



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2024 – 11:57 PM EDT

PDB ID : 6ZOD
Title : Fusidic acid binding to the allosteric deep transmembrane domain binding pocket, TM7/TM8 groove, and TM1/TM2 groove of the fully induced AcrB T protomer
Authors : Oswald, C.; Tam, H.K.; Pos, K.M.
Deposited on : 2020-07-07
Resolution : 2.85 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

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	:	4.02b-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

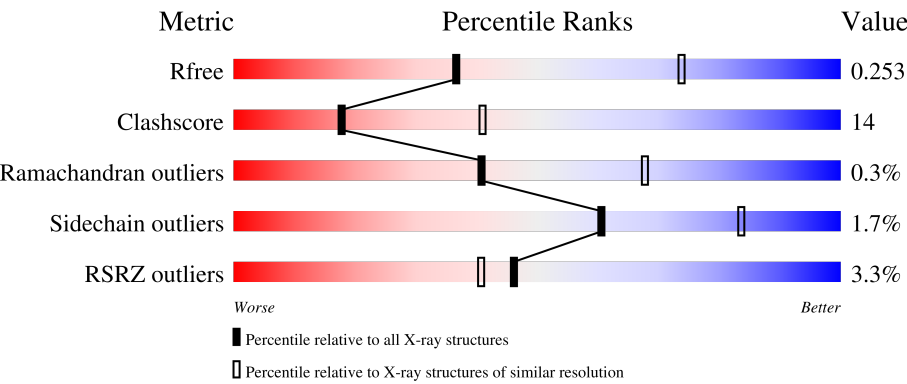
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	<div><div>2%</div><div>70%28%</div><div></div></div>
1	B	1057	<div><div>2%</div><div>71%25%</div><div></div></div>
1	C	1057	<div><div>2%</div><div>71%26%</div><div></div></div>
2	D	169	<div><div>10%</div><div>72%18%9%</div><div></div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	169	<div><div></div><div>21%</div><div>56%</div><div>33%</div><div>10%</div></div>

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 26706 atoms, of which 126 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	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	B	1020	Total	C	N	O	S	0	0	0
			7771	5007	1280	1440	44			
1	C	1032	Total	C	N	O	S	0	0	0
			7838	5043	1294	1457	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...

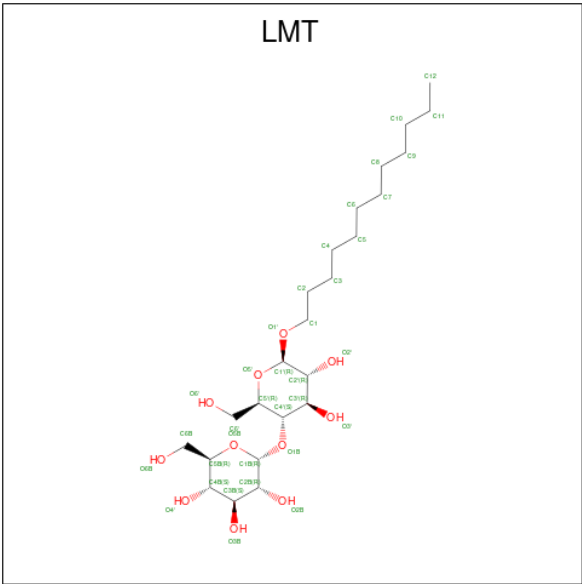
Continued from previous page...

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	154	Total	C	N	O	S	0	0	0
			1167	736	204	226	1			
2	E	152	Total	C	N	O	S	0	0	0
			1150	727	201	221	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



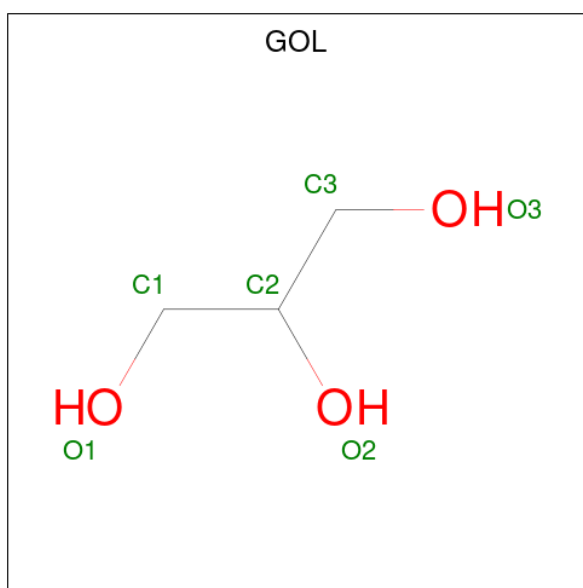
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	O		0	0
			4	2	2			
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	O		0	0
			4	2	2			
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

Continued on next page...

Continued from previous page...

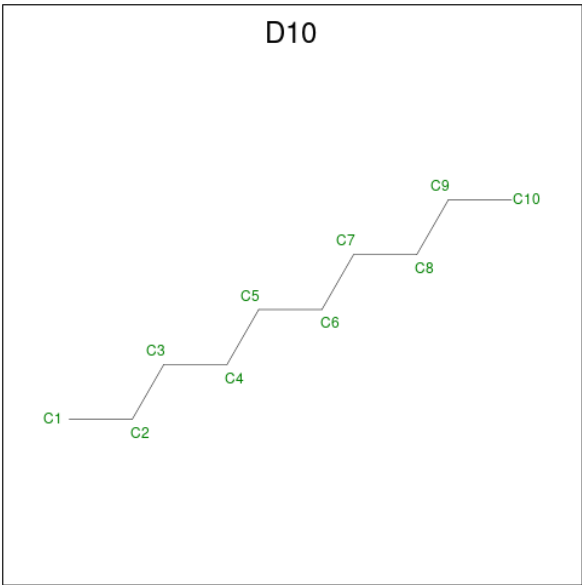
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C H O 10 2 6 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



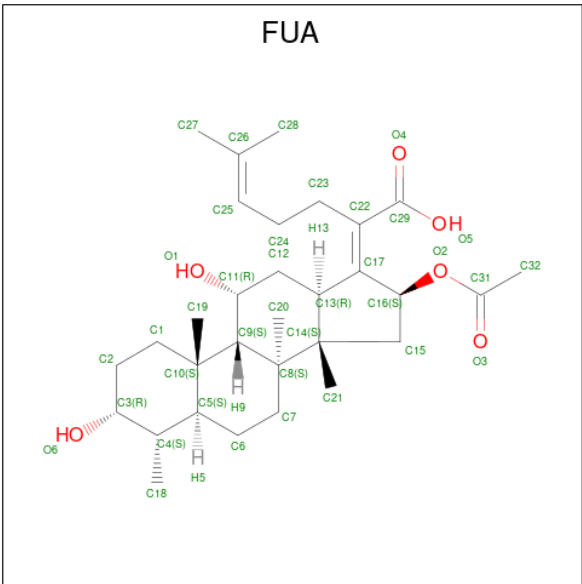
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is DECANE (three-letter code: D10) (formula: $C_{10}H_{22}$).



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		

- Molecule 7 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆) (labeled as "Ligand of Interest" by depositor).



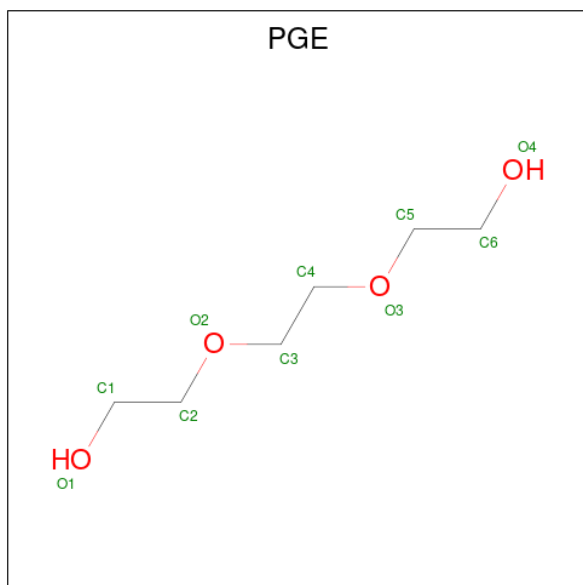
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			37	31	6		

Continued on next page...

Continued from previous page...

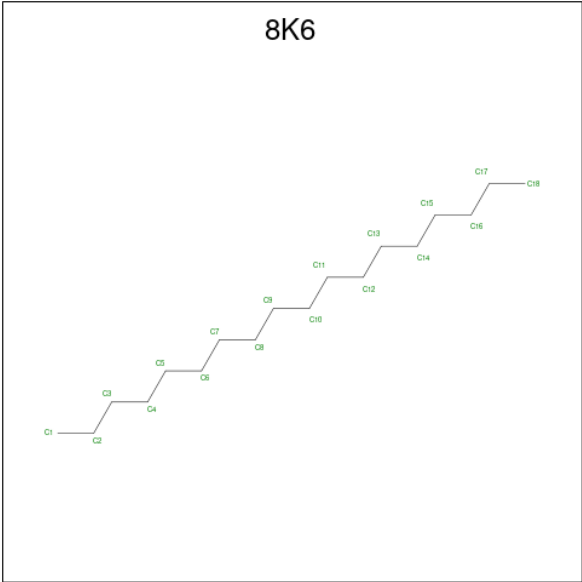
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			37	31	6		
7	B	1	Total	C	O	0	0
			37	31	6		
7	B	1	Total	C	O	0	0
			37	31	6		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



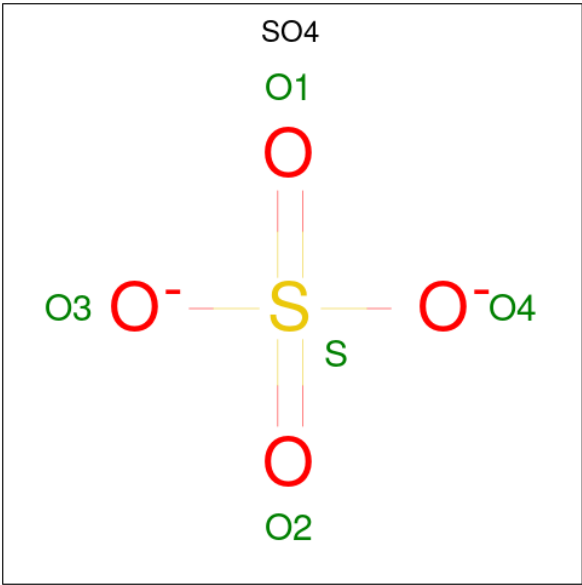
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is Octadecane (three-letter code: 8K6) (formula: $C_{18}H_{38}$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	C	0	0
			18	18		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



