LEU:HD13	2.44	0.47
1:A:418:ARG:CZ	1:A:970:MET:HE2	2.45	0.47
4:A:1102:LMT:C4B	4:B:1110:LMT:H3B	2.45	0.47
1:A:456:MET:HE2	1:A:467:TYR:HD1	1.76	0.47
1:A:546:LEU:N	1:A:546:LEU:HD23	2.29	0.47
1:A:866:GLU:OE1	1:A:866:GLU:CA	2.58	0.47
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.96	0.47
1:C:489:THR:HB	1:C:490:PRO:HD3	1.95	0.47
1:C:987:MET:HG3	1:C:1008:MET:HE1	1.95	0.47
1:A:418:ARG:CZ	1:A:970:MET:CE	2.92	0.47
1:A:405:LEU:N	1:A:405:LEU:HD23	2.28	0.47
1:A:544:LEU:HD12	1:A:544:LEU:O	2.14	0.47
1:A:1043:SER:HA	1:A:1044:HIS:HA	1.49	0.47
3:D:202:GOL:O3	3:D:202:GOL:O1	2.30	0.47
1:A:214:VAL:HG22	1:A:236:ALA:HB3	1.96	0.47
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.39	0.47
1:A:631:LEU:HD11	1:A:644:VAL:HG22	1.97	0.47
1:A:507:GLU:OE1	1:A:518:ARG:NH1	2.44	0.47
1:A:987:MET:N	1:A:988:PRO:CD	2.78	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
1:A:504:ASP:C	1:A:505:HIS:ND1	2.69	0.47
1:A:865:GLN:HB2	1:A:868:LEU:HG	1.96	0.47
4:A:1109:LMT:O2B	4:A:1109:LMT:H4'	2.13	0.47
1:C:329:THR:HB	15:C:1558:HOH:O	2.15	0.47
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.44	0.47
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.97	0.46
1:C:659:LYS:NZ	1:C:660:ASP:HB2	2.30	0.46
1:A:55:LYS:NZ	1:A:59:ASP:OD2	2.47	0.46
1:A:1035:ARG:CA	1:A:1036:LYS:HE2	2.40	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:ASP:OD1	1:C:182:TYR:HB2	2.15	0.46
1:C:564:LEU:HD23	1:C:670:ALA:HB1	1.97	0.46
1:B:127:VAL:N	3:B:1102:GOL:O1	2.42	0.46
1:B:669:PRO:HD3	11:B:1114:LMU:O6'	2.15	0.46
1:B:919:ARG:HB3	1:B:921:LEU:HD22	1.96	0.46
1:C:1011:MET:HA	1:C:1011:MET:CE	2.41	0.46
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.96	0.46
1:A:355:MET:HE1	1:A:410:ILE:HD11	1.98	0.46
1:A:1036:LYS:O	1:A:1037:ASN:OD1	2.33	0.46
1:A:1042:HIS:HD2	1:A:1043:SER:CA	2.27	0.46
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.74	0.46
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.96	0.46
2:E:49:THR:HB	2:E:50:PRO:CD	2.45	0.46
1:B:563:PHE:CE2	1:B:677:ALA:HB2	2.51	0.46
1:C:778:LYS:NZ	15:C:1454:HOH:O	2.49	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.31	0.46
1:A:673:GLU:H	1:A:673:GLU:CD	2.23	0.46
1:B:247:GLY:CA	1:B:268:ILE:HD12	2.45	0.46
1:B:563:PHE:CE2	1:B:677:ALA:N	2.84	0.46
1:B:999:ALA:O	1:B:1003:VAL:HG13	2.15	0.46
1:C:83:ASP:OD1	1:C:83:ASP:C	2.58	0.46
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.16	0.46
1:C:901:VAL:O	1:C:904:VAL:HG12	2.16	0.46
1:B:375:VAL:HG11	1:B:405:LEU:HD13	1.97	0.46
1:B:554:TYR:O	1:B:558:ARG:HG3	2.15	0.46
1:C:277:ILE:C	1:C:278:ILE:HG13	2.40	0.46
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.51	0.46
1:C:360:GLN:HG2	1:C:513:PHE:CE1	2.51	0.46
1:C:895:TRP:CD2	5:C:1103:OCT:H13	2.51	0.46
1:A:356:TYR:HA	1:A:365:THR:HG21	1.98	0.46
1:A:393:LEU:HD11	1:A:466:ILE:HG13	1.98	0.46
1:A:463:THR:HG23	1:A:467:TYR:CE2	2.50	0.46
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.97	0.46
1:B:189:ASN:OD1	1:B:189:ASN:C	2.58	0.46
1:C:111:LEU:HD23	1:C:129:VAL:CG2	2.46	0.46
1:C:195:LYS:HE3	1:C:196:PHE:CZ	2.51	0.46
1:A:554:TYR:CZ	1:A:558:ARG:HD2	2.51	0.45
1:B:83:ASP:C	1:B:83:ASP:OD1	2.59	0.45
1:A:501:ALA:O	1:A:502:LYS:C	2.58	0.45
1:A:1031:ARG:O	1:A:1033:PHE:N	2.49	0.45
1:B:11:PHE:O	1:B:11:PHE:HD1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:PHE:HB3	1:B:388:PHE:HE1	1.78	0.45
1:C:977:MET:HE2	1:C:977:MET:HB3	1.70	0.45
1:A:875:SER:O	1:A:879:ILE:HG23	2.15	0.45
1:B:428:LYS:HE2	1:B:432:ARG:CZ	2.47	0.45
1:B:655:PHE:C	1:B:657:GLN:N	2.72	0.45
1:B:866:GLU:C	1:B:868:LEU:N	2.72	0.45
1:C:32:VAL:HG12	1:C:337:ILE:CD1	2.47	0.45
1:C:395:MET:HE2	1:C:395:MET:HA	1.97	0.45
1:A:910:ILE:HG23	1:A:911:GLY:N	2.31	0.45
1:A:987:MET:N	1:A:988:PRO:HD2	2.31	0.45
1:B:135:SER:OG	15:B:1652:HOH:O	2.16	0.45
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.99	0.45
2:D:93:LEU:HB3	2:D:94:GLU:OE2	2.17	0.45
1:A:956:GLU:OE2	1:A:956:GLU:HA	2.14	0.45
1:A:1030:ARG:O	1:A:1034:SER:HB3	2.16	0.45
1:A:1040:ILE:CG2	1:A:1041:GLU:HB3	2.40	0.45
1:B:645:GLU:OE1	1:B:649:MET:CE	2.65	0.45
1:B:918:PHE:CD1	1:B:918:PHE:C	2.94	0.45
1:B:426:PRO:HD2	1:B:429:GLU:CG	2.46	0.45
1:A:537:SER:HB2	1:A:538:THR:H	1.47	0.45
1:A:449:LEU:O	1:A:452:VAL:HG13	2.16	0.45
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.99	0.44
1:B:564:LEU:CD1	1:B:671:ILE:HD12	2.47	0.44
1:C:774:MET:SD	3:C:1115:GOL:O3	2.75	0.44
1:A:346:GLU:HG2	4:A:1109:LMT:H122	1.99	0.44
1:A:372:VAL:HB	1:A:373:PRO:CD	2.47	0.44
1:A:416:VAL:O	1:A:419:VAL:HB	2.17	0.44
1:A:892:TYR:CZ	1:A:946:VAL:HG22	2.53	0.44
1:C:479:ALA:O	1:C:483:LEU:HD23	2.17	0.44
1:C:670:ALA:HB3	1:C:862:MET:HE2	1.99	0.44
1:A:866:GLU:C	1:A:868:LEU:CB	2.71	0.44
4:A:1104:LMT:H5B	4:A:1104:LMT:O6'	2.18	0.44
1:B:426:PRO:HB2	1:B:429:GLU:OE1	2.17	0.44
2:E:17:LYS:HD2	2:E:17:LYS:HA	1.59	0.44
1:A:16:ALA:HB2	1:A:488:LEU:HD22	2.00	0.44
1:A:712:MET:HA	1:A:835:LYS:HG3	1.98	0.44
1:B:75:LEU:HD13	3:B:1101:GOL:C3	2.39	0.44
1:C:195:LYS:HE3	1:C:196:PHE:CE2	2.52	0.44
1:A:808:ARG:HA	2:E:79:LEU:HD23	2.00	0.44
1:A:881:LEU:CD1	4:A:1103:LMT:C12	2.96	0.44
1:B:127:VAL:H	3:B:1102:GOL:C1	2.29	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:LEU:HD11	1:C:402:ILE:CD1	2.47	0.44
1:C:671:ILE:CD1	1:C:674:LEU:CG	2.96	0.44
1:C:889:ALA:HA	1:C:894:SER:O	2.18	0.44
1:A:420:MET:HE1	1:A:498:LYS:O	2.16	0.44
1:B:187:TRP:HB3	1:B:776:GLU:HG3	1.98	0.44
1:B:349:ILE:O	1:B:353:LEU:HD22	2.17	0.44
1:C:894:SER:O	1:C:898:PRO:HG2	2.17	0.44
1:A:127:VAL:HG22	1:B:113:LEU:HD22	1.99	0.44
1:C:876:LEU:CD1	1:C:932:LEU:HD11	2.48	0.44
1:C:897:ILE:N	1:C:897:ILE:CD1	2.81	0.44
1:A:1030:ARG:NE	1:A:1030:ARG:HA	2.33	0.44
1:B:696:THR:OG1	1:B:825:MET:HE1	2.18	0.44
1:A:38:ILE:HD12	1:A:674:LEU:HD21	1.97	0.43
1:A:728:LYS:O	1:A:807:SER:HA	2.18	0.43
4:B:1110:LMT:O5B	4:B:1110:LMT:H6D	2.17	0.43
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.97	0.43
1:C:254:ASN:N	1:C:258:SER:O	2.39	0.43
2:E:32:ILE:N	2:E:32:ILE:HD13	2.33	0.43
1:A:57:VAL:HG11	1:A:88:VAL:HG22	1.94	0.43
1:A:489:THR:N	1:A:490:PRO:CD	2.81	0.43
1:B:873:ALA:CB	1:B:874:PRO:CD	2.81	0.43
1:C:719:ASN:HB2	1:C:828:LEU:HD22	1.99	0.43
1:A:56:THR:O	1:A:60:THR:HB	2.18	0.43
4:A:1109:LMT:H1B	4:A:1109:LMT:H4B	1.57	0.43
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.70	0.43
1:B:593:GLU:OE2	1:B:658:ILE:HD13	2.17	0.43
1:C:631:LEU:HD11	1:C:644:VAL:HG22	1.98	0.43
1:A:8:ARG:NH2	8:A:1111:D12:H13	2.33	0.43
1:A:537:SER:CB	1:A:540:ARG:HH11	2.26	0.43
1:B:138:MET:CE	1:B:140:VAL:HG22	2.43	0.43
3:B:1116:GOL:H12	15:B:1469:HOH:O	2.17	0.43
1:A:909:VAL:HA	1:A:931:LEU:HD21	2.00	0.43
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.18	0.43
1:B:8:ARG:HG3	1:B:8:ARG:HH11	1.84	0.43
1:A:368:PRO:HA	1:A:409:ALA:HB1	2.00	0.43
1:A:687:GLN:NE2	15:A:1616:HOH:O	2.51	0.43
1:A:778:LYS:NZ	15:A:1496:HOH:O	2.43	0.43
1:B:987:MET:N	1:B:988:PRO:CD	2.81	0.43
1:A:366:LEU:HD12	1:A:366:LEU:HA	1.71	0.43
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.49	0.43
1:A:879:ILE:HD12	1:A:883:VAL:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:ARG:NH1	4:B:1104:LMT:O2B	2.51	0.43
