Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 12:10 AM EDT

PDB ID	:	6ZOF
Title	:	Fusidic acid binding to the TM7/TM8 groove of AcrB-F380A T protomer
Authors	:	Tam, H.K.; Foong, W.E.; Pos, K.M.
Deposited on	:	2020-07-07
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

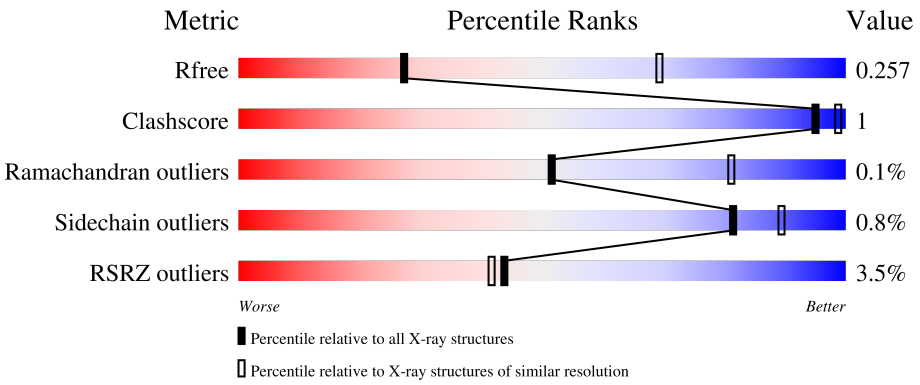
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2% 95%
1	B	1057	3% 93%
1	C	1057	2% 95%
2	D	169	5% 92% 8%
2	E	169	20% 91% 9%

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
10	PTY	C	1101	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26308 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
			Total	C	N	O	S			
1	A	1042	7921	5091	1311	1475	44	0	0	0
1	B	1034	7849	5049	1296	1460	44	0	0	0
1	C	1035	7860	5055	1300	1461	44	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ALA	PHE	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	380	ALA	PHE	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	380	ALA	PHE	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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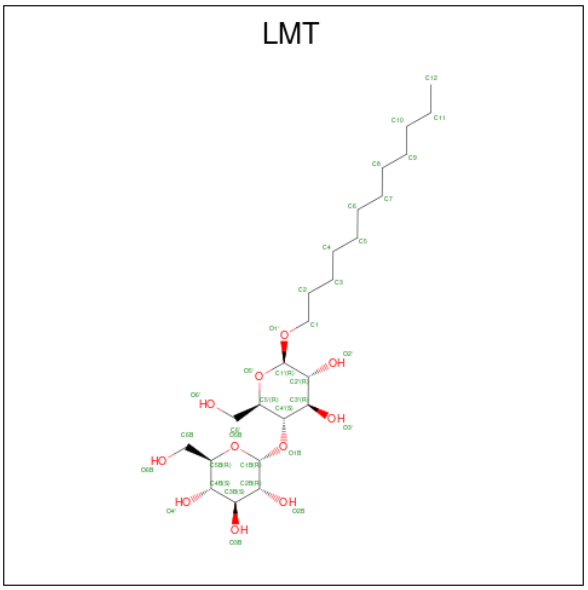
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

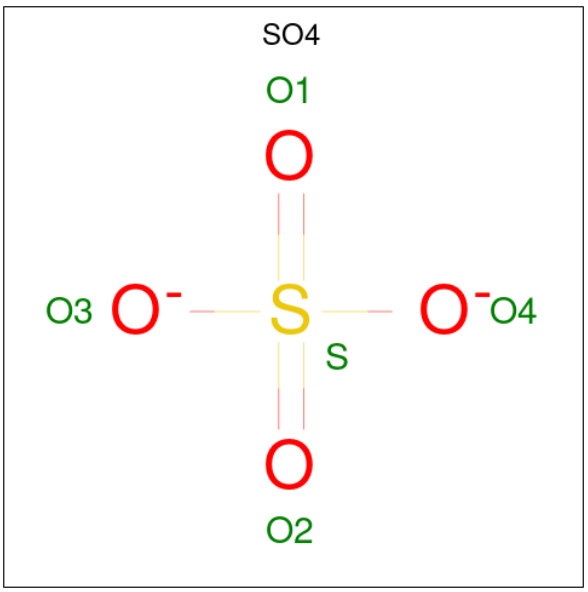
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	155	1173	739	205	228	1	0	0	0
			Total	C	N	O	S			
2	E	154	1167	736	204	226	1	0	0	0

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



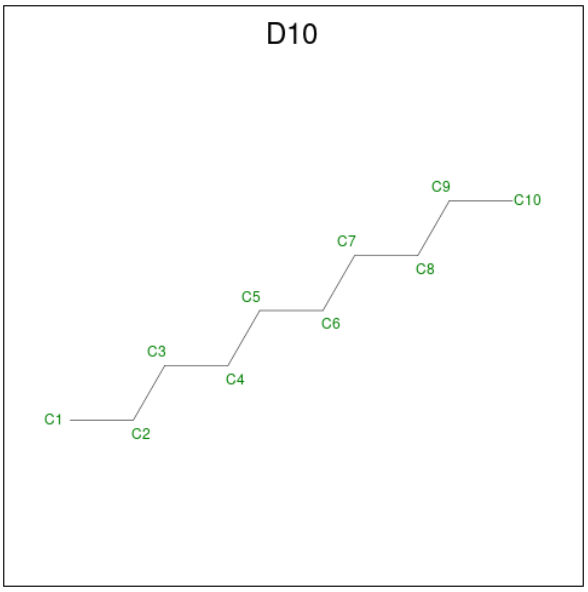
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	A	1	35	24	11	0	0
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	B	1	35	24	11	0	0
			Total	C	O		
3	C	1	35	24	11	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



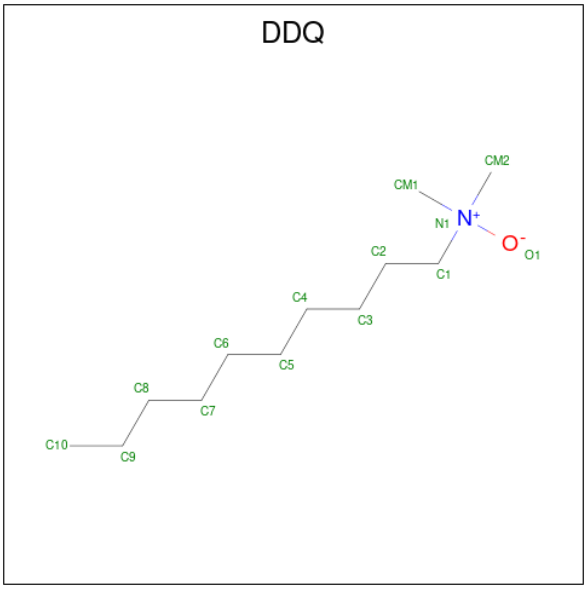
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

- Molecule 5 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



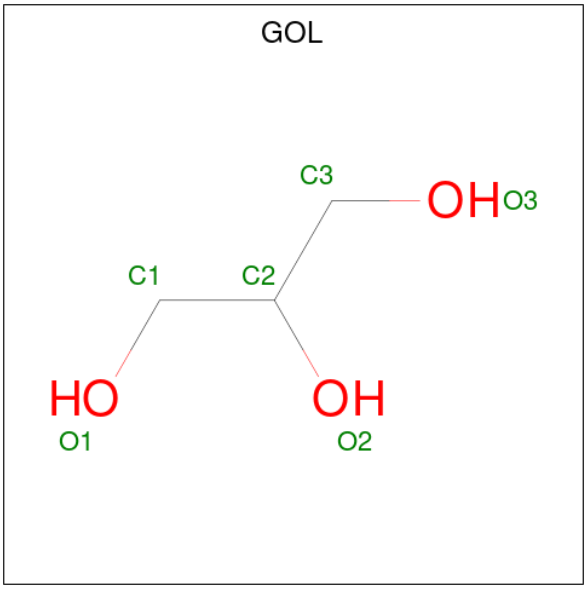
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C 10 10	0	0

- Molecule 6 is DECYLAMINE-N,N-DIMETHYL-N-OXIDE (three-letter code: DDQ) (formula: $C_{12}H_{27}NO$).



