



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 04:14 pm BST

PDB ID : 8B17  
Title : DtpB-Nb132-AWA  
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Deposited on : 2022-09-09  
Resolution : 2.50 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)  
Xtrriage (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

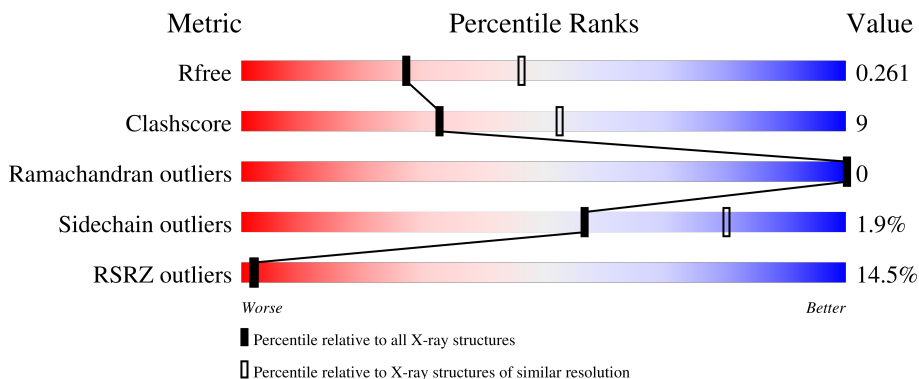
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	
2	B	127	
3	C	3	

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
11	HEX	A	814	-	-	-	X
6	PG4	A	806	-	-	-	X
7	1PE	A	811	-	-	-	X
8	D12	A	809	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 4791 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

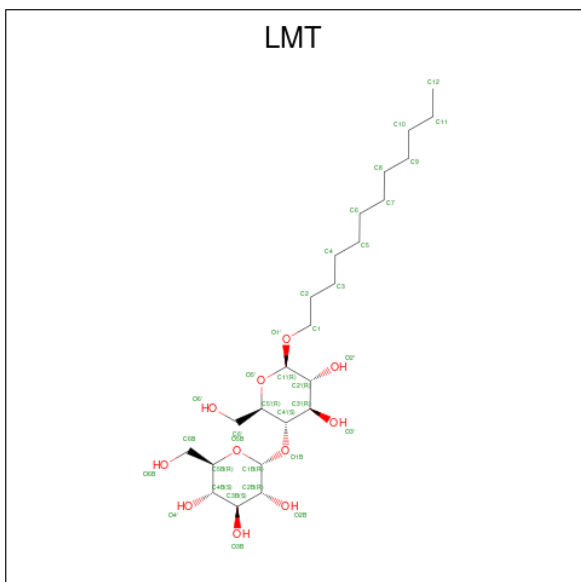
- Molecule 2 is a protein called Nanobody 132.

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-TRP-ALA.

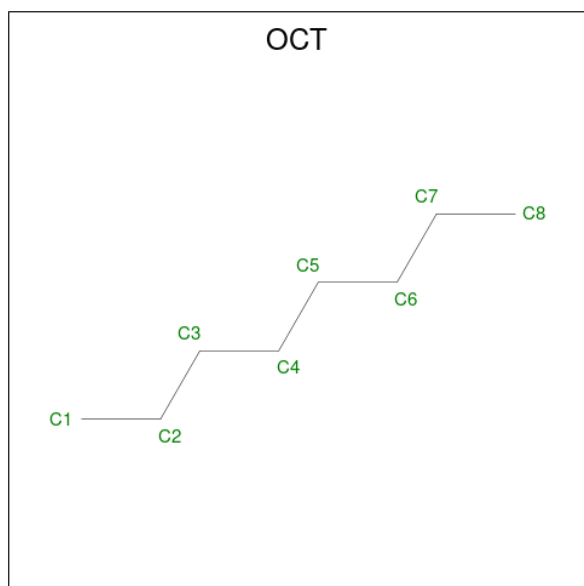
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	3	25	17	4	4	0	0	0

- 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).



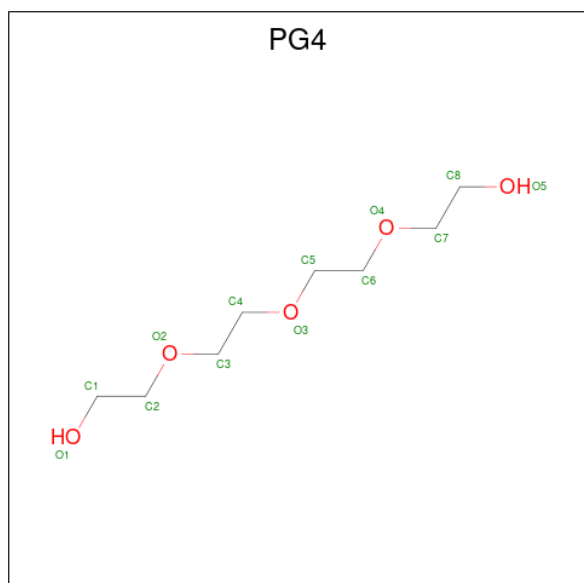
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	24	11		

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



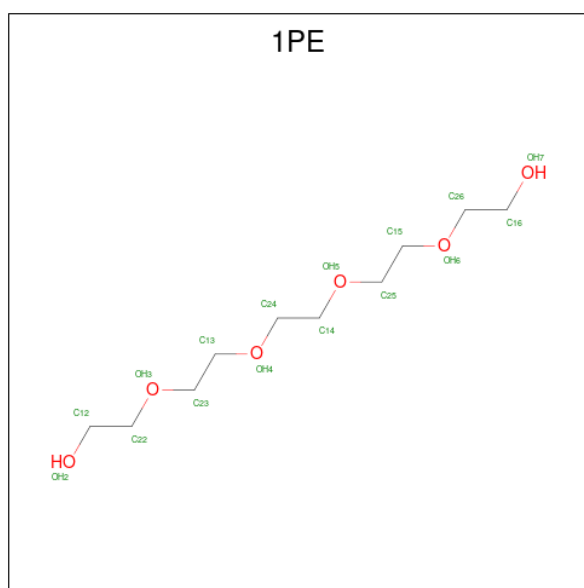
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	C	0	0
			8	8		

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



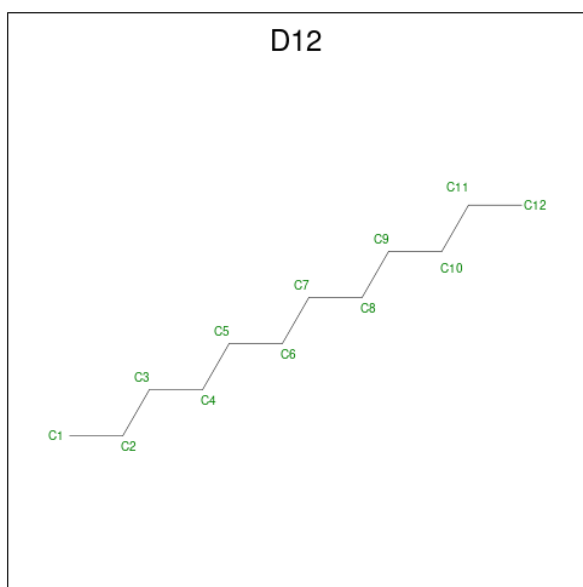
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C<sub>10</sub>H<sub>22</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



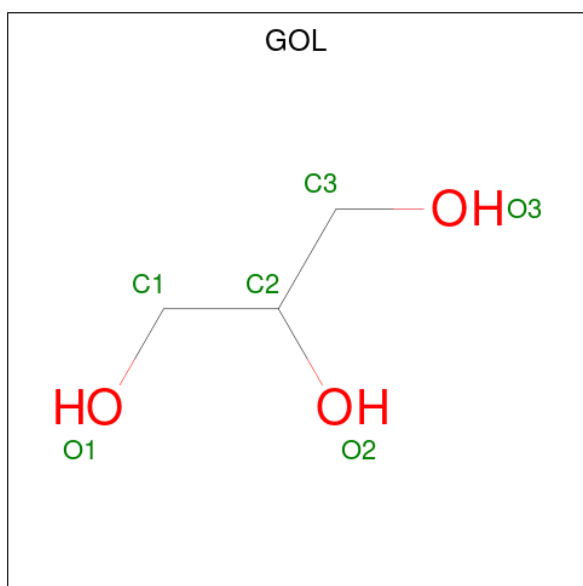
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			16	10	6		
7	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 8 is DODECANE (three-letter code: D12) (formula: C<sub>12</sub>H<sub>26</sub>) (labeled as "Ligand of Interest" by depositor).



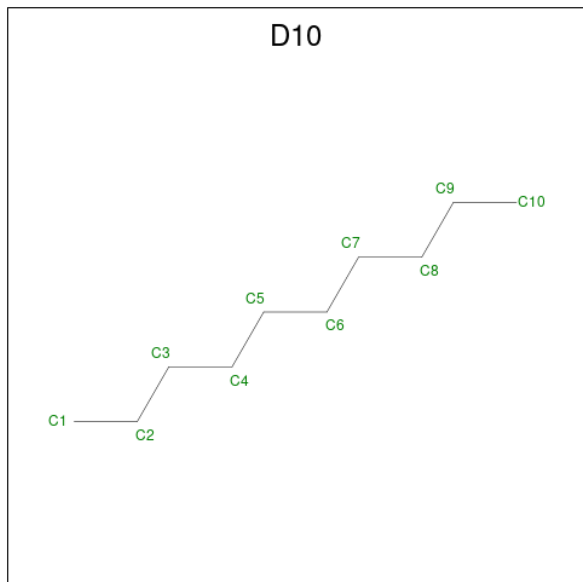
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 12 12	0	0

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



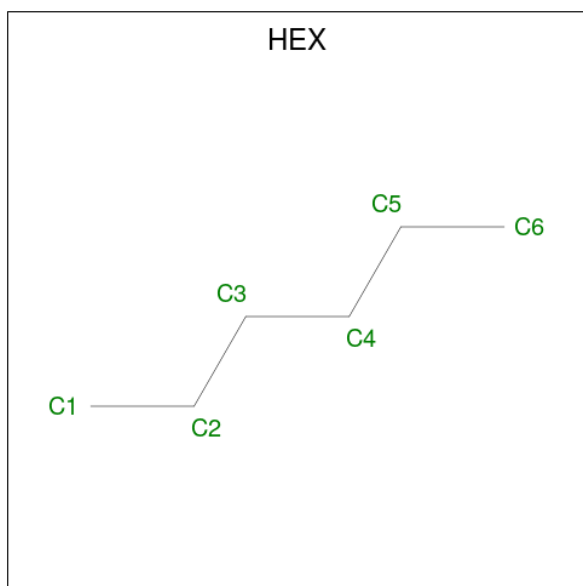
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0

