Full wwPDB X-ray Structure Validation Report ⓘ

Jul 31, 2023 – 04:19 pm BST

PDB ID	:	8B1C
Title	:	DtpB-Nb132-ALA
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Deposited on	:	2022-09-09
Resolution	:	2.56 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

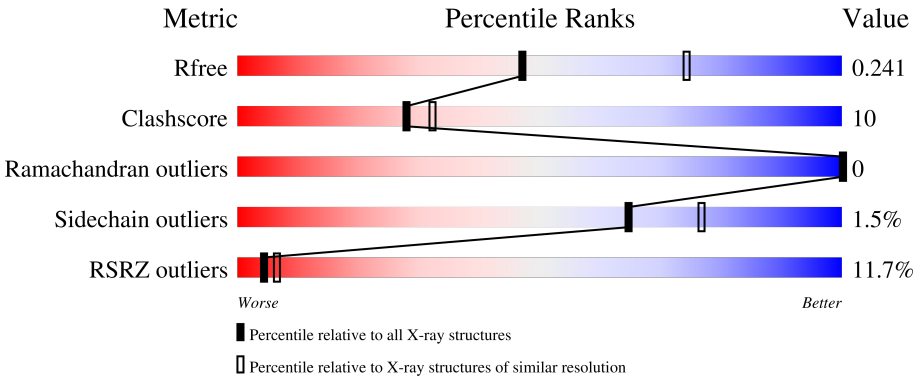
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	12% 74% 18% · 8%
2	B	127	7% 82% 17% ·
3	C	3	33% 67%

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
11	HEX	A	815	-	-	-	X
5	OCT	A	802	-	-	-	X
6	PG4	A	805	-	-	-	X
6	PG4	A	806	-	-	-	X
7	1PE	A	804	-	-	-	X
7	1PE	A	811	-	-	-	X
8	D12	A	809	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4781 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
1	A	451	Total	C	N	O	S	4	0	0
			3480	2349	531	573	27			

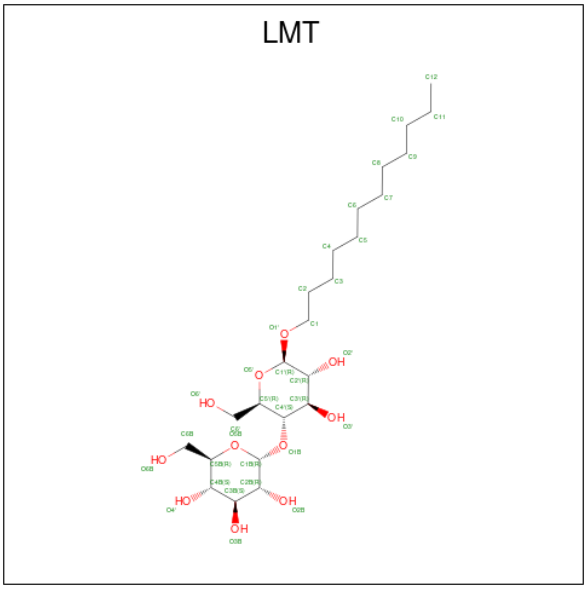
- Molecule 2 is a protein called Nanobody 132.

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

- Molecule 3 is a protein called ALA-LEU-ALA.

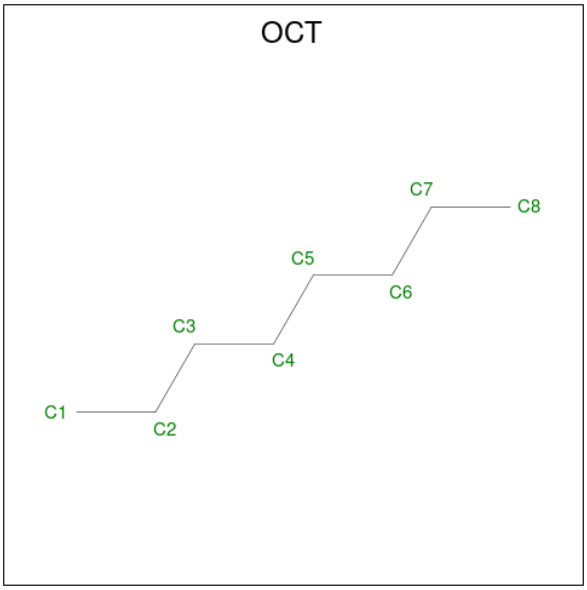
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			19	12	3	4			

- Molecule 4 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



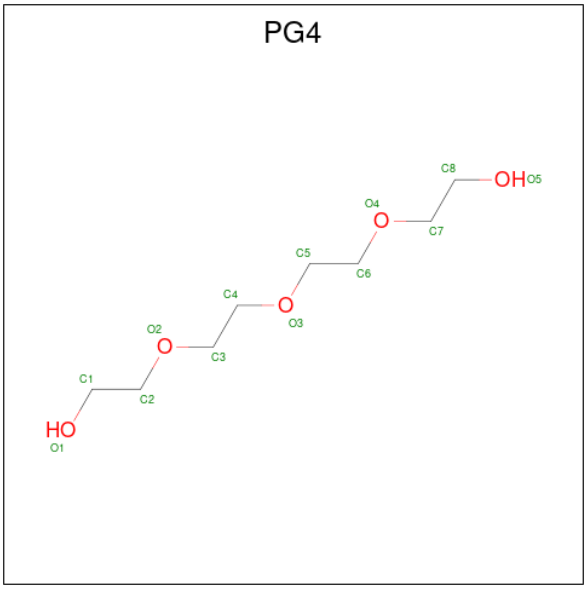
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0

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



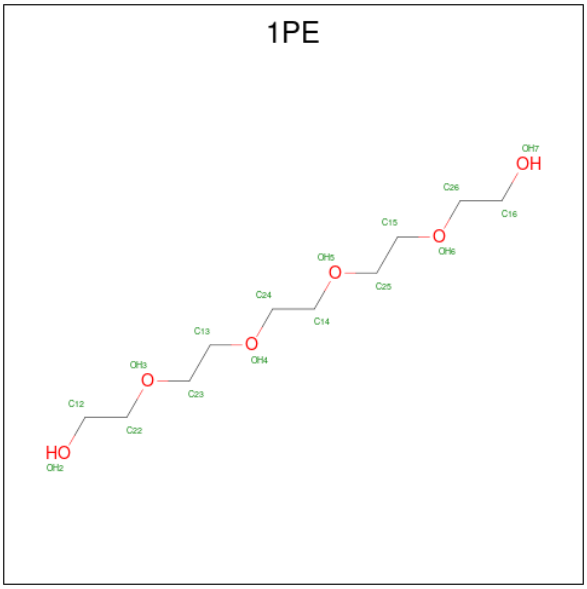
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C 8 8	0	0

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



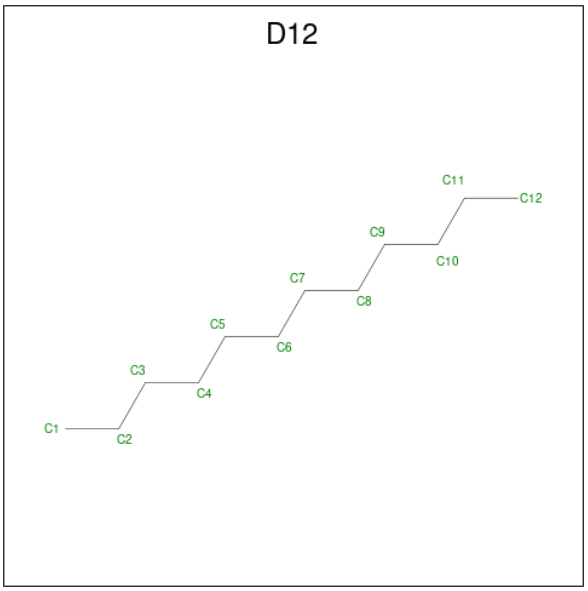
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0
6	A	1	Total C O 13 8 5	0	0

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



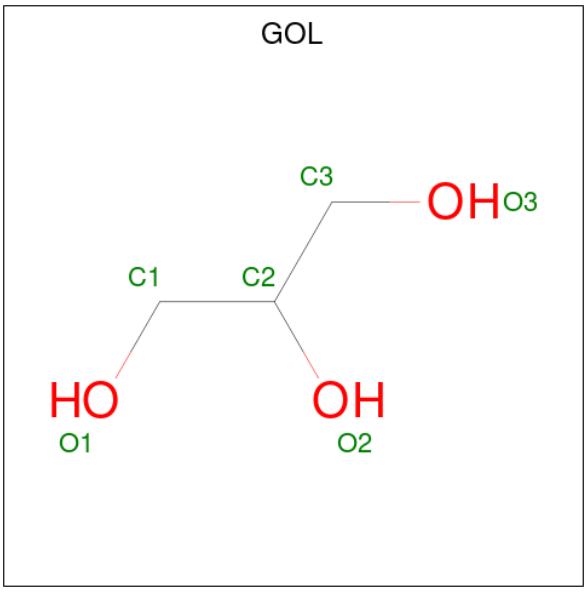
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 16 10 6	0	0
7	A	1	Total C O 16 10 6	0	0