1:C:671:ILE:N	1:C:862:MET:HE1	2.33	0.43
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.19	0.43
2:D:110:ASP:C	2:D:110:ASP:OD1	2.61	0.43
1:A:109:ASN:O	1:A:112:GLN:HG3	2.18	0.43
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.43
1:B:645:GLU:HG2	1:B:649:MET:CE	2.40	0.43
1:B:896:SER:C	1:B:898:PRO:HD2	2.43	0.43
1:A:681:ASP:OD1	1:A:826:GLU:OE1	2.36	0.43
1:B:489:THR:HG21	15:B:1728:HOH:O	2.19	0.43
1:B:885:PHE:CZ	8:B:1106:D12:H112	2.54	0.43
1:A:671:ILE:O	1:A:674:LEU:HB2	2.19	0.43
1:A:991:ILE:O	1:A:991:ILE:HG23	2.17	0.43
1:A:1038:GLU:CB	1:A:1039:ASP:CA	2.62	0.43
4:A:1102:LMT:H6'	4:A:1102:LMT:C5B	2.30	0.43
1:A:1:MET:N	1:A:2:PRO:CD	2.82	0.42
1:A:554:TYR:OH	1:A:558:ARG:NE	2.51	0.42
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.84	0.42
1:C:398:MET:O	1:C:402:ILE:HG12	2.18	0.42
1:A:372:VAL:HB	1:A:373:PRO:HD3	2.00	0.42
1:C:1013:THR:HB	1:C:1017:LEU:HD22	2.00	0.42
1:A:618:ALA:HB3	1:A:619:GLY:C	2.39	0.42
1:A:712:MET:HE2	1:A:712:MET:HB2	1.98	0.42
1:C:57:VAL:HG11	1:C:88:VAL:CG2	2.44	0.42
1:C:463:THR:CG2	1:C:467:TYR:CZ	3.02	0.42
1:A:672:VAL:HG23	1:A:673:GLU:OE2	2.19	0.42
1:A:672:VAL:O	1:A:673:GLU:C	2.60	0.42
1:A:684:LEU:HD23	1:A:695:LEU:HD22	2.01	0.42
1:A:1038:GLU:HB2	1:A:1040:ILE:O	2.20	0.42
1:B:670:ALA:C	1:B:671:ILE:HG13	2.43	0.42
1:B:809:TRP:CD1	2:D:79:LEU:HD22	2.54	0.42
1:A:9:PRO:HD2	1:B:893:GLU:OE1	2.19	0.42
1:A:990:VAL:HG12	1:A:1004:GLY:C	2.43	0.42
1:B:600:THR:HG22	1:B:601:LYS:HD3	2.01	0.42
1:B:776:GLU:HB3	15:B:1321:HOH:O	2.19	0.42
1:B:895:TRP:CD1	6:B:1105:D10:H32	2.55	0.42
1:B:973:ARG:HG2	1:B:977:MET:CE	2.37	0.42
1:C:121:GLU:HB2	15:C:1336:HOH:O	2.19	0.42
1:C:509:LYS:HG2	1:C:510:LYS:HE3	2.00	0.42
1:A:879:ILE:HG13	1:A:880:SER:N	2.34	0.42
1:B:314:GLU:N	1:B:315:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:662:MET:HE3	1:B:664:PHE:HE1	1.84	0.42
1:A:500:ILE:N	15:A:1731:HOH:O	2.53	0.42
1:B:578:LEU:N	1:B:578:LEU:HD23	2.35	0.42
1:B:885:PHE:CG	1:B:902:MET:HE1	2.55	0.42
1:C:1029:VAL:O	1:C:1033:PHE:HD2	2.02	0.42
2:D:91:GLY:HA2	2:D:128:ILE:CD1	2.49	0.42
2:E:32:ILE:HB	2:E:33:LEU:H	1.49	0.42
2:E:142:GLN:HB3	2:E:146:GLY:HA2	2.00	0.42
1:A:736:ALA:HA	1:A:741:VAL:HG22	2.01	0.42
1:A:892:TYR:OH	1:A:946:VAL:HG22	2.19	0.42
1:B:135:SER:N	15:B:1652:HOH:O	2.50	0.42
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.55	0.42
1:C:193:LEU:CD1	1:C:265:VAL:HB	2.49	0.42
1:B:429:GLU:CD	1:B:429:GLU:H	2.27	0.42
1:B:564:LEU:HD12	1:B:671:ILE:HD12	2.01	0.42
1:C:165:ALA:HB3	1:C:313:MET:CE	2.50	0.42
2:D:91:GLY:HA2	2:D:128:ILE:HD12	2.02	0.42
1:A:351:VAL:O	1:A:355:MET:HG2	2.20	0.42
1:A:777:ALA:O	1:A:781:MET:HG2	2.20	0.42
4:A:1109:LMT:H2B	4:A:1109:LMT:C6'	2.50	0.42
1:B:124:GLN:HG2	1:B:758:TYR:CE2	2.55	0.42
1:B:447:MET:HE2	1:B:447:MET:CA	2.40	0.42
1:A:489:THR:HB	1:A:490:PRO:HD3	2.01	0.41
1:A:867:ARG:HA	1:A:869:SER:N	2.34	0.41
1:B:330:THR:N	1:B:331:PRO:CD	2.83	0.41
1:C:947:GLU:HG3	1:C:948:PHE:N	2.31	0.41
2:D:14:LEU:HD23	2:D:14:LEU:HA	1.79	0.41
2:E:31:ARG:HH12	2:E:65:VAL:CG2	2.32	0.41
1:A:416:VAL:HG22	1:A:431:THR:HA	2.01	0.41
1:B:446:ALA:HB2	1:B:482:VAL:HG21	2.02	0.41
1:C:447:MET:SD	1:C:887:CYS:HB3	2.61	0.41
1:C:456:MET:HG3	1:C:467:TYR:HB3	2.02	0.41
1:A:355:MET:HE1	1:A:410:ILE:CD1	2.50	0.41
1:A:539:GLY:N	1:A:542:LEU:CD1	2.84	0.41
1:A:986:VAL:O	1:A:989:LEU:HB2	2.20	0.41
1:C:425:LEU:HA	1:C:426:PRO:HD3	1.91	0.41
2:E:74:ASN:ND2	2:E:105:ASP:HB2	2.35	0.41
1:A:8:ARG:HH22	8:A:1111:D12:H13	1.85	0.41
1:B:347:ALA:O	1:B:351:VAL:HG23	2.19	0.41
1:B:645:GLU:CD	1:B:649:MET:HE3	2.44	0.41
1:B:866:GLU:C	1:B:868:LEU:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:907:LEU:HG	1:B:1017:LEU:HB3	2.02	0.41
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.89	0.41
1:C:544:LEU:HD12	1:C:544:LEU:HA	1.70	0.41
1:C:732:ASP:CG	1:C:735:LYS:HG3	2.46	0.41
1:C:873:ALA:N	1:C:874:PRO:CD	2.83	0.41
1:A:875:SER:O	1:A:878:ALA:HB3	2.20	0.41
1:B:566:ASP:OD1	11:B:1114:LMU:O6B	2.38	0.41
1:B:744:ASN:O	1:B:748:THR:CG2	2.63	0.41
1:C:404:LEU:HD13	1:C:982:PHE:CD1	2.55	0.41
2:E:31:ARG:O	2:E:32:ILE:O	2.38	0.41
2:E:34:MET:HE2	2:E:40:VAL:CG1	2.50	0.41
1:A:8:ARG:CZ	8:A:1111:D12:H13	2.50	0.41
1:A:578:LEU:HB3	1:A:579:PRO:HD2	2.03	0.41
1:A:845:GLU:HG2	1:A:857:TYR:CZ	2.55	0.41
2:D:142:GLN:HA	2:D:147:LYS:O	2.20	0.41
1:A:448:VAL:O	1:A:451:ALA:HB3	2.21	0.41
1:A:449:LEU:HD23	1:A:478:MET:SD	2.60	0.41
1:A:507:GLU:CD	1:A:518:ARG:HH11	2.26	0.41
1:B:760:ASN:HB2	3:B:1116:GOL:O1	2.21	0.41
1:C:154:ILE:O	1:C:158:VAL:HG23	2.20	0.41
2:E:110:ASP:OD1	2:E:110:ASP:C	2.63	0.41
1:A:38:ILE:HD11	1:A:674:LEU:CD2	2.42	0.41
1:A:372:VAL:N	1:A:373:PRO:HD2	2.35	0.41
1:A:407:ASP:O	1:A:411:VAL:HG23	2.20	0.41
1:A:709:HIS:N	1:A:710:PRO:CD	2.80	0.41
1:B:8:ARG:N	1:B:9:PRO:CD	2.84	0.41
1:B:342:LYS:HD3	1:B:346:GLU:OE2	2.20	0.41
1:B:888:LEU:HB3	1:B:898:PRO:HB3	2.03	0.41
1:C:376:LEU:HD11	1:C:402:ILE:HD11	2.02	0.41
1:A:63:GLN:CD	1:C:768:VAL:HG23	2.46	0.41
1:A:121:GLU:CD	1:A:121:GLU:H	2.28	0.41
1:A:438:ILE:O	1:A:441:ALA:N	2.53	0.41
1:A:674:LEU:N	1:A:674:LEU:HD23	2.36	0.41
1:A:865:GLN:O	1:A:865:GLN:CG	2.69	0.41
1:A:1040:ILE:H	1:A:1040:ILE:HG12	1.51	0.41
1:B:70:ASN:O	1:B:110:LYS:HE3	2.21	0.41
1:B:426:PRO:HD2	1:B:429:GLU:HG3	2.03	0.41
1:C:2:PRO:O	1:C:6:ILE:HG13	2.21	0.41
1:C:368:PRO:HD3	1:C:413:VAL:HG21	2.02	0.41
1:A:335:ILE:HG23	4:A:1109:LMT:H6D	2.03	0.41
1:A:575:MET:SD	1:A:664:PHE:CZ	3.14	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:LEU:HD12	1:A:921:LEU:HA	1.83	0.41
1:B:169:THR:O	1:B:172:VAL:HG13	2.21	0.41
2:D:93:LEU:O	2:D:97:GLU:HG3	2.21	0.41
1:B:489:THR:N	1:B:490:PRO:CD	2.84	0.40
1:B:645:GLU:OE1	1:B:649:MET:HE3	2.21	0.40
1:C:507:GLU:HG2	1:C:518:ARG:HG2	2.02	0.40
1:C:919:ARG:NH2	15:C:1637:HOH:O	2.55	0.40
1:A:115:MET:HB2	1:A:116:PRO:HD3	2.03	0.40
1:A:756:GLY:HA3	3:A:1110:GOL:H32	2.03	0.40
1:A:897:ILE:N	1:A:898:PRO:HD2	2.37	0.40
1:A:1038:GLU:CG	1:A:1039:ASP:CA	2.94	0.40
1:C:53:ASP:O	1:C:57:VAL:HG23	2.22	0.40
1:C:111:LEU:HD23	1:C:129:VAL:HG21	2.04	0.40
1:B:386:PHE:HB3	1:B:388:PHE:HD1	1.77	0.40
1:B:454:VAL:N	1:B:455:PRO:CD	2.84	0.40
1:C:13:TRP:NE1	8:C:1104:D12:H92	2.37	0.40
1:C:326:PRO:O	1:C:630:SER:HB2	2.21	0.40
1:C:404:LEU:HG	1:C:449:LEU:HD13	2.04	0.40
2:E:62:ILE:O	2:E:66:LEU:HG	2.20	0.40
1:A:460:GLY:N	1:A:872:GLN:HE22	2.18	0.40
1:B:352:PHE:HE2	1:B:365:THR:CG2	2.25	0.40
1:B:712:MET:HG3	1:B:713:LEU:HD13	2.03	0.40
1:A:538:THR:CG2	1:A:539:GLY:H	2.00	0.40
1:A:876:LEU:HD23	1:A:876:LEU:HA	1.90	0.40
1:B:126:GLY:CA	1:C:116:PRO:HB3	2.51	0.40
1:B:138:MET:HE1	1:B:325:TYR:CE2	2.57	0.40
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.95	0.40
1:C:111:LEU:HD22	1:C:129:VAL:HG22	2.03	0.40
1:C:632:LYS:NZ	15:C:1778:HOH:O	2.45	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%)	986 (95%)	40 (4%)	16 (2%)	8	2
1	B	1031/1057 (98%)	1004 (97%)	22 (2%)	5 (0%)	24	16
1	C	1031/1057 (98%)	1002 (97%)	26 (2%)	3 (0%)	36	29
2	D	154/169 (91%)	152 (99%)	2 (1%)	0	100	100
2	E	150/169 (89%)	145 (97%)	2 (1%)	3 (2%)	6	1
All	All	3408/3509 (97%)	3289 (96%)	92 (3%)	27 (1%)	16	8