- 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

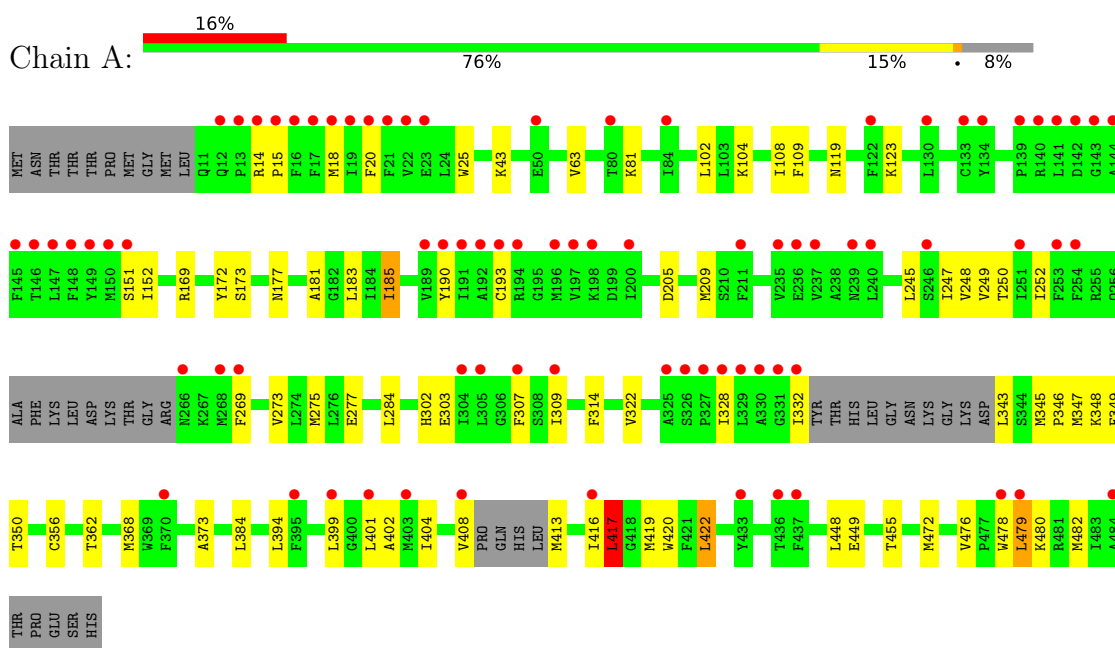
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	68	Total O 68 68	0	0
12	B	56	Total O 56 56	0	0

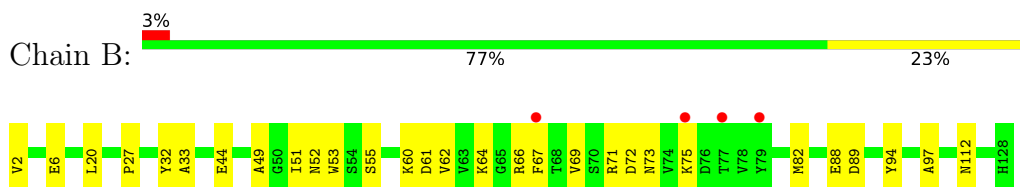
### 3 Residue-property plots [i](#)

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-TRP-ALA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.60Å 125.36Å 168.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.41 – 2.50 84.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (84.41-2.50) 98.7 (84.41-2.50)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.234 , 0.269 0.231 , 0.261	Depositor DCC
$R_{free}$ test set	2000 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.7	Xtrriage
Anisotropy	0.076	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 78.3	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	0.88	EDS
Total number of atoms	4791	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: LMT, PG4, 1PE, HEX, D12, D10, GOL, OCT

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	0.53	0/3572	0.70	2/4859 (0.0%)
2	B	0.55	0/1004	0.71	0/1361
3	C	0.81	0/26	0.58	0/34
All	All	0.54	0/4602	0.70	2/6254 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	417	LEU	CA-CB-CG	6.16	129.47	115.30
1	A	479	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3480	0	3605	60	0
2	B	976	0	939	21	0
3	C	25	0	22	2	0
4	A	35	0	46	3	0
5	A	8	0	18	0	0
6	A	65	0	90	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	32	0	44	0	0
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	0	0
11	A	12	0	28	0	0
12	A	68	0	0	4	0
12	B	56	0	0	2	0
All	All	4791	0	4856	83	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 9.

All (83) 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:25:TRP:CE2	1:A:185:ILE:HD11	2.19	0.78
1:A:368:MET:HG3	1:A:455:THR:HG21	1.71	0.73
1:A:177:ASN:OD1	12:A:901:HOH:O	2.08	0.70
1:A:449:GLU:OE2	12:A:902:HOH:O	2.10	0.68
2:B:2:VAL:HA	2:B:112:ASN:HD22	1.59	0.68
1:A:284:LEU:HD12	1:A:356:CYS:HB3	1.75	0.68
1:A:273:VAL:O	1:A:277:GLU:HG3	1.95	0.67
1:A:416:ILE:HA	1:A:419:MET:HG2	1.76	0.67
1:A:348:LYS:HD3	1:A:399:LEU:HD21	1.77	0.66
2:B:2:VAL:HA	2:B:112:ASN:ND2	2.12	0.65
1:A:119:ASN:HD21	1:A:123:LYS:CE	2.09	0.65
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.27	0.64
2:B:60:LYS:HD3	2:B:62:VAL:HG22	1.81	0.61
1:A:348:LYS:HD3	1:A:399:LEU:CD2	2.30	0.61
1:A:362:THR:HG21	1:A:384:LEU:HD23	1.82	0.61
1:A:413:MET:O	1:A:416:ILE:HG13	2.01	0.60
4:A:801:LMT:H4B	2:B:32:TYR:OH	2.01	0.59
4:A:801:LMT:H3'	4:A:801:LMT:H5B	1.85	0.58
1:A:269:PHE:O	1:A:273:VAL:HG22	2.03	0.58
1:A:413:MET:SD	1:A:417:LEU:HD11	2.44	0.58
1:A:81:LYS:HB3	1:A:190:TYR:OH	2.05	0.57
1:A:347:MET:HE2	1:A:476:VAL:HG11	1.87	0.56
2:B:61[A]:ASP:HA	2:B:64:LYS:HE2	1.88	0.56
1:A:181:ALA:O	1:A:185:ILE:HG23	2.05	0.55
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.89	0.55
1:A:275:MET:HG3	1:A:420:TRP:HD1	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:HG3	1:A:420:TRP:CD1	2.43	0.54
1:A:63:VAL:HG13	1:A:119:ASN:ND2	2.23	0.53
1:A:249:VAL:HG21	1:A:422:LEU:HD13	1.90	0.53
1:A:302:HIS:HD2	12:B:213:HOH:O	1.92	0.52
1:A:322:VAL:HG13	1:A:394:LEU:HD21	1.91	0.52
1:A:401:LEU:HB2	1:A:420:TRP:CH2	2.45	0.52
2:B:61[B]:ASP:HA	2:B:64:LYS:HE2	1.93	0.51
1:A:368:MET:HG3	1:A:455:THR:CG2	2.40	0.51
2:B:44:GLU:HA	2:B:44:GLU:OE1	2.11	0.50
2:B:51:ILE:HD13	2:B:71:ARG:HB2	1.93	0.50
1:A:309:ILE:HD11	1:A:314:PHE:CZ	2.47	0.50
1:A:102:LEU:HD21	1:A:172:TYR:HB2	1.93	0.49
1:A:328:ILE:O	1:A:332:ILE:HG12	2.12	0.49
2:B:67:PHE:CE1	2:B:82:MET:HB3	2.47	0.49
1:A:169:ARG:NH1	2:B:27:PRO:HD3	2.28	0.48
1:A:413:MET:O	1:A:417:LEU:HD12	2.13	0.48
2:B:6:GLU:OE2	2:B:94:TYR:HA	2.12	0.48
1:A:245:LEU:O	1:A:249:VAL:HG23	2.14	0.48
1:A:20:PHE:CE2	1:A:151:SER:HB2	2.48	0.48
1:A:119:ASN:HD21	1:A:123:LYS:HE2	1.77	0.48
1:A:247:ILE:O	1:A:250:THR:HG22	2.14	0.48
1:A:343:LEU:N	1:A:480:LYS:HZ3	2.13	0.47
1:A:349:PHE:CZ	1:A:404:ILE:HD11	2.50	0.47
1:A:152:ILE:HD13	3:C:3:ALA:HA	1.97	0.46
1:A:346:PRO:HB3	1:A:479:LEU:HD22	1.95	0.46
1:A:362:THR:CG2	1:A:384:LEU:HD23	2.45	0.46
2:B:33:ALA:CB	2:B:52:ASN:HA	2.46	0.46
1:A:43:LYS:HA	1:A:43:LYS:HD2	1.69	0.46
2:B:49:ALA:HB1	2:B:69:VAL:CG2	2.46	0.45
1:A:20:PHE:CD2	1:A:151:SER:HB2	2.51	0.45
2:B:71:ARG:HD3	2:B:73:ASN:OD1	2.16	0.45
4:A:801:LMT:H3'	4:A:801:LMT:C5B	2.45	0.44
2:B:72:ASP:OD2	2:B:75:LYS:HB2	2.18	0.43
3:C:2:TRP:O	3:C:3:ALA:C	2.57	0.43
1:A:14:ARG:N	1:A:15:PRO:HD2	2.34	0.43
2:B:20:LEU:HG	2:B:82:MET:HE2	2.01	0.43
2:B:55:SER:N	12:B:204:HOH:O	2.49	0.43
1:A:25:TRP:CD2	1:A:185:ILE:HD11	2.53	0.43
1:A:277:GLU:OE2	1:A:472:MET:HG2	2.19	0.43
1:A:402:ALA:HA	12:A:961:HOH:O	2.19	0.42
1:A:119:ASN:ND2	1:A:123:LYS:HE2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:GLU:CD	1:A:472:MET:HG2	2.40	0.42
1:A:401:LEU:HB2	1:A:420:TRP:CZ3	2.54	0.42
1:A:102:LEU:HD22	12:A:957:HOH:O	2.20	0.42
2:B:88:GLU:H	2:B:88:GLU:CD	2.23	0.42
1:A:108:ILE:HG23	1:A:109:PHE:N	2.35	0.42
1:A:25:TRP:NE1	1:A:185:ILE:HD11	2.33	0.42
1:A:408:VAL:HG11	1:A:416:ILE:HG12	2.01	0.41
1:A:303:GLU:HA	1:A:307:PHE:O	2.21	0.41
1:A:373:ALA:O	1:A:448:LEU:HD11	2.20	0.41
1:A:248:VAL:O	1:A:252:ILE:HG22	2.20	0.41
1:A:350:THR:HA	1:A:472:MET:HE2	2.02	0.41
1:A:478:TRP:HE1	1:A:482:MET:HE1	1.86	0.41
2:B:20:LEU:HG	2:B:82:MET:CE	2.51	0.41
1:A:478:TRP:C	1:A:478:TRP:CD1	2.95	0.40
2:B:97:ALA:HB3	2:B:112:ASN:HB2	2.03	0.40
1:A:183:LEU:HD13	1:A:183:LEU:HA	1.87	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	443/489 (91%)	433 (98%)	10 (2%)	0	100	100
2	B	126/127 (99%)	122 (97%)	4 (3%)	0	100	100
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	570/619 (92%)	556 (98%)	14 (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%)	360 (98%)	8 (2%)	52	77
2	B	102/101 (101%)	101 (99%)	1 (1%)	76	90
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	471/503 (94%)	462 (98%)	9 (2%)	57	80

