



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 04:15 pm BST

PDB ID : 8B1D  
Title : DtpB-Nb132-APF  
Authors : Killer, M.; Finocchio, G.; Lei, J.; Jungnickel, K.; Kotov, V.; Steinke, J.; Bartels, K.; Strauss, J.; Dupeux, F.; Humm, A.S.; Cornaciu, I.; Marquez, J.; Pardon, E.; Steyeart, J.; Loew, C.  
Deposited on : 2022-09-09  
Resolution : 2.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

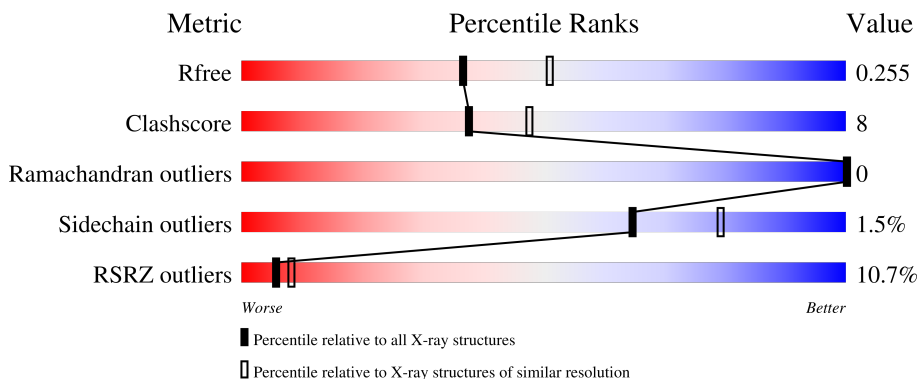
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	489	 10% 76% 14% 8%
2	B	127	 8% 87% 13%
3	C	3	 33% 67% 33%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
11	HEX	A	814	-	-	-	X
8	D12	A	809	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4792 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 Dipeptide and tripeptide permease B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	3480	2349	531	573	27	4	0	0

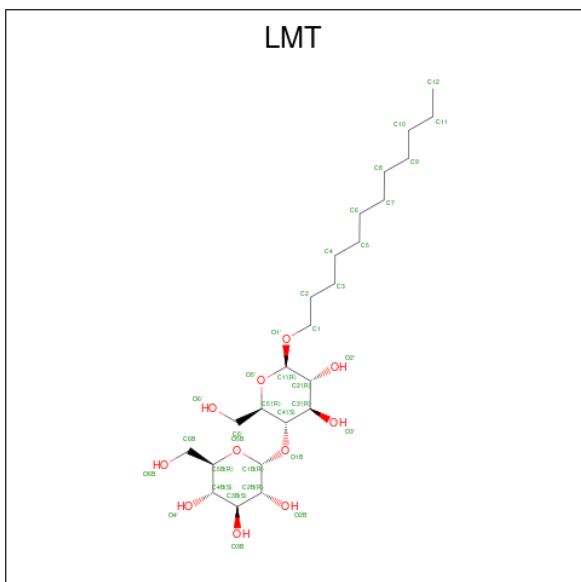
- Molecule 2 is a protein called Nanobody 132.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	127	976	613	178	181	4	5	1	0

- Molecule 3 is a protein called ALA-PRO-PHE.

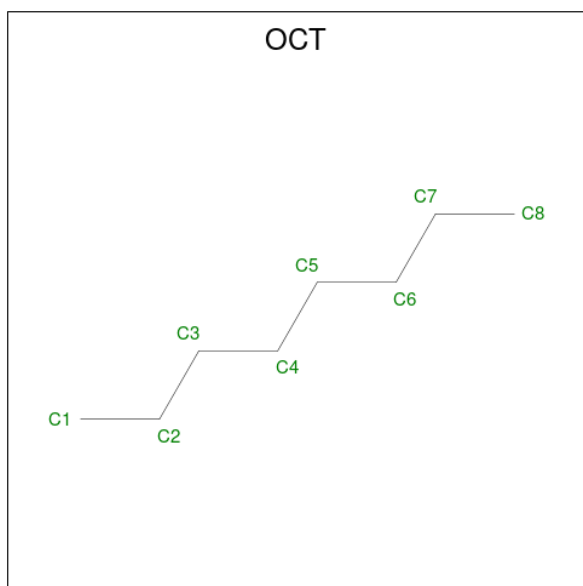
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	24	17	3	4	0	0	0

- Molecule 4 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>) (labeled as "Ligand of Interest" by depositor).



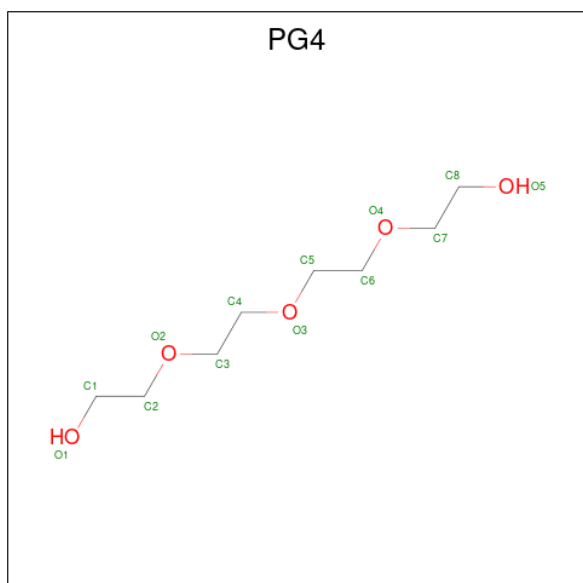
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

- Molecule 5 is N-OCTANE (three-letter code: OCT) (formula:  $C_8H_{18}$ ) (labeled as "Ligand of Interest" by depositor).



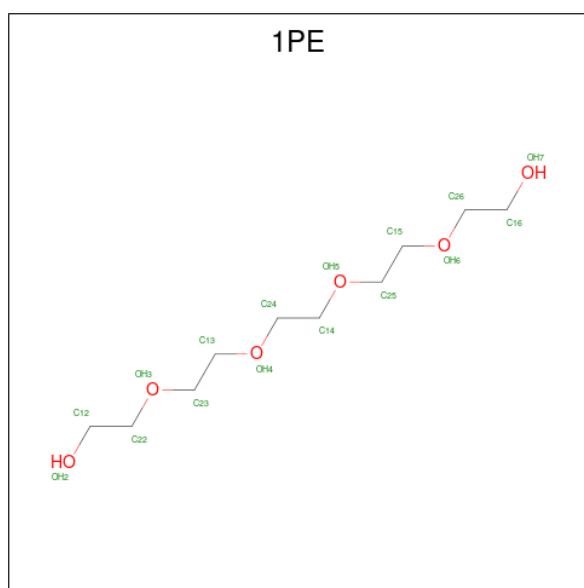
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ) (labeled as "Ligand of Interest" by depositor).



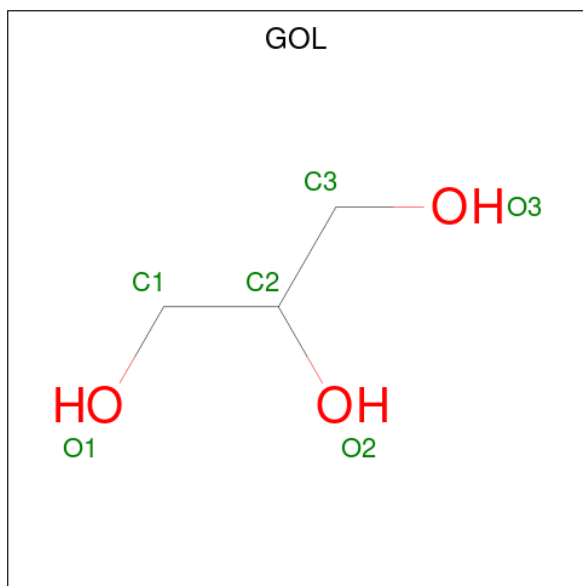
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is DODECANE (three-letter code: D12) (formula:  $C_{12}H_{26}$ ) (labeled as "Ligand of Interest" by depositor).



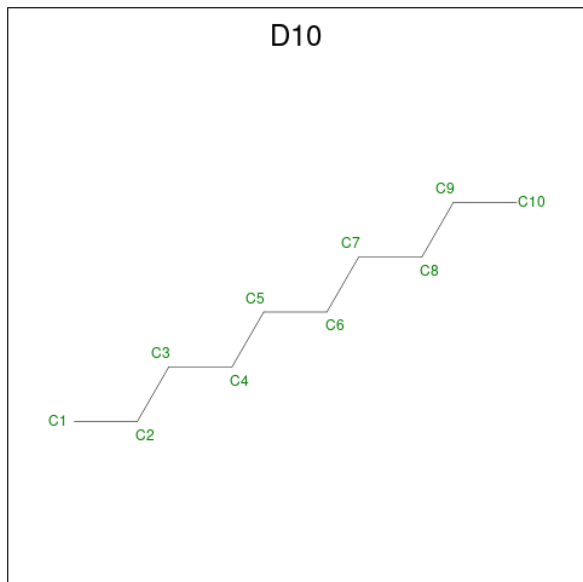
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 12 12	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ) (labeled as "Ligand of Interest" by depositor).



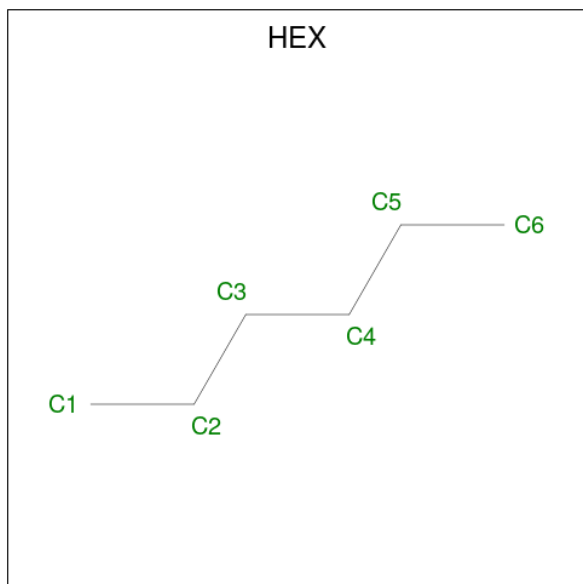
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0

- Molecule 10 is DECANE (three-letter code: D10) (formula:  $C_{10}H_{22}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C 10 10	0	0

- Molecule 11 is HEXANE (three-letter code: HEX) (formula:  $C_6H_{14}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 6 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C 6 6	0	0

