



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:25 PM UTC

PDB ID : 9G14 / pdb_00009g14
Title : Human LTC4 synthase in complex with compound 2
Authors : Srinivas, H.
Deposited on : 2024-07-09
Resolution : 2.24 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

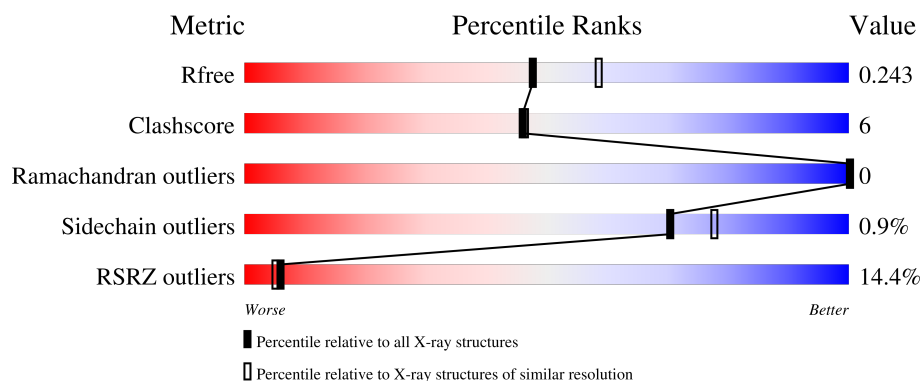
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	157	

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
6	PAM	A	214	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 1447 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 Leukotriene C4 synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	146	1130	751	195	182	2	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q16873
A	-5	HIS	-	expression tag	UNP Q16873
A	-4	HIS	-	expression tag	UNP Q16873
A	-3	HIS	-	expression tag	UNP Q16873
A	-2	HIS	-	expression tag	UNP Q16873
A	-1	HIS	-	expression tag	UNP Q16873
A	0	HIS	-	expression tag	UNP Q16873
A	1	GLY	-	expression tag	UNP Q16873

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



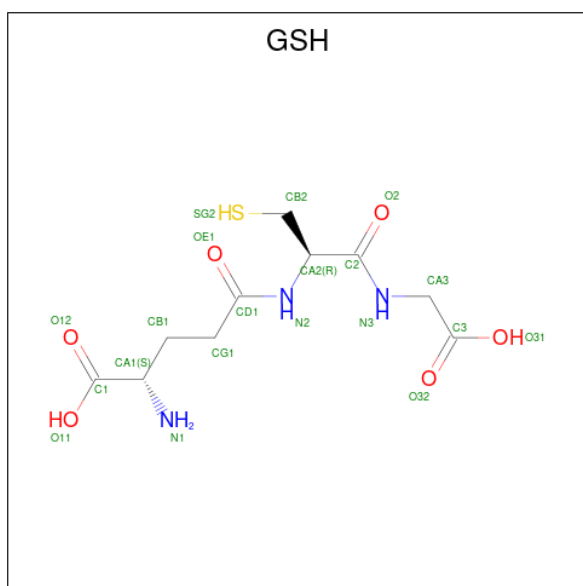
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



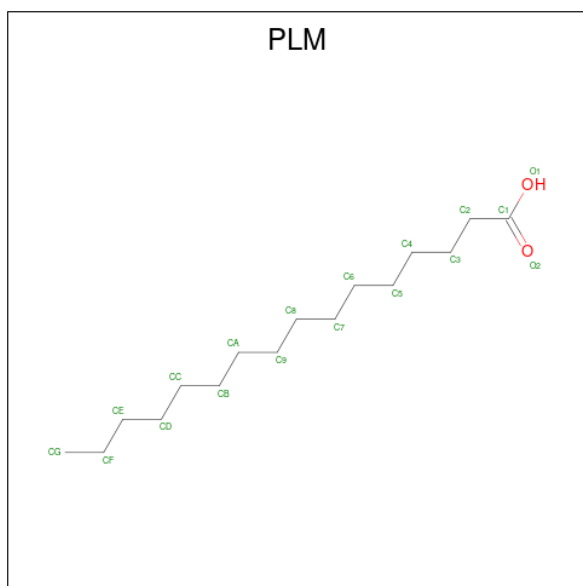
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



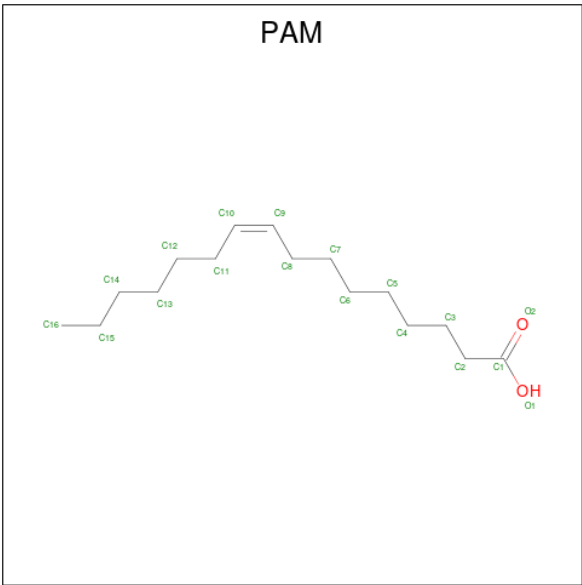
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 5 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



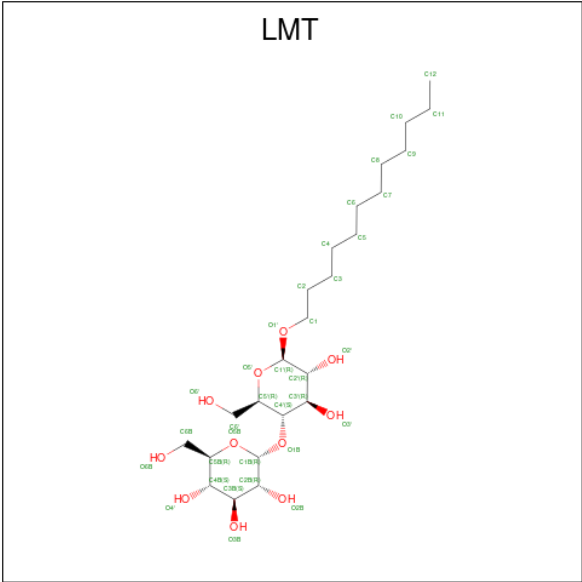
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	10	2		
5	A	1	Total	C		0	0
			8	8			
5	A	1	Total	C		0	0
			10	10			
5	A	1	Total	C		0	0
			7	7			
5	A	1	Total	C		0	0
			7	7			
5	A	1	Total	C		0	0
			11	11			
5	A	1	Total	C	O	0	0
			9	7	2		
5	A	1	Total	C		0	0
			8	8			
5	A	1	Total	C		0	0
			6	6			
5	A	1	Total	C		0	0
			8	8			

- Molecule 6 is PALMITOLEIC ACID (CCD ID: PAM) (formula: $C_{16}H_{30}O_2$).



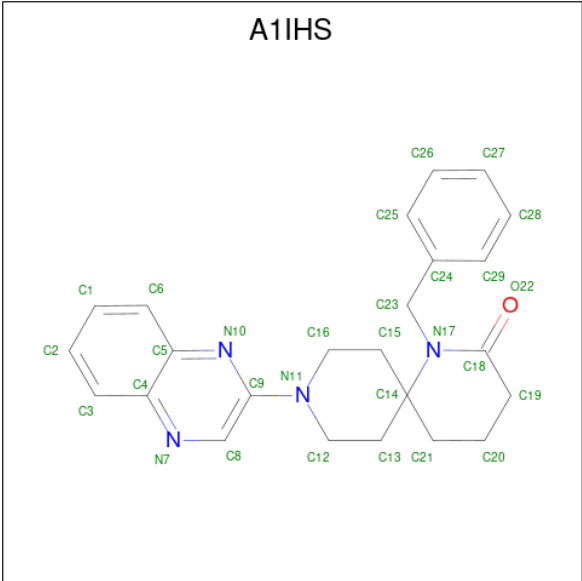
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 14 12 2	0	0
6	A	1	Total C 10 10	0	0
6	A	1	Total C 10 10	0	0
6	A	1	Total C O 18 16 2	0	0
6	A	1	Total C 10 10	0	0
6	A	1	Total C 6 6	0	0
6	A	1	Total C 7 7	0	0

- Molecule 7 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			24	18	6		
7	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 8 is 1-(phenylmethyl)-9-quinoxalin-2-yl-1,9-diazaspiro[5.5]undecan-2-one (CCD ID: A1IHS) (formula: C₂₄H₂₆N₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			29	24	4	1		

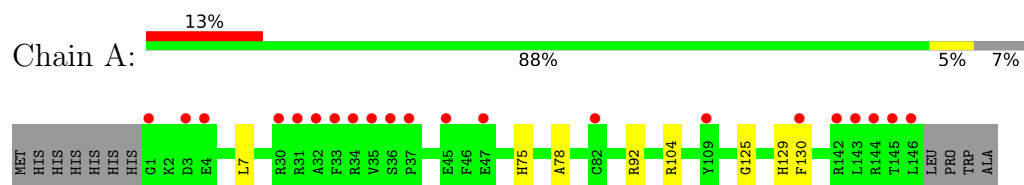
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	37	Total 37	O 37	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: Leukotriene C4 synthase



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	178.56Å 178.56Å 178.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.23 – 2.24 28.23 – 2.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.23-2.24) 99.9 (28.23-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.11.8 (26-JUL-2023)	Depositor
R, R_{free}	0.216 , 0.245 0.218 , 0.243	Depositor DCC
R_{free} test set	1137 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.5	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1447	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GSH, SO4, LMT, A1IHS, PLM, GOL, PAM

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	0.74	0/1159	1.03	0/1580

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

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	1130	0	1175	12	0
2	A	6	0	8	1	0
3	A	5	0	0	0	0
4	A	20	0	15	2	0
5	A	86	0	133	8	0
6	A	75	0	114	3	0
7	A	59	0	81	3	0
8	A	29	0	0	0	0
9	A	37	0	0	0	0
All	All	1447	0	1526	17	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.