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	173	SER
1	A	185	ILE
1	A	205	ASP
1	A	209	MET
1	A	345	MET
1	A	417	LEU
1	A	422	LEU
2	B	53	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	389	GLN
1	A	424	GLN
1	A	456	ASN

### 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	$\# Z  > 2$
8	D12	A	809	-	11,11,11	0.42	0	10,10,10	0.70	0
7	1PE	A	811	-	15,15,15	0.51	0	14,14,14	0.41	0
6	PG4	A	805	-	12,12,12	0.50	0	11,11,11	0.38	0
6	PG4	A	808	-	12,12,12	0.55	0	11,11,11	0.53	0
9	GOL	A	810	-	5,5,5	0.98	0	5,5,5	0.88	0
10	D10	A	812	-	9,9,9	0.33	0	8,8,8	0.92	0
7	1PE	A	804	-	15,15,15	0.50	0	14,14,14	0.33	0
6	PG4	A	806	-	12,12,12	0.55	0	11,11,11	0.36	0
6	PG4	A	807	-	12,12,12	0.49	0	11,11,11	0.37	0
4	LMT	A	801	-	36,36,36	1.20	3 (8%)	47,47,47	1.63	12 (25%)
11	HEX	A	815	-	5,5,5	0.36	0	4,4,4	0.50	0
5	OCT	A	802	-	7,7,7	0.39	0	6,6,6	0.66	0
6	PG4	A	803	-	12,12,12	0.54	0	11,11,11	0.26	0
11	HEX	A	814	-	5,5,5	0.39	0	4,4,4	0.51	0
9	GOL	A	813	-	5,5,5	1.21	0	5,5,5	0.84	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	D12	A	809	-	-	1/9/9/9	-
7	1PE	A	811	-	-	7/13/13/13	-
6	PG4	A	805	-	-	3/10/10/10	-
6	PG4	A	808	-	-	6/10/10/10	-
9	GOL	A	810	-	-	0/4/4/4	-
10	D10	A	812	-	-	2/7/7/7	-
7	1PE	A	804	-	-	6/13/13/13	-
6	PG4	A	806	-	-	8/10/10/10	-
6	PG4	A	807	-	-	6/10/10/10	-
4	LMT	A	801	-	-	15/21/61/61	0/2/2/2
11	HEX	A	815	-	-	0/3/3/3	-
5	OCT	A	802	-	-	3/5/5/5	-
6	PG4	A	803	-	-	5/10/10/10	-
11	HEX	A	814	-	-	0/3/3/3	-
9	GOL	A	813	-	-	0/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5B-C1B	3.49	1.50	1.41
4	A	801	LMT	O5'-C1'	3.21	1.50	1.41
4	A	801	LMT	O5B-C5B	2.27	1.49	1.44

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	LMT	C4B-C3B-C2B	-3.48	104.74	110.82
4	A	801	LMT	O1'-C1'-C2'	3.39	113.59	108.30
4	A	801	LMT	C1'-O5'-C5'	-3.31	107.19	113.69
4	A	801	LMT	C1'-C2'-C3'	2.96	116.15	110.00
4	A	801	LMT	C2'-C3'-C4'	2.75	115.95	109.68
4	A	801	LMT	O5B-C1B-C2B	-2.57	104.92	110.35
4	A	801	LMT	O1B-C4'-C5'	2.38	115.98	109.45
4	A	801	LMT	O3B-C3B-C4B	2.18	115.38	110.35
4	A	801	LMT	O6'-C6'-C5'	-2.16	103.88	111.29
4	A	801	LMT	O1B-C4'-C3'	2.10	112.86	107.28
4	A	801	LMT	C1B-C2B-C3B	-2.10	105.63	110.00
4	A	801	LMT	C1B-O1B-C4'	2.08	123.10	117.96

There are no chirality outliers.

All (62) 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
4	A	801	LMT	O5B-C5B-C6B-O6B
4	A	801	LMT	C4B-C5B-C6B-O6B
6	A	806	PG4	O3-C5-C6-O4
6	A	803	PG4	O3-C5-C6-O4
6	A	806	PG4	O2-C3-C4-O3
6	A	805	PG4	O3-C5-C6-O4
4	A	801	LMT	O5'-C5'-C6'-O6'
6	A	805	PG4	O2-C3-C4-O3
6	A	807	PG4	O3-C5-C6-O4
6	A	808	PG4	O2-C3-C4-O3
4	A	801	LMT	C5-C6-C7-C8
4	A	801	LMT	C4'-C5'-C6'-O6'
4	A	801	LMT	C3-C4-C5-C6
4	A	801	LMT	C5'-C4'-O1B-C1B
5	A	802	OCT	C4-C5-C6-C7
4	A	801	LMT	C9-C10-C11-C12
4	A	801	LMT	C4-C5-C6-C7
4	A	801	LMT	C3'-C4'-O1B-C1B
7	A	811	1PE	OH2-C12-C22-OH3
7	A	811	1PE	OH6-C15-C25-OH5
7	A	804	1PE	OH7-C16-C26-OH6
10	A	812	D10	C3-C4-C5-C6
4	A	801	LMT	C11-C10-C9-C8
6	A	808	PG4	C1-C2-O2-C3
7	A	811	1PE	C13-C23-OH3-C22
6	A	803	PG4	C4-C3-O2-C2
6	A	806	PG4	C6-C5-O3-C4
7	A	811	1PE	C15-C25-OH5-C14
6	A	807	PG4	C3-C4-O3-C5
6	A	806	PG4	C1-C2-O2-C3
6	A	805	PG4	C5-C6-O4-C7
7	A	804	1PE	OH4-C13-C23-OH3
5	A	802	OCT	C3-C4-C5-C6
6	A	807	PG4	O1-C1-C2-O2
6	A	806	PG4	C4-C3-O2-C2
4	A	801	LMT	C1-C2-C3-C4
6	A	808	PG4	C4-C3-O2-C2
8	A	809	D12	C1-C2-C3-C4
7	A	811	1PE	C16-C26-OH6-C15
6	A	806	PG4	O4-C7-C8-O5

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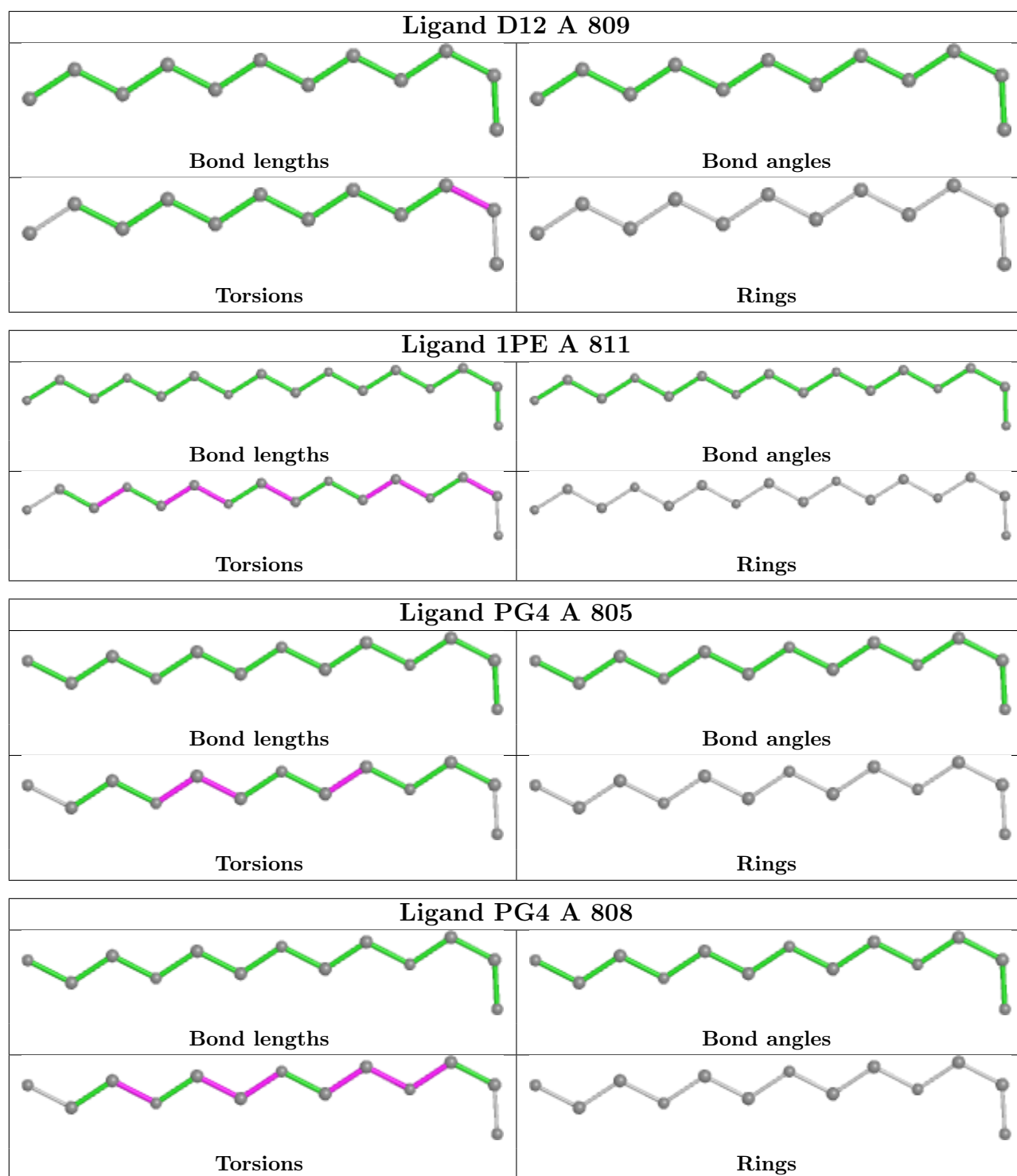
Mol	Chain	Res	Type	Atoms
5	A	802	OCT	C2-C3-C4-C5
6	A	807	PG4	O2-C3-C4-O3
6	A	808	PG4	C8-C7-O4-C6
6	A	806	PG4	C3-C4-O3-C5
6	A	807	PG4	C6-C5-O3-C4
6	A	803	PG4	C1-C2-O2-C3
6	A	808	PG4	C6-C5-O3-C4
6	A	807	PG4	C1-C2-O2-C3
10	A	812	D10	C1-C2-C3-C4
7	A	811	1PE	OH4-C13-C23-OH3
7	A	804	1PE	OH5-C14-C24-OH4
6	A	803	PG4	O2-C3-C4-O3
7	A	811	1PE	OH5-C14-C24-OH4
7	A	804	1PE	C23-C13-OH4-C24
6	A	806	PG4	C5-C6-O4-C7
4	A	801	LMT	C2B-C1B-O1B-C4'
7	A	804	1PE	C25-C15-OH6-C26
6	A	803	PG4	O4-C7-C8-O5
7	A	804	1PE	OH2-C12-C22-OH3
6	A	808	PG4	O3-C5-C6-O4

