



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2020 – 10:10 AM JST

PDB ID : 6L4K  
Title : Human serum albumin-Palmitic acid-Cu compound  
Authors : Zhang, Z.L.  
Deposited on : 2019-10-17  
Resolution : 2.09 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

i

## X-RAY DIFFRACTION

A.

 $R_{free}$ 1

## 2 Entry composition [i](#)

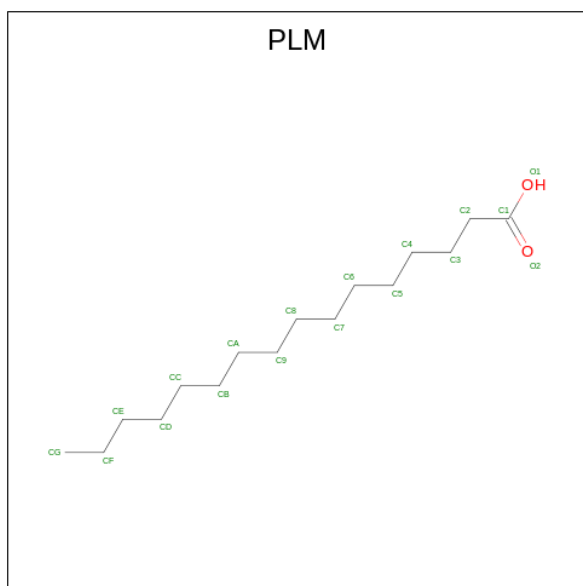
There are 3 unique types of molecules in this entry. The entry contains 9106 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4443	2819	744	839	41			
1	I	581	Total	C	N	O	S	0	0	0
			4443	2819	744	839	41			

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



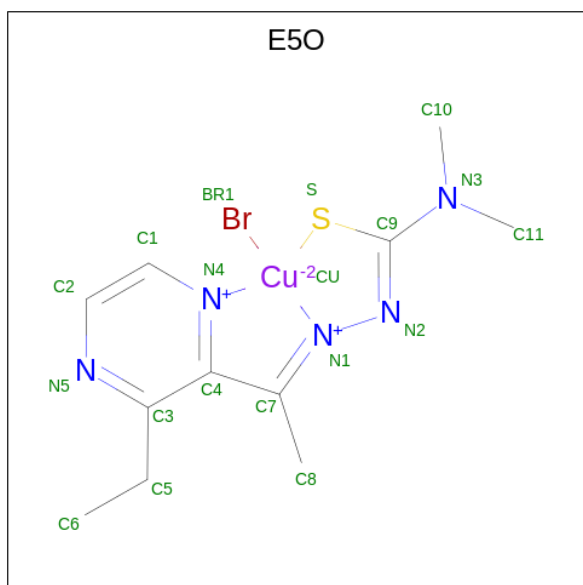
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	11	2		
2	A	1	Total	C	O	0	0
			18	16	2		
2	A	1	Total	C	O	0	0
			17	15	2		
2	A	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	15	2		
2	A	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			13	11	2		
2	I	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			17	15	2		
2	I	1	Total	C	O	0	0
			18	16	2		
2	I	1	Total	C	O	0	0
			17	15	2		
2	I	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is 2-bromanyl-9-ethyl- {N}, {N},7-trimethyl-3-thia-1 $\lambda^4$ ,5,6 $\lambda^4$ ,10-tetraza-2 $\lambda^4$ -cupratricyclo[6.4.0.0 $^{2,6}$ ]dodeca-1(8),4,6,9,11-pentaen-4-amine (three-letter code: E5O) (formula: C<sub>11</sub>H<sub>16</sub>BrCuN<sub>5</sub>S) (labeled as "Ligand of Interest" by author).

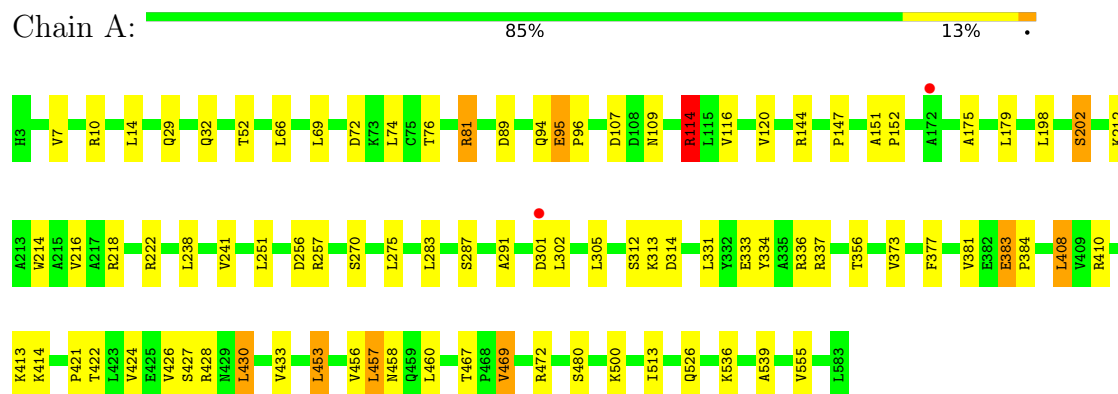


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cu	N	S	0	0
			18	11	1	5	1		

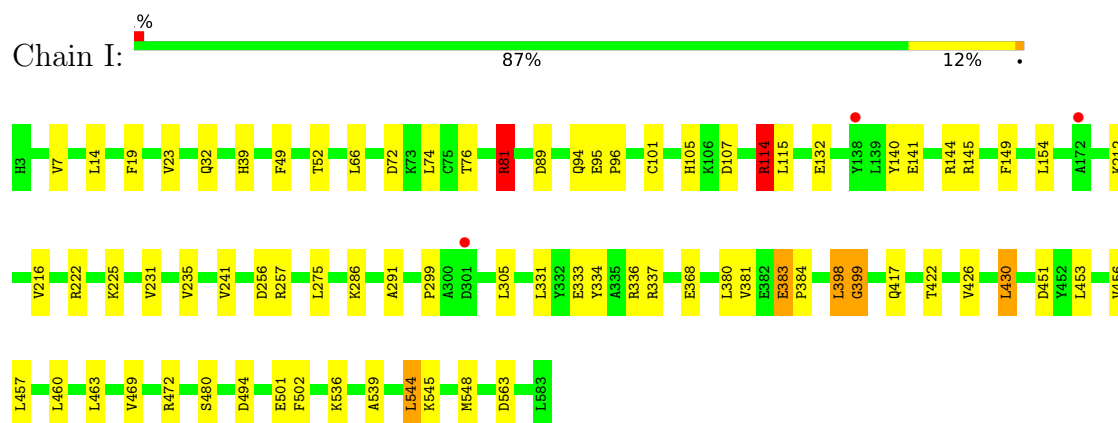
### 3 Residue-property plots

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

#### • Molecule 1: Serum albumin



#### • Molecule 1: Serum albumin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.36Å 93.52Å 96.36Å 74.89° 89.68° 80.04°	Depositor
Resolution (Å)	46.53 – 2.09 46.53 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.9 (46.53-2.09) 87.9 (46.53-2.09)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.10.1	Depositor
R, $R_{free}$	0.236 , 0.290 0.235 , 0.283	Depositor DCC
$R_{free}$ test set	3379 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 18.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.136 for h,h-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9106	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: E5O, PLM

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	0.69	0/4532	0.86	10/6148 (0.2%)
1	I	0.71	0/4532	0.88	11/6148 (0.2%)
All	All	0.70	0/9064	0.87	21/12296 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	I	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	A	336	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	I	114	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	I	144	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	I	472	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	I	144	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	472	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	I	81	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	I	336	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	I	145	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	I	81	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	I	336	ARG	NE-CZ-NH1	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	I	337	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	81	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	144	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	337	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	81	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	114	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	I	114	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	337	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	GLN	Peptide
1	I	94	GLN	Peptide

## 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	4443	0	4193	45	0
1	I	4443	0	4193	30	0
2	A	101	0	163	3	0
2	I	101	0	163	1	0
3	A	18	0	0	2	0
All	All	9106	0	8712	75	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 4.