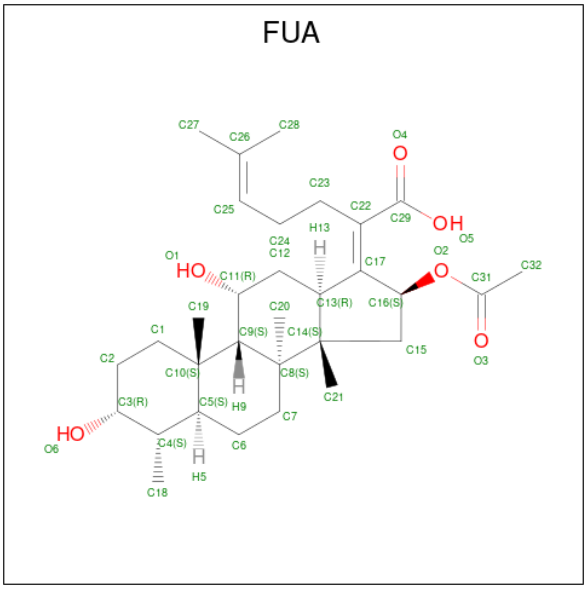
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	B	1	14	12	1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



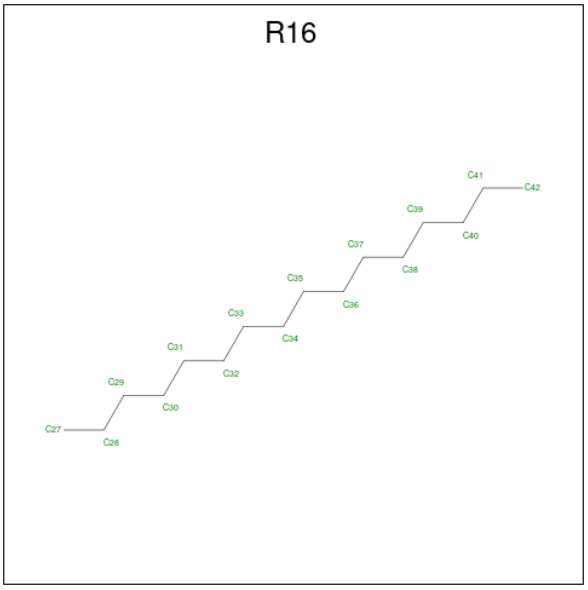
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
7	B	1	6	3	3		0	0

- Molecule 8 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



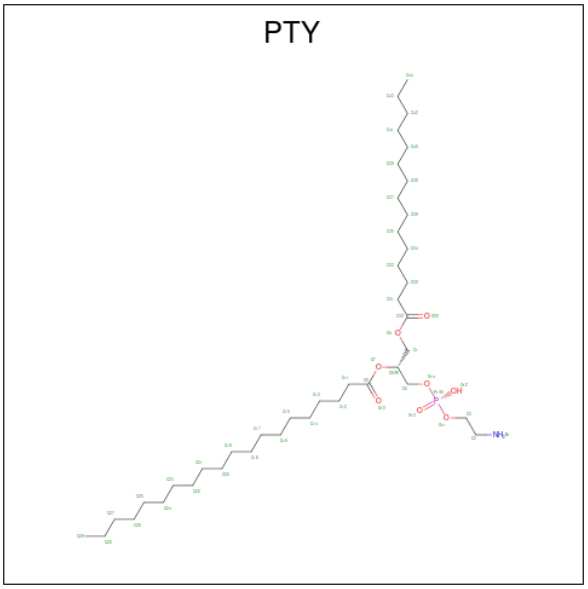
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	37	31	6	0	0

- Molecule 9 is HEXADECANE (three-letter code: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
9	B	1	16	16	0	0

- Molecule 10 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
10	C	1	50	40	1	8	1	0	0

- Molecule 11 is water.

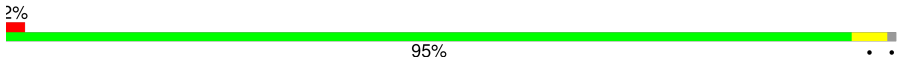
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	5	5	5	0	0
11	B	9	9	9	0	0
11	C	6	6	6	0	0

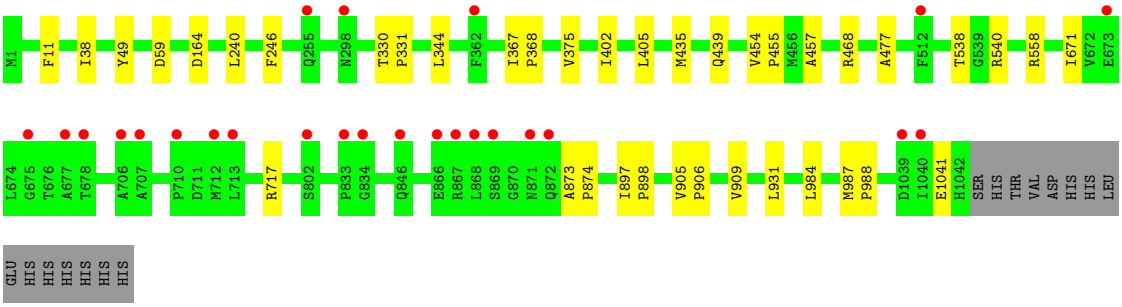
3 Residue-property plots (i)

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: Multidrug efflux pump subunit AcrB

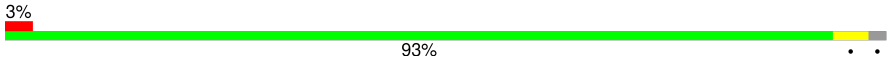
Chain A:

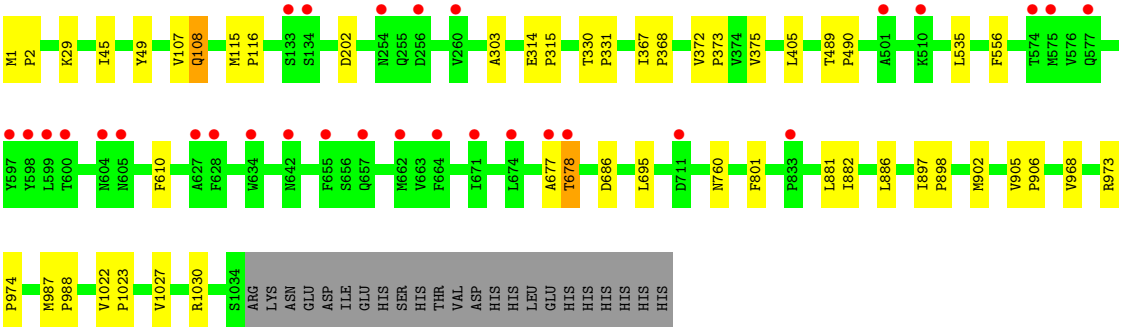




• Molecule 1: Multidrug efflux pump subunit AcrB

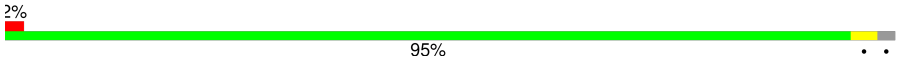
Chain B:

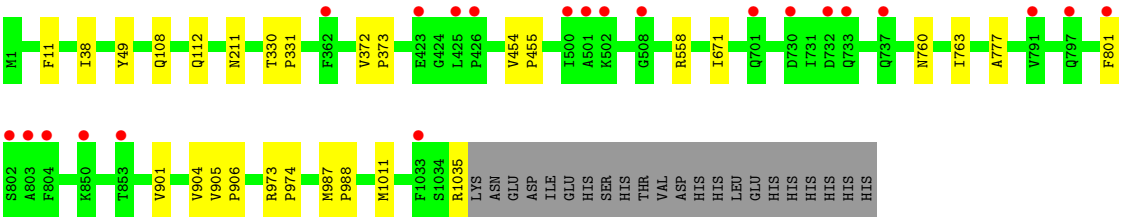




• Molecule 1: Multidrug efflux pump subunit AcrB

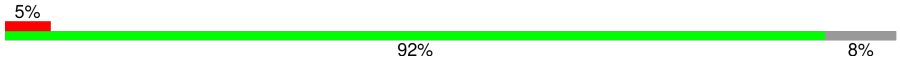
Chain C:

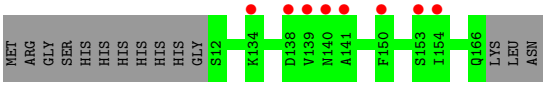




• Molecule 2: DARPIN

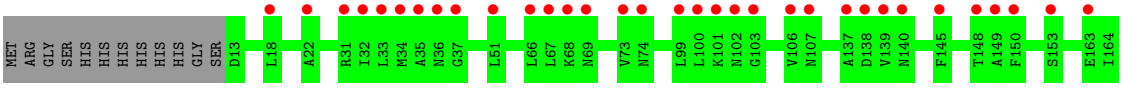
Chain D:





• Molecule 2: DARPIN

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	145.10Å 162.33Å 244.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.65 – 3.30 49.65 – 3.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.65-3.30) 100.0 (49.65-3.30)	Depositor EDS
R_{merge}	0.42	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.236 , 0.258 0.237 , 0.257	Depositor DCC
R_{free} test set	4369 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.812	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	26308	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: R16, SO4, FUA, DDQ, GOL, PTY, LMT, D10

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	0.67	0/8071	0.70	0/10959
1	B	0.67	0/7998	0.70	0/10862
1	C	0.67	0/8009	0.70	0/10876
2	D	0.68	0/1192	0.71	0/1621
2	E	0.68	0/1186	0.71	0/1613
All	All	0.67	0/26456	0.70	0/35931

There are no bond length outliers.