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



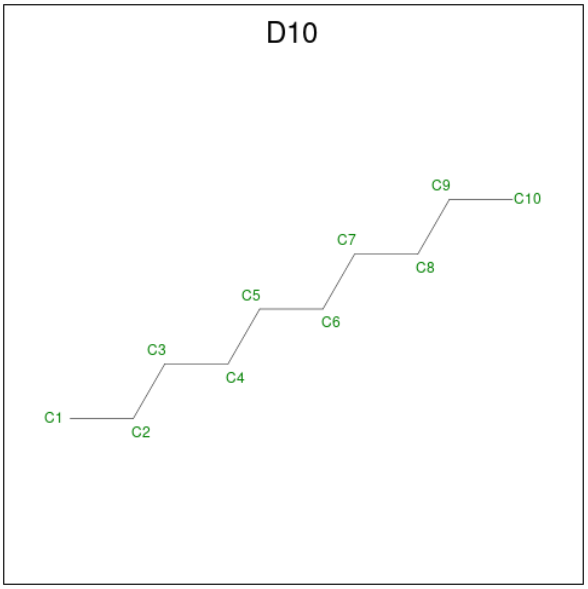
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C 12 12	0	0

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



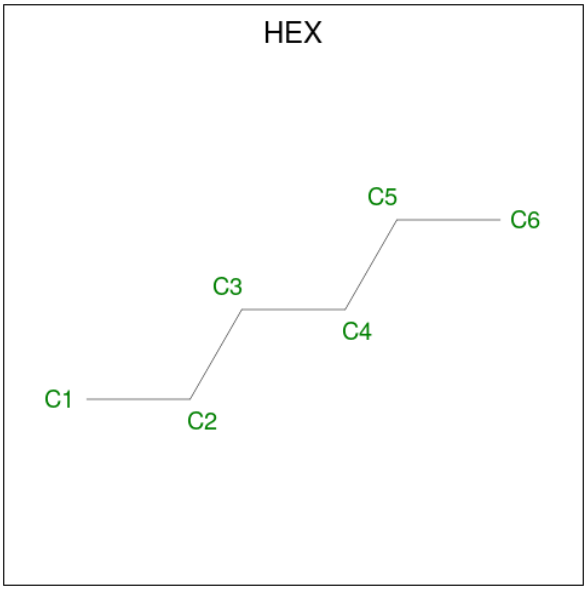
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C O 6 3 3	0	0
9	A	1	Total C O 6 3 3	0	0

- 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

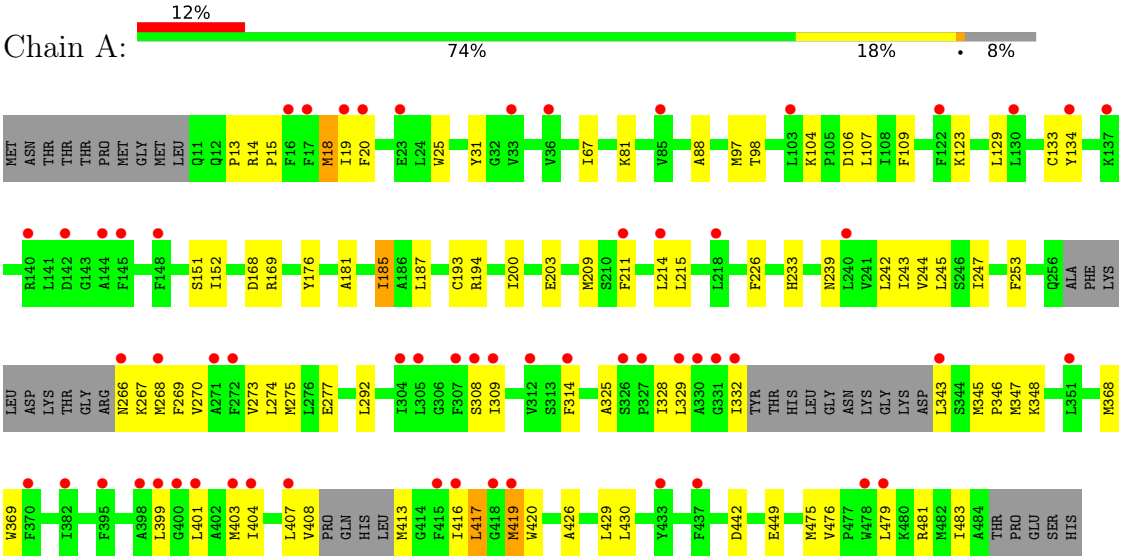
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	67	Total O 67 67	0	0
12	B	52	Total O 52 52	0	0
12	C	1	Total O 1 1	0	0

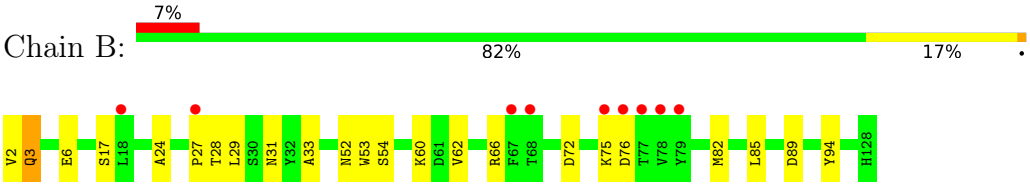
3 Residue-property plots (i)

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-LEU-ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.40Å 123.54Å 169.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.79 – 2.56 99.80 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.79-2.56) 93.0 (99.80-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.215 , 0.241 0.215 , 0.241	Depositor DCC
R_{free} test set	1892 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4781	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, 1PE, HEX, OCT, D10, LMT, PG4, D12

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	0.54	0/3572	0.77	1/4859 (0.0%)
2	B	0.49	0/1004	0.73	0/1361
3	C	0.38	0/18	0.43	0/22
All	All	0.53	0/4594	0.76	1/6242 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	417	LEU	CA-CB-CG	8.07	133.86	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	82	0
2	B	976	0	939	13	0
3	C	19	0	23	2	0
4	A	35	0	46	5	0
5	A	8	0	18	0	0
6	A	65	0	90	1	0
7	A	32	0	44	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	12	0	26	0	0
9	A	12	0	16	0	0
10	A	10	0	22	2	0
11	A	12	0	28	0	0
12	A	67	0	0	5	0
12	B	52	0	0	0	0
12	C	1	0	0	0	0
All	All	4781	0	4857	94	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 10.