All (75) 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:I:398:LEU:O	1:I:399:GLY:O	2.02	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:NH2	1:A:89:ASP:OD1	2.20	0.74
1:I:222:ARG:NH1	1:I:291:ALA:O	2.23	0.72
1:I:81:ARG:NH2	1:I:89:ASP:OD1	2.26	0.66
1:A:426:VAL:HG11	1:A:460:LEU:CD1	2.29	0.63
1:I:426:VAL:HG11	1:I:460:LEU:CD1	2.28	0.63
1:A:95:GLU:O	1:A:96:PRO:C	2.36	0.63
1:I:426:VAL:HG11	1:I:460:LEU:HD11	1.82	0.62
1:A:408:LEU:HD13	1:A:427:SER:CB	2.31	0.61
1:I:383:GLU:HG3	1:I:384:PRO:HD3	1.82	0.61
1:A:222:ARG:NH1	1:A:291:ALA:O	2.33	0.60
1:A:120:VAL:HG21	1:A:175:ALA:HB2	1.83	0.60
1:I:149:PHE:CD2	1:I:154:LEU:HD13	2.36	0.59
1:I:430:LEU:HD13	1:I:456:VAL:HG11	1.83	0.59
1:I:305:LEU:CD2	1:I:333:GLU:HB3	2.33	0.58
1:I:212:LYS:O	1:I:216:VAL:HG23	2.03	0.57
1:A:424:VAL:O	1:A:428:ARG:HG3	2.03	0.57
1:A:120:VAL:HG21	1:A:175:ALA:CB	2.35	0.57
1:A:430:LEU:HD13	1:A:456:VAL:HG11	1.87	0.56
1:I:72:ASP:O	1:I:76:THR:HG23	2.05	0.55
1:I:49:PHE:O	1:I:52:THR:HB	2.05	0.55
1:A:32:GLN:HE22	1:A:107:ASP:H	1.53	0.55
1:I:95:GLU:O	1:I:96:PRO:C	2.38	0.55
1:A:457:LEU:HD11	2:A:1004:PLM:H51	1.89	0.55
1:I:114:ARG:HH11	1:I:114:ARG:HG3	1.72	0.55
1:A:257:ARG:NH1	1:A:287:SER:OG	2.40	0.54
1:I:501:GLU:OE1	1:I:502:PHE:N	2.42	0.53
1:I:241:VAL:HG22	1:I:256:ASP:HB3	1.90	0.52
1:A:212:LYS:O	1:A:216:VAL:HG23	2.10	0.52
1:I:257:ARG:NH1	2:I:1002:PLM:O1	2.43	0.52
1:A:513:ILE:HD11	1:A:555:VAL:HG13	1.93	0.51
1:A:305:LEU:HD21	1:A:333:GLU:HB3	1.93	0.51
1:A:383:GLU:HG3	1:A:384:PRO:HD3	1.93	0.50
1:I:422:THR:O	1:I:426:VAL:HG13	2.12	0.50
1:A:377:PHE:O	1:A:381:VAL:HG23	2.12	0.50
1:A:410:ARG:O	1:A:414:LYS:HG3	2.12	0.49
1:A:356:THR:HG21	1:A:373:VAL:HG23	1.94	0.49
1:A:114:ARG:HH11	1:A:116:VAL:HG12	1.78	0.49
1:I:7:VAL:HA	1:I:66:LEU:HD21	1.95	0.49
1:A:460:LEU:HD11	2:A:1004:PLM:HC2	1.95	0.48
1:A:313:LYS:O	1:A:314:ASP:CB	2.61	0.48
1:A:72:ASP:O	1:A:76:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:VAL:HG11	1:A:453:LEU:HD13	1.96	0.47
1:A:218:ARG:HG3	3:A:1007:E5O:C11	2.45	0.47
1:I:417:GLN:NE2	1:I:494:ASP:OD2	2.40	0.46
1:A:241:VAL:HG22	1:A:256:ASP:HB3	1.98	0.46
1:A:214:TRP:CZ3	3:A:1007:E5O:C10	2.99	0.46
1:A:198:LEU:HD13	1:A:458:ASN:OD1	2.15	0.46
1:I:545:LYS:HA	1:I:548:MET:HE2	1.98	0.46
1:A:408:LEU:HD13	1:A:427:SER:HB2	1.98	0.45
1:A:413:LYS:NZ	1:A:539:ALA:O	2.48	0.45
1:A:305:LEU:HD21	1:A:333:GLU:CB	2.46	0.45
1:I:19:PHE:O	1:I:23:VAL:HG23	2.17	0.45
1:A:7:VAL:HG11	1:A:69:LEU:HD13	1.99	0.44
1:A:408:LEU:HD21	1:A:526:GLN:HB3	1.98	0.44
1:A:10:ARG:HG3	1:A:66:LEU:HD11	1.98	0.44
1:A:198:LEU:O	1:A:202:SER:OG	2.37	0.43
1:A:114:ARG:NH1	1:A:116:VAL:HG12	2.33	0.43
1:I:115:LEU:HD11	1:I:141:GLU:HB3	2.00	0.43
1:A:29:GLN:HG2	1:A:147:PRO:HA	2.01	0.43
1:I:32:GLN:HE22	1:I:107:ASP:H	1.68	0.42
1:I:381:VAL:O	1:I:384:PRO:HD2	2.19	0.42
1:I:225:LYS:HG3	1:I:299:PRO:HD3	2.02	0.42
1:A:422:THR:O	1:A:426:VAL:HG13	2.20	0.41
1:I:231:VAL:O	1:I:235:VAL:HG23	2.20	0.41
1:A:381:VAL:O	1:A:384:PRO:HD2	2.20	0.41
1:A:383:GLU:HG3	1:A:384:PRO:CD	2.50	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.91	0.41
1:A:151:ALA:HB3	1:A:152:PRO:HD3	2.02	0.41
1:A:383:GLU:CG	1:A:384:PRO:HD3	2.51	0.41
1:I:101:CYS:O	1:I:105:HIS:HD2	2.04	0.41
1:A:251:LEU:HD21	2:A:1002:PLM:HA2	2.04	0.40
1:A:301:ASP:O	1:A:302:LEU:HD23	2.22	0.40
1:I:114:ARG:HH11	1:I:114:ARG:CG	2.31	0.40
1:I:539:ALA:CB	1:I:544:LEU:HD13	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/581 (100%)	561 (97%)	17 (3%)	1 (0%)	47	49
1	I	579/581 (100%)	555 (96%)	22 (4%)	2 (0%)	41	41
All	All	1158/1162 (100%)	1116 (96%)	39 (3%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	399	GLY
1	A	469	VAL
1	I	563	ASP

### 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	455/509 (89%)	430 (94%)	25 (6%)	21	19
1	I	455/509 (89%)	431 (95%)	24 (5%)	22	20
All	All	910/1018 (89%)	861 (95%)	49 (5%)	22	20

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	52	THR
1	A	74	LEU

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Mol	Chain	Res	Type
1	A	95	GLU
1	A	109	ASN
1	A	114	ARG
1	A	179	LEU
1	A	202	SER
1	A	270	SER
1	A	275	LEU
1	A	283	LEU
1	A	312	SER
1	A	331	LEU
1	A	334	TYR
1	A	383	GLU
1	A	408	LEU
1	A	421	PRO
1	A	430	LEU
1	A	453	LEU
1	A	457	LEU
1	A	467	THR
1	A	469	VAL
1	A	480	SER
1	A	500	LYS
1	A	536	LYS
1	I	14	LEU
1	I	39	HIS
1	I	74	LEU
1	I	81	ARG
1	I	114	ARG
1	I	132	GLU
1	I	140	TYR
1	I	275	LEU
1	I	286	LYS
1	I	331	LEU
1	I	334	TYR
1	I	368	GLU
1	I	380	LEU
1	I	383	GLU
1	I	398	LEU
1	I	430	LEU
1	I	451	ASP
1	I	453	LEU
1	I	457	LEU
1	I	463	LEU

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Mol	Chain	Res	Type
1	I	469	VAL
1	I	480	SER
1	I	536	LYS
1	I	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	105	HIS
1	A	318	ASN
1	A	459	GLN
1	A	580	GLN
1	I	32	GLN
1	I	105	HIS
1	I	318	ASN
1	I	459	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no 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	$\# Z  > 2$
2	PLM	A	1001	-	9,12,17	0.42	0	8,12,17	0.55	0
2	PLM	I	1004	-	14,17,17	0.21	0	13,17,17	0.83	0
2	PLM	A	1006	-	14,17,17	0.42	0	13,17,17	0.54	0
2	PLM	I	1005	-	13,16,17	0.29	0	12,16,17	0.69	0
2	PLM	A	1002	-	14,17,17	0.21	0	13,17,17	0.78	0
2	PLM	I	1001	-	9,12,17	0.39	0	8,12,17	0.98	0
2	PLM	I	1006	-	14,17,17	0.38	0	13,17,17	0.41	0
2	PLM	I	1002	-	14,17,17	0.30	0	13,17,17	0.52	0
2	PLM	A	1003	-	13,16,17	0.41	0	12,16,17	0.66	0
3	E5O	A	1007	1	17,20,21	2.50	6 (35%)	18,30,33	4.09	11 (61%)
2	PLM	A	1004	-	14,17,17	0.19	0	13,17,17	0.61	0
2	PLM	I	1003	-	13,16,17	0.31	0	12,16,17	0.77	1 (8%)
2	PLM	A	1005	-	13,16,17	0.47	0	12,16,17	0.88	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
2	PLM	A	1001	-	-	6/8/10/15	-
2	PLM	I	1004	-	-	8/13/15/15	-
2	PLM	A	1006	-	-	6/13/15/15	-
2	PLM	I	1005	-	-	7/12/14/15	-
2	PLM	A	1002	-	-	7/13/15/15	-
2	PLM	I	1001	-	-	3/8/10/15	-
2	PLM	I	1006	-	-	8/13/15/15	-
2	PLM	I	1002	-	-	4/13/15/15	-
2	PLM	A	1003	-	-	6/12/14/15	-
3	E5O	A	1007	1	-	2/6/30/35	0/3/3/3
2	PLM	A	1004	-	-	6/13/15/15	-
2	PLM	I	1003	-	-	6/12/14/15	-
2	PLM	A	1005	-	-	5/12/14/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	E5O	C4-N4	6.11	1.44	1.35
3	A	1007	E5O	C9-N3	-4.54	1.28	1.35
3	A	1007	E5O	C4-C3	3.91	1.51	1.41
3	A	1007	E5O	C4-C7	3.04	1.52	1.48
3	A	1007	E5O	C5-C3	-2.52	1.46	1.51
3	A	1007	E5O	C9-S	-2.12	1.71	1.73

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1007	E5O	C3-C4-N4	-10.72	113.84	118.82
3	A	1007	E5O	C5-C3-C4	6.19	133.75	125.32
3	A	1007	E5O	C8-C7-N1	-5.02	114.36	123.64
3	A	1007	E5O	S-C9-N2	-4.89	120.25	124.85
3	A	1007	E5O	C6-C5-C3	4.85	126.82	114.88
3	A	1007	E5O	C8-C7-C4	4.44	133.25	123.62
3	A	1007	E5O	C5-C3-N5	-4.42	106.73	114.83
3	A	1007	E5O	C2-N5-C3	3.15	121.77	117.81
3	A	1007	E5O	C3-C4-C7	3.04	130.27	127.53
3	A	1007	E5O	C1-N4-C4	2.55	121.81	118.27
3	A	1007	E5O	C11-N3-C9	2.22	125.51	121.39
2	I	1003	PLM	C6-C5-C4	-2.01	104.21	114.42

There are no chirality outliers.