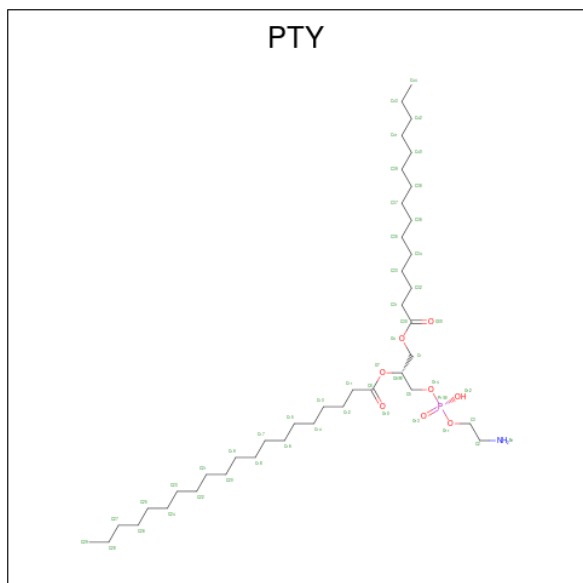
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		
10	B	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

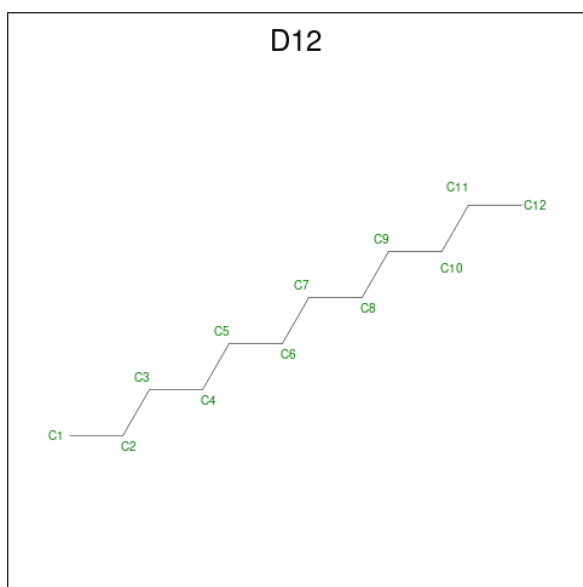
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



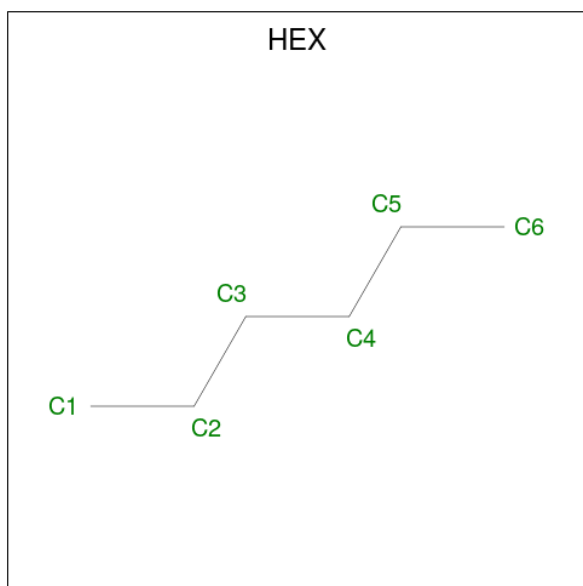
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			50	40	1	8	1		

- Molecule 12 is DODECANE (three-letter code: D12) (formula: $C_{12}H_{26}$).



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

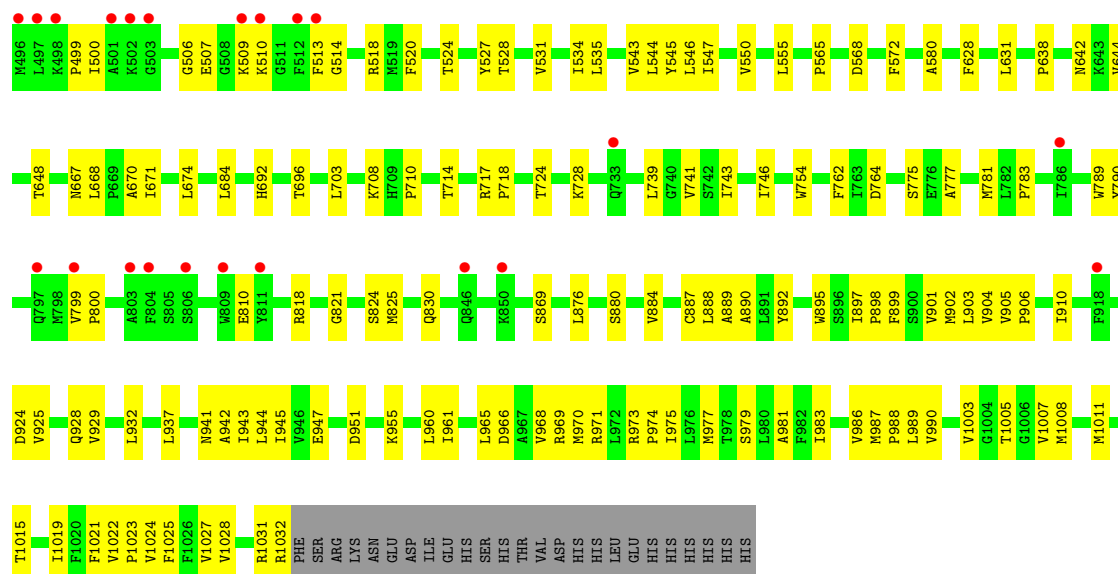
- Molecule 13 is HEXANE (three-letter code: HEX) (formula: C₆H₁₄).



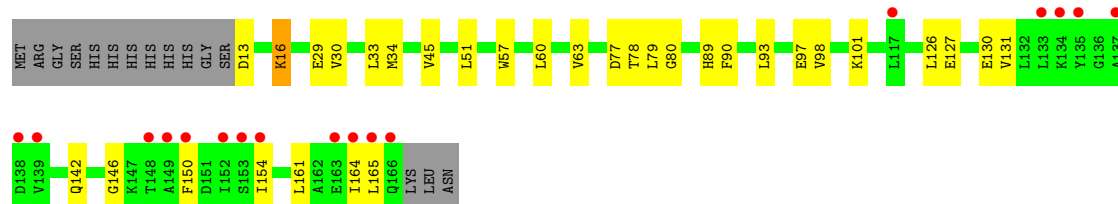
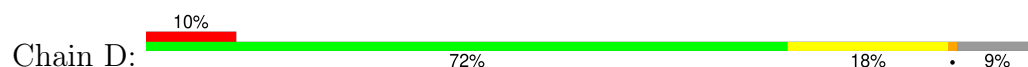
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	H	0	0
			20	6	14		

- Molecule 14 is water.

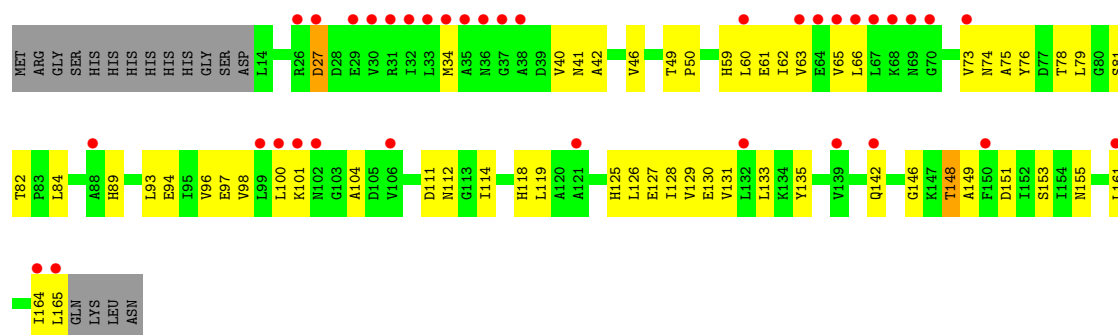
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	54	Total 54	O 54	0	0
14	B	45	Total 45	O 45	0	0
14	C	45	Total 45	O 45	0	0
14	D	3	Total 3	O 3	0	0
14	E	2	Total 2	O 2	0	0



• 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 166.13Å 243.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.85 49.12 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.12-2.85) 97.4 (49.12-2.85)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.86Å)	Xtriage
Refinement program	PHENIX 3707	Depositor
R, R_{free}	0.205 , 0.247 0.210 , 0.253	Depositor DCC
R_{free} test set	6708 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	69.8	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	26706	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: D12, D10, PGE, FUA, 8K6, EDO, LMT, GOL, PTY, SO4, HEX

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	0.32	0/7999	0.50	1/10863 (0.0%)
1	B	0.31	0/7920	0.48	0/10754
1	C	0.34	0/7987	0.50	0/10847
2	D	0.32	0/1186	0.49	0/1613
2	E	0.29	0/1169	0.47	0/1590
All	All	0.32	0/26261	0.49	1/35667 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	LEU	CA-CB-CG	5.72	128.46	115.30

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	7849	0	8001	228	0
1	B	7771	0	7925	217	0
1	C	7838	0	7992	209	0
2	D	1167	0	1151	25	0
2	E	1150	0	1139	40	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	140	0	184	18	0
3	C	105	0	138	6	0
4	A	24	24	36	0	0
4	B	20	18	30	2	0
4	C	8	0	12	0	0
4	D	8	0	12	0	0
5	A	6	0	8	1	0
5	B	6	0	8	1	0
6	A	10	22	22	1	0
6	B	10	22	22	0	0
7	A	37	0	47	8	0
7	B	111	0	141	27	0
8	B	10	0	14	1	0
9	B	18	0	38	3	0
10	B	20	0	0	0	0
10	C	5	0	0	0	0
11	C	100	0	158	7	0
12	C	12	26	26	0	0
13	C	6	14	14	0	0
14	A	54	0	0	0	0
14	B	45	0	0	0	0
14	C	45	0	0	0	0
14	D	3	0	0	0	0
14	E	2	0	0	0	0
All	All	26580	126	27118	727	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 14.