There are no bond angle outliers.

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	7921	0	8068	18	0
1	B	7849	0	8002	26	0
1	C	7860	0	8015	15	0
2	D	1173	0	1156	0	0
2	E	1167	0	1151	0	0
3	A	70	0	92	0	0
3	B	70	0	92	0	0
3	C	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	5	0	0	0	0
4	C	5	0	0	0	0
5	B	10	0	22	1	0
6	B	14	0	27	0	0
7	B	6	0	8	2	0
8	B	37	0	47	7	0
9	B	16	0	34	1	0
10	C	50	0	79	1	0
11	A	5	0	0	0	0
11	B	9	0	0	0	0
11	C	6	0	0	0	0
All	All	26308	0	26839	65	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 1.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:968:VAL:HG11	1:B:1023:PRO:HG3	1.65	0.77
1:C:38:ILE:HD11	1:C:671:ILE:HD12	1.72	0.72
8:B:1104:FUA:H232	8:B:1104:FUA:H122	1.73	0.70
8:B:1104:FUA:H202	8:B:1104:FUA:H5	1.76	0.67
9:B:1105:R16:H382	9:B:1105:R16:H341	1.80	0.64
8:B:1104:FUA:O2	8:B:1104:FUA:H211	2.02	0.60
1:C:1035:ARG:NH2	10:C:1101:PTY:O13	2.37	0.58
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.87	0.57
1:A:344:LEU:HD12	1:A:402:ILE:HD11	1.87	0.57
8:B:1104:FUA:H232	8:B:1104:FUA:C12	2.34	0.56
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.87	0.55
1:C:973:ARG:HB3	1:C:974:PRO:HD3	1.89	0.55
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.90	0.54
1:C:38:ILE:HD11	1:C:671:ILE:CD1	2.39	0.52
1:A:435:MET:O	1:A:439:GLN:HB2	2.11	0.50
1:A:38:ILE:HD11	1:A:671:ILE:HG21	1.94	0.49
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.95	0.49
1:B:902:MET:HA	8:B:1104:FUA:H273	1.95	0.48
1:B:29:LYS:O	5:B:1101:D10:H101	2.13	0.48
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.95	0.48
8:B:1104:FUA:O4	8:B:1104:FUA:H16	2.14	0.48
7:B:1103:GOL:O3	7:B:1103:GOL:O1	2.21	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.96	0.47
1:B:677:ALA:O	1:B:678:THR:OG1	2.26	0.47
1:B:882:ILE:O	1:B:886:LEU:HG	2.14	0.47
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.97	0.46
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.96	0.46
1:B:686:ASP:HB2	1:B:695:LEU:HD22	1.97	0.46
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.97	0.46
1:B:108:GLN:CD	1:C:112:GLN:HG3	2.36	0.45
1:A:987:MET:N	1:A:988:PRO:CD	2.80	0.45
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.45
8:B:1104:FUA:O4	8:B:1104:FUA:C16	2.64	0.45
1:B:115:MET:N	1:B:116:PRO:CD	2.80	0.44
1:C:108:GLN:O	1:C:112:GLN:HG2	2.17	0.44
1:A:457:ALA:O	1:A:468:ARG:NH1	2.51	0.44
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.99	0.44
1:B:489:THR:N	1:B:490:PRO:CD	2.81	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.99	0.44
1:A:344:LEU:CD1	1:A:402:ILE:HD11	2.47	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.81	0.43
1:C:330:THR:N	1:C:331:PRO:CD	2.81	0.43
1:B:897:ILE:N	1:B:898:PRO:HD2	2.33	0.43
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.53	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.00	0.43
1:A:330:THR:OG1	1:A:331:PRO:HD3	2.18	0.43
1:A:454:VAL:N	1:A:455:PRO:CD	2.82	0.43
1:A:897:ILE:N	1:A:898:PRO:CD	2.82	0.43
1:B:897:ILE:N	1:B:898:PRO:CD	2.82	0.42
1:B:760:ASN:HA	7:B:1103:GOL:H32	2.00	0.42
1:C:901:VAL:O	1:C:904:VAL:HG12	2.20	0.42
1:C:987:MET:HB3	1:C:988:PRO:HD3	2.01	0.42
1:B:973:ARG:N	1:B:974:PRO:HD2	2.35	0.42
1:B:987:MET:N	1:B:988:PRO:CD	2.83	0.42
1:B:375:VAL:HG11	1:B:405:LEU:HD22	2.01	0.41
1:B:314:GLU:N	1:B:315:PRO:CD	2.82	0.41
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.35	0.41
1:A:59:ASP:HB3	1:C:763:ILE:HD11	2.03	0.41
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.03	0.41
1:C:987:MET:N	1:C:988:PRO:CD	2.84	0.41
1:A:873:ALA:HB3	1:A:874:PRO:HD3	2.02	0.41
1:C:211:ASN:O	1:C:760:ASN:ND2	2.53	0.41
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HD11	1:B:107:VAL:HG13	2.03	0.40
1:B:330:THR:N	1:B:331:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1040/1057 (98%)	994 (96%)	45 (4%)	1 (0%)	51	81
1	B	1032/1057 (98%)	996 (96%)	35 (3%)	1 (0%)	51	81
1	C	1033/1057 (98%)	989 (96%)	43 (4%)	1 (0%)	51	81
2	D	153/169 (90%)	147 (96%)	6 (4%)	0	100	100
2	E	152/169 (90%)	143 (94%)	9 (6%)	0	100	100
All	All	3410/3509 (97%)	3269 (96%)	138 (4%)	3 (0%)	51	81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	B	678	THR
1	C	777	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	847/862 (98%)	839 (99%)	8 (1%)	78	87
1	B	839/862 (97%)	831 (99%)	8 (1%)	76	86
1	C	840/862 (97%)	835 (99%)	5 (1%)	86	91
2	D	120/132 (91%)	120 (100%)	0	100	100
2	E	119/132 (90%)	119 (100%)	0	100	100
All	All	2765/2850 (97%)	2744 (99%)	21 (1%)	81	89

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	PHE
1	A	49	TYR
1	A	164	ASP
1	A	540	ARG
1	A	558	ARG
1	A	717	ARG
1	A	984	LEU
1	A	1041	GLU
1	B	49	TYR
1	B	108	GLN
1	B	202	ASP
1	B	556	PHE
1	B	610	PHE
1	B	801	PHE
1	B	881	LEU
1	B	1030	ARG
1	C	11	PHE
1	C	49	TYR
1	C	558	ARG
1	C	801	PHE
1	C	1011	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LMT	B	1106	-	36,36,36	0.43	0	47,47,47	0.50	0
3	LMT	A	1102	-	36,36,36	0.43	0	47,47,47	0.48	0
5	D10	B	1101	-	9,9,9	0.09	0	8,8,8	0.09	0
8	FUA	B	1104	-	39,40,40	1.54	2 (5%)	50,64,64	0.85	1 (2%)
7	GOL	B	1103	-	5,5,5	0.09	0	5,5,5	0.43	0
9	R16	B	1105	-	15,15,15	0.10	0	14,14,14	0.15	0
4	SO4	C	1103	-	4,4,4	0.34	0	6,6,6	0.07	0
6	DDQ	B	1102	-	11,13,13	0.18	0	12,15,15	0.27	0
3	LMT	B	1107	-	36,36,36	0.47	0	47,47,47	0.61	0
10	PTY	C	1101	-	49,49,49	0.26	0	52,54,54	0.39	0
3	LMT	A	1101	-	36,36,36	0.48	0	47,47,47	0.64	1 (2%)
4	SO4	A	1103	-	4,4,4	0.34	0	6,6,6	0.07	0
3	LMT	C	1102	-	36,36,36	0.43	0	47,47,47	0.55	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
3	LMT	B	1106	-	-	10/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	1102	-	-	9/21/61/61	0/2/2/2
5	D10	B	1101	-	-	1/7/7/7	-
8	FUA	B	1104	-	-	6/16/92/92	0/4/4/4
7	GOL	B	1103	-	-	4/4/4/4	-
9	R16	B	1105	-	-	6/13/13/13	-
6	DDQ	B	1102	-	-	4/11/11/11	-
3	LMT	B	1107	-	-	11/21/61/61	0/2/2/2
10	PTY	C	1101	-	-	21/53/53/53	-
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
3	LMT	C	1102	-	-	8/21/61/61	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1104	FUA	C29-C22	-8.73	1.35	1.47
8	B	1104	FUA	O5-C29	-2.68	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1104	FUA	C14-C8-C9	-2.61	104.72	109.30
3	A	1101	LMT	O1B-C4'-C5'	2.08	114.92	109.48

There are no chirality outliers.