All (74) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	PLM	C1-C2-C3-C4
2	I	1004	PLM	C1-C2-C3-C4
2	A	1006	PLM	C1-C2-C3-C4
2	I	1005	PLM	C1-C2-C3-C4
2	I	1001	PLM	C1-C2-C3-C4
2	A	1003	PLM	C1-C2-C3-C4
3	A	1007	E5O	C4-C3-C5-C6
3	A	1007	E5O	N5-C3-C5-C6
2	I	1003	PLM	C1-C2-C3-C4
2	I	1001	PLM	C4-C5-C6-C7
2	I	1004	PLM	C2-C3-C4-C5
2	A	1002	PLM	C2-C3-C4-C5
2	I	1005	PLM	C9-CA-CB-CC
2	I	1006	PLM	C2-C3-C4-C5
2	I	1006	PLM	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
2	A	1004	PLM	C8-C9-CA-CB
2	A	1001	PLM	C5-C6-C7-C8
2	I	1004	PLM	C9-CA-CB-CC
2	I	1002	PLM	C2-C3-C4-C5
2	I	1004	PLM	C3-C4-C5-C6
2	I	1004	PLM	C8-C9-CA-CB
2	I	1002	PLM	C8-C9-CA-CB
2	I	1003	PLM	CB-CC-CD-CE
2	A	1003	PLM	C8-C9-CA-CB
2	A	1003	PLM	CB-CC-CD-CE
2	A	1004	PLM	C9-CA-CB-CC
2	I	1005	PLM	CA-CB-CC-CD
2	A	1002	PLM	C3-C4-C5-C6
2	A	1002	PLM	CC-CD-CE-CF
2	A	1004	PLM	C5-C6-C7-C8
2	A	1001	PLM	C6-C7-C8-C9
2	A	1004	PLM	C6-C7-C8-C9
2	I	1005	PLM	CC-CD-CE-CF
2	A	1002	PLM	C7-C8-C9-CA
2	I	1005	PLM	C4-C5-C6-C7
2	I	1005	PLM	C5-C6-C7-C8
2	A	1002	PLM	C5-C6-C7-C8
2	A	1005	PLM	CB-CC-CD-CE
2	A	1006	PLM	C6-C7-C8-C9
2	A	1004	PLM	C4-C5-C6-C7
2	A	1005	PLM	CC-CD-CE-CF
2	A	1001	PLM	C3-C4-C5-C6
2	I	1002	PLM	CB-CC-CD-CE
2	I	1006	PLM	CD-CE-CF-CG
2	I	1006	PLM	C6-C7-C8-C9
2	A	1002	PLM	CA-CB-CC-CD
2	A	1005	PLM	C3-C4-C5-C6
2	I	1006	PLM	C9-CA-CB-CC
2	I	1005	PLM	C6-C7-C8-C9
2	A	1002	PLM	CB-CC-CD-CE
2	I	1002	PLM	C7-C8-C9-CA
2	A	1005	PLM	C9-CA-CB-CC
2	A	1003	PLM	C9-CA-CB-CC
2	I	1004	PLM	C6-C7-C8-C9
2	I	1003	PLM	C2-C3-C4-C5
2	A	1006	PLM	C2-C3-C4-C5
2	I	1003	PLM	CA-CB-CC-CD

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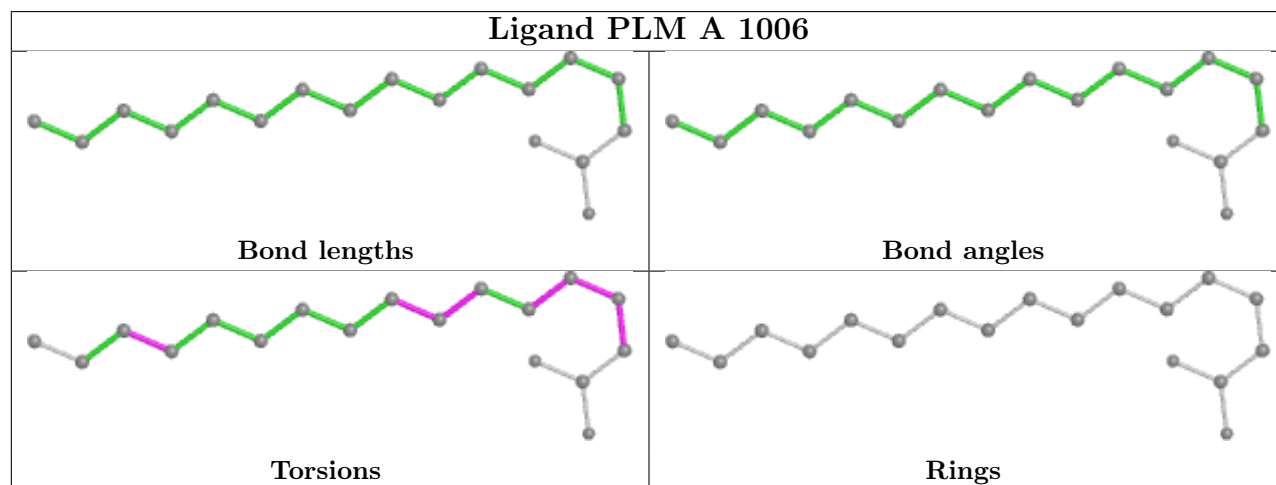
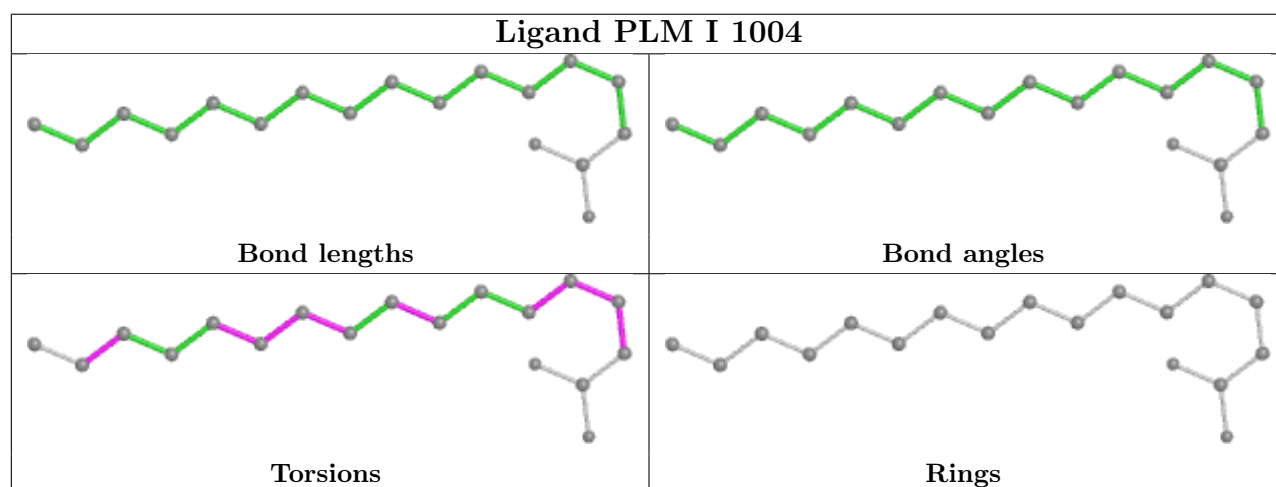
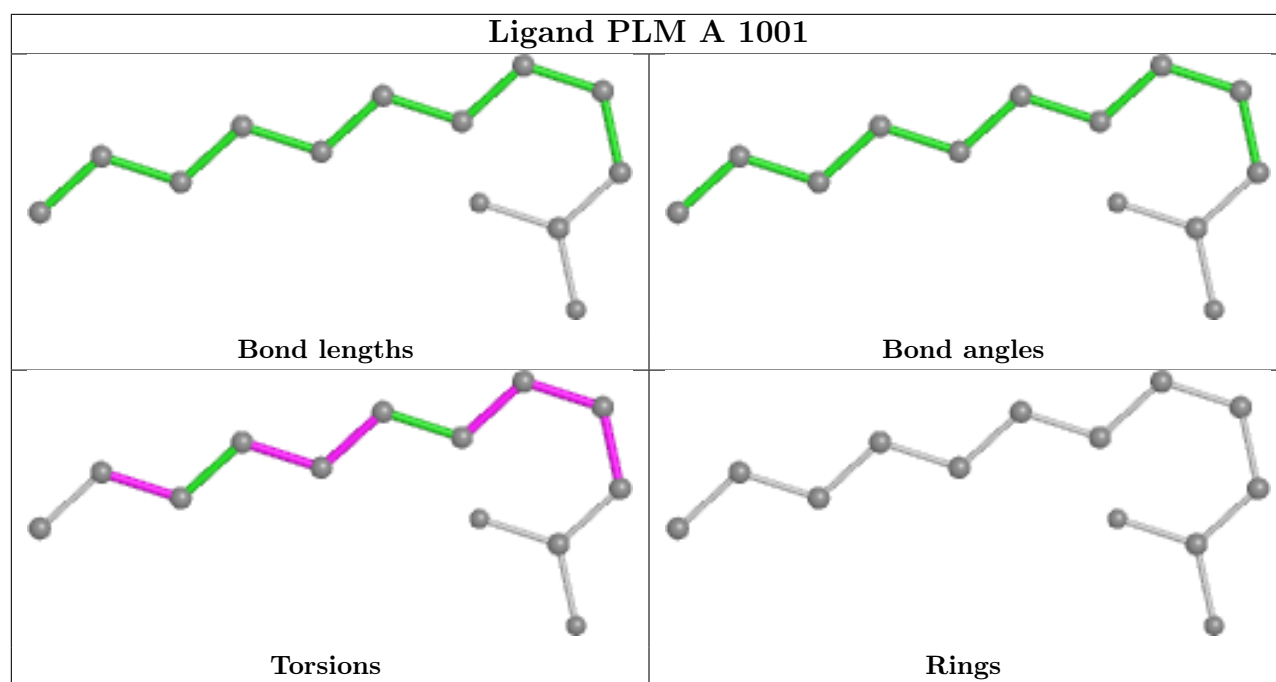
Mol	Chain	Res	Type	Atoms
2	I	1003	PLM	CC-CD-CE-CF
2	A	1003	PLM	CC-CD-CE-CF
2	A	1001	PLM	C2-C3-C4-C5
2	A	1001	PLM	C8-C9-CA-CB
2	A	1005	PLM	C8-C9-CA-CB
2	I	1006	PLM	CC-CD-CE-CF
2	A	1006	PLM	C3-C4-C5-C6
2	I	1003	PLM	C6-C7-C8-C9
2	A	1006	PLM	CC-CD-CE-CF
2	A	1003	PLM	C2-C3-C4-C5
2	A	1004	PLM	C2-C3-C4-C5
2	A	1006	PLM	C5-C6-C7-C8
2	I	1006	PLM	C1-C2-C3-C4
2	I	1006	PLM	C7-C8-C9-CA
2	I	1004	PLM	CD-CE-CF-CG
2	I	1004	PLM	CA-CB-CC-CD
2	I	1001	PLM	C6-C7-C8-C9