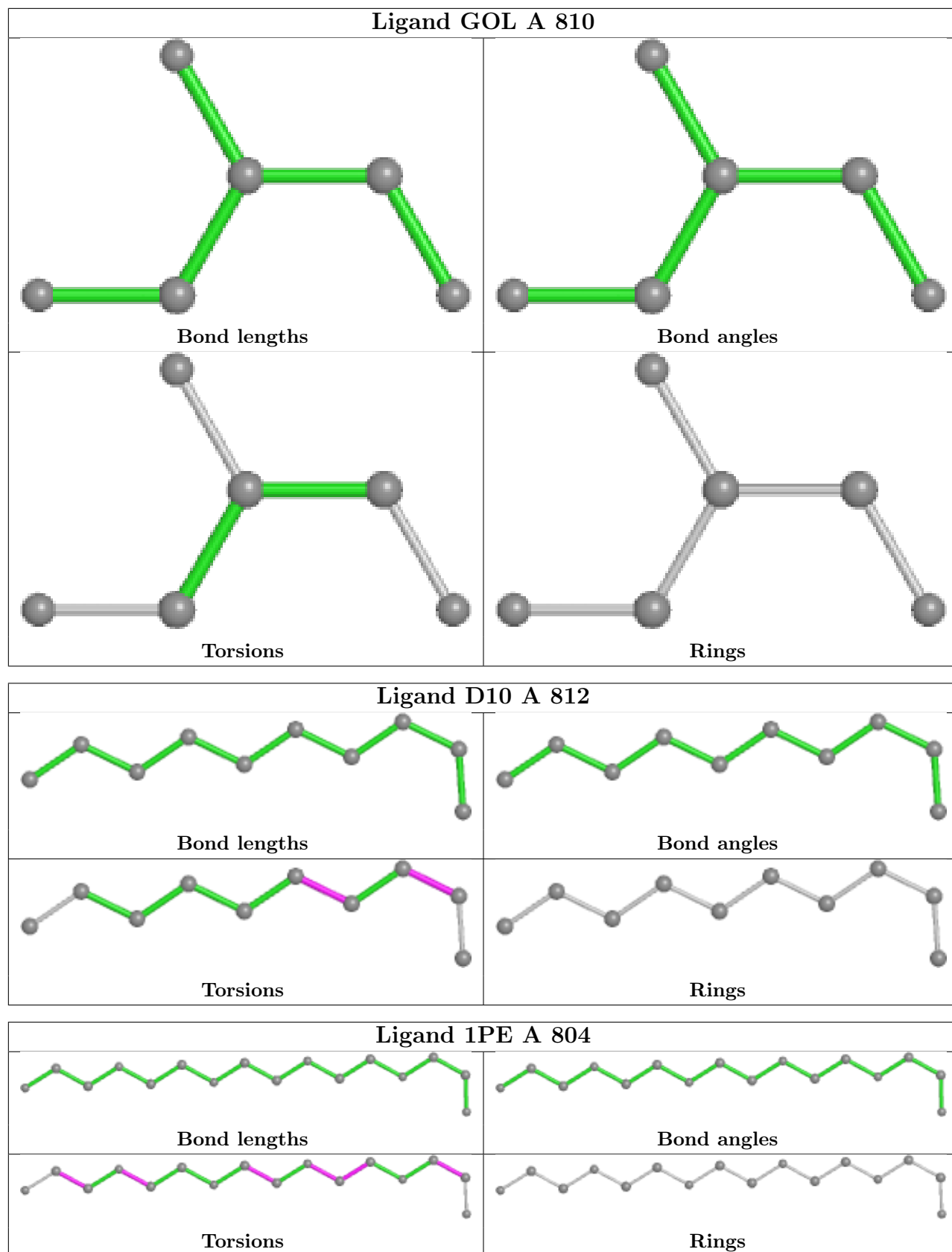
There are no ring outliers.

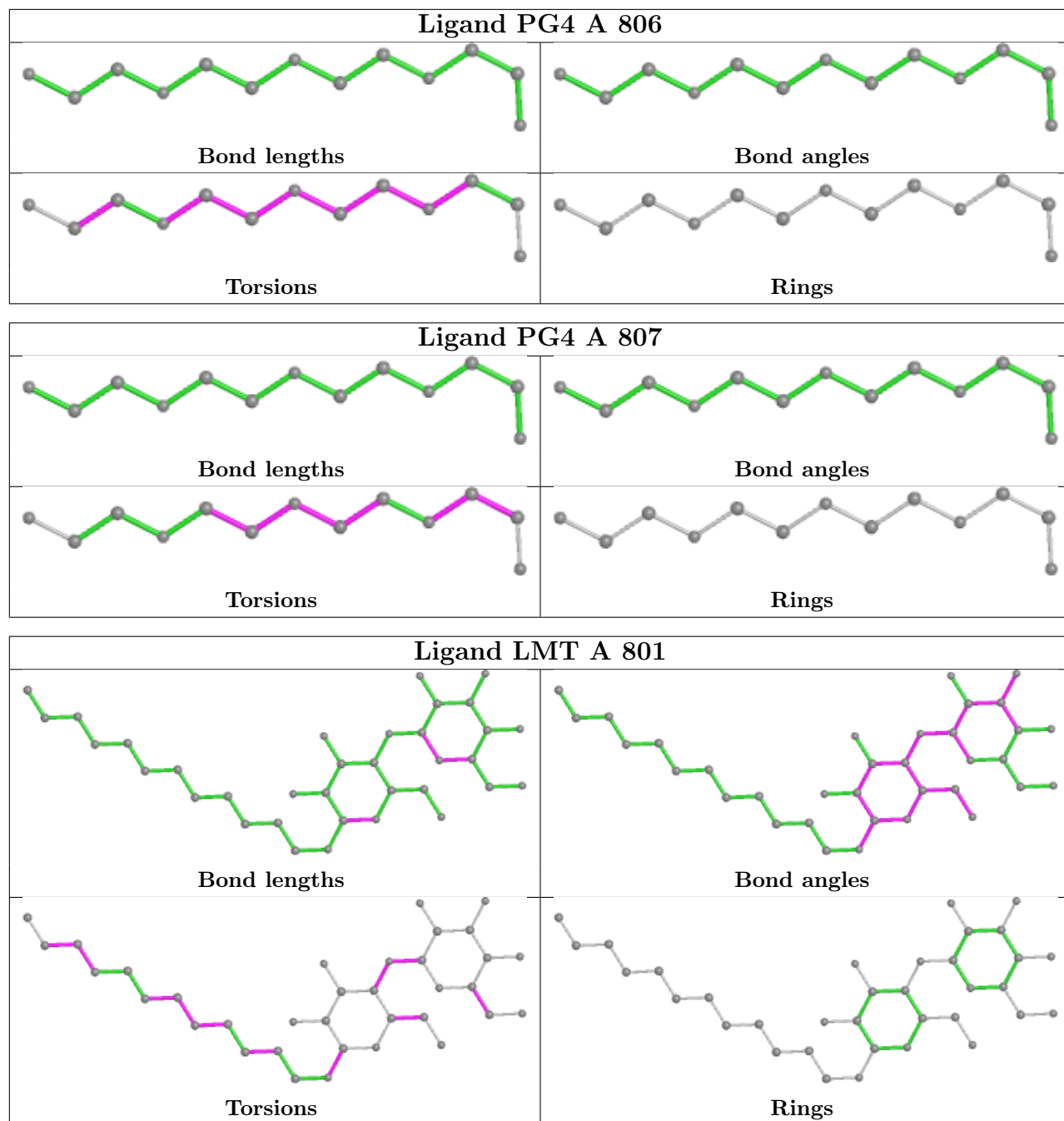
1 monomer is involved in 3 short contacts:

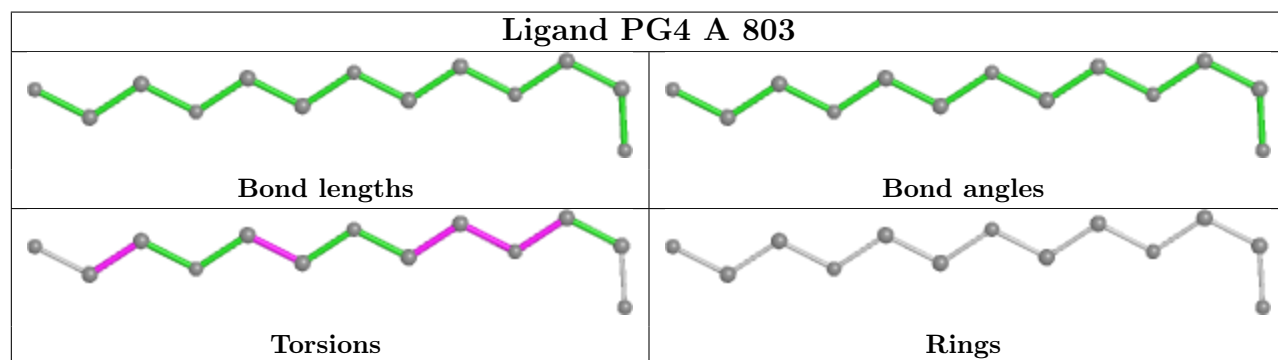
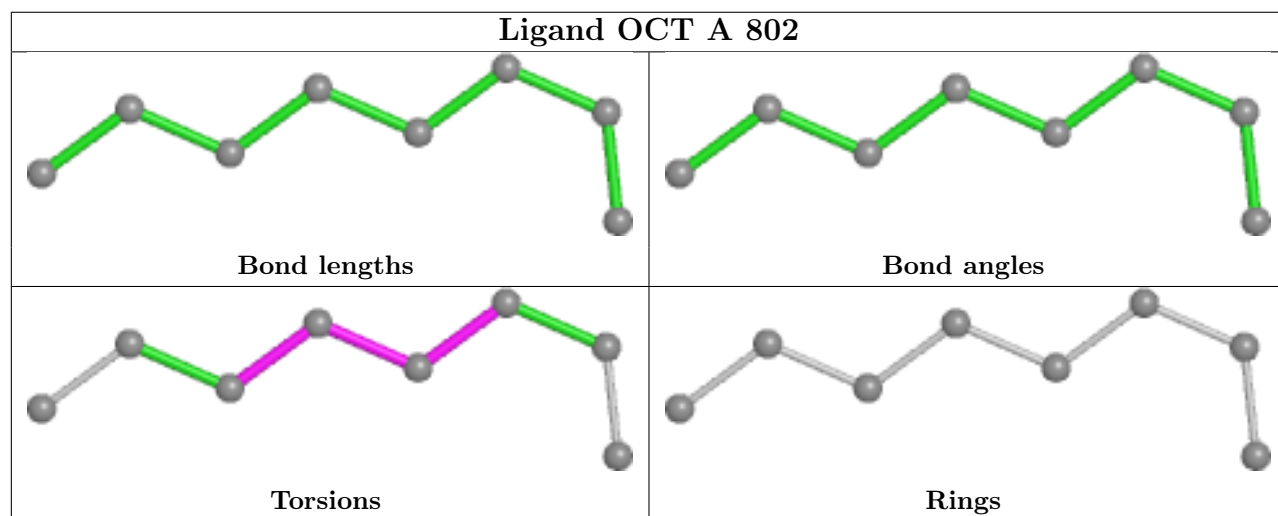
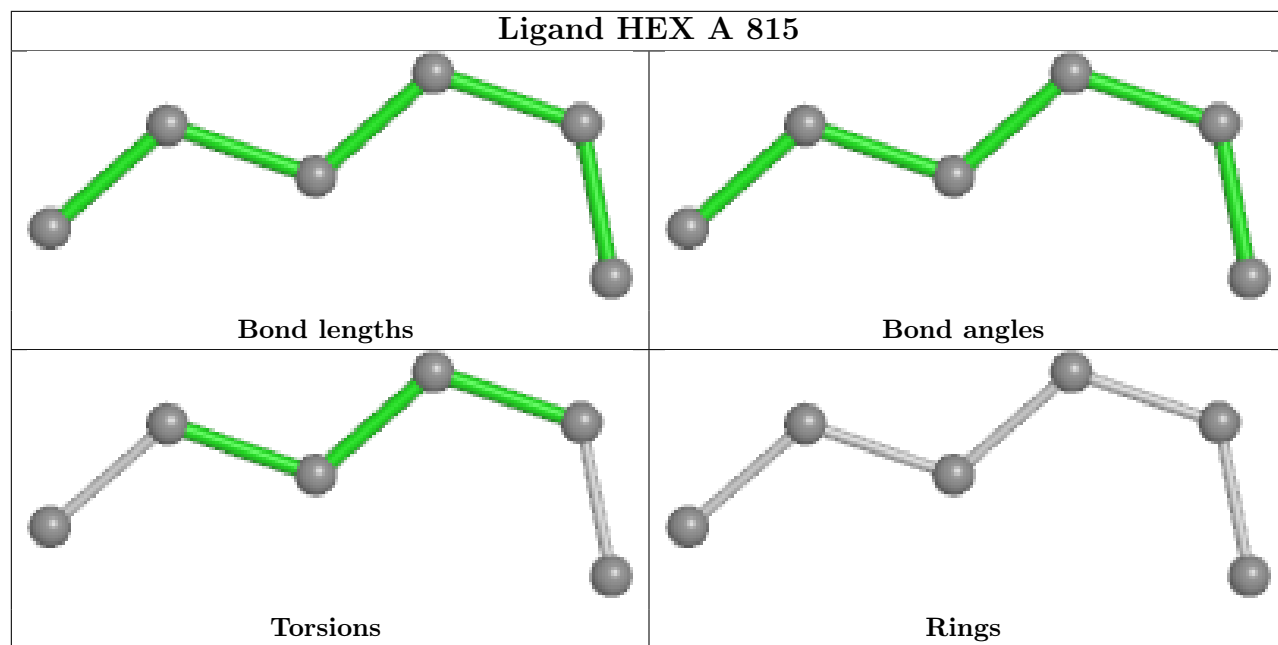
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	LMT	3	0

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.

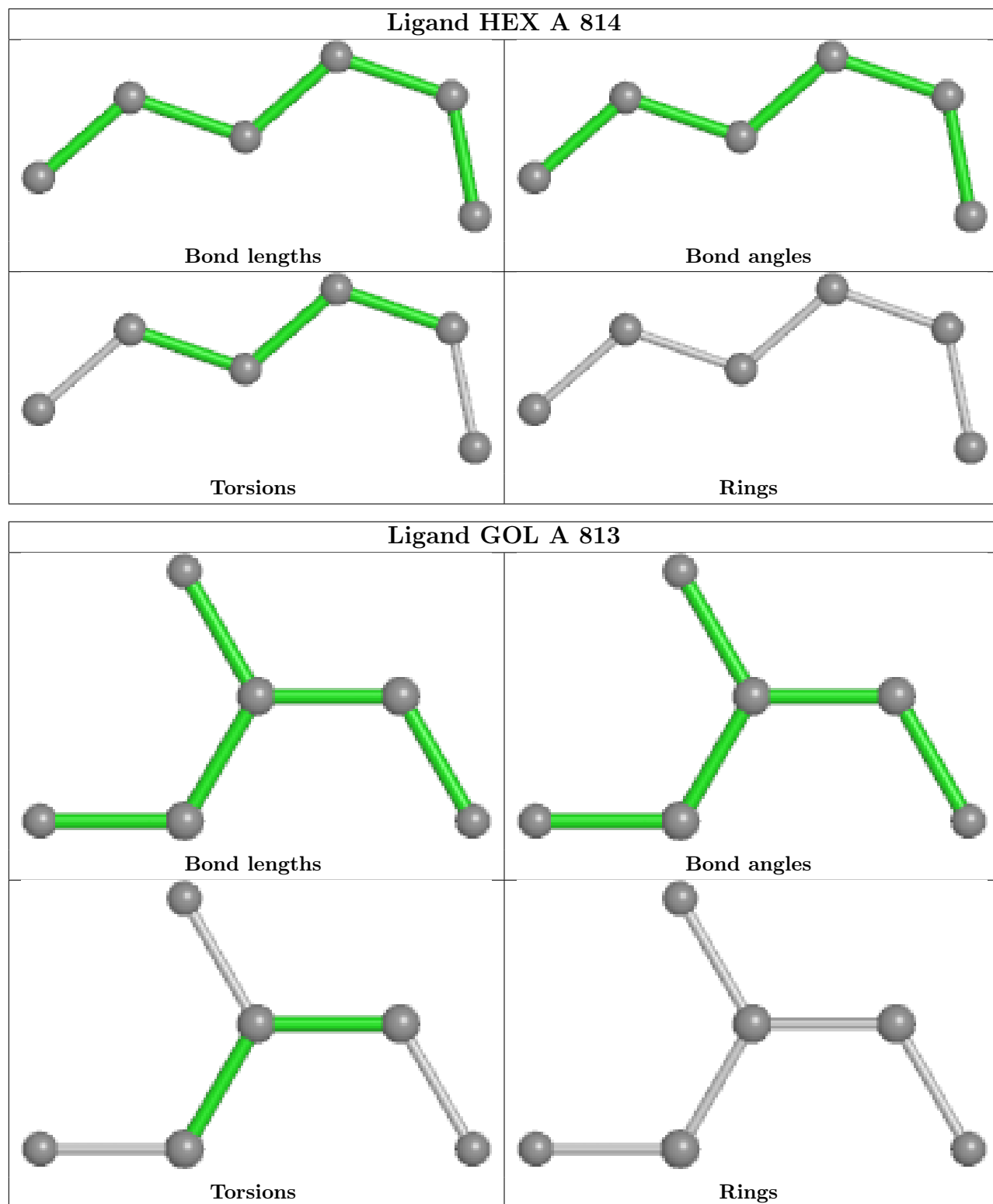












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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%)	1.08	80 (17%) <b>1</b> <b>1</b>	51, 69, 118, 143	1 (0%)
2	B	127/127 (100%)	0.51	4 (3%) 49 52	52, 68, 97, 105	1 (0%)
3	C	3/3 (100%)	-0.00	0 <b>100</b> <b>100</b>	73, 73, 81, 91	0
All	All	581/619 (93%)	0.95	84 (14%) <b>2</b> <b>2</b>	51, 69, 113, 143	2 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	PHE	11.2
1	A	144	ALA	11.0
1	A	17	PHE	9.8
1	A	20	PHE	8.9
1	A	330	ALA	8.4
1	A	329	LEU	8.2
1	A	148	PHE	7.1
1	A	16	PHE	6.8
1	A	15	PRO	6.5
1	A	326	SER	6.3
1	A	18	MET	6.3
1	A	145	PHE	6.3
1	A	305	LEU	6.3
1	A	134	TYR	6.2
1	A	19	ILE	6.1
1	A	21	PHE	6.1
1	A	147	LEU	5.9
1	A	198	LYS	5.9
2	B	79	TYR	5.8
1	A	240	LEU	5.7
1	A	327	PRO	5.6
1	A	332	ILE	5.3
1	A	399	LEU	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	200	ILE	5.2
1	A	143	GLY	5.2
1	A	139	PRO	5.2
1	A	146	THR	4.9
1	A	191	ILE	4.9
1	A	197	VAL	4.9
1	A	236	GLU	4.7
1	A	253	PHE	4.6
1	A	196	MET	4.5
1	A	189	VAL	4.5
1	A	14	ARG	4.3
1	A	130	LEU	4.1
1	A	141	LEU	4.1
1	A	401	LEU	4.0
1	A	12	GLN	4.0
1	A	133	CYS	3.8
1	A	192	ALA	3.8
1	A	304	ILE	3.7
2	B	77	THR	3.6
1	A	237	VAL	3.6
1	A	22	VAL	3.6
1	A	140	ARG	3.6
1	A	142	ASP	3.5
1	A	235	VAL	3.5
1	A	194	ARG	3.4
1	A	151	SER	3.4
1	A	150	MET	3.4
1	A	23	GLU	3.3
1	A	433	TYR	3.2
1	A	190	TYR	3.2
1	A	331	GLY	3.2
1	A	254	PHE	3.0
1	A	328	ILE	3.0
2	B	67	PHE	2.8
1	A	403	MET	2.7
1	A	246	SER	2.7
1	A	437	PHE	2.6
1	A	13	PRO	2.6
1	A	268	MET	2.6
1	A	193	CYS	2.6
1	A	479	LEU	2.6
1	A	239	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	478	TRP	2.4
1	A	436	THR	2.4
1	A	269	PHE	2.4
1	A	251	ILE	2.3
1	A	325	ALA	2.3
1	A	408	VAL	2.3
1	A	84	ILE	2.3
1	A	211	PHE	2.3
1	A	309	ILE	2.2
1	A	50	GLU	2.2
2	B	75	LYS	2.1
1	A	80	THR	2.1
1	A	416	ILE	2.1
1	A	266	ASN	2.1
1	A	484	ALA	2.0
1	A	370	PHE	2.0
1	A	149	TYR	2.0
1	A	122	PHE	2.0
1	A	395	PHE	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.

