



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 10, 2025 – 12:18 pm GMT

PDB ID : 9HCI / pdb\_00009hci  
Title : structure of the double Cys-substituted cross-linked AcrB variant  
S562C\_T837C  
Authors : Brandstaetter, L.; Mueller, R.T.; Pos, K.M.  
Deposited on : 2024-11-10  
Resolution : 2.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

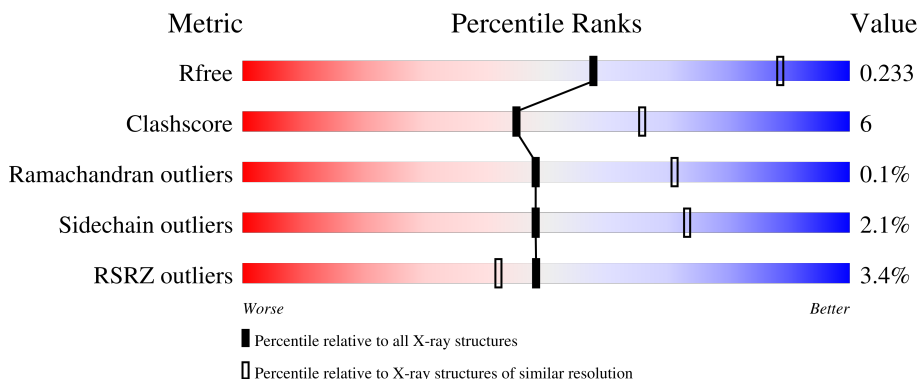
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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  $\geq 3$ , 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	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	1057	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	1057	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
2	D	169	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
2	E	169	<div> <div>%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	D10	C	1117	-	-	-	X

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27769 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7942	5105	1315	1476	46			
1	B	1033	Total	C	N	O	S	0	1	0
			7856	5056	1296	1457	47			
1	C	1033	Total	C	N	O	S	0	0	0
			7848	5051	1295	1456	46			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	562	CYS	SER	engineered mutation	UNP P31224
A	837	CYS	THR	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	562	CYS	SER	engineered mutation	UNP P31224
B	837	CYS	THR	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	562	CYS	SER	engineered mutation	UNP P31224
C	837	CYS	THR	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224

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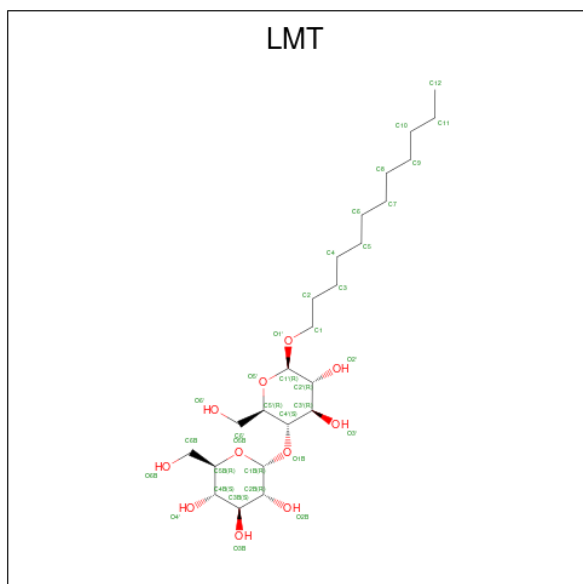
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Chain	Residue	Modelled	Actual	Comment	Reference
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	155	Total	C	N	O	S	0	0	0
			1173	739	205	228	1			
2	E	153	Total	C	N	O	S	0	0	0
			1159	732	203	223	1			

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



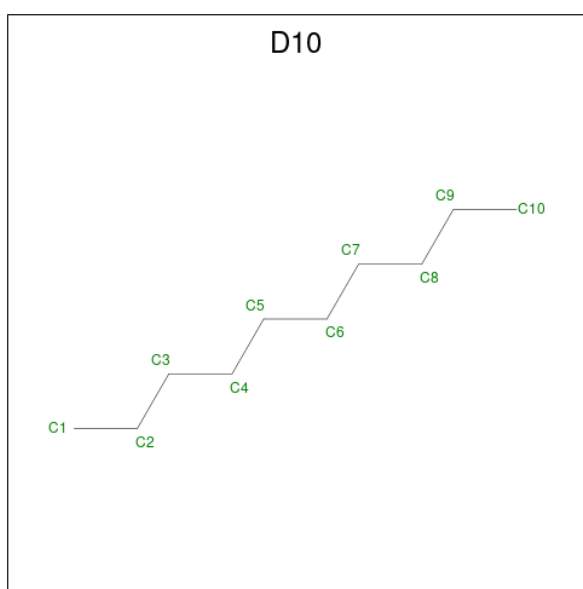
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		
3	A	1	Total	C	O	0	0
			35	24	11		

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

- Molecule 4 is DECANE (CCD ID: D10) (formula:  $C_{10}H_{22}$ ).



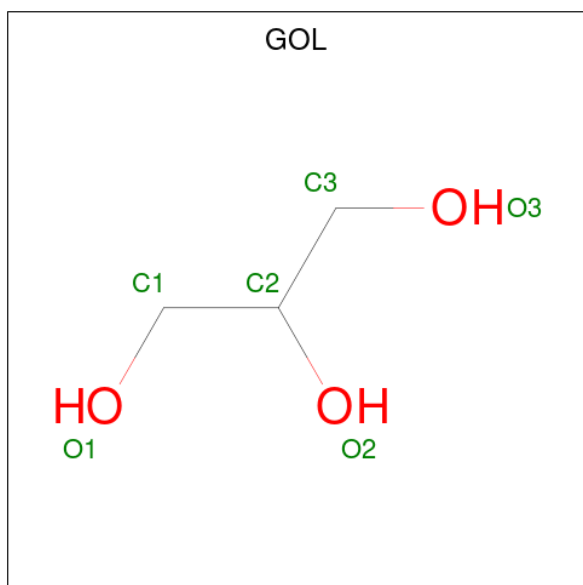
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	B	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		
4	C	1	Total	C	0	0
			10	10		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C 10 10	0	0
4	C	1	Total C 10 10	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



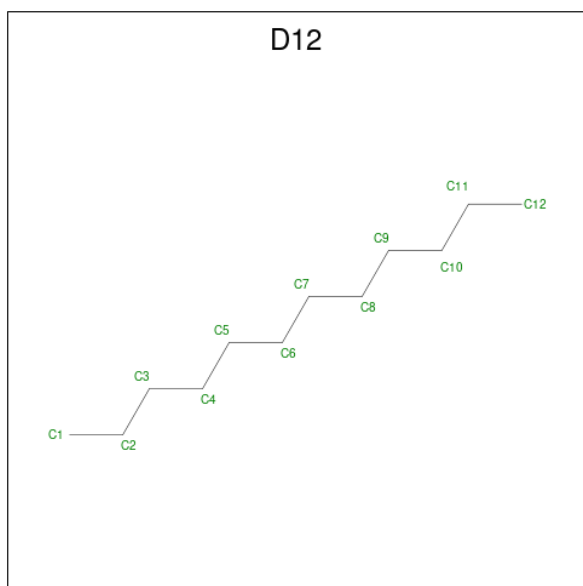
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

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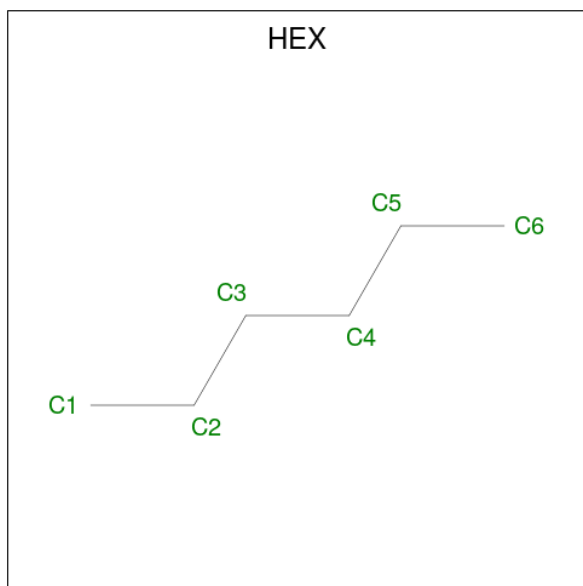
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DODECANE (CCD ID: D12) (formula:  $C_{12}H_{26}$ ).