All (17) 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)
7:A:220:LMT:H5B	7:A:220:LMT:H6D	1.54	0.87
1:A:104:ARG:HH11	4:A:203:GSH:HB23	1.38	0.85
1:A:92:ARG:HE	5:A:217:PLM:H51	1.44	0.80
1:A:75:HIS:HB3	5:A:204:PLM:H51	1.68	0.74
1:A:125:GLY:O	1:A:129:HIS:HD2	1.79	0.66
7:A:220:LMT:H6D	7:A:220:LMT:C5B	2.28	0.61
1:A:92:ARG:HH21	5:A:217:PLM:H31	1.66	0.61
1:A:104:ARG:HH12	2:A:201:GOL:H31	1.65	0.60
1:A:92:ARG:NE	5:A:217:PLM:H51	2.15	0.60
1:A:78:ALA:HB2	5:A:204:PLM:H71	1.89	0.54
1:A:130:PHE:HB2	6:A:205:PAM:H51	1.91	0.51
1:A:78:ALA:HB1	7:A:220:LMT:O4'	2.12	0.48
6:A:213:PAM:H162	6:A:214:PAM:H141	1.97	0.47
1:A:104:ARG:HH11	4:A:203:GSH:CB2	2.20	0.45
1:A:92:ARG:HE	5:A:217:PLM:C5	2.21	0.44
6:A:205:PAM:H81	5:A:209:PLM:H71	2.02	0.42
5:A:206:PLM:HB2	5:A:207:PLM:HC2	2.02	0.41

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	144/157 (92%)	142 (99%)	2 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	108/120 (90%)	107 (99%)	1 (1%)	70	78

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	55	ASN
1	A	75	HIS
1	A	95	GLN
1	A	129	HIS

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](#)

23 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
5	PLM	A	222	-	7,7,17	0.71	0	6,6,17	0.41	0
8	A1IHS	A	223	-	33,33,33	1.57	5 (15%)	39,47,47	1.88	9 (23%)
5	PLM	A	218	-	5,5,17	0.75	0	4,4,17	0.36	0
3	SO4	A	202	-	4,4,4	0.29	0	6,6,6	0.17	0
4	GSH	A	203	-	18,19,19	0.75	0	21,24,24	0.88	0
6	PAM	A	212	-	9,9,17	0.64	0	8,8,17	0.58	0
6	PAM	A	213	-	17,17,17	0.74	0	17,17,17	0.45	0
6	PAM	A	211	-	9,9,17	0.68	0	8,8,17	0.49	0
7	LMT	A	219	-	24,24,36	1.08	1 (4%)	29,29,47	0.77	1 (3%)
2	GOL	A	201	-	5,5,5	0.03	0	5,5,5	0.22	0
6	PAM	A	215	-	5,5,17	0.70	0	4,4,17	0.47	0
5	PLM	A	210	-	10,10,17	0.74	0	9,9,17	0.51	0
6	PAM	A	214	-	9,9,17	0.64	0	8,8,17	0.34	0
5	PLM	A	206	-	7,7,17	0.77	0	6,6,17	0.44	0
5	PLM	A	217	-	7,7,17	0.79	0	6,6,17	0.43	0
5	PLM	A	208	-	6,6,17	0.77	0	5,5,17	0.33	0
5	PLM	A	209	-	6,6,17	0.75	0	5,5,17	0.40	0
5	PLM	A	216	-	8,8,17	0.75	0	8,8,17	0.43	0
5	PLM	A	204	-	11,11,17	0.87	0	11,11,17	0.37	0
5	PLM	A	207	-	9,9,17	0.75	0	8,8,17	0.52	0
7	LMT	A	220	-	36,36,36	0.98	1 (2%)	47,47,47	0.69	0
6	PAM	A	205	-	13,13,17	0.75	0	13,13,17	0.43	0
6	PAM	A	221	-	6,6,17	0.66	0	5,5,17	0.49	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
5	PLM	A	222	-	-	3/5/5/15	-
8	A1IHS	A	223	-	-	0/8/37/37	0/5/5/5
5	PLM	A	218	-	-	0/3/3/15	-
4	GSH	A	203	-	-	5/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PAM	A	212	-	-	4/7/7/15	-
6	PAM	A	213	-	-	10/15/15/15	-
6	PAM	A	211	-	-	3/7/7/15	-
7	LMT	A	219	-	-	8/15/35/61	0/1/1/2
2	GOL	A	201	-	-	0/4/4/4	-
6	PAM	A	215	-	-	2/3/3/15	-
5	PLM	A	210	-	-	5/8/8/15	-
6	PAM	A	214	-	-	3/7/7/15	-
5	PLM	A	206	-	-	2/5/5/15	-
5	PLM	A	217	-	-	3/5/5/15	-
5	PLM	A	208	-	-	2/4/4/15	-
5	PLM	A	209	-	-	2/4/4/15	-
5	PLM	A	216	-	-	4/6/6/15	-
5	PLM	A	204	-	-	4/9/9/15	-
5	PLM	A	207	-	-	4/7/7/15	-
7	LMT	A	220	-	-	9/21/61/61	0/2/2/2
6	PAM	A	205	-	-	4/11/11/15	-
6	PAM	A	221	-	-	3/4/4/15	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	223	A1IHS	C13-C14	3.61	1.58	1.53
8	A	223	A1IHS	C15-C14	3.23	1.58	1.53
8	A	223	A1IHS	C21-C14	3.02	1.57	1.53
7	A	219	LMT	O1'-C1'	2.89	1.45	1.40
7	A	220	LMT	O1'-C1'	2.67	1.44	1.40
8	A	223	A1IHS	C9-N10	2.64	1.36	1.32
8	A	223	A1IHS	C8-N7	2.14	1.35	1.31

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	223	A1IHS	C9-N10-C5	4.59	122.54	117.54
8	A	223	A1IHS	C19-C18-N17	3.83	123.91	118.00
8	A	223	A1IHS	C15-C16-N11	-3.78	103.69	110.53
8	A	223	A1IHS	C8-N7-C4	3.73	121.28	116.96
8	A	223	A1IHS	O22-C18-C19	-3.72	113.04	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	223	A1IHS	C21-C14-C13	-3.07	104.30	110.14
8	A	223	A1IHS	C8-C9-N10	-2.76	117.78	121.23
8	A	223	A1IHS	C13-C12-N11	-2.51	105.98	110.53
7	A	219	LMT	O1B-C4'-C3'	2.38	116.00	110.38
8	A	223	A1IHS	C5-C4-N7	-2.05	119.15	121.00

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	203	GSH	C1-CA1-CB1-CG1
7	A	219	LMT	C2'-C1'-O1'-C1
7	A	219	LMT	O5'-C1'-O1'-C1
7	A	220	LMT	O1'-C1-C2-C3
7	A	220	LMT	O5B-C5B-C6B-O6B
5	A	216	PLM	C1-C2-C3-C4
4	A	203	GSH	CA1-CB1-CG1-CD1
6	A	213	PAM	C1-C2-C3-C4
5	A	207	PLM	C8-C9-CA-CB
6	A	213	PAM	C3-C4-C5-C6
5	A	216	PLM	C3-C4-C5-C6
5	A	217	PLM	C5-C6-C7-C8
5	A	209	PLM	C6-C7-C8-C9
7	A	219	LMT	C2-C1-O1'-C1'
7	A	220	LMT	C2-C1-O1'-C1'
5	A	207	PLM	CA-CB-CC-CD
5	A	204	PLM	C1-C2-C3-C4
5	A	210	PLM	C9-CA-CB-CC
7	A	220	LMT	C4'-C5'-C6'-O6'
7	A	219	LMT	C3-C4-C5-C6
5	A	208	PLM	CB-CC-CD-CE
5	A	210	PLM	CA-CB-CC-CD
5	A	210	PLM	CB-CC-CD-CE
6	A	212	PAM	C11-C12-C13-C14
5	A	216	PLM	C2-C3-C4-C5
6	A	212	PAM	C7-C8-C9-C10
5	A	210	PLM	CC-CD-CE-CF
6	A	205	PAM	C6-C7-C8-C9
6	A	213	PAM	C6-C7-C8-C9
6	A	211	PAM	C11-C12-C13-C14
6	A	205	PAM	C1-C2-C3-C4
6	A	212	PAM	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
7	A	220	LMT	O5'-C5'-C6'-O6'
7	A	219	LMT	C5-C6-C7-C8
6	A	221	PAM	C13-C14-C15-C16
5	A	206	PLM	C8-C9-CA-CB
5	A	222	PLM	C2-C3-C4-C5
5	A	204	PLM	C7-C8-C9-CA
5	A	208	PLM	CA-CB-CC-CD
5	A	210	PLM	CD-CE-CF-CG
6	A	214	PAM	C12-C13-C14-C15
6	A	213	PAM	C4-C5-C6-C7
5	A	204	PLM	C3-C4-C5-C6
7	A	220	LMT	C1-C2-C3-C4
5	A	207	PLM	CC-CD-CE-CF
7	A	220	LMT	C9-C10-C11-C12
5	A	207	PLM	C9-CA-CB-CC
6	A	211	PAM	C7-C8-C9-C10
6	A	205	PAM	C5-C6-C7-C8
7	A	219	LMT	C11-C10-C9-C8
5	A	206	PLM	CA-CB-CC-CD
6	A	221	PAM	C11-C12-C13-C14
7	A	220	LMT	C3-C4-C5-C6
6	A	213	PAM	C13-C14-C15-C16
6	A	221	PAM	C12-C13-C14-C15
4	A	203	GSH	C2-CA2-N2-CD1
6	A	205	PAM	C9-C10-C11-C12
6	A	215	PAM	C7-C8-C9-C10
6	A	215	PAM	C9-C10-C11-C12
5	A	204	PLM	C5-C6-C7-C8
7	A	219	LMT	C4-C5-C6-C7
6	A	214	PAM	C10-C11-C12-C13
6	A	213	PAM	C12-C13-C14-C15
4	A	203	GSH	O12-C1-CA1-N1
5	A	222	PLM	C5-C6-C7-C8
6	A	213	PAM	O2-C1-C2-C3
5	A	217	PLM	C3-C4-C5-C6
6	A	213	PAM	O1-C1-C2-C3
6	A	213	PAM	C11-C12-C13-C14
6	A	212	PAM	C9-C10-C11-C12
5	A	222	PLM	C3-C4-C5-C6
6	A	213	PAM	C7-C8-C9-C10
5	A	209	PLM	C5-C6-C7-C8
4	A	203	GSH	O2-C2-CA2-N2