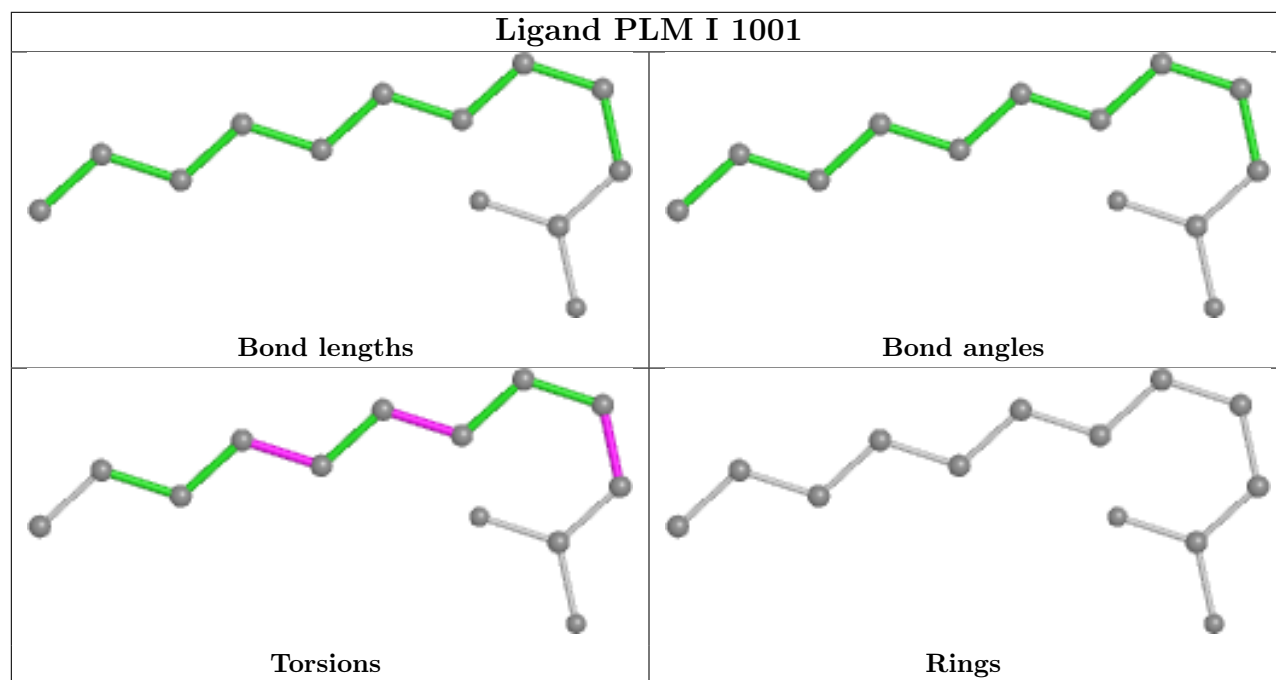
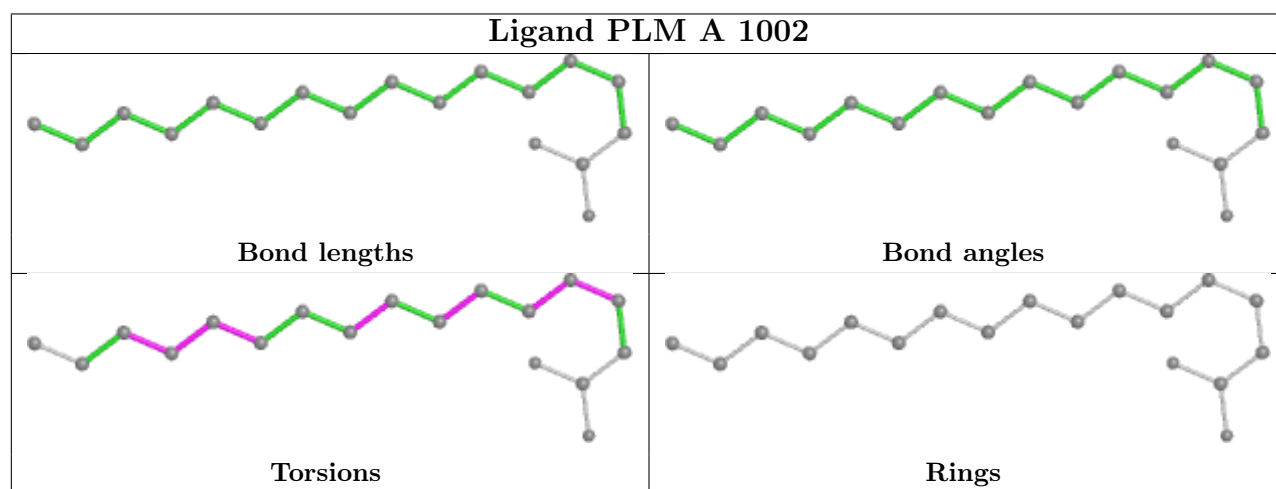
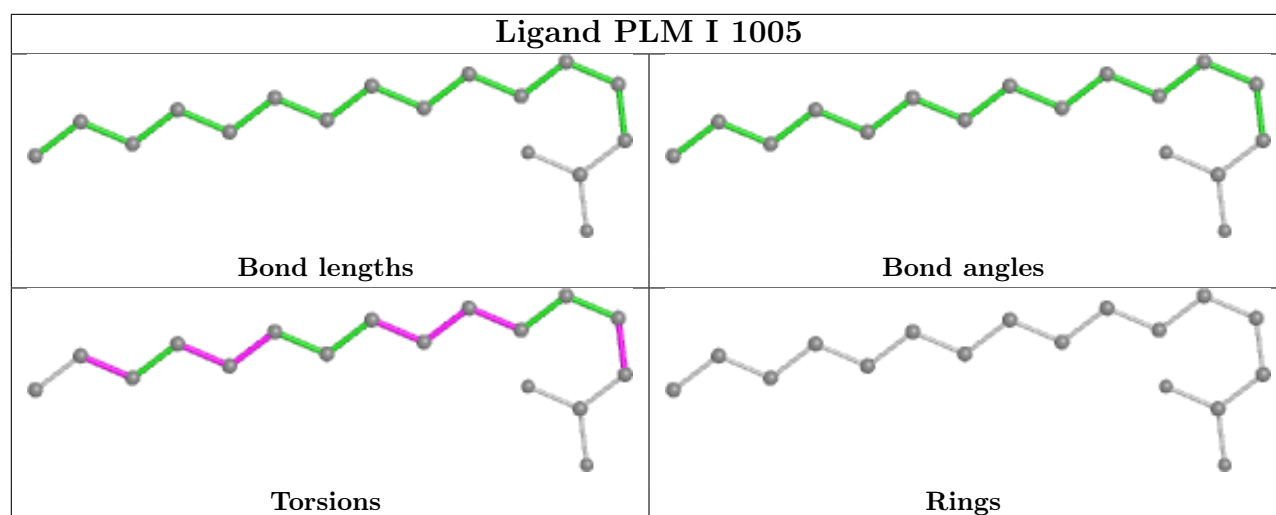
There are no ring outliers.