All (94) 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:194:ARG:NH1	12:A:902:HOH:O	2.02	0.91
1:A:25:TRP:CE2	1:A:185:ILE:HD11	2.15	0.81
1:A:203:GLU:OE1	12:A:901:HOH:O	2.00	0.80
1:A:348:LYS:HD3	1:A:399:LEU:HD21	1.66	0.76
1:A:292:LEU:HB3	12:A:921:HOH:O	1.84	0.75
2:B:66:ARG:NH2	2:B:89:ASP:OD2	2.18	0.70
1:A:18:MET:HG3	1:A:193:CYS:HB2	1.73	0.70
1:A:169:ARG:HH22	4:A:801:LMT:H1'	1.56	0.70
1:A:104:LYS:NZ	12:A:907:HOH:O	2.27	0.67
1:A:346:PRO:HB2	1:A:476:VAL:HG13	1.78	0.66
2:B:60:LYS:HD3	2:B:62:VAL:HG12	1.78	0.65
1:A:346:PRO:HG3	1:A:479:LEU:HD22	1.77	0.64
1:A:267:LYS:HD3	1:A:407:LEU:HD23	1.79	0.63
1:A:181:ALA:O	1:A:185:ILE:HG23	1.99	0.62
1:A:481:ARG:HG3	1:A:481:ARG:HH11	1.63	0.62
1:A:401:LEU:HD22	1:A:420:TRP:CG	2.36	0.61
1:A:270:VAL:HG13	1:A:479:LEU:HD21	1.83	0.60
1:A:253:PHE:CZ	1:A:268:MET:HB3	2.36	0.60
1:A:408:VAL:HG21	1:A:416:ILE:HG12	1.84	0.60
2:B:2:VAL:N	2:B:27:PRO:HG2	2.17	0.59
1:A:242:LEU:HD22	1:A:429:LEU:HD22	1.84	0.58
1:A:104:LYS:HB3	10:A:812:D10:H42	1.85	0.58
1:A:273:VAL:HG21	1:A:475:MET:HE1	1.86	0.58
1:A:401:LEU:HD12	1:A:404:ILE:HB	1.86	0.58
1:A:401:LEU:HD22	1:A:420:TRP:CD1	2.39	0.58
1:A:18:MET:CE	1:A:19:ILE:HG13	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:CD1	1:A:123:LYS:HD2	2.36	0.56
1:A:343:LEU:HA	1:A:347:MET:HB3	1.86	0.56
1:A:129:LEU:HD11	1:A:200:ILE:HG22	1.90	0.54
1:A:25:TRP:CD2	1:A:185:ILE:HD11	2.43	0.54
1:A:169:ARG:NH2	4:A:801:LMT:H1'	2.23	0.53
1:A:346:PRO:CG	1:A:479:LEU:HD22	2.39	0.53
1:A:328:ILE:O	1:A:332:ILE:HD12	2.09	0.53
1:A:430:LEU:HG	7:A:811:1PE:H251	1.91	0.52
2:B:6:GLU:OE1	2:B:94:TYR:HA	2.09	0.52
1:A:368:MET:HE2	1:A:369:TRP:CE2	2.44	0.52
1:A:168:ASP:OD1	2:B:31:ASN:ND2	2.35	0.52
1:A:347:MET:HE2	1:A:476:VAL:HG21	1.93	0.51
1:A:442:ASP:HB3	2:B:54:SER:OG	2.10	0.51
1:A:273:VAL:O	1:A:277:GLU:HG3	2.10	0.51
1:A:408:VAL:HG11	1:A:416:ILE:HG12	1.92	0.51
1:A:25:TRP:CZ2	1:A:185:ILE:HD11	2.46	0.50
1:A:88:ALA:HB3	1:A:187:LEU:HD13	1.94	0.50
1:A:274:LEU:HB2	1:A:404:ILE:HD11	1.93	0.50
1:A:18:MET:HG3	1:A:193:CYS:CB	2.42	0.49
1:A:81:LYS:HE2	1:A:200:ILE:O	2.11	0.49
1:A:168:ASP:O	2:B:28:THR:HG22	2.11	0.49
1:A:266:ASN:HA	1:A:269:PHE:CD1	2.48	0.49
1:A:13:PRO:HD2	1:A:134:TYR:CE2	2.47	0.49
1:A:106:ASP:HB2	10:A:812:D10:H41	1.94	0.48
1:A:346:PRO:HG3	1:A:479:LEU:CD2	2.43	0.48
2:B:17:SER:HA	2:B:82:MET:O	2.13	0.48
1:A:109:PHE:CE2	1:A:233:HIS:HD2	2.31	0.48
1:A:211:PHE:O	1:A:215:LEU:HD23	2.13	0.48
1:A:479:LEU:O	1:A:483:ILE:HD12	2.14	0.48
1:A:18:MET:HE2	1:A:19:ILE:HG13	1.97	0.47
1:A:97:MET:CE	1:A:107:LEU:HD11	2.45	0.47
1:A:404:ILE:HG22	1:A:416:ILE:HD13	1.96	0.47
1:A:244:VAL:O	1:A:247:ILE:HG12	2.15	0.46
1:A:20:PHE:CE2	1:A:151:SER:HB2	2.50	0.46
1:A:309:ILE:HD11	1:A:314:PHE:CZ	2.51	0.46
2:B:24:ALA:HB2	2:B:29:LEU:HD13	1.98	0.46
2:B:72:ASP:OD2	2:B:75:LYS:HG3	2.15	0.46
1:A:14:ARG:N	1:A:15:PRO:HD2	2.30	0.46
1:A:239:ASN:O	1:A:243:ILE:HG13	2.17	0.45
1:A:270:VAL:HA	1:A:273:VAL:HG12	1.98	0.45
1:A:325:ALA:O	1:A:329:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLN:HA	2:B:3:GLN:OE1	2.17	0.45
4:A:801:LMT:H41	4:A:801:LMT:H12	1.47	0.45
1:A:347:MET:HE2	1:A:476:VAL:HG11	1.99	0.45
1:A:481:ARG:HG3	1:A:481:ARG:NH1	2.30	0.44
1:A:449:GLU:OE2	12:A:903:HOH:O	2.21	0.44
1:A:98:THR:HG22	1:A:176:TYR:CD2	2.52	0.44
1:A:200:ILE:HD13	1:A:200:ILE:HA	1.64	0.44
1:A:266:ASN:HA	1:A:269:PHE:CE1	2.53	0.44
1:A:475:MET:HB3	1:A:475:MET:HE3	1.61	0.44
1:A:209:MET:SD	1:A:214:LEU:HD22	2.57	0.44
1:A:242:LEU:HD23	1:A:426:ALA:HA	2.00	0.43
1:A:413:MET:O	1:A:416:ILE:HG13	2.18	0.43
1:A:308:SER:O	4:A:801:LMT:H4'	2.19	0.42
1:A:343:LEU:HA	1:A:347:MET:CB	2.49	0.42
1:A:185:ILE:HD13	1:A:185:ILE:HG21	1.74	0.42
2:B:33:ALA:HA	2:B:52:ASN:HA	2.02	0.42
2:B:82:MET:HE2	2:B:85:LEU:HD21	2.02	0.42
1:A:152:ILE:HD13	3:C:3:ALA:HA	2.02	0.41
1:A:345:MET:CE	1:A:403:MET:HB3	2.50	0.41
4:A:801:LMT:H41	4:A:801:LMT:H2'	2.02	0.41
1:A:67:ILE:HD13	1:A:123:LYS:HD2	2.03	0.41
1:A:15:PRO:HB2	1:A:133:CYS:SG	2.61	0.41
1:A:267:LYS:O	1:A:407:LEU:HB3	2.20	0.41
1:A:275:MET:HE1	1:A:419:MET:HG2	2.03	0.41
1:A:31:TYR:CZ	3:C:1:ALA:HB1	2.56	0.41
1:A:226:PHE:CE2	6:A:806:PG4:H41	2.55	0.41
1:A:401:LEU:HD21	1:A:417:LEU:HD23	2.03	0.40

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%)	364 (99%)	4 (1%)	73	83
2	B	102/101 (101%)	99 (97%)	3 (3%)	42	55
3	C	1/1 (100%)	1 (100%)	0	100	100
All	All	471/503 (94%)	464 (98%)	7 (2%)	65	77

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

Mol	Chain	Res	Type
1	A	18	MET
1	A	185	ILE
1	A	245	LEU
1	A	419	MET
2	B	3	GLN
2	B	53	TRP
2	B	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	233	HIS
1	A	389	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
11	HEX	A	815	-	5,5,5	0.46	0	4,4,4	0.41	0
10	D10	A	812	-	9,9,9	0.38	0	8,8,8	0.61	0
9	GOL	A	810	-	5,5,5	1.03	0	5,5,5	0.83	0
5	OCT	A	802	-	7,7,7	0.45	0	6,6,6	0.55	0
7	1PE	A	804	-	15,15,15	0.51	0	14,14,14	0.37	0
6	PG4	A	806	-	12,12,12	0.59	0	11,11,11	0.83	0
6	PG4	A	803	-	12,12,12	0.52	0	11,11,11	0.67	0
6	PG4	A	805	-	12,12,12	0.51	0	11,11,11	0.52	0
6	PG4	A	807	-	12,12,12	0.51	0	11,11,11	0.49	0
6	PG4	A	808	-	12,12,12	0.53	0	11,11,11	0.58	0
11	HEX	A	814	-	5,5,5	0.37	0	4,4,4	0.57	0
9	GOL	A	813	-	5,5,5	1.04	0	5,5,5	1.03	0
4	LMT	A	801	-	36,36,36	1.20	4 (11%)	47,47,47	1.55	8 (17%)
8	D12	A	809	-	11,11,11	0.47	0	10,10,10	0.58	0
7	1PE	A	811	-	15,15,15	0.52	0	14,14,14	0.46	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
11	HEX	A	815	-	-	0/3/3/3	-
10	D10	A	812	-	-	0/7/7/7	-
9	GOL	A	810	-	-	2/4/4/4	-
5	OCT	A	802	-	-	2/5/5/5	-
7	1PE	A	804	-	-	5/13/13/13	-
6	PG4	A	806	-	-	6/10/10/10	-
6	PG4	A	803	-	-	4/10/10/10	-
6	PG4	A	805	-	-	5/10/10/10	-
6	PG4	A	807	-	-	4/10/10/10	-
6	PG4	A	808	-	-	4/10/10/10	-
11	HEX	A	814	-	-	0/3/3/3	-
9	GOL	A	813	-	-	0/4/4/4	-
4	LMT	A	801	-	-	15/21/61/61	0/2/2/2
8	D12	A	809	-	-	3/9/9/9	-
7	1PE	A	811	-	-	5/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	LMT	O5B-C1B	3.61	1.51	1.41
4	A	801	LMT	O5'-C1'	3.18	1.49	1.41
4	A	801	LMT	O3B-C3B	2.25	1.48	1.43
4	A	801	LMT	O1B-C4'	2.09	1.49	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	LMT	C1'-C2'-C3'	3.58	117.45	110.00
4	A	801	LMT	C3'-C4'-C5'	2.91	117.60	110.93
4	A	801	LMT	C2'-C3'-C4'	2.82	116.12	109.68
4	A	801	LMT	C1B-O1B-C4'	2.74	124.75	117.96
4	A	801	LMT	O3B-C3B-C2B	2.49	116.11	110.35
4	A	801	LMT	C4B-C3B-C2B	-2.05	107.24	110.82
4	A	801	LMT	O5B-C5B-C6B	2.04	111.51	106.44
4	A	801	LMT	C1'-O5'-C5'	-2.00	109.76	113.69

There are no chirality outliers.