The worst 5 of 727 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:C:356:TYR:HA	1:C:365:THR:HG21	1.41	1.01
3:C:1305:LMT:H3O2	3:C:1305:LMT:H2O1	1.10	0.99
1:A:356:TYR:HA	1:A:365:THR:HG21	1.52	0.90
1:A:376:LEU:HD11	1:A:402:ILE:HD11	1.54	0.89
1:B:1013:THR:HA	1:B:1016:VAL:HG22	1.55	0.88

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	1031/1057 (98%)	996 (97%)	30 (3%)	5 (0%)	29	57
1	B	1016/1057 (96%)	988 (97%)	24 (2%)	4 (0%)	34	62
1	C	1030/1057 (97%)	1002 (97%)	28 (3%)	0	100	100
2	D	152/169 (90%)	147 (97%)	5 (3%)	0	100	100
2	E	150/169 (89%)	142 (95%)	8 (5%)	0	100	100
All	All	3379/3509 (96%)	3275 (97%)	95 (3%)	9 (0%)	41	68

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	538	THR
1	A	869	SER
1	B	313	MET
1	B	216	ALA
1	A	677	ALA

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	839/863 (97%)	827 (99%)	12 (1%)	67	86
1	B	832/863 (96%)	814 (98%)	18 (2%)	52	79
1	C	838/863 (97%)	828 (99%)	10 (1%)	71	89
2	D	119/132 (90%)	117 (98%)	2 (2%)	60	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	117/132 (89%)	113 (97%)	4 (3%)	37 67
All	All	2745/2853 (96%)	2699 (98%)	46 (2%)	60 83

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	938	SER
1	C	180	SER
1	B	1032	ARG
1	C	104	GLN
1	C	510	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	604	ASN
1	C	104	GLN
1	C	726	GLN
1	C	697	GLN
1	A	923	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

41 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	$\# Z > 2$
9	8K6	B	1208	-	17,17,17	0.14	0	16,16,16	0.10	0
4	EDO	A	1110	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	A	1106	-	3,3,3	0.48	0	2,2,2	0.46	0
7	FUA	B	1213	-	39,40,40	1.29	2 (5%)	50,64,64	1.99	13 (26%)
10	SO4	B	1209	-	4,4,4	0.24	0	6,6,6	0.12	0
6	D10	A	1107	-	9,9,9	0.10	0	8,8,8	0.38	0
10	SO4	B	1212	-	4,4,4	0.28	0	6,6,6	0.17	0
3	LMT	C	1306	-	36,36,36	0.42	0	47,47,47	0.74	0
3	LMT	A	1101	-	36,36,36	0.40	0	47,47,47	1.39	7 (14%)
5	GOL	A	1105	-	5,5,5	1.03	0	5,5,5	0.88	0
6	D10	B	1207	-	9,9,9	0.13	0	8,8,8	0.26	0
4	EDO	D	202	-	3,3,3	0.49	0	2,2,2	0.20	0
4	EDO	B	1205	-	3,3,3	0.44	0	2,2,2	0.44	0
4	EDO	A	1108	-	3,3,3	0.48	0	2,2,2	0.34	0
11	PTY	C	1307	-	49,49,49	0.95	2 (4%)	52,54,54	1.03	3 (5%)
10	SO4	B	1210	-	4,4,4	0.26	0	6,6,6	0.07	0
5	GOL	B	1202	-	5,5,5	0.91	0	5,5,5	1.13	0
4	EDO	A	1109	-	3,3,3	0.48	0	2,2,2	0.31	0
8	PGE	B	1204	-	9,9,9	0.33	0	8,8,8	0.25	0
4	EDO	B	1203	-	3,3,3	0.43	0	2,2,2	0.41	0
3	LMT	A	1103	-	36,36,36	0.48	1 (2%)	47,47,47	0.96	1 (2%)
7	FUA	B	1214	-	39,40,40	1.24	3 (7%)	50,64,64	1.91	8 (16%)
4	EDO	C	1301	-	3,3,3	0.46	0	2,2,2	0.25	0
4	EDO	A	1102	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	A	1104	-	3,3,3	0.43	0	2,2,2	0.45	0
3	LMT	C	1302	-	36,36,36	0.48	0	47,47,47	1.06	4 (8%)
4	EDO	D	201	-	3,3,3	0.41	0	2,2,2	0.50	0
13	HEX	C	1309	-	5,5,5	0.14	0	4,4,4	0.33	0
3	LMT	C	1305	-	36,36,36	0.45	0	47,47,47	0.78	1 (2%)
11	PTY	C	1303	-	49,49,49	0.93	2 (4%)	52,54,54	1.04	4 (7%)
3	LMT	A	1111	-	36,36,36	0.51	0	47,47,47	1.16	5 (10%)
7	FUA	B	1215	-	39,40,40	1.35	4 (10%)	50,64,64	2.13	12 (24%)
4	EDO	B	1216	-	3,3,3	0.47	0	2,2,2	0.47	0
12	D12	C	1308	-	11,11,11	0.23	0	10,10,10	0.64	0
10	SO4	C	1310	-	4,4,4	0.25	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	1304	-	3,3,3	0.47	0	2,2,2	0.35	0
3	LMT	A	1112	-	36,36,36	0.52	0	47,47,47	1.15	5 (10%)
7	FUA	A	1113	-	39,40,40	1.28	2 (5%)	50,64,64	1.79	9 (18%)
4	EDO	B	1206	-	3,3,3	0.49	0	2,2,2	0.38	0
4	EDO	B	1201	-	3,3,3	0.44	0	2,2,2	0.41	0
10	SO4	B	1211	-	4,4,4	0.26	0	6,6,6	0.08	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
9	8K6	B	1208	-	-	4/15/15/15	-
4	EDO	A	1110	-	-	0/1/1/1	-
4	EDO	A	1106	-	-	1/1/1/1	-
7	FUA	B	1213	-	-	4/16/92/92	0/4/4/4
6	D10	A	1107	-	-	2/7/7/7	-
3	LMT	C	1306	-	-	9/21/61/61	0/2/2/2
3	LMT	A	1101	-	-	12/21/61/61	0/2/2/2
5	GOL	A	1105	-	-	0/4/4/4	-
6	D10	B	1207	-	-	0/7/7/7	-
4	EDO	D	202	-	-	0/1/1/1	-
4	EDO	B	1205	-	-	0/1/1/1	-
4	EDO	A	1108	-	-	0/1/1/1	-
11	PTY	C	1307	-	-	29/53/53/53	-
5	GOL	B	1202	-	-	2/4/4/4	-
4	EDO	A	1109	-	-	0/1/1/1	-
8	PGE	B	1204	-	-	2/7/7/7	-
4	EDO	B	1203	-	-	1/1/1/1	-
3	LMT	A	1103	-	-	8/21/61/61	0/2/2/2
7	FUA	B	1214	-	-	6/16/92/92	0/4/4/4
4	EDO	C	1301	-	-	0/1/1/1	-
4	EDO	A	1102	-	-	0/1/1/1	-
4	EDO	A	1104	-	-	0/1/1/1	-
3	LMT	C	1302	-	-	6/21/61/61	0/2/2/2
4	EDO	D	201	-	-	0/1/1/1	-
13	HEX	C	1309	-	-	1/3/3/3	-
3	LMT	C	1305	-	-	10/21/61/61	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	PTY	C	1303	-	-	19/53/53/53	-
3	LMT	A	1111	-	-	14/21/61/61	0/2/2/2
7	FUA	B	1215	-	-	5/16/92/92	0/4/4/4
4	EDO	B	1216	-	-	1/1/1/1	-
12	D12	C	1308	-	-	4/9/9/9	-
4	EDO	C	1304	-	-	0/1/1/1	-
3	LMT	A	1112	-	-	5/21/61/61	0/2/2/2
7	FUA	A	1113	-	-	6/16/92/92	0/4/4/4
4	EDO	B	1206	-	-	0/1/1/1	-
4	EDO	B	1201	-	-	0/1/1/1	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1214	FUA	O2-C31	5.29	1.46	1.35
7	A	1113	FUA	O2-C31	5.12	1.46	1.35
7	B	1215	FUA	O2-C31	5.06	1.46	1.35
7	B	1213	FUA	O2-C31	4.98	1.46	1.35
11	C	1307	PTY	O4-C30	4.33	1.46	1.33

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1215	FUA	C21-C14-C8	-6.22	107.07	112.23
7	B	1214	FUA	O2-C31-C32	5.57	121.03	111.09
7	A	1113	FUA	O2-C31-C32	5.48	120.86	111.09
7	B	1214	FUA	C21-C14-C8	-5.38	107.77	112.23
7	B	1213	FUA	C16-O2-C31	-5.35	109.06	117.00

There are no chirality outliers.

5 of 151 torsion outliers are listed below:

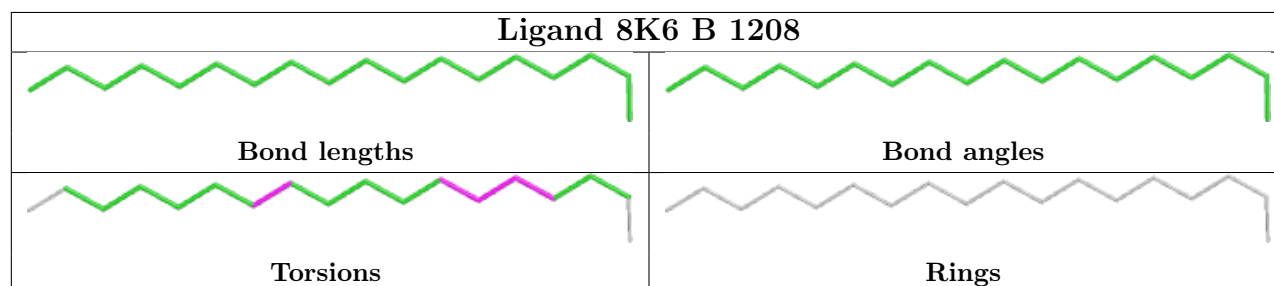
Mol	Chain	Res	Type	Atoms
3	A	1112	LMT	C2'-C1'-O1'-C1
3	C	1305	LMT	C2-C1-O1'-C1'
7	A	1113	FUA	C17-C22-C23-C24
7	A	1113	FUA	C29-C22-C23-C24
7	A	1113	FUA	C23-C22-C29-O4

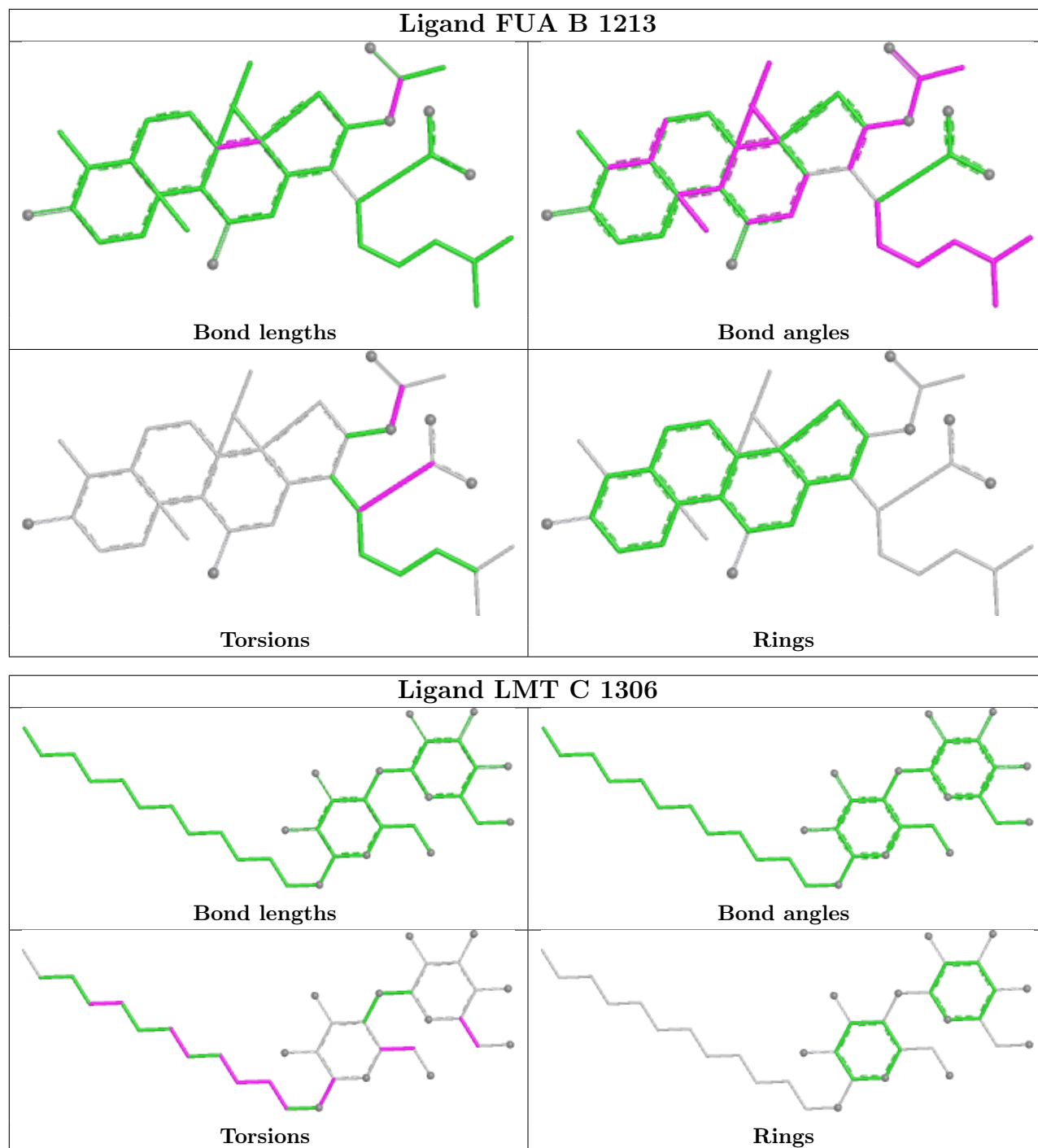
There are no ring outliers.

