



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2020 – 08:49 pm BST

PDB ID : 4Z69
Title : Human serum albumin complexed with palmitic acid and diclofenac
Authors : Zhang, Y.; Yang, F.
Deposited on : 2015-04-04
Resolution : 2.19 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 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 : 2.11
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) : 2.11

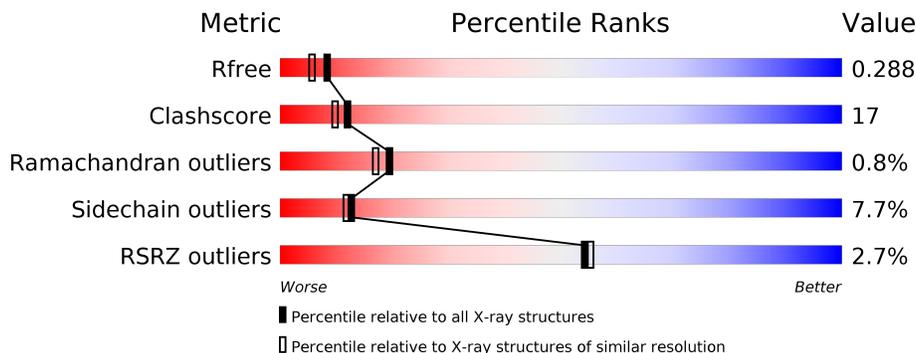
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 on 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	585	 3% 66% 29% . .
1	I	585	 2% 68% 29% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DIF	A	1006	-	-	X	-
4	DIF	A	1008	-	-	X	-

2 Entry composition [i](#)

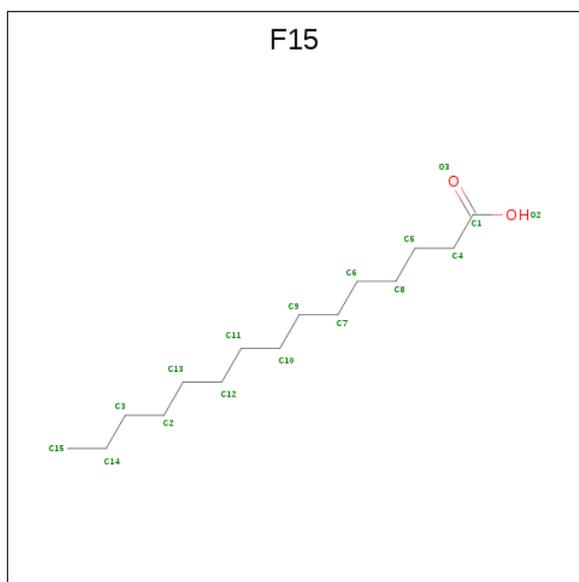
There are 5 unique types of molecules in this entry. The entry contains 9315 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	581	Total 4453	C 2823	N 744	O 845	S 41	0	0	0
1	I	581	Total 4443	C 2819	N 744	O 839	S 41	0	0	0

- Molecule 2 is PENTADECANOIC ACID (three-letter code: F15) (formula: C₁₅H₃₀O₂).



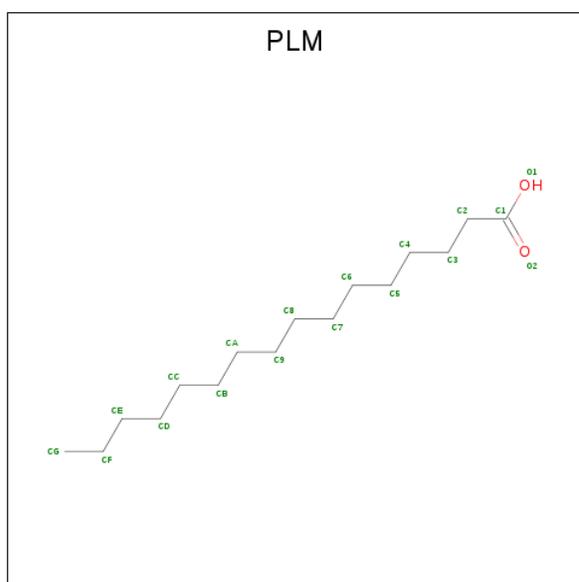
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 13	C 11	O 2	0	0
2	A	1	Total 17	C 15	O 2	0	0
2	A	1	Total 17	C 15	O 2	0	0
2	I	1	Total 13	C 11	O 2	0	0

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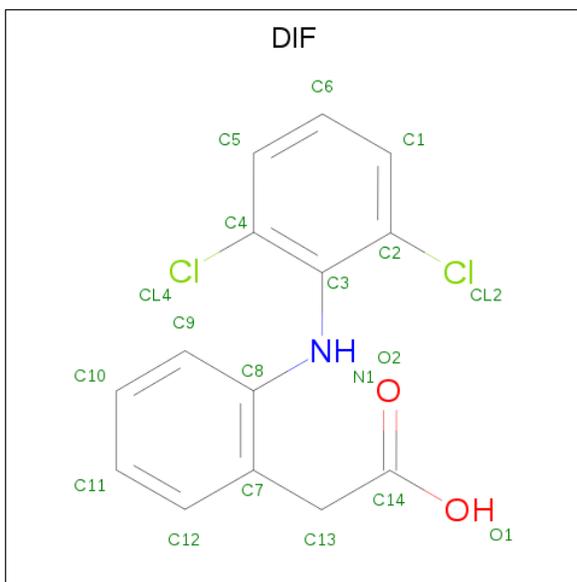
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			17	15	2		
2	I	1	Total	C	O	0	0
			17	15	2		

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	A	1	Total	C	O	0	0
			18	16	2		
3	I	1	Total	C	O	0	0
			18	16	2		
3	I	1	Total	C	O	0	0
			18	16	2		

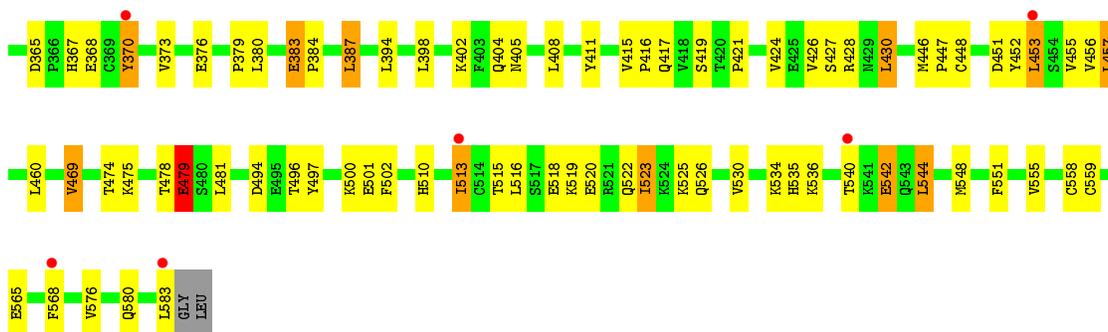
- Molecule 4 is 2-[2,6-DICHLOROPHENYL)AMINO]BENZENEACETIC ACID (three-letter code: DIF) (formula: C₁₄H₁₁Cl₂NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
4	A	1	19	14	2	1	2	0	0
4	A	1	19	14	2	1	2	0	0
4	A	1	19	14	2	1	2	0	0
4	I	1	19	14	2	1	2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	I	95	Total	O	0	0
			95	95		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.40Å 95.00Å 96.34Å 105.00° 101.45° 89.97°	Depositor
Resolution (Å)	45.82 – 2.19 46.11 – 2.19	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.82-2.19) 93.1 (46.11-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.18Å)	Xtrriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.225 , 0.293 0.219 , 0.288	Depositor DCC
R_{free} test set	3160 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtrriage
Anisotropy	0.190	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.457 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9315	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: DIF, PLM, F15

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	0.42	0/4542	0.57	0/6161
1	I	0.42	0/4532	0.59	0/6148
All	All	0.42	0/9074	0.58	0/12309

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	I	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
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	4453	0	4201	162	0
1	I	4443	0	4193	132	0
2	A	47	0	76	3	0
2	I	47	0	76	7	0
3	A	36	0	62	5	0
3	I	36	0	62	5	0
4	A	57	0	30	34	0
4	I	19	0	10	4	0
5	A	82	0	0	5	0
5	I	95	0	0	6	0
All	All	9315	0	8710	307	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 17.