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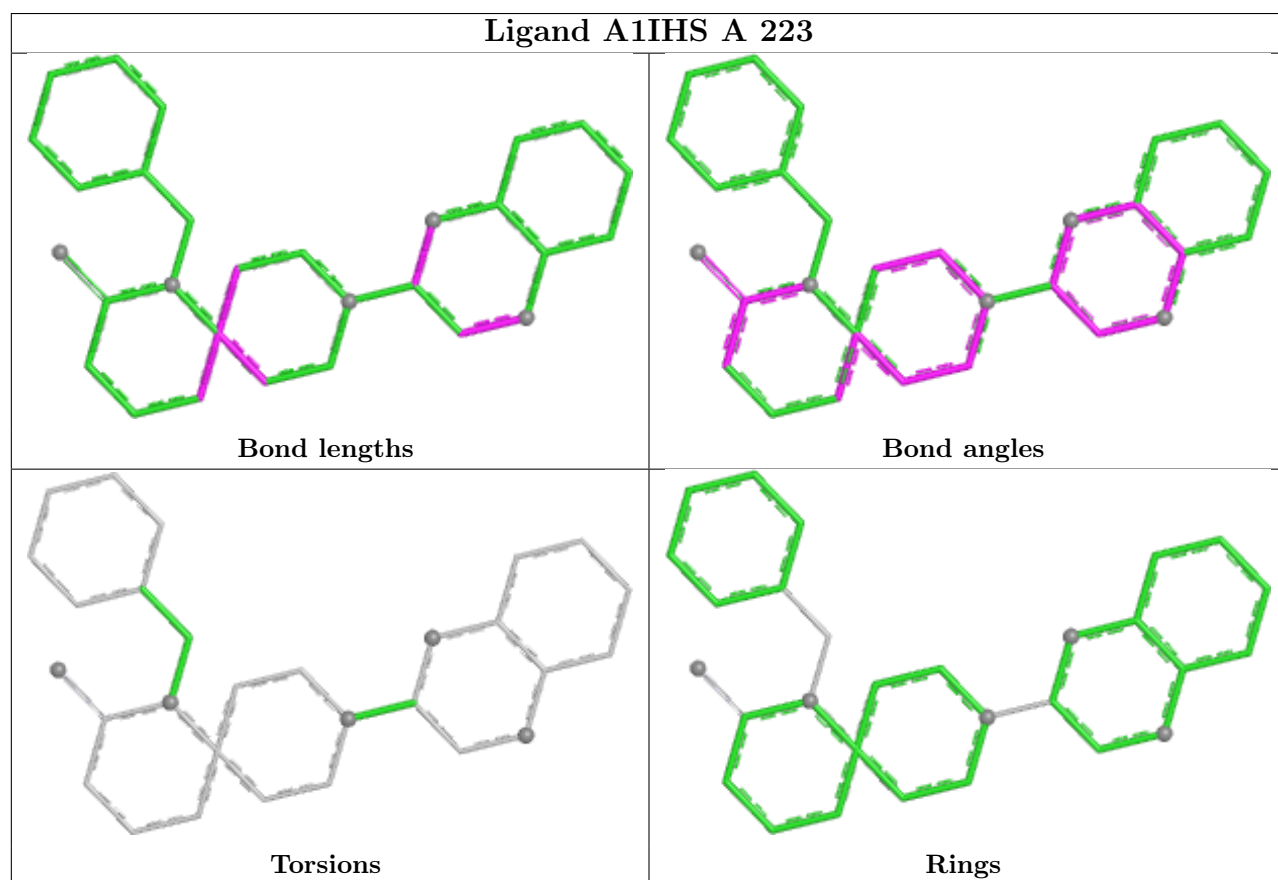
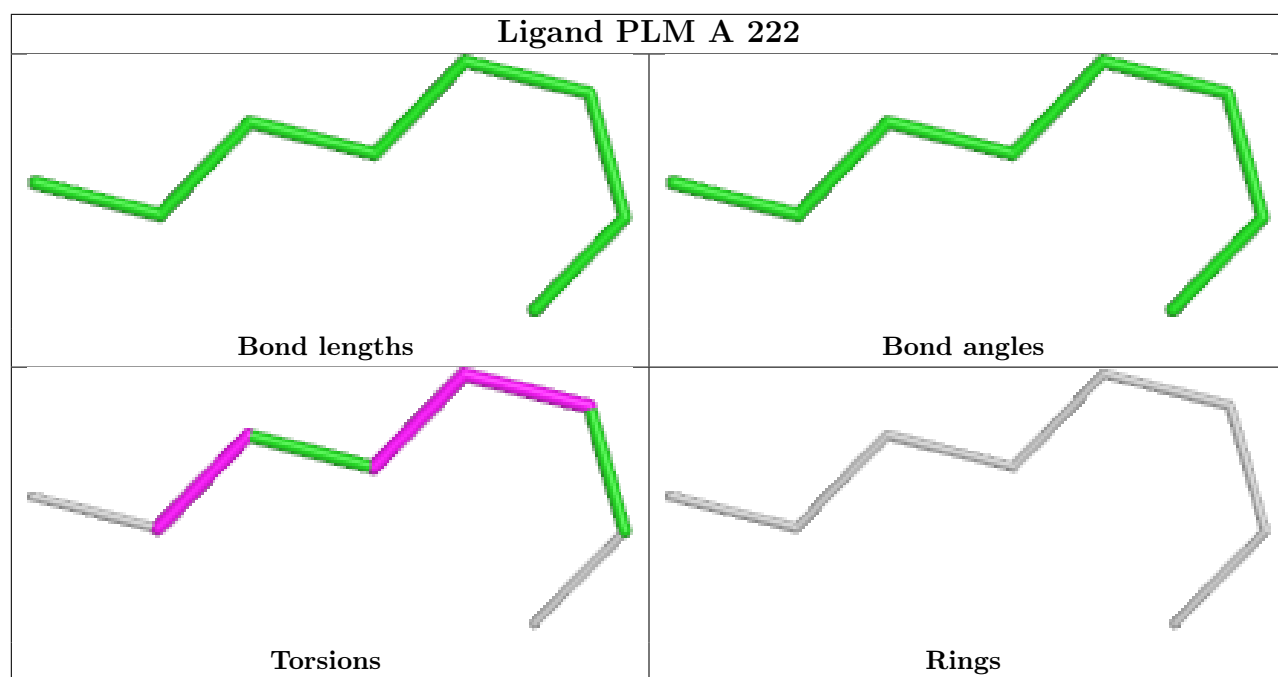
Mol	Chain	Res	Type	Atoms
6	A	214	PAM	C7-C8-C9-C10
6	A	211	PAM	C13-C14-C15-C16
5	A	217	PLM	C4-C5-C6-C7
7	A	219	LMT	C7-C8-C9-C10
7	A	220	LMT	C2-C3-C4-C5
5	A	216	PLM	C4-C5-C6-C7

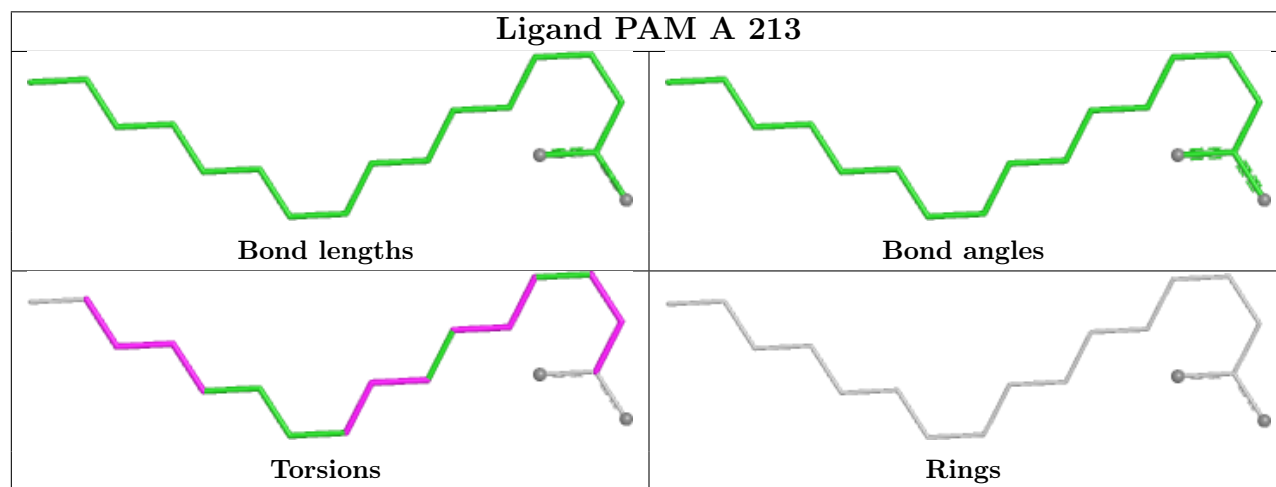
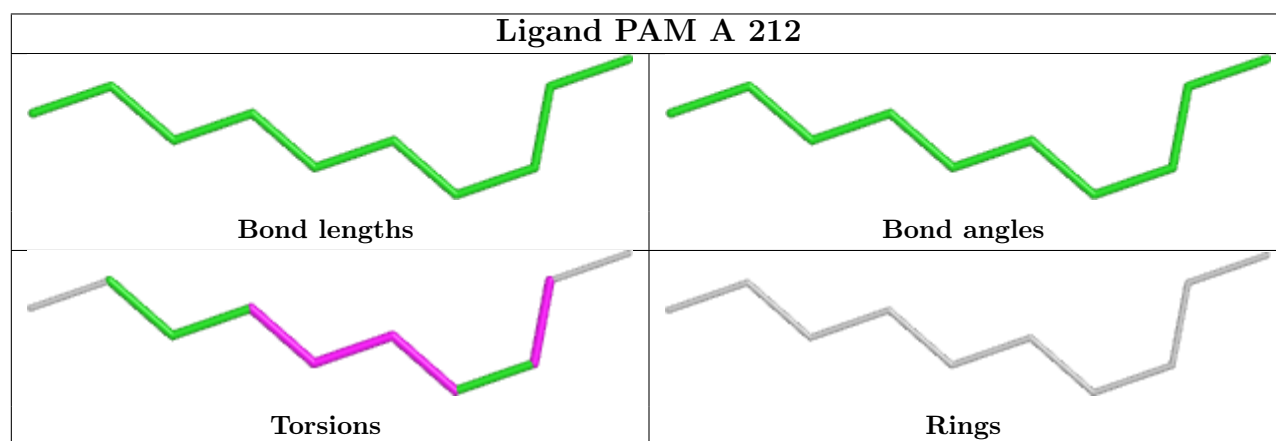
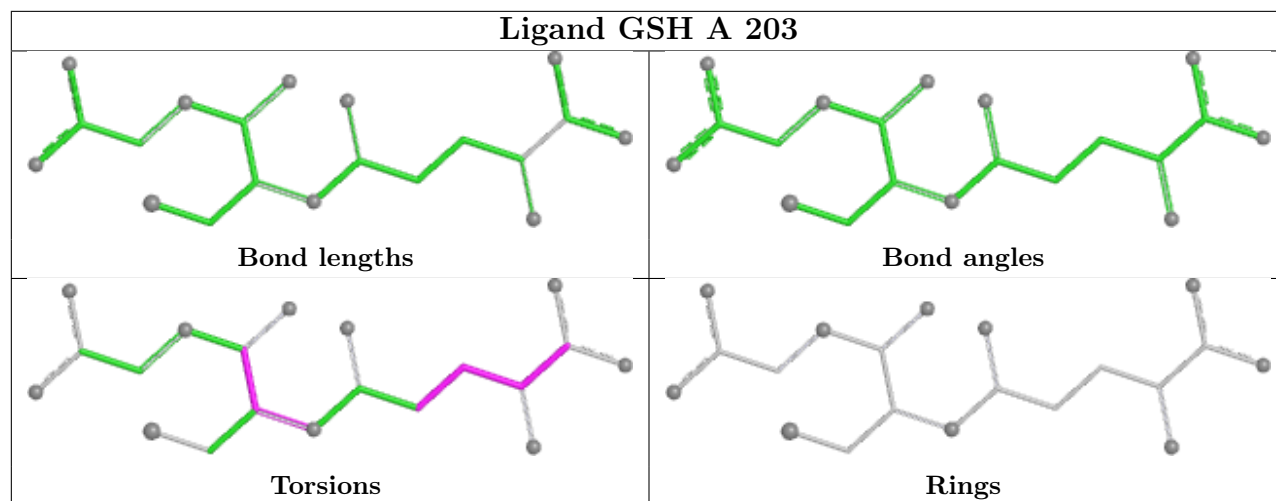
There are no ring outliers.