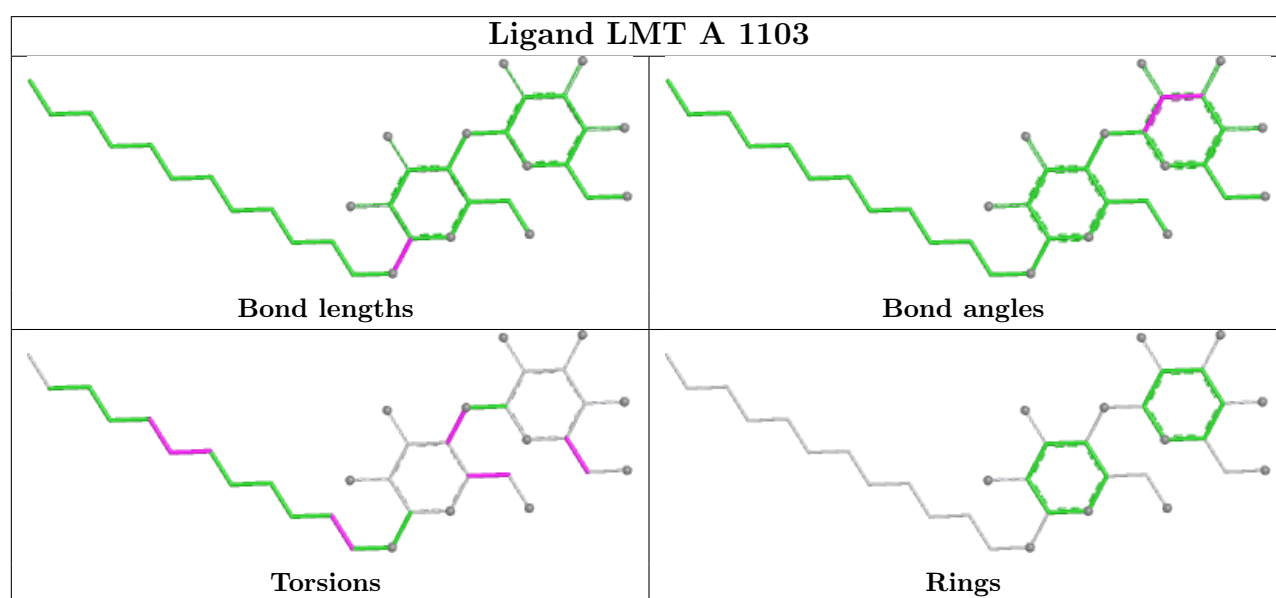
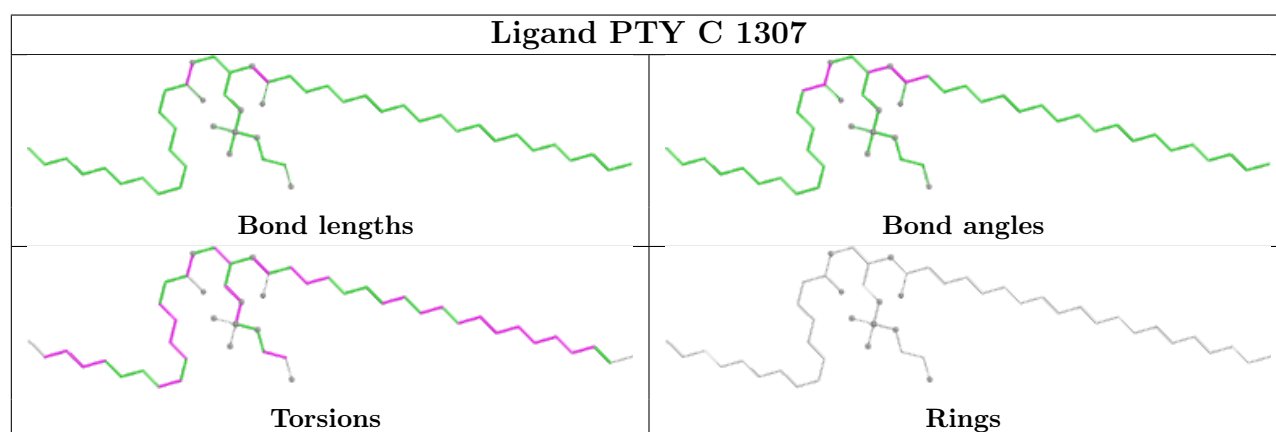
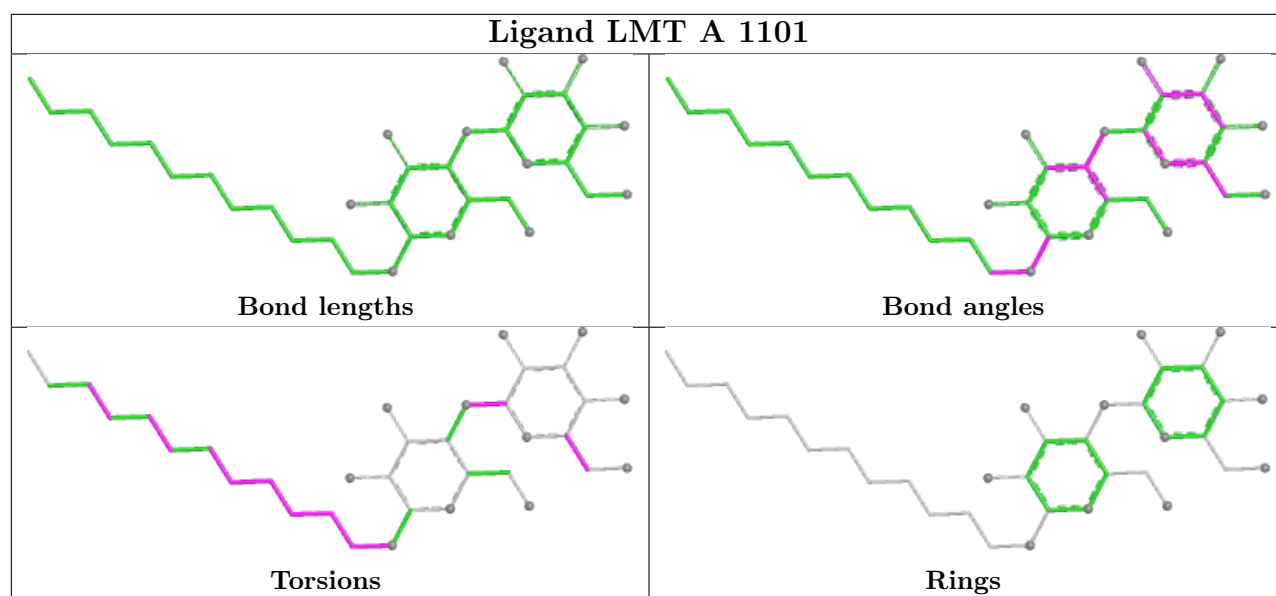
19 monomers are involved in 72 short contacts:

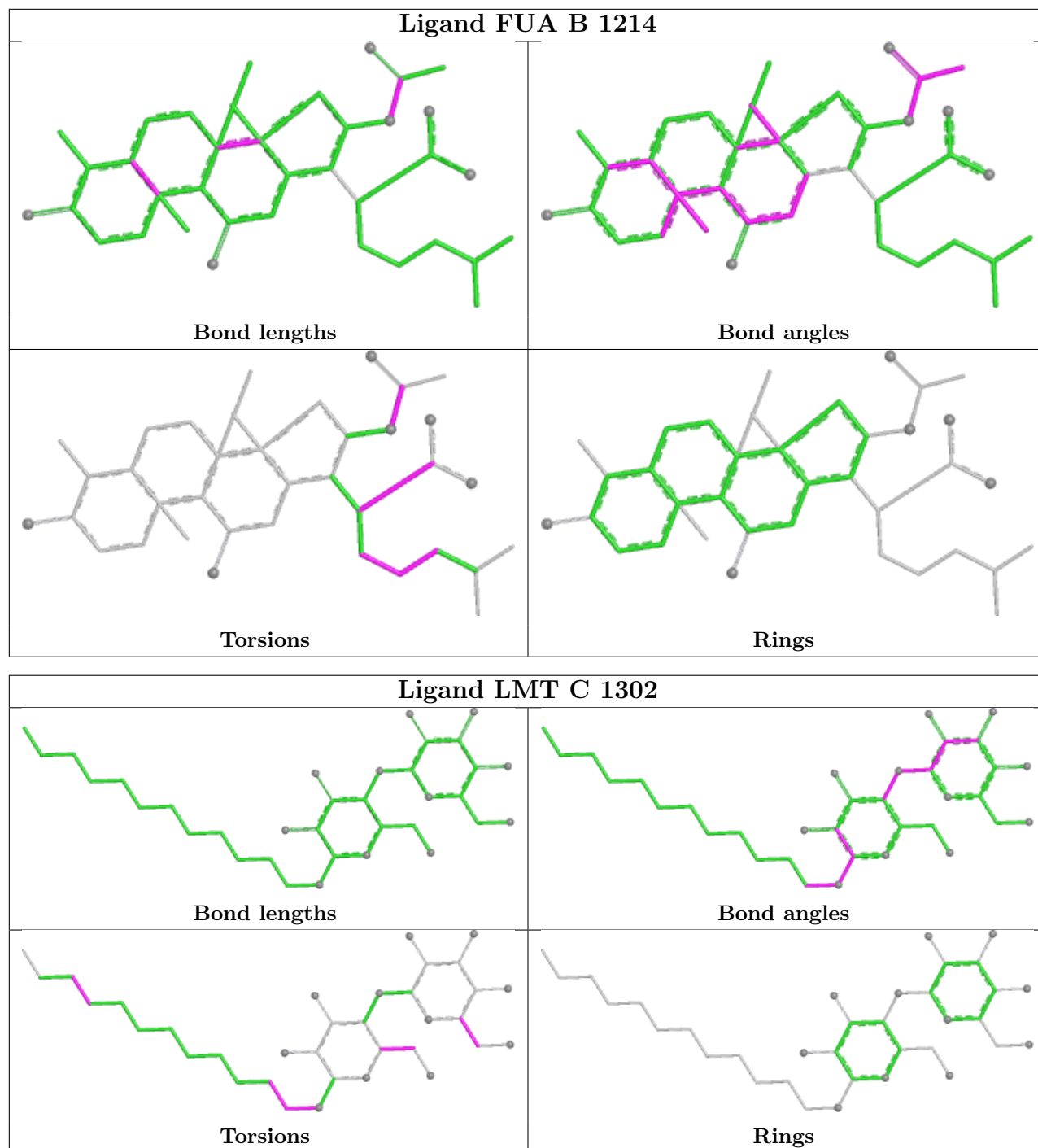
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	1208	8K6	3	0
7	B	1213	FUA	11	0
6	A	1107	D10	1	0
3	C	1306	LMT	4	0
3	A	1101	LMT	4	0
5	A	1105	GOL	1	0
4	B	1205	EDO	1	0
11	C	1307	PTY	4	0
5	B	1202	GOL	1	0
8	B	1204	PGE	1	0
3	A	1103	LMT	5	0
7	B	1214	FUA	8	0
3	C	1305	LMT	2	0
11	C	1303	PTY	3	0
3	A	1111	LMT	7	0
7	B	1215	FUA	8	0
3	A	1112	LMT	2	0
7	A	1113	FUA	8	0
4	B	1206	EDO	1	0