All (92) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1106	LMT	C2-C1-O1'-C1'
7	B	1103	GOL	O1-C1-C2-O2
7	B	1103	GOL	O1-C1-C2-C3
10	C	1101	PTY	N1-C2-C3-O11
10	C	1101	PTY	C11-C8-O7-C6
10	C	1101	PTY	O30-C30-O4-C1
3	A	1101	LMT	C5'-C4'-O1B-C1B
10	C	1101	PTY	O10-C8-O7-C6
10	C	1101	PTY	C31-C30-O4-C1
3	B	1107	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	O5B-C5B-C6B-O6B
3	A	1102	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	A	1101	LMT	O5'-C1'-O1'-C1
3	C	1102	LMT	O5'-C5'-C6'-O6'
9	B	1105	R16	C38-C39-C40-C41
3	A	1101	LMT	C2'-C1'-O1'-C1
3	A	1102	LMT	C4'-C5'-C6'-O6'
3	C	1102	LMT	C4'-C5'-C6'-O6'
3	A	1101	LMT	O5'-C5'-C6'-O6'
3	B	1106	LMT	O1'-C1-C2-C3
3	A	1101	LMT	C4B-C5B-C6B-O6B
3	A	1101	LMT	C4'-C5'-C6'-O6'
3	B	1107	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	O1'-C1-C2-C3
9	B	1105	R16	C34-C35-C36-C37
8	B	1104	FUA	C32-C31-O2-C16
3	B	1106	LMT	C2'-C1'-O1'-C1
7	B	1103	GOL	C1-C2-C3-O3
5	B	1101	D10	C4-C5-C6-C7
3	B	1106	LMT	O5'-C1'-O1'-C1
10	C	1101	PTY	C11-C12-C13-C14
3	A	1102	LMT	C3-C4-C5-C6
3	A	1102	LMT	C11-C10-C9-C8
3	B	1106	LMT	C11-C10-C9-C8
10	C	1101	PTY	C35-C36-C37-C38
10	C	1101	PTY	C30-C31-C32-C33
6	B	1102	DDQ	C5-C6-C7-C8
3	B	1107	LMT	C1-C2-C3-C4
3	A	1102	LMT	C7-C8-C9-C10
3	B	1107	LMT	O5B-C5B-C6B-O6B
3	A	1101	LMT	C3-C4-C5-C6
10	C	1101	PTY	C39-C40-C41-C42
8	B	1104	FUA	C22-C23-C24-C25
3	B	1106	LMT	C6-C7-C8-C9
3	C	1102	LMT	C1-C2-C3-C4
3	B	1107	LMT	C6-C7-C8-C9
3	C	1102	LMT	O1'-C1-C2-C3
3	B	1106	LMT	C4'-C5'-C6'-O6'
3	A	1102	LMT	C9-C10-C11-C12
10	C	1101	PTY	C36-C37-C38-C39
3	B	1107	LMT	C9-C10-C11-C12
3	B	1107	LMT	C2-C1-O1'-C1'
3	C	1102	LMT	C2-C1-O1'-C1'
8	B	1104	FUA	O3-C31-O2-C16

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Mol	Chain	Res	Type	Atoms
3	C	1102	LMT	C4-C5-C6-C7
10	C	1101	PTY	C26-C27-C28-C29
10	C	1101	PTY	C19-C20-C21-C22
8	B	1104	FUA	C15-C16-O2-C31
9	B	1105	R16	C32-C33-C34-C35
7	B	1103	GOL	O2-C2-C3-O3
10	C	1101	PTY	C12-C11-C8-O7
10	C	1101	PTY	O14-C5-C6-C1
3	A	1102	LMT	C4-C5-C6-C7
6	B	1102	DDQ	C2-C1-N1-CM2
3	B	1107	LMT	O1'-C1-C2-C3
3	C	1102	LMT	C9-C10-C11-C12
9	B	1105	R16	C35-C36-C37-C38
10	C	1101	PTY	C34-C35-C36-C37
10	C	1101	PTY	O14-C5-C6-O7
10	C	1101	PTY	C25-C26-C27-C28
6	B	1102	DDQ	C2-C1-N1-O1
3	B	1106	LMT	C4-C5-C6-C7
3	B	1107	LMT	C4-C5-C6-C7
10	C	1101	PTY	C23-C24-C25-C26
10	C	1101	PTY	C31-C32-C33-C34
6	B	1102	DDQ	C7-C8-C9-C10
3	A	1102	LMT	C6-C7-C8-C9
3	B	1107	LMT	C3-C4-C5-C6
3	B	1107	LMT	C2-C3-C4-C5
3	A	1101	LMT	C9-C10-C11-C12
3	C	1102	LMT	C11-C10-C9-C8
3	B	1106	LMT	C9-C10-C11-C12
10	C	1101	PTY	C33-C34-C35-C36
3	A	1101	LMT	C3'-C4'-O1B-C1B
3	B	1106	LMT	O5'-C5'-C6'-O6'
3	A	1101	LMT	C2-C3-C4-C5
3	A	1101	LMT	C7-C8-C9-C10
9	B	1105	R16	C28-C29-C30-C31
9	B	1105	R16	C37-C38-C39-C40
8	B	1104	FUA	C24-C25-C26-C27
10	C	1101	PTY	C12-C11-C8-O10
8	B	1104	FUA	C24-C25-C26-C28

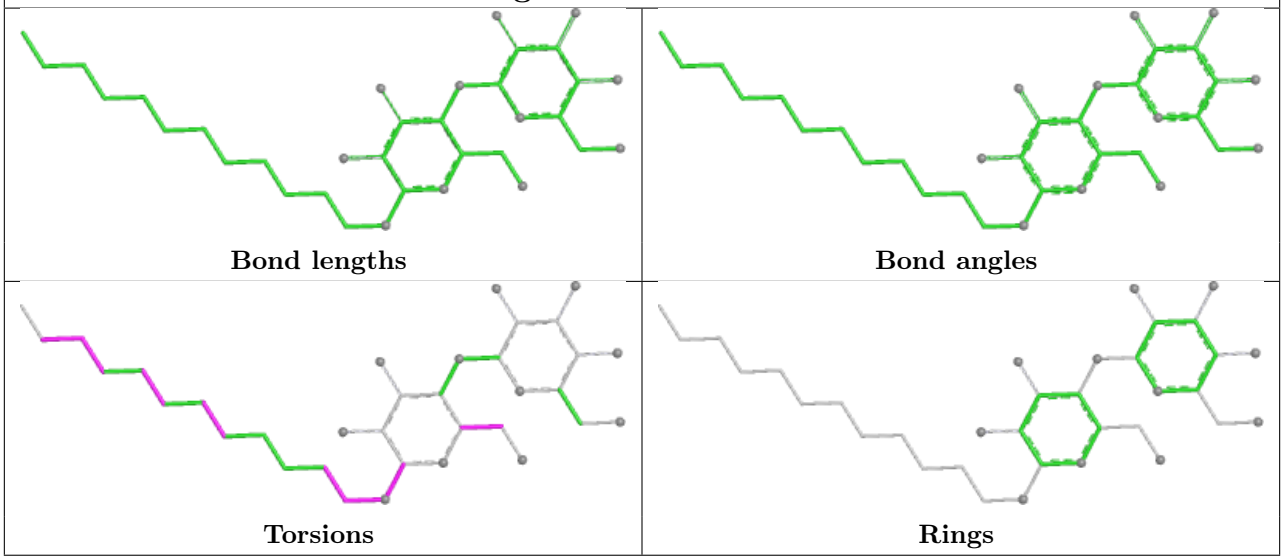
There are no ring outliers.

5 monomers are involved in 12 short contacts:

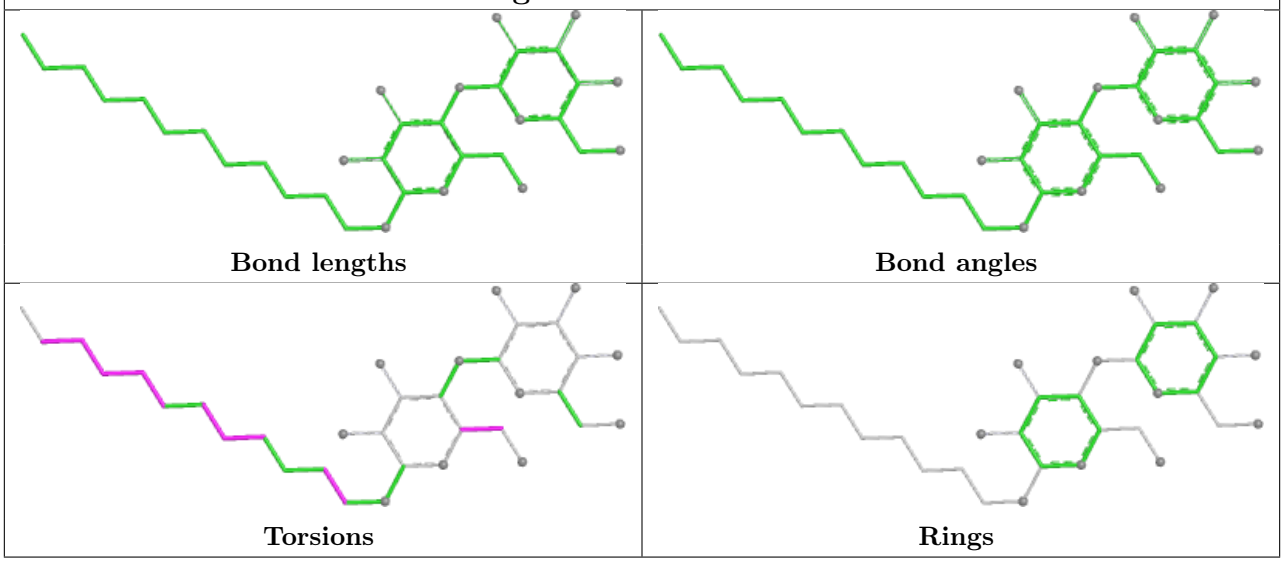
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1101	D10	1	0
8	B	1104	FUA	7	0
7	B	1103	GOL	2	0
9	B	1105	R16	1	0
10	C	1101	PTY	1	0

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 then 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.