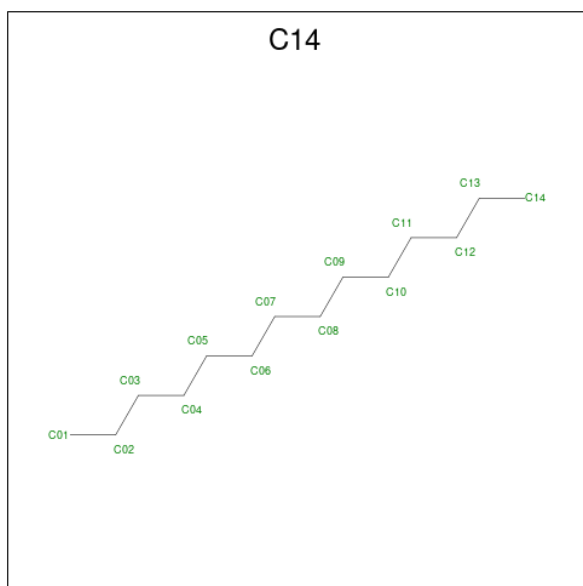
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	C	0	0
			12	12		
6	B	1	Total	C	0	0
			12	12		
6	C	1	Total	C	0	0
			12	12		
6	C	1	Total	C	0	0
			12	12		

- Molecule 7 is HEXANE (CCD ID: HEX) (formula:  $C_6H_{14}$ ).



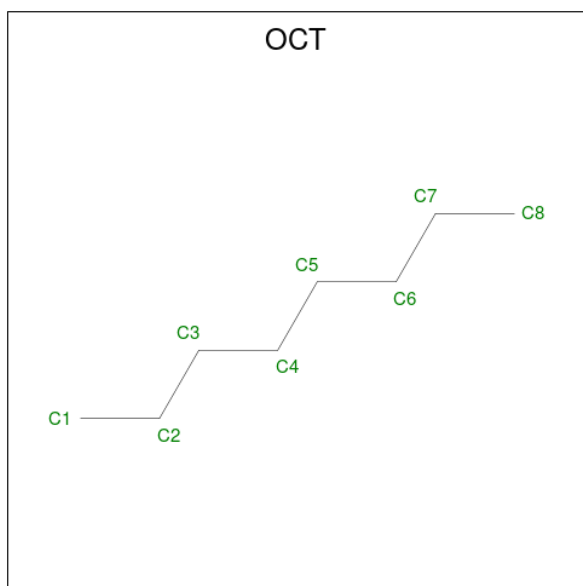
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0
7	C	1	Total C 6 6	0	0

- Molecule 8 is TETRADECANE (CCD ID: C14) (formula:  $C_{14}H_{30}$ ).



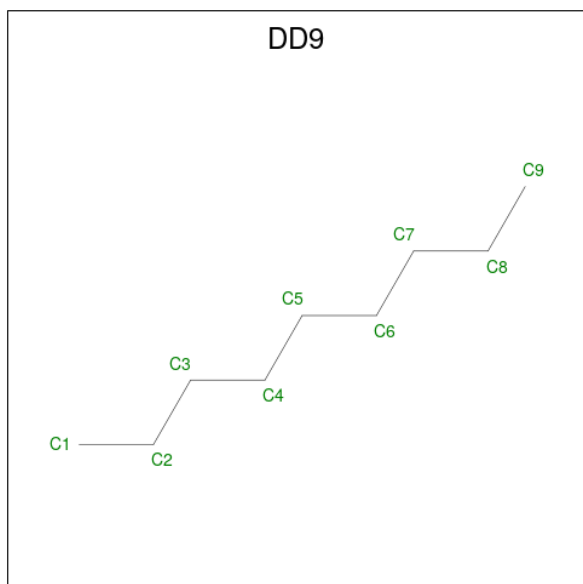
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C 14 14	0	0

- Molecule 9 is N-OCTANE (CCD ID: OCT) (formula:  $C_8H_{18}$ ).



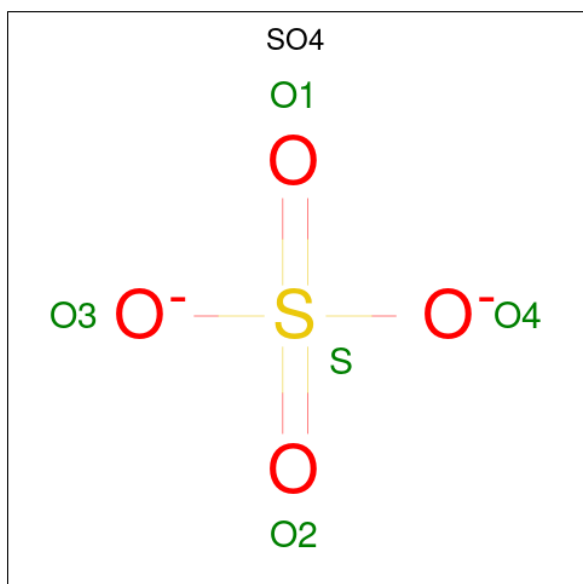
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C 8 8	0	0
9	C	1	Total C 8 8	0	0

- Molecule 10 is nonane (CCD ID: DD9) (formula:  $C_9H_{20}$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total C 9 9	0	0

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	434	Total O 434 434	0	0
12	B	288	Total O 288 288	0	0
12	C	389	Total O 389 389	0	0
12	D	53	Total O 53 53	0	0
12	E	51	Total O 51 51	0	0

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.

[illegible]

Chain B:

4% 85% 12% ..