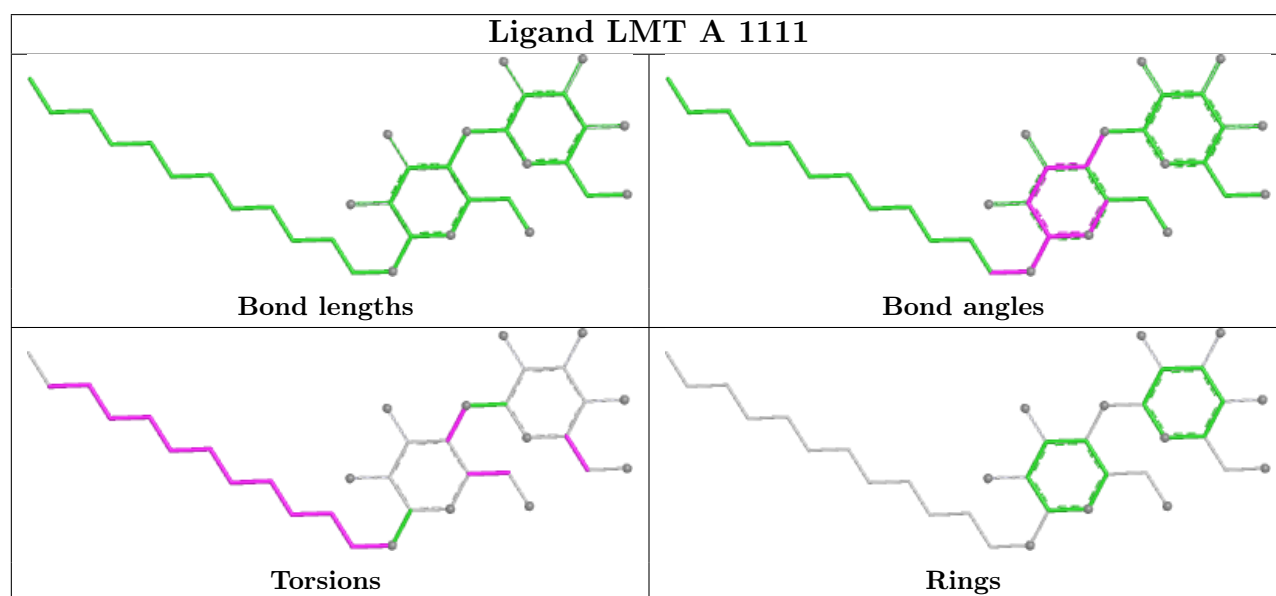
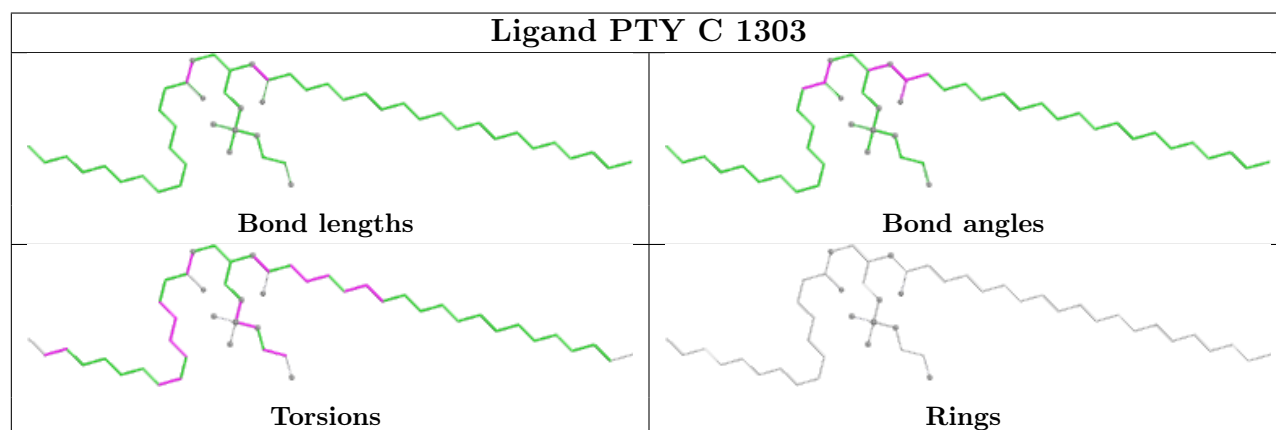
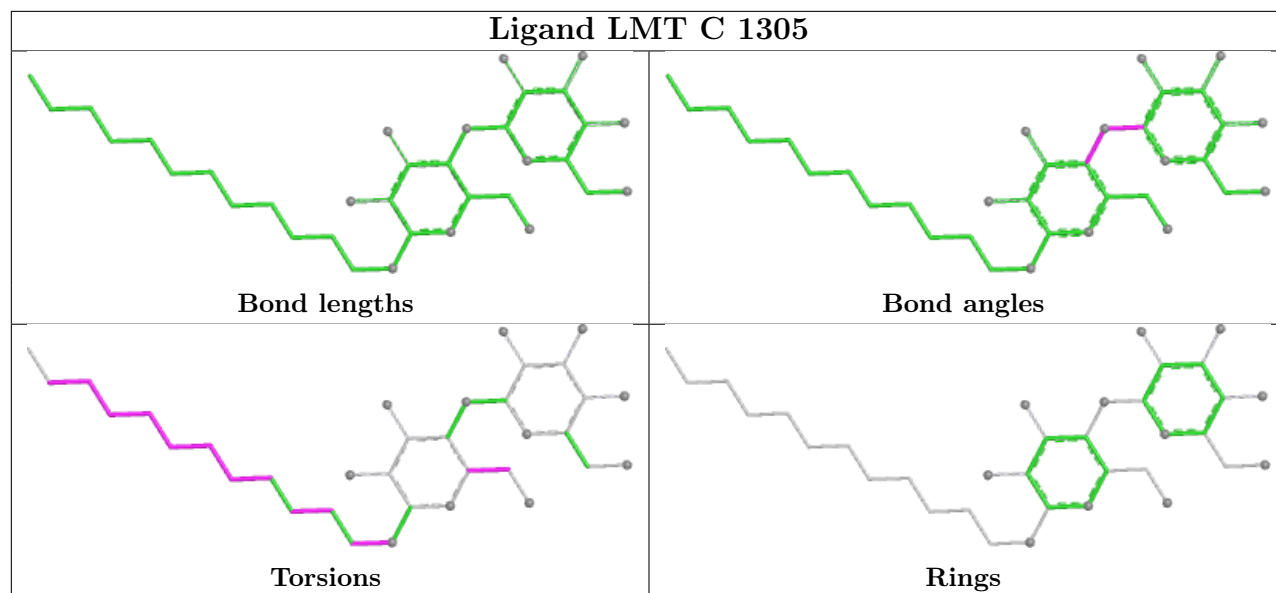
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