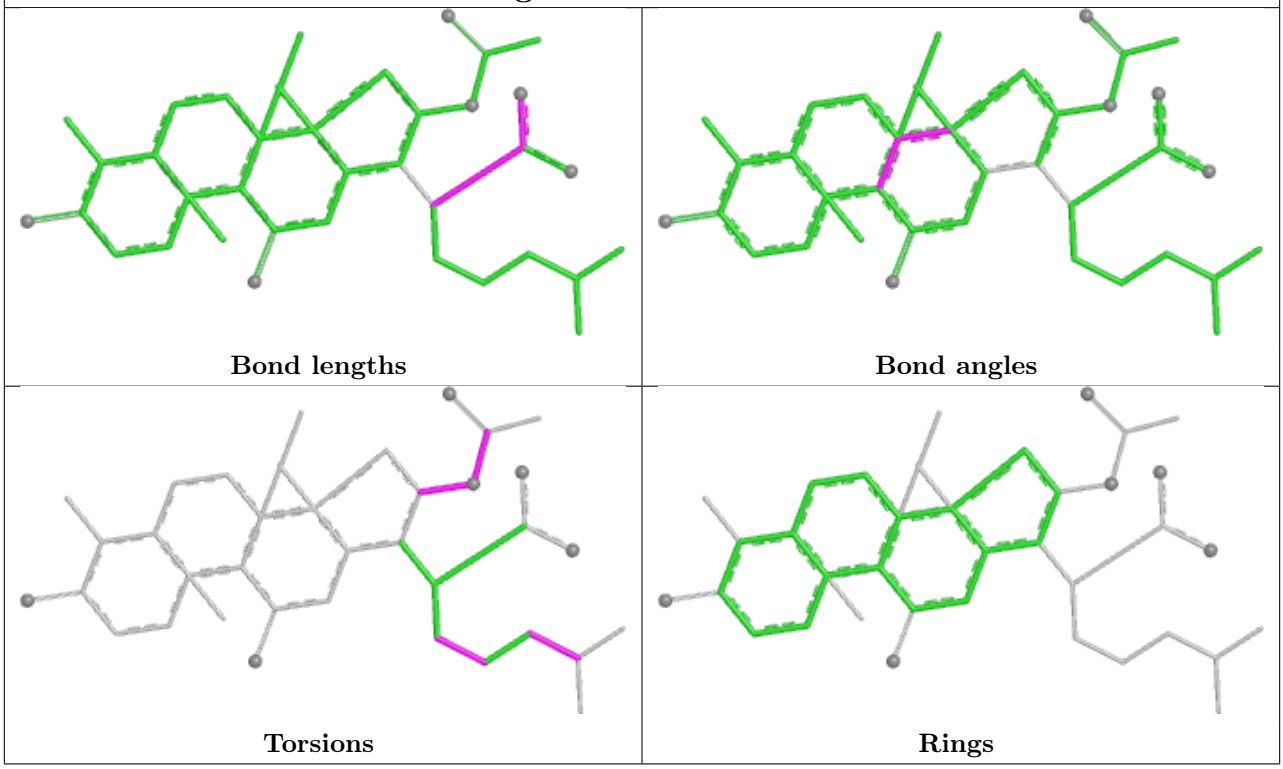
Ligand LMT B 1106



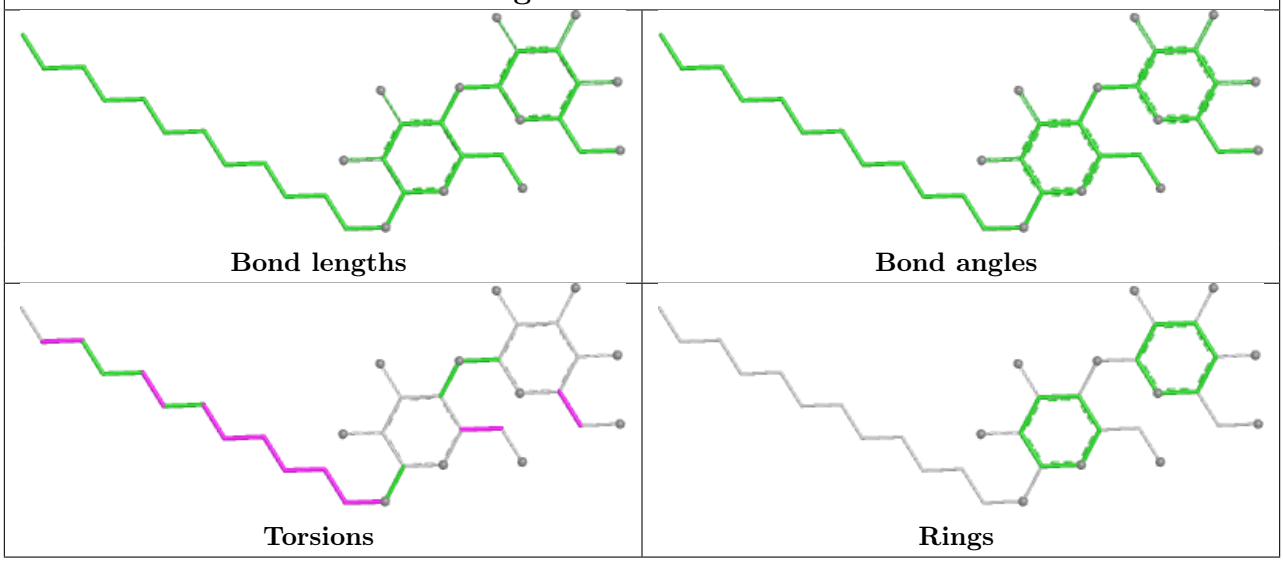
Ligand LMT A 1102



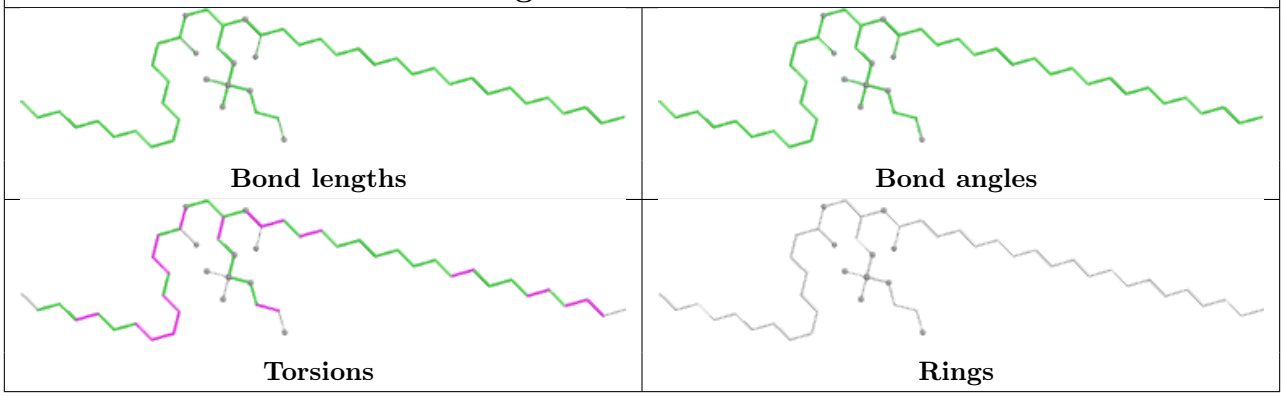
Ligand FUA B 1104



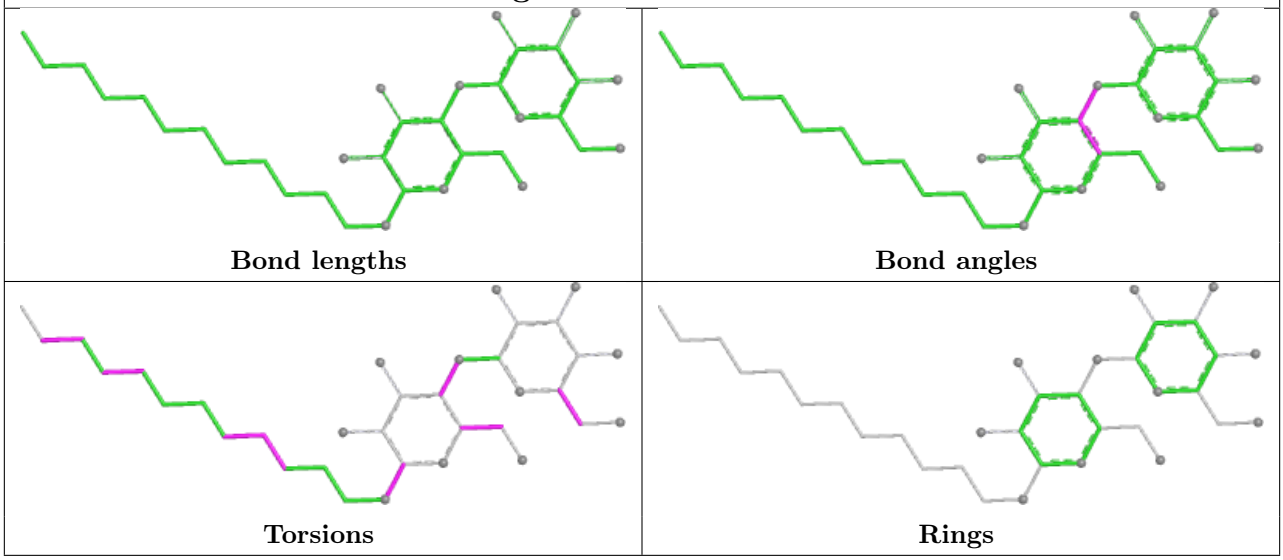
Ligand LMT B 1107

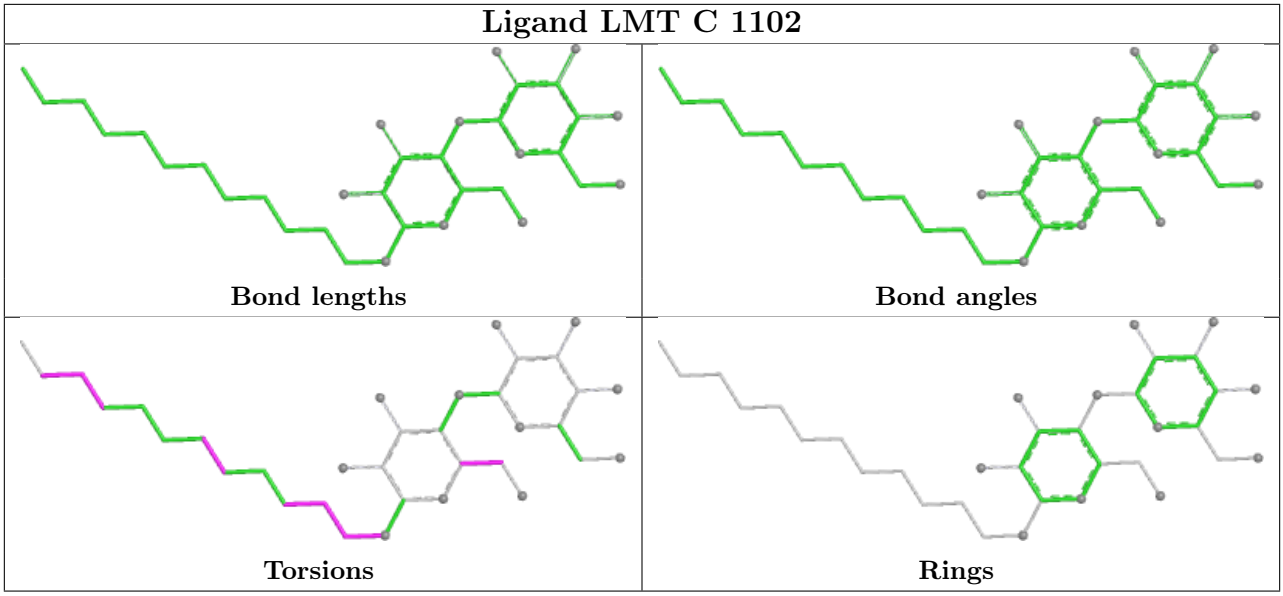


Ligand PTY C 1101



Ligand LMT A 1101





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1042/1057 (98%)	0.10	25 (2%)	59	56	33, 61, 96, 131	0
1	B	1034/1057 (97%)	0.06	30 (2%)	51	50	35, 59, 86, 110	0
1	C	1035/1057 (97%)	-0.02	22 (2%)	63	62	40, 52, 73, 97	0
2	D	155/169 (91%)	0.43	8 (5%)	27	25	49, 62, 77, 86	0
2	E	154/169 (91%)	1.23	34 (22%)	0	1	57, 71, 91, 101	0
All	All	3420/3509 (97%)	0.12	119 (3%)	44	42	33, 58, 87, 131	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	678	THR	4.4
2	D	141	ALA	4.1
2	E	139	VAL	4.0
2	E	66	LEU	3.8
2	E	69	ASN	3.6
1	B	134	SER	3.5
1	B	677	ALA	3.5
1	A	675	GLY	3.4
1	B	642	ASN	3.3
2	E	99	LEU	3.3
2	E	150	PHE	3.2
2	E	67	LEU	3.2
1	A	869	SER	3.2
2	E	36	ASN	3.1
1	A	673	GLU	3.1
2	D	140	ASN	3.1
2	E	32	ILE	3.0
1	A	868	LEU	3.0
1	A	871	ASN	3.0
2	E	35	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	73	VAL	3.0
2	E	74	ASN	2.9
2	E	33	LEU	2.9
2	E	37	GLY	2.8
2	E	153	SER	2.8
2	E	34	MET	2.7
2	E	51	LEU	2.7
1	A	833	PRO	2.7
1	B	604	ASN	2.7
1	B	711	ASP	2.7
2	D	154	ILE	2.7
2	E	31	ARG	2.7
2	E	68	LYS	2.7
1	C	1033	PHE	2.6
1	A	255	GLN	2.6
1	C	502	LYS	2.6
1	C	733	GLN	2.6
1	C	730	ASP	2.6
2	E	148	THR	2.6
1	B	662	MET	2.6
1	C	850	LYS	2.6
1	C	804	PHE	2.5
1	C	732	ASP	2.5
2	E	102	ASN	2.5
1	A	1040	ILE	2.5
2	E	106	VAL	2.5
1	B	628	PHE	2.5
2	E	103	GLY	2.5
2	E	140	ASN	2.5
1	A	866	GLU	2.5
2	D	153	SER	2.5
1	A	846	GLN	2.5