L492	L497	L498	K510	S530	L546	Y554	R558	L559	C562	F563	L564	P565	D568	V571	M575	A580	T583	K589	T595	H596	Y597	V609	F610	F615	G616	F617	R620	G621	T624	I626	S630	D633	W634	A635	S644						
P331	K334	V340	L343	L359	K361	R362	R363	L367	P368	K391	T392	L393	T394	K395	L400	A401	L402	V412	V413	E414	R415	V416	E417	E423	P426	P427	K428	E429	A430	T431	R432	K433	S434	M435	V448	M456	G464	Y467	R469	A485	T489
W1	K29	I38	A47	M68	M69	N70	N81	S82	D83	V88	K110	M115	P116	G126	S133	S134	S135	I143	D146	R185	L219	P223	R239	E244	G247	K252	V253	K254	Q255	I268	A303	E314	P315	D328	T329	T330					



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.71Å 165.30Å 244.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.69 – 2.60 47.69 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.69-2.60) 100.0 (47.69-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.61Å)	Xtriage
Refinement program	PDB-REDO 8.11	Depositor
R, $R_{free}$	0.190 , 0.230 0.197 , 0.233	Depositor DCC
$R_{free}$ test set	9291 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.905	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	27769	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D12, GOL, DD9, SO4, D10, HEX, OCT, C14, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.70	3/8094 (0.0%)	0.93	5/10989 (0.0%)
1	B	0.69	3/8006 (0.0%)	0.94	9/10871 (0.1%)
1	C	0.69	3/7998 (0.0%)	0.91	3/10861 (0.0%)
2	D	0.69	1/1192 (0.1%)	0.93	1/1621 (0.1%)
2	E	0.64	0/1178	0.96	1/1602 (0.1%)
All	All	0.69	10/26468 (0.0%)	0.93	19/35944 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	6
1	C	0	5
2	D	0	1
All	All	0	17

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	34	MET	SD-CE	-9.91	1.54	1.79
1	A	552	MET	SD-CE	-8.35	1.58	1.79
1	C	420	MET	SD-CE	-8.28	1.58	1.79
1	B	435	MET	SD-CE	-7.93	1.59	1.79
1	A	445	ILE	CG1-CD1	-6.18	1.27	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	ASN	CA-CB-CG	-7.26	105.34	112.60
1	C	83	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	244	GLU	CB-CG-CD	5.85	122.54	112.60
2	E	110	ASP	CA-CB-CG	5.84	118.44	112.60
1	B	610	PHE	CA-CB-CG	5.78	119.58	113.80

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	468	ARG	Sidechain
1	A	620	ARG	Sidechain
1	A	699	ARG	Sidechain
1	A	8	ARG	Sidechain
1	A	957	GLY	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7942	0	8080	121	0
1	B	7856	0	8007	91	0
1	C	7848	0	7999	85	0
2	D	1173	0	1156	9	0
2	E	1159	0	1147	9	0
3	A	175	0	230	9	0
3	B	70	0	92	3	0
3	C	35	0	46	0	0
4	A	10	0	22	0	0
4	B	40	0	88	0	0
4	C	40	0	88	0	0
5	A	12	0	16	1	0
5	B	48	0	64	0	0
5	C	18	0	24	2	0
5	D	18	0	24	0	0
6	A	12	0	26	0	0
6	B	12	0	26	0	0
6	C	24	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	6	0	14	0	0
7	C	12	0	28	0	0
8	C	14	0	30	0	0
9	C	16	0	36	0	0
10	C	9	0	20	0	0
11	C	5	0	0	0	0
12	A	434	0	0	12	0
12	B	288	0	0	7	0
12	C	389	0	0	4	0
12	D	53	0	0	1	0
12	E	51	0	0	0	0
All	All	27769	0	27315	311	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 6.

The worst 5 of 311 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:343:THR:HG21	1:A:989:LEU:CD1	1.74	1.17
1:A:580:ALA:HB1	1:A:724:THR:HG22	1.30	1.13
1:A:580:ALA:CB	1:A:724:THR:HG22	2.00	0.90
1:C:146:ASP:OD1	1:C:148:THR:HG23	1.73	0.88
1:A:445:ILE:CD1	1:A:943:ILE:HG21	2.04	0.87

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%)	1024 (98%)	16 (2%)	2 (0%)	44 66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1032/1057 (98%)	1011 (98%)	21 (2%)	0	100	100
1	C	1031/1057 (98%)	1009 (98%)	22 (2%)	0	100	100
2	D	153/169 (90%)	152 (99%)	1 (1%)	0	100	100
2	E	151/169 (89%)	149 (99%)	2 (1%)	0	100	100
All	All	3409/3509 (97%)	3345 (98%)	62 (2%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1034	SER
1	A	1036	LYS

### 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%)	827 (97%)	23 (3%)	40	66
1	B	840/863 (97%)	821 (98%)	19 (2%)	45	71
1	C	839/863 (97%)	827 (99%)	12 (1%)	62	82
2	D	120/132 (91%)	118 (98%)	2 (2%)	56	78
2	E	118/132 (89%)	117 (99%)	1 (1%)	79	91
All	All	2767/2853 (97%)	2710 (98%)	57 (2%)	48	73

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	530	SER
2	D	61	GLU
1	B	673	GLU
2	D	53	LEU
1	C	481	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	104	GLN
1	C	274	ASN
2	E	92	HIS
1	C	108	GLN
1	C	197	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