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	539	GLY
1	A	673	GLU
1	A	677	ALA
1	A	1036	LYS
1	A	1038	GLU
1	A	1043	SER
1	B	659	LYS
1	B	869	SER
1	C	510	LYS
1	C	618	ALA
2	E	32	ILE
2	E	33	LEU
2	E	165	LEU
1	A	620	ARG
1	A	869	SER
1	A	1032	ARG
1	A	1041	GLU
1	A	1042	HIS
1	B	678	THR
1	B	873	ALA
1	A	871	ASN
1	A	1031	ARG
1	A	1037	ASN
1	B	603	LYS
1	A	868	LEU
1	C	669	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	850/863 (98%)	782 (92%)	68 (8%)	11	5
1	B	839/863 (97%)	780 (93%)	59 (7%)	14	7
1	C	839/863 (97%)	790 (94%)	49 (6%)	18	10
2	D	120/132 (91%)	114 (95%)	6 (5%)	22	14
2	E	117/132 (89%)	106 (91%)	11 (9%)	8	3
All	All	2765/2853 (97%)	2572 (93%)	193 (7%)	14	7

All (193) 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	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	270	LEU
1	A	293	LEU
1	A	310	LEU
1	A	321	LEU
1	A	366	LEU
1	A	376	LEU
1	A	431	THR
1	A	437	GLN
1	A	447	MET
1	A	448	VAL
1	A	452	VAL
1	A	456	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	462	SER
1	A	483	LEU
1	A	486	LEU
1	A	498	LYS
1	A	522	LYS
1	A	523	SER
1	A	536	ARG
1	A	537	SER
1	A	540	ARG
1	A	542	LEU
1	A	557	VAL
1	A	617	PHE
1	A	649	MET
1	A	659	LYS
1	A	673	GLU
1	A	674	LEU
1	A	676	THR
1	A	678	THR
1	A	695	LEU
1	A	713	LEU
1	A	828	LEU
1	A	865	GLN
1	A	868	LEU
1	A	879	ILE
1	A	919	ARG
1	A	921	LEU
1	A	931	LEU
1	A	946	VAL
1	A	956	GLU
1	A	961	ILE
1	A	968	VAL
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	A	987	MET
1	A	990	VAL
1	A	991	ILE
1	A	1005	THR
1	A	1017	LEU
1	A	1027	VAL
1	A	1035	ARG
1	A	1036	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1040	ILE
1	A	1042	HIS
1	A	1044	HIS
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	132	SER
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	293	LEU
1	B	314	GLU
1	B	353	LEU
1	B	365	THR
1	B	366	LEU
1	B	377	LEU
1	B	399	VAL
1	B	429	GLU
1	B	480	LEU
1	B	483	LEU
1	B	497	LEU
1	B	519	MET
1	B	522	LYS
1	B	555	LEU
1	B	574	THR
1	B	578	LEU
1	B	600	THR
1	B	633	ASP
1	B	658	ILE
1	B	659	LYS
1	B	673	GLU
1	B	695	LEU
1	B	713	LEU
1	B	714	THR
1	B	748	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	778	LYS
1	B	801	PHE
1	B	868	LEU
1	B	875	SER
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	907	LEU
1	B	914	LEU
1	B	921	LEU
1	B	937	LEU
1	B	960	LEU
1	B	965	LEU
1	B	968	VAL
1	B	972	LEU
1	B	980	LEU
1	B	986	VAL
1	B	987	MET
1	B	1003	VAL
1	B	1022	VAL
1	C	1	MET
1	C	38	ILE
1	C	75	LEU
1	C	96	SER
1	C	121	GLU
1	C	127	VAL
1	C	152	GLU
1	C	177	LEU
1	C	193	LEU
1	C	253	VAL
1	C	256	ASP
1	C	258	SER
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	544	LEU
1	C	558	ARG
1	C	564	LEU
1	C	660	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	676	THR
1	C	690	LEU
1	C	693	GLU
1	C	695	LEU
1	C	702	LEU
1	C	717	ARG
1	C	739	LEU
1	C	742	SER
1	C	743	ILE
1	C	750	LEU
1	C	799	VAL
1	C	822	LEU
1	C	828	LEU
1	C	850	LYS
1	C	867	ARG
1	C	876	LEU
1	C	891	LEU
1	C	897	ILE
1	C	910	ILE
1	C	948	PHE
1	C	951	ASP
1	C	960	LEU
1	C	968	VAL
1	C	976	LEU
1	C	980	LEU
1	C	1011	MET
1	C	1017	LEU
2	D	45	VAL
2	D	61	GLU
2	D	79	LEU
2	D	94	GLU
2	D	139	VAL
2	D	154	ILE
2	E	29	GLU
2	E	32	ILE
2	E	34	MET
2	E	45	VAL
2	E	61	GLU
2	E	65	VAL
2	E	79	LEU
2	E	94	GLU
2	E	119	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	126	LEU
2	E	159	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	151	GLN
1	A	194	ASN
1	A	1042	HIS
1	B	58	GLN
1	B	70	ASN
1	B	81	ASN
1	B	274	ASN
1	B	577	GLN
1	B	584	GLN
1	B	687	GLN
1	B	872	GLN
1	C	81	ASN
1	C	605	ASN
1	C	642	ASN
1	C	709	HIS
1	C	1001	ASN
2	E	112	ASN
2	E	122	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

51 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$
4	LMT	B	1104	-	36,36,36	1.14	3 (8%)	47,47,47	1.30	5 (10%)
3	GOL	C	1117	-	5,5,5	0.52	0	5,5,5	0.44	0
8	D12	C	1104	-	11,11,11	0.36	0	10,10,10	0.80	0
6	D10	C	1107	-	9,9,9	0.47	0	8,8,8	1.02	0
3	GOL	B	1113	-	5,5,5	0.36	0	5,5,5	0.63	0
11	LMU	B	1114	-	36,36,36	1.12	4 (11%)	47,47,47	2.31	14 (29%)
5	OCT	C	1112	-	7,7,7	0.31	0	6,6,6	0.76	0
6	D10	C	1120	-	9,9,9	0.32	0	8,8,8	0.72	0
14	UND	C	1119	-	10,10,10	0.32	0	9,9,9	0.74	0
6	D10	B	1107	-	9,9,9	0.40	0	8,8,8	0.97	0
3	GOL	B	1115	-	5,5,5	0.39	0	5,5,5	0.34	0
7	HEX	B	1108	-	5,5,5	0.32	0	4,4,4	0.67	0
7	HEX	C	1113	-	5,5,5	0.25	0	4,4,4	0.54	0
5	OCT	C	1103	-	7,7,7	0.37	0	6,6,6	0.79	0
3	GOL	C	1114	-	5,5,5	0.35	0	5,5,5	0.35	0
6	D10	A	1107	-	9,9,9	0.33	0	8,8,8	0.72	0
4	LMT	A	1103	-	36,36,36	1.16	3 (8%)	47,47,47	1.16	3 (6%)
5	OCT	C	1105	-	7,7,7	0.39	0	6,6,6	1.20	1 (16%)
4	LMT	B	1110	-	36,36,36	1.21	3 (8%)	47,47,47	1.40	6 (12%)
5	OCT	C	1116	-	7,7,7	0.38	0	6,6,6	0.90	0
7	HEX	A	1108	-	5,5,5	0.30	0	4,4,4	0.77	0
8	D12	B	1106	-	11,11,11	0.29	0	10,10,10	0.75	0
8	D12	C	1108	-	11,11,11	0.49	0	10,10,10	1.13	1 (10%)
3	GOL	B	1102	-	5,5,5	0.41	0	5,5,5	0.35	0
7	HEX	C	1110	-	5,5,5	0.30	0	4,4,4	0.79	0
6	D10	C	1109	-	9,9,9	0.35	0	8,8,8	0.82	0
13	SO4	C	1118	-	4,4,4	0.21	0	6,6,6	0.12	0
3	GOL	B	1101	-	5,5,5	0.34	0	5,5,5	0.44	0
3	GOL	D	202	-	5,5,5	0.36	0	5,5,5	0.51	0
3	GOL	A	1101	-	5,5,5	0.33	0	5,5,5	0.59	0
3	GOL	E	201	-	5,5,5	0.33	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	LMT	A	1109	-	36,36,36	1.11	3 (8%)	47,47,47	1.53	11 (23%)
3	GOL	C	1115	-	5,5,5	0.49	0	5,5,5	0.79	0
4	LMT	A	1104	-	36,36,36	1.20	3 (8%)	47,47,47	1.15	4 (8%)
10	C14	B	1109	-	13,13,13	0.36	0	12,12,12	0.93	0
12	DD9	C	1111	-	8,8,8	0.30	0	7,7,7	0.76	0
4	LMT	C	1102	-	36,36,36	1.16	3 (8%)	47,47,47	1.10	2 (4%)
3	GOL	D	201	-	5,5,5	0.35	0	5,5,5	0.41	0
3	GOL	A	1110	-	5,5,5	0.38	0	5,5,5	0.81	0
5	OCT	A	1105	-	7,7,7	0.43	0	6,6,6	0.84	0
3	GOL	B	1117	-	5,5,5	0.47	0	5,5,5	0.46	0
4	LMT	A	1102	-	36,36,36	1.16	3 (8%)	47,47,47	1.49	7 (14%)
5	OCT	A	1106	-	7,7,7	0.29	0	6,6,6	0.65	0
5	OCT	C	1106	-	7,7,7	0.31	0	6,6,6	0.66	0
4	LMT	B	1111	-	36,36,36	1.18	3 (8%)	47,47,47	1.06	3 (6%)
3	GOL	B	1116	-	5,5,5	0.39	0	5,5,5	0.14	0
7	HEX	B	1112	-	5,5,5	0.26	0	4,4,4	0.57	0
8	D12	A	1111	-	11,11,11	0.53	0	10,10,10	1.12	0
9	MIY	B	1103	-	36,36,36	3.52	17 (47%)	42,58,58	2.33	15 (35%)
3	GOL	C	1101	-	5,5,5	0.32	0	5,5,5	0.46	0
6	D10	B	1105	-	9,9,9	0.45	0	8,8,8	0.91	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LMT	B	1104	-	-	13/21/61/61	0/2/2/2
3	GOL	C	1117	-	-	2/4/4/4	-
8	D12	C	1104	-	-	1/9/9/9	-
6	D10	C	1107	-	-	1/7/7/7	-
3	GOL	B	1113	-	-	0/4/4/4	-
11	LMU	B	1114	-	-	10/21/61/61	0/2/2/2
5	OCT	C	1112	-	-	1/5/5/5	-
6	D10	C	1120	-	-	3/7/7/7	-
14	UND	C	1119	-	-	1/8/8/8	-
6	D10	B	1107	-	-	5/7/7/7	-
3	GOL	B	1115	-	-	2/4/4/4	-
7	HEX	B	1108	-	-	2/3/3/3	-
7	HEX	C	1113	-	-	1/3/3/3	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	OCT	C	1103	-	-	0/5/5/5	-
3	GOL	C	1114	-	-	3/4/4/4	-
6	D10	A	1107	-	-	2/7/7/7	-
4	LMT	A	1103	-	-	12/21/61/61	0/2/2/2
5	OCT	C	1105	-	-	1/5/5/5	-
4	LMT	B	1110	-	-	11/21/61/61	0/2/2/2
5	OCT	C	1116	-	-	1/5/5/5	-
7	HEX	A	1108	-	-	2/3/3/3	-
8	D12	B	1106	-	-	3/9/9/9	-
8	D12	C	1108	-	-	0/9/9/9	-
3	GOL	B	1102	-	-	2/4/4/4	-
7	HEX	C	1110	-	-	1/3/3/3	-
6	D10	C	1109	-	-	3/7/7/7	-
3	GOL	B	1101	-	-	1/4/4/4	-
3	GOL	D	202	-	-	0/4/4/4	-
3	GOL	A	1101	-	-	3/4/4/4	-
3	GOL	E	201	-	-	2/4/4/4	-
4	LMT	A	1109	-	-	12/21/61/61	0/2/2/2
3	GOL	C	1115	-	-	4/4/4/4	-
4	LMT	A	1104	-	-	11/21/61/61	0/2/2/2
10	C14	B	1109	-	-	5/11/11/11	-
12	DD9	C	1111	-	-	5/6/6/6	-
4	LMT	C	1102	-	-	6/21/61/61	0/2/2/2
3	GOL	D	201	-	-	0/4/4/4	-
3	GOL	A	1110	-	-	2/4/4/4	-
5	OCT	A	1105	-	-	0/5/5/5	-
3	GOL	B	1117	-	-	2/4/4/4	-
4	LMT	A	1102	-	-	8/21/61/61	0/2/2/2
5	OCT	A	1106	-	-	0/5/5/5	-
5	OCT	C	1106	-	-	3/5/5/5	-
4	LMT	B	1111	-	-	14/21/61/61	0/2/2/2
3	GOL	B	1116	-	-	2/4/4/4	-
7	HEX	B	1112	-	-	0/3/3/3	-
8	D12	A	1111	-	-	3/9/9/9	-
9	MIY	B	1103	-	-	3/12/70/70	0/4/4/4
3	GOL	C	1101	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	D10	B	1105	-	-	0/7/7/7	-

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1103	MIY	C10-C9	10.98	1.53	1.40
9	B	1103	MIY	O1-C1	8.26	1.36	1.22
9	B	1103	MIY	O5-C15	7.40	1.38	1.23
9	B	1103	MIY	C18-C1	-4.92	1.48	1.55
9	B	1103	MIY	C14-C13	4.59	1.48	1.41
9	B	1103	MIY	C11-C12	4.54	1.46	1.38
4	B	1110	LMT	O5B-C1B	3.88	1.51	1.41
9	B	1103	MIY	C16-C17	3.87	1.40	1.36
9	B	1103	MIY	C8-C9	3.85	1.57	1.51
4	B	1111	LMT	O5B-C1B	3.80	1.51	1.41
9	B	1103	MIY	C14-C9	-3.78	1.34	1.40
4	A	1104	LMT	O5B-C1B	3.68	1.51	1.41
4	A	1103	LMT	O5B-C1B	3.66	1.51	1.41
9	B	1103	MIY	O7-C18	-3.64	1.36	1.42
4	C	1102	LMT	O5B-C1B	3.60	1.51	1.41
4	A	1102	LMT	O5B-C1B	3.56	1.51	1.41
9	B	1103	MIY	C21-N2	3.53	1.43	1.33
4	B	1104	LMT	O5B-C1B	3.37	1.50	1.41
4	A	1109	LMT	O5B-C1B	3.36	1.50	1.41
11	B	1114	LMU	C4B-C5B	3.31	1.60	1.53
4	B	1110	LMT	C3'-C4'	-3.30	1.43	1.52
9	B	1103	MIY	C7-C16	-3.25	1.48	1.51
4	A	1104	LMT	C3'-C4'	-3.23	1.43	1.52
4	B	1111	LMT	C3'-C4'	-3.21	1.43	1.52
4	A	1103	LMT	C3'-C4'	-3.11	1.43	1.52
4	C	1102	LMT	C3'-C4'	-3.07	1.43	1.52
4	A	1102	LMT	O5'-C5'	3.00	1.51	1.44
4	B	1104	LMT	O5'-C5'	2.99	1.51	1.44
11	B	1114	LMU	O4'-C4B	2.97	1.50	1.43
9	B	1103	MIY	O6-C17	2.95	1.42	1.32
4	A	1102	LMT	C3'-C4'	-2.95	1.44	1.52
9	B	1103	MIY	C11-C10	2.91	1.44	1.39
4	A	1109	LMT	C3'-C4'	-2.91	1.44	1.52
4	B	1104	LMT	C3'-C4'	-2.91	1.44	1.52
4	A	1104	LMT	O5'-C5'	2.82	1.51	1.44
4	A	1109	LMT	O5'-C5'	2.81	1.51	1.44
4	B	1110	LMT	O5'-C5'	2.76	1.51	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1111	LMT	O5'-C5'	2.71	1.51	1.44
4	C	1102	LMT	O5'-C5'	2.67	1.50	1.44
4	A	1103	LMT	O5'-C5'	2.64	1.50	1.44
11	B	1114	LMU	C4B-C3B	2.58	1.59	1.52
9	B	1103	MIY	C5-C4	2.29	1.56	1.54
9	B	1103	MIY	C2-C21	2.29	1.52	1.47
9	B	1103	MIY	C10-N7	2.22	1.48	1.42
11	B	1114	LMU	O2B-C2B	-2.07	1.37	1.43