1	B	256	ASP	2.5
2	D	150	PHE	2.5
1	A	834	GLY	2.4
1	B	600	THR	2.4
2	E	138	ASP	2.4
2	E	165	LEU	2.4
2	E	101	LYS	2.4
1	A	362	PHE	2.4
1	B	574	THR	2.4
1	C	426	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	137	ALA	2.4
1	B	597	TYR	2.4
2	E	163	GLU	2.4
2	E	18	LEU	2.4
1	B	133	SER	2.4
1	C	803	ALA	2.4
1	C	737	GLN	2.4
1	B	627	ALA	2.4
2	E	107	ASN	2.4
1	B	655	PHE	2.3
1	A	713	LEU	2.3
1	C	801	PHE	2.3
1	B	254	ASN	2.3
2	D	138	ASP	2.3
1	B	671	ILE	2.3
1	B	833	PRO	2.3
2	E	145	PHE	2.3
1	B	260	VAL	2.2
1	C	425	LEU	2.2
1	C	501	ALA	2.2
1	B	605	ASN	2.2
1	A	512	PHE	2.2
1	C	802	SER	2.2
1	C	701	GLN	2.2
1	A	706	ALA	2.2
1	A	872	GLN	2.2
1	A	802	SER	2.2
1	B	657	GLN	2.2
1	B	598	TYR	2.1
1	C	500	ILE	2.1
1	C	791	VAL	2.1
2	D	139	VAL	2.1
1	A	710	PRO	2.1
1	A	712	MET	2.1
1	C	362	PHE	2.1
1	B	634	TRP	2.1
2	E	100	LEU	2.1
1	A	1039	ASP	2.1
1	C	423	GLU	2.1
1	C	508	GLY	2.1
1	A	678	THR	2.1
1	A	707	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	867	ARG	2.1
1	B	501	ALA	2.1
2	E	22	ALA	2.0
1	B	599	LEU	2.0
1	B	575	MET	2.0
1	A	298	ASN	2.0
1	B	510	LYS	2.0
1	B	664	PHE	2.0
1	C	853	THR	2.0
1	C	797	GLN	2.0
1	B	674	LEU	2.0
2	D	134	LYS	2.0
1	B	577	GLN	2.0
1	A	677	ALA	2.0
2	E	149	ALA	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 monosaccharides 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(Å^2)	Q<0.9
3	LMT	B	1107	35/35	0.73	0.38	92,115,122,124	0
9	R16	B	1105	16/16	0.78	0.29	58,61,61,61	0
6	DDQ	B	1102	14/14	0.80	0.31	64,68,73,74	0
10	PTY	C	1101	50/50	0.80	0.46	81,87,105,106	0
3	LMT	A	1101	35/35	0.84	0.29	75,90,101,103	0
3	LMT	A	1102	35/35	0.86	0.49	94,98,101,101	0
3	LMT	B	1106	35/35	0.86	0.33	86,88,92,92	0
8	FUA	B	1104	37/37	0.87	0.33	74,76,91,93	0