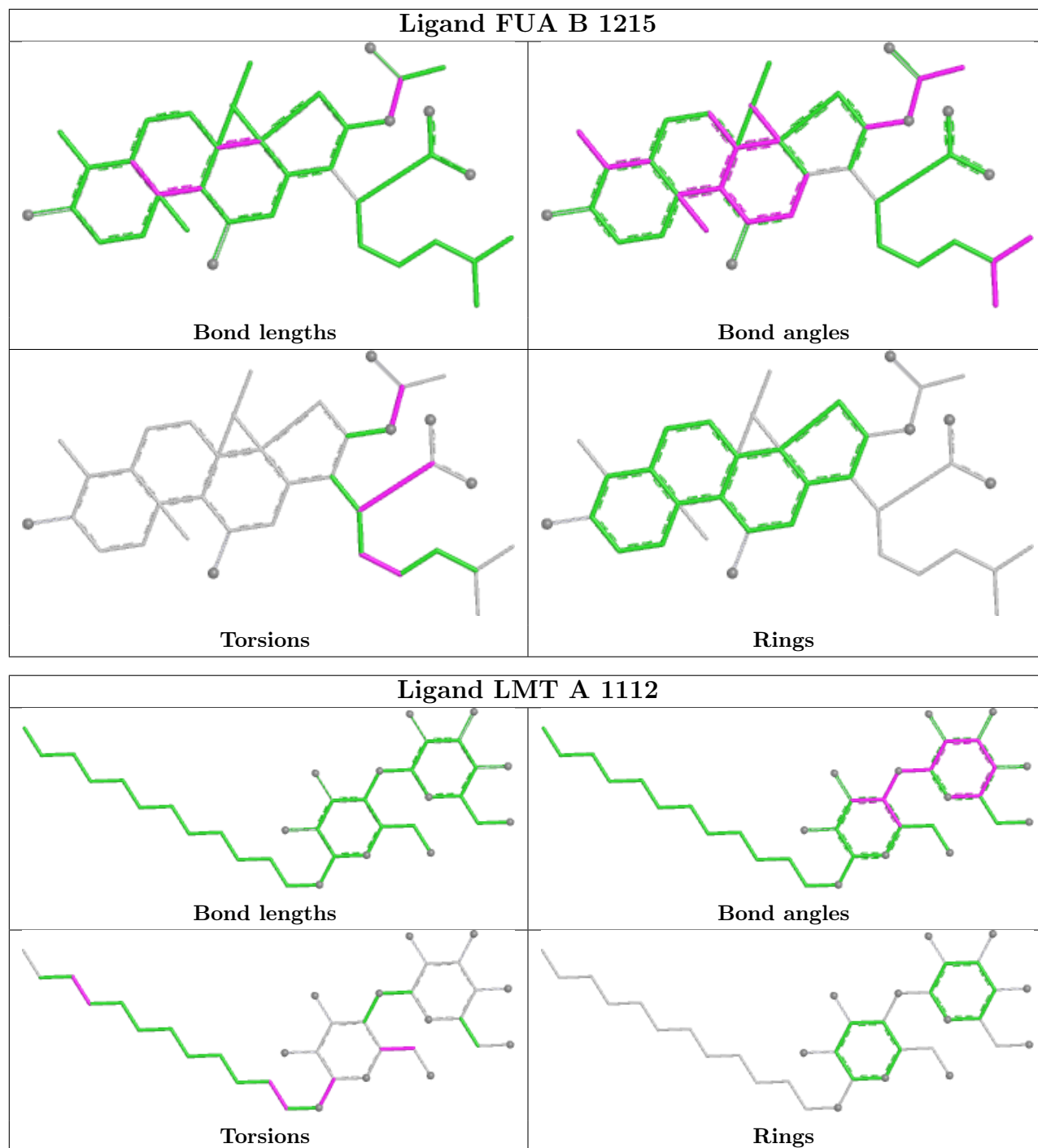


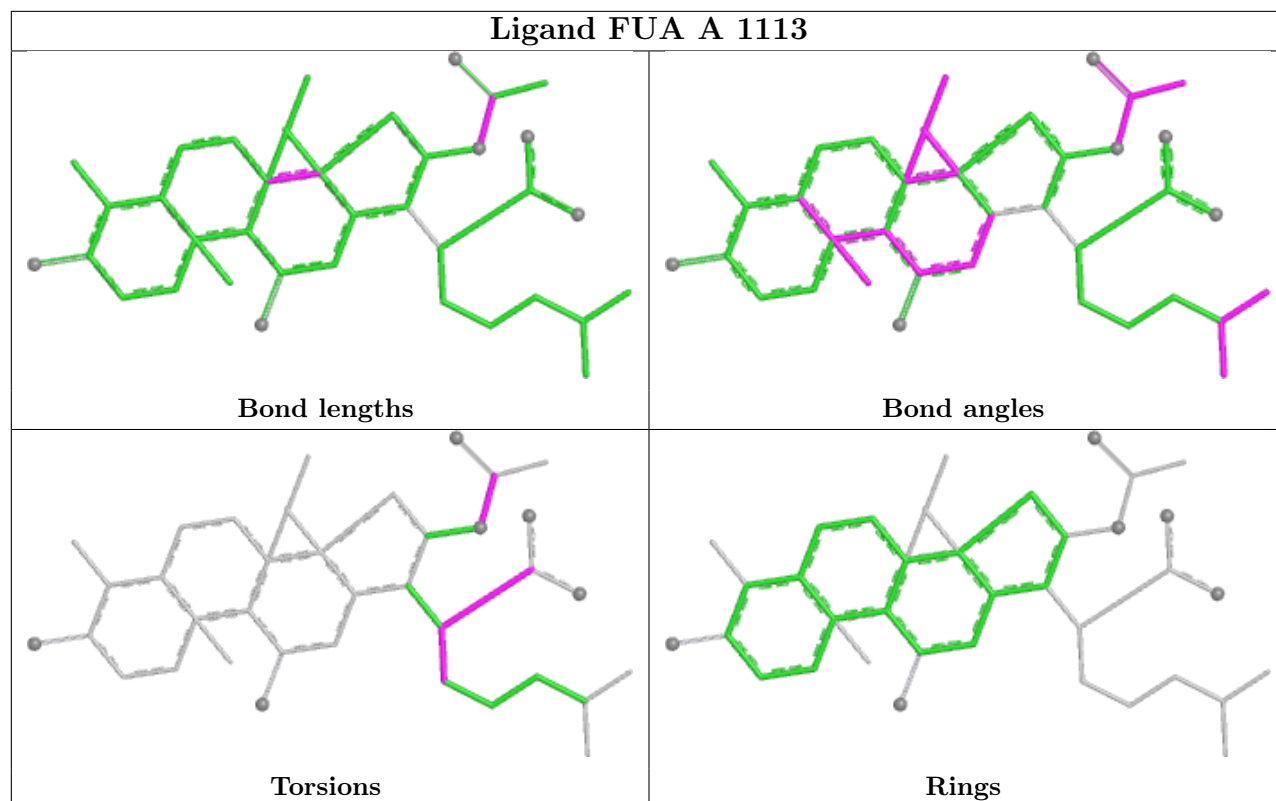












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	1033/1057 (97%)	-0.10	18 (1%) 70 68	35, 72, 122, 157	0
1	B	1020/1057 (96%)	-0.10	18 (1%) 68 66	37, 77, 113, 180	0
1	C	1032/1057 (97%)	-0.11	23 (2%) 62 59	36, 69, 109, 144	0
2	D	154/169 (91%)	0.31	17 (11%) 5 4	62, 78, 114, 146	0
2	E	152/169 (89%)	1.10	36 (23%) 0 0	57, 91, 122, 167	0
All	All	3391/3509 (96%)	-0.03	112 (3%) 46 41	35, 74, 115, 180	0

The worst 5 of 112 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	34	MET	6.3
1	B	316	PHE	5.2
2	E	66	LEU	5.0
1	B	1005	THR	4.8
2	E	35	ALA	4.2

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,

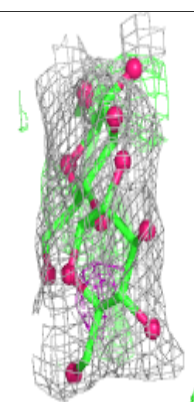
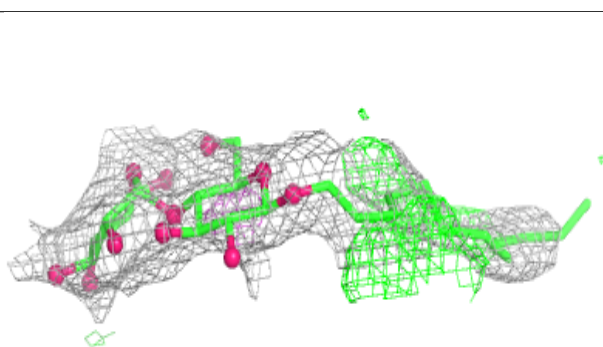
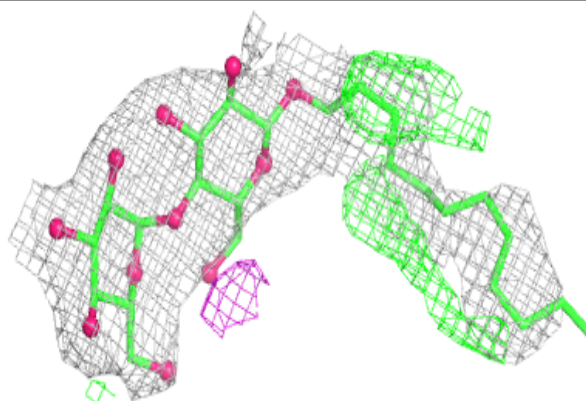
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	A	1108	4/4	0.68	0.19	111,133,148,148	0
3	LMT	C	1305	35/35	0.72	0.26	102,136,145,147	0
13	HEX	C	1309	6/6	0.75	0.34	80,99,112,112	0
7	FUA	B	1215	37/37	0.77	0.40	136,166,177,183	0
3	LMT	C	1302	35/35	0.77	0.37	91,138,155,156	0
11	PTY	C	1307	50/50	0.79	0.32	88,123,167,172	0
6	D10	A	1107	10/10	0.79	0.31	88,112,127,131	0
7	FUA	B	1214	37/37	0.81	0.34	134,158,168,171	0
3	LMT	C	1306	35/35	0.81	0.29	109,119,140,140	0
5	GOL	B	1202	6/6	0.82	0.32	82,86,92,94	0
12	D12	C	1308	12/12	0.82	0.31	72,105,126,127	0
4	EDO	C	1304	4/4	0.82	0.20	78,80,81,84	0
4	EDO	A	1110	4/4	0.83	0.30	95,114,135,135	0
3	LMT	A	1103	35/35	0.84	0.32	72,128,151,154	0
4	EDO	A	1106	4/4	0.84	0.13	88,106,114,114	0
3	LMT	A	1112	35/35	0.84	0.36	85,126,147,153	0
11	PTY	C	1303	50/50	0.86	0.35	79,107,141,156	0
3	LMT	A	1101	35/35	0.86	0.24	70,118,148,150	0
3	LMT	A	1111	35/35	0.86	0.27	81,123,137,145	0
10	SO4	B	1212	5/5	0.86	0.26	107,110,115,122	0
6	D10	B	1207	10/10	0.87	0.37	65,88,106,106	0
4	EDO	D	202	4/4	0.87	0.18	80,82,83,84	0
4	EDO	C	1301	4/4	0.87	0.40	82,86,87,89	0
4	EDO	B	1216	4/4	0.87	0.40	112,135,140,140	0
8	PGE	B	1204	10/10	0.88	0.20	83,95,105,107	0
7	FUA	A	1113	37/37	0.88	0.38	87,122,131,132	37
9	8K6	B	1208	18/18	0.90	0.21	64,89,102,104	0
7	FUA	B	1213	37/37	0.90	0.43	104,134,156,164	0
4	EDO	A	1109	4/4	0.92	0.11	67,87,96,106	0
4	EDO	A	1104	4/4	0.92	0.28	70,70,73,75	0
4	EDO	B	1201	4/4	0.93	0.32	72,74,75,80	0
10	SO4	C	1310	5/5	0.93	0.14	111,112,115,124	0
10	SO4	B	1211	5/5	0.93	0.19	121,127,135,137	0
10	SO4	B	1210	5/5	0.94	0.14	113,114,127,128	0
5	GOL	A	1105	6/6	0.94	0.36	71,83,89,90	0
4	EDO	B	1205	4/4	0.94	0.22	94,113,114,115	0
10	SO4	B	1209	5/5	0.94	0.20	121,133,135,141	0
4	EDO	D	201	4/4	0.95	0.21	74,75,78,82	0
4	EDO	A	1102	4/4	0.95	0.23	62,63,64,68	0
4	EDO	B	1203	4/4	0.95	0.23	80,80,90,95	0
4	EDO	B	1206	4/4	0.97	0.27	56,85,98,102	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.