The worst 5 of 307 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)
4:A:1008:DIF:H9	4:A:1008:DIF:CL2	1.81	1.16
1:A:161:TYR:OH	4:A:1006:DIF:H10	1.59	1.03
4:A:1008:DIF:CL2	4:A:1008:DIF:C9	2.55	0.92
1:I:540:THR:HG22	1:I:542:GLU:H	1.32	0.90
1:I:32:GLN:HE22	1:I:107:ASP:H	1.23	0.87

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	579/585 (99%)	545 (94%)	31 (5%)	3 (0%)	29 28
1	I	579/585 (99%)	549 (95%)	24 (4%)	6 (1%)	15 12
All	All	1158/1170 (99%)	1094 (94%)	55 (5%)	9 (1%)	19 17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	469	VAL
1	I	190	LYS
1	I	469	VAL
1	I	110	PRO

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	458/511 (90%)	421 (92%)	37 (8%)	11	10
1	I	455/511 (89%)	422 (93%)	33 (7%)	14	13
All	All	913/1022 (89%)	843 (92%)	70 (8%)	13	12

5 of 70 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	481	LEU
1	I	103	LEU
1	I	481	LEU
1	A	500	LYS
1	A	544	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	GLN
1	A	580	GLN
1	I	109	ASN
1	A	318	ASN
1	I	242	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	F15	A	1001	-	9,12,16	0.48	0	8,12,16	0.33	0
3	PLM	I	1002	-	14,17,17	0.28	0	13,17,17	0.74	0
2	F15	I	1003	-	13,16,16	0.24	0	12,16,16	0.68	0
4	DIF	A	1006	-	17,20,20	0.84	0	23,27,27	1.97	5 (21%)
3	PLM	A	1002	-	14,17,17	0.24	0	13,17,17	0.73	0
4	DIF	A	1007	-	17,20,20	0.81	1 (5%)	23,27,27	2.58	6 (26%)
3	PLM	I	1004	-	14,17,17	0.27	0	13,17,17	0.66	0
2	F15	A	1003	-	13,16,16	0.26	0	12,16,16	0.64	0
2	F15	I	1005	-	13,16,16	0.29	0	12,16,16	0.70	0
3	PLM	A	1004	-	14,17,17	0.23	0	13,17,17	0.80	0
2	F15	I	1001	-	9,12,16	0.43	0	8,12,16	0.38	0
4	DIF	A	1008	-	17,20,20	0.72	0	23,27,27	1.42	3 (13%)
4	DIF	I	1006	-	17,20,20	0.73	0	23,27,27	2.04	6 (26%)
2	F15	A	1005	-	13,16,16	0.31	0	12,16,16	0.71	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	F15	A	1001	-	-	5/8/10/14	-
3	PLM	I	1002	-	-	8/13/15/15	-
2	F15	I	1003	-	-	8/12/14/14	-
4	DIF	A	1006	-	-	1/6/8/8	0/2/2/2
3	PLM	A	1002	-	-	4/13/15/15	-
4	DIF	A	1007	-	-	1/6/8/8	0/2/2/2
3	PLM	I	1004	-	-	8/13/15/15	-
2	F15	A	1003	-	-	9/12/14/14	-
2	F15	I	1005	-	-	6/12/14/14	-
3	PLM	A	1004	-	-	7/13/15/15	-
2	F15	I	1001	-	-	4/8/10/14	-
4	DIF	A	1008	-	-	2/6/8/8	0/2/2/2
4	DIF	I	1006	-	-	0/6/8/8	0/2/2/2
2	F15	A	1005	-	-	7/12/14/14	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	DIF	C8-C7	-2.25	1.37	1.40

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1007	DIF	C7-C8-N1	-8.14	112.15	118.60
4	A	1006	DIF	C3-N1-C8	-6.67	109.09	123.01
4	I	1006	DIF	C14-C13-C7	5.78	128.15	114.71
4	A	1007	DIF	C14-C13-C7	4.65	125.53	114.71
4	A	1008	DIF	C4-C3-N1	-4.24	116.53	122.04

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	1002	PLM	C1-C2-C3-C4
2	I	1003	F15	C1-C4-C5-C8
4	A	1007	DIF	C14-C13-C7-C12
3	I	1004	PLM	C1-C2-C3-C4

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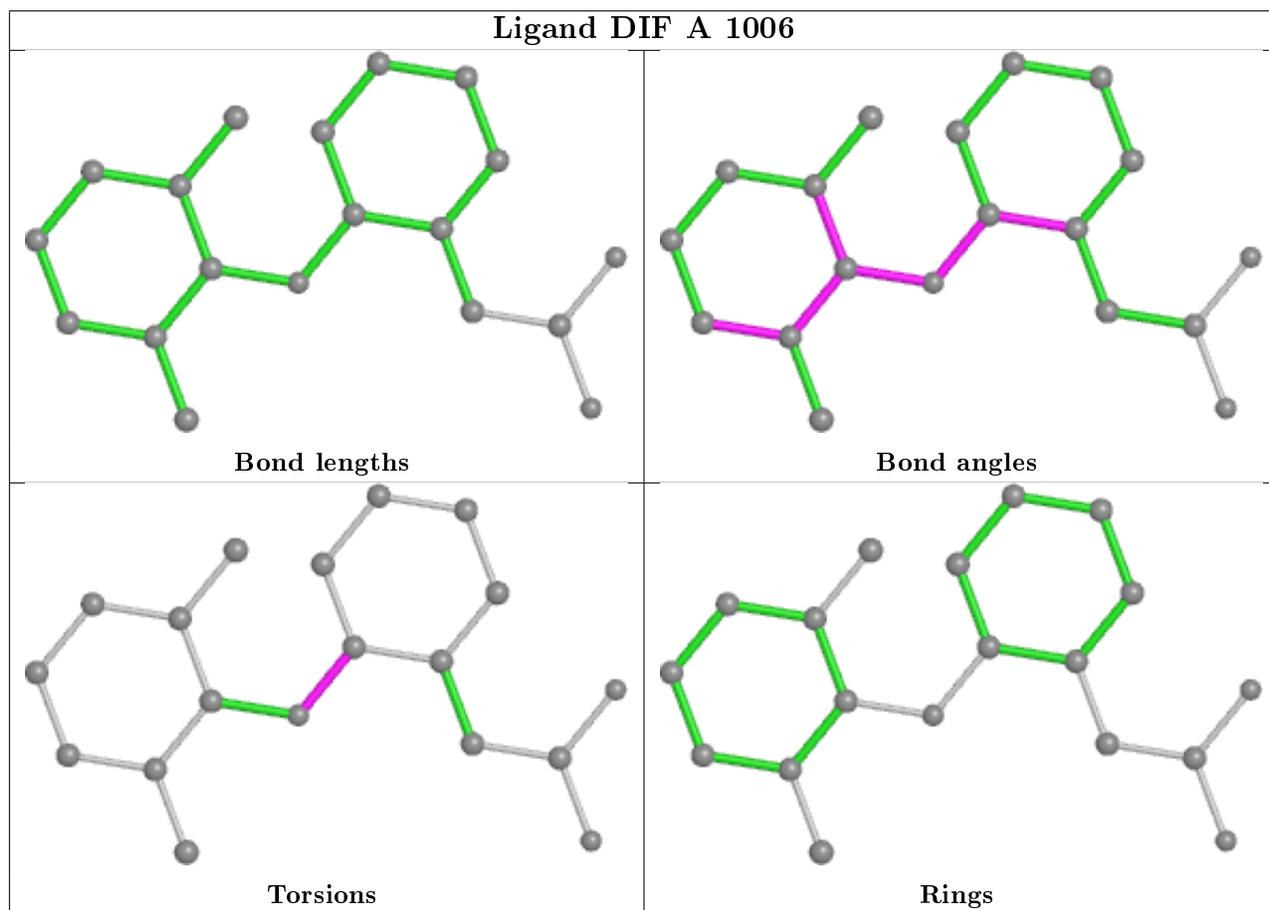
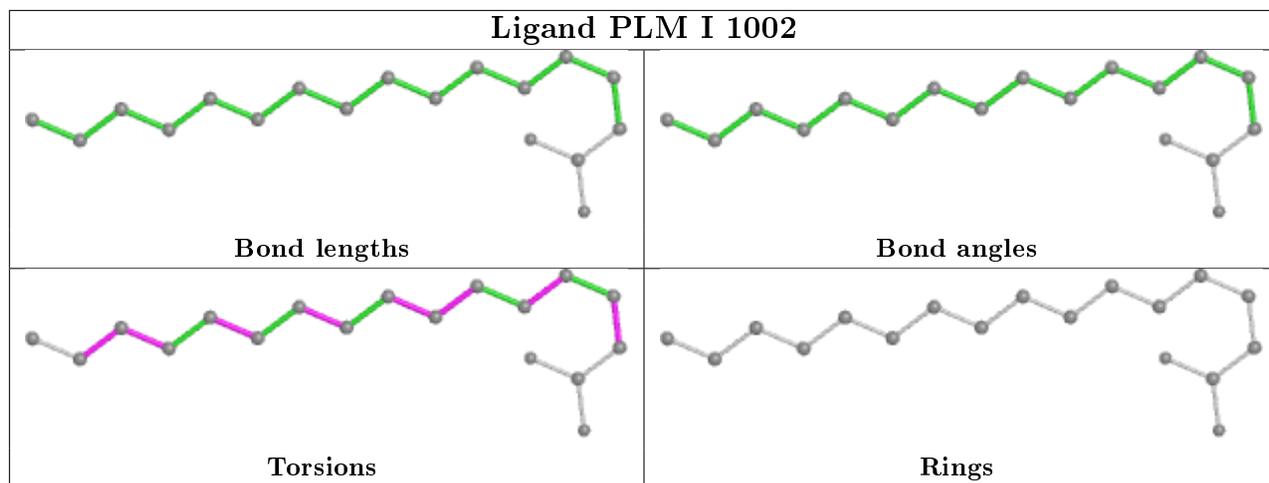
Mol	Chain	Res	Type	Atoms
2	A	1003	F15	C1-C4-C5-C8