45 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	D10	C	1117	-	9,9,9	0.50	0	8,8,8	0.54	0
7	HEX	B	1113	-	5,5,5	0.62	0	4,4,4	0.25	0
6	D12	A	1107	-	11,11,11	0.53	0	10,10,10	0.39	0
6	D12	C	1108	-	11,11,11	0.68	0	10,10,10	0.23	0
3	LMT	B	1109	-	36,36,36	0.41	0	47,47,47	0.67	0
5	GOL	B	1115	-	5,5,5	0.08	0	5,5,5	0.22	0
5	GOL	A	1108	-	5,5,5	0.10	0	5,5,5	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	1104	-	5,5,5	0.08	0	5,5,5	0.29	0
9	OCT	C	1106	-	7,7,7	0.36	0	6,6,6	0.82	0
4	D10	B	1103	-	9,9,9	0.72	0	8,8,8	0.39	0
10	DD9	C	1111	-	8,8,8	0.48	0	7,7,7	0.56	0
5	GOL	D	201	-	5,5,5	0.12	0	5,5,5	0.39	0
3	LMT	A	1103	-	36,36,36	0.28	0	47,47,47	0.59	0
3	LMT	A	1102	-	36,36,36	0.26	0	47,47,47	0.49	0
5	GOL	D	202	-	5,5,5	0.08	0	5,5,5	0.23	0
9	OCT	C	1104	-	7,7,7	0.73	0	6,6,6	0.70	0
4	D10	A	1104	-	9,9,9	0.58	0	8,8,8	0.43	0
4	D10	C	1116	-	9,9,9	0.60	0	8,8,8	0.51	0
5	GOL	B	1102	-	5,5,5	0.14	0	5,5,5	0.31	0
5	GOL	B	1106	-	5,5,5	0.08	0	5,5,5	0.18	0
3	LMT	A	1101	-	36,36,36	0.33	0	47,47,47	0.53	0
7	HEX	C	1112	-	5,5,5	0.49	0	4,4,4	0.26	0
5	GOL	B	1101	-	5,5,5	0.11	0	5,5,5	0.28	0
3	LMT	A	1109	-	36,36,36	0.25	0	47,47,47	0.72	1 (2%)
5	GOL	C	1114	-	5,5,5	0.16	0	5,5,5	0.53	0
5	GOL	C	1113	-	5,5,5	0.10	0	5,5,5	0.27	0
5	GOL	D	203	-	5,5,5	0.12	0	5,5,5	0.39	0
8	C14	C	1101	-	13,13,13	0.51	0	12,12,12	0.51	0
5	GOL	B	1107	-	5,5,5	0.19	0	5,5,5	0.61	0
4	D10	C	1109	-	9,9,9	0.59	0	8,8,8	0.30	0
3	LMT	C	1103	-	36,36,36	0.42	0	47,47,47	0.53	0
4	D10	C	1107	-	9,9,9	0.55	0	8,8,8	0.48	0
4	D10	B	1105	-	9,9,9	0.57	0	8,8,8	0.18	0
7	HEX	C	1110	-	5,5,5	0.50	0	4,4,4	0.34	0
4	D10	B	1110	-	9,9,9	0.48	0	8,8,8	0.57	0
5	GOL	A	1106	-	5,5,5	0.13	0	5,5,5	0.26	0
5	GOL	B	1108	-	5,5,5	0.09	0	5,5,5	0.32	0
5	GOL	C	1102	-	5,5,5	0.18	0	5,5,5	0.69	0
6	D12	C	1105	-	11,11,11	0.59	0	10,10,10	0.52	0
11	SO4	C	1115	-	4,4,4	0.36	0	6,6,6	0.07	0
5	GOL	B	1116	-	5,5,5	0.15	0	5,5,5	0.35	0
3	LMT	A	1105	-	36,36,36	0.43	0	47,47,47	0.80	1 (2%)
3	LMT	B	1114	-	36,36,36	0.26	0	47,47,47	0.79	2 (4%)
4	D10	B	1112	-	9,9,9	0.61	0	8,8,8	0.42	0
6	D12	B	1111	-	11,11,11	0.69	0	10,10,10	0.23	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	D10	C	1117	-	-	3/7/7/7	-
7	HEX	B	1113	-	-	0/3/3/3	-
6	D12	A	1107	-	-	5/9/9/9	-
6	D12	C	1108	-	-	2/9/9/9	-
3	LMT	B	1109	-	-	10/21/61/61	0/2/2/2
5	GOL	B	1115	-	-	2/4/4/4	-
5	GOL	A	1108	-	-	2/4/4/4	-
5	GOL	B	1104	-	-	1/4/4/4	-
9	OCT	C	1106	-	-	1/5/5/5	-
4	D10	B	1103	-	-	2/7/7/7	-
10	DD9	C	1111	-	-	3/6/6/6	-
5	GOL	D	201	-	-	0/4/4/4	-
3	LMT	A	1103	-	-	11/21/61/61	0/2/2/2
3	LMT	A	1102	-	-	6/21/61/61	0/2/2/2
5	GOL	D	202	-	-	0/4/4/4	-
9	OCT	C	1104	-	-	0/5/5/5	-
4	D10	A	1104	-	-	2/7/7/7	-
4	D10	C	1116	-	-	0/7/7/7	-
5	GOL	B	1102	-	-	2/4/4/4	-
5	GOL	B	1106	-	-	2/4/4/4	-
3	LMT	A	1101	-	-	6/21/61/61	0/2/2/2
7	HEX	C	1112	-	-	3/3/3/3	-
5	GOL	B	1101	-	-	2/4/4/4	-
3	LMT	A	1109	-	-	11/21/61/61	0/2/2/2
5	GOL	C	1114	-	-	4/4/4/4	-
5	GOL	C	1113	-	-	2/4/4/4	-
5	GOL	D	203	-	-	0/4/4/4	-
8	C14	C	1101	-	-	3/11/11/11	-
5	GOL	B	1107	-	-	2/4/4/4	-
4	D10	C	1109	-	-	2/7/7/7	-
3	LMT	C	1103	-	-	8/21/61/61	0/2/2/2
4	D10	C	1107	-	-	0/7/7/7	-
4	D10	B	1105	-	-	5/7/7/7	-
7	HEX	C	1110	-	-	0/3/3/3	-
4	D10	B	1110	-	-	0/7/7/7	-
5	GOL	A	1106	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1108	-	-	2/4/4/4	-
5	GOL	C	1102	-	-	0/4/4/4	-
6	D12	C	1105	-	-	1/9/9/9	-
5	GOL	B	1116	-	-	0/4/4/4	-
3	LMT	A	1105	-	-	9/21/61/61	0/2/2/2
3	LMT	B	1114	-	-	13/21/61/61	0/2/2/2
4	D10	B	1112	-	-	2/7/7/7	-
6	D12	B	1111	-	-	0/9/9/9	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1114	LMT	C1B-O1B-C4'	2.68	124.59	117.96
3	B	1114	LMT	C1'-O5'-C5'	2.38	118.37	113.69
3	A	1109	LMT	O1'-C1'-C2'	2.24	111.80	108.30
3	A	1105	LMT	C2'-C3'-C4'	2.10	114.48	109.68

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

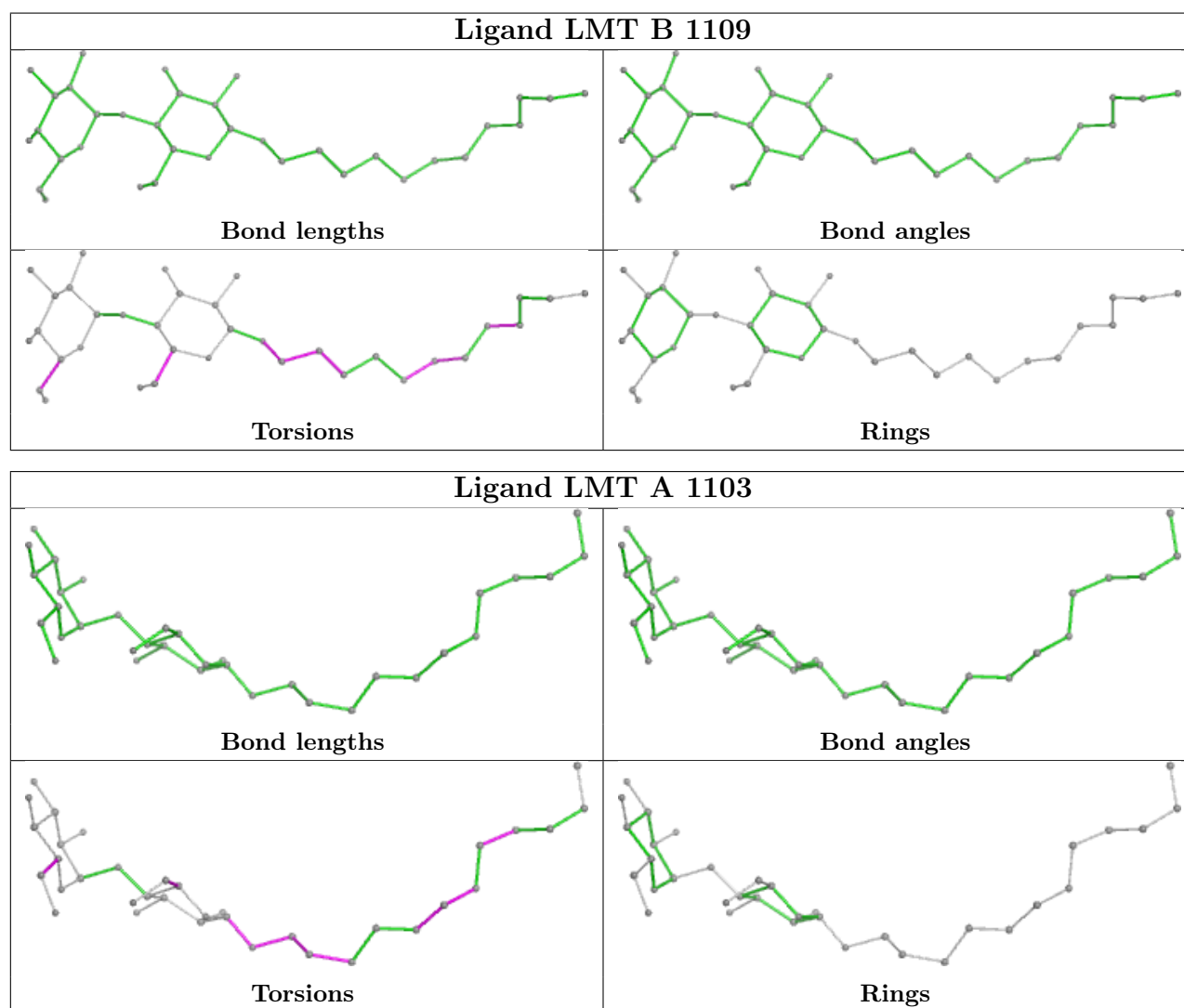
Mol	Chain	Res	Type	Atoms
3	A	1103	LMT	C2-C1-O1'-C1'
3	A	1105	LMT	C2B-C1B-O1B-C4'
3	A	1105	LMT	O5'-C1'-O1'-C1
3	A	1105	LMT	C2-C1-O1'-C1'
3	A	1109	LMT	C2'-C1'-O1'-C1