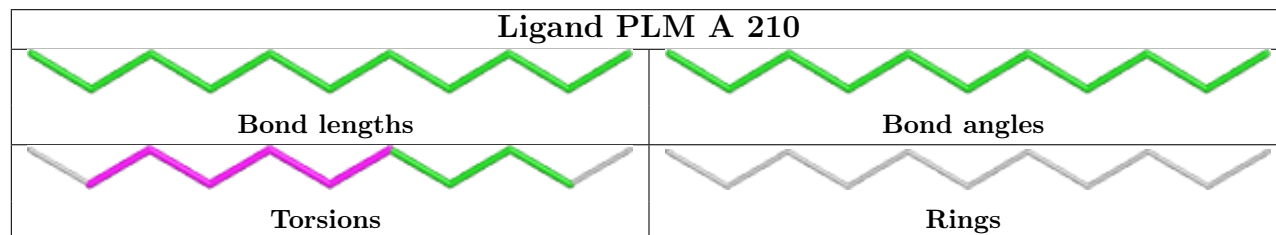
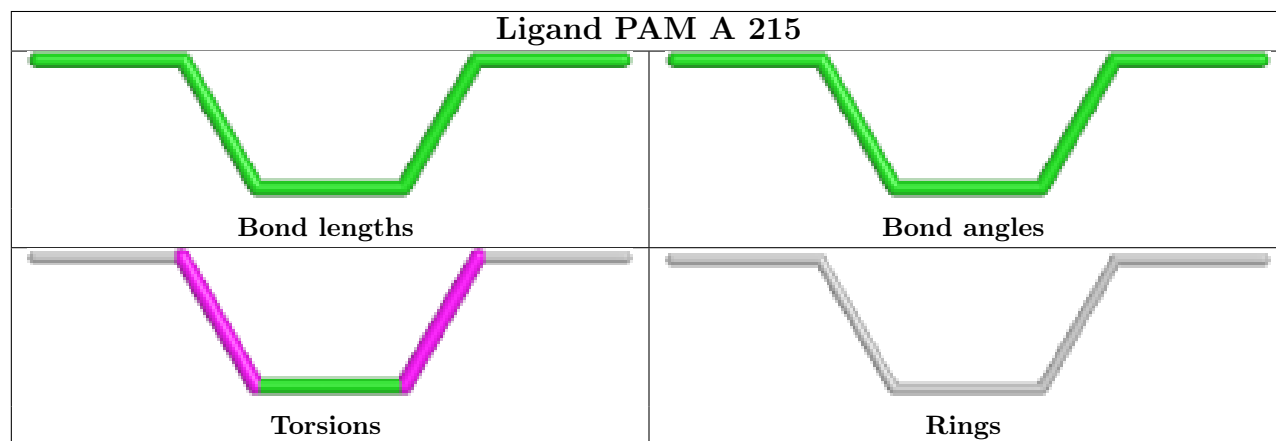
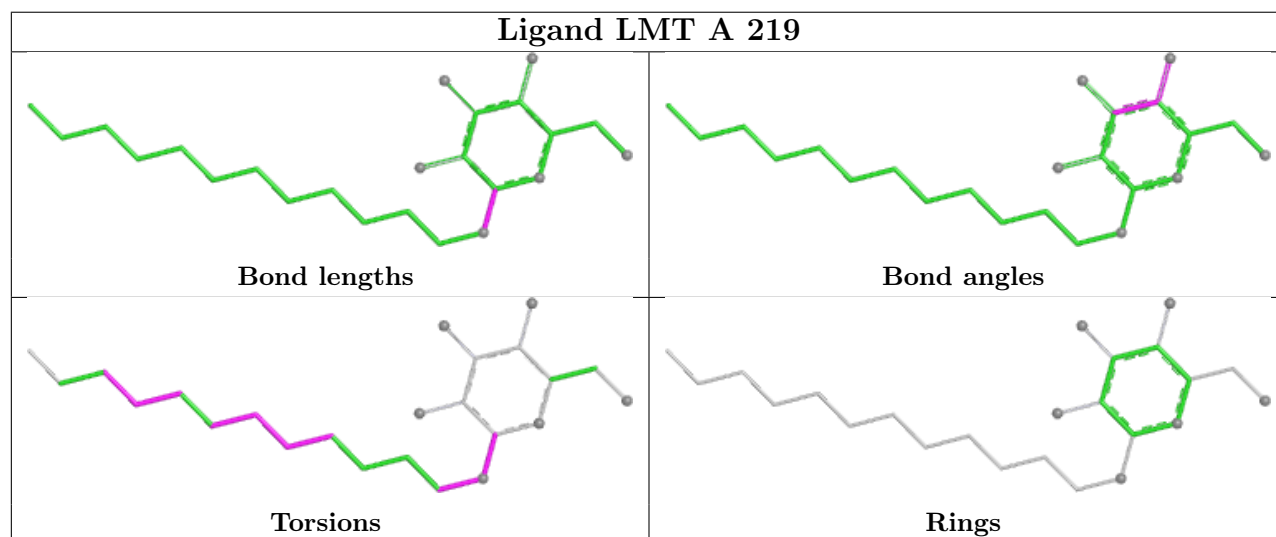
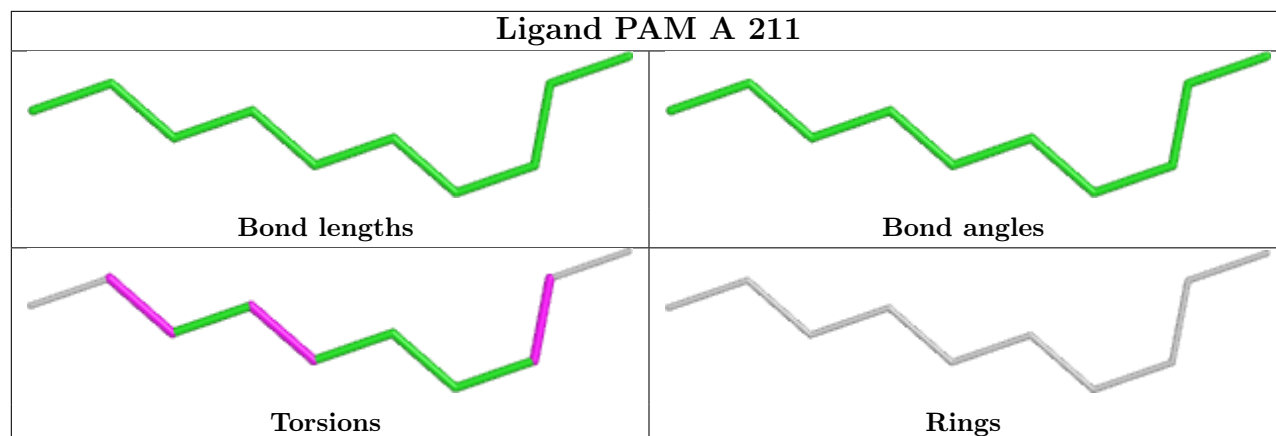
11 monomers are involved in 16 short contacts:

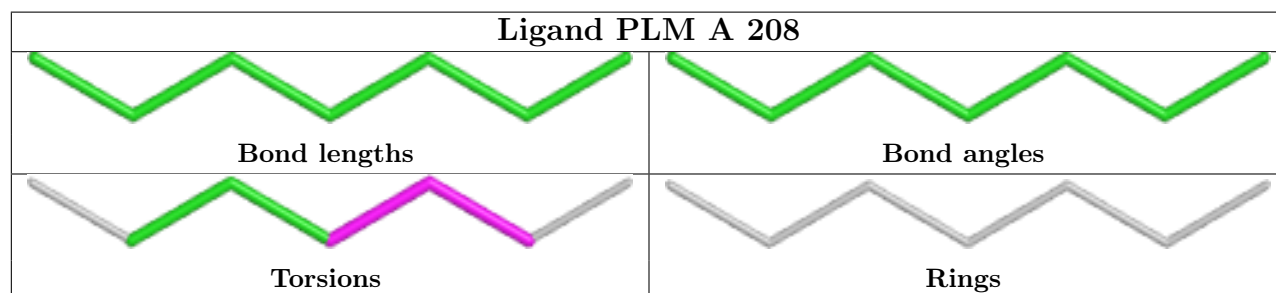
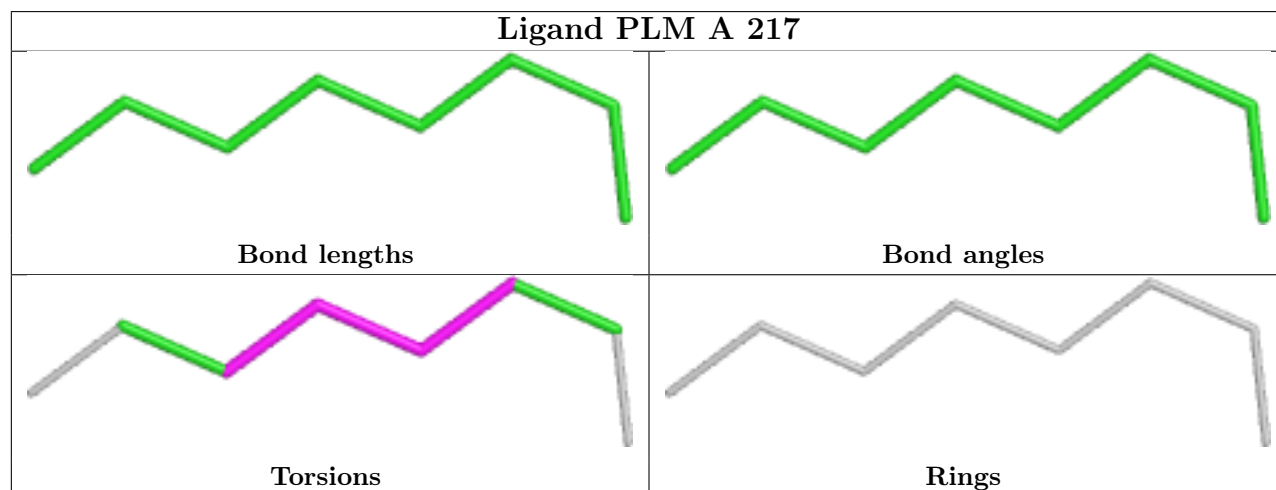
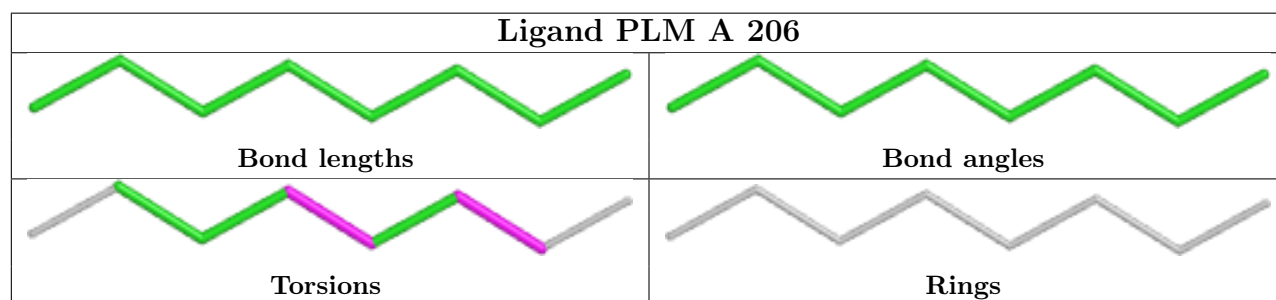
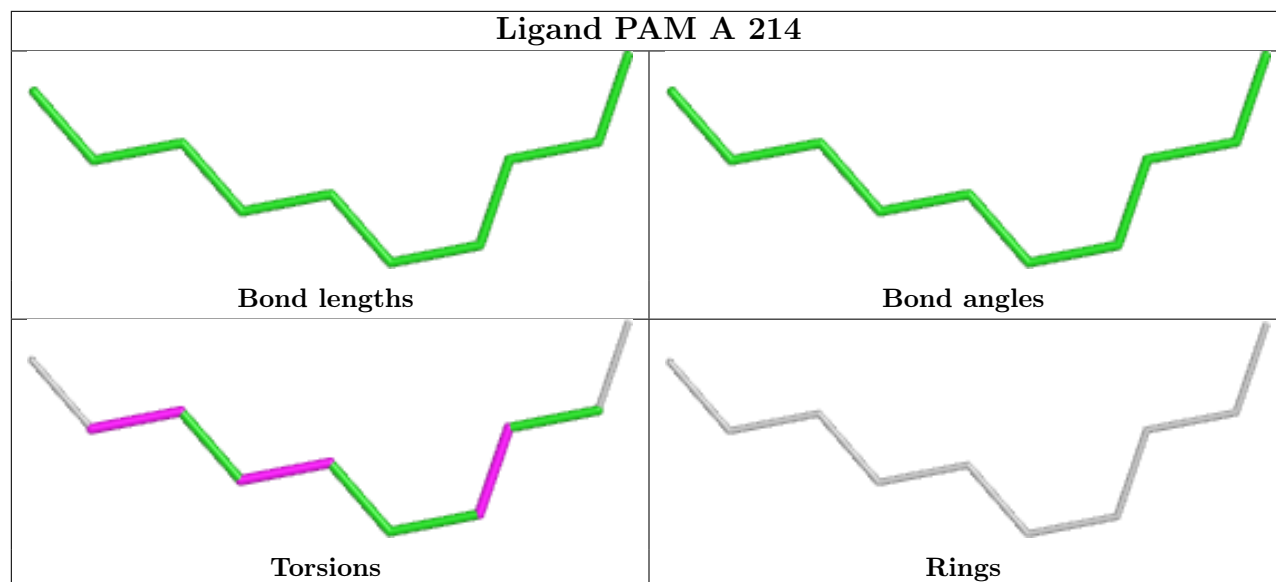
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	203	GSH	2	0
6	A	213	PAM	1	0
2	A	201	GOL	1	0
6	A	214	PAM	1	0
5	A	206	PLM	1	0
5	A	217	PLM	4	0
5	A	209	PLM	1	0
5	A	204	PLM	2	0
5	A	207	PLM	1	0
7	A	220	LMT	3	0
6	A	205	PAM	2	0

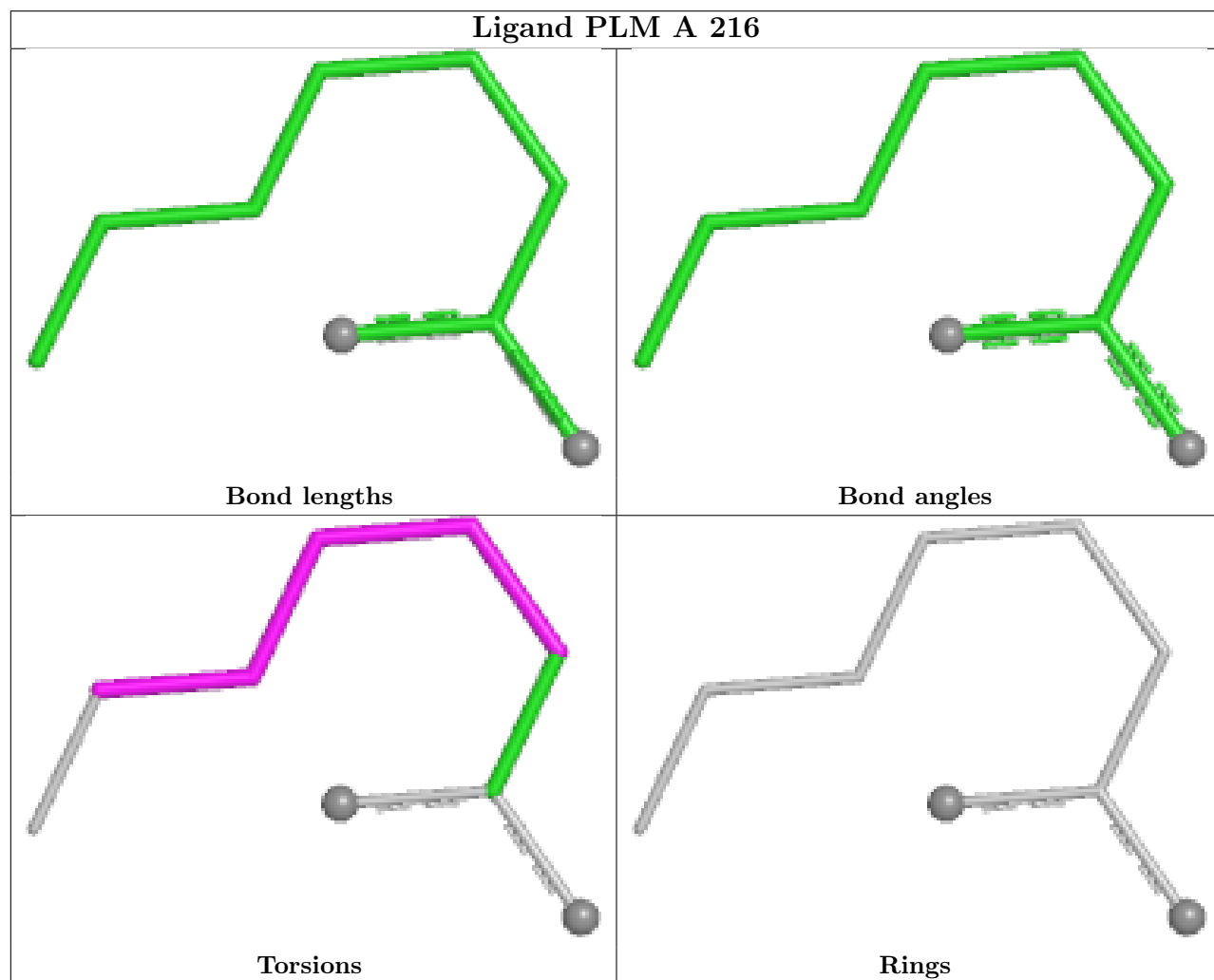
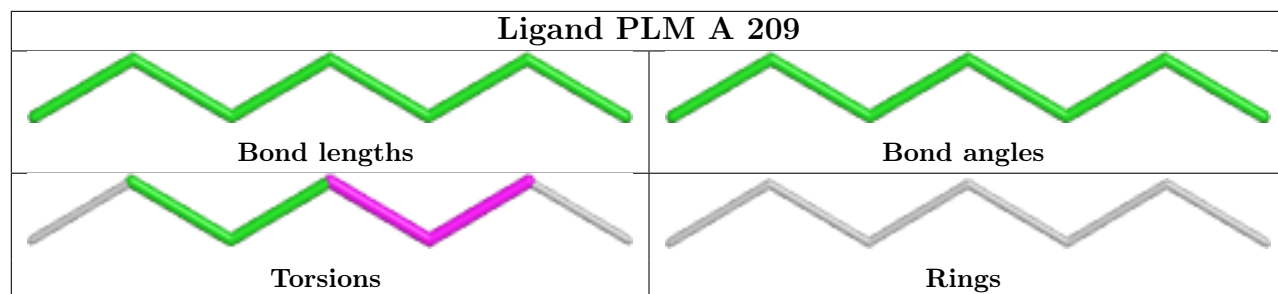
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