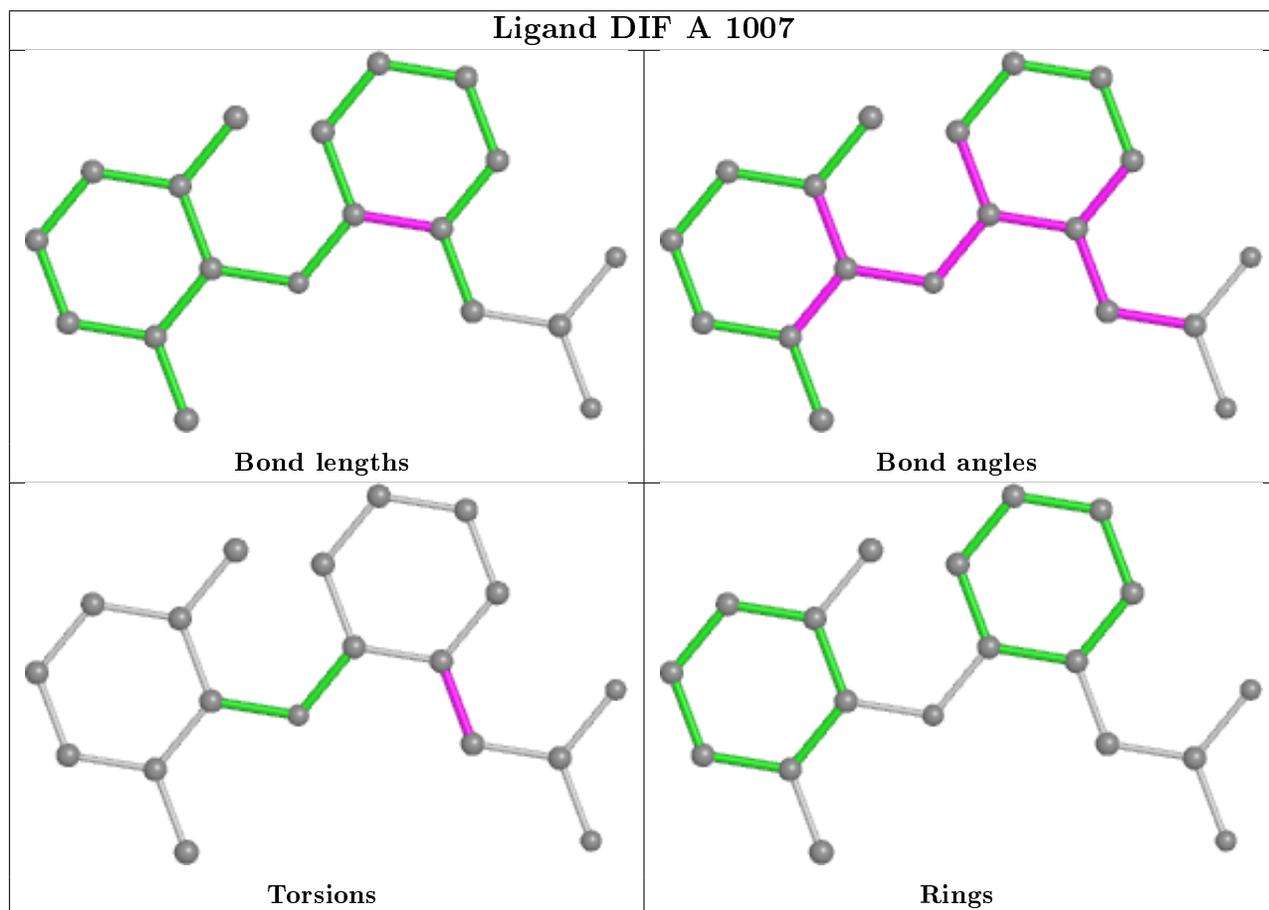
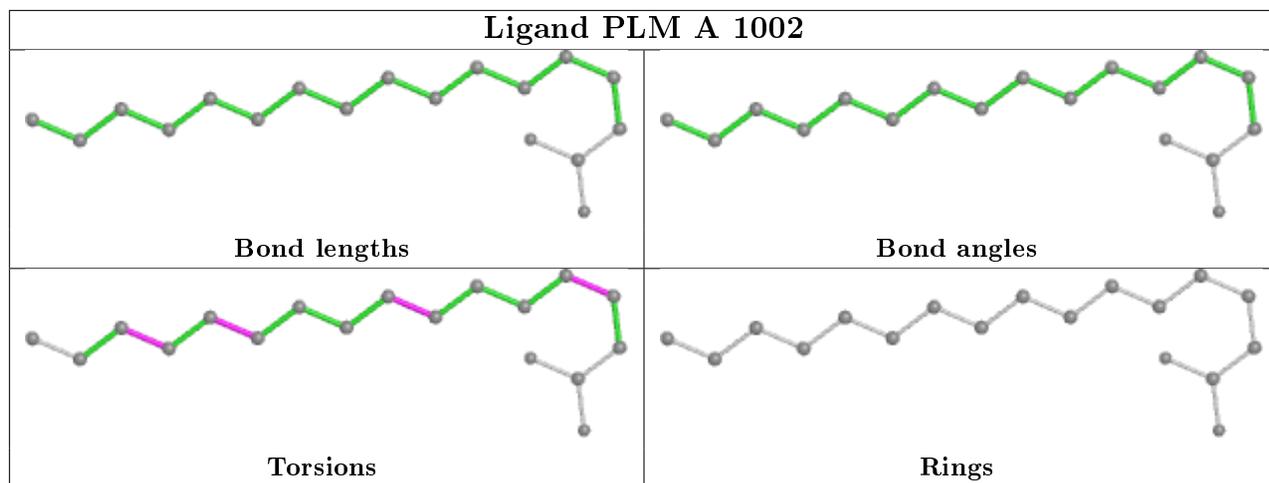
There are no ring outliers.