All (55) 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
4	A	801	LMT	O5'-C5'-C6'-O6'
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	C4'-C5'-C6'-O6'
7	A	811	1PE	OH5-C14-C24-OH4
6	A	806	PG4	O3-C5-C6-O4
4	A	801	LMT	C3-C4-C5-C6
7	A	811	1PE	OH4-C13-C23-OH3
4	A	801	LMT	C7-C8-C9-C10
4	A	801	LMT	C5-C6-C7-C8
7	A	811	1PE	OH6-C15-C25-OH5
5	A	802	OCT	C4-C5-C6-C7
4	A	801	LMT	C5'-C4'-O1B-C1B
4	A	801	LMT	C1-C2-C3-C4
6	A	805	PG4	O3-C5-C6-O4
4	A	801	LMT	C6-C7-C8-C9
7	A	804	1PE	OH7-C16-C26-OH6
5	A	802	OCT	C3-C4-C5-C6
4	A	801	LMT	C3'-C4'-O1B-C1B
8	A	809	D12	C9-C10-C11-C12
4	A	801	LMT	C11-C10-C9-C8
6	A	805	PG4	O4-C7-C8-O5
8	A	809	D12	C3-C4-C5-C6
4	A	801	LMT	C4-C5-C6-C7
6	A	808	PG4	C3-C4-O3-C5
6	A	807	PG4	C3-C4-O3-C5
6	A	807	PG4	C8-C7-O4-C6
9	A	810	GOL	O2-C2-C3-O3
7	A	811	1PE	C25-C15-OH6-C26
6	A	806	PG4	C4-C3-O2-C2
7	A	804	1PE	OH2-C12-C22-OH3
6	A	805	PG4	C3-C4-O3-C5
6	A	805	PG4	C5-C6-O4-C7
6	A	806	PG4	C3-C4-O3-C5
6	A	808	PG4	O2-C3-C4-O3
6	A	808	PG4	O3-C5-C6-O4
6	A	803	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	A	803	PG4	C1-C2-O2-C3
6	A	806	PG4	C6-C5-O3-C4
6	A	803	PG4	C4-C3-O2-C2
6	A	805	PG4	O2-C3-C4-O3
6	A	808	PG4	C6-C5-O3-C4
6	A	806	PG4	C1-C2-O2-C3
7	A	804	1PE	OH4-C13-C23-OH3
6	A	807	PG4	O2-C3-C4-O3
8	A	809	D12	C1-C2-C3-C4
7	A	804	1PE	OH6-C15-C25-OH5
7	A	811	1PE	C15-C25-OH5-C14
9	A	810	GOL	C1-C2-C3-O3
7	A	804	1PE	OH5-C14-C24-OH4

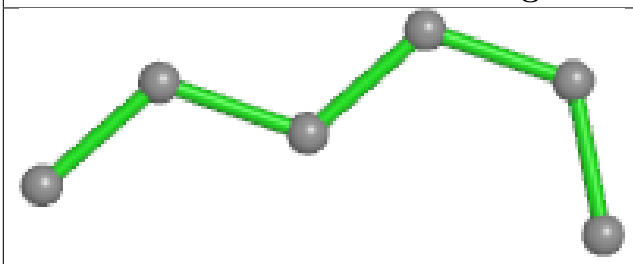
There are no ring outliers.

4 monomers are involved in 9 short contacts:

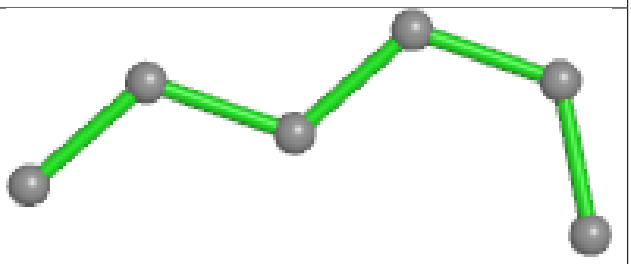
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	812	D10	2	0
6	A	806	PG4	1	0
4	A	801	LMT	5	0
7	A	811	1PE	1	0

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 then 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.