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1103	MIY	C11-C12-C13	-6.48	114.02	120.50
11	B	1114	LMU	O5'-C5'-C6'	5.50	120.07	106.44
11	B	1114	LMU	O5B-C5B-C6B	5.26	119.46	106.44
11	B	1114	LMU	O1'-C1'-C2'	5.24	116.24	108.27
11	B	1114	LMU	O5B-C5B-C4B	5.04	118.78	109.70
4	B	1110	LMT	C1-O1'-C1'	4.91	122.07	113.68
4	B	1104	LMT	C1-O1'-C1'	4.85	121.96	113.68
9	B	1103	MIY	O6-C17-C18	4.82	120.35	113.37
11	B	1114	LMU	O4'-C4B-C3B	4.55	121.11	110.38
9	B	1103	MIY	C18-C17-C16	-4.50	118.49	123.06
4	A	1102	LMT	O5B-C5B-C4B	4.41	117.65	109.70
4	A	1102	LMT	C3B-C4B-C5B	4.41	118.23	110.23
9	B	1103	MIY	C9-C10-N7	4.40	124.13	118.87
11	B	1114	LMU	O4'-C4B-C5B	4.21	119.68	109.32
4	A	1109	LMT	C1B-O5B-C5B	-4.20	105.51	113.72
4	A	1103	LMT	C1-O1'-C1'	3.94	120.41	113.68
11	B	1114	LMU	C3B-C4B-C5B	3.93	117.35	110.23
11	B	1114	LMU	C1'-O5'-C5'	-3.89	106.12	113.72
4	C	1102	LMT	C1-O1'-C1'	3.83	120.22	113.68
4	A	1104	LMT	C1-O1'-C1'	3.71	120.01	113.68
9	B	1103	MIY	C12-C13-C14	3.63	124.78	120.15
9	B	1103	MIY	C6-C5-C4	-3.57	108.57	113.73
4	A	1109	LMT	C3'-C4'-C5'	3.51	118.71	110.93
4	A	1104	LMT	C1B-O1B-C4'	-3.45	109.80	117.98
4	B	1111	LMT	C1-O1'-C1'	3.35	119.40	113.68
4	A	1109	LMT	C2'-C3'-C4'	3.34	117.25	109.68
11	B	1114	LMU	C6'-C5'-C4'	3.31	122.69	113.38
4	A	1109	LMT	O1B-C1B-C2B	3.27	116.13	108.09
11	B	1114	LMU	C1B-O1B-C4'	-3.16	110.48	117.98
4	B	1110	LMT	C1B-O1B-C4'	-3.04	110.76	117.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1103	MIY	C9-C8-C7	-3.03	109.11	113.12
9	B	1103	MIY	C18-C5-C4	3.03	115.78	111.64
11	B	1114	LMU	O5B-C1B-C2B	3.01	116.56	110.37
9	B	1103	MIY	O7-C18-C17	-2.91	105.48	110.14
4	A	1109	LMT	O5'-C5'-C4'	2.86	115.64	109.72
4	A	1102	LMT	C1B-O1B-C4'	-2.77	111.41	117.98
4	A	1103	LMT	C2'-C3'-C4'	2.75	115.91	109.68
11	B	1114	LMU	C6B-C5B-C4B	2.70	119.65	113.02
4	A	1109	LMT	O6'-C6'-C5'	2.69	120.49	111.33
4	B	1110	LMT	O5B-C5B-C4B	2.65	114.48	109.70
4	A	1102	LMT	O1'-C1-C2	2.62	118.27	109.37
9	B	1103	MIY	C20-N1-C4	-2.53	108.33	114.10
4	C	1102	LMT	O1'-C1-C2	2.49	117.81	109.37
9	B	1103	MIY	C12-C11-C10	2.47	124.06	119.10
5	C	1105	OCT	C6-C5-C4	-2.47	101.88	114.37
4	A	1109	LMT	C1-O1'-C1'	2.45	117.86	113.68
11	B	1114	LMU	O1B-C4'-C3'	2.44	113.44	107.23
4	B	1110	LMT	C1B-O5B-C5B	2.44	118.49	113.72
4	B	1104	LMT	C2'-C3'-C4'	2.43	115.19	109.68
9	B	1103	MIY	C11-C10-N7	-2.39	118.36	121.65
4	A	1103	LMT	O1'-C1-C2	2.39	117.47	109.37
4	A	1102	LMT	C1-O1'-C1'	2.37	117.73	113.68
4	B	1111	LMT	O6B-C6B-C5B	2.36	119.38	111.33
4	A	1109	LMT	C3B-C4B-C5B	2.33	114.45	110.23
4	A	1102	LMT	O6'-C6'-C5'	2.32	119.24	111.33
8	C	1108	D12	C9-C8-C7	-2.28	102.83	114.37
9	B	1103	MIY	C11-C10-C9	-2.27	117.50	120.59
4	B	1104	LMT	O1'-C1-C2	2.26	117.04	109.37
4	B	1110	LMT	O1'-C1'-C2'	2.23	111.66	108.27
4	A	1104	LMT	O6'-C6'-C5'	2.20	118.83	111.33
4	A	1109	LMT	O1'-C1-C2	2.20	116.84	109.37
4	B	1110	LMT	O1'-C1-C2	2.19	116.80	109.37
11	B	1114	LMU	O5'-C5'-C4'	2.18	114.23	109.72
4	A	1109	LMT	O1B-C4'-C3'	-2.15	101.77	107.23
4	A	1104	LMT	O6B-C6B-C5B	2.14	118.61	111.33
9	B	1103	MIY	O5-C15-C16	-2.13	117.45	121.14
4	B	1104	LMT	O1B-C1B-C2B	2.12	113.31	108.09
4	A	1102	LMT	C1B-O5B-C5B	2.10	117.81	113.72
4	B	1104	LMT	O6B-C6B-C5B	2.09	118.46	111.33
4	A	1109	LMT	C1B-C2B-C3B	-2.08	105.64	110.01
4	B	1111	LMT	O5'-C5'-C6'	2.03	111.48	106.44
9	B	1103	MIY	C5-C18-C1	-2.01	108.75	111.05

There are no chirality outliers.

All (173) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1102	GOL	O1-C1-C2-O2
3	B	1102	GOL	O1-C1-C2-C3
3	B	1116	GOL	O1-C1-C2-O2
3	B	1116	GOL	O1-C1-C2-C3
3	B	1117	GOL	O1-C1-C2-O2
3	B	1117	GOL	O1-C1-C2-C3
3	C	1115	GOL	O1-C1-C2-C3
3	C	1115	GOL	C1-C2-C3-O3
3	C	1117	GOL	O1-C1-C2-C3
3	E	201	GOL	O1-C1-C2-C3
4	A	1109	LMT	C2B-C1B-O1B-C4'
4	A	1109	LMT	O5'-C1'-O1'-C1
4	B	1110	LMT	C2'-C1'-O1'-C1
4	B	1110	LMT	O5'-C1'-O1'-C1
4	B	1111	LMT	C2-C1-O1'-C1'
4	C	1102	LMT	O5'-C1'-O1'-C1
4	C	1102	LMT	C2-C1-O1'-C1'
9	B	1103	MIY	C5-C4-N1-C19
11	B	1114	LMU	C2-C1-O1'-C1'
4	B	1111	LMT	O5B-C1B-O1B-C4'
4	B	1111	LMT	C4B-C5B-C6B-O6B
4	B	1104	LMT	O5B-C5B-C6B-O6B
4	B	1111	LMT	O5B-C5B-C6B-O6B
4	A	1102	LMT	C4'-C5'-C6'-O6'
4	A	1109	LMT	O5B-C5B-C6B-O6B
4	A	1103	LMT	O5B-C5B-C6B-O6B
4	B	1111	LMT	O5'-C5'-C6'-O6'
4	B	1104	LMT	C4B-C5B-C6B-O6B
11	B	1114	LMU	C4'-C5'-C6'-O6'
4	A	1102	LMT	O5'-C5'-C6'-O6'
4	A	1109	LMT	C4B-C5B-C6B-O6B
4	A	1109	LMT	C4-C5-C6-C7
5	C	1105	OCT	C2-C3-C4-C5
4	B	1111	LMT	C5'-C4'-O1B-C1B
4	B	1104	LMT	C7-C8-C9-C10
4	A	1103	LMT	O5'-C5'-C6'-O6'
4	C	1102	LMT	O5B-C5B-C6B-O6B
4	B	1110	LMT	O5'-C5'-C6'-O6'
3	C	1117	GOL	O1-C1-C2-O2
3	E	201	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1109	LMT	C11-C10-C9-C8
4	A	1104	LMT	C4B-C5B-C6B-O6B
4	A	1104	LMT	O5B-C5B-C6B-O6B
4	A	1103	LMT	C4B-C5B-C6B-O6B
4	C	1102	LMT	O1'-C1-C2-C3
4	A	1102	LMT	O1'-C1-C2-C3
4	A	1109	LMT	C2'-C1'-O1'-C1
4	B	1104	LMT	O1'-C1-C2-C3
3	A	1110	GOL	O1-C1-C2-C3
3	B	1115	GOL	O1-C1-C2-C3
3	C	1101	GOL	O1-C1-C2-C3
3	C	1101	GOL	C1-C2-C3-O3
3	C	1114	GOL	O1-C1-C2-C3
11	B	1114	LMU	O1'-C1-C2-C3
4	A	1103	LMT	C7-C8-C9-C10
5	C	1116	OCT	C2-C3-C4-C5
7	A	1108	HEX	C2-C3-C4-C5
7	B	1108	HEX	C2-C3-C4-C5
7	C	1113	HEX	C2-C3-C4-C5
10	B	1109	C14	C03-C04-C05-C06
3	C	1101	GOL	O1-C1-C2-O2
3	C	1101	GOL	O2-C2-C3-O3
3	C	1115	GOL	O1-C1-C2-O2
3	C	1115	GOL	O2-C2-C3-O3
4	A	1109	LMT	O5'-C5'-C6'-O6'
4	B	1111	LMT	C4'-C5'-C6'-O6'
4	B	1111	LMT	C2-C3-C4-C5
6	A	1107	D10	C2-C3-C4-C5
4	B	1104	LMT	C1-C2-C3-C4
4	B	1104	LMT	C2-C3-C4-C5
4	B	1111	LMT	C3-C4-C5-C6
12	C	1111	DD9	C4-C5-C6-C7
4	A	1104	LMT	C6-C7-C8-C9
4	B	1111	LMT	C1-C2-C3-C4
4	B	1104	LMT	C3-C4-C5-C6
4	B	1104	LMT	C9-C10-C11-C12
4	B	1111	LMT	C3'-C4'-O1B-C1B
4	A	1103	LMT	C9-C10-C11-C12
4	B	1110	LMT	C11-C10-C9-C8
6	B	1107	D10	C3-C4-C5-C6
4	A	1109	LMT	O1'-C1-C2-C3
4	B	1111	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1104	LMT	C1-C2-C3-C4
11	B	1114	LMU	C4-C5-C6-C7
4	A	1103	LMT	C5-C6-C7-C8
4	A	1102	LMT	C7-C8-C9-C10
4	A	1104	LMT	C7-C8-C9-C10
11	B	1114	LMU	C4B-C5B-C6B-O6B
10	B	1109	C14	C07-C08-C09-C10
8	B	1106	D12	C11-C10-C9-C8
4	A	1109	LMT	C2-C3-C4-C5
8	A	1111	D12	C6-C7-C8-C9
8	B	1106	D12	C6-C7-C8-C9
4	A	1104	LMT	O5B-C1B-O1B-C4'
10	B	1109	C14	C11-C12-C13-C14
4	A	1102	LMT	C1-C2-C3-C4
4	A	1103	LMT	C2-C1-O1'-C1'
4	B	1104	LMT	C2-C1-O1'-C1'
4	B	1110	LMT	C2-C1-O1'-C1'
4	B	1110	LMT	C3-C4-C5-C6
6	C	1120	D10	C4-C5-C6-C7
11	B	1114	LMU	C6-C7-C8-C9
12	C	1111	DD9	C2-C3-C4-C5
6	B	1107	D10	C7-C8-C9-C10
4	A	1104	LMT	C3-C4-C5-C6
7	C	1110	HEX	C2-C3-C4-C5
12	C	1111	DD9	C5-C6-C7-C8
4	B	1104	LMT	C4-C5-C6-C7
4	B	1104	LMT	C5-C6-C7-C8
4	A	1104	LMT	C11-C10-C9-C8
3	B	1115	GOL	O1-C1-C2-O2
3	C	1114	GOL	O1-C1-C2-O2
4	A	1103	LMT	C3'-C4'-O1B-C1B
6	B	1107	D10	C5-C6-C7-C8
11	B	1114	LMU	C7-C8-C9-C10
12	C	1111	DD9	C1-C2-C3-C4
3	A	1101	GOL	O1-C1-C2-C3
14	C	1119	UND	C11-C10-C9-C8
4	A	1103	LMT	C4'-C5'-C6'-O6'
4	B	1110	LMT	C4'-C5'-C6'-O6'
6	C	1109	D10	C3-C4-C5-C6
4	C	1102	LMT	C4B-C5B-C6B-O6B
4	A	1104	LMT	C9-C10-C11-C12
4	A	1103	LMT	C5'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1107	D10	C4-C5-C6-C7
8	A	1111	D12	C7-C8-C9-C10
4	C	1102	LMT	C3-C4-C5-C6
5	C	1106	OCT	C2-C3-C4-C5
4	B	1110	LMT	C5-C6-C7-C8
5	C	1106	OCT	C5-C6-C7-C8
11	B	1114	LMU	C9-C10-C11-C12
4	A	1104	LMT	C2B-C1B-O1B-C4'
4	A	1102	LMT	C11-C10-C9-C8
4	A	1104	LMT	C5-C6-C7-C8
6	B	1107	D10	C2-C3-C4-C5
6	B	1107	D10	C1-C2-C3-C4
12	C	1111	DD9	C6-C7-C8-C9
7	A	1108	HEX	C3-C4-C5-C6
6	C	1109	D10	C2-C3-C4-C5
11	B	1114	LMU	C3-C4-C5-C6
5	C	1106	OCT	C3-C4-C5-C6
4	B	1111	LMT	C4-C5-C6-C7
10	B	1109	C14	C09-C10-C11-C12
4	B	1110	LMT	C2-C3-C4-C5
6	C	1120	D10	C5-C6-C7-C8
11	B	1114	LMU	C11-C10-C9-C8
4	A	1102	LMT	C6-C7-C8-C9
8	C	1104	D12	C6-C7-C8-C9
5	C	1112	OCT	C5-C6-C7-C8
3	B	1101	GOL	C1-C2-C3-O3
3	C	1114	GOL	C1-C2-C3-O3
3	A	1110	GOL	O1-C1-C2-O2
4	A	1103	LMT	C3-C4-C5-C6
9	B	1103	MIY	C9-C10-N7-CN7
8	A	1111	D12	C5-C6-C7-C8
4	B	1110	LMT	C1-C2-C3-C4
3	A	1101	GOL	O2-C2-C3-O3
6	C	1120	D10	C7-C8-C9-C10
4	B	1104	LMT	O5B-C1B-O1B-C4'
4	B	1104	LMT	C2B-C1B-O1B-C4'
10	B	1109	C14	C10-C11-C12-C13
4	A	1109	LMT	C6-C7-C8-C9
4	A	1109	LMT	C4'-C5'-C6'-O6'
9	B	1103	MIY	C11-C10-N7-CN7
6	C	1109	D10	C7-C8-C9-C10
4	B	1111	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	B	1110	LMT	C6-C7-C8-C9
3	A	1101	GOL	C1-C2-C3-O3
7	B	1108	HEX	C1-C2-C3-C4
6	C	1107	D10	C1-C2-C3-C4
4	A	1103	LMT	C2-C3-C4-C5
4	A	1102	LMT	C2-C3-C4-C5
8	B	1106	D12	C1-C2-C3-C4