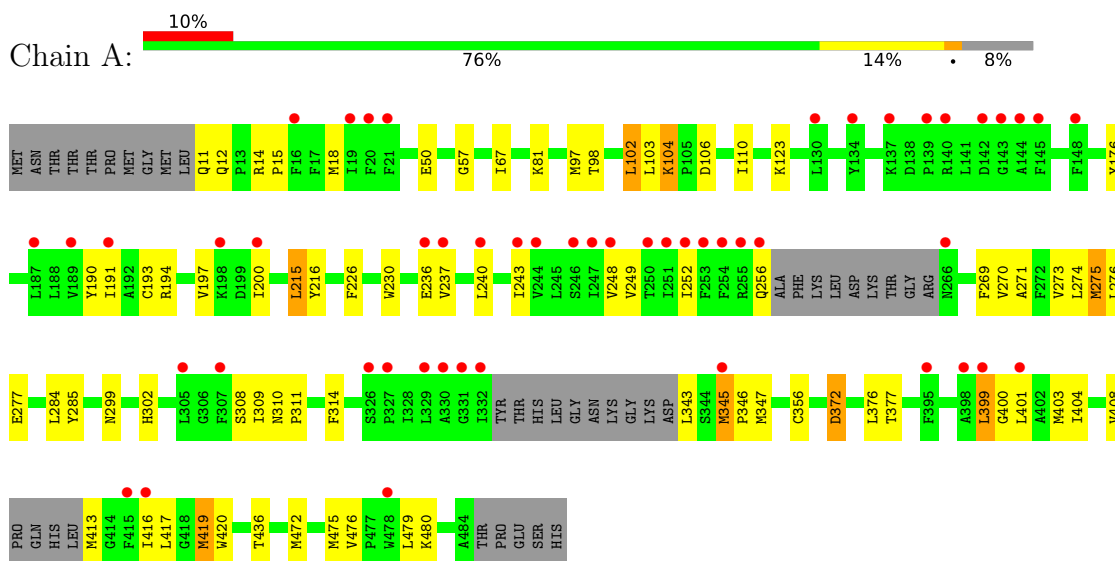
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	71	Total O 71 71	0	0
12	B	54	Total O 54 54	0	0
12	C	1	Total O 1 1	0	0

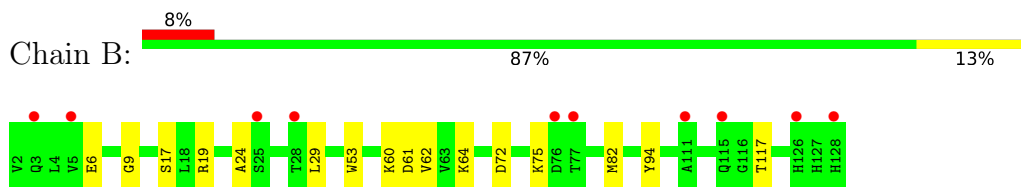
### 3 Residue-property plots [i](#)

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.

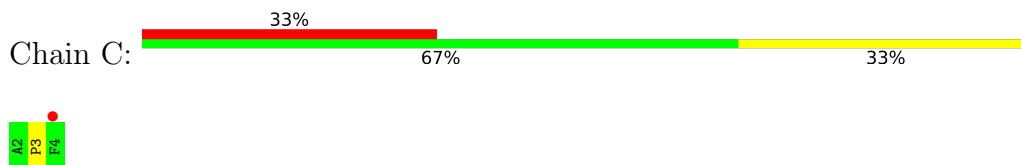
- Molecule 1: Dipeptide and tripeptide permease B



- Molecule 2: Nanobody 132



- Molecule 3: ALA-PRO-PHE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.76Å 125.16Å 169.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.58 – 2.30 100.77 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.58-2.30) 91.8 (100.77-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.68 (at 2.29Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.230 , 0.258 0.227 , 0.255	Depositor DCC
$R_{free}$ test set	2649 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 67.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PG4, 1PE, OCT, LMT, D12, D10, HEX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/3572	0.74	8/4859 (0.2%)
2	B	0.48	0/1004	0.70	0/1361
3	C	0.56	0/25	0.65	0/32
All	All	0.51	0/4601	0.73	8/6252 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	LEU	CA-CB-CG	9.53	137.22	115.30
1	A	103	LEU	CA-CB-CG	8.54	134.95	115.30
1	A	276	LEU	CA-CB-CG	7.11	131.64	115.30
1	A	275	MET	CA-CB-CG	6.54	124.41	113.30
1	A	345	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	215	LEU	CB-CG-CD1	-5.84	101.07	111.00
1	A	399	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	102	LEU	CA-CB-CG	-5.24	103.26	115.30

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	3480	0	3605	62	0
2	B	976	0	939	9	0
3	C	24	0	20	1	0
4	A	35	0	46	6	0
5	A	8	0	18	0	0
6	A	65	0	90	2	0
7	A	32	0	44	4	0
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	1	0
11	A	12	0	28	1	0
12	A	71	0	0	2	0
12	B	54	0	0	1	0
12	C	1	0	0	0	0
All	All	4792	0	4854	73	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 8.

All (73) 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:A:345:MET:HB3	1:A:346:PRO:HD3	1.54	0.87
1:A:197:VAL:HA	1:A:200:ILE:HD13	1.66	0.78
1:A:346:PRO:HB2	1:A:476:VAL:HG22	1.67	0.76
1:A:273:VAL:HG11	1:A:479:LEU:HD11	1.69	0.73
1:A:243:ILE:HG13	7:A:811:1PE:H151	1.71	0.73
2:B:19:ARG:NH1	12:B:201:HOH:O	2.21	0.73
1:A:237:VAL:HA	1:A:240:LEU:HD12	1.72	0.71
1:A:345:MET:HB3	1:A:346:PRO:CD	2.21	0.70
2:B:72:ASP:OD2	2:B:75:LYS:HG3	1.97	0.65
1:A:277:GLU:OE2	1:A:472:MET:HG2	1.98	0.64
1:A:413:MET:O	1:A:416:ILE:HG13	2.00	0.61
1:A:284:LEU:HD12	1:A:356:CYS:HB3	1.83	0.61
1:A:248:VAL:O	1:A:252:ILE:HG23	2.02	0.59
1:A:345:MET:SD	1:A:403:MET:HG3	2.44	0.58
1:A:343:LEU:N	1:A:480:LYS:HZ3	2.02	0.58
2:B:24:ALA:HB2	2:B:29:LEU:HD13	1.86	0.57
1:A:271:ALA:O	1:A:275:MET:HG2	2.05	0.57
1:A:401:LEU:HA	1:A:404:ILE:HB	1.86	0.56
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.86	0.56
1:A:401:LEU:HD21	1:A:417:LEU:CD1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLN:HG3	1:A:12:GLN:HG2	1.88	0.55
1:A:343:LEU:HA	1:A:347:MET:CB	2.37	0.54
1:A:310:ASN:HB2	4:A:801:LMT:H6'1	1.90	0.53
1:A:191:ILE:O	1:A:194:ARG:NH1	2.43	0.51
1:A:243:ILE:CG1	7:A:811:1PE:H151	2.41	0.51
1:A:230:TRP:CZ3	1:A:237:VAL:HG21	2.46	0.51
1:A:475:MET:HB3	1:A:479:LEU:HD23	1.91	0.51
1:A:273:VAL:O	1:A:277:GLU:HG3	2.11	0.51
1:A:308:SER:O	4:A:801:LMT:H4'	2.10	0.51
1:A:249:VAL:HA	1:A:252:ILE:HG12	1.92	0.50
1:A:416:ILE:HA	1:A:419:MET:HG2	1.92	0.50
1:A:310:ASN:ND2	4:A:801:LMT:H6'1	2.26	0.50
1:A:401:LEU:HD21	1:A:417:LEU:HD11	1.94	0.49
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.93	0.49
1:A:285:TYR:CE2	3:C:3:PRO:HD3	2.47	0.49
1:A:343:LEU:HA	1:A:347:MET:HB3	1.95	0.49
1:A:57:GLY:HA3	12:A:951:HOH:O	2.14	0.48
1:A:226:PHE:CE2	6:A:806:PG4:H41	2.48	0.48
2:B:6:GLU:OE2	2:B:94:TYR:HA	2.14	0.48
1:A:104:LYS:HG2	10:A:812:D10:H62	1.95	0.47
1:A:269:PHE:O	1:A:273:VAL:HG12	2.14	0.47
1:A:347:MET:HE2	1:A:476:VAL:HG11	1.96	0.47
2:B:61[B]:ASP:OD1	2:B:62:VAL:N	2.45	0.47
1:A:309:ILE:HD11	1:A:314:PHE:CZ	2.50	0.46
1:A:401:LEU:HD22	1:A:420:TRP:CD1	2.51	0.46
1:A:475:MET:HE3	1:A:479:LEU:HD21	1.98	0.46
1:A:67:ILE:HD11	1:A:123:LYS:HD3	1.99	0.45
1:A:400:GLY:O	1:A:404:ILE:HG12	2.17	0.45
1:A:302:HIS:CE1	1:A:311:PRO:HG3	2.52	0.45
1:A:273:VAL:HG21	1:A:475:MET:HE1	1.99	0.45
1:A:50:GLU:HG3	1:A:436:THR:HB	1.99	0.44
1:A:97:MET:HE2	1:A:110:ILE:HG22	1.99	0.44
2:B:9:GLY:H	2:B:117:THR:HG21	1.83	0.44
2:B:61[A]:ASP:HA	2:B:64:LYS:HD2	1.99	0.44
1:A:372:ASP:HB2	1:A:376:LEU:H	1.82	0.44
1:A:275:MET:HE1	1:A:420:TRP:HB2	2.00	0.43
1:A:236:GLU:OE2	7:A:811:1PE:OH2	2.35	0.43
1:A:401:LEU:HD21	1:A:417:LEU:HD13	1.98	0.43
1:A:270:VAL:O	1:A:274:LEU:HG	2.19	0.43
1:A:472:MET:O	1:A:476:VAL:HG23	2.17	0.43
1:A:399:LEU:O	1:A:403:MET:HE2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:HB3	6:A:807:PG4:H42	2.01	0.42
1:A:310:ASN:HD22	4:A:801:LMT:H6'1	1.84	0.42
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.19	0.42
4:A:801:LMT:H41	4:A:801:LMT:H12	1.61	0.42
7:A:811:1PE:OH7	11:A:814:HEX:H12	2.20	0.42
1:A:98:THR:HG22	1:A:176:TYR:CD2	2.55	0.42
1:A:102:LEU:HD22	12:A:963:HOH:O	2.19	0.42
1:A:299:ASN:O	1:A:377:THR:HG22	2.20	0.41
1:A:310:ASN:CB	4:A:801:LMT:H6'1	2.50	0.41
1:A:408:VAL:HG11	1:A:413:MET:HA	2.03	0.41
1:A:14:ARG:N	1:A:15:PRO:HD2	2.35	0.41
2:B:17:SER:HA	2:B:82:MET:O	2.21	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	443/489 (91%)	435 (98%)	8 (2%)	0	100	100
2	B	126/127 (99%)	125 (99%)	1 (1%)	0	100	100
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	570/619 (92%)	561 (98%)	9 (2%)	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	368/401 (92%)	362 (98%)	6 (2%)	62	78
2	B	102/101 (101%)	101 (99%)	1 (1%)	76	87
3	C	2/2 (100%)	2 (100%)	0	100	100
All	All	472/504 (94%)	465 (98%)	7 (2%)	65	79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	106	ASP
1	A	215	LEU
1	A	256	GLN
1	A	372	ASP
1	A	419	MET
2	B	53	TRP