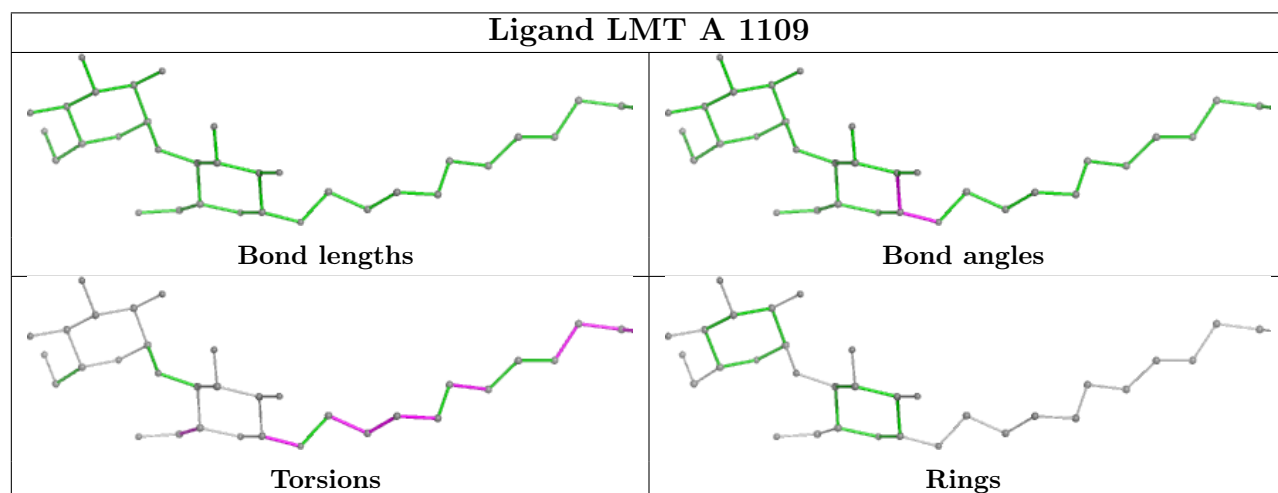
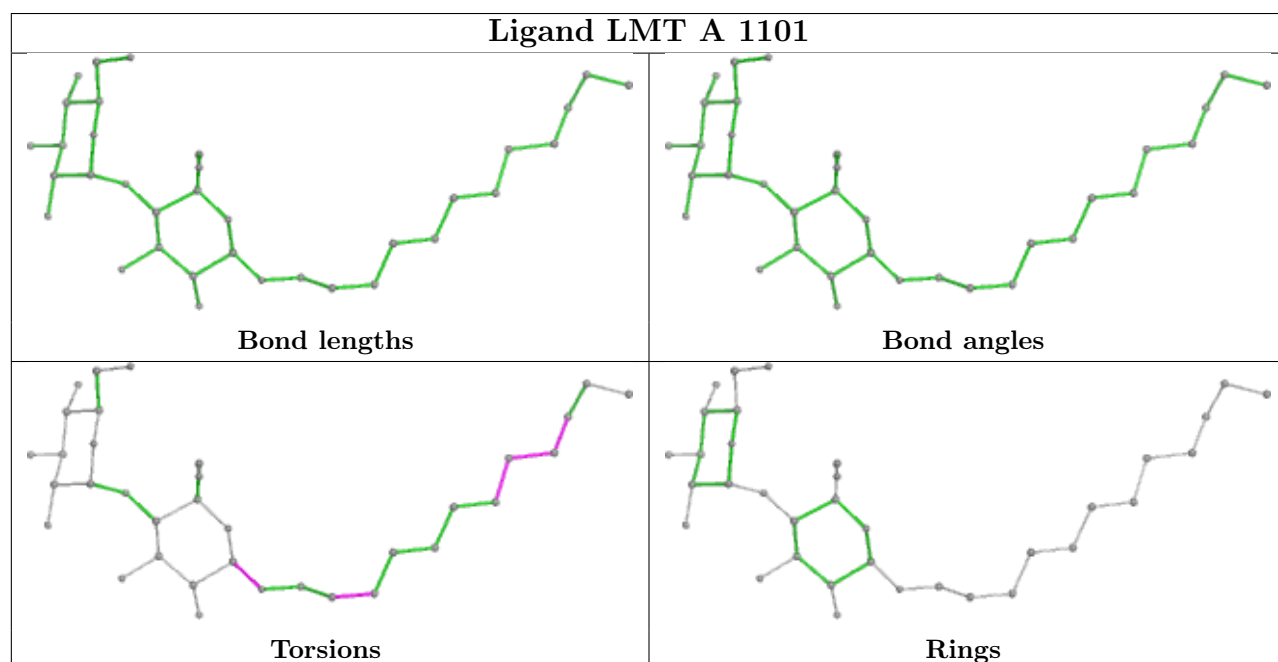
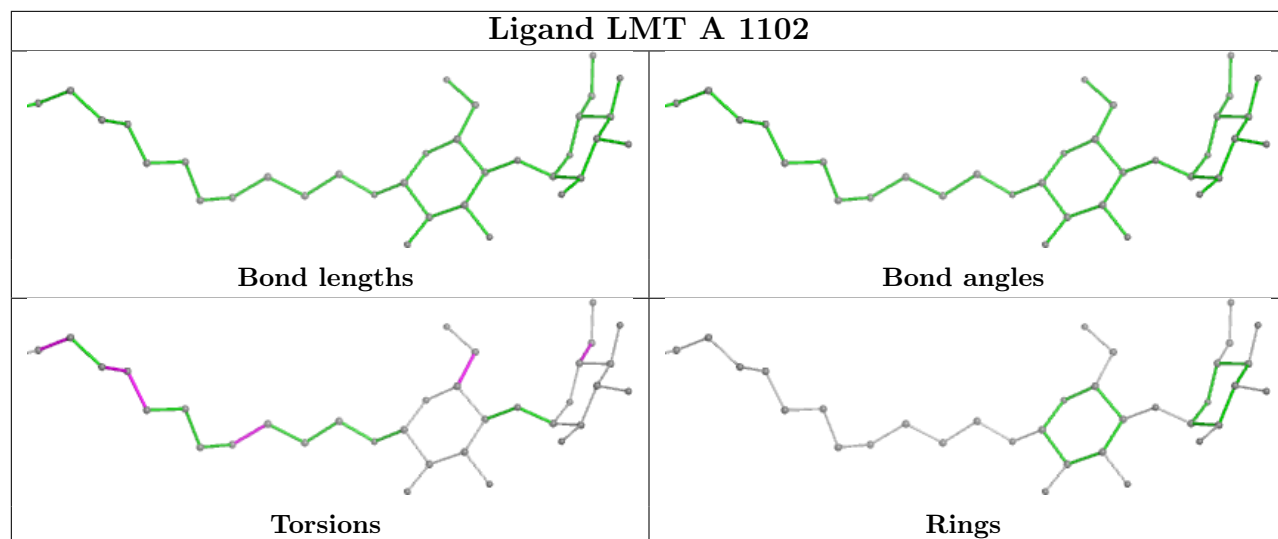
There are no ring outliers.