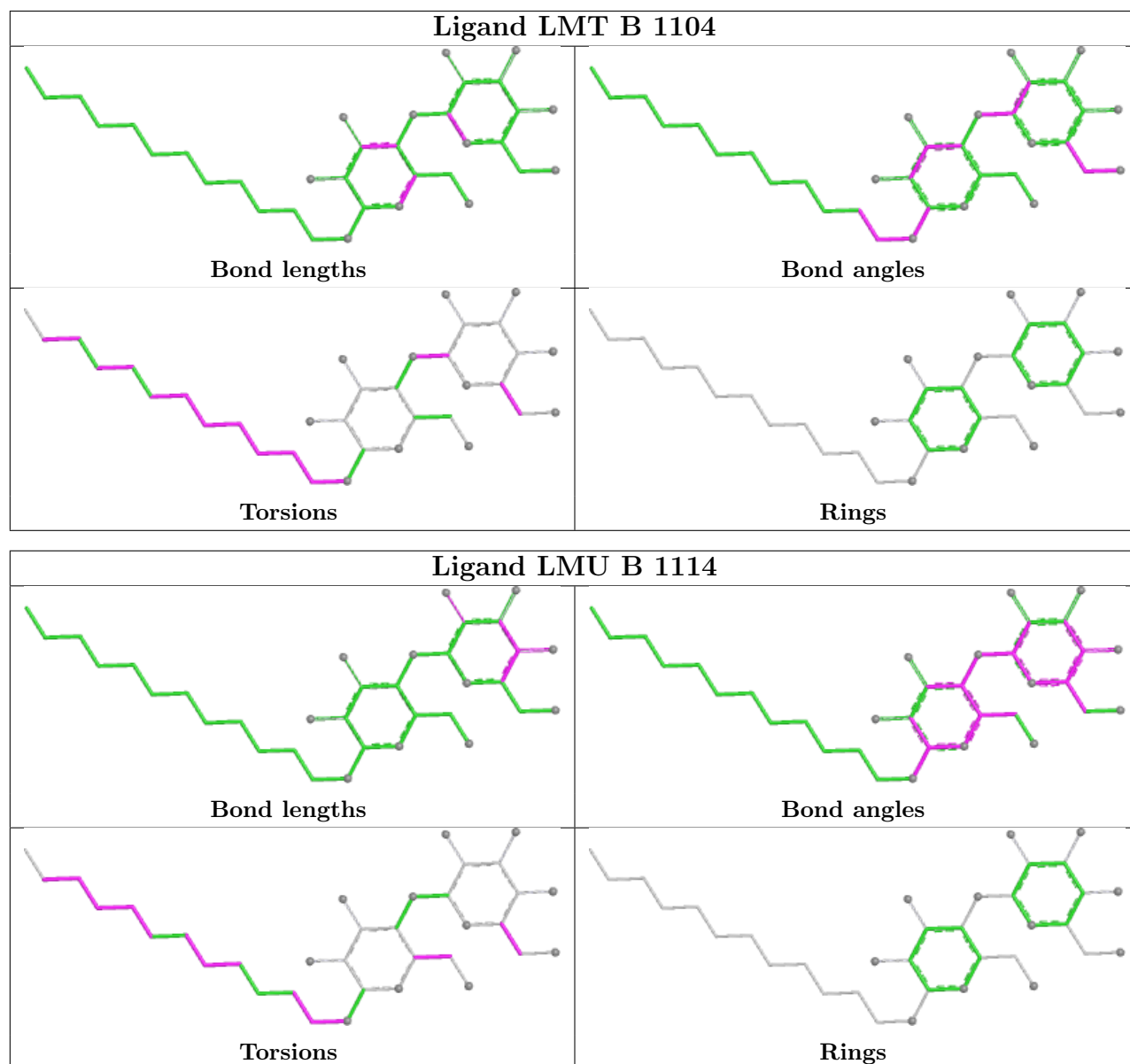
There are no ring outliers.

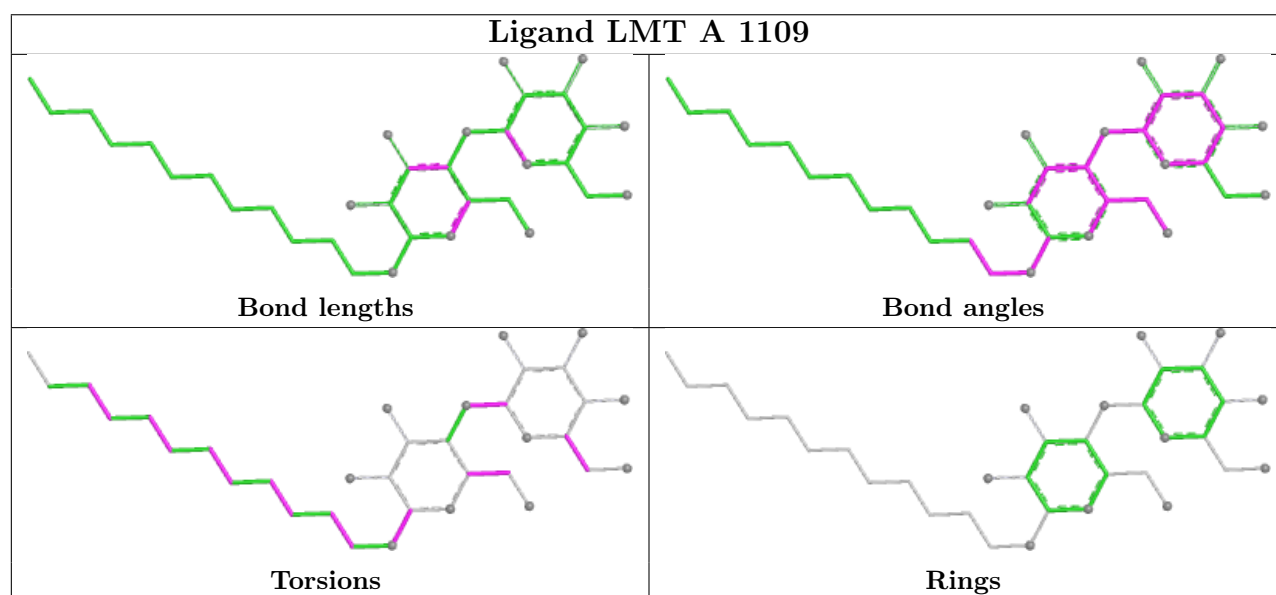
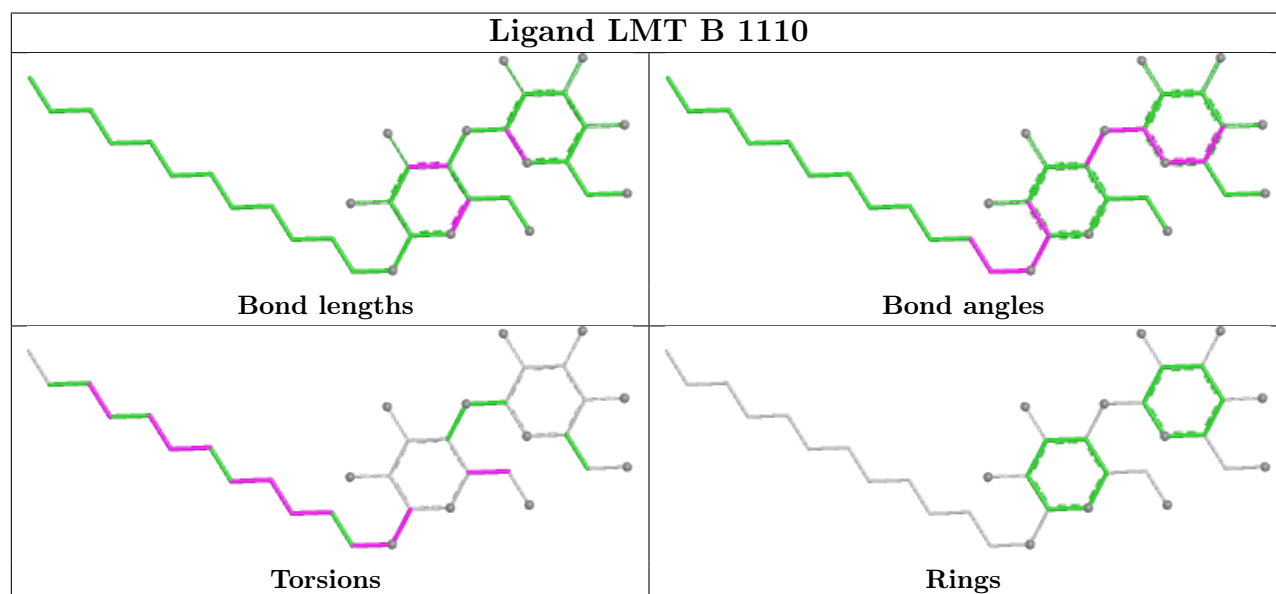
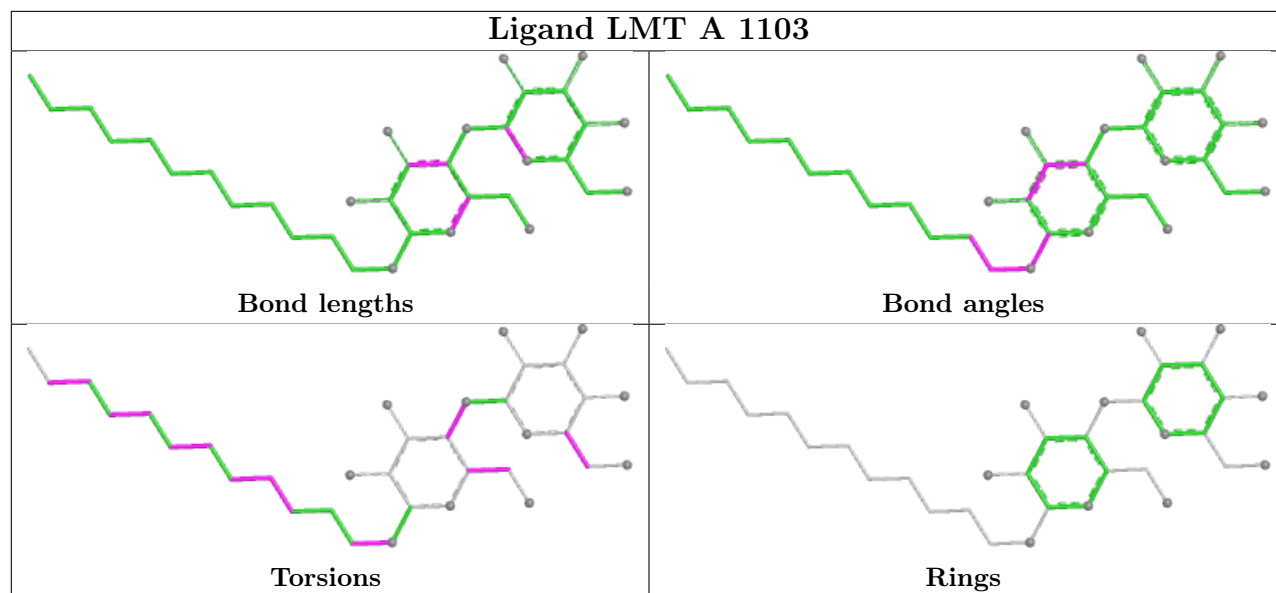
28 monomers are involved in 86 short contacts:

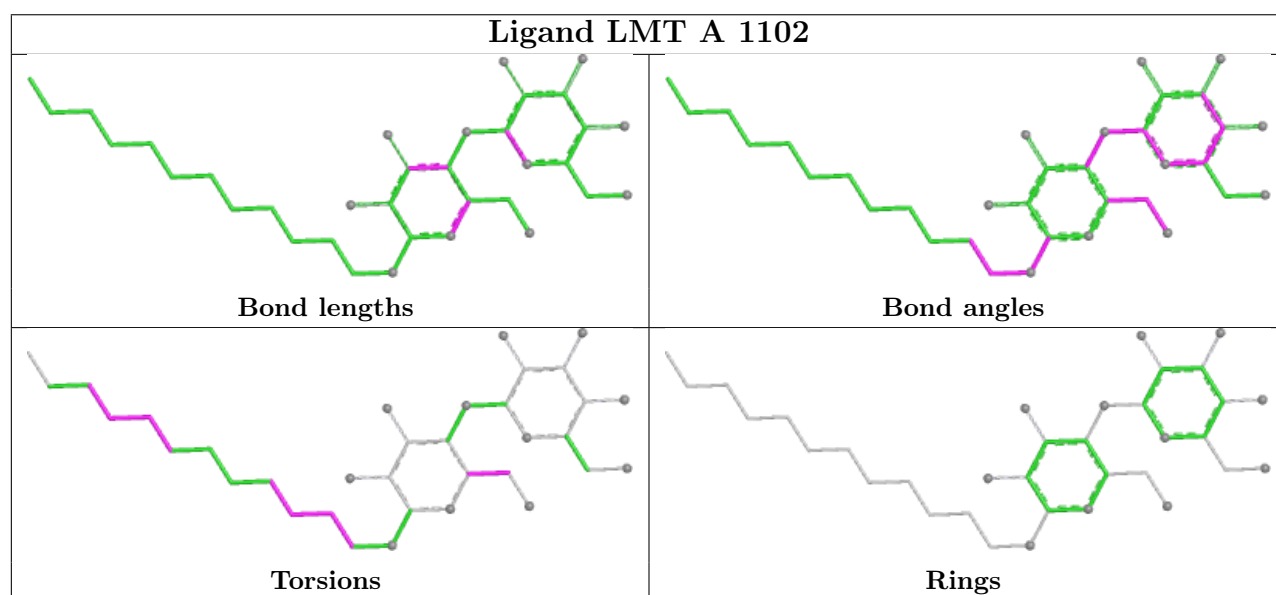
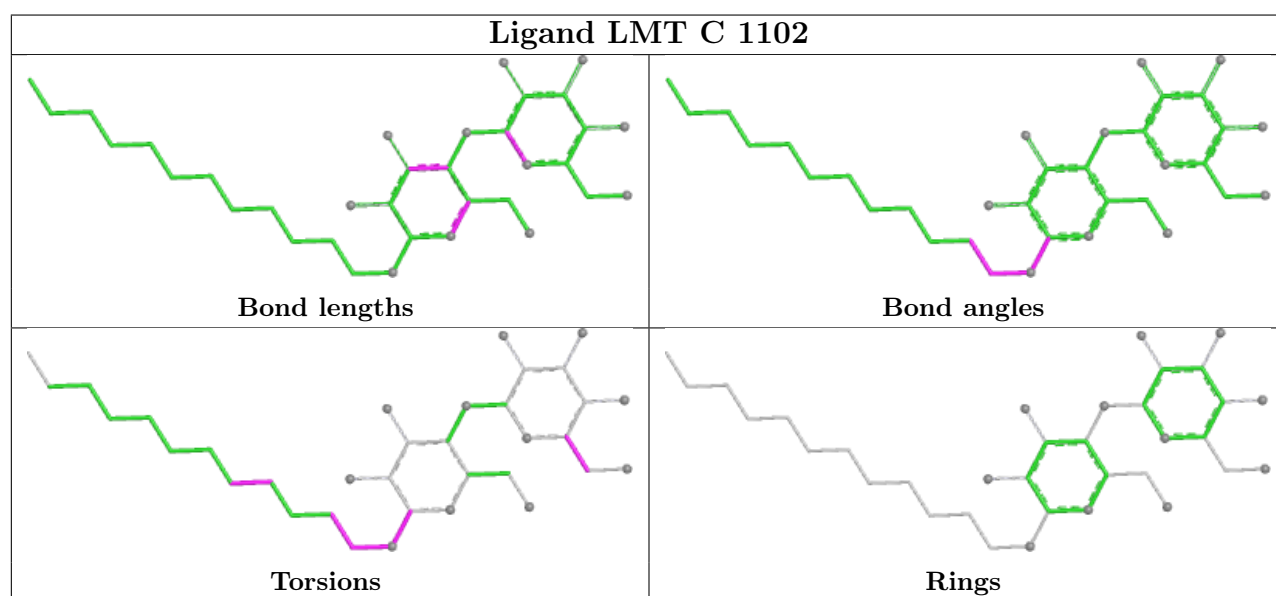
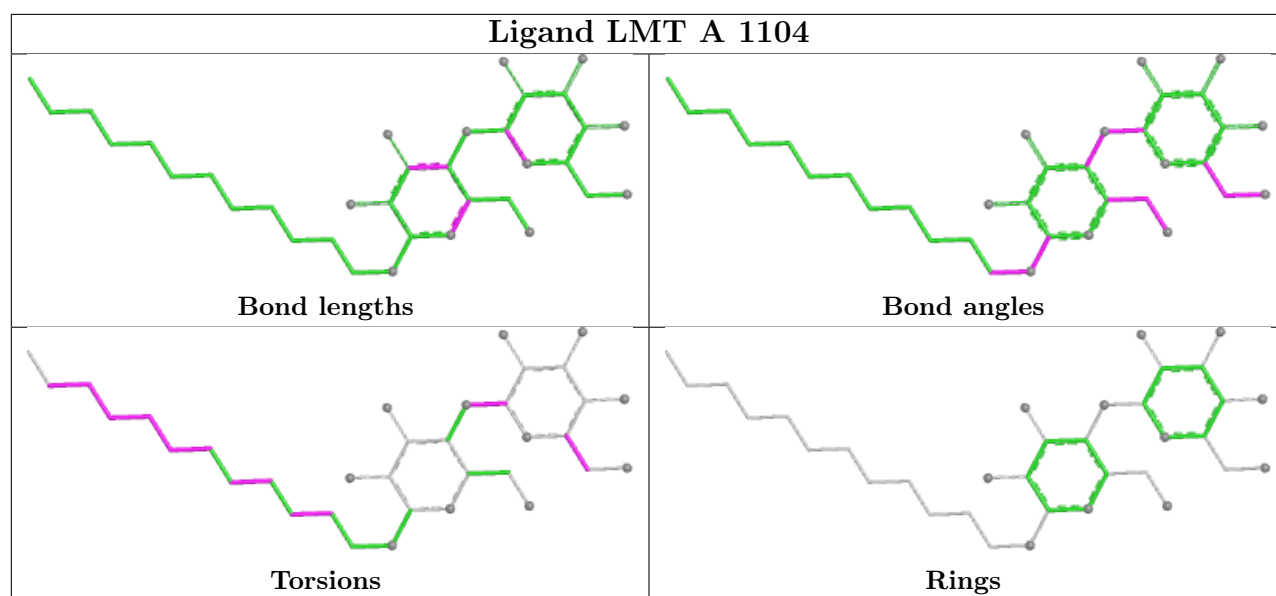
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	LMT	4	0
3	C	1117	GOL	1	0
8	C	1104	D12	1	0
3	B	1113	GOL	1	0
11	B	1114	LMU	3	0
3	B	1115	GOL	1	0
5	C	1103	OCT	1	0
6	A	1107	D10	1	0
4	A	1103	LMT	11	0
4	B	1110	LMT	9	0
8	B	1106	D12	1	0
3	B	1102	GOL	2	0
3	B	1101	GOL	2	0
3	D	202	GOL	1	0
3	E	201	GOL	1	0
4	A	1109	LMT	14	0
3	C	1115	GOL	3	0
4	A	1104	LMT	2	0
10	B	1109	C14	2	0
4	C	1102	LMT	1	0
3	A	1110	GOL	1	0
4	A	1102	LMT	6	0
4	B	1111	LMT	4	0
3	B	1116	GOL	5	0
8	A	1111	D12	8	0
9	B	1103	MIY	2	0
3	C	1101	GOL	1	0
6	B	1105	D10	1	0

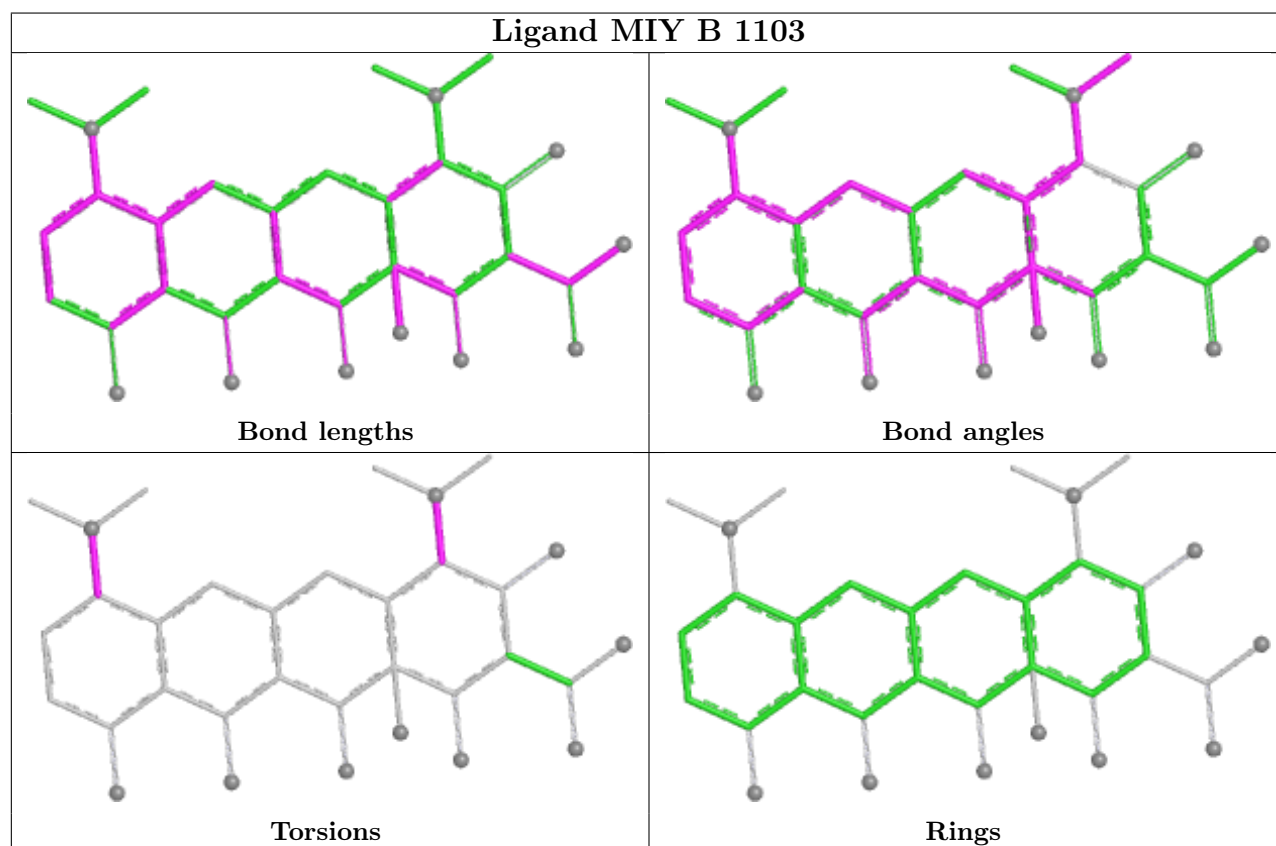
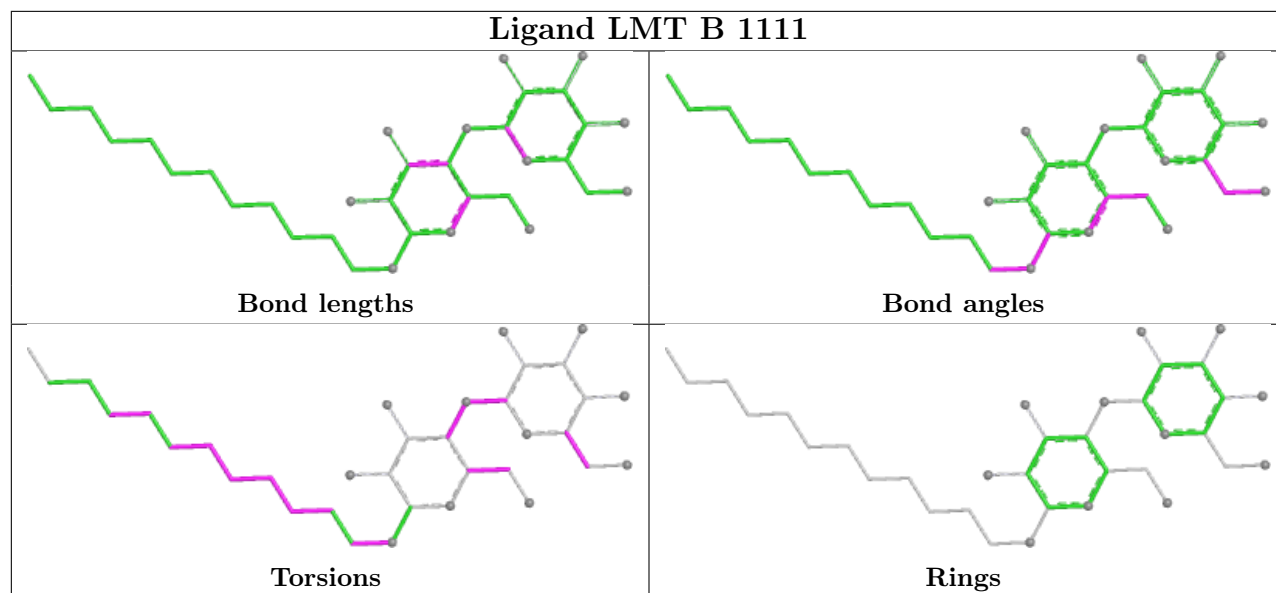
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 ⓘ