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

15 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
7	1PE	A	804	-	15,15,15	0.27	0	14,14,14	0.36	0
6	PG4	A	803	-	12,12,12	0.22	0	11,11,11	0.63	0
4	LMT	A	801	-	36,36,36	1.06	3 (8%)	47,47,47	1.39	7 (14%)
6	PG4	A	806	-	12,12,12	0.23	0	11,11,11	0.37	0
5	OCT	A	802	-	7,7,7	0.33	0	6,6,6	0.78	0
6	PG4	A	807	-	12,12,12	0.18	0	11,11,11	0.33	0
8	D12	A	809	-	11,11,11	0.39	0	10,10,10	0.71	0
9	GOL	A	810	-	5,5,5	0.94	0	5,5,5	0.88	0
6	PG4	A	805	-	12,12,12	0.19	0	11,11,11	0.44	0
11	HEX	A	814	-	5,5,5	0.35	0	4,4,4	0.58	0
11	HEX	A	815	-	5,5,5	0.34	0	4,4,4	0.54	0
10	D10	A	812	-	9,9,9	0.33	0	8,8,8	0.90	0
7	1PE	A	811	-	15,15,15	0.15	0	14,14,14	0.34	0
9	GOL	A	813	-	5,5,5	0.92	0	5,5,5	0.91	0
6	PG4	A	808	-	12,12,12	0.23	0	11,11,11	0.58	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. <sup>2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	A	804	-	-	5/13/13/13	-
6	PG4	A	803	-	-	4/10/10/10	-
4	LMT	A	801	-	-	15/21/61/61	0/2/2/2
6	PG4	A	806	-	-	6/10/10/10	-
5	OCT	A	802	-	-	2/5/5/5	-
6	PG4	A	807	-	-	5/10/10/10	-
8	D12	A	809	-	-	3/9/9/9	-
9	GOL	A	810	-	-	2/4/4/4	-
6	PG4	A	805	-	-	4/10/10/10	-
11	HEX	A	814	-	-	0/3/3/3	-
11	HEX	A	815	-	-	0/3/3/3	-
10	D10	A	812	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	1PE	A	811	-	-	6/13/13/13	-
9	GOL	A	813	-	-	0/4/4/4	-
6	PG4	A	808	-	-	4/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O2B-C2B	-2.45	1.37	1.43
4	A	801	LMT	O2'-C2'	-2.33	1.37	1.43
4	A	801	LMT	C3'-C2'	2.33	1.58	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	O5B-C5B-C4B	3.41	115.88	109.69
4	A	801	LMT	C1B-O1B-C4'	2.94	125.23	117.96
4	A	801	LMT	C1'-O5'-C5'	-2.86	108.08	113.69
4	A	801	LMT	C1'-C2'-C3'	2.48	115.16	110.00
4	A	801	LMT	C2'-C3'-C4'	2.24	114.79	109.68
4	A	801	LMT	O1B-C4'-C5'	2.14	115.31	109.45
4	A	801	LMT	O1B-C4'-C3'	2.04	112.70	107.28

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C2'-C1'-O1'-C1
4	A	801	LMT	O5'-C1'-O1'-C1
6	A	803	PG4	O3-C5-C6-O4
6	A	806	PG4	O2-C3-C4-O3
6	A	807	PG4	O3-C5-C6-O4
4	A	801	LMT	O5B-C5B-C6B-O6B
4	A	801	LMT	O5'-C5'-C6'-O6'
7	A	811	1PE	OH5-C14-C24-OH4
4	A	801	LMT	C4'-C5'-C6'-O6'
6	A	806	PG4	O3-C5-C6-O4
4	A	801	LMT	C5'-C4'-O1B-C1B
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C3-C4-C5-C6
4	A	801	LMT	C7-C8-C9-C10
4	A	801	LMT	C5-C6-C7-C8

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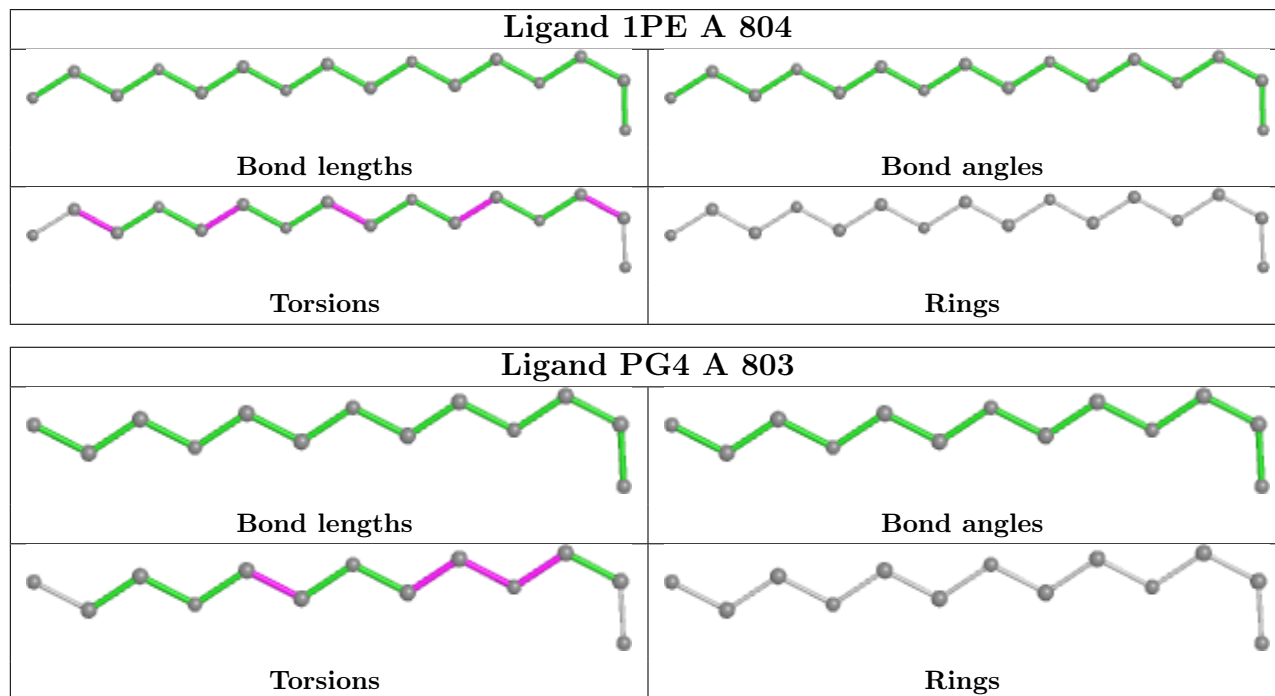
Mol	Chain	Res	Type	Atoms
4	A	801	LMT	C1-C2-C3-C4
5	A	802	OCT	C4-C5-C6-C7
7	A	811	1PE	OH6-C15-C25-OH5
4	A	801	LMT	C3'-C4'-O1B-C1B
4	A	801	LMT	C6-C7-C8-C9
6	A	805	PG4	O3-C5-C6-O4
7	A	804	1PE	OH7-C16-C26-OH6
5	A	802	OCT	C3-C4-C5-C6
8	A	809	D12	C9-C10-C11-C12
9	A	810	GOL	O2-C2-C3-O3
4	A	801	LMT	C11-C10-C9-C8
8	A	809	D12	C3-C4-C5-C6
6	A	805	PG4	O4-C7-C8-O5
6	A	803	PG4	C1-C2-O2-C3
6	A	807	PG4	C8-C7-O4-C6
6	A	805	PG4	C5-C6-O4-C7
6	A	808	PG4	C3-C4-O3-C5
6	A	806	PG4	C1-C2-O2-C3
7	A	811	1PE	C12-C22-OH3-C23
7	A	811	1PE	C25-C15-OH6-C26
4	A	801	LMT	C4-C5-C6-C7
6	A	806	PG4	C4-C3-O2-C2
6	A	807	PG4	C1-C2-O2-C3
6	A	806	PG4	C3-C4-O3-C5
7	A	804	1PE	OH2-C12-C22-OH3
6	A	808	PG4	O2-C3-C4-O3
6	A	808	PG4	O3-C5-C6-O4
6	A	806	PG4	C6-C5-O3-C4
6	A	807	PG4	C3-C4-O3-C5
4	A	801	LMT	C4B-C5B-C6B-O6B
6	A	803	PG4	O2-C3-C4-O3
6	A	803	PG4	C4-C3-O2-C2
6	A	808	PG4	C6-C5-O3-C4
6	A	805	PG4	O2-C3-C4-O3
6	A	807	PG4	O2-C3-C4-O3
7	A	804	1PE	OH4-C13-C23-OH3
8	A	809	D12	C1-C2-C3-C4
7	A	804	1PE	OH6-C15-C25-OH5
9	A	810	GOL	C1-C2-C3-O3
10	A	812	D10	C5-C6-C7-C8
7	A	811	1PE	C15-C25-OH5-C14
7	A	804	1PE	OH5-C14-C24-OH4