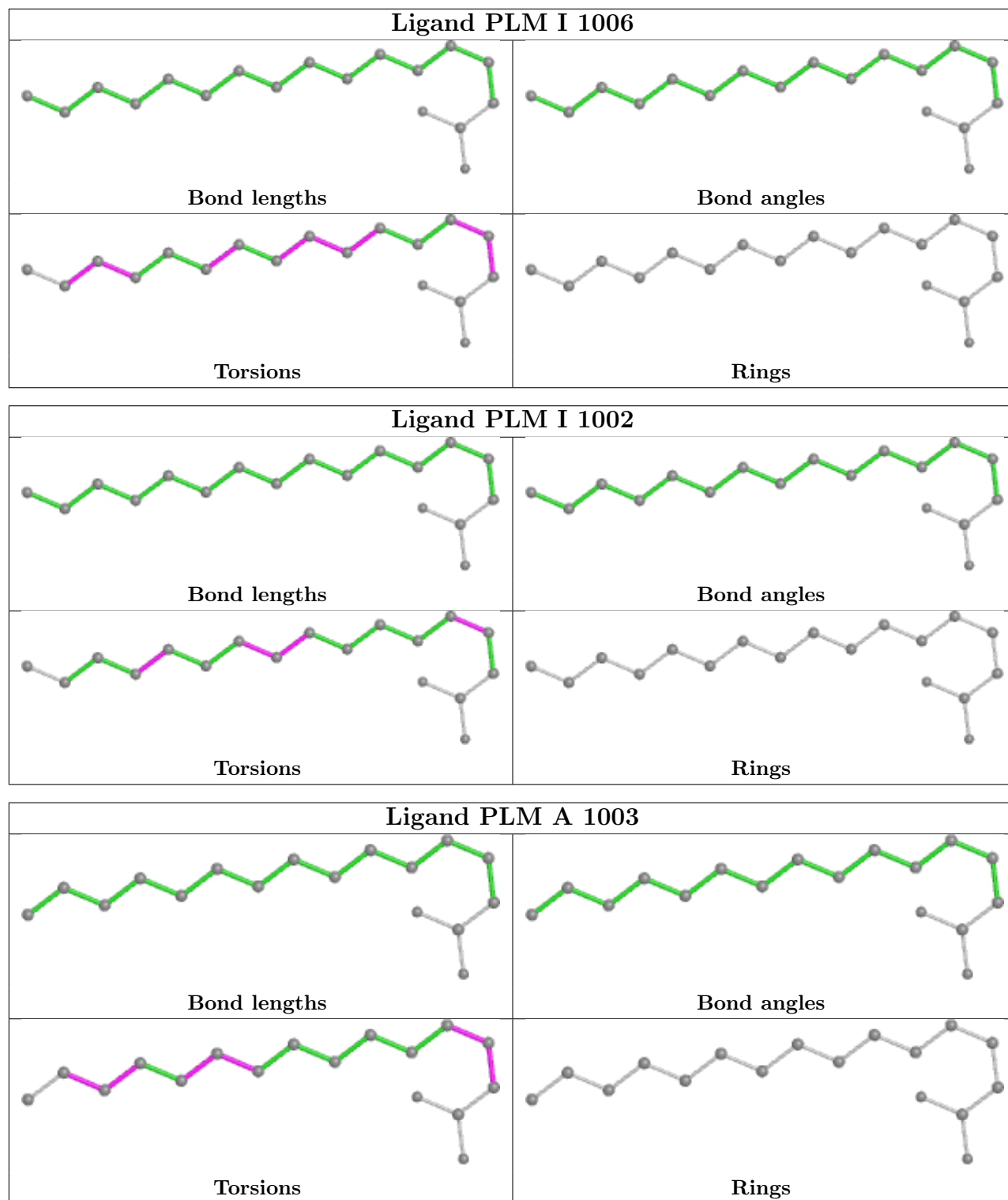
4 monomers are involved in 6 short contacts:

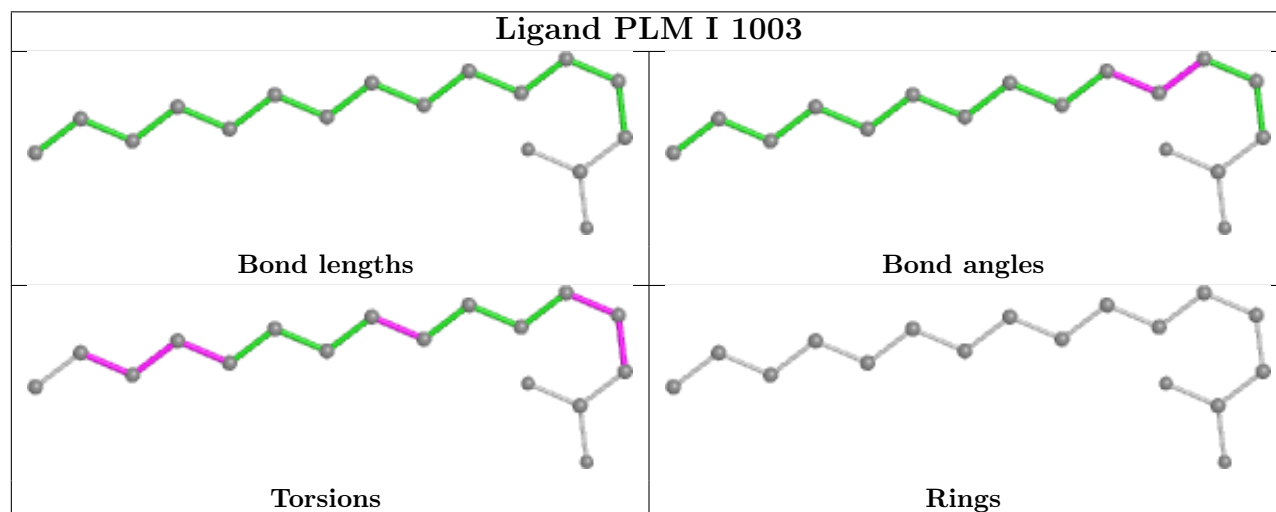
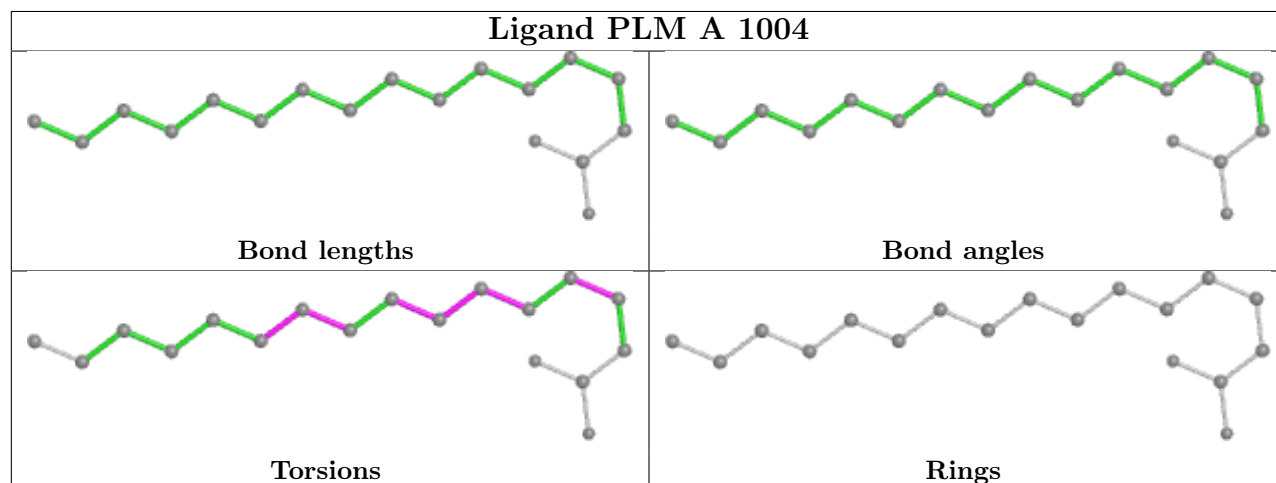
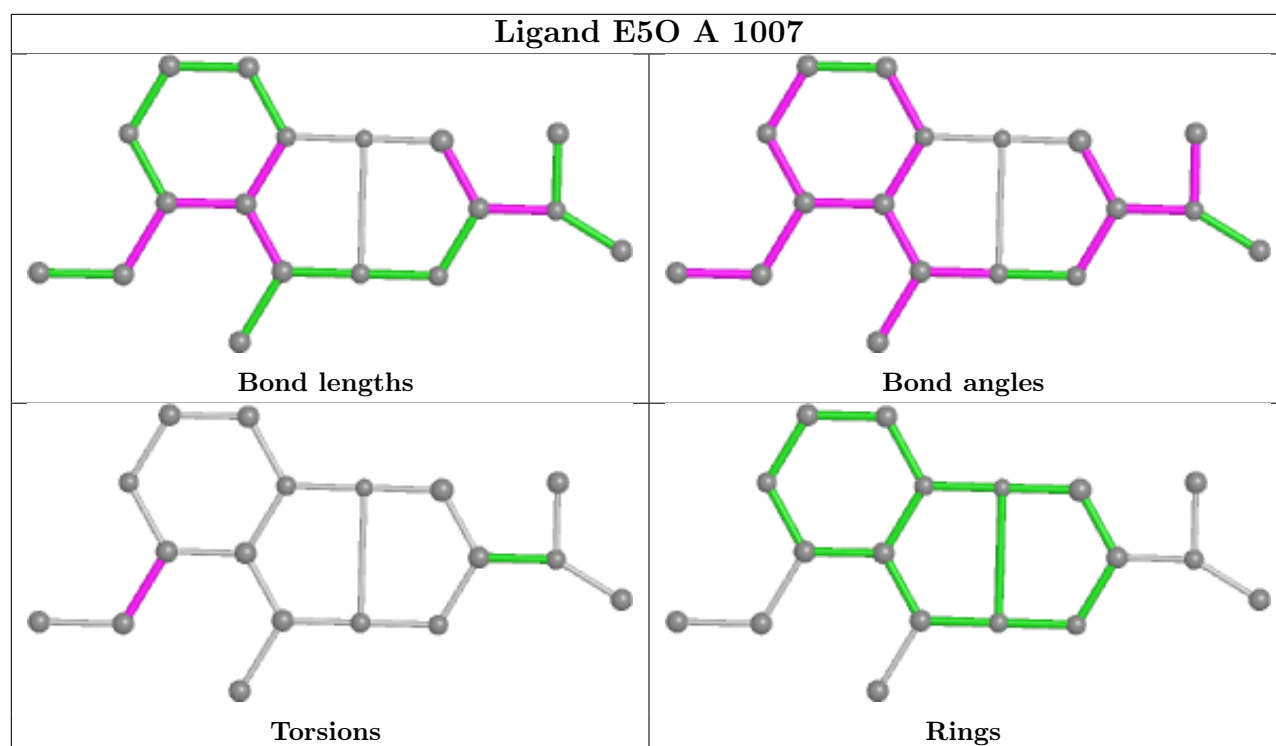
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	PLM	1	0
2	I	1002	PLM	1	0
3	A	1007	E5O	2	0
2	A	1004	PLM	2	0