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%)	0.43	86 (8%) 17 18	17, 43, 87, 136	0
1	B	1033/1057 (97%)	0.32	56 (5%) 31 33	19, 41, 69, 133	0
1	C	1033/1057 (97%)	0.12	48 (4%) 37 40	20, 36, 61, 104	0
2	D	156/169 (92%)	0.20	8 (5%) 33 36	30, 39, 66, 110	0
2	E	152/169 (89%)	0.79	14 (9%) 14 15	34, 50, 83, 106	0
All	All	3418/3509 (97%)	0.31	212 (6%) 26 28	17, 40, 75, 136	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	677	ALA	10.6
2	D	11	GLY	7.6
1	A	617	PHE	7.6
1	C	617	PHE	7.3
1	B	678	THR	6.0
1	B	563	PHE	5.4
1	A	1040	ILE	5.4
1	C	672	VAL	5.3
1	A	672	VAL	5.3
1	A	674	LEU	5.2
1	B	877	TYR	5.1
2	D	12	SER	5.0
1	A	868	LEU	5.0
1	A	677	ALA	4.7
1	B	870	GLY	4.7
1	A	678	THR	4.6
1	C	618	ALA	4.6
1	A	1043	SER	4.5
1	A	436	GLY	4.5
1	B	871	ASN	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	811	TYR	4.4
1	C	1033	PHE	4.4
1	A	618	ALA	4.4
1	C	671	ILE	4.3
1	A	459	PHE	4.3
1	B	868	LEU	4.3
1	A	918	PHE	4.2
1	A	539	GLY	4.2
1	A	362	PHE	4.2
1	B	874	PRO	4.1
1	A	676	THR	4.1
1	B	660	ASP	3.9
1	A	668	LEU	3.9
1	A	518	ARG	3.9
1	A	956	GLU	3.9
2	E	33	LEU	3.8
1	C	670	ALA	3.7
1	C	510	LYS	3.6
1	A	1042	HIS	3.6
1	C	362	PHE	3.6
1	A	1035	ARG	3.6
1	B	676	THR	3.5
1	A	619	GLY	3.5
1	A	1044	HIS	3.5
1	C	951	ASP	3.5
1	B	674	LEU	3.4
1	A	865	GLN	3.3
2	D	13	ASP	3.3
2	E	15	GLY	3.3
1	B	873	ALA	3.3
1	B	386	PHE	3.3
1	A	463	THR	3.3
1	A	675	GLY	3.3
1	A	872	GLN	3.2
1	B	867	ARG	3.2
1	A	1036	LYS	3.2
1	B	134	SER	3.2
1	B	659	LYS	3.2
1	C	28	LEU	3.2
1	B	620	ARG	3.1
1	C	676	THR	3.1
1	B	133	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	511	GLY	3.1
2	E	164	ILE	3.1
1	A	955	LYS	3.1
1	A	662	MET	3.1
1	C	954	ASP	3.0
1	A	542	LEU	3.0
1	A	460	GLY	3.0
1	B	671	ILE	3.0
1	C	918	PHE	3.0
1	A	833	PRO	3.0
1	B	872	GLN	2.9
1	C	955	LYS	2.9
1	B	617	PHE	2.9
1	A	836	SER	2.9
1	A	425	LEU	2.9
1	A	538	THR	2.9
1	B	635	ALA	2.9
1	B	244	GLU	2.9
1	B	255	GLN	2.8
1	B	618	ALA	2.8
1	B	628	PHE	2.8
1	B	633	ASP	2.8
1	A	1033	PHE	2.8
1	A	867	ARG	2.8
1	A	510	LYS	2.8
1	C	361	ASN	2.8
1	A	526	HIS	2.8
1	C	497	LEU	2.8
1	A	961	ILE	2.7
1	C	494	ALA	2.7
2	E	35	ALA	2.7
1	B	918	PHE	2.7
1	A	980	LEU	2.7
1	A	38	ILE	2.7
1	B	510	LYS	2.7
1	A	515	TRP	2.7
1	C	71	GLY	2.7
1	B	672	VAL	2.7
1	A	712	MET	2.6
1	C	259	ARG	2.6
1	A	697	GLN	2.6
1	A	922	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	877	TYR	2.6
1	C	674	LEU	2.6
1	C	620	ARG	2.6
1	A	464	GLY	2.6
1	C	957	GLY	2.6
1	A	866	GLU	2.6
1	B	993	THR	2.6
1	A	895	TRP	2.6
1	B	662	MET	2.6
2	E	34	MET	2.6
1	A	671	ILE	2.6
1	C	498	LYS	2.6
1	C	429	GLU	2.5
1	B	600	THR	2.5
1	A	422	GLU	2.5
1	B	136	PHE	2.5
1	B	459	PHE	2.5
1	C	503	GLY	2.5
1	A	361	ASN	2.5
1	A	498	LYS	2.5
1	A	835	LYS	2.5
1	C	124	GLN	2.5
1	A	670	ALA	2.5
1	C	146	ASP	2.5
1	B	638	PRO	2.5
2	E	31	ARG	2.4
1	A	876	LEU	2.4
1	B	332	PHE	2.4
1	C	21	LEU	2.4
1	A	669	PRO	2.4
2	D	154	ILE	2.4
1	C	853	THR	2.4
1	A	874	PRO	2.4
1	C	737	GLN	2.4
1	A	1039	ASP	2.3
1	B	28	LEU	2.3
2	D	166	GLN	2.3
2	E	166	GLN	2.3
1	C	743	ILE	2.3
1	C	575	MET	2.3
1	A	71	GLY	2.3
1	B	561	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	258	SER	2.3
1	A	1038	GLU	2.3
1	A	993	THR	2.3
2	E	36	ASN	2.3
1	C	29	LYS	2.3
1	A	483	LEU	2.3
1	B	230	LEU	2.3
1	B	508	GLY	2.3
1	A	1016	VAL	2.3
1	A	359	LEU	2.3
1	A	386	PHE	2.2
1	A	501	ALA	2.2
1	A	556	PHE	2.2
2	E	37	GLY	2.2
2	E	163	GLU	2.2
1	B	875	SER	2.2
1	B	601	LYS	2.2
1	A	544	LEU	2.2
1	C	675	GLY	2.2
2	D	164	ILE	2.2
1	C	952	LEU	2.2
1	A	616	GLY	2.2
1	C	116	PRO	2.2
1	C	871	ASN	2.2
1	B	549	VAL	2.2
2	E	45	VAL	2.2
1	B	463	THR	2.2
1	B	135	SER	2.2
1	A	960	LEU	2.2
1	B	668	LEU	2.2
2	D	14	LEU	2.2
1	C	114	ALA	2.2
1	B	1033	PHE	2.1
1	B	991	ILE	2.1
1	A	37	THR	2.1
1	C	508	GLY	2.1
1	C	619	GLY	2.1
1	B	366	LEU	2.1
2	E	66	LEU	2.1
1	A	657	GLN	2.1
1	B	657	GLN	2.1
1	A	541	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	27	ILE	2.1
1	B	634	TRP	2.1
1	B	869	SER	2.1
1	A	536	ARG	2.1
1	B	557	VAL	2.1
1	A	680	PHE	2.1
1	A	356	TYR	2.1
1	A	438	ILE	2.1
1	C	152	GLU	2.1
1	C	659	LYS	2.1
1	A	871	ASN	2.1
1	A	21	LEU	2.1
1	A	873	ALA	2.1
1	C	501	ALA	2.1
1	C	673	GLU	2.0
2	E	32	ILE	2.0
1	A	914	LEU	2.0
1	A	352	PHE	2.0
1	A	514	GLY	2.0
1	A	920	GLY	2.0
1	C	148	THR	2.0
2	D	15	GLY	2.0
2	E	70	GLY	2.0
1	B	597	TYR	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	1107	10/10	0.49	0.28	75,92,106,108	0
5	OCT	C	1106	8/8	0.60	0.28	73,88,101,101	0
8	D12	B	1106	12/12	0.61	0.24	74,92,108,109	0
5	OCT	C	1112	8/8	0.64	0.24	79,97,102,103	0
6	D10	C	1107	10/10	0.66	0.25	72,92,96,99	0
5	OCT	A	1105	8/8	0.66	0.19	73,89,93,94	0
6	D10	C	1109	10/10	0.67	0.23	73,90,102,102	0
8	D12	C	1104	12/12	0.67	0.23	68,85,98,99	0
7	HEX	B	1112	6/6	0.68	0.24	79,96,103,103	0
6	D10	C	1120	10/10	0.69	0.27	72,94,116,116	0
10	C14	B	1109	14/14	0.71	0.22	70,87,106,109	0
4	LMT	B	1111	35/35	0.73	0.24	78,120,130,131	0
7	HEX	C	1113	6/6	0.74	0.29	71,89,105,105	0
8	D12	C	1108	12/12	0.74	0.17	40,63,90,90	0
6	D10	B	1107	10/10	0.74	0.26	64,94,113,113	0
3	GOL	C	1117	6/6	0.76	0.23	41,53,58,61	0
14	UND	C	1119	11/11	0.76	0.20	64,98,118,118	0
4	LMT	B	1110	35/35	0.77	0.22	65,121,126,129	0
7	HEX	C	1110	6/6	0.77	0.22	77,93,98,98	0
4	LMT	A	1109	35/35	0.77	0.19	70,95,104,105	0
11	LMU	B	1114	35/35	0.77	0.16	76,100,115,118	0
7	HEX	B	1108	6/6	0.77	0.19	66,79,87,87	0
6	D10	B	1105	10/10	0.78	0.18	69,85,88,88	0
7	HEX	A	1108	6/6	0.78	0.35	89,110,112,112	0
12	DD9	C	1111	9/9	0.78	0.25	56,80,98,101	0
5	OCT	A	1106	8/8	0.78	0.17	66,82,86,86	0
4	LMT	A	1103	35/35	0.79	0.16	68,88,105,106	0
3	GOL	C	1114	6/6	0.80	0.21	59,67,69,70	0
8	D12	A	1111	12/12	0.80	0.20	53,73,98,98	0
3	GOL	B	1116	6/6	0.80	0.23	67,75,82,87	0
5	OCT	C	1103	8/8	0.81	0.18	65,80,84,86	0
3	GOL	D	202	6/6	0.83	0.19	53,69,83,88	0
9	MIY	B	1103	33/33	0.83	0.14	52,74,112,116	0
3	GOL	B	1117	6/6	0.84	0.24	55,55,64,75	0
5	OCT	C	1105	8/8	0.84	0.23	67,83,101,105	0
3	GOL	C	1101	6/6	0.85	0.20	50,57,69,74	0
5	OCT	C	1116	8/8	0.85	0.19	61,75,84,85	0
3	GOL	B	1115	6/6	0.86	0.22	56,68,71,72	0
4	LMT	B	1104	35/35	0.87	0.17	53,68,98,99	0
3	GOL	B	1101	6/6	0.87	0.16	34,41,52,58	0
4	LMT	A	1104	35/35	0.88	0.14	51,74,104,108	0
3	GOL	A	1101	6/6	0.88	0.15	38,47,54,58	0
3	GOL	E	201	6/6	0.88	0.16	56,59,64,68	0

Continued on next page...