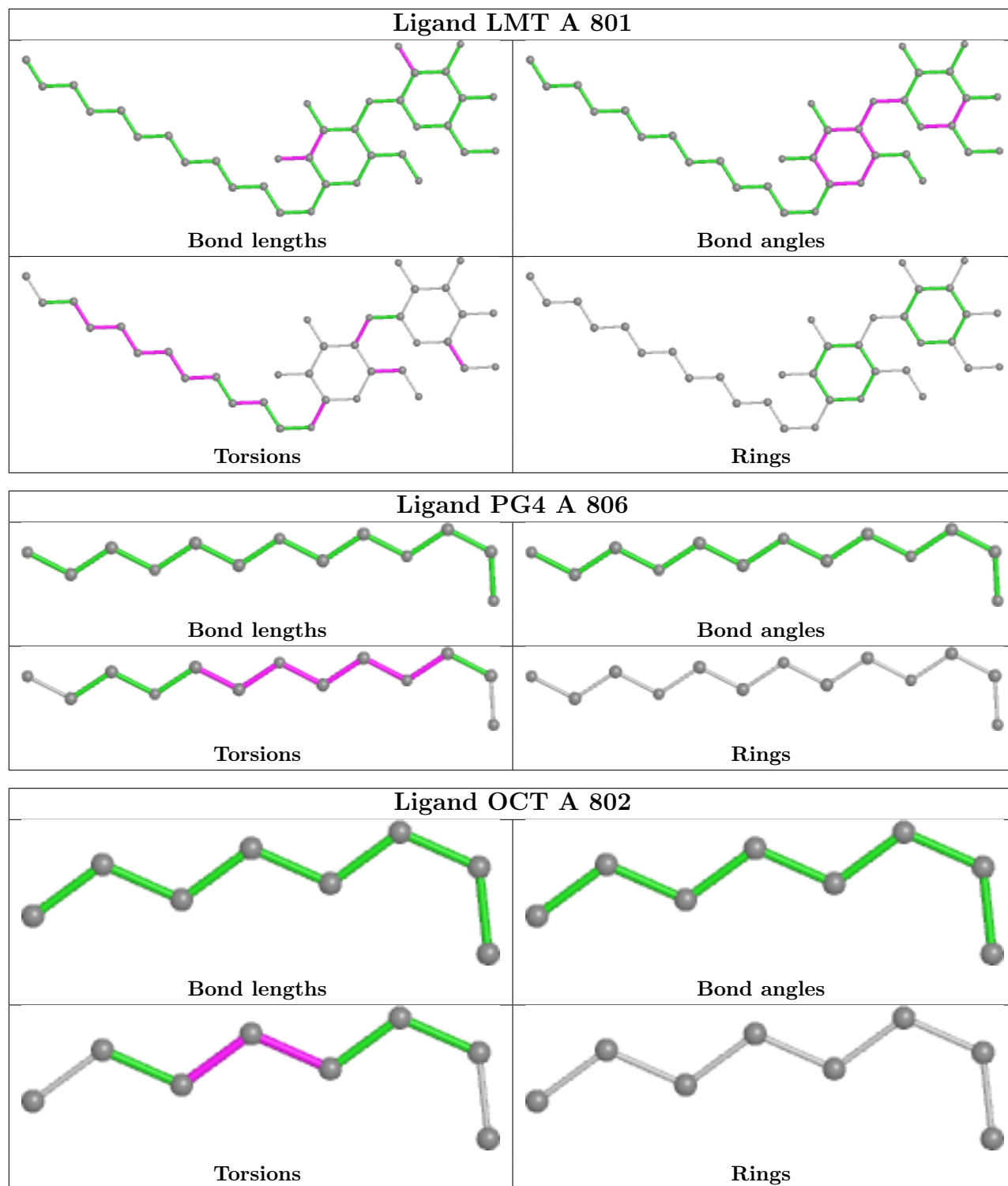
There are no ring outliers.

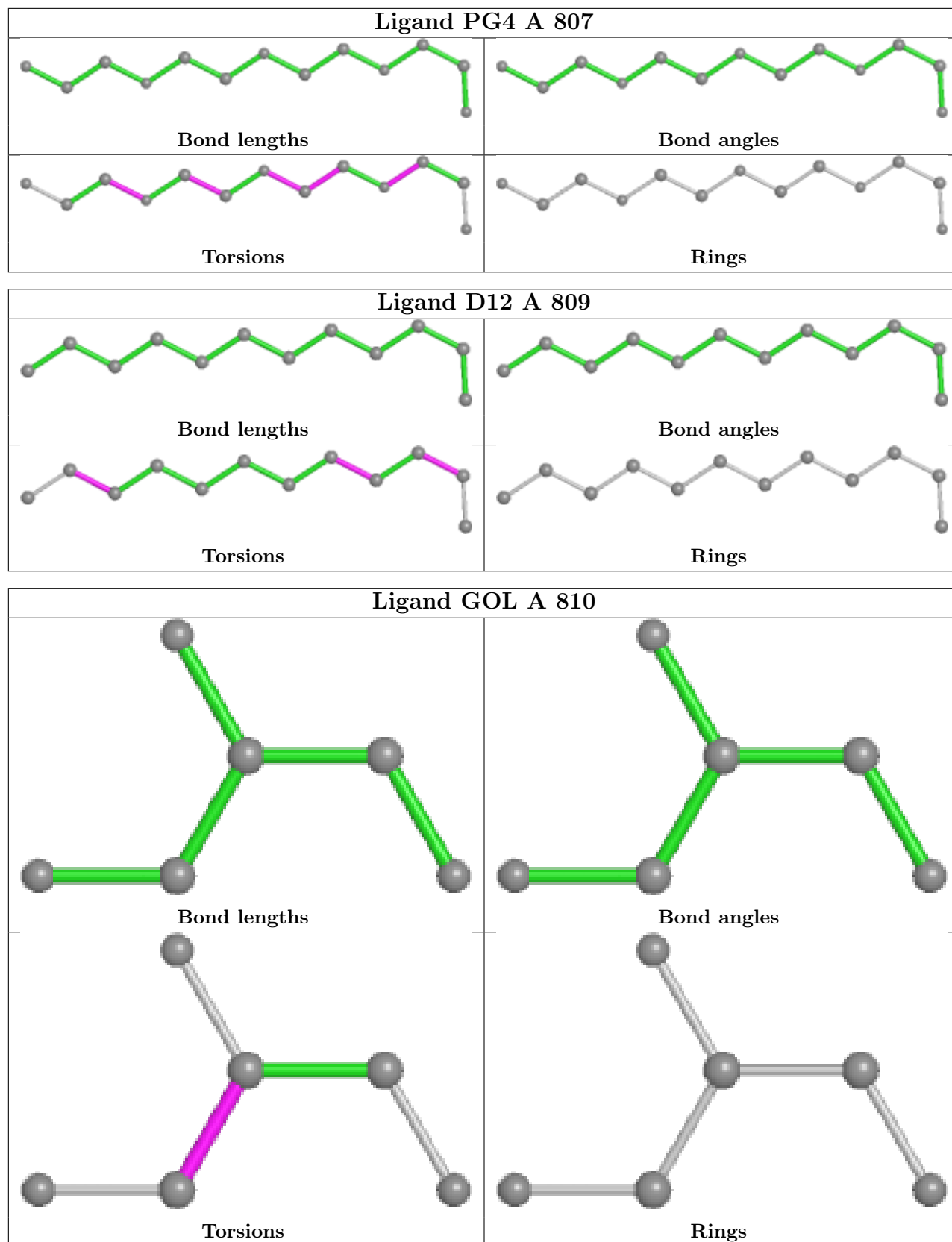
6 monomers are involved in 13 short contacts:

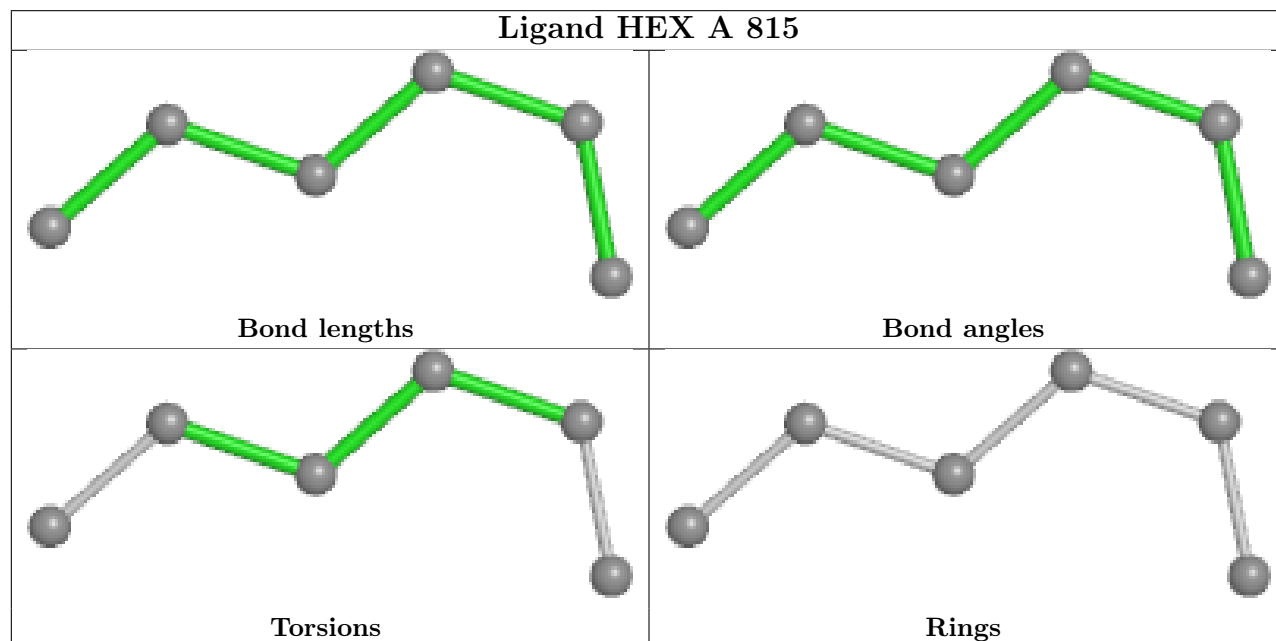
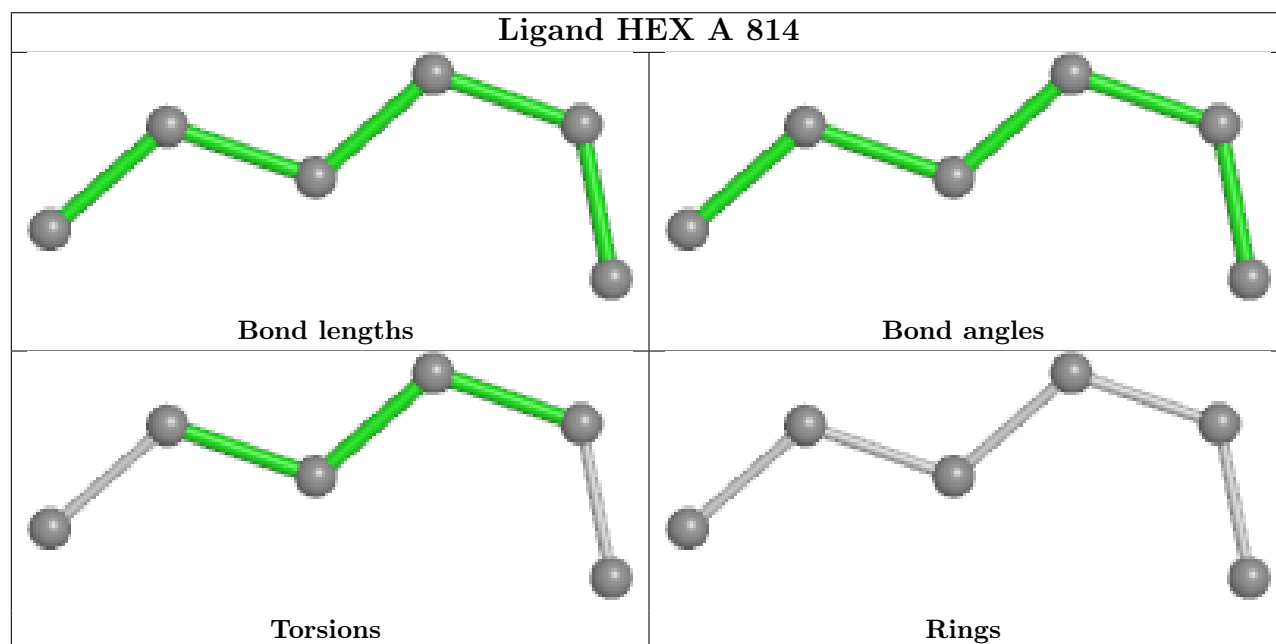
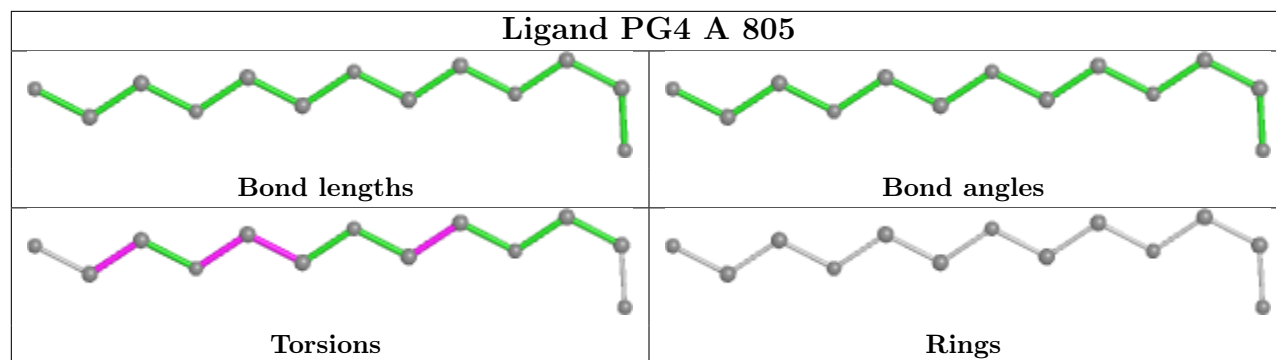
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	LMT	6	0
6	A	806	PG4	1	0
6	A	807	PG4	1	0
11	A	814	HEX	1	0
10	A	812	D10	1	0
7	A	811	1PE	4	0