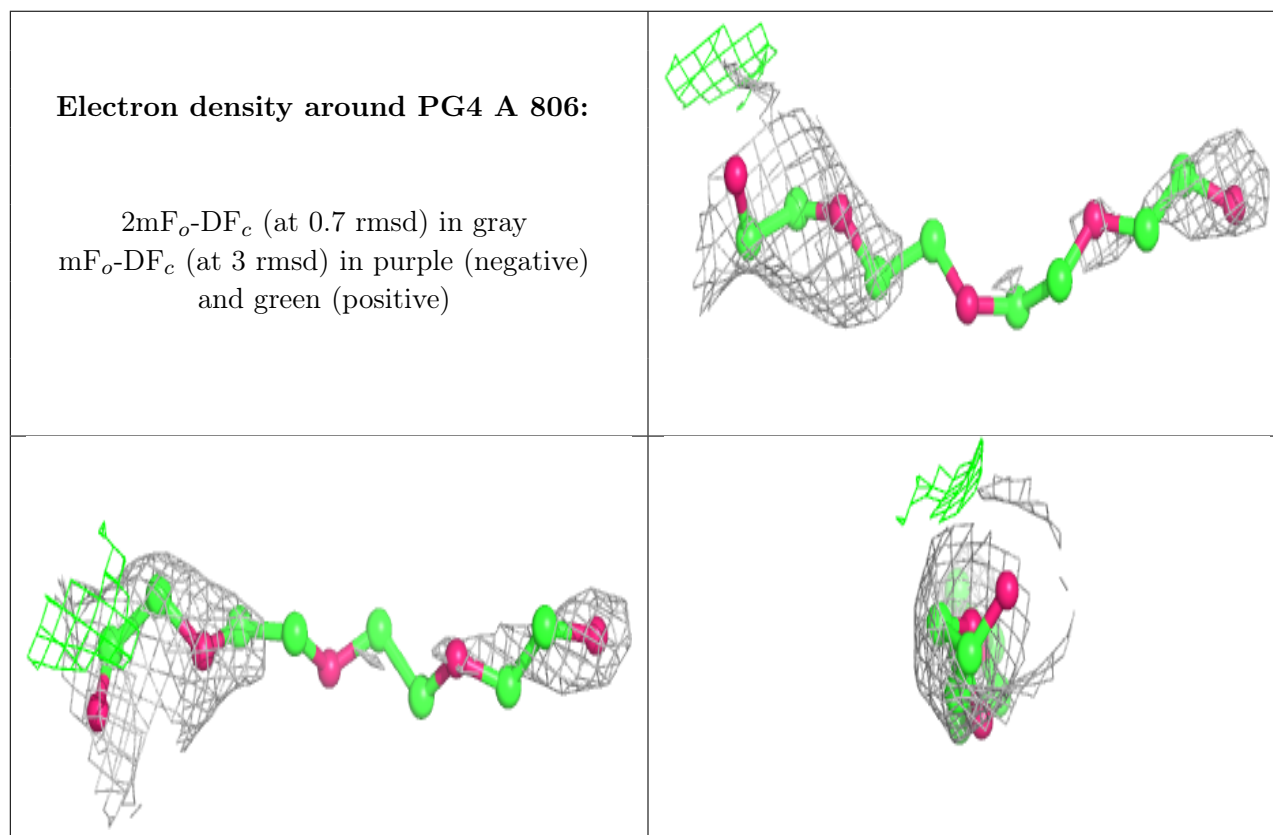
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	PG4	A	806	13/13	0.36	0.64	82,100,118,119	0
10	D10	A	812	10/10	0.43	0.31	79,84,90,92	0
9	GOL	A	810	6/6	0.51	0.20	120,121,127,127	0
6	PG4	A	805	13/13	0.51	0.39	77,94,113,113	0

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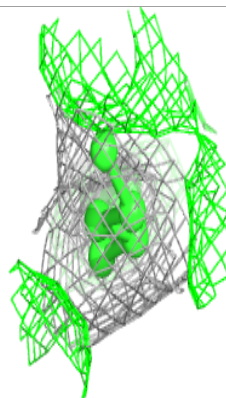
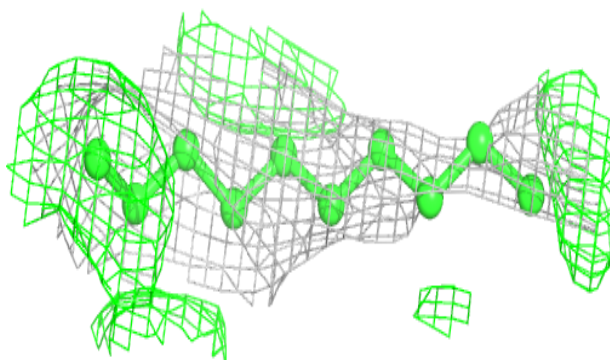
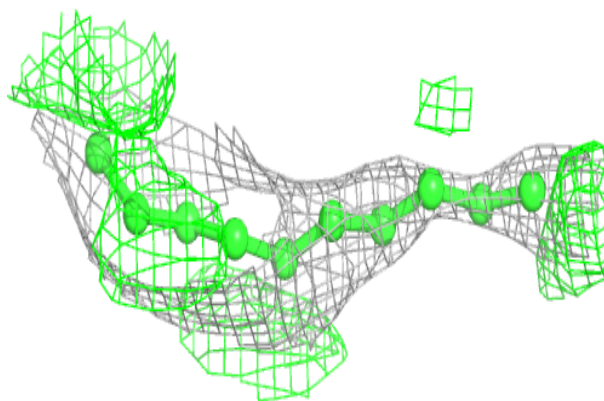
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	1PE	A	811	16/16	0.58	0.56	97,101,105,110	0
9	GOL	A	813	6/6	0.64	0.18	87,89,92,92	0
8	D12	A	809	12/12	0.68	0.68	84,92,104,105	0
5	OCT	A	802	8/8	0.71	0.28	73,76,79,80	0
6	PG4	A	808	13/13	0.74	0.30	81,89,97,100	0
11	HEX	A	814	6/6	0.74	0.52	85,86,87,91	0
6	PG4	A	807	13/13	0.75	0.23	77,87,103,110	0
4	LMT	A	801	35/35	0.80	0.39	68,86,100,102	0
7	1PE	A	804	16/16	0.81	0.54	71,84,109,111	0
6	PG4	A	803	13/13	0.82	0.24	78,85,110,110	0
11	HEX	A	815	6/6	0.82	0.46	77,88,94,96	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.

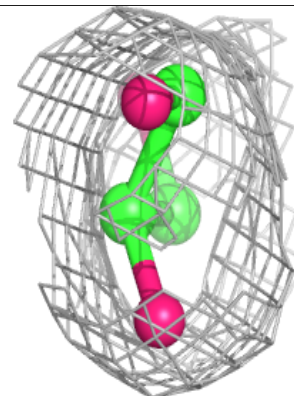
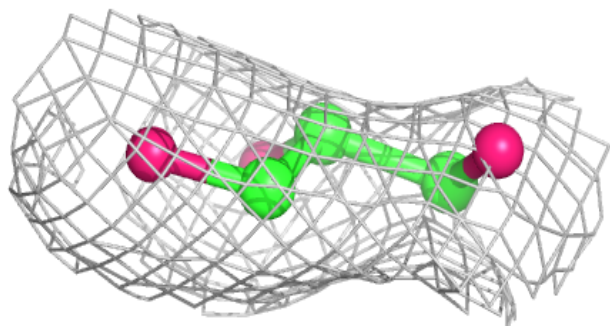
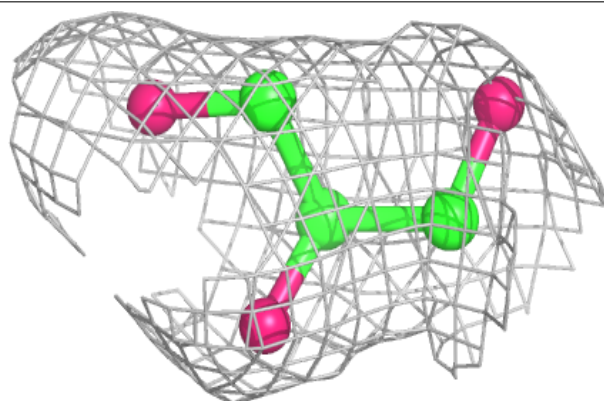


**Electron density around D10 A 812:**

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

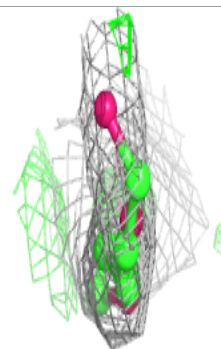
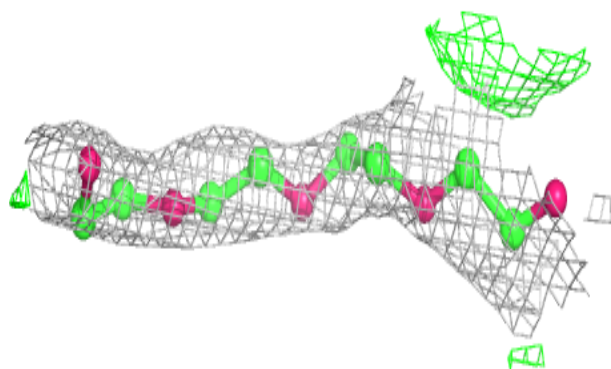
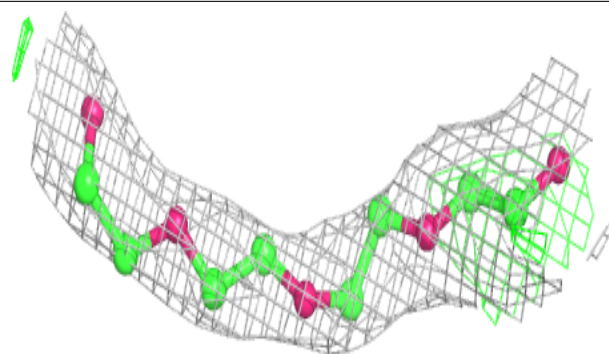
**Electron density around GOL A 810:**