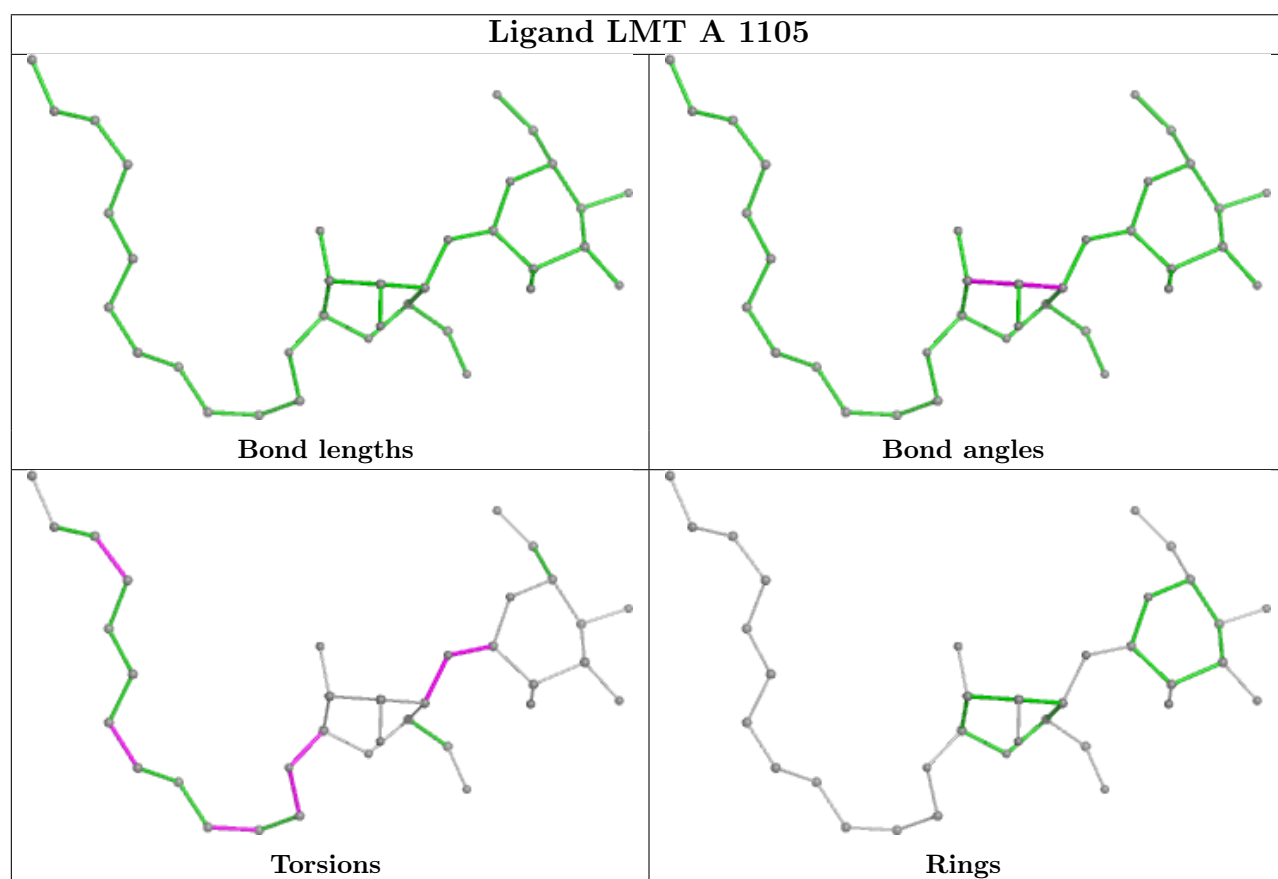
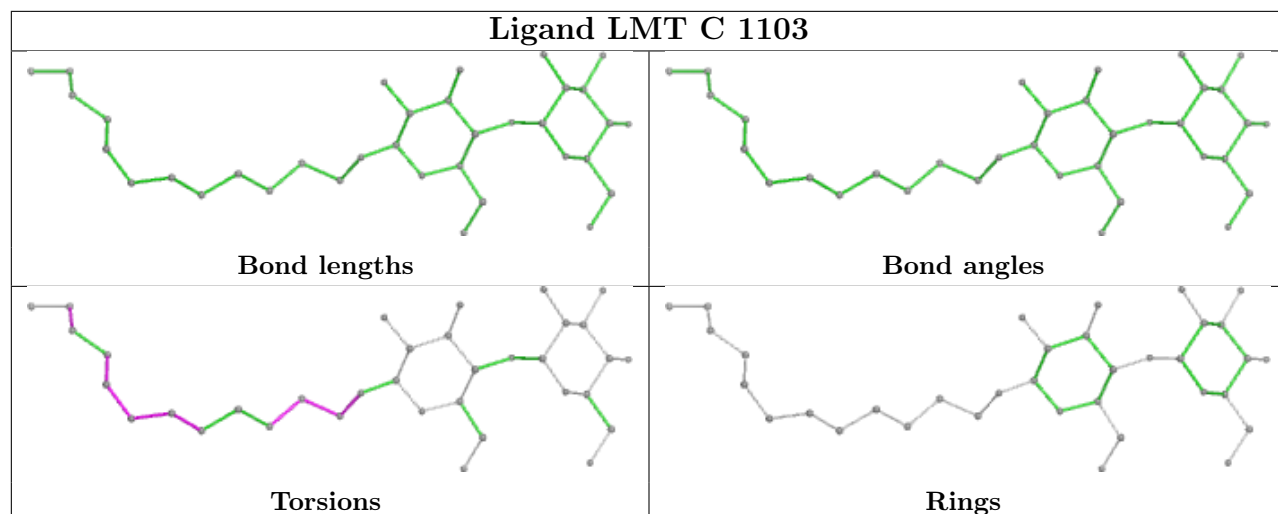
7 monomers are involved in 15 short contacts:

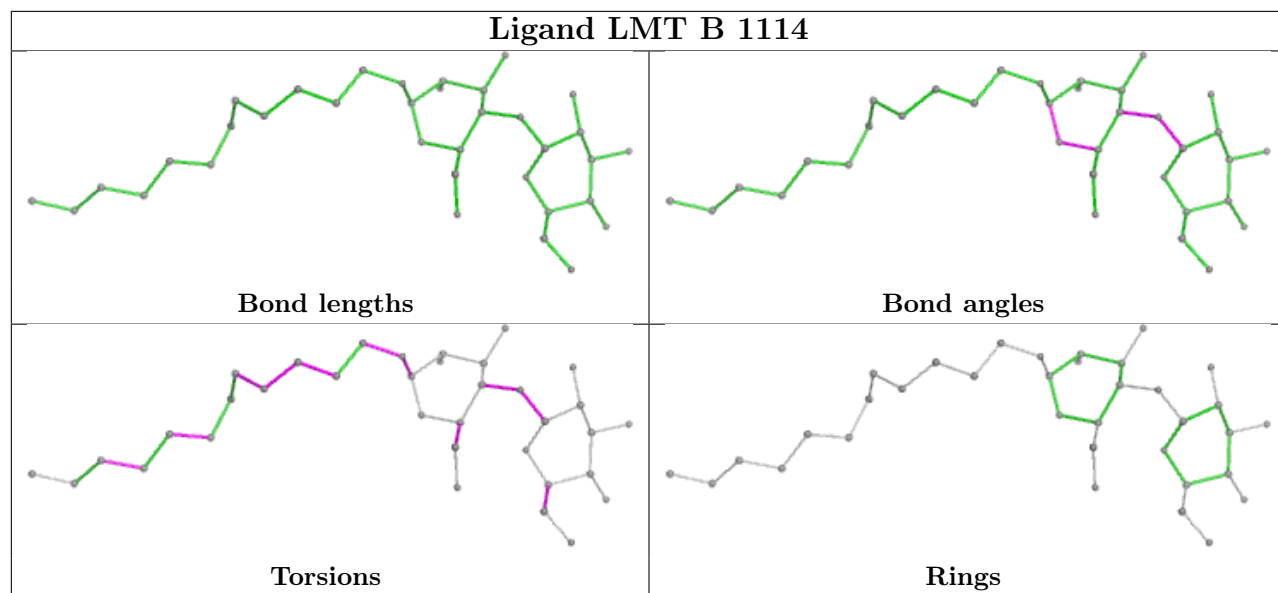
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	LMT	1	0
3	A	1102	LMT	4	0
3	A	1109	LMT	2	0
5	C	1114	GOL	2	0
5	A	1106	GOL	1	0
3	A	1105	LMT	2	0
3	B	1114	LMT	3	0

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









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1044/1057 (98%)	0.03	52 (4%)	35	30	15, 41, 104, 177	0
1	B	1033/1057 (97%)	-0.12	41 (3%)	43	37	13, 43, 79, 124	1 (0%)
1	C	1033/1057 (97%)	-0.31	20 (1%)	66	61	13, 38, 75, 123	0
2	D	155/169 (91%)	-0.43	2 (1%)	74	70	26, 38, 64, 90	0
2	E	153/169 (90%)	-0.15	2 (1%)	74	70	26, 46, 86, 106	0
All	All	3418/3509 (97%)	-0.15	117 (3%)	48	42	13, 41, 88, 177	1 (0%)

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	618	ALA	5.7
1	A	1040	ILE	5.4
1	B	868	LEU	4.8
1	A	659	LYS	4.3
1	A	539	GLY	4.3

### 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, 95<sup>th</sup> 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
4	D10	C	1117	10/10	0.67	0.41	53,72,96,104	0
6	D12	A	1107	12/12	0.67	0.33	44,57,82,93	0
5	GOL	A	1108	6/6	0.68	0.17	73,93,100,108	0
6	D12	C	1105	12/12	0.68	0.29	42,63,86,88	0
4	D10	B	1103	10/10	0.70	0.30	40,55,67,71	0
9	OCT	C	1104	8/8	0.70	0.24	41,53,64,70	0
4	D10	B	1112	10/10	0.71	0.35	41,64,97,100	0
6	D12	B	1111	12/12	0.71	0.27	43,59,74,75	0
4	D10	C	1107	10/10	0.72	0.34	53,76,87,98	0
4	D10	C	1116	10/10	0.72	0.39	31,76,92,97	0
7	HEX	B	1113	6/6	0.75	0.24	46,51,57,60	0
4	D10	B	1105	10/10	0.78	0.33	41,69,78,98	0
6	D12	C	1108	12/12	0.78	0.21	37,47,65,73	0
8	C14	C	1101	14/14	0.80	0.29	62,75,90,96	0
4	D10	C	1109	10/10	0.80	0.28	52,63,98,107	0
5	GOL	B	1104	6/6	0.82	0.15	57,70,74,76	0
7	HEX	C	1112	6/6	0.83	0.29	47,58,71,76	0
4	D10	A	1104	10/10	0.83	0.26	33,56,93,99	0
7	HEX	C	1110	6/6	0.83	0.26	32,41,50,55	0
5	GOL	B	1101	6/6	0.84	0.15	40,47,61,65	0
3	LMT	A	1103	35/35	0.86	0.14	49,76,113,136	0
3	LMT	B	1109	35/35	0.86	0.17	46,75,105,109	0
4	D10	B	1110	10/10	0.86	0.17	45,55,65,70	0
3	LMT	B	1114	35/35	0.86	0.20	59,120,173,188	0
3	LMT	A	1102	35/35	0.86	0.22	69,112,167,197	0
9	OCT	C	1106	8/8	0.86	0.27	27,39,58,59	0
10	DD9	C	1111	9/9	0.86	0.25	26,59,78,85	0
5	GOL	B	1102	6/6	0.88	0.24	38,65,91,115	0
3	LMT	A	1105	35/35	0.89	0.17	36,85,136,148	0
5	GOL	C	1102	6/6	0.89	0.19	45,53,72,98	0
5	GOL	C	1113	6/6	0.89	0.18	61,67,68,70	0
5	GOL	D	202	6/6	0.89	0.14	31,47,68,74	0
3	LMT	A	1109	35/35	0.89	0.15	47,87,138,155	0
5	GOL	B	1108	6/6	0.91	0.14	39,53,69,73	0
5	GOL	D	203	6/6	0.92	0.14	43,50,57,84	0
3	LMT	C	1103	35/35	0.92	0.15	33,58,127,128	0
5	GOL	C	1114	6/6	0.92	0.10	14,18,20,22	0
3	LMT	A	1101	35/35	0.92	0.11	30,50,119,133	0
11	SO4	C	1115	5/5	0.92	0.19	56,59,73,135	0
5	GOL	B	1116	6/6	0.93	0.15	43,51,64,112	0
5	GOL	D	201	6/6	0.94	0.11	45,56,59,78	0

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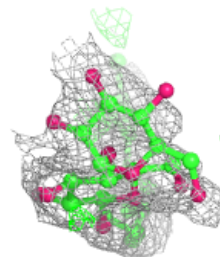
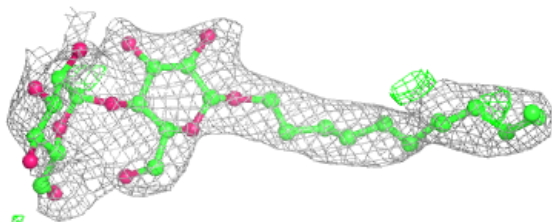
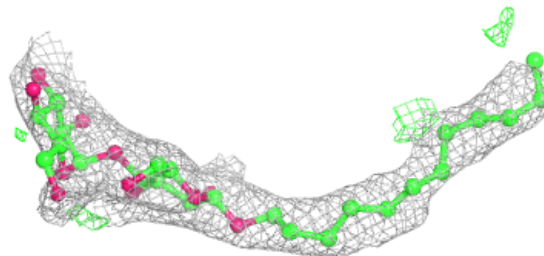
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	1107	6/6	0.94	0.09	22,29,35,37	0
5	GOL	B	1115	6/6	0.94	0.15	44,56,70,81	0
5	GOL	A	1106	6/6	0.96	0.10	19,34,47,56	0
5	GOL	B	1106	6/6	0.96	0.14	29,43,53,110	0