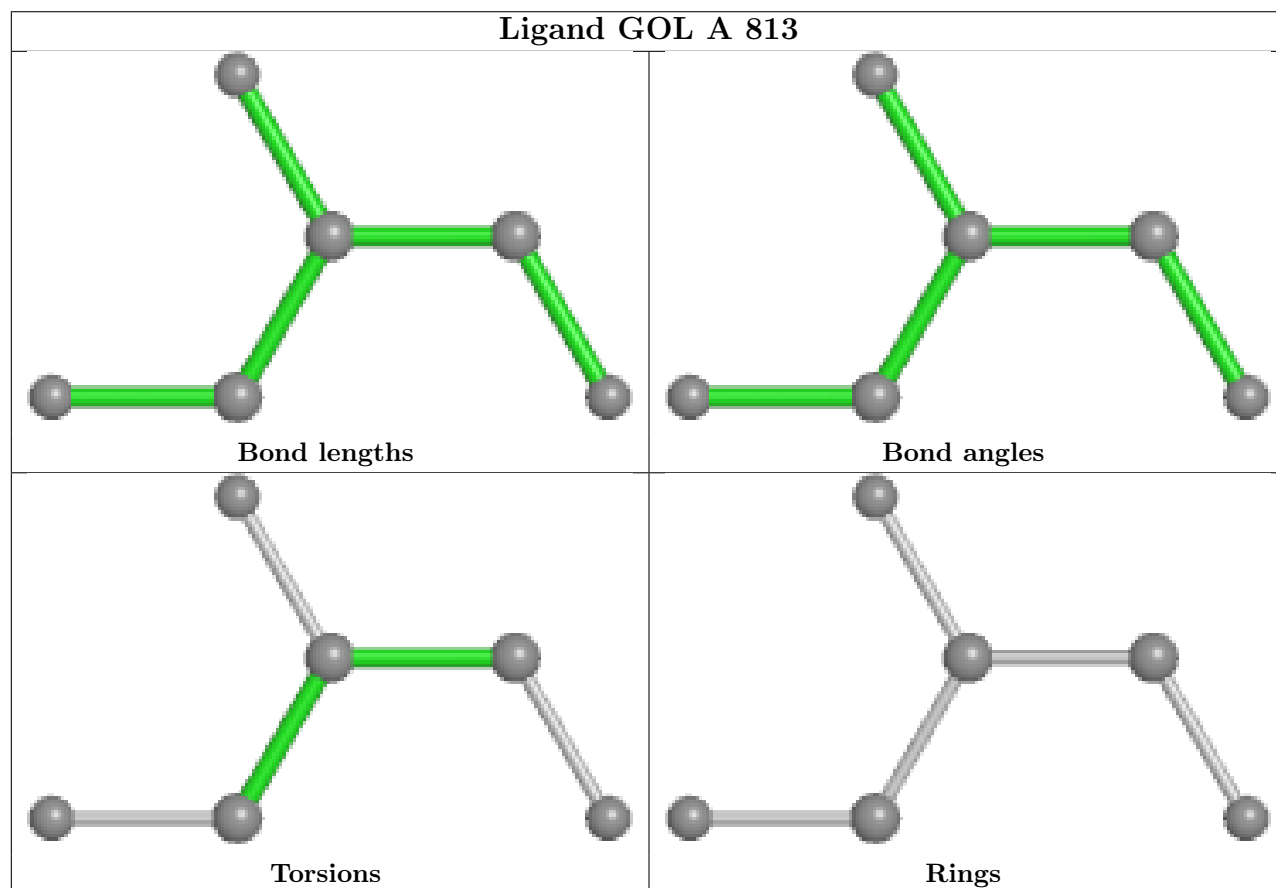
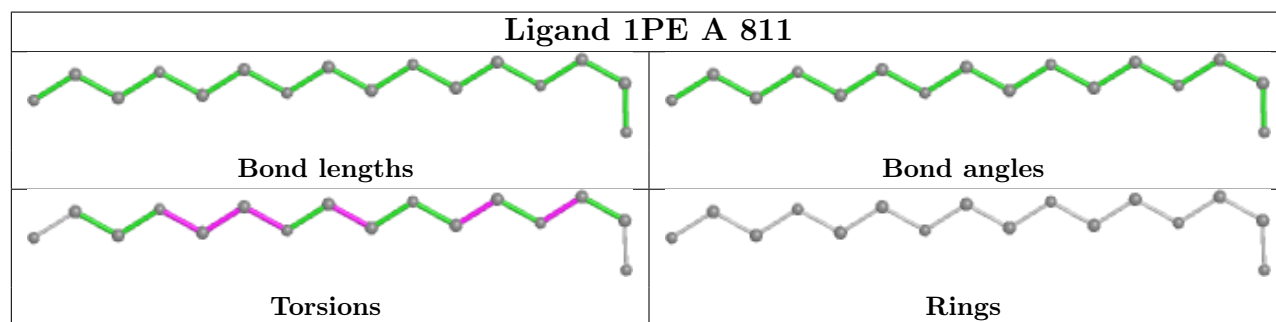
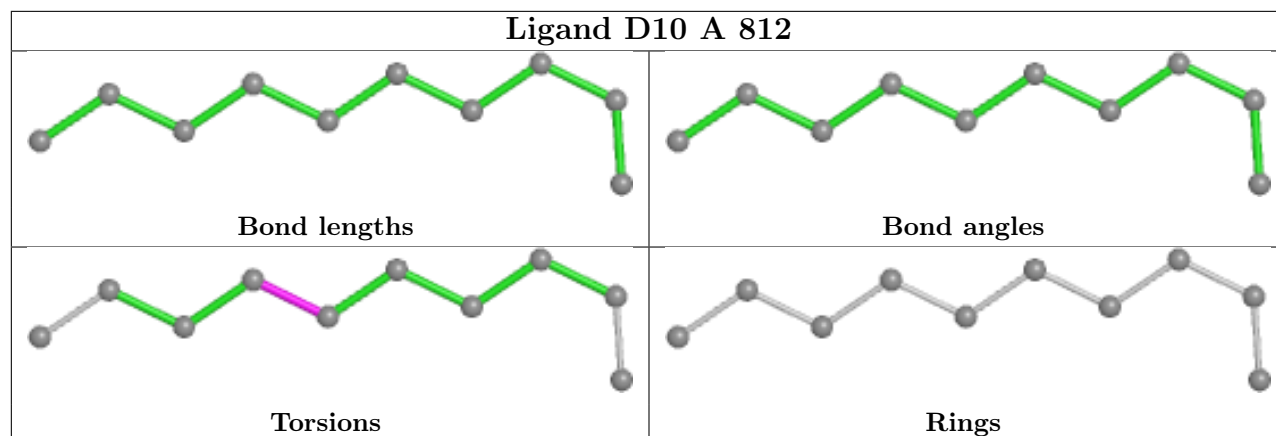
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