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

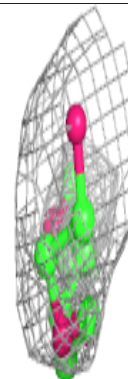
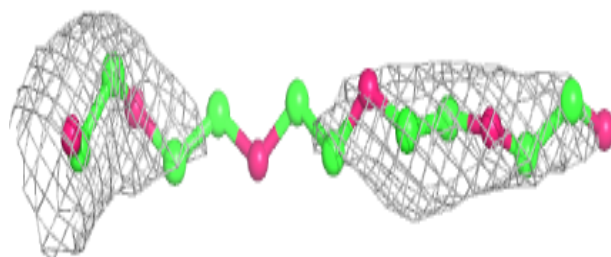
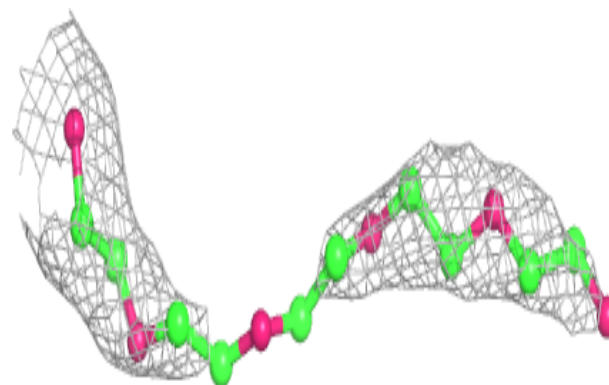


**Electron density around PG4 A 805:**

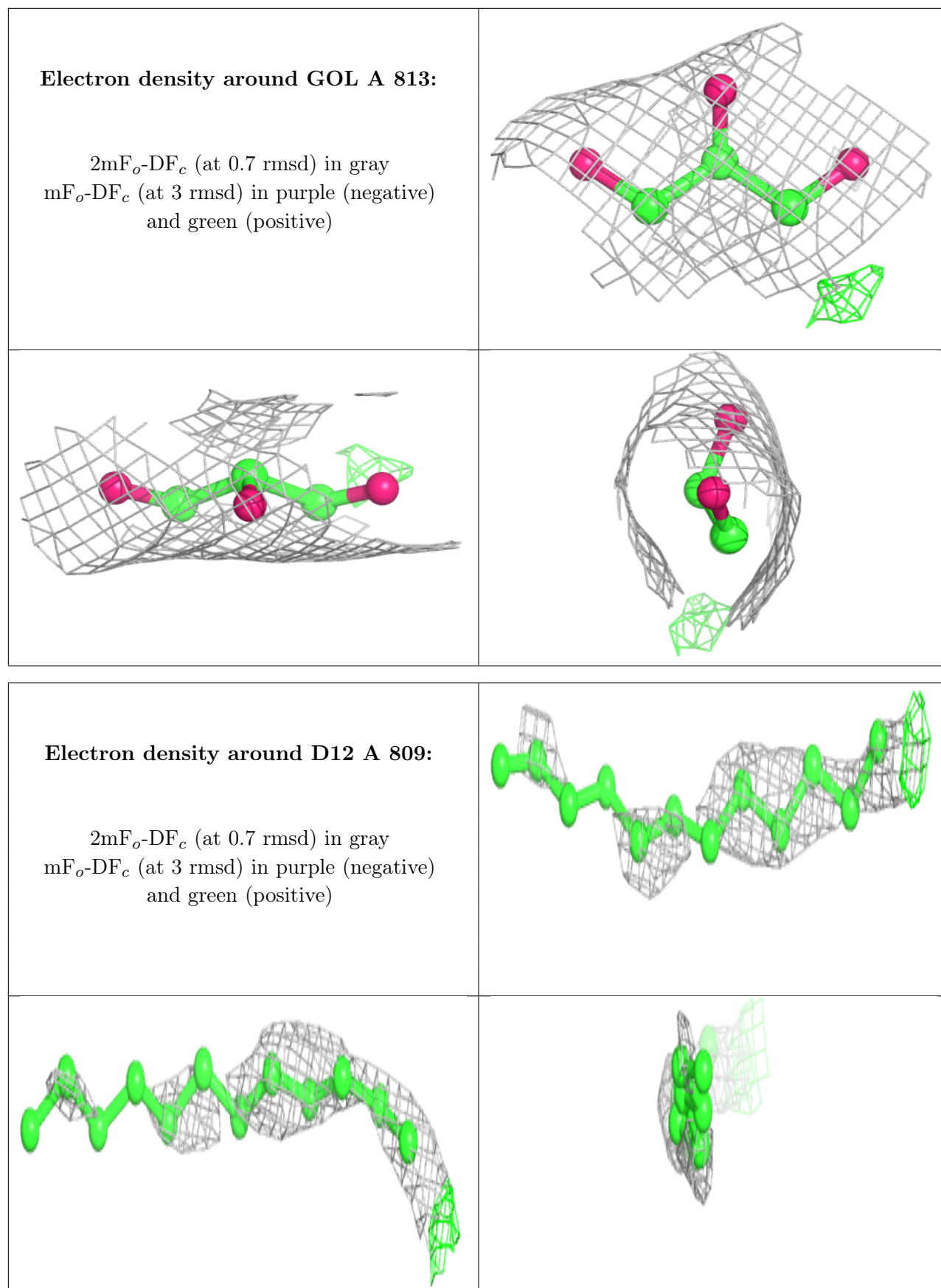
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

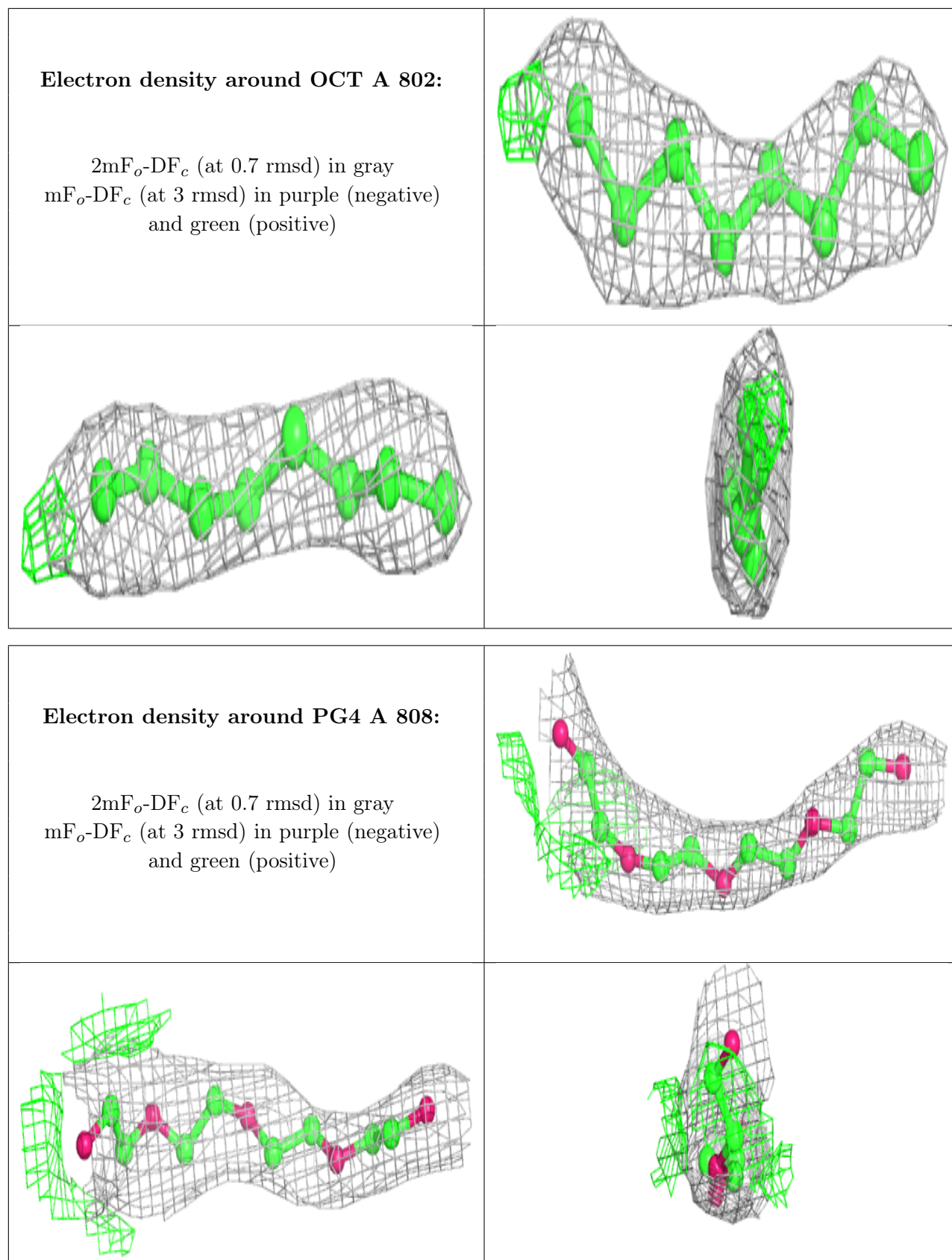
**Electron density around 1PE A 811:**

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



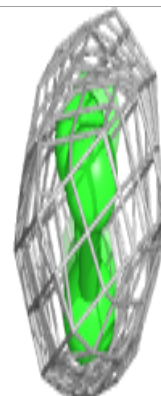
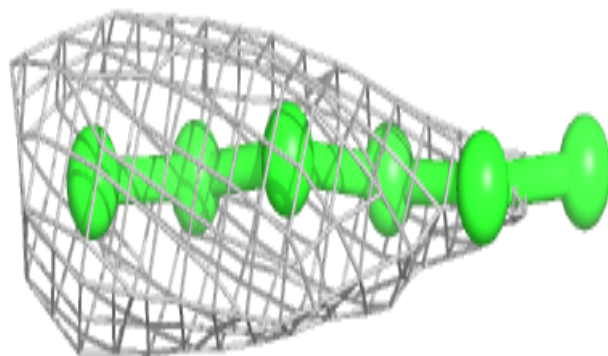
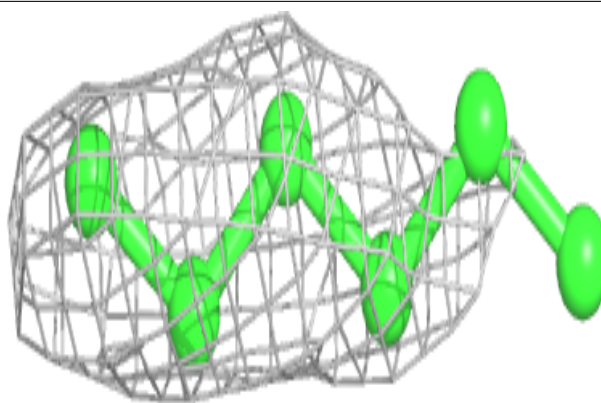