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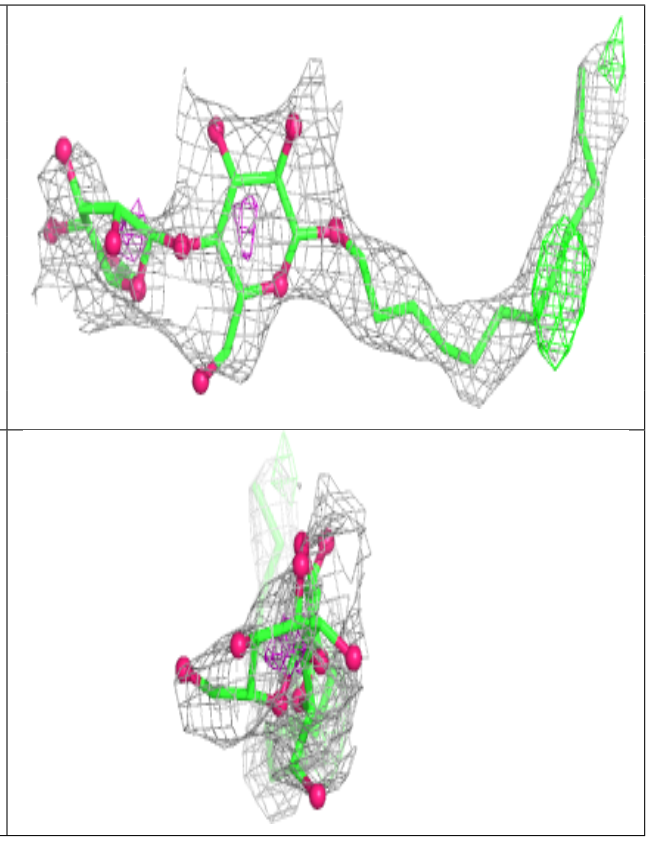
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1103	5/5	0.89	0.24	140,140,141,141	0
5	D10	B	1101	10/10	0.89	0.19	48,49,49,49	0
3	LMT	C	1102	35/35	0.90	0.27	63,65,67,68	0
4	SO4	C	1103	5/5	0.93	0.17	75,75,75,75	0
7	GOL	B	1103	6/6	0.95	0.22	47,48,48,48	0

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.

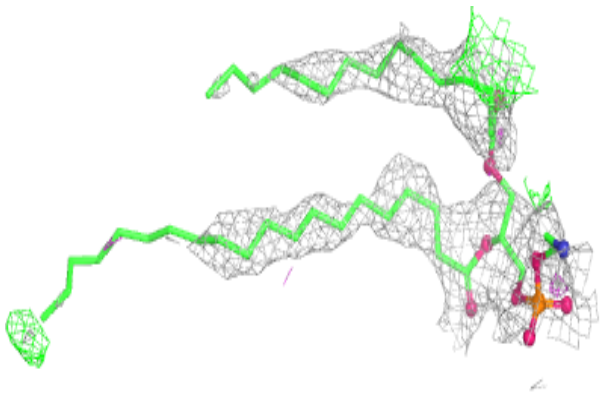
Electron density around LMT B 1107:

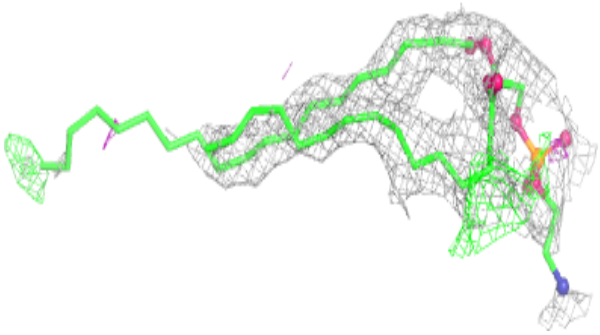
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

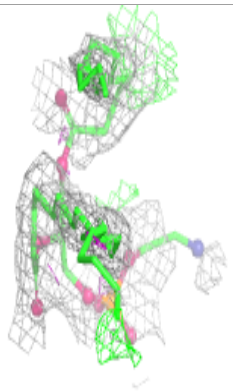


Electron density around PTY C 1101:

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

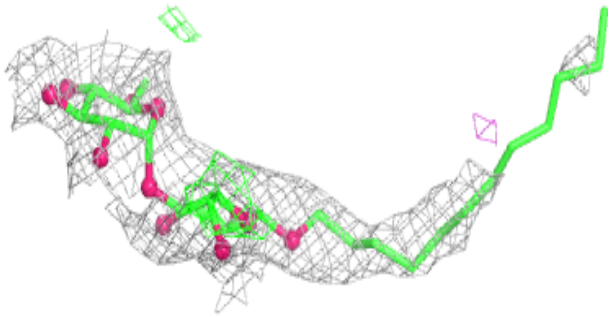


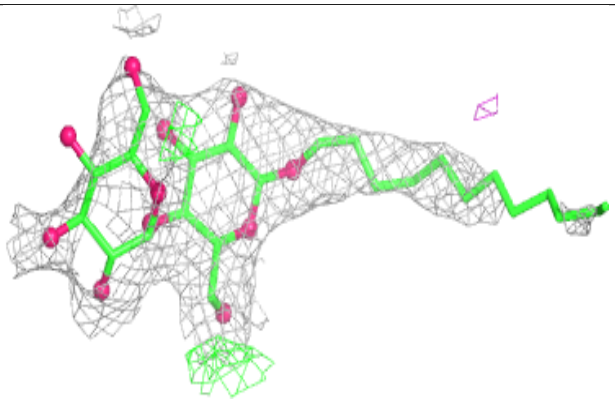


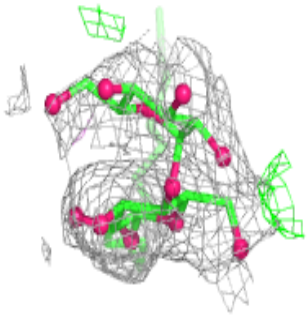


Electron density around LMT A 1101:

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

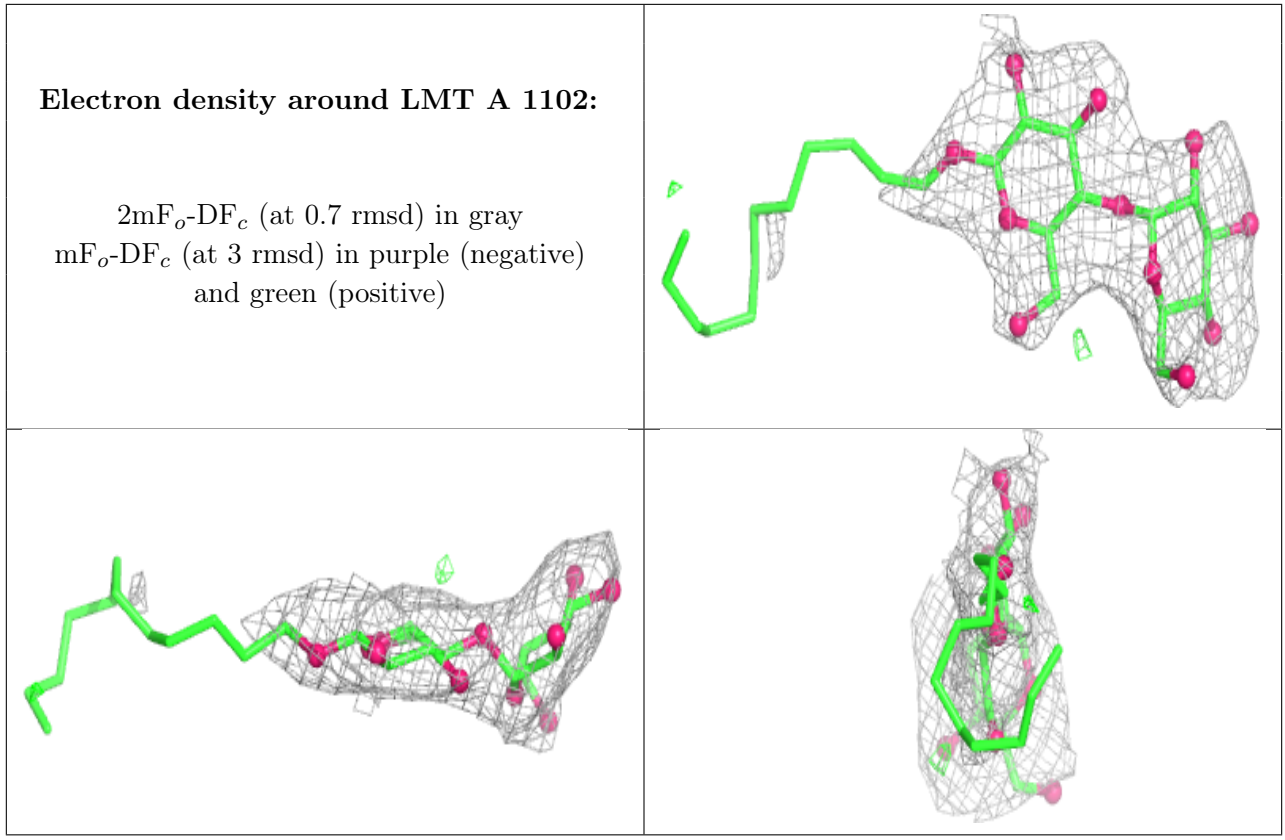






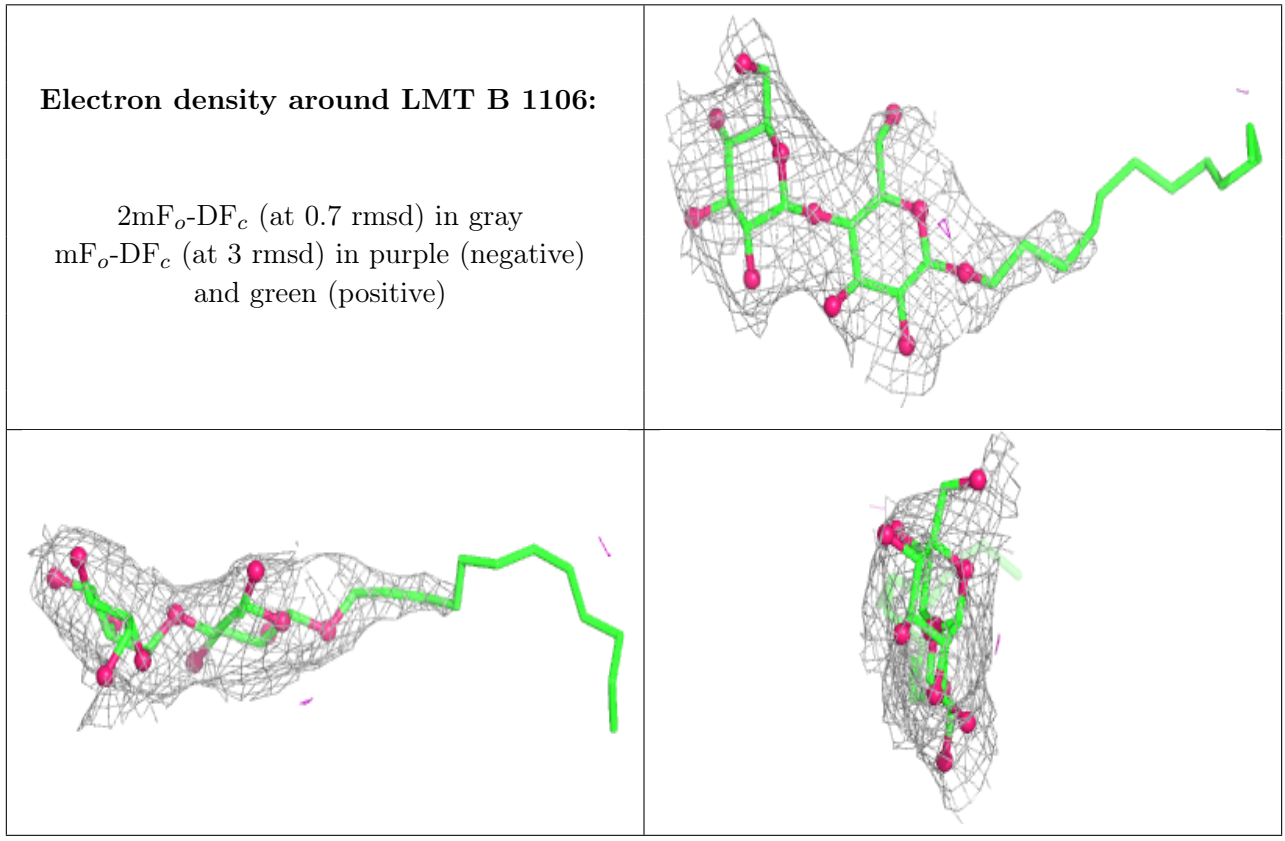
Electron density around LMT A 1102:

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



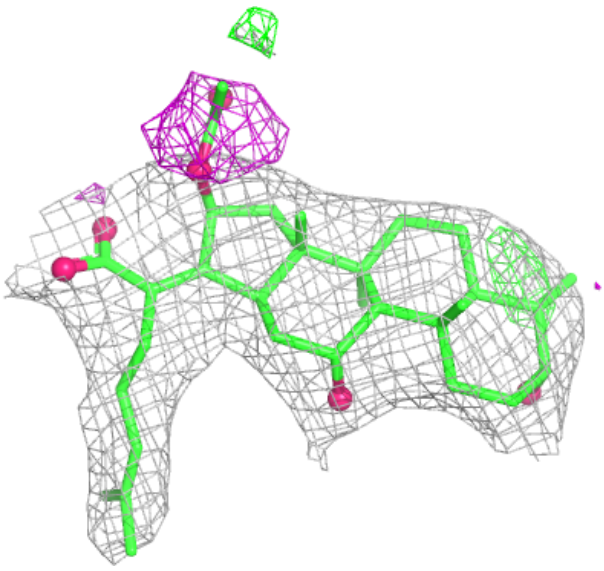
Electron density around LMT B 1106:

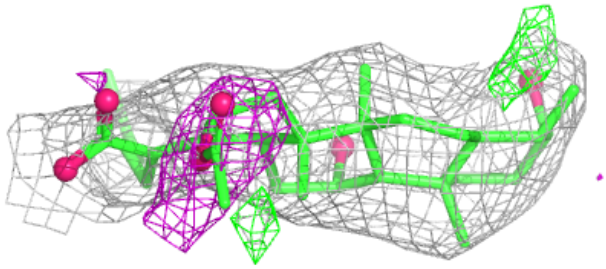
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

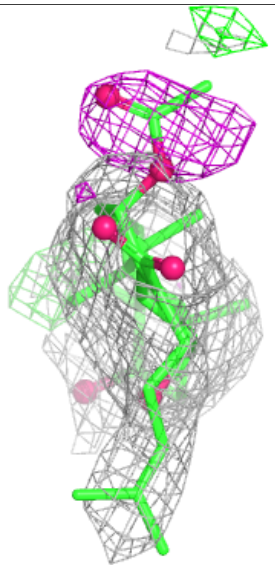


Electron density around FUA B 1104:

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

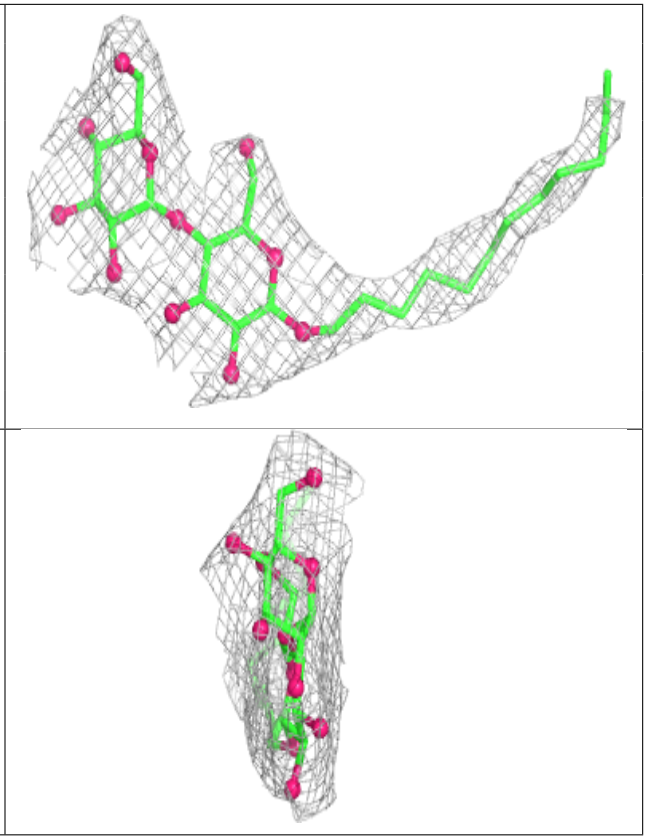






Electron density around LMT C 1102:

$2mF_o$-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 (i)

There are no such residues in this entry.