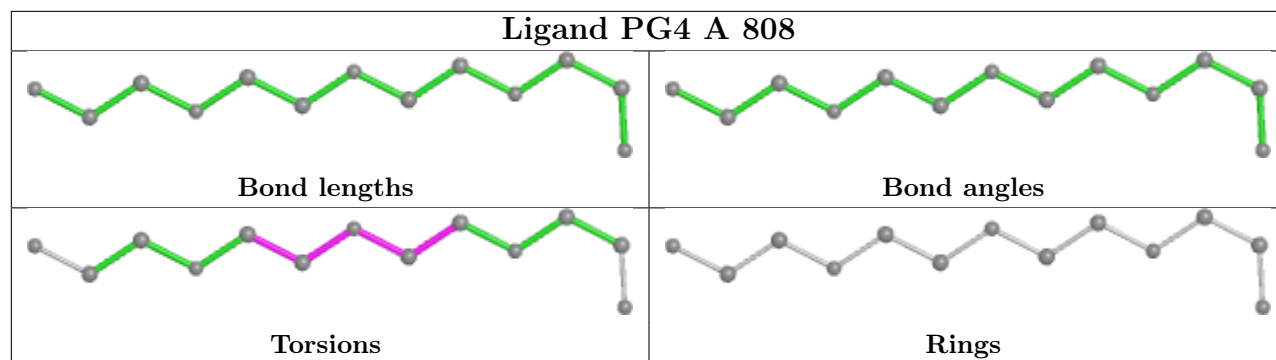












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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	451/489 (92%)	0.96	51 (11%) <b>5</b> <b>7</b>	43, 58, 109, 147	1 (0%)
2	B	127/127 (100%)	0.54	10 (7%) <b>12</b> <b>17</b>	47, 64, 94, 101	1 (0%)
3	C	3/3 (100%)	2.54	1 (33%) <b>0</b> <b>0</b>	57, 57, 70, 83	0
All	All	581/619 (93%)	0.87	62 (10%) <b>6</b> <b>8</b>	43, 60, 105, 147	2 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	PHE	22.0
1	A	251	ILE	18.0
1	A	330	ALA	14.4
1	A	250	THR	12.2
1	A	255	ARG	11.3
1	A	329	LEU	7.6
3	C	4	PHE	7.5
1	A	247	ILE	6.8
1	A	401	LEU	6.3
1	A	331	GLY	6.2
1	A	307	PHE	5.9
1	A	134	TYR	5.7
1	A	326	SER	5.3
1	A	244	VAL	5.2
1	A	240	LEU	5.2
1	A	327	PRO	5.0
1	A	248	VAL	4.8
2	B	115	GLN	4.5
2	B	25	SER	4.3
1	A	395	PHE	4.1
1	A	252	ILE	4.1
1	A	266	ASN	3.8
1	A	137	LYS	3.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	198	LYS	3.7
1	A	16	PHE	3.5
1	A	332	ILE	3.5
2	B	77	THR	3.4
1	A	144	ALA	3.4
1	A	142	ASP	3.4
1	A	130	LEU	3.4
1	A	243	ILE	3.3
2	B	76	ASP	3.2
1	A	253	PHE	3.2
1	A	140	ARG	3.2
2	B	5	VAL	3.0
2	B	3	GLN	3.0
1	A	143	GLY	3.0
1	A	478	TRP	2.9
1	A	200	ILE	2.8
1	A	415	PHE	2.8
1	A	398	ALA	2.8
1	A	399	LEU	2.7
1	A	145	PHE	2.7
1	A	148	PHE	2.7
1	A	246	SER	2.6
1	A	237	VAL	2.6
1	A	345	MET	2.6
1	A	236	GLU	2.6
1	A	416	ILE	2.6
2	B	128	HIS	2.6
1	A	139	PRO	2.4
1	A	20	PHE	2.4
1	A	21	PHE	2.3
1	A	305	LEU	2.2
1	A	19	ILE	2.2
2	B	126	HIS	2.1
2	B	111	ALA	2.1
1	A	189	VAL	2.1
1	A	191	ILE	2.1
1	A	256	GLN	2.0
1	A	187	LEU	2.0
2	B	28	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

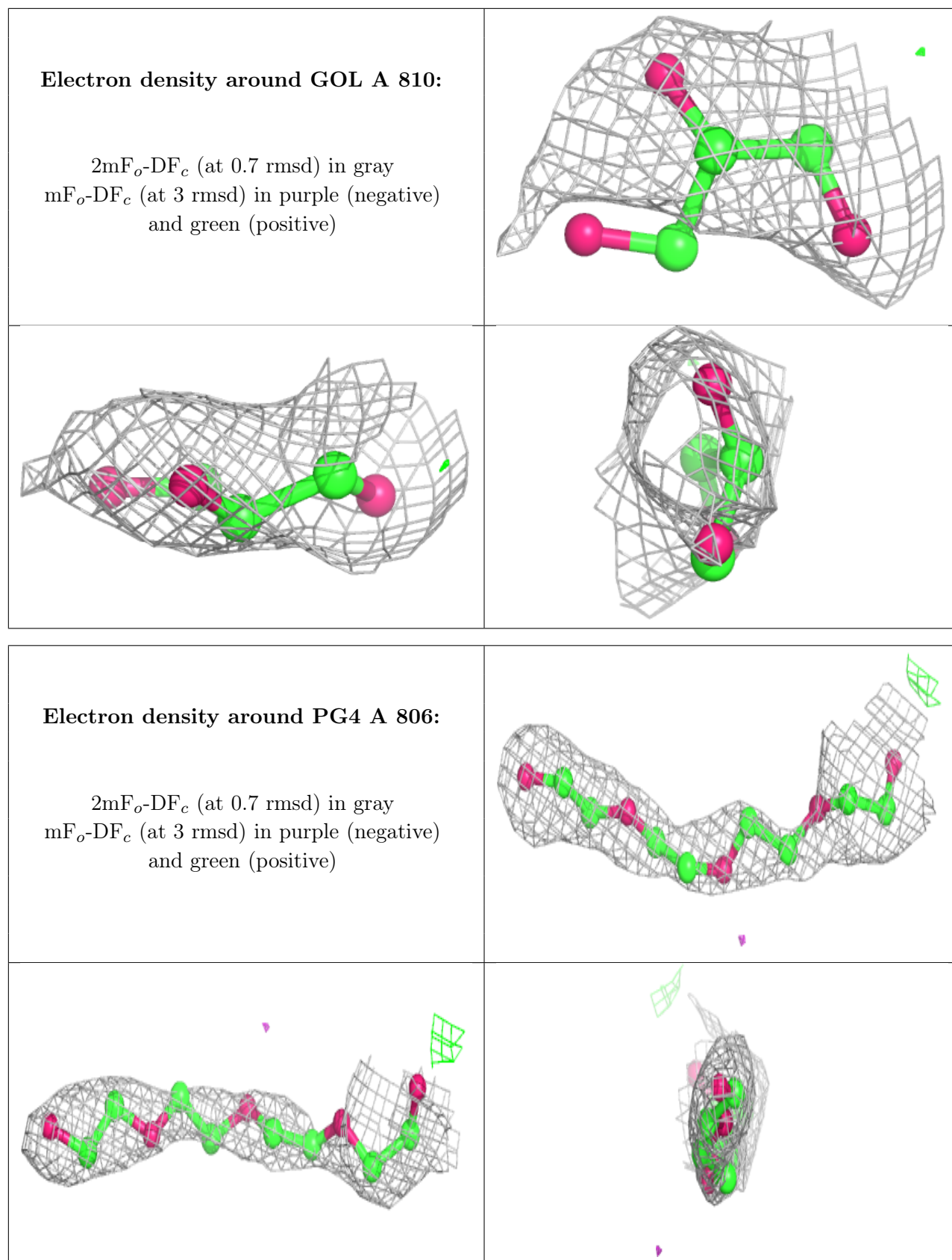
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

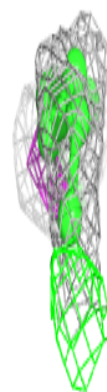
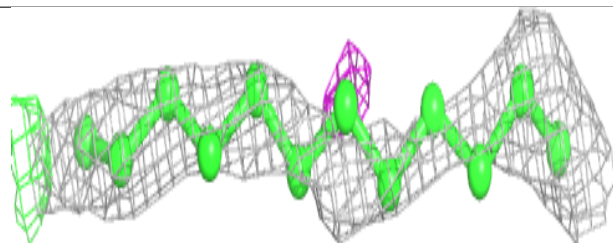
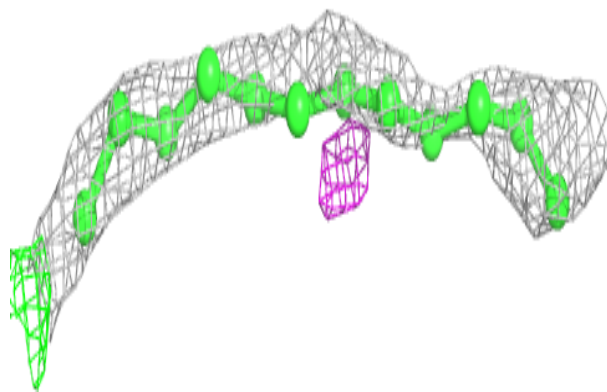
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	GOL	A	810	6/6	0.38	0.32	112,115,117,121	0
6	PG4	A	806	13/13	0.46	0.39	74,84,108,109	0
8	D12	A	809	12/12	0.54	0.60	68,79,82,83	0
11	HEX	A	814	6/6	0.61	0.57	81,84,85,86	0
11	HEX	A	815	6/6	0.64	0.32	71,75,77,78	0
6	PG4	A	805	13/13	0.65	0.21	75,84,99,100	0
9	GOL	A	813	6/6	0.72	0.14	77,81,84,85	0
6	PG4	A	808	13/13	0.73	0.17	73,79,95,96	0
5	OCT	A	802	8/8	0.76	0.28	62,64,66,68	0
7	1PE	A	811	16/16	0.77	0.35	79,84,94,94	0
10	D10	A	812	10/10	0.77	0.18	61,68,83,89	0
4	LMT	A	801	35/35	0.81	0.33	61,83,103,106	0
6	PG4	A	807	13/13	0.84	0.13	66,75,86,93	0
7	1PE	A	804	16/16	0.87	0.26	61,71,89,92	0
6	PG4	A	803	13/13	0.90	0.13	67,75,88,92	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.

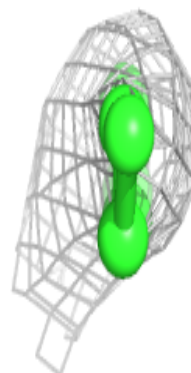
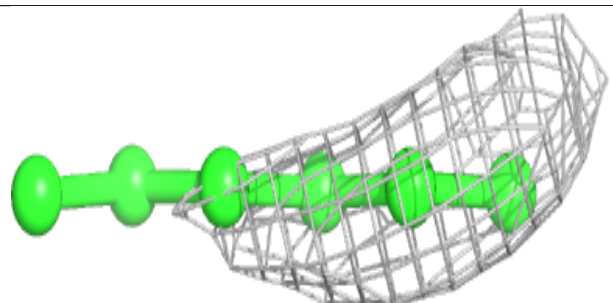
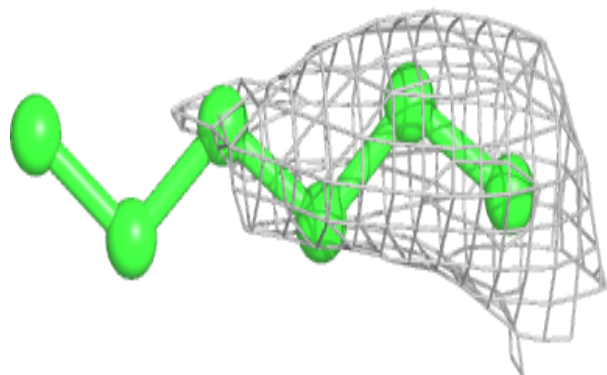


**Electron density around D12 A 809:**

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

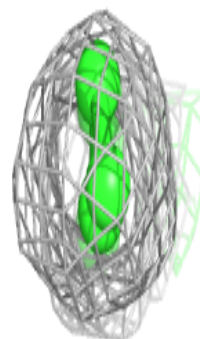
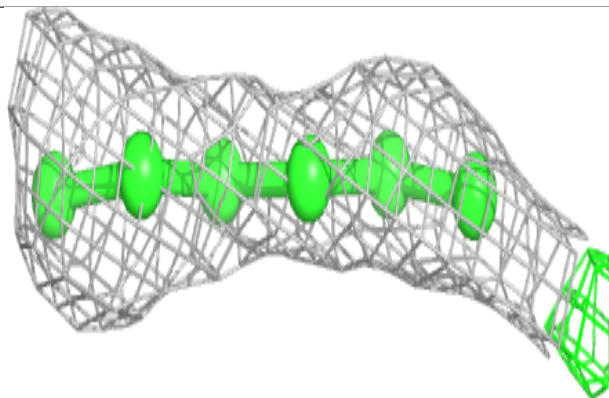
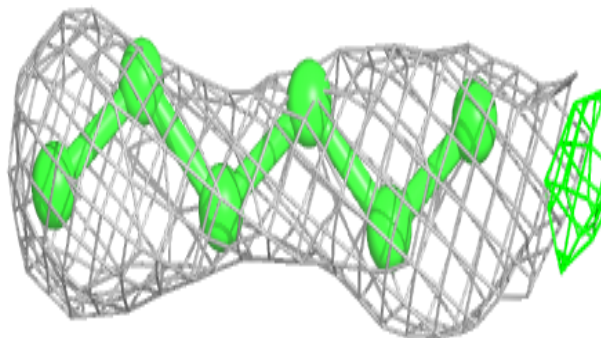
**Electron density around HEX A 814:**