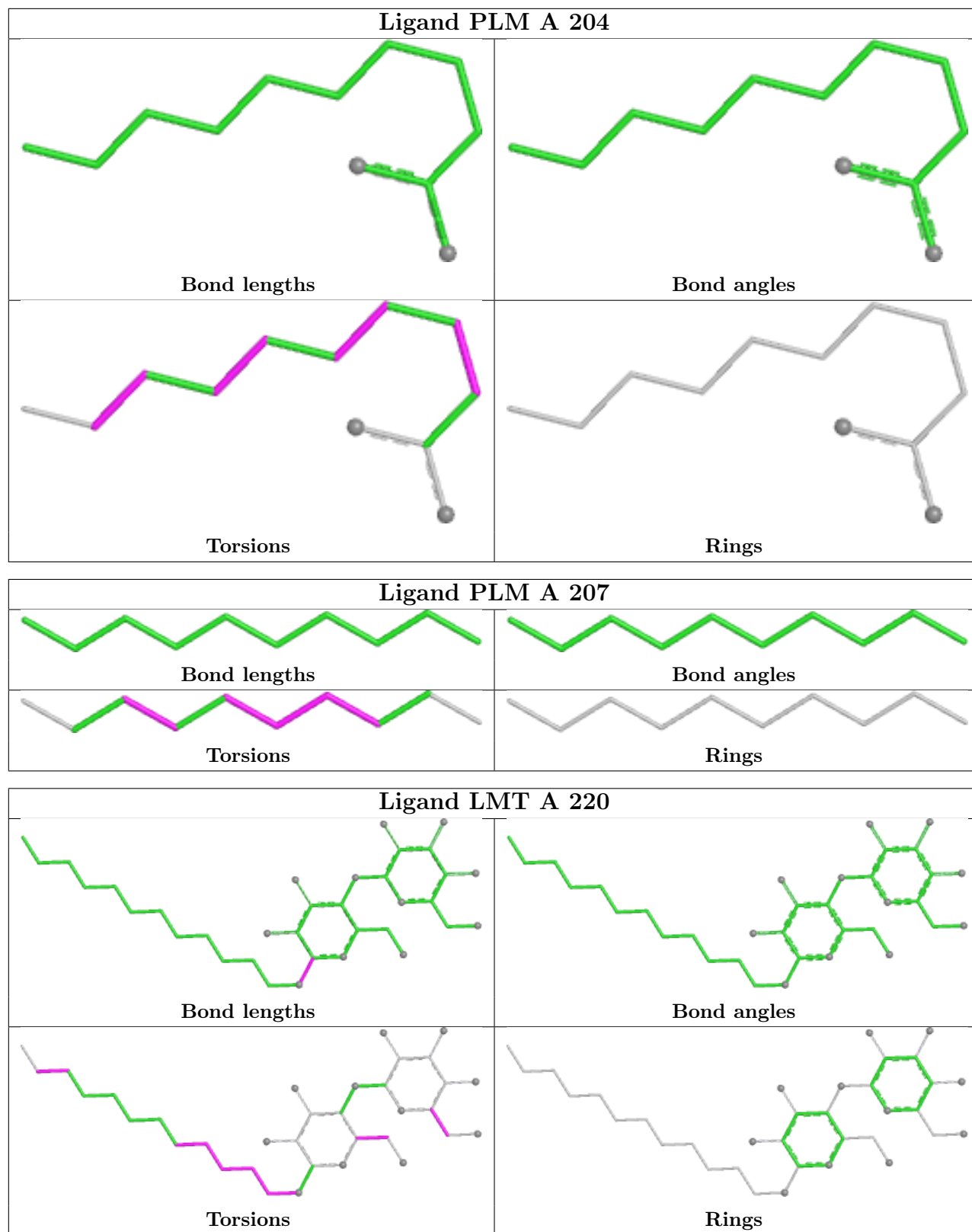


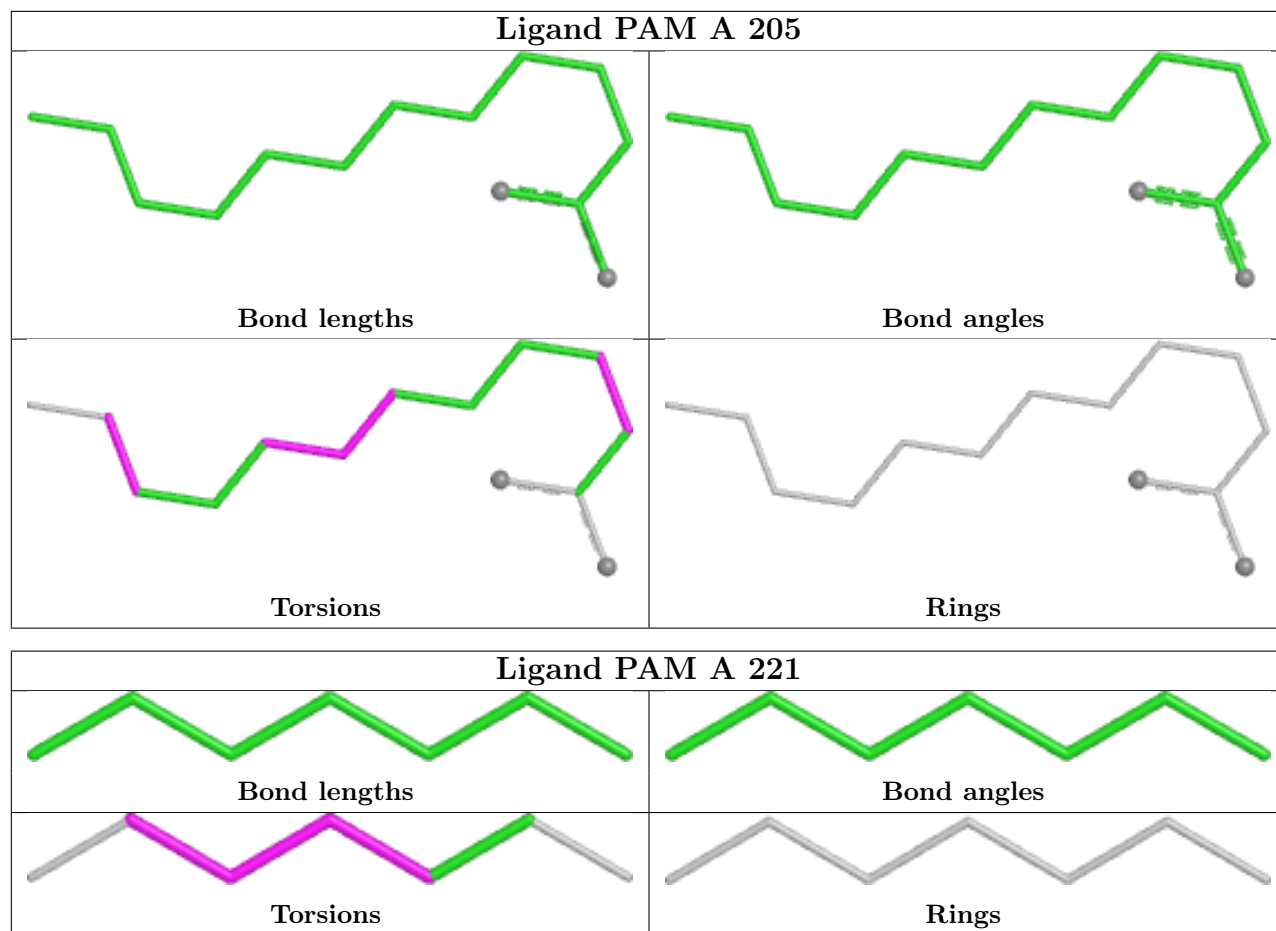












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	146/157 (92%)	0.75	21 (14%) 6 5	36, 51, 89, 104	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	31	ARG	5.2
1	A	146	LEU	5.2
1	A	144	ARG	4.8
1	A	3	ASP	4.3
1	A	145	THR	4.3
1	A	34	ARG	4.1
1	A	32	ALA	3.6
1	A	47	GLU	3.6
1	A	109	TYR	3.2
1	A	35	VAL	3.0
1	A	4	GLU	3.0
1	A	143	LEU	2.9
1	A	82	CYS	2.6
1	A	130	PHE	2.6
1	A	33	PHE	2.5
1	A	1	GLY	2.5
1	A	30	ARG	2.3
1	A	45	GLU	2.2
1	A	142	ARG	2.1
1	A	36	SER	2.0
1	A	37	PRO	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

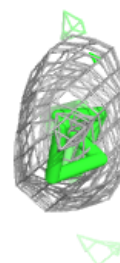
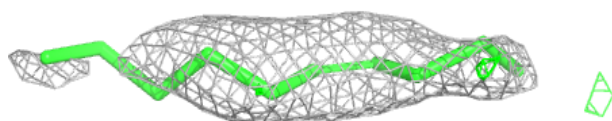
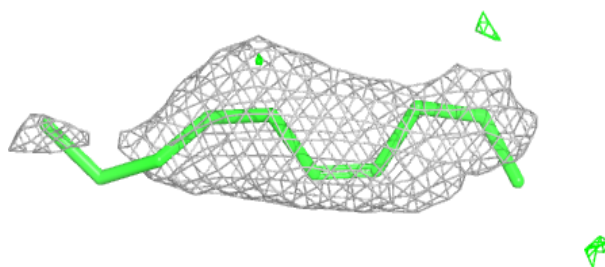
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PAM	A	214	10/18	0.70	0.42	122,122,122,122	0
6	PAM	A	215	6/18	0.73	0.40	117,117,117,117	0
7	LMT	A	219	24/35	0.73	0.32	98,108,111,112	0
5	PLM	A	218	6/18	0.76	0.34	106,106,106,106	0
3	SO4	A	202	5/5	0.76	0.18	122,122,122,122	0
6	PAM	A	213	18/18	0.77	0.26	105,107,107,107	0
5	PLM	A	204	12/18	0.77	0.27	70,71,72,72	0
5	PLM	A	209	7/18	0.77	0.33	92,92,92,92	0
2	GOL	A	201	6/6	0.77	0.35	115,115,115,115	0
5	PLM	A	216	9/18	0.78	0.27	98,99,99,99	0
5	PLM	A	217	8/18	0.80	0.28	72,73,75,75	0
5	PLM	A	206	8/18	0.80	0.30	103,103,103,103	0
4	GSH	A	203	20/20	0.81	0.27	82,87,90,91	0
6	PAM	A	205	14/18	0.81	0.28	79,81,83,83	0
5	PLM	A	208	7/18	0.84	0.26	77,77,78,78	0
7	LMT	A	220	35/35	0.85	0.19	93,96,97,97	0
6	PAM	A	211	10/18	0.86	0.23	80,80,81,81	0
5	PLM	A	207	10/18	0.87	0.24	85,86,86,86	0
5	PLM	A	222	8/18	0.87	0.22	83,83,83,83	0
5	PLM	A	210	11/18	0.87	0.25	72,74,75,75	0
6	PAM	A	212	10/18	0.90	0.17	68,69,70,70	0
6	PAM	A	221	7/18	0.92	0.17	75,76,76,76	0
8	A1IHS	A	223	29/29	0.92	0.12	47,50,54,55	0

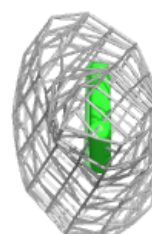
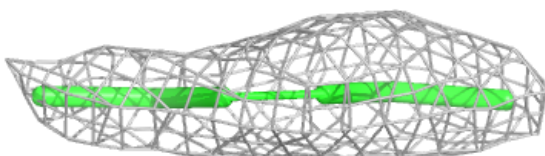
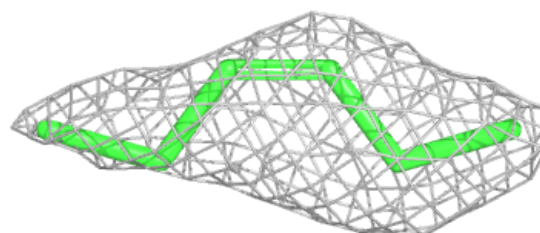
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PAM A 214:

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

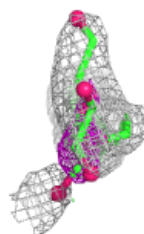
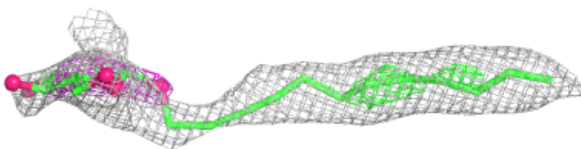
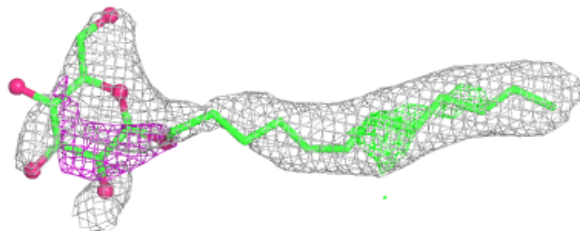
**Electron density around PAM A 215:**

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

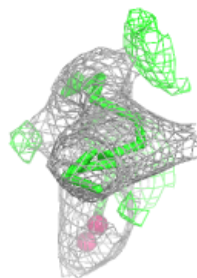
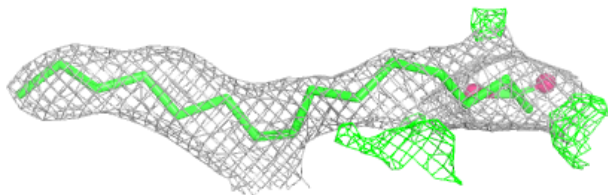
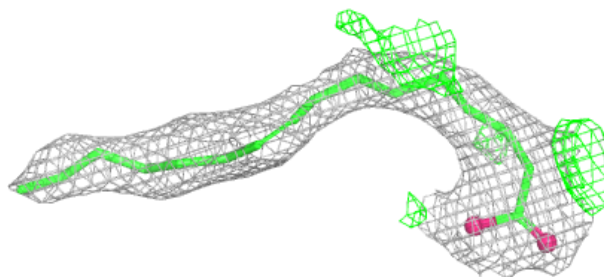


Electron density around LMT A 219:

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

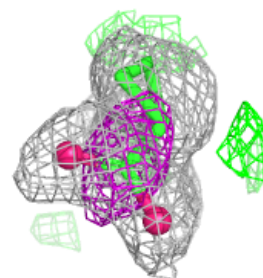
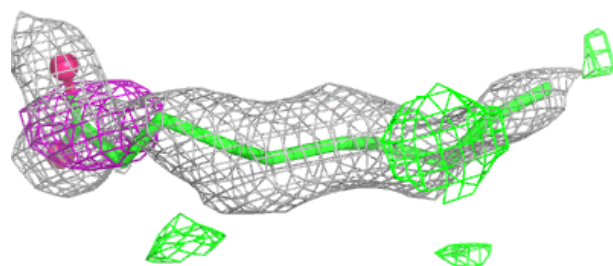
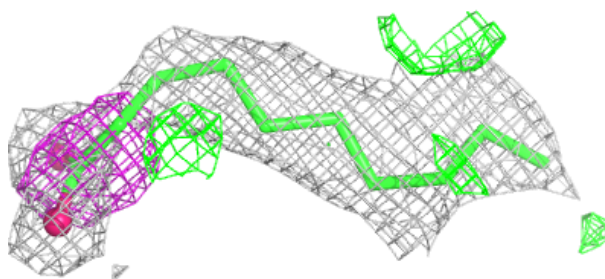
**Electron density around PAM A 213:**

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

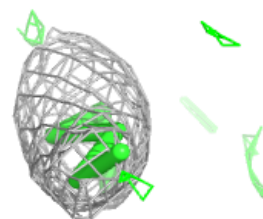
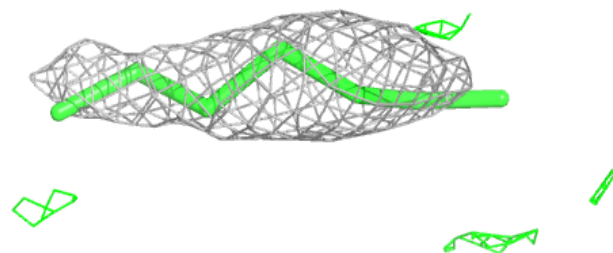
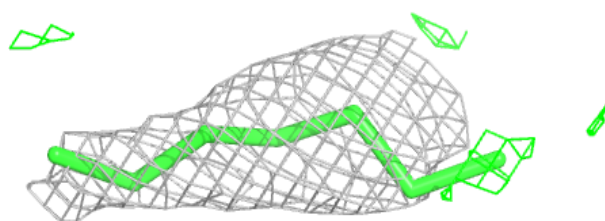


Electron density around PLM A 204:

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

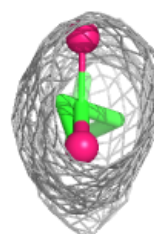
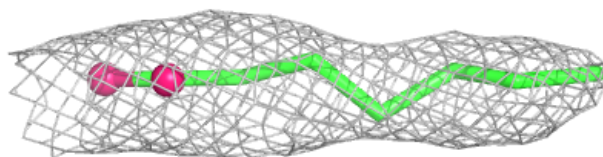
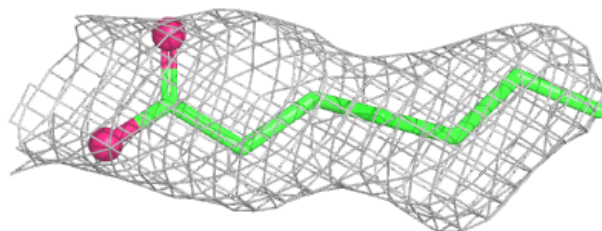
**Electron density around PLM A 209:**

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

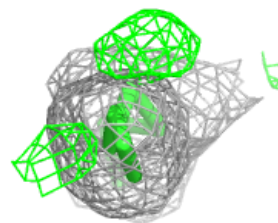
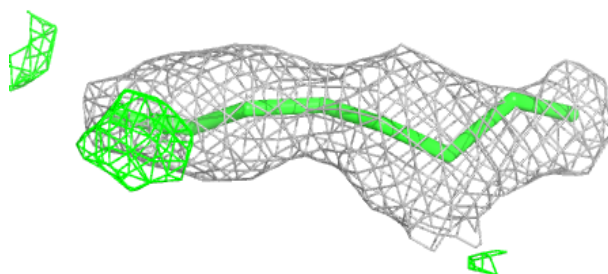
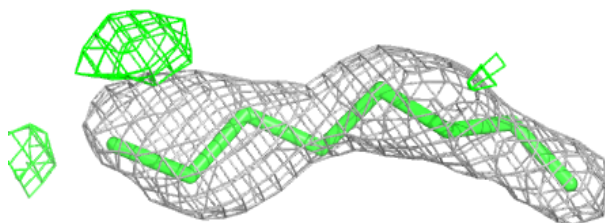


Electron density around PLM A 216:

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

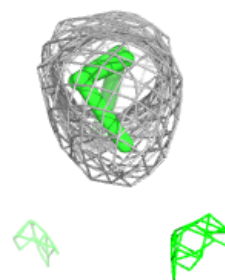
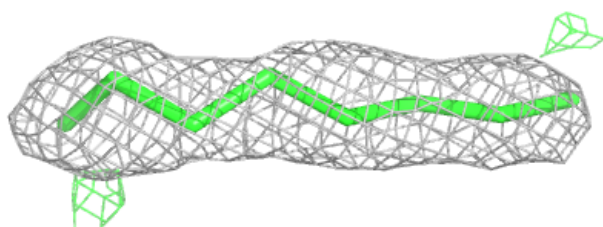
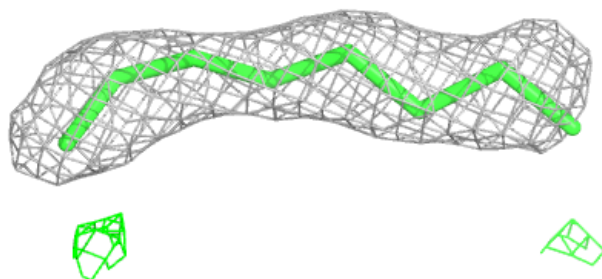
**Electron density around PLM A 217:**

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

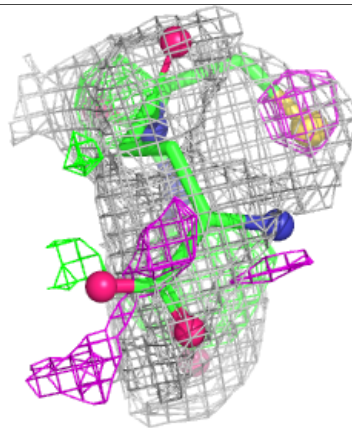
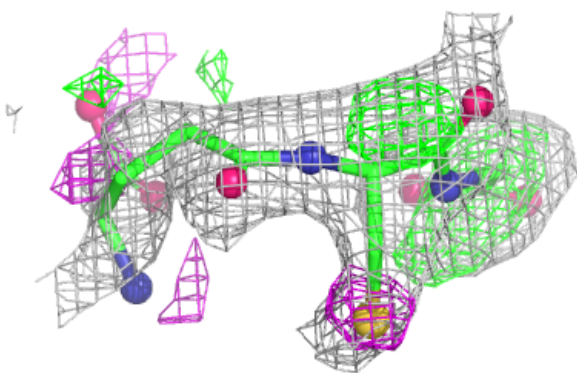
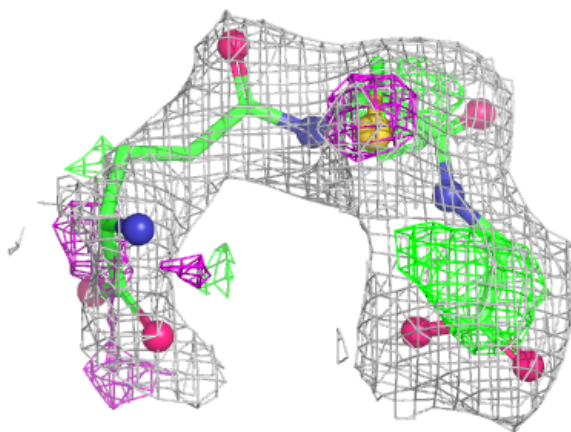


Electron density around PLM A 206:

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

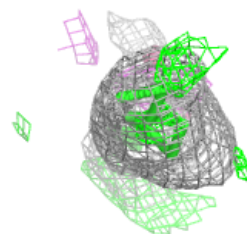
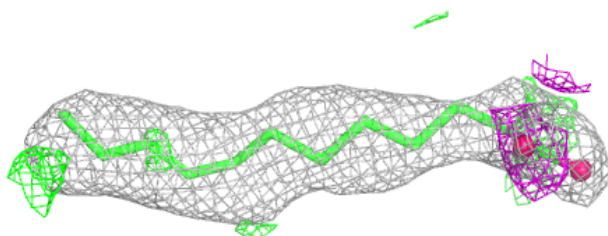
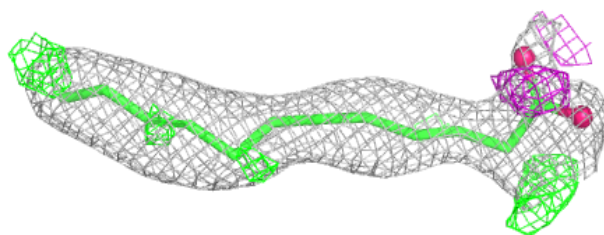
**Electron density around GSH A 203:**

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

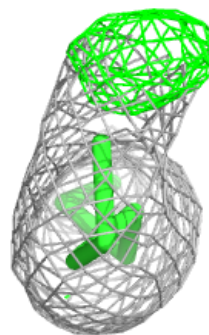
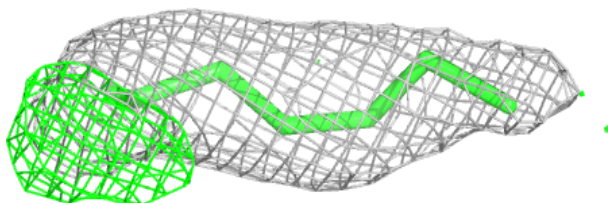
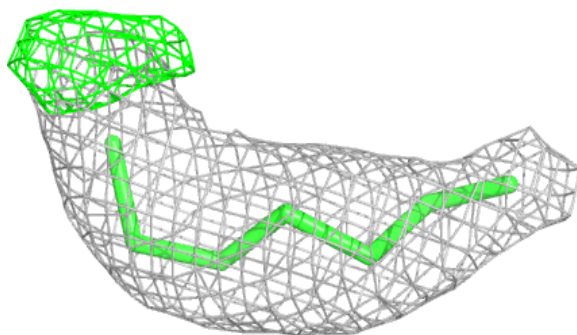


Electron density around PAM A 205:

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

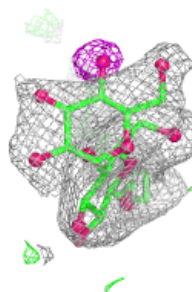
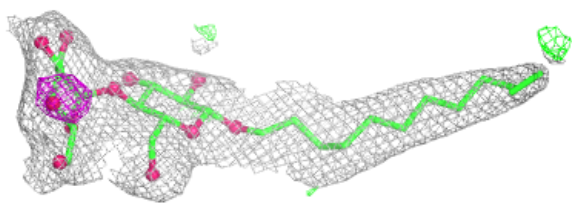
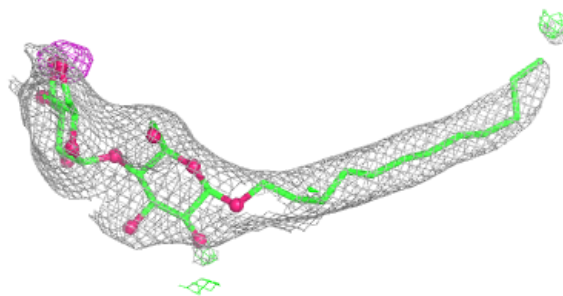
**Electron density around PLM A 208:**

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

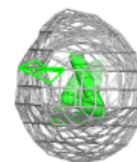
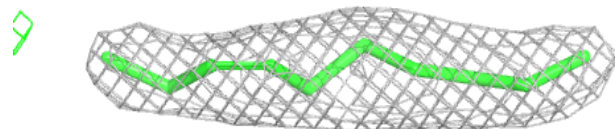
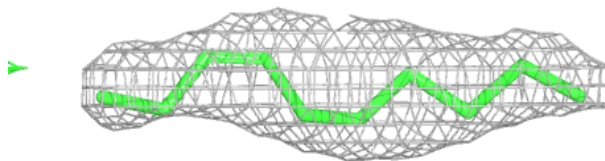


Electron density around LMT A 220:

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

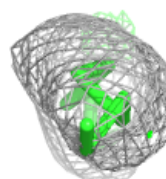
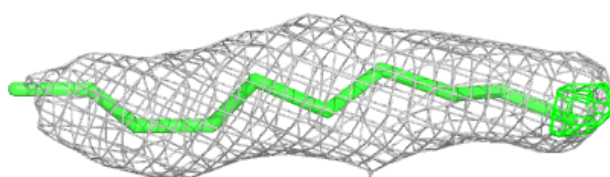
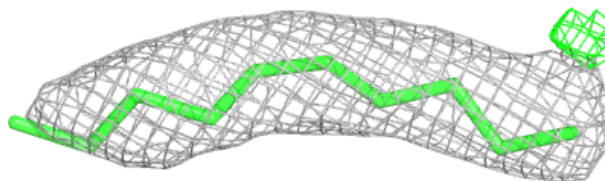
**Electron density around PAM A 211:**

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

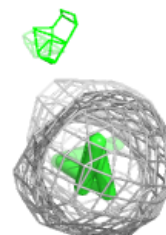
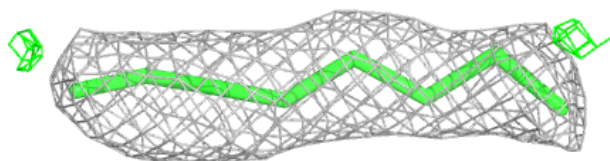
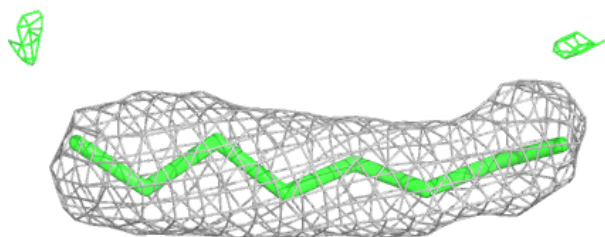


Electron density around PLM A 207:

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

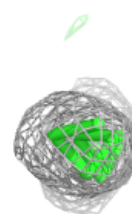
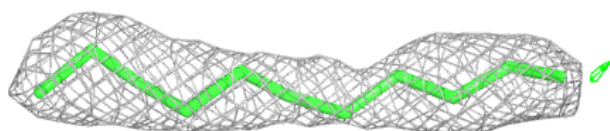
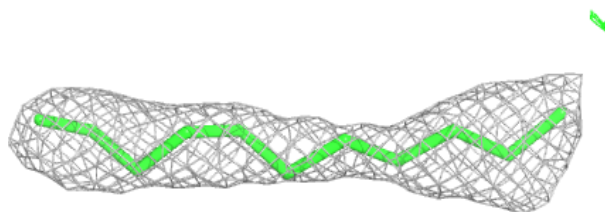
**Electron density around PLM A 222:**

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

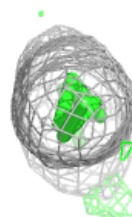
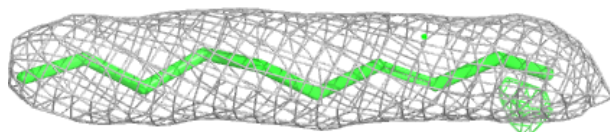
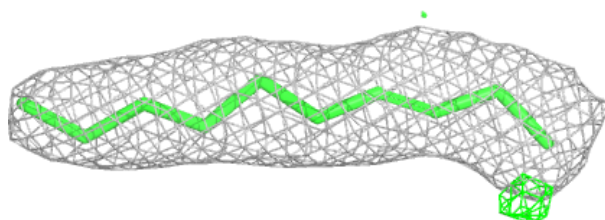


Electron density around PLM A 210:

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

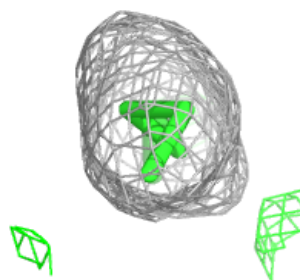
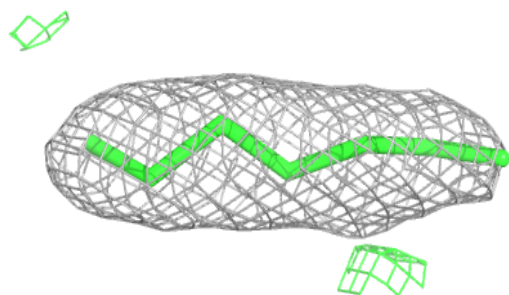
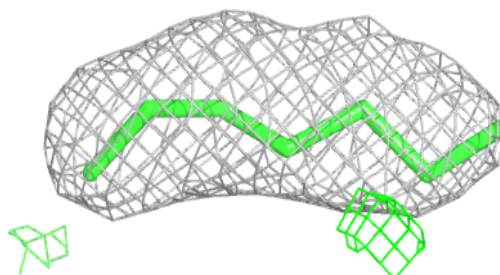
**Electron density around PAM A 212:**

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

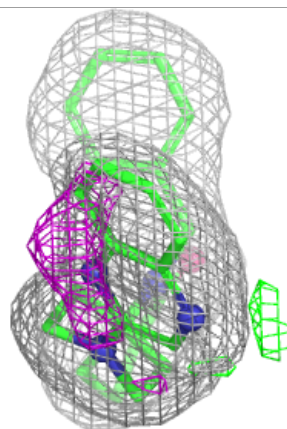
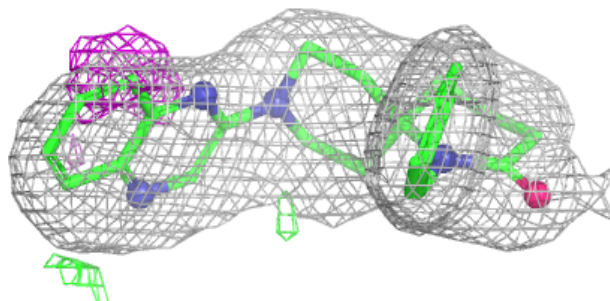
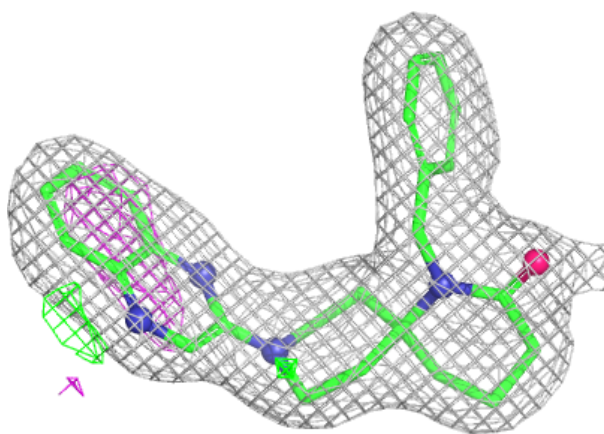


Electron density around PAM A 221:

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

**Electron density around A1IHS A 223:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.