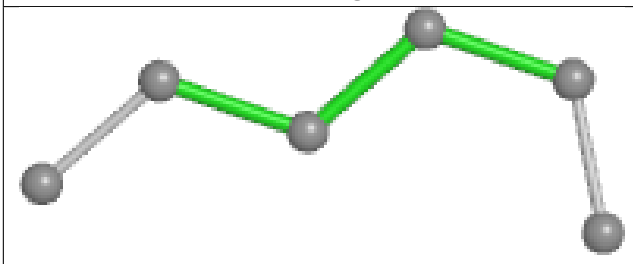
Ligand HEX A 815



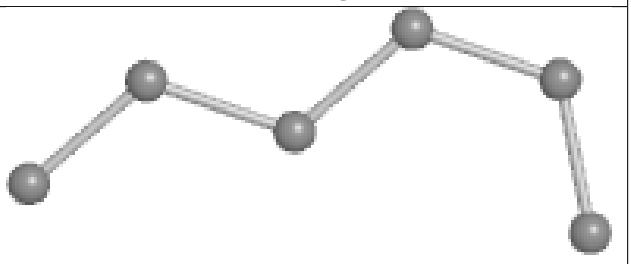
Bond lengths



Bond angles

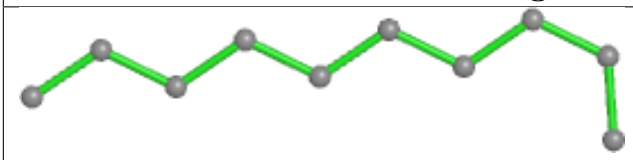


Torsions

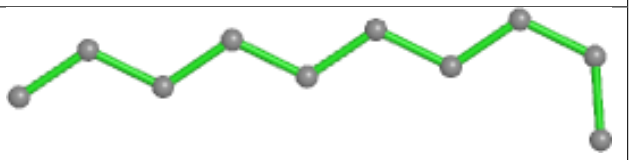


Rings

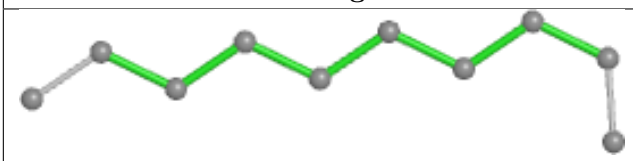
Ligand D10 A 812



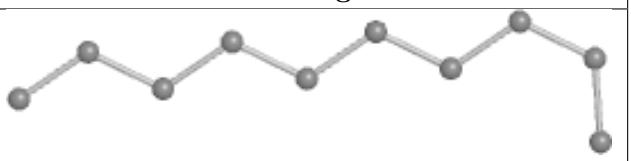
Bond lengths



Bond angles

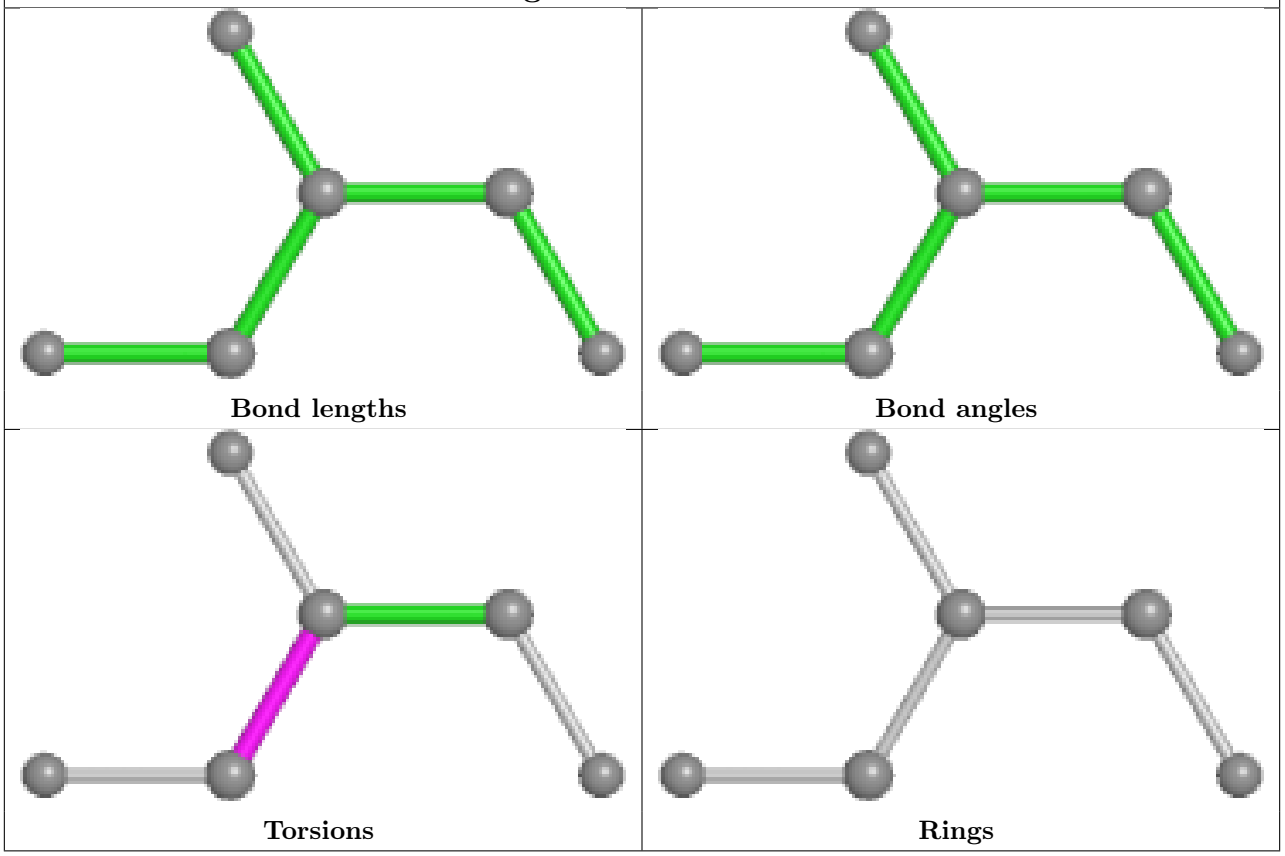


Torsions

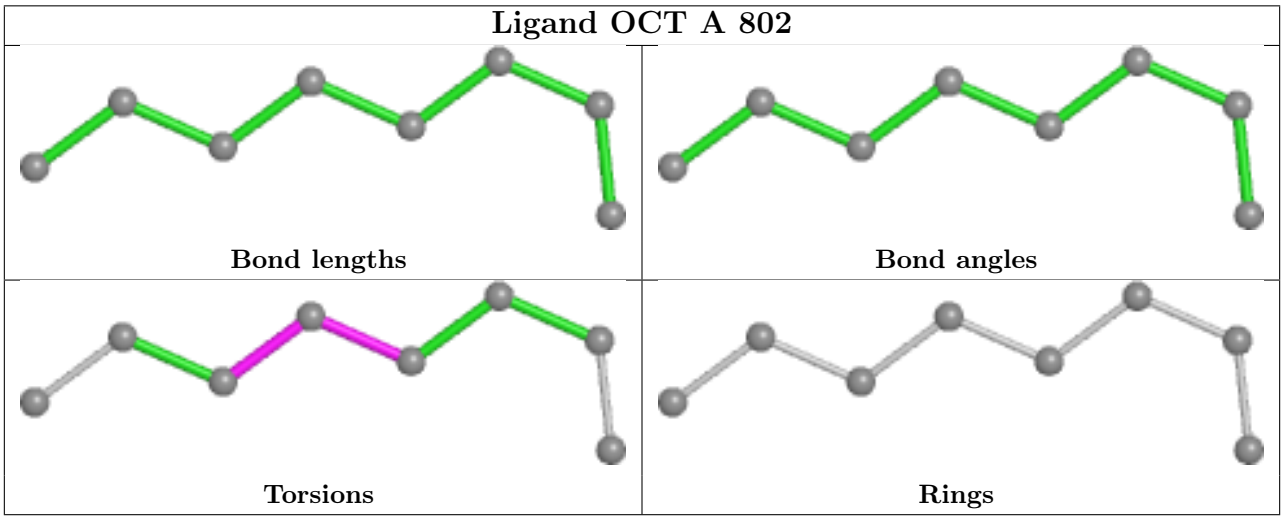


Rings

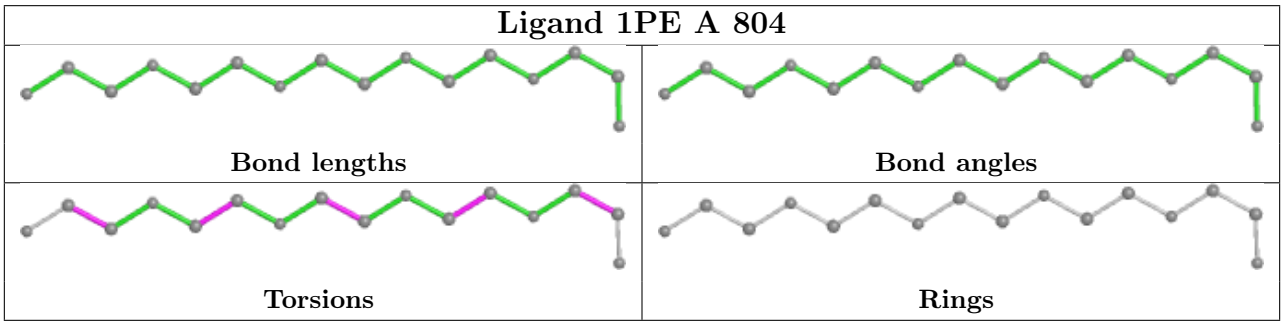
Ligand GOL A 810



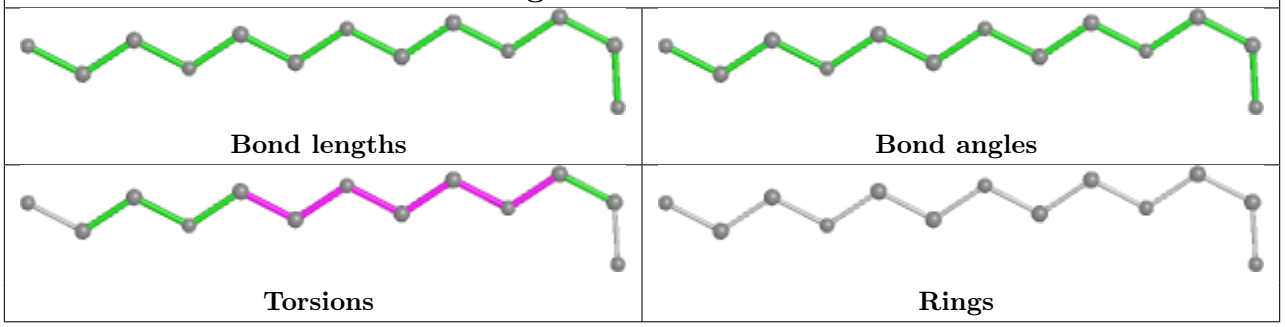
Ligand OCT A 802



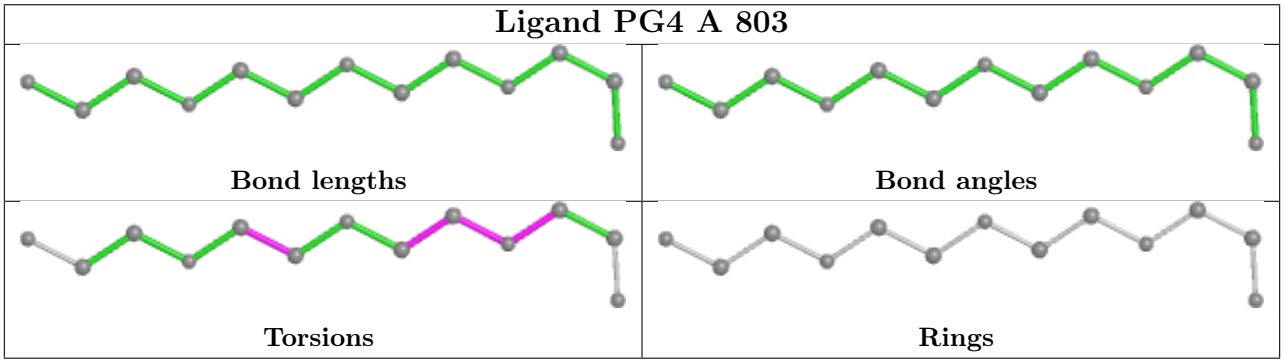
Ligand 1PE A 804



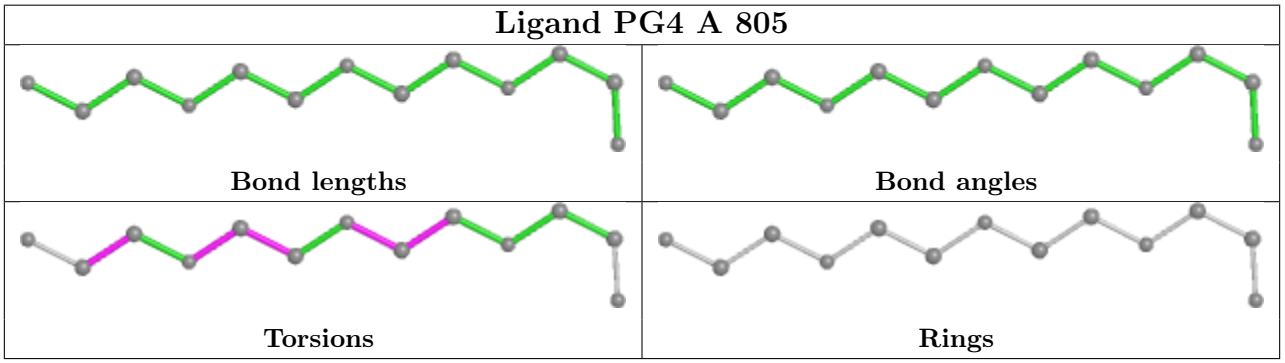
Ligand PG4 A 806



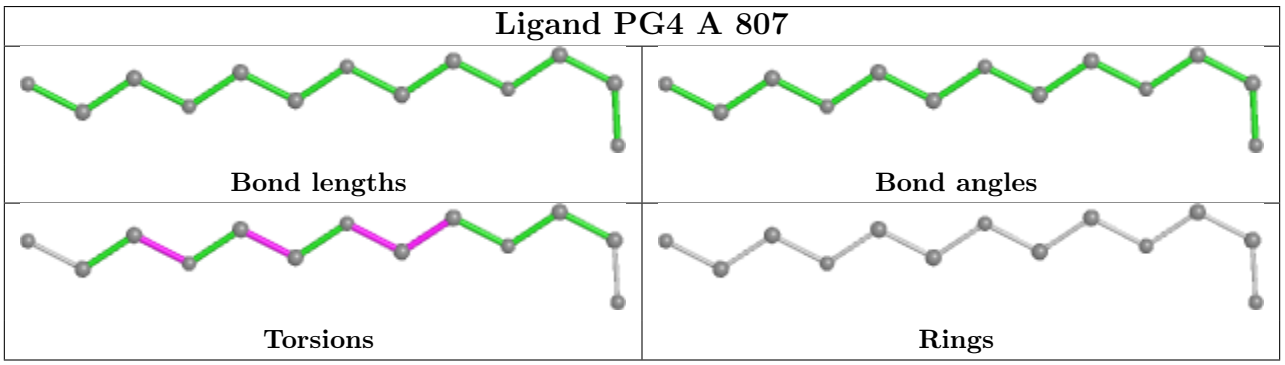
Ligand PG4 A 803



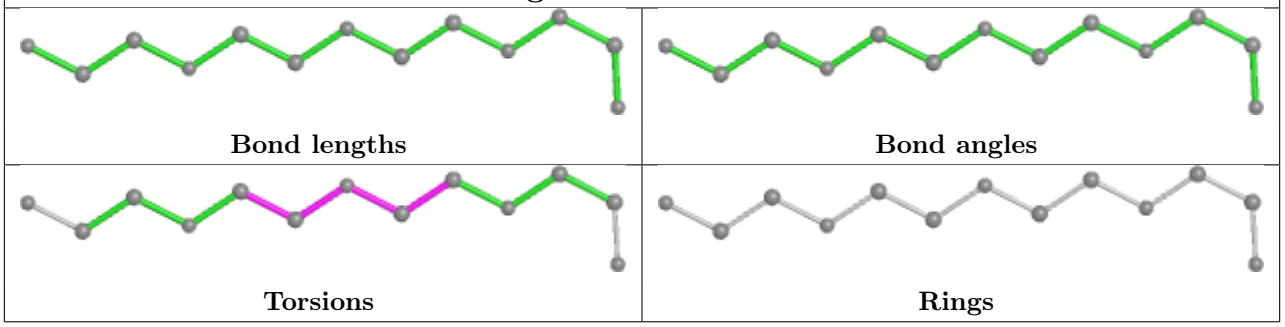
Ligand PG4 A 805



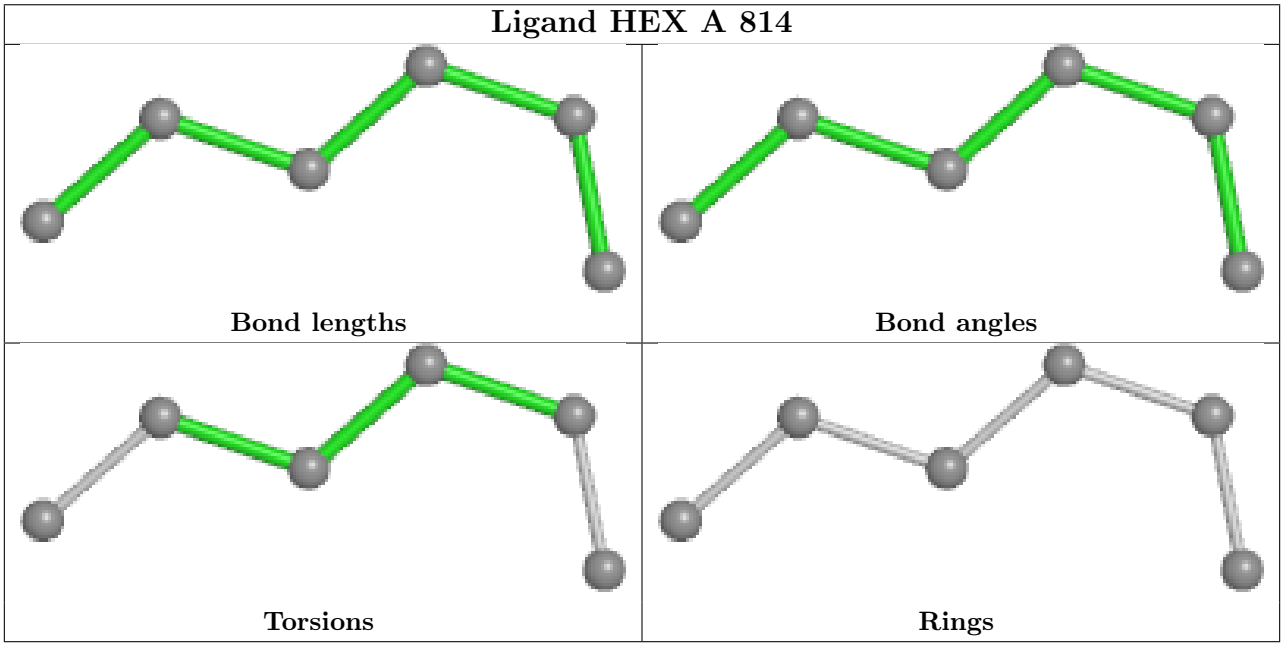
Ligand PG4 A 807



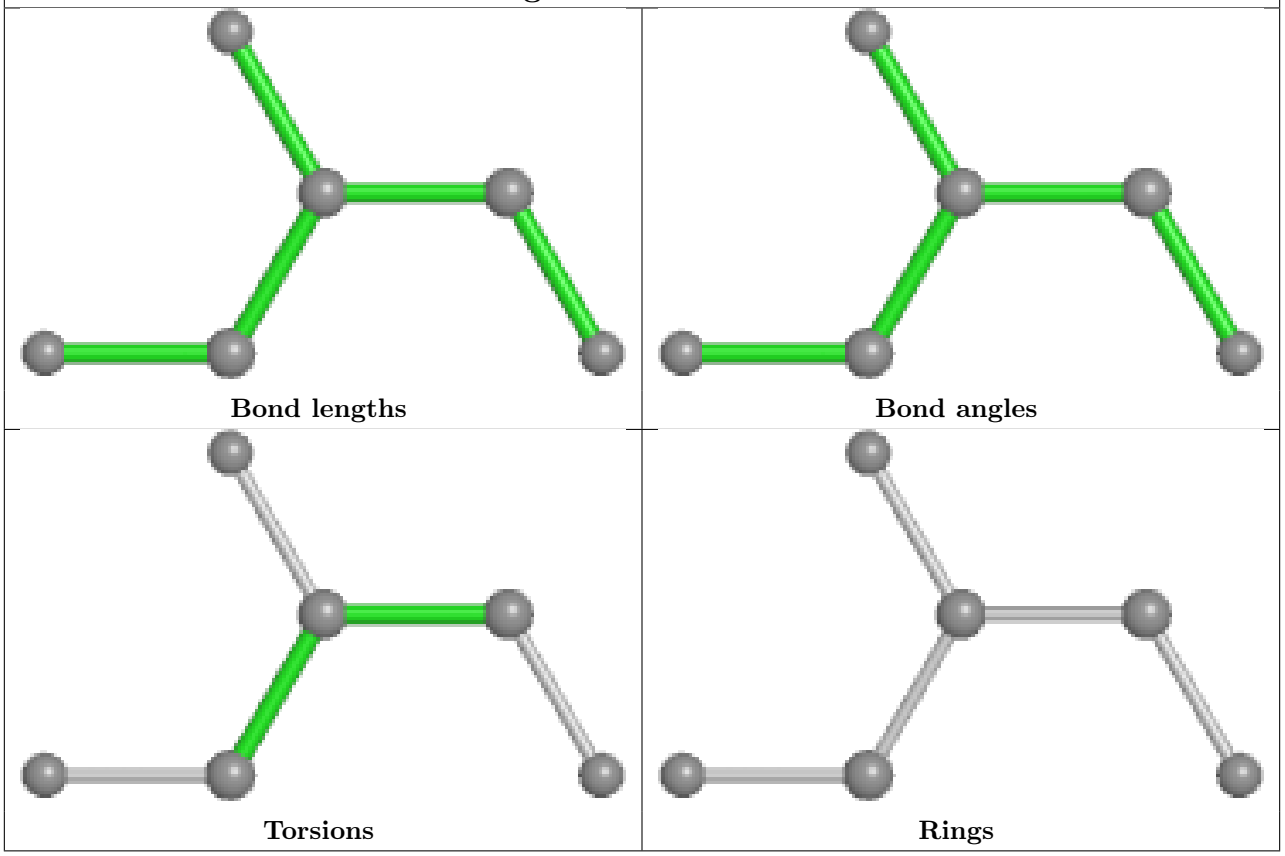
Ligand PG4 A 808



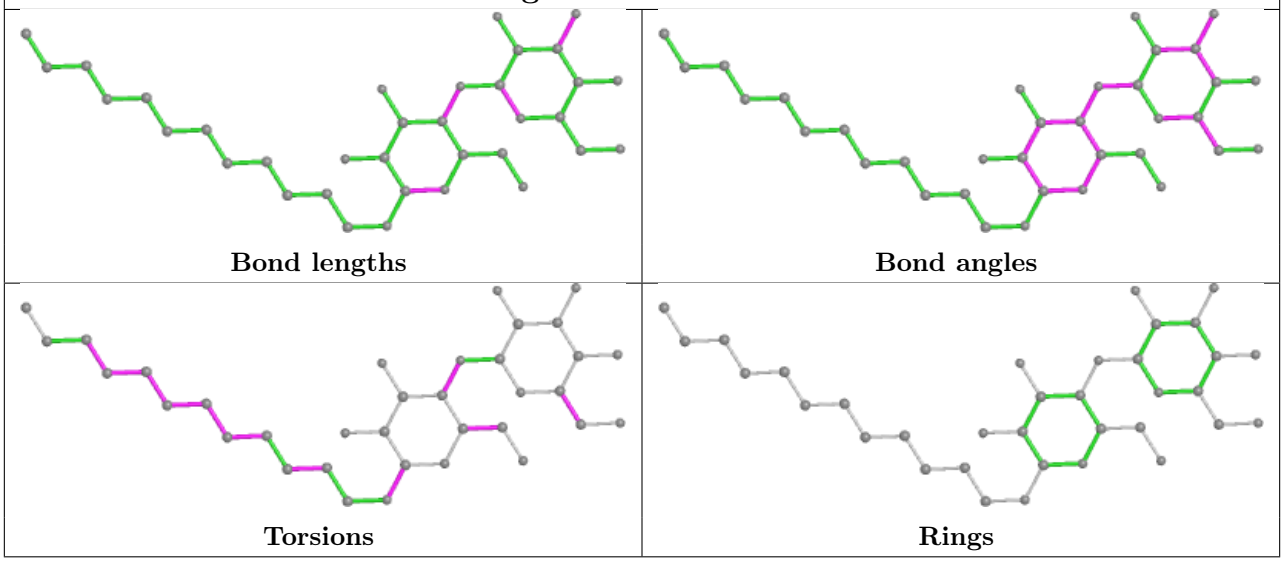
Ligand HEX A 814

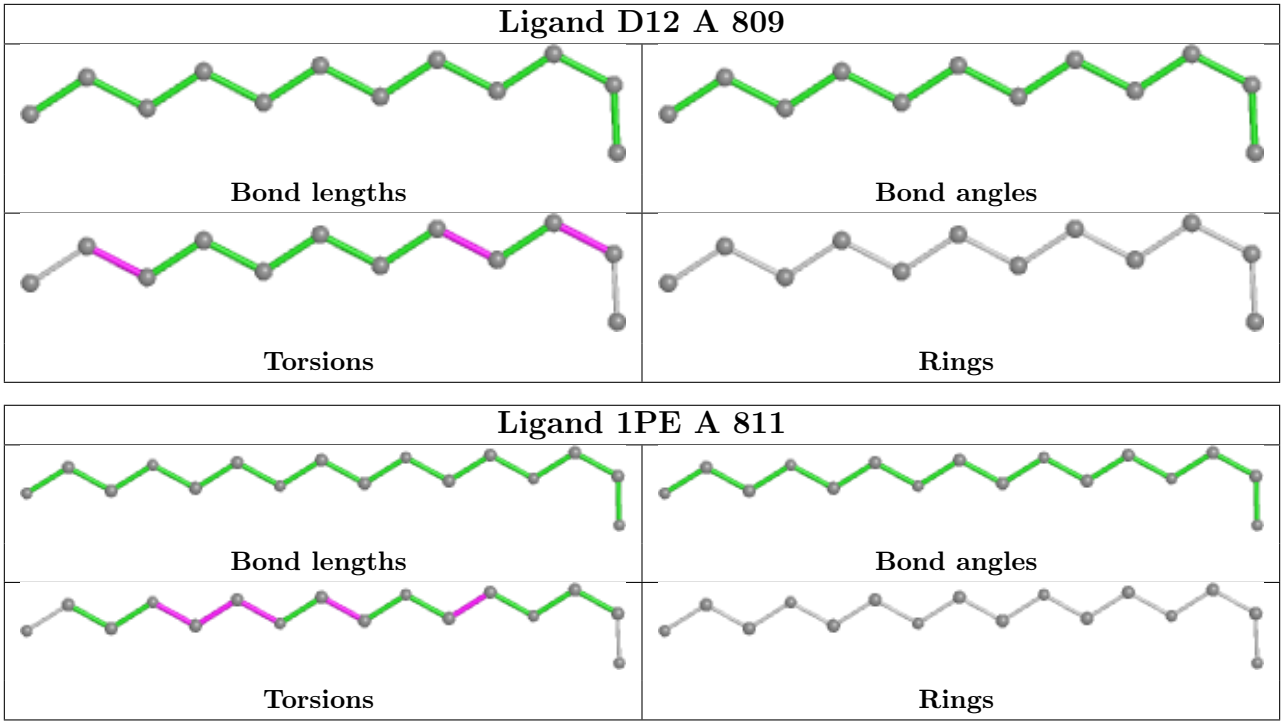


Ligand GOL A 813



Ligand LMT A 801





5.7 Other polymers