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

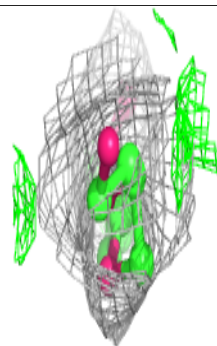
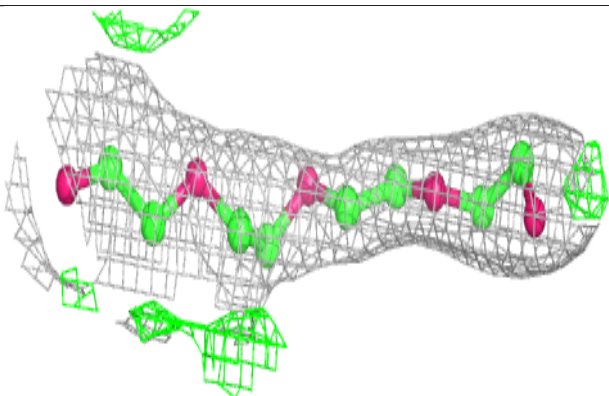
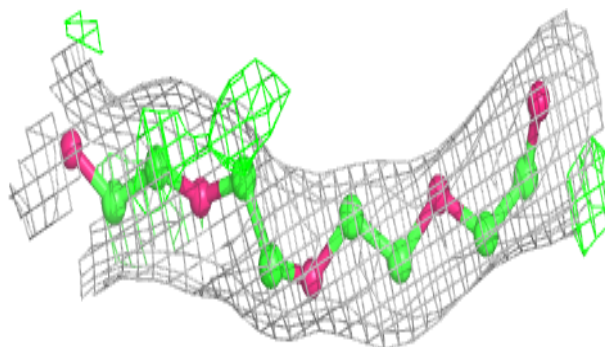


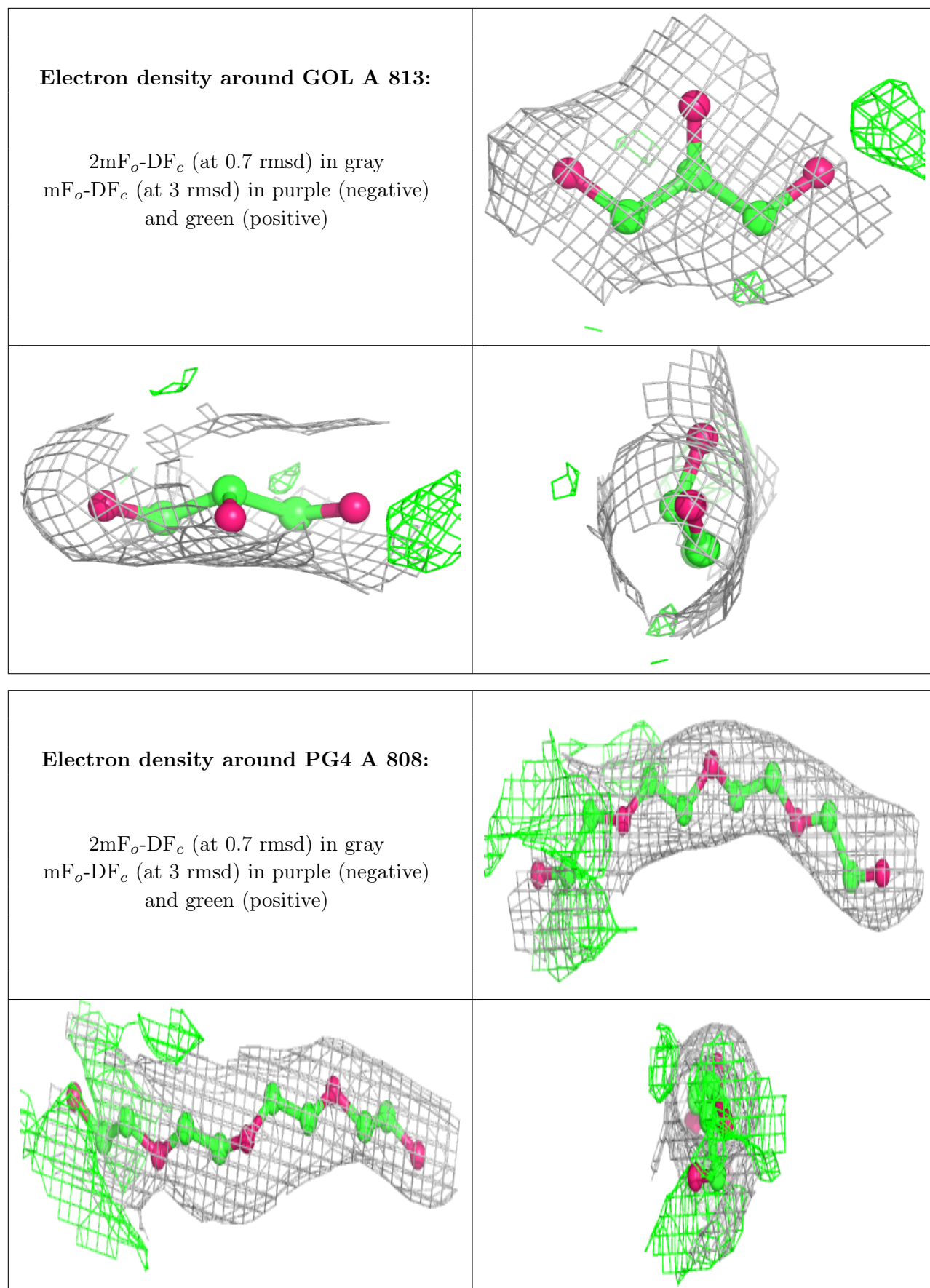
**Electron density around HEX A 815:**

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

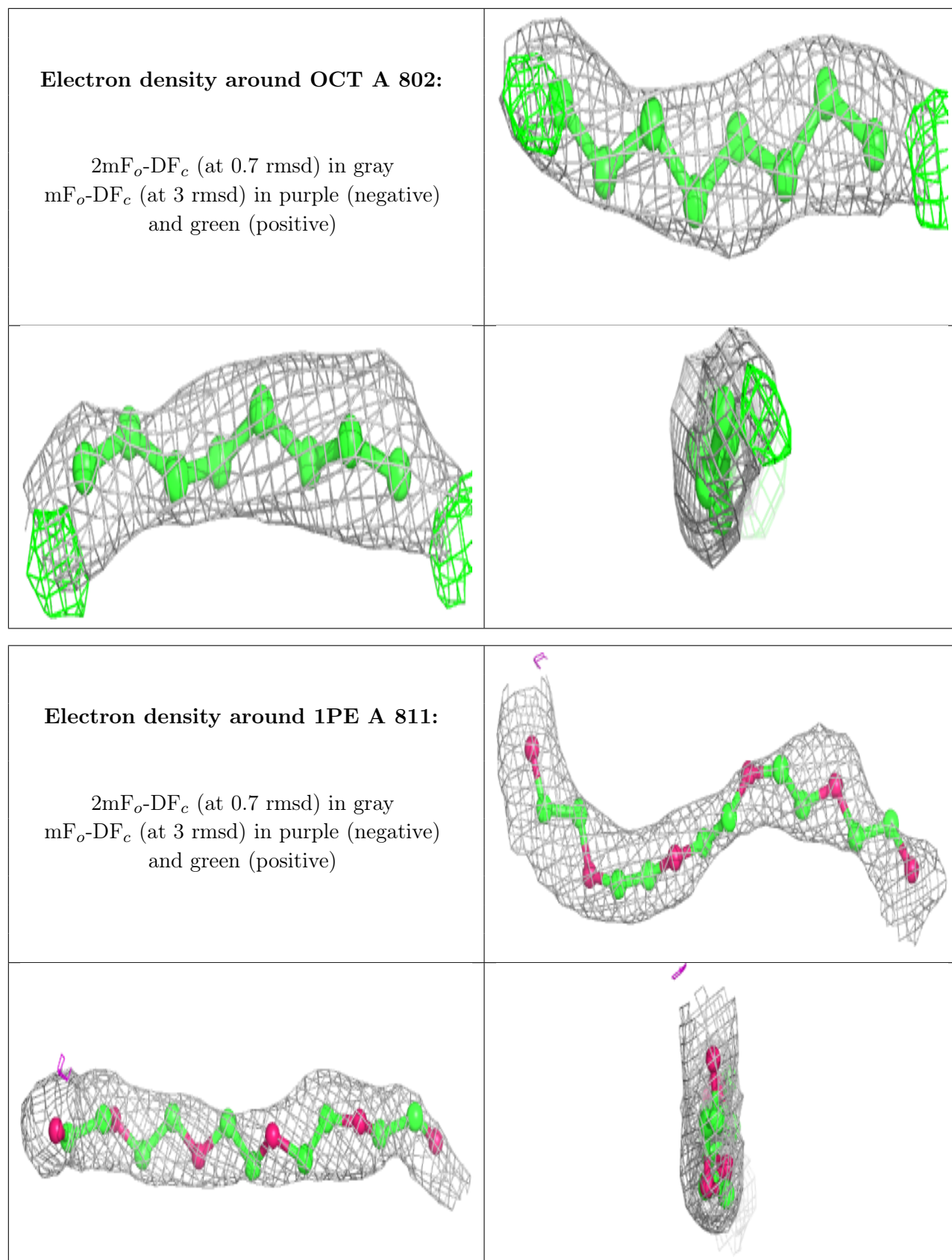
**Electron density around PG4 A 805:**

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



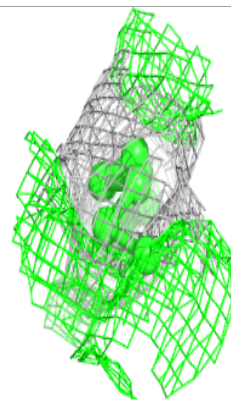
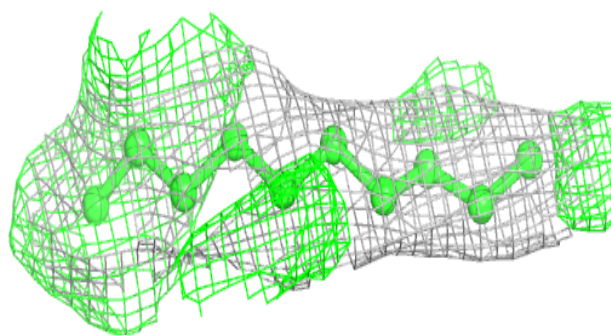
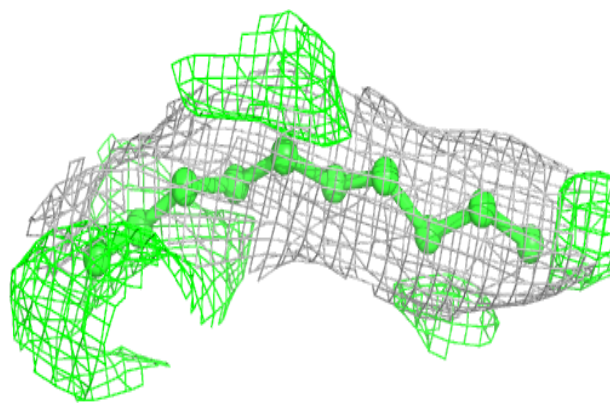