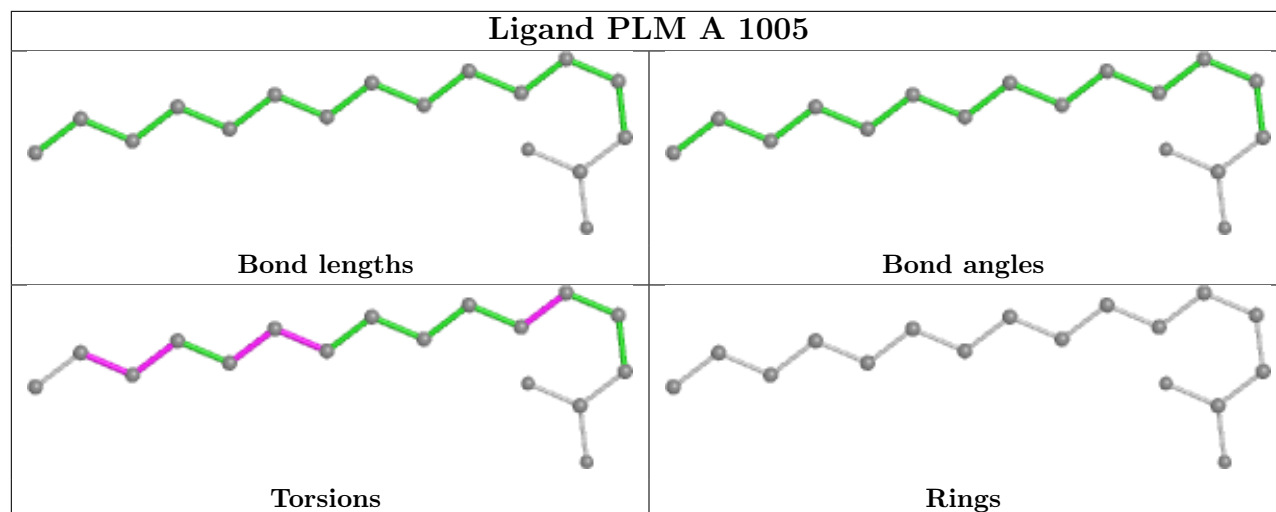
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	581/581 (100%)	-0.35	2 (0%) 94 94	27, 45, 64, 88	0
1	I	581/581 (100%)	-0.35	3 (0%) 91 92	28, 44, 65, 101	0
All	All	1162/1162 (100%)	-0.35	5 (0%) 92 93	27, 45, 65, 101	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	172	ALA	5.1
1	I	301	ASP	4.9
1	A	172	ALA	4.6
1	A	301	ASP	2.8
1	I	138	TYR	2.3

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

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

### 6.3 Carbohydrates [i](#)

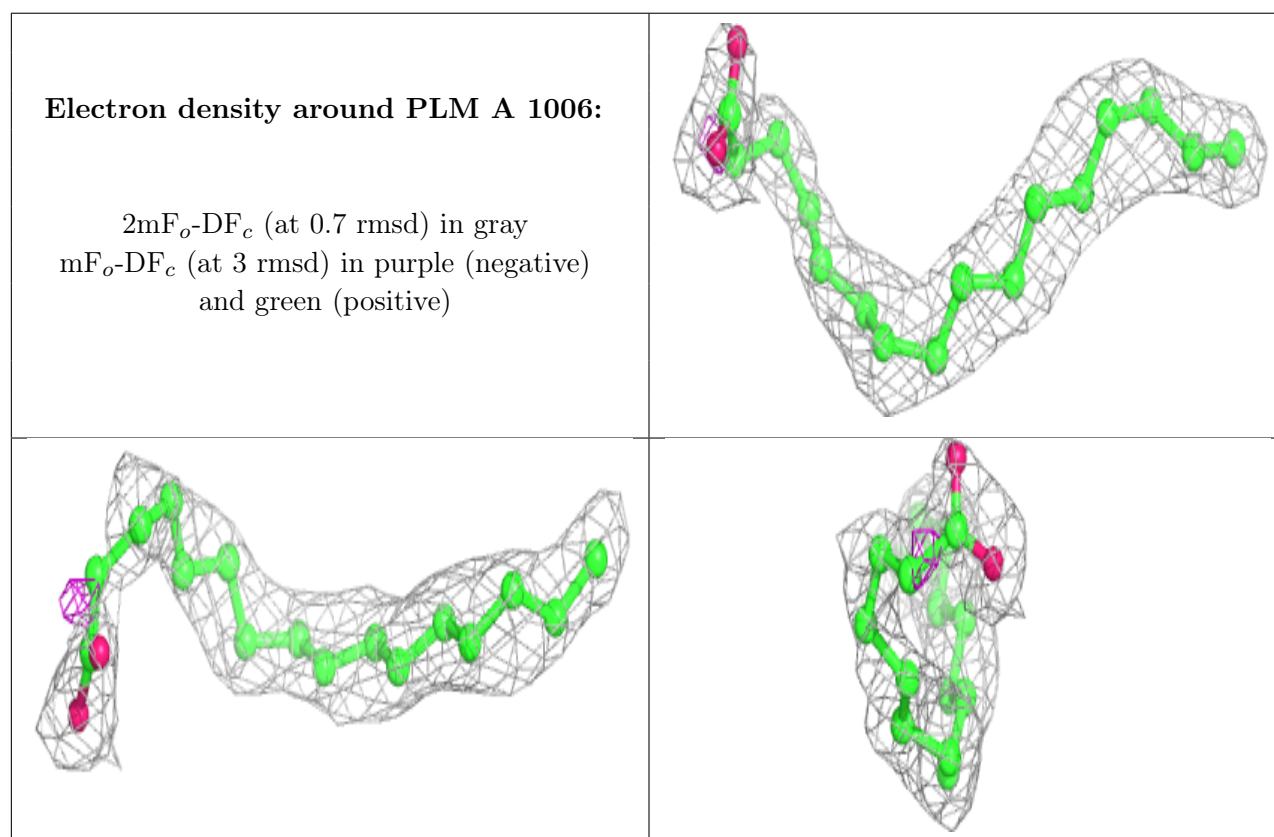
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PLM	A	1006	18/18	0.80	0.21	44,48,64,67	0
2	PLM	A	1001	13/18	0.81	0.26	50,67,74,76	0
2	PLM	I	1001	13/18	0.81	0.24	47,58,73,75	0
2	PLM	I	1006	18/18	0.83	0.22	49,55,84,89	0
2	PLM	I	1002	18/18	0.83	0.20	48,56,68,68	0
2	PLM	A	1002	18/18	0.87	0.26	46,56,60,60	0
2	PLM	I	1004	18/18	0.88	0.23	46,48,54,55	0
2	PLM	A	1003	17/18	0.88	0.23	32,54,82,85	0
2	PLM	I	1005	17/18	0.91	0.13	39,44,54,54	0
3	E5O	A	1007	18/19	0.91	0.16	62,65,88,89	0
2	PLM	A	1004	18/18	0.91	0.33	48,61,69,70	0
2	PLM	A	1005	17/18	0.92	0.16	41,46,53,53	0
2	PLM	I	1003	17/18	0.93	0.15	32,44,55,56	0

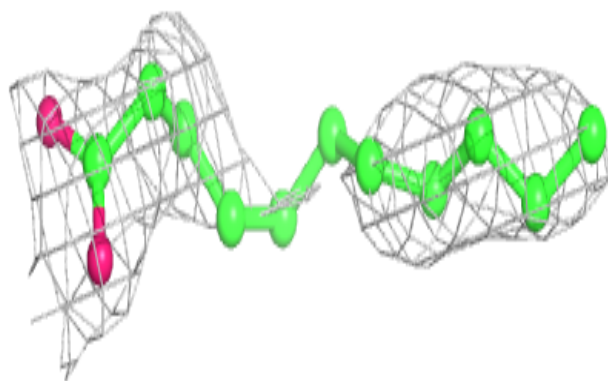
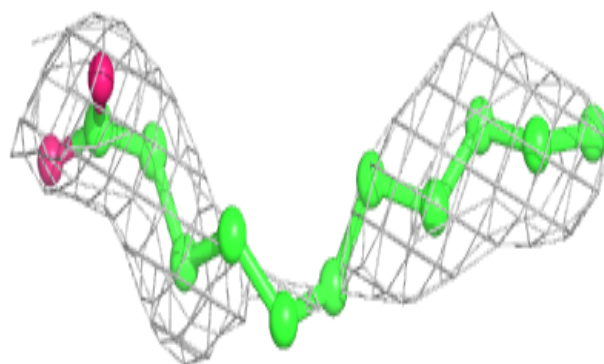
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