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^{th} 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	451/489 (92%)	1.13	59 (13%) 3 4	54, 69, 111, 138	1 (0%)
2	B	127/127 (100%)	0.61	9 (7%) 16 20	55, 70, 97, 108	1 (0%)
3	C	3/3 (100%)	1.04	0 100 100	64, 64, 65, 75	0
All	All	581/619 (93%)	1.02	68 (11%) 4 6	54, 69, 108, 138	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	18.2
1	A	404	ILE	8.1
1	A	332	ILE	7.9
1	A	330	ALA	7.7
1	A	478	TRP	7.5
1	A	331	GLY	7.2
1	A	395	PHE	7.1
1	A	307	PHE	6.0
1	A	272	PHE	5.7
1	A	329	LEU	5.2
1	A	148	PHE	5.0
1	A	416	ILE	4.5
2	B	76	ASP	4.3
1	A	17	PHE	3.9
1	A	240	LEU	3.9
1	A	137	LYS	3.9
1	A	351	LEU	3.8
1	A	407	LEU	3.8
1	A	19	ILE	3.8
1	A	144	ALA	3.8
1	A	479	LEU	3.6
1	A	134	TYR	3.5
1	A	433	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	437	PHE	3.4
1	A	266	ASN	3.3
2	B	79	TYR	3.2
1	A	343	LEU	3.1
1	A	398	ALA	3.1
1	A	399	LEU	2.9
1	A	419	MET	2.9
1	A	85	VAL	2.8
1	A	370	PHE	2.8
2	B	68	THR	2.8
2	B	77	THR	2.7
1	A	308	SER	2.7
1	A	309	ILE	2.7
1	A	130	LEU	2.7
1	A	314	PHE	2.6
1	A	326	SER	2.6
1	A	304	ILE	2.6
1	A	268	MET	2.6
1	A	218	LEU	2.5
1	A	142	ASP	2.5
1	A	312	VAL	2.5
1	A	327	PRO	2.5
1	A	400	GLY	2.5
2	B	75	LYS	2.5
1	A	415	PHE	2.4
1	A	403	MET	2.4
1	A	140	ARG	2.4