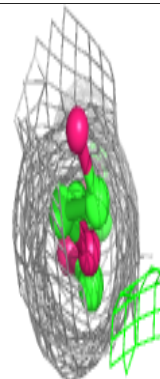
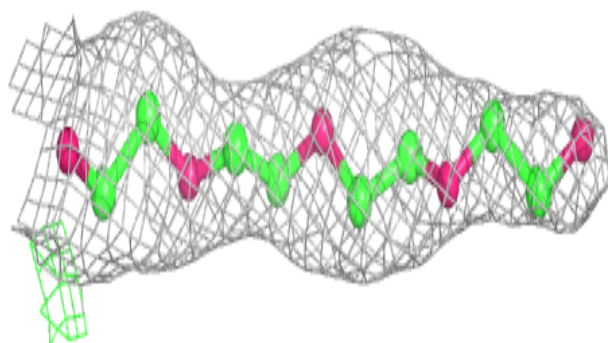
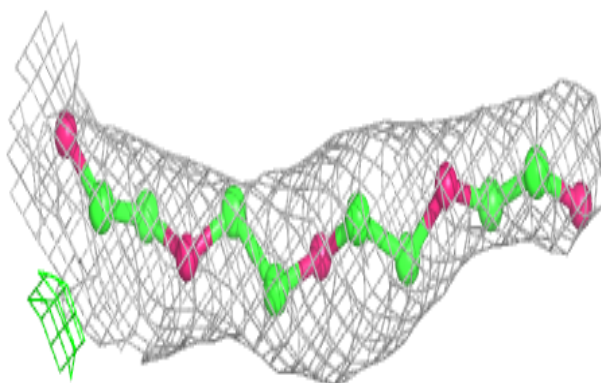


**Electron density around HEX A 814:**

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

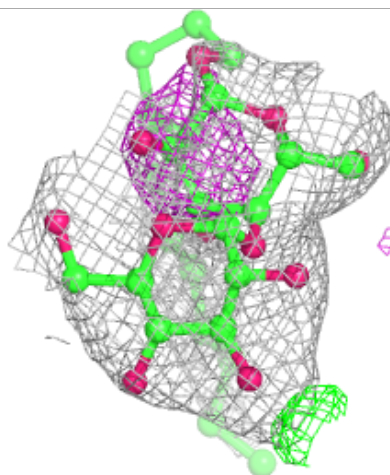
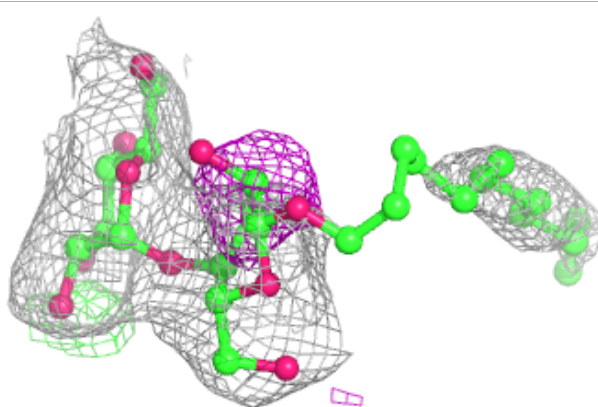
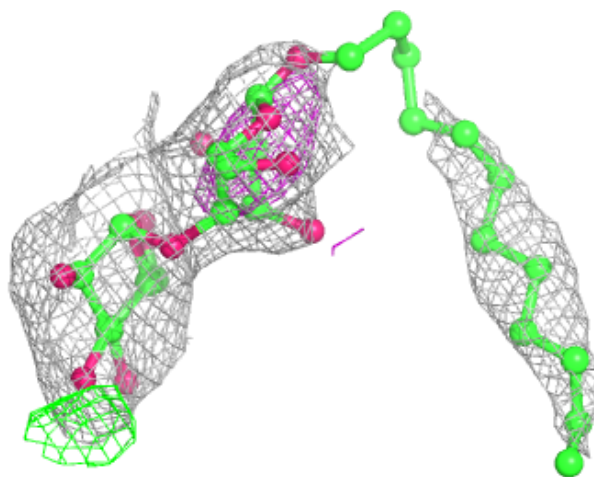
**Electron density around PG4 A 807:**

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



**Electron density around LMT A 801:**

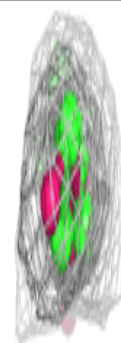
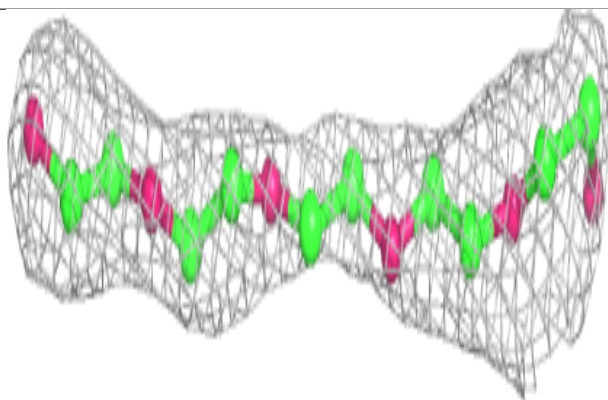
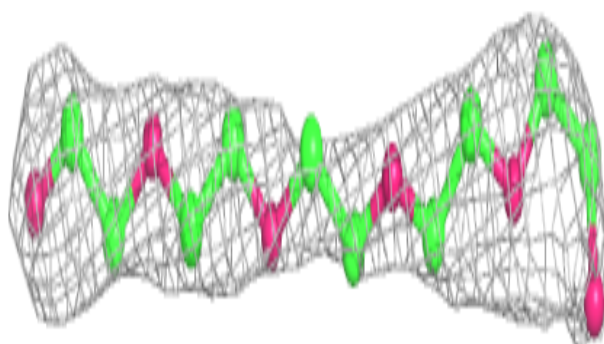
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



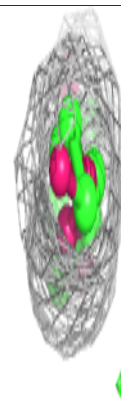
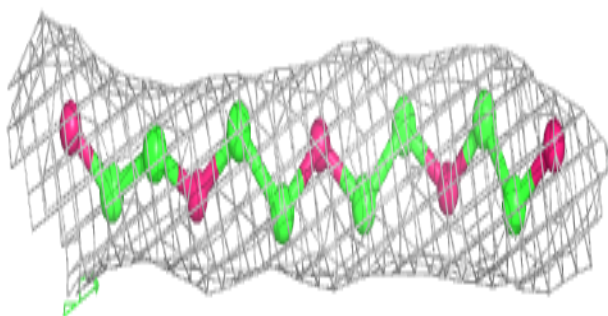
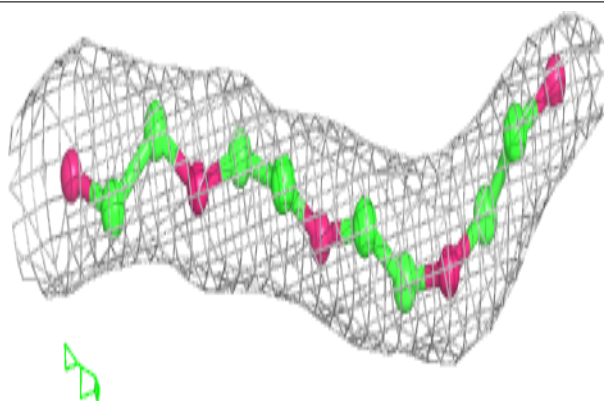


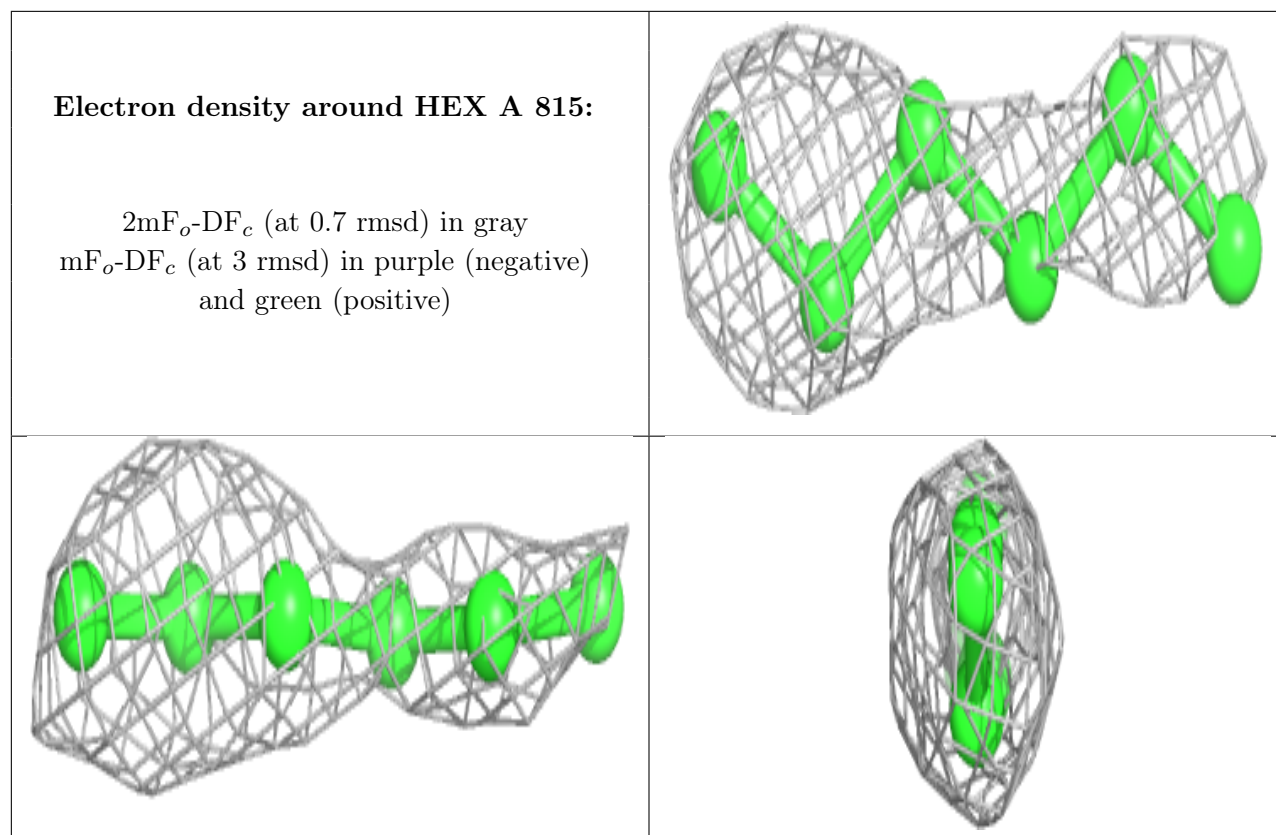
**Electron density around 1PE A 804:**

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

**Electron density around PG4 A 803:**

$2mF_o-DF_c$  (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.