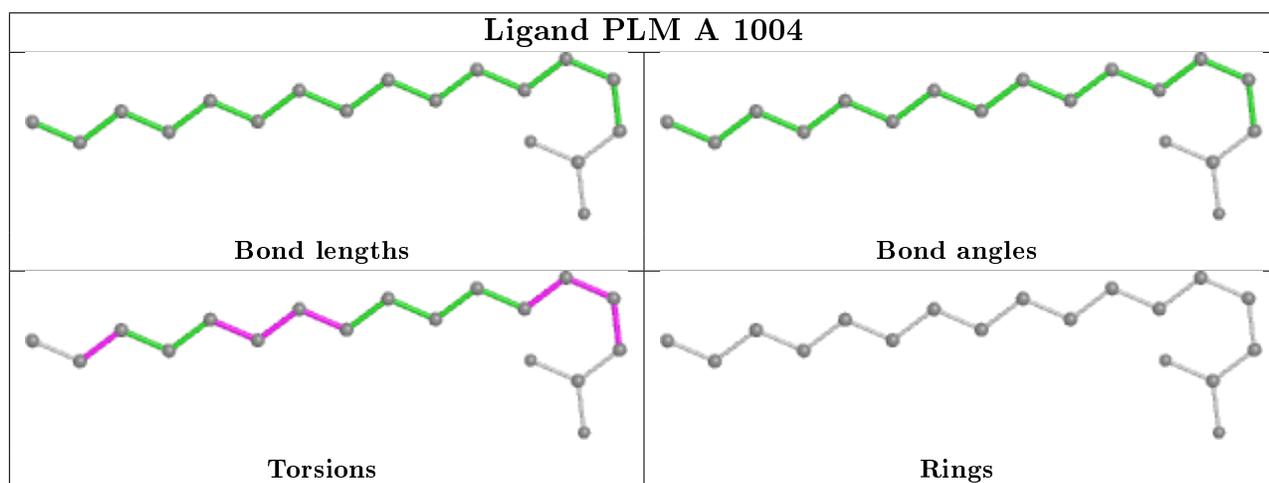
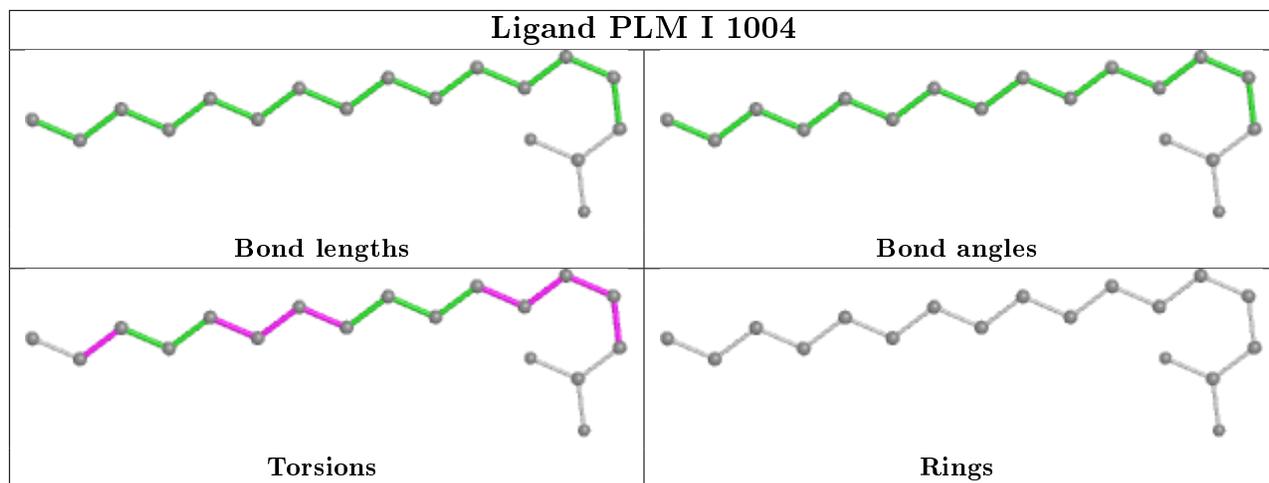
14 monomers are involved in 57 short contacts:

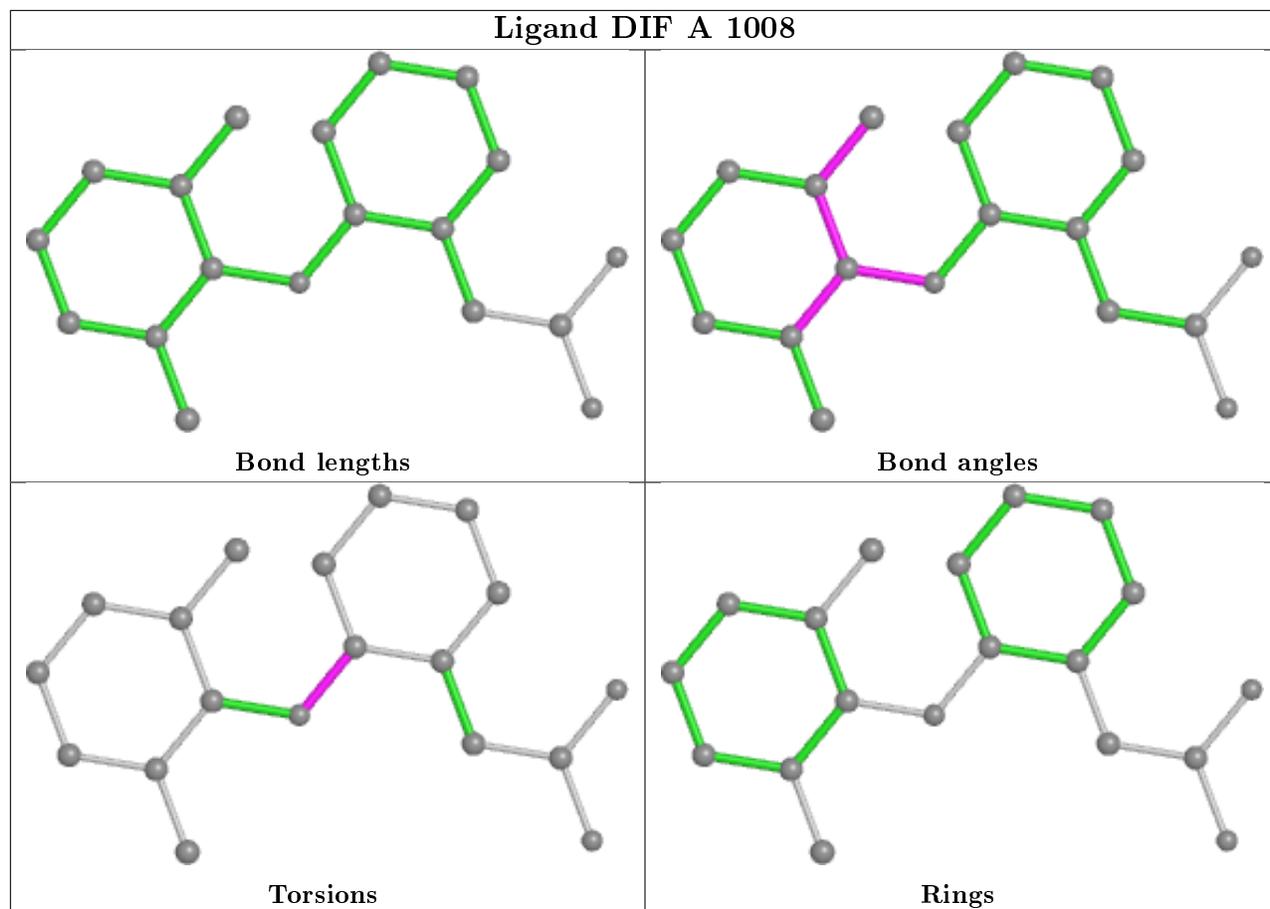
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	F15	1	0
3	I	1002	PLM	4	0
2	I	1003	F15	2	0
4	A	1006	DIF	17	0
3	A	1002	PLM	3	0
4	A	1007	DIF	1	0
3	I	1004	PLM	1	0
2	A	1003	F15	1	0
2	I	1005	F15	3	0
3	A	1004	PLM	2	0
2	I	1001	F15	2	0
4	A	1008	DIF	16	0
4	I	1006	DIF	4	0
2	A	1005	F15	1	0