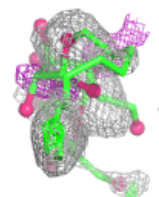
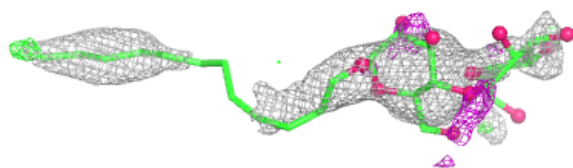
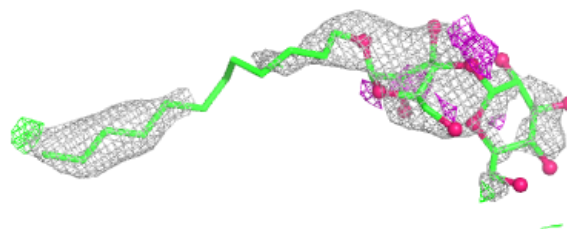
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1113	6/6	0.88	0.16	56,64,67,68	0
3	GOL	C	1115	6/6	0.89	0.17	30,39,51,52	0
3	GOL	D	201	6/6	0.89	0.15	55,60,64,71	0
4	LMT	A	1102	35/35	0.89	0.13	50,71,95,101	0
3	GOL	B	1102	6/6	0.90	0.15	40,58,64,69	0
4	LMT	C	1102	35/35	0.91	0.13	50,64,79,80	0
3	GOL	A	1110	6/6	0.96	0.10	28,40,54,56	0
13	SO4	C	1118	5/5	0.97	0.05	62,67,76,78	0

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

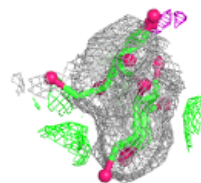
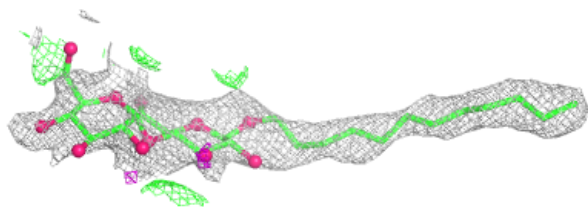
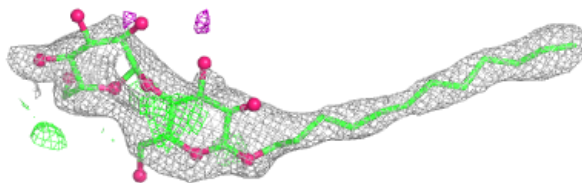
Electron density around LMT B 1111:

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

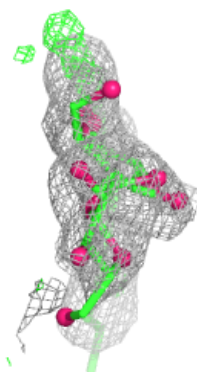
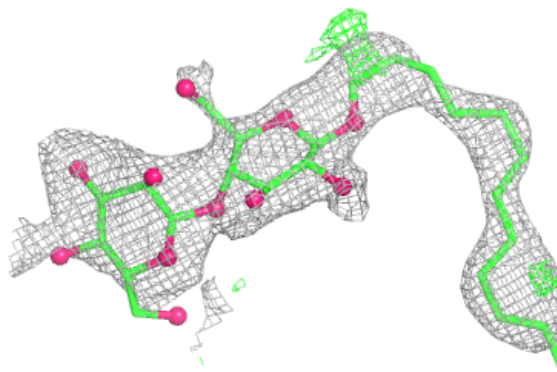


Electron density around LMT B 1110:

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

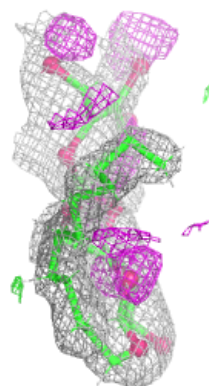
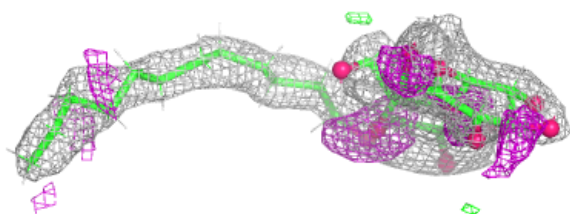
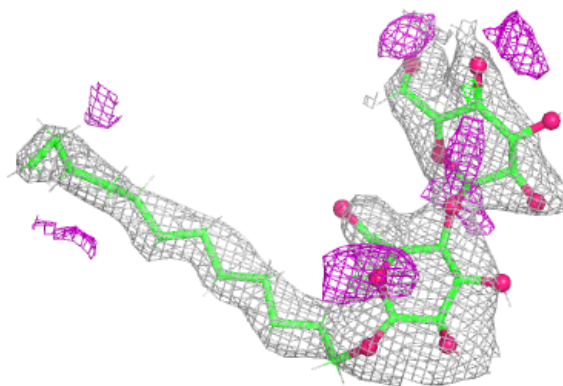
**Electron density around LMT A 1109:**

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

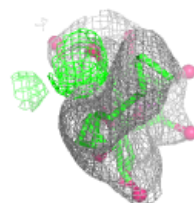
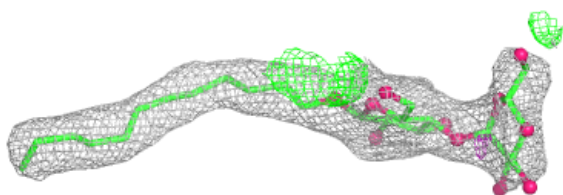
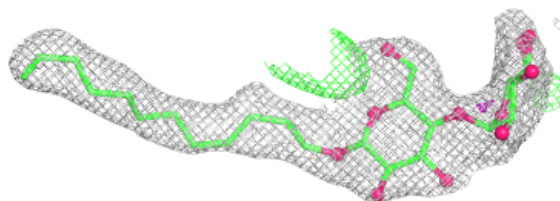


Electron density around LMU B 1114:

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

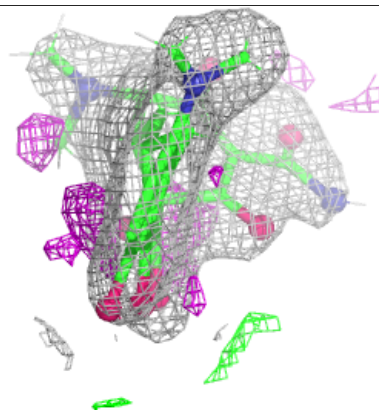
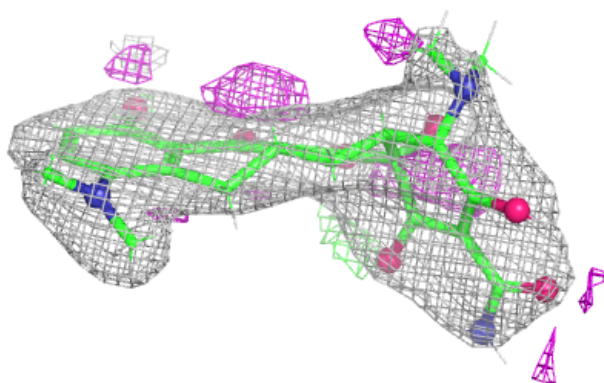
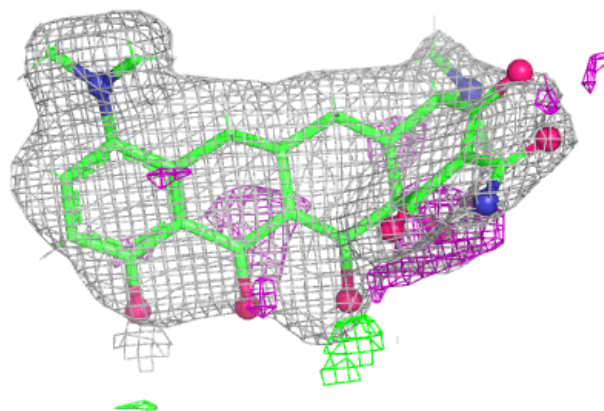
**Electron density around LMT A 1103:**

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

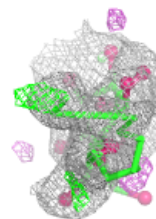
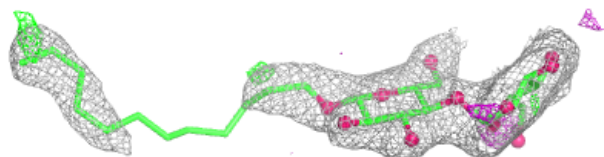
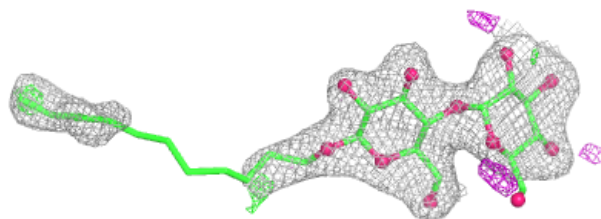


Electron density around MIY B 1103:

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

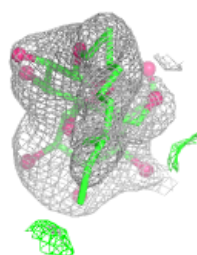
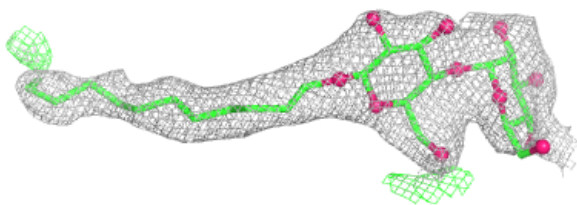
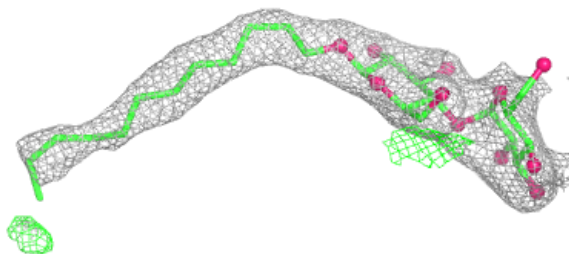
**Electron density around LMT B 1104:**

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

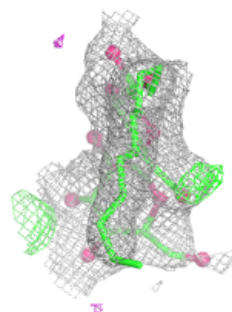
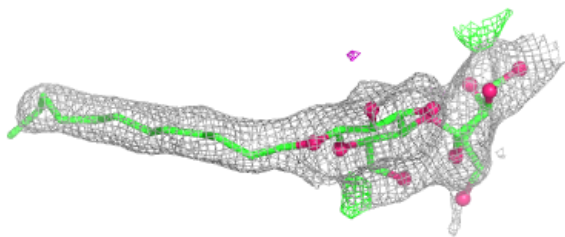
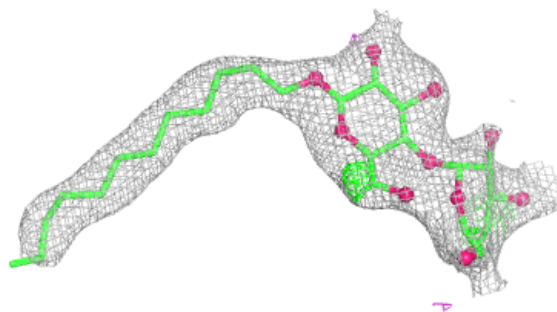


Electron density around LMT A 1104:

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

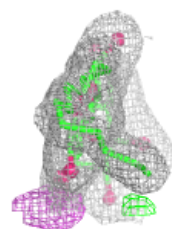
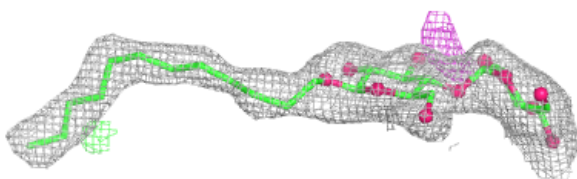
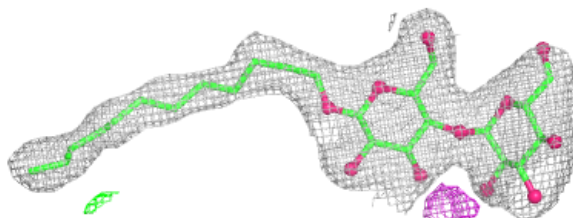
**Electron density around LMT A 1102:**

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



Electron density around LMT C 1102:

$2mF_o-DF_c$ (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.