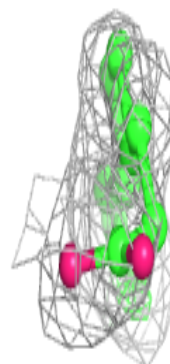
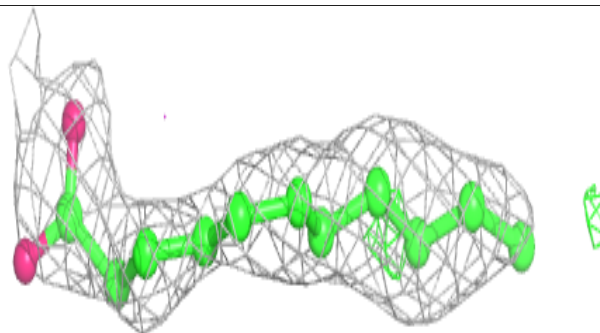
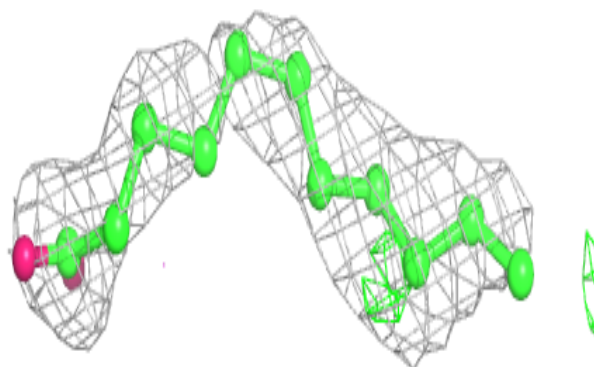


**Electron density around PLM A 1001:**

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

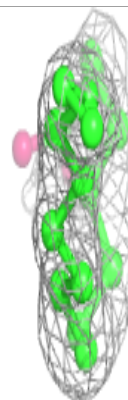
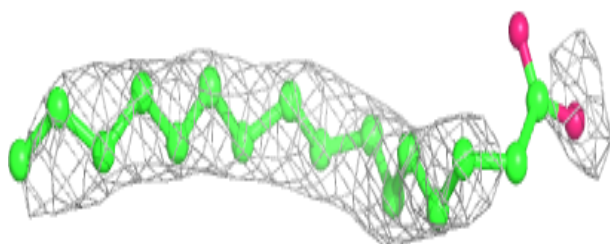
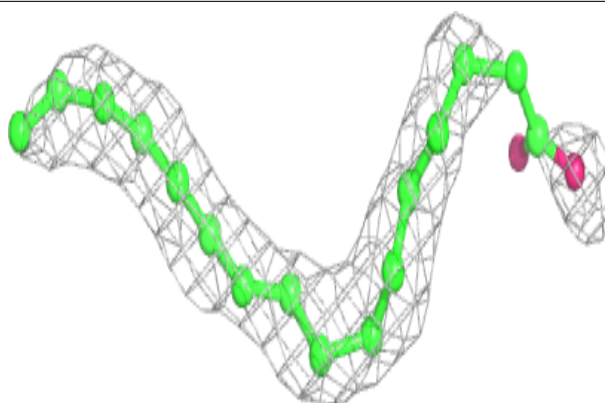
**Electron density around PLM I 1001:**

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and green (positive)

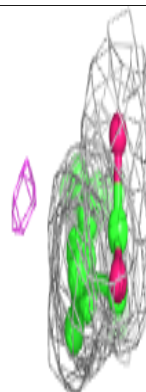
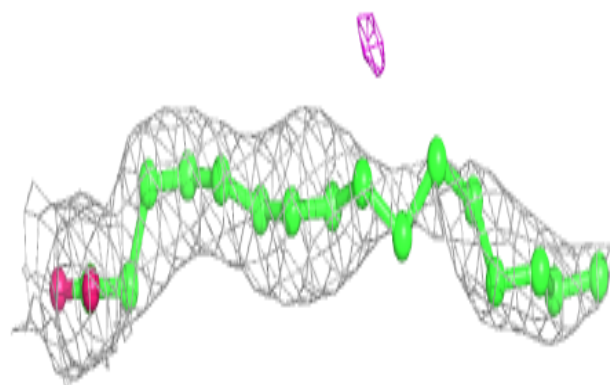
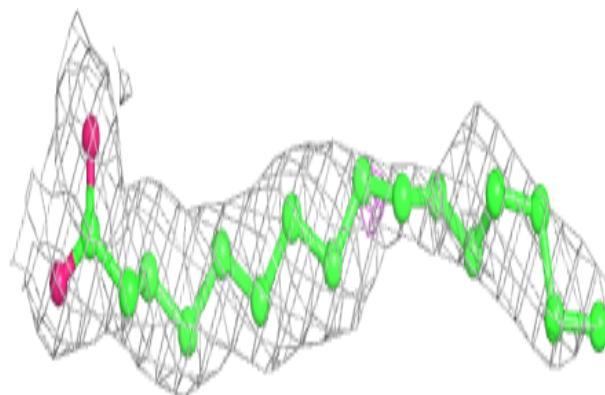


**Electron density around PLM I 1006:**

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

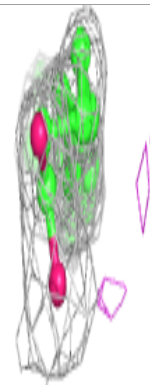
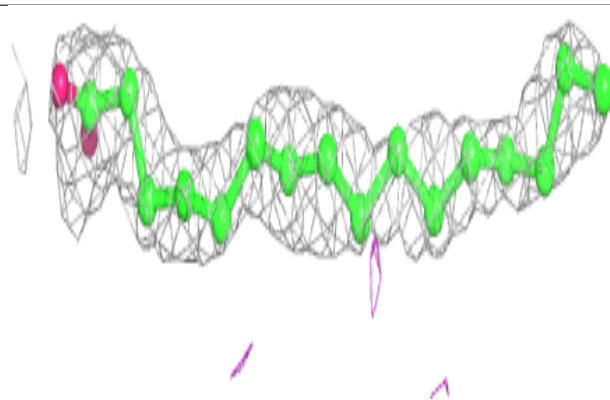
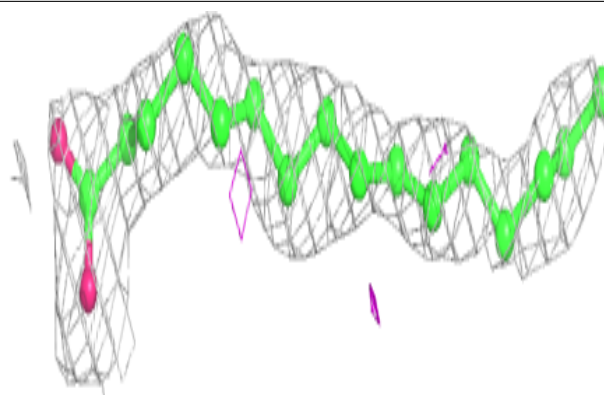
**Electron density around PLM I 1002:**

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and green (positive)

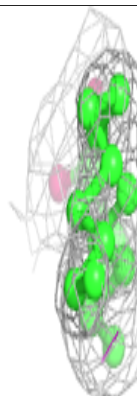
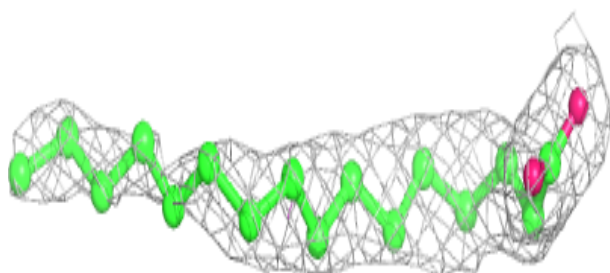
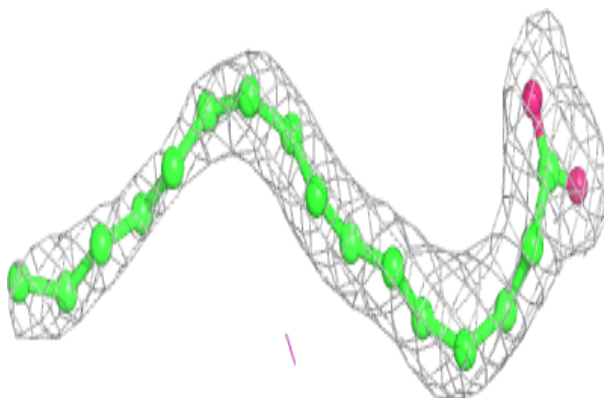


**Electron density around PLM A 1002:**

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

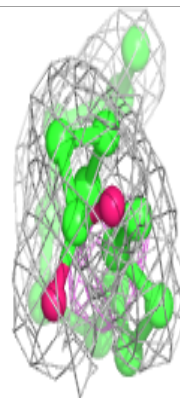
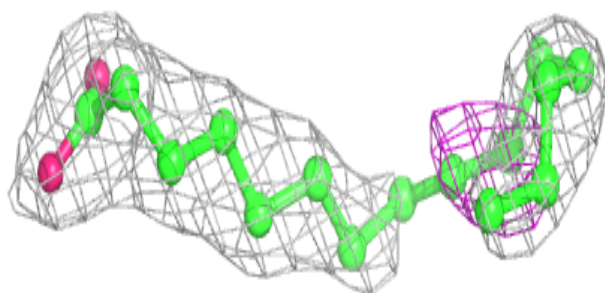
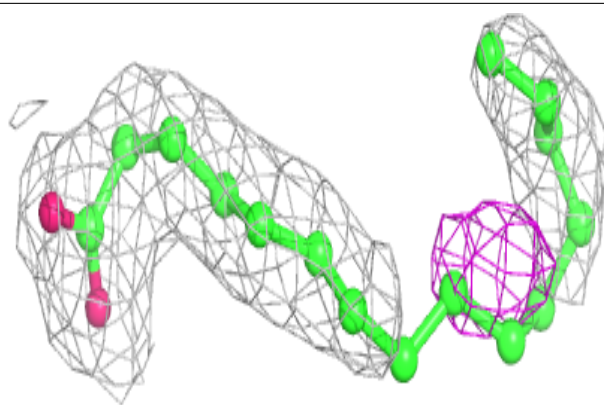
**Electron density around PLM I 1004:**