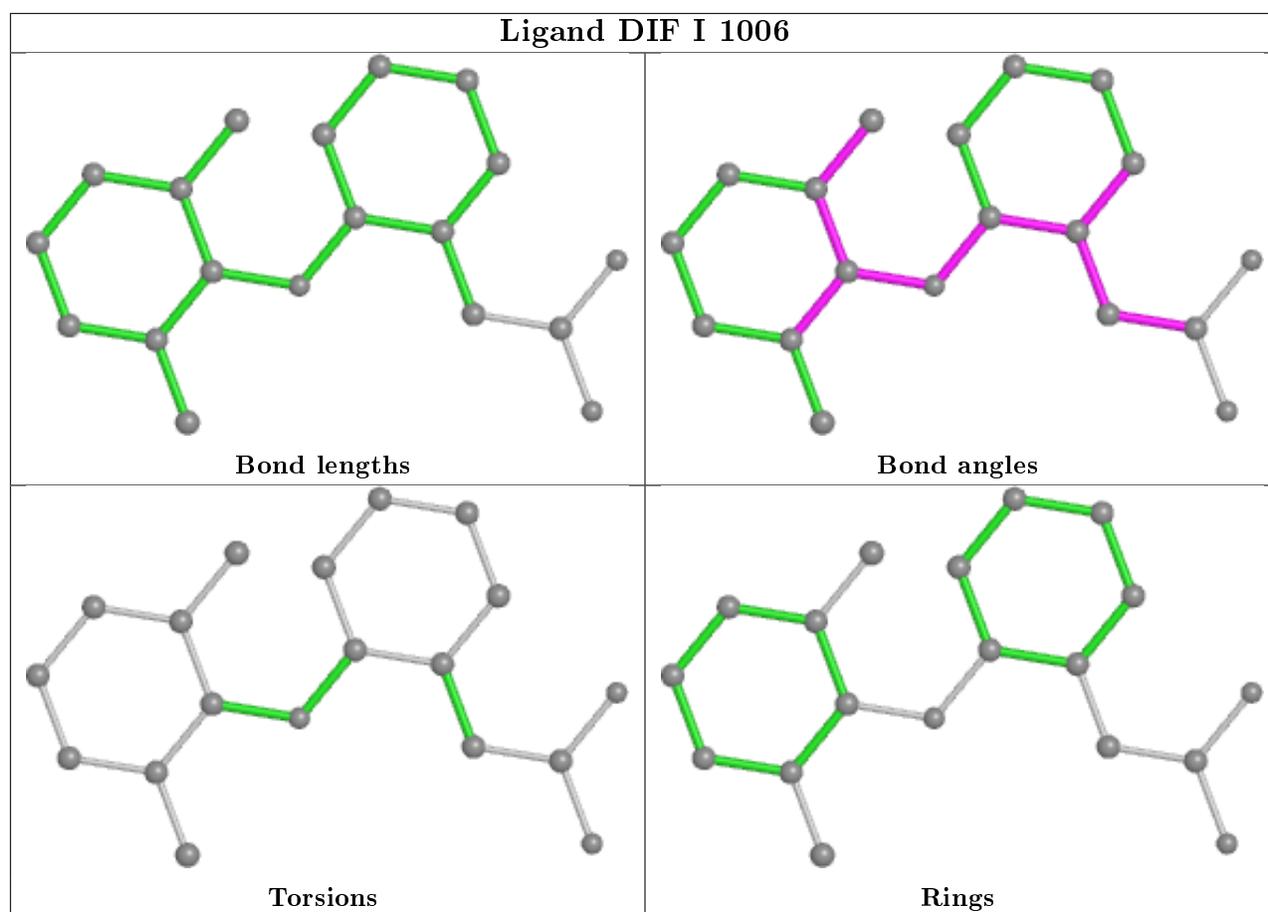
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	581/585 (99%)	0.33	17 (2%) 51 52	33, 55, 78, 98	0
1	I	581/585 (99%)	0.35	14 (2%) 59 59	31, 55, 77, 105	0
All	All	1162/1170 (99%)	0.34	31 (2%) 54 55	31, 55, 77, 105	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	109	ASN	4.2
1	A	388	ILE	3.7
1	A	310	VAL	3.7
1	A	381	VAL	3.1
1	A	555	VAL	3.0

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

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

6.3 Carbohydrates [i](#)

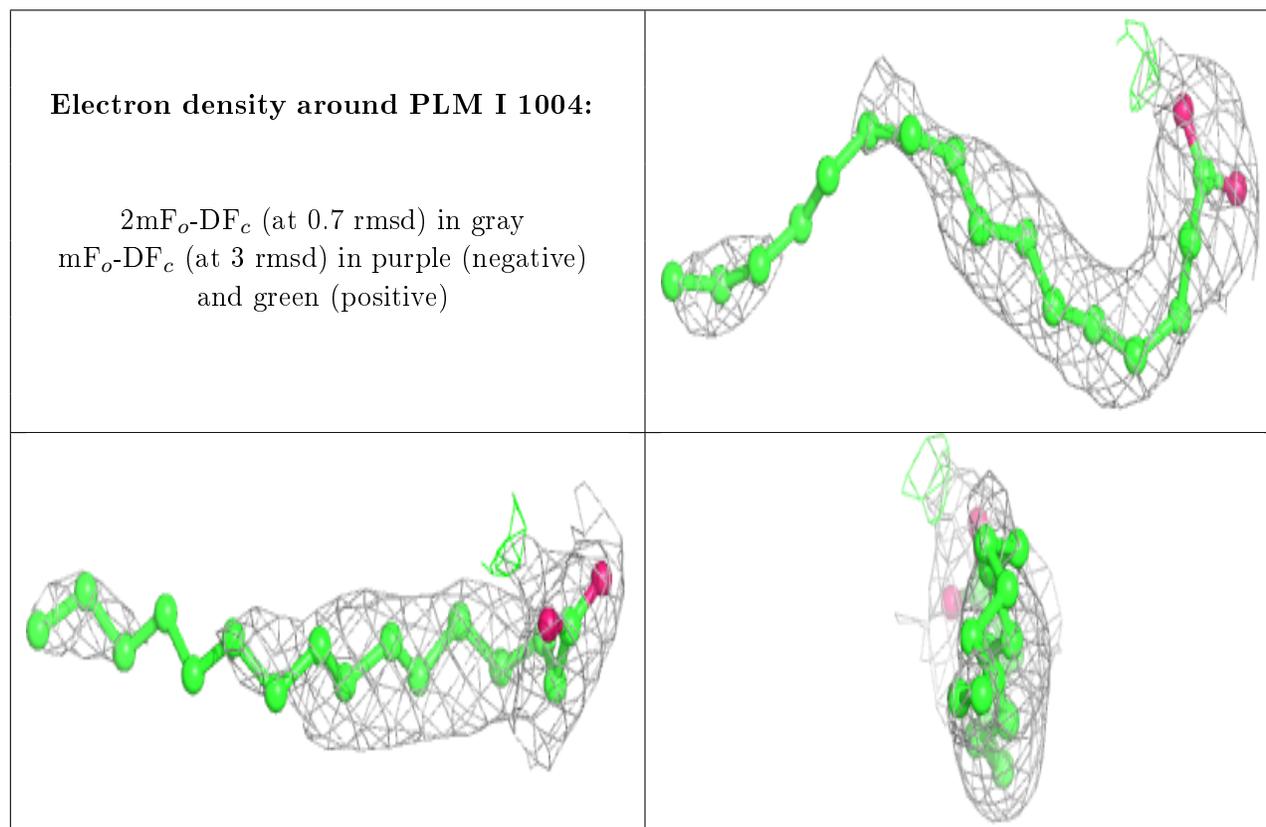
There are no carbohydrates in this entry.