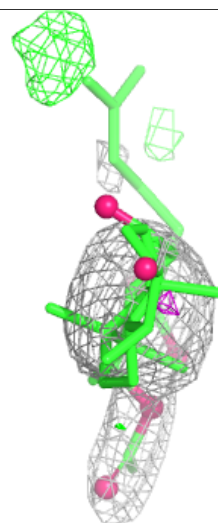
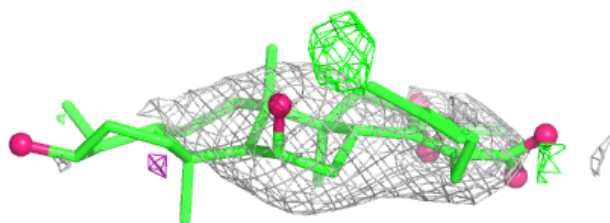
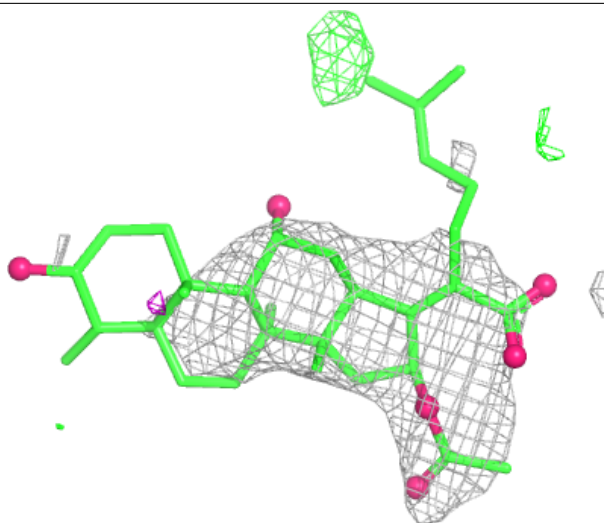
Electron density around LMT C 1305:

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



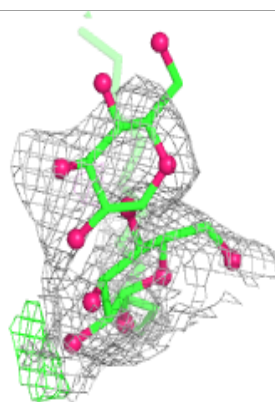
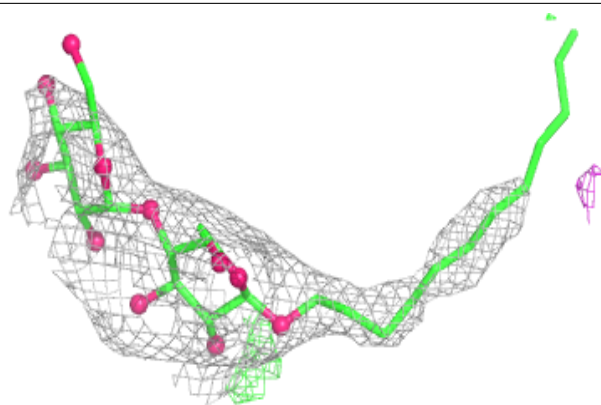
Electron density around FUA B 1215:

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

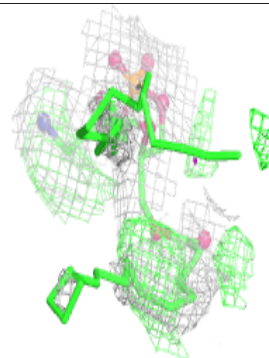
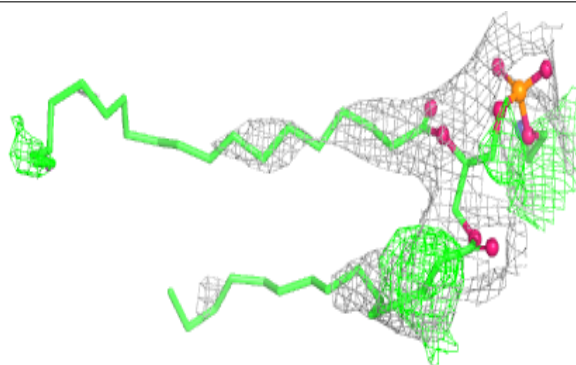


Electron density around LMT C 1302:

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

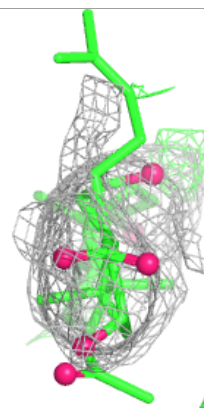
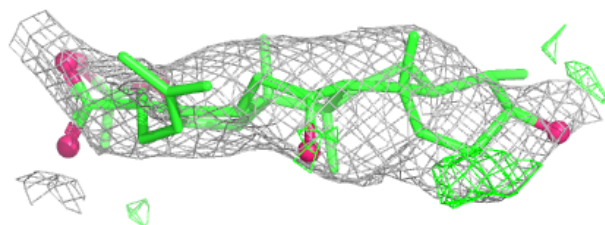
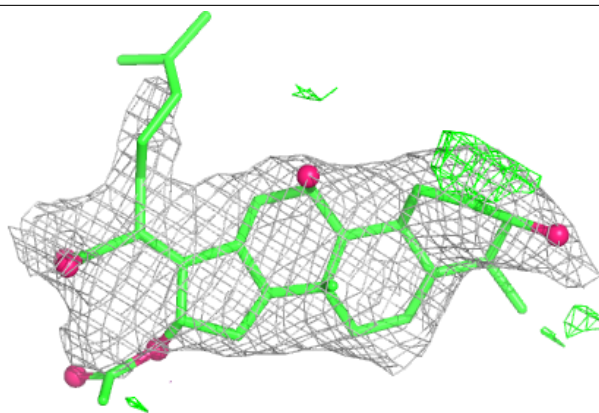
**Electron density around PTY C 1307:**

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

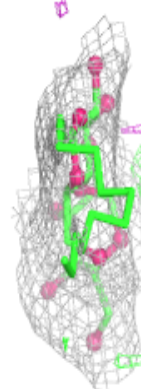
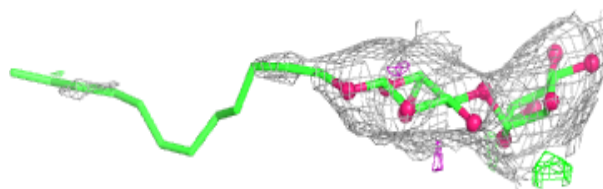
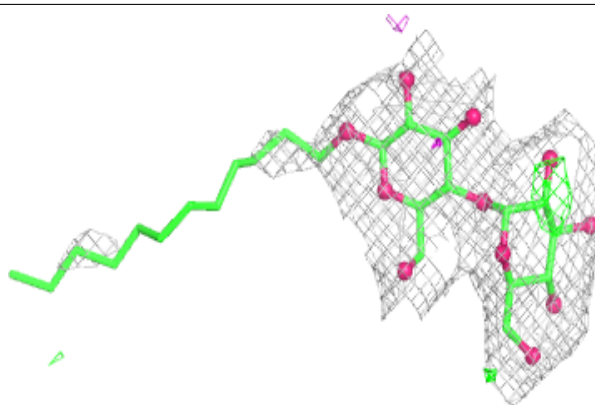


Electron density around FUA B 1214:

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

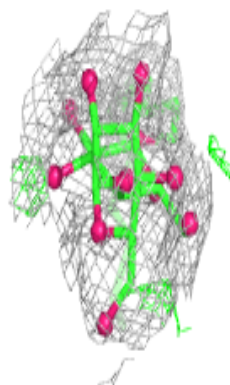
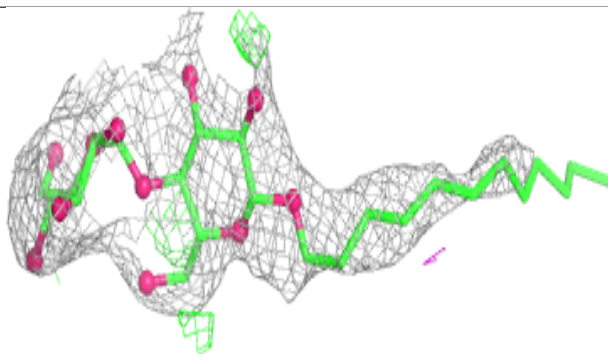
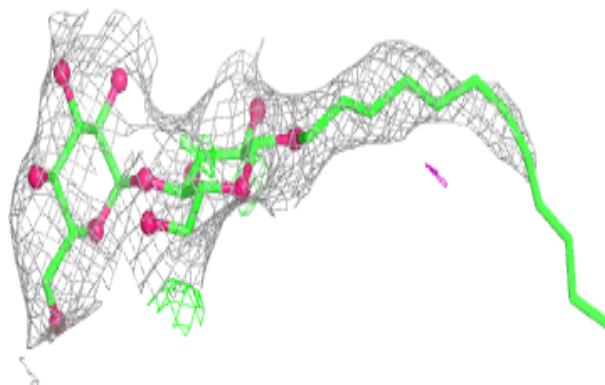
**Electron density around LMT C 1306:**

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

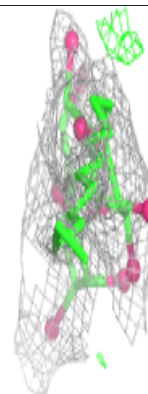
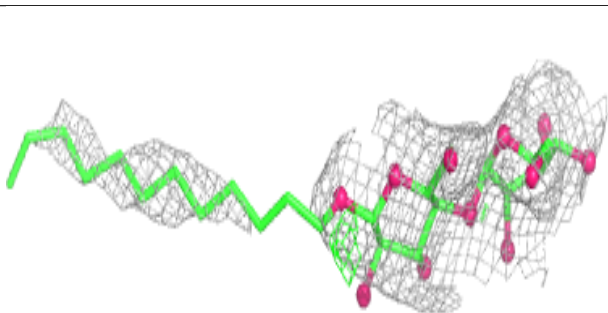
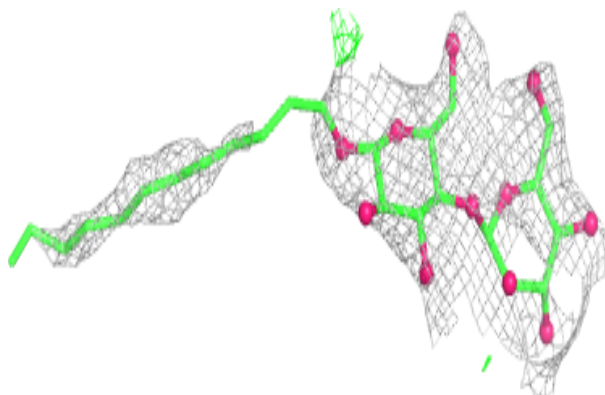


Electron density around LMT A 1103:

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

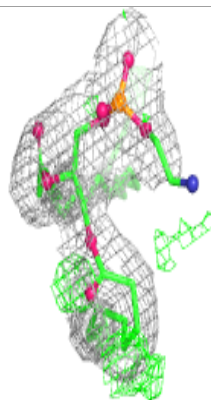
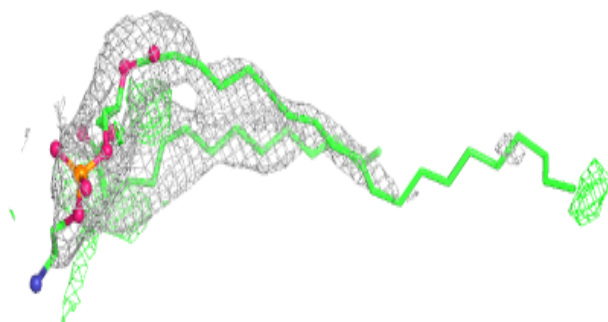
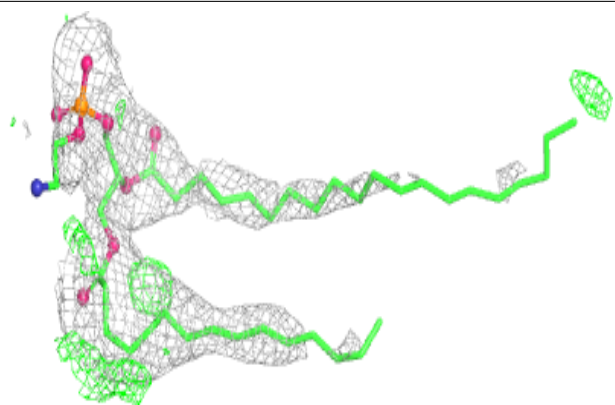
**Electron density around LMT A 1112:**

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

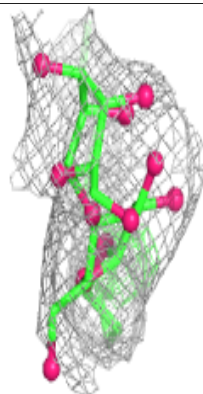
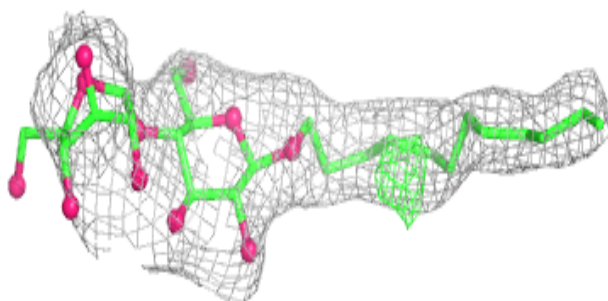
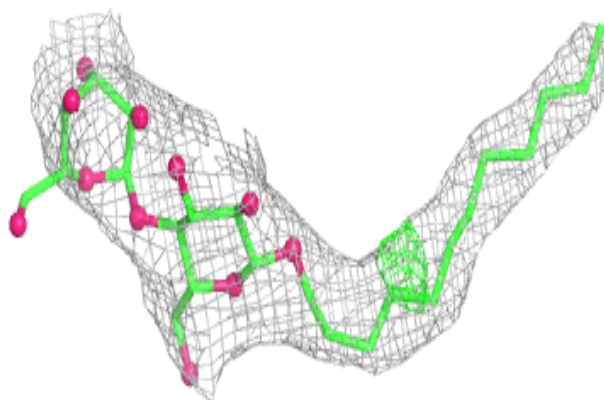


Electron density around PTY C 1303:

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

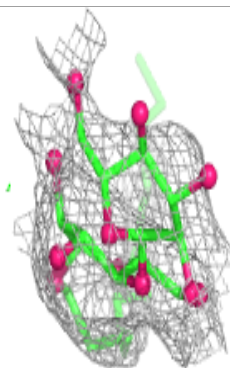
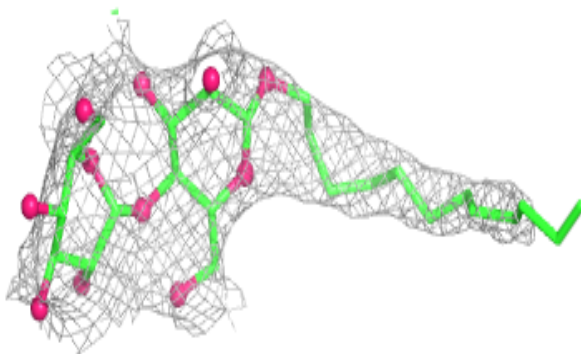
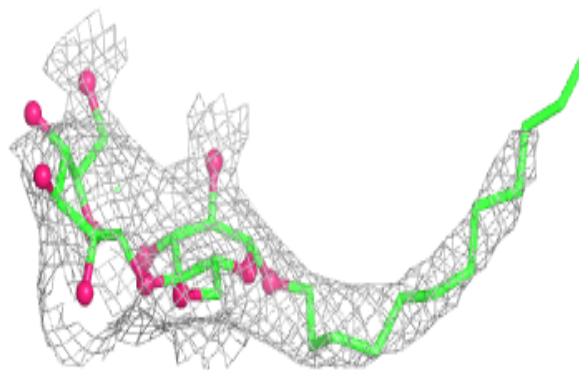
**Electron density around LMT A 1101:**

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



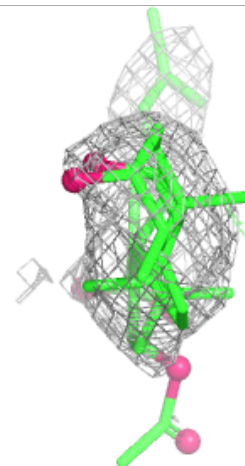
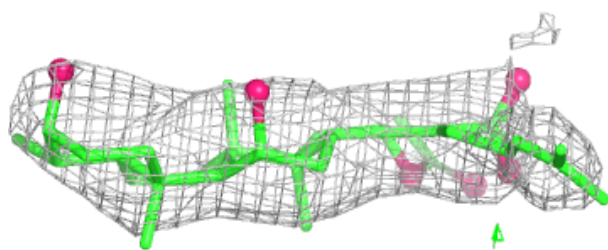
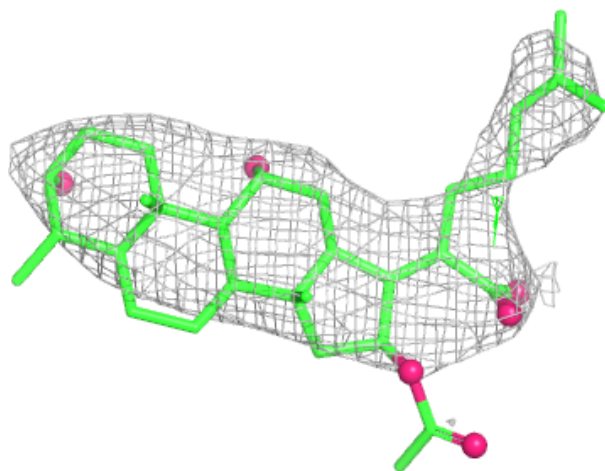
Electron density around LMT A 1111:

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



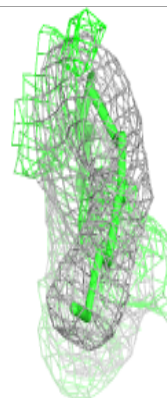
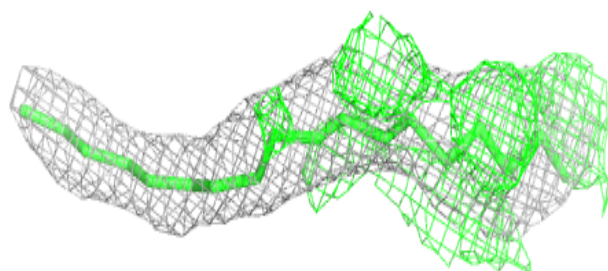
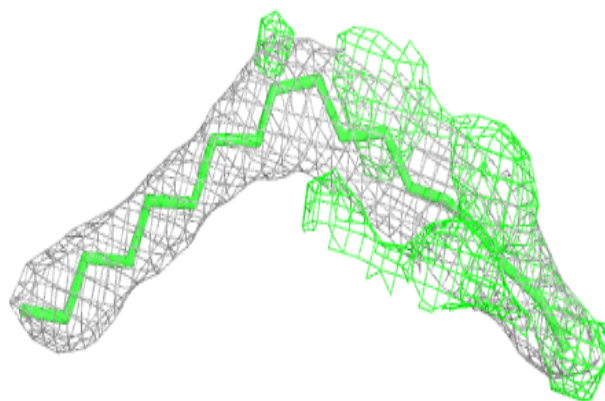
Electron density around FUA A 1113:

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



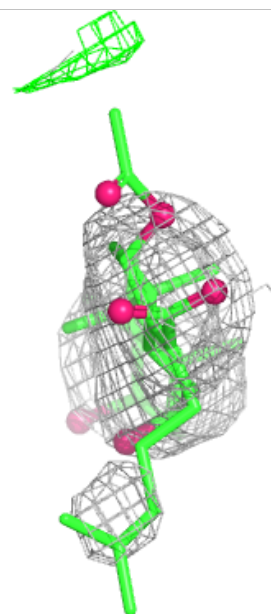
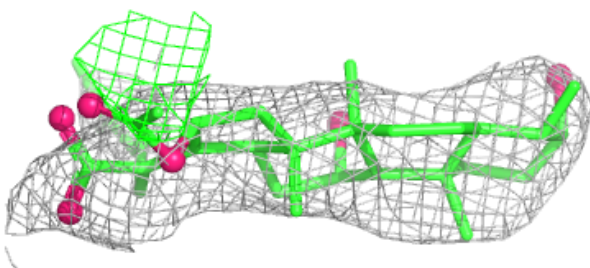
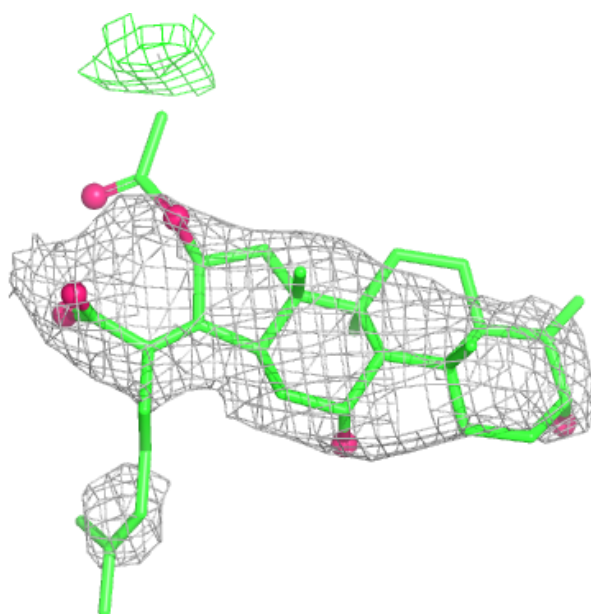
Electron density around 8K6 B 1208:

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



Electron density around FUA B 1213:

$2mF_o-DF_c$ (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.