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and green (positive)

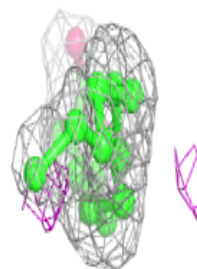
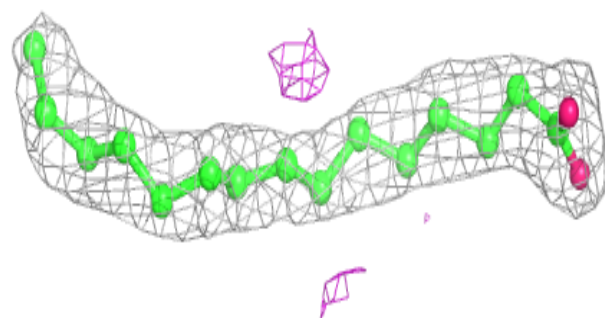
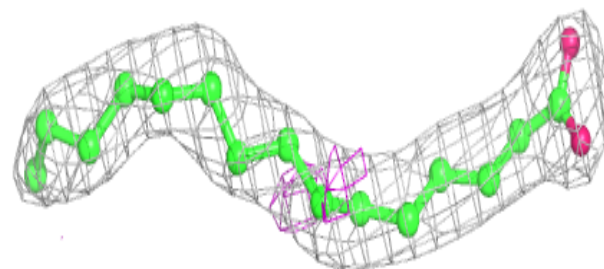


**Electron density around PLM A 1003:**

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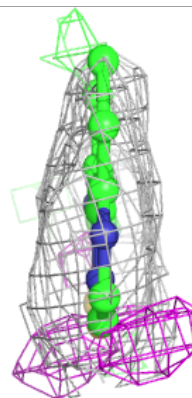
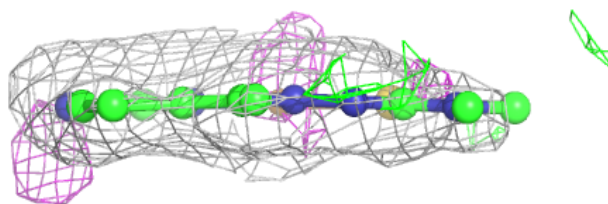
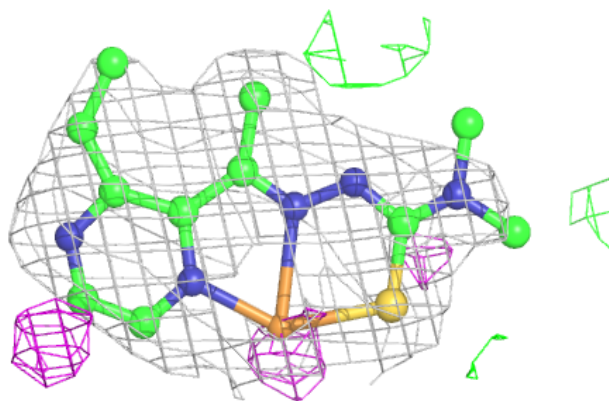
**Electron density around PLM I 1005:**

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and green (positive)

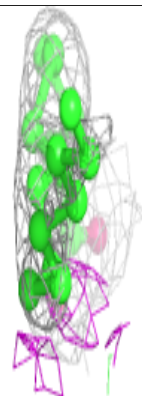
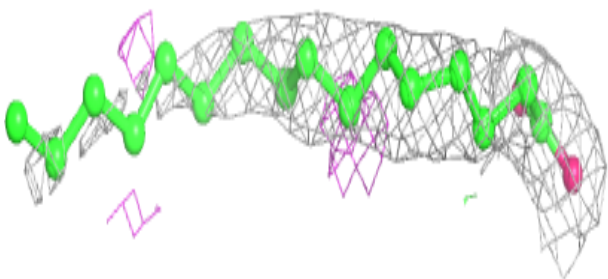
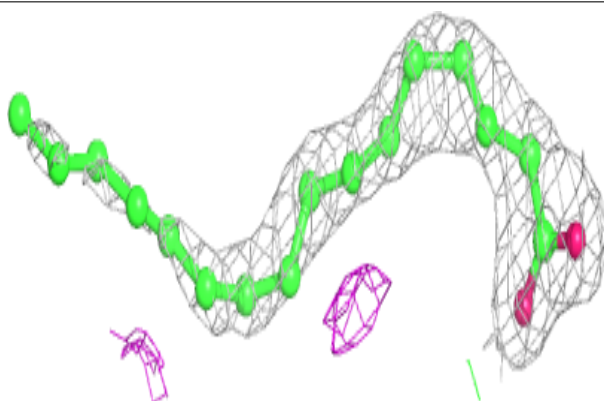


**Electron density around E5O A 1007:**

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

**Electron density around PLM A 1004:**

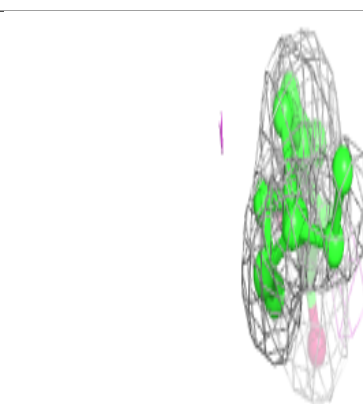
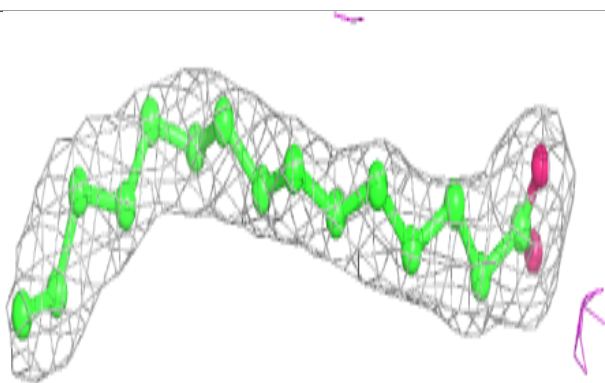
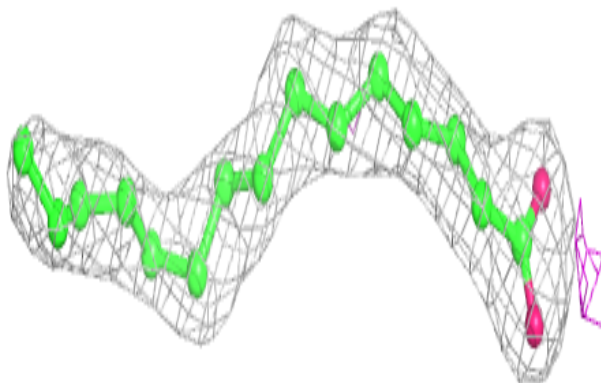
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



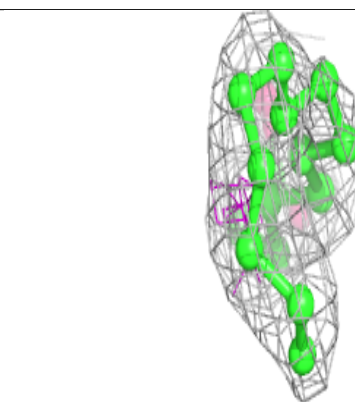
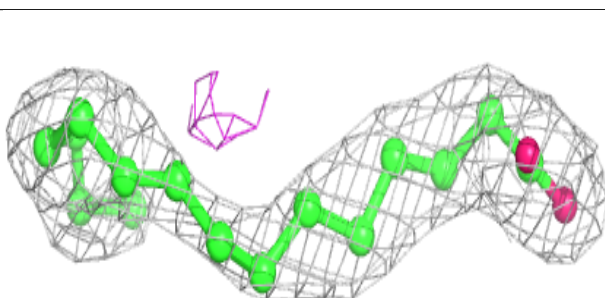
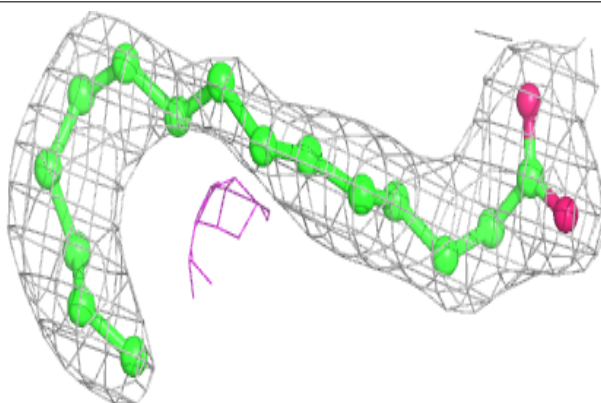


**Electron density around PLM A 1005:**

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

**Electron density around PLM I 1003:**

$2mF_o-DF_c$  (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.