1	A	122	PHE	2.3
1	A	103	LEU	2.3
1	A	20	PHE	2.3
2	B	67	PHE	2.2
1	A	305	LEU	2.2
1	A	145	PHE	2.2
1	A	271	ALA	2.2
2	B	78	VAL	2.2
1	A	382	ILE	2.2
1	A	16	PHE	2.2
1	A	36	VAL	2.1
1	A	214	LEU	2.1
2	B	27	PRO	2.1
1	A	211	PHE	2.1
1	A	23	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	18	LEU	2.1
1	A	33	VAL	2.1
1	A	418	GLY	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)

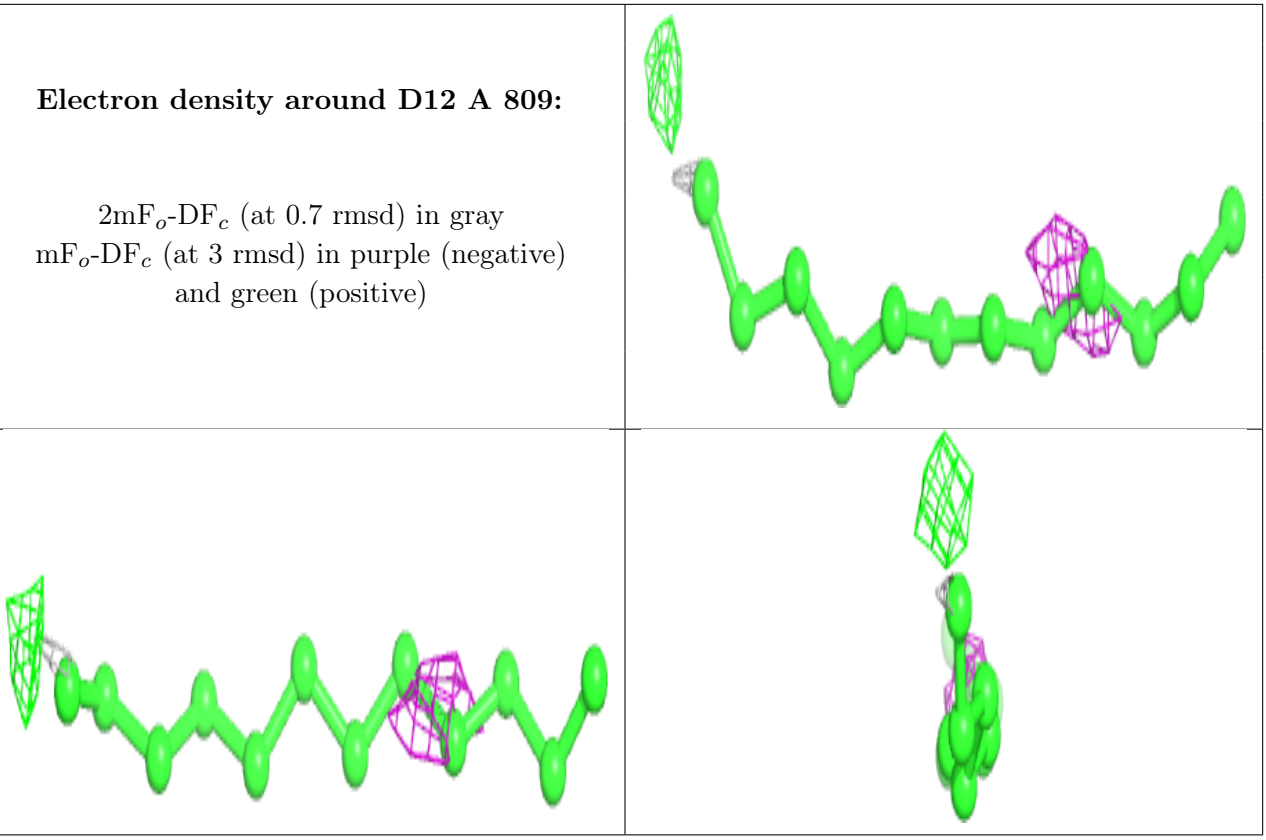
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	D12	A	809	12/12	0.47	1.78	82,90,92,93	0
6	PG4	A	806	13/13	0.49	0.90	82,91,114,115	0
6	PG4	A	805	13/13	0.58	0.41	75,88,105,106	0
7	1PE	A	811	16/16	0.59	0.53	87,95,112,113	0
5	OCT	A	802	8/8	0.64	0.84	70,78,83,84	0
6	PG4	A	808	13/13	0.65	0.28	78,90,102,108	0
7	1PE	A	804	16/16	0.67	0.68	70,80,108,110	0
11	HEX	A	814	6/6	0.69	0.72	79,85,88,90	0
11	HEX	A	815	6/6	0.69	0.52	74,82,85,86	0
9	GOL	A	810	6/6	0.74	0.12	115,117,120,121	0
10	D10	A	812	10/10	0.76	0.26	70,82,91,94	0
6	PG4	A	807	13/13	0.80	0.42	79,89,102,109	0
9	GOL	A	813	6/6	0.81	0.11	87,90,96,101	0
4	LMT	A	801	35/35	0.81	0.49	68,88,103,106	0
6	PG4	A	803	13/13	0.90	0.25	71,80,98,108	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.