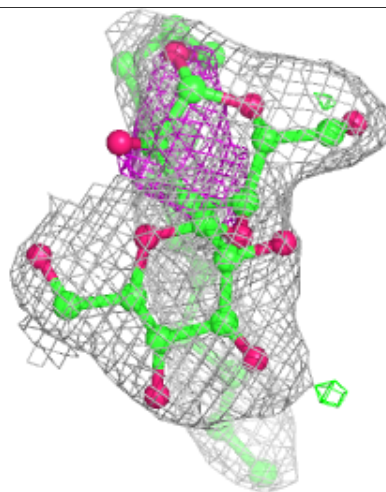
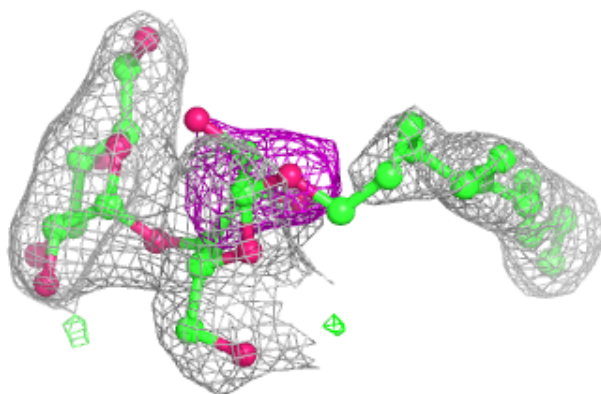
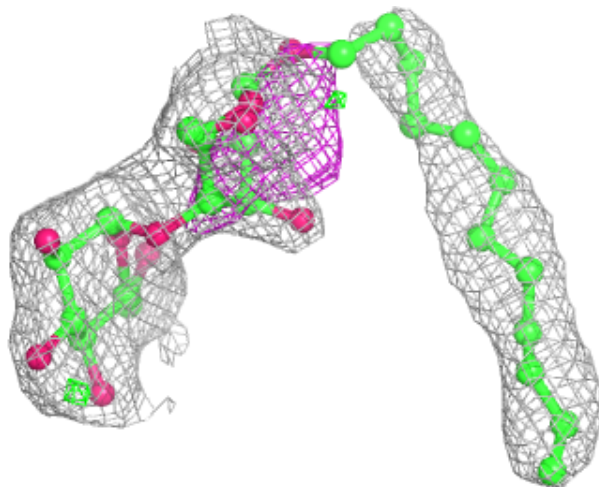
**Electron density around D10 A 812:**

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



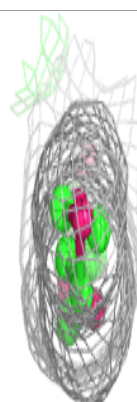
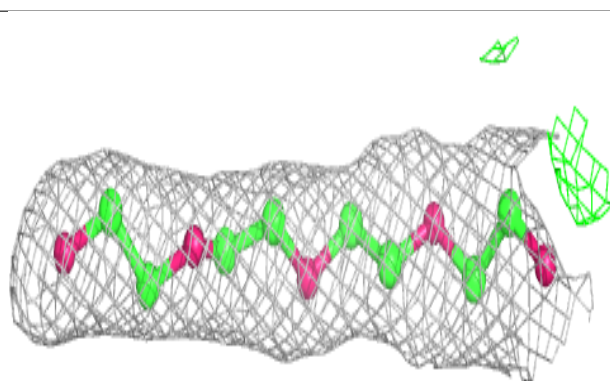
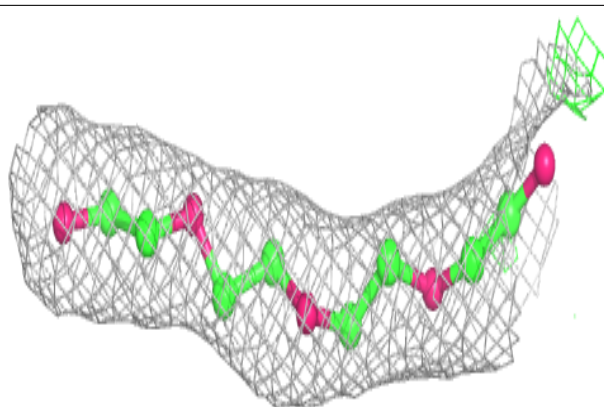
**Electron density around LMT A 801:**

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

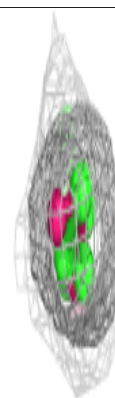
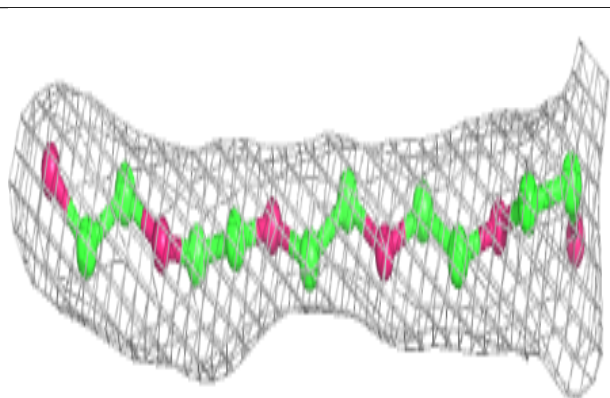
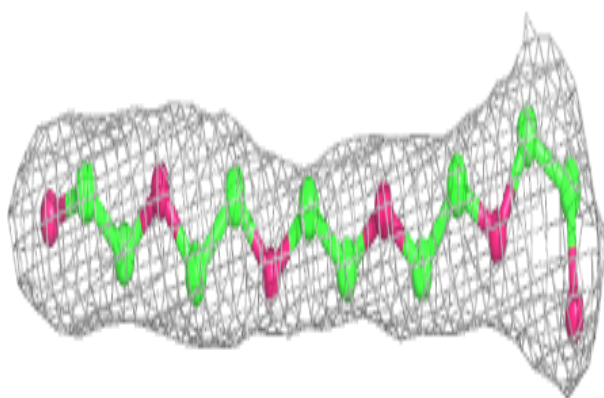


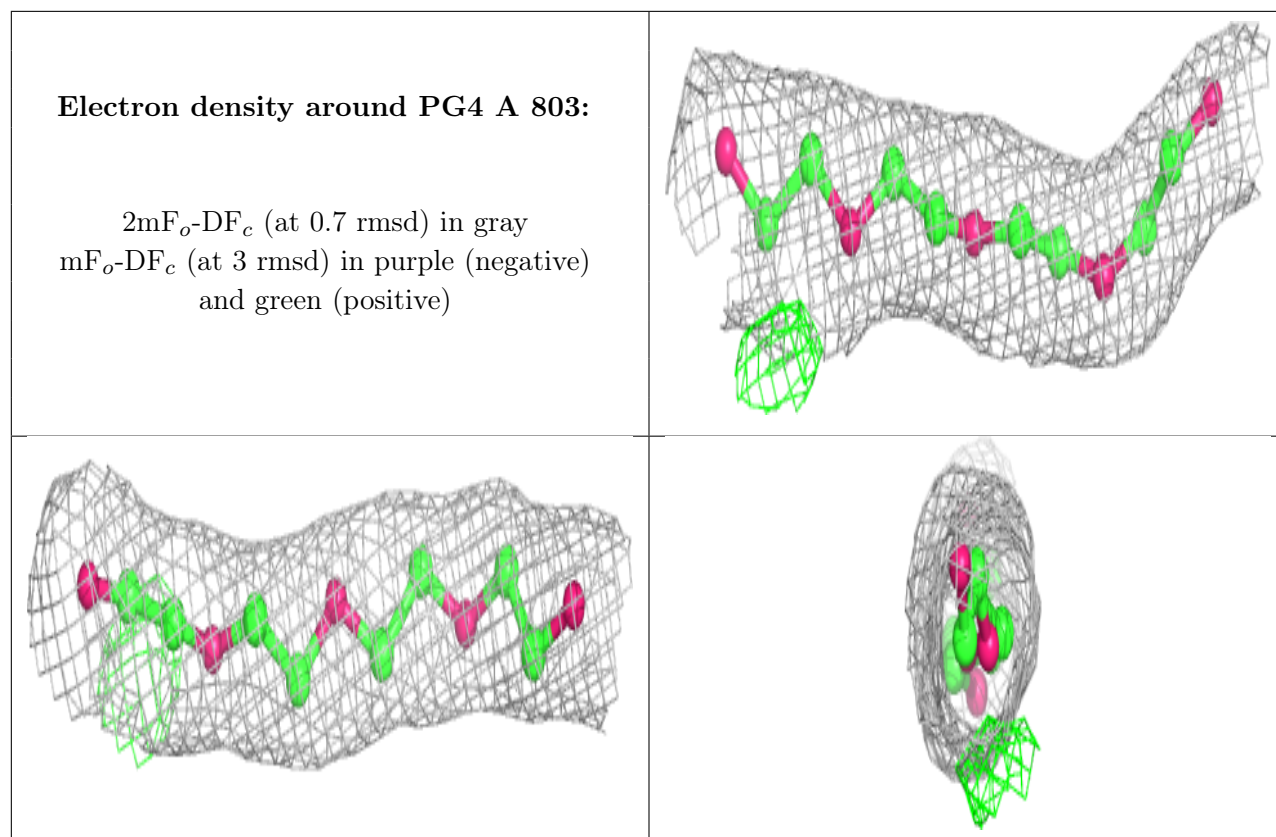
**Electron density around PG4 A 807:**

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

**Electron density around 1PE A 804:**

$2mF_o-DF_c$  (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.