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.

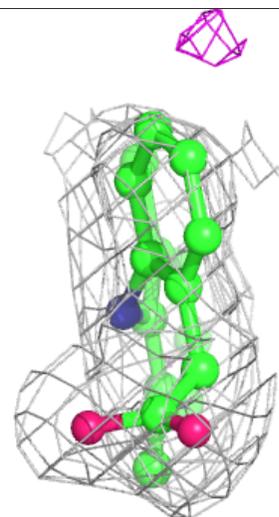
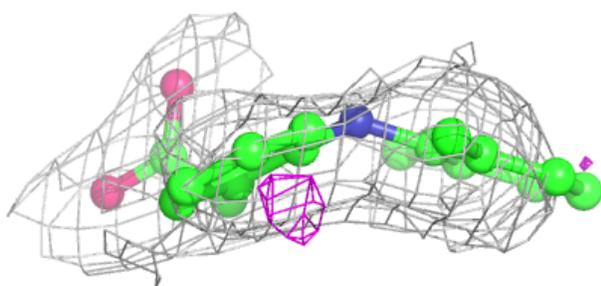
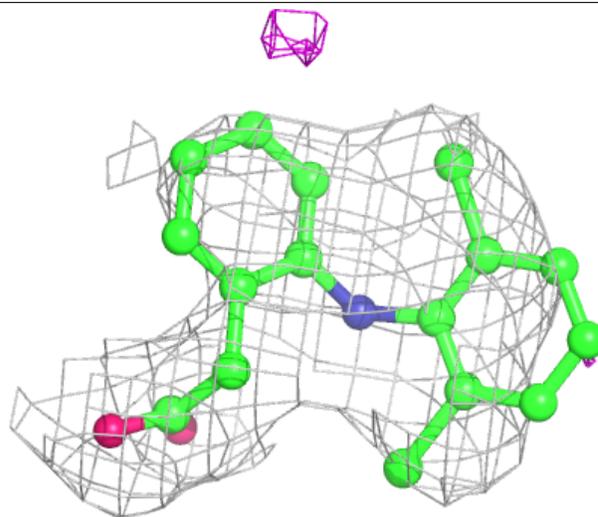
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	F15	I	1001	13/17	0.57	0.40	36,74,91,91	0
2	F15	A	1001	13/17	0.76	0.27	44,67,85,86	0
3	PLM	I	1004	18/18	0.81	0.28	45,66,84,85	0
4	DIF	A	1008	19/19	0.81	0.26	67,85,101,153	0
3	PLM	A	1004	18/18	0.85	0.35	48,66,83,91	0
4	DIF	I	1006	19/19	0.86	0.19	45,56,78,84	0
4	DIF	A	1007	19/19	0.87	0.17	42,59,92,100	0
2	F15	I	1005	17/17	0.87	0.18	35,50,63,64	0
2	F15	A	1003	17/17	0.88	0.33	52,68,83,83	0
2	F15	A	1005	17/17	0.90	0.30	43,52,61,61	0
3	PLM	A	1002	18/18	0.91	0.34	36,46,102,105	0
4	DIF	A	1006	19/19	0.91	0.20	39,76,97,218	0
2	F15	I	1003	17/17	0.92	0.23	56,73,83,86	0
3	PLM	I	1002	18/18	0.93	0.17	38,56,81,82	0

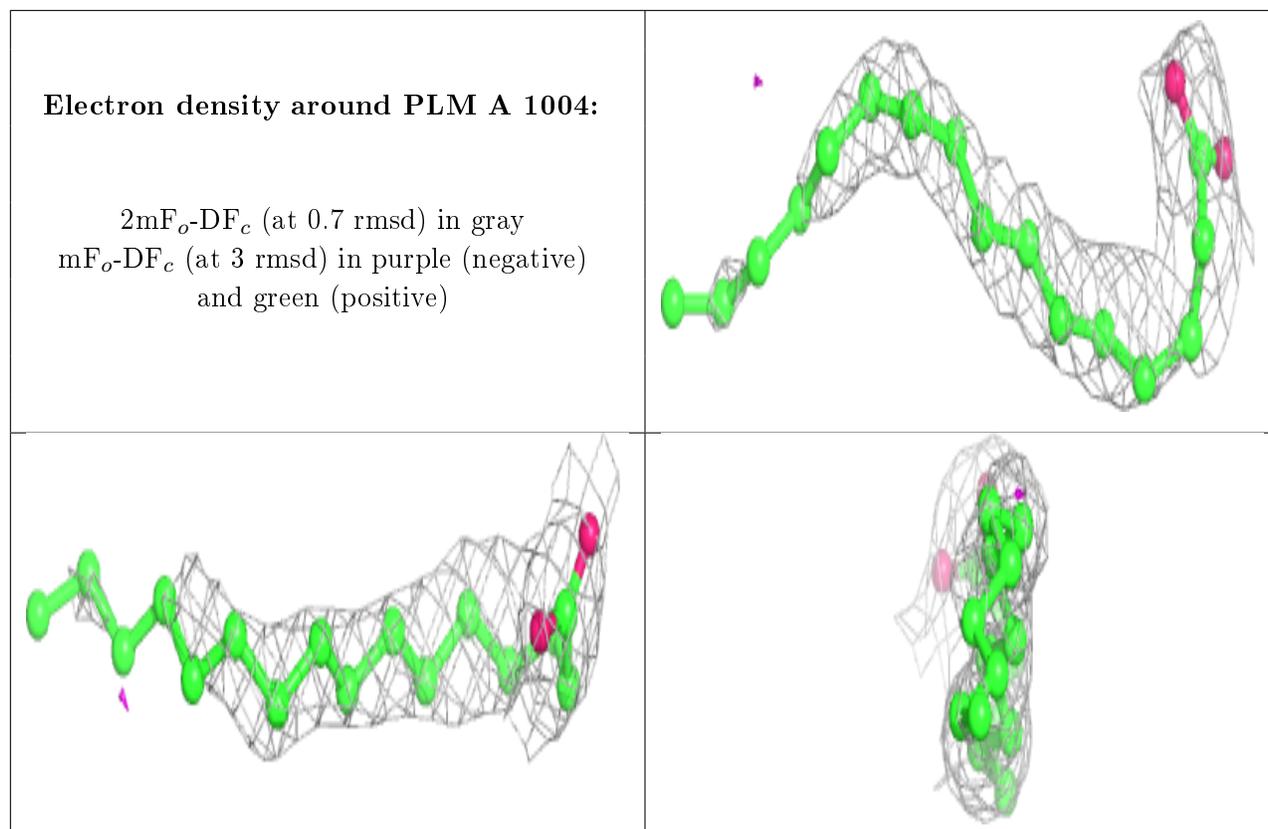
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around DIF A 1008:

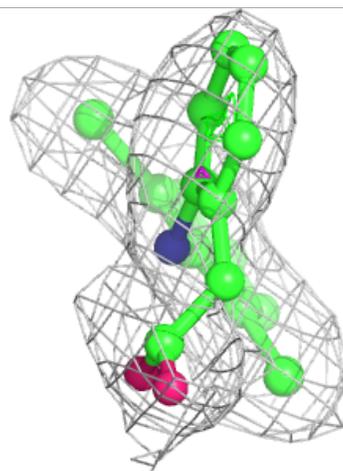
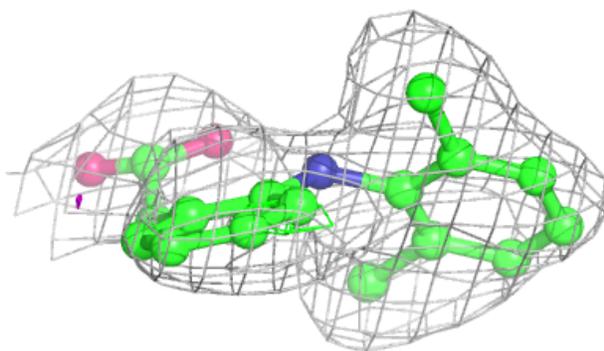
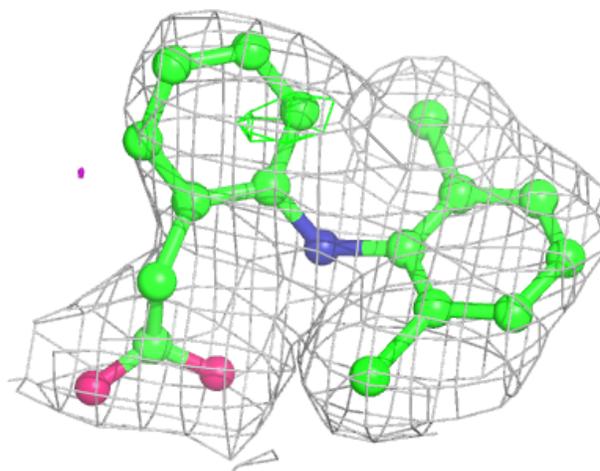
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