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

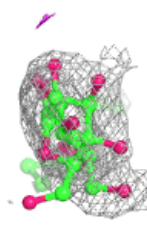
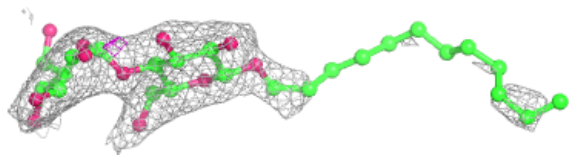
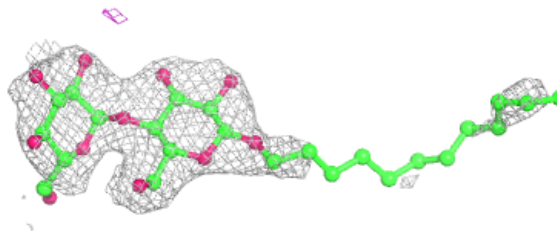
**Electron density around LMT A 1103:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

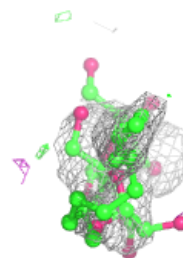
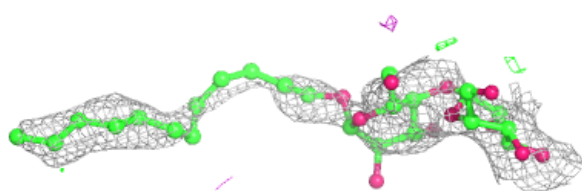
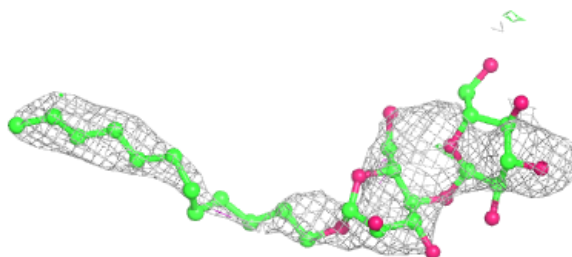


**Electron density around LMT B 1109:**

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

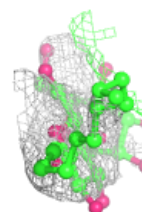
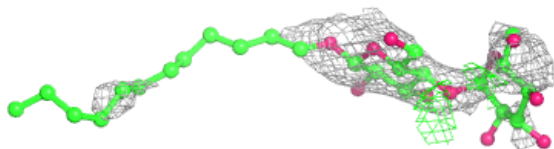
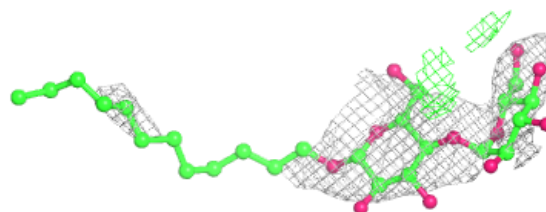
**Electron density around LMT B 1114:**

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

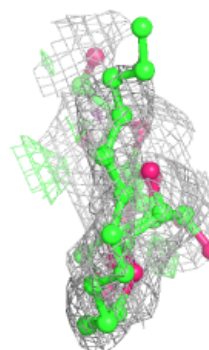
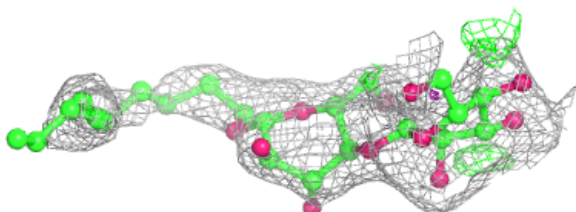
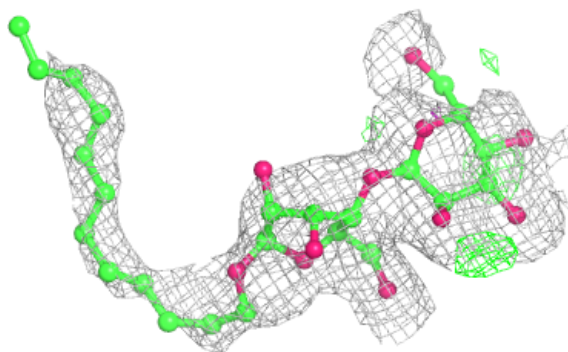


**Electron density around LMT A 1102:**

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

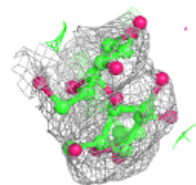
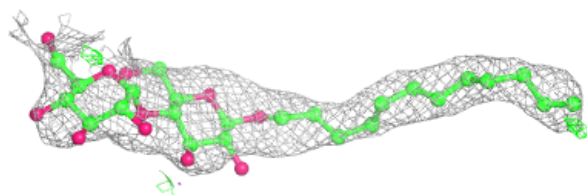
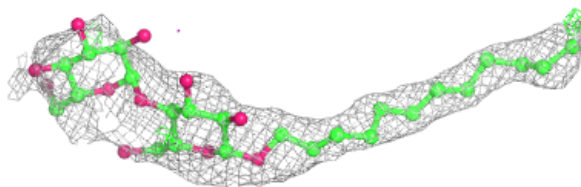
**Electron density around LMT A 1105:**

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

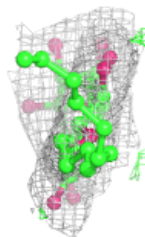
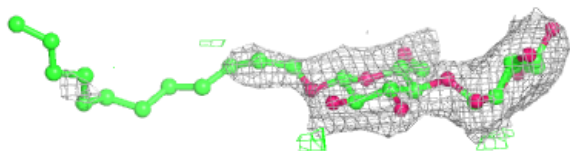
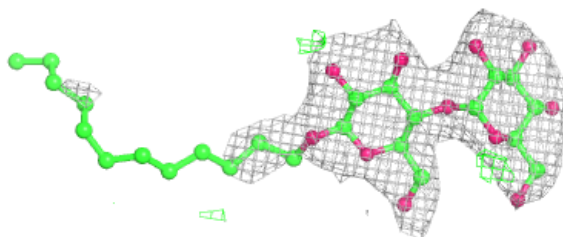


**Electron density around LMT A 1109:**

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

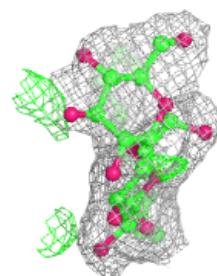
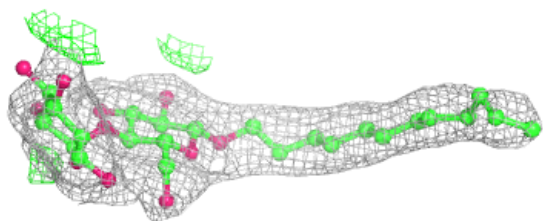
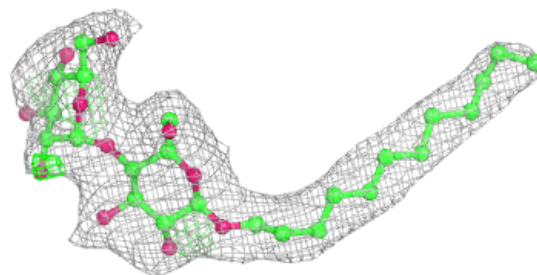
**Electron density around LMT C 1103:**

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



**Electron density around LMT A 1101:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.