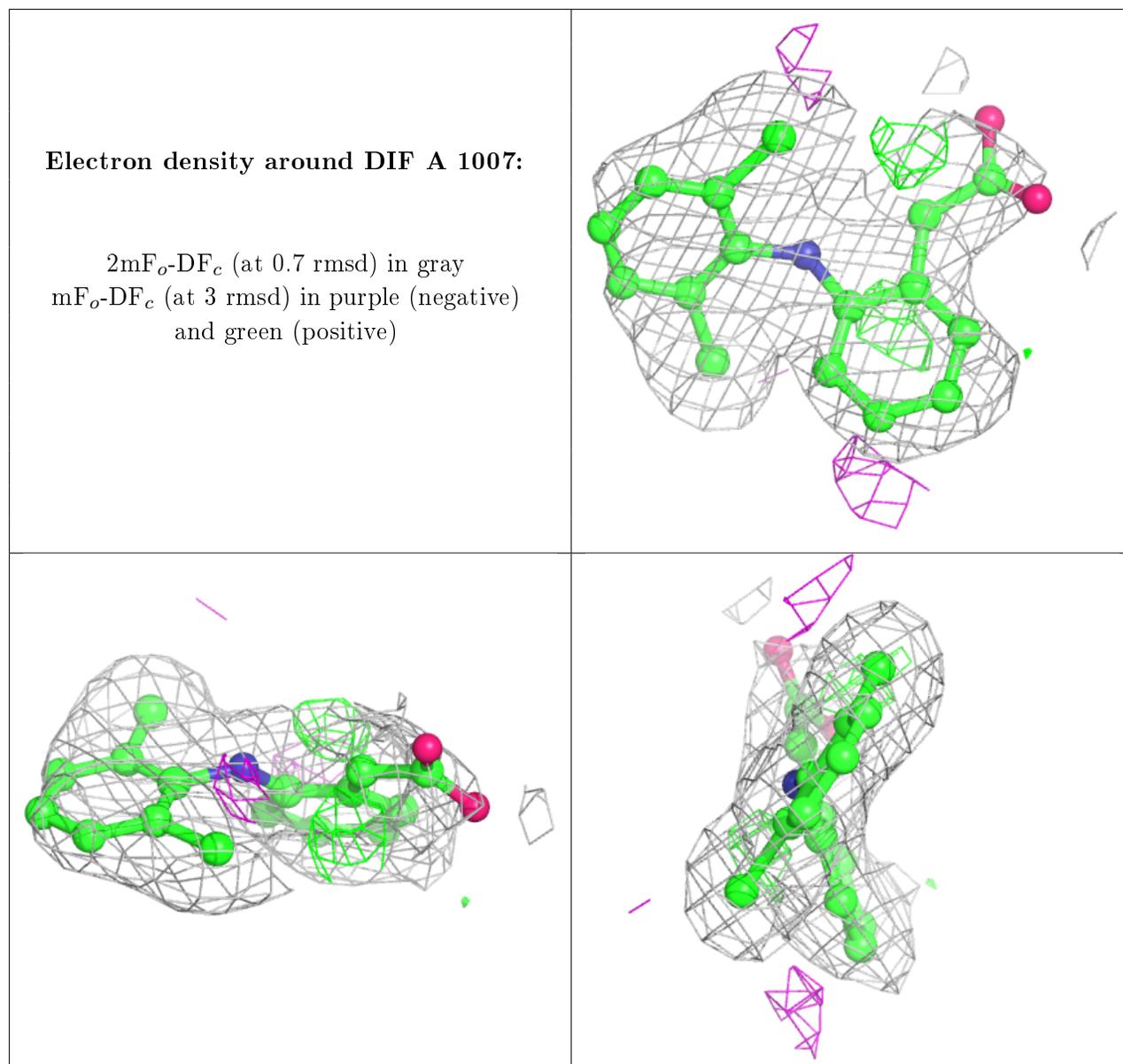


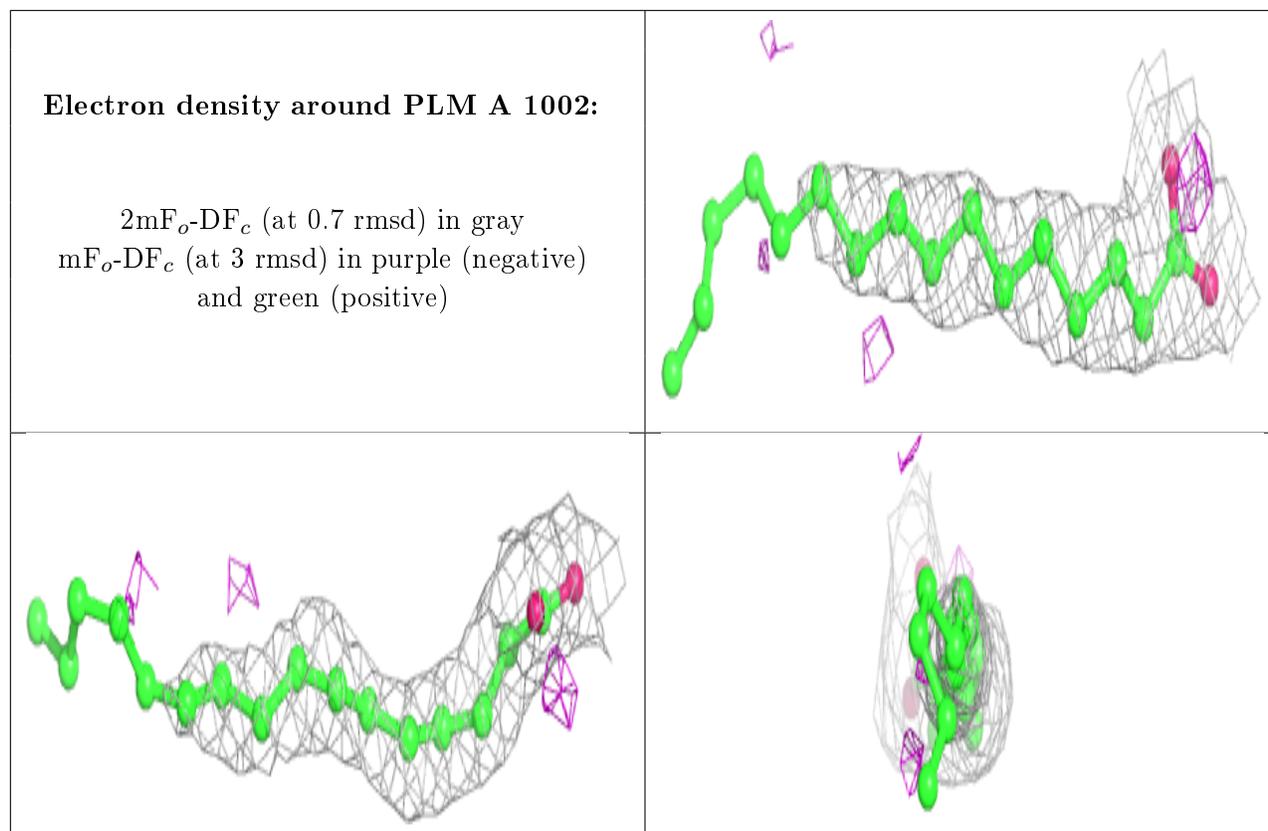


Electron density around DIF I 1006:

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

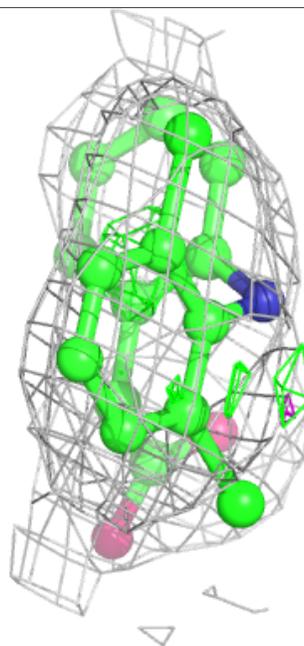
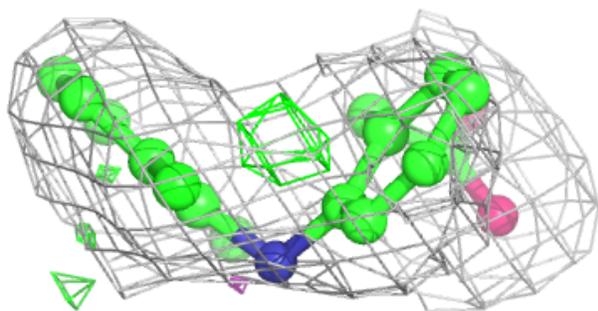
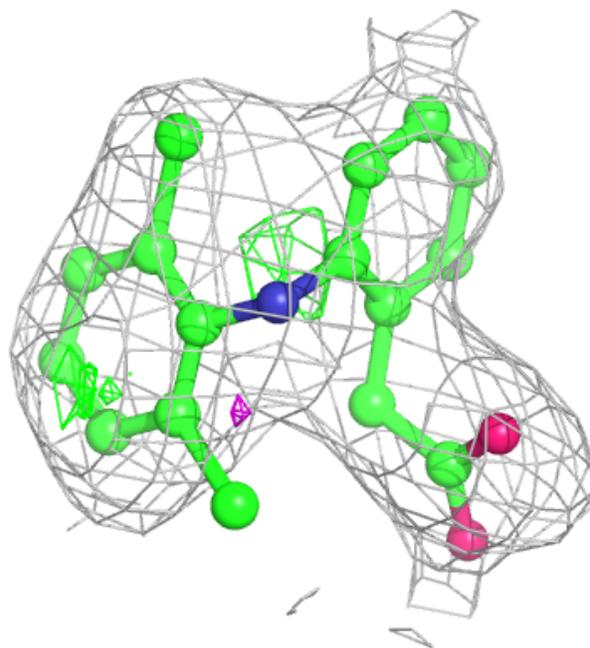


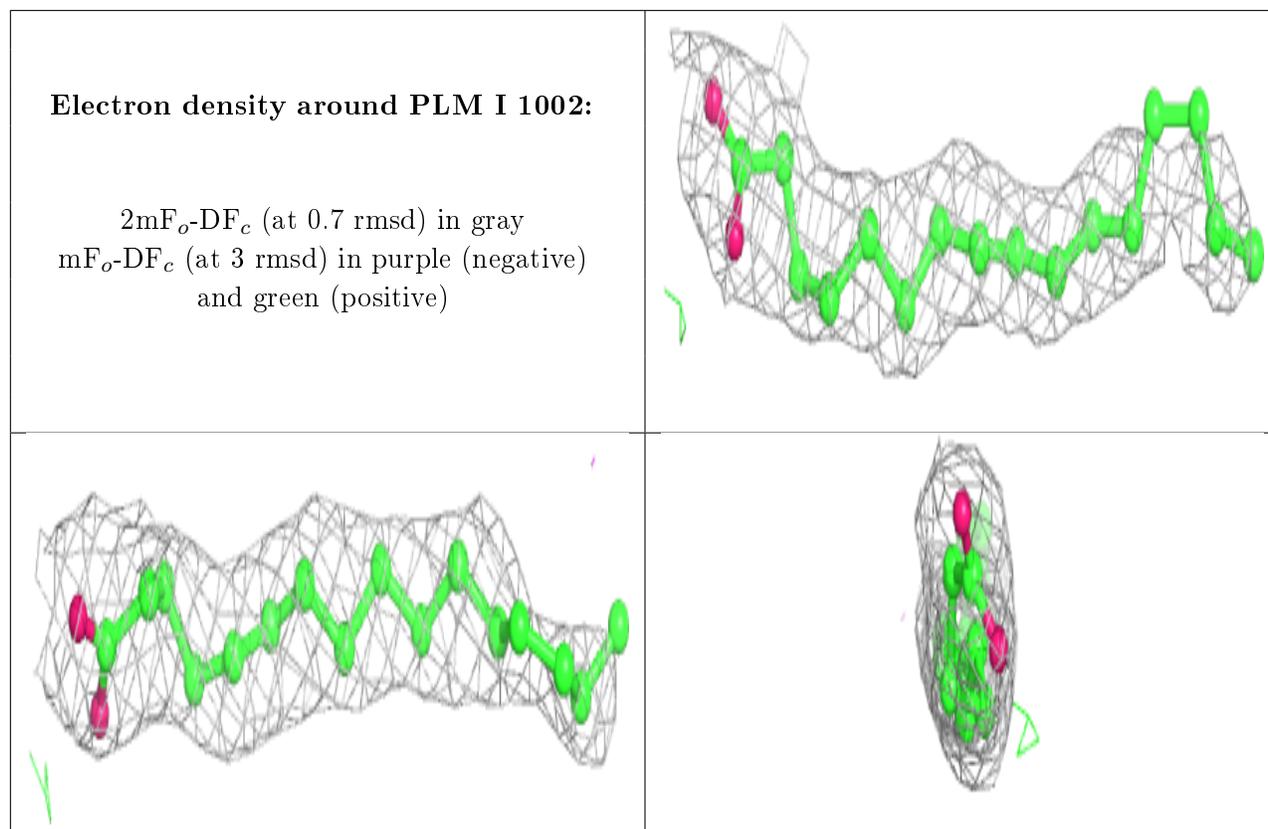




Electron density around DIF A 1006:

$2mF_o-DF_c$ (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.