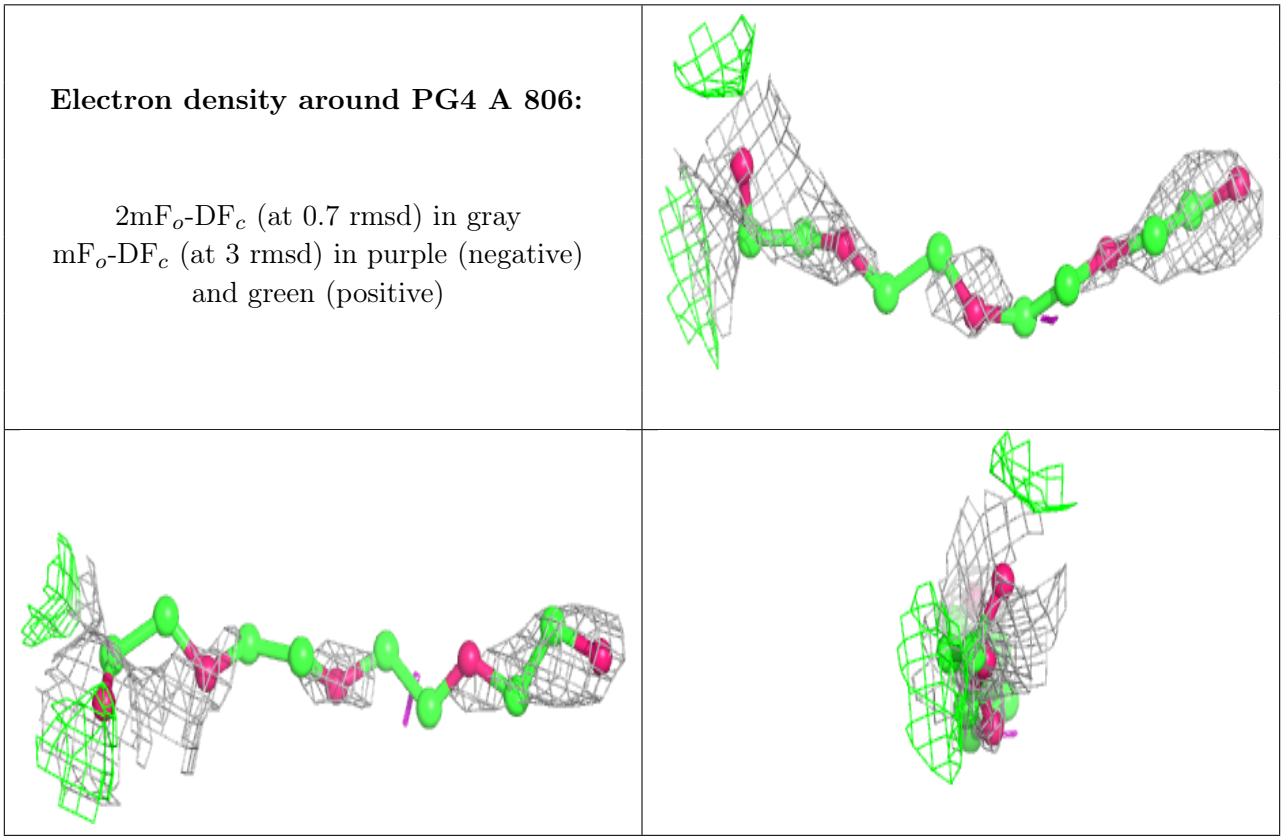
Electron density around D12 A 809:

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



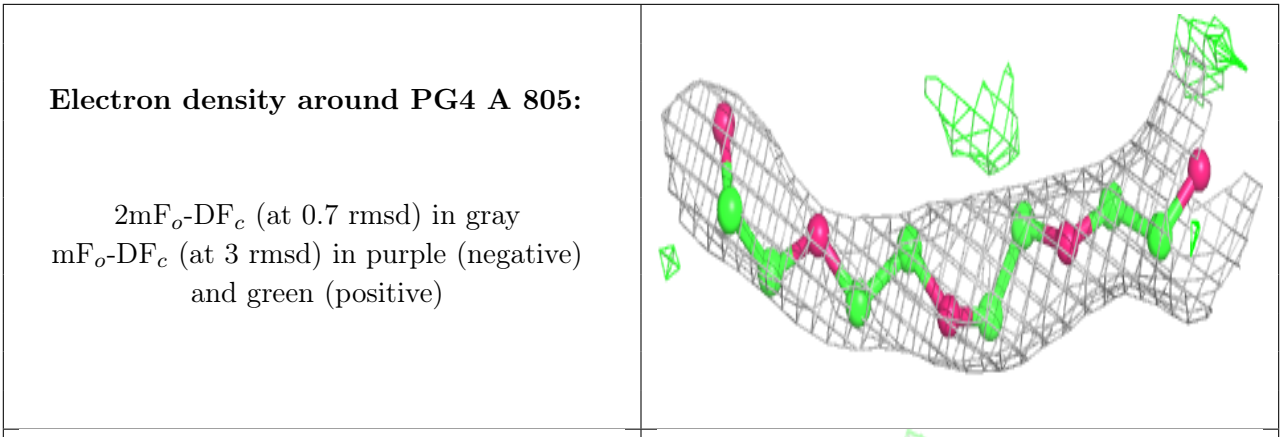
Electron density around PG4 A 806:

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



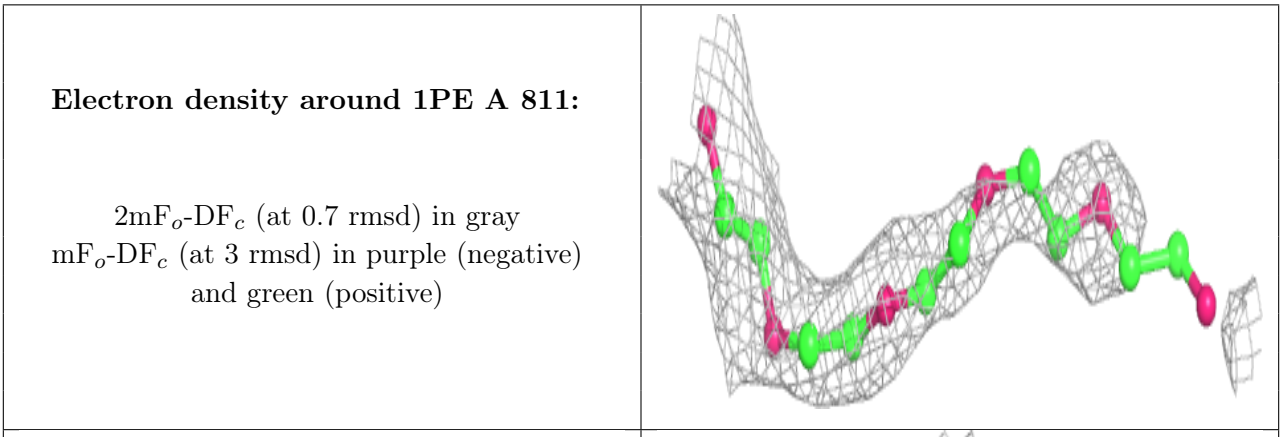
Electron density around PG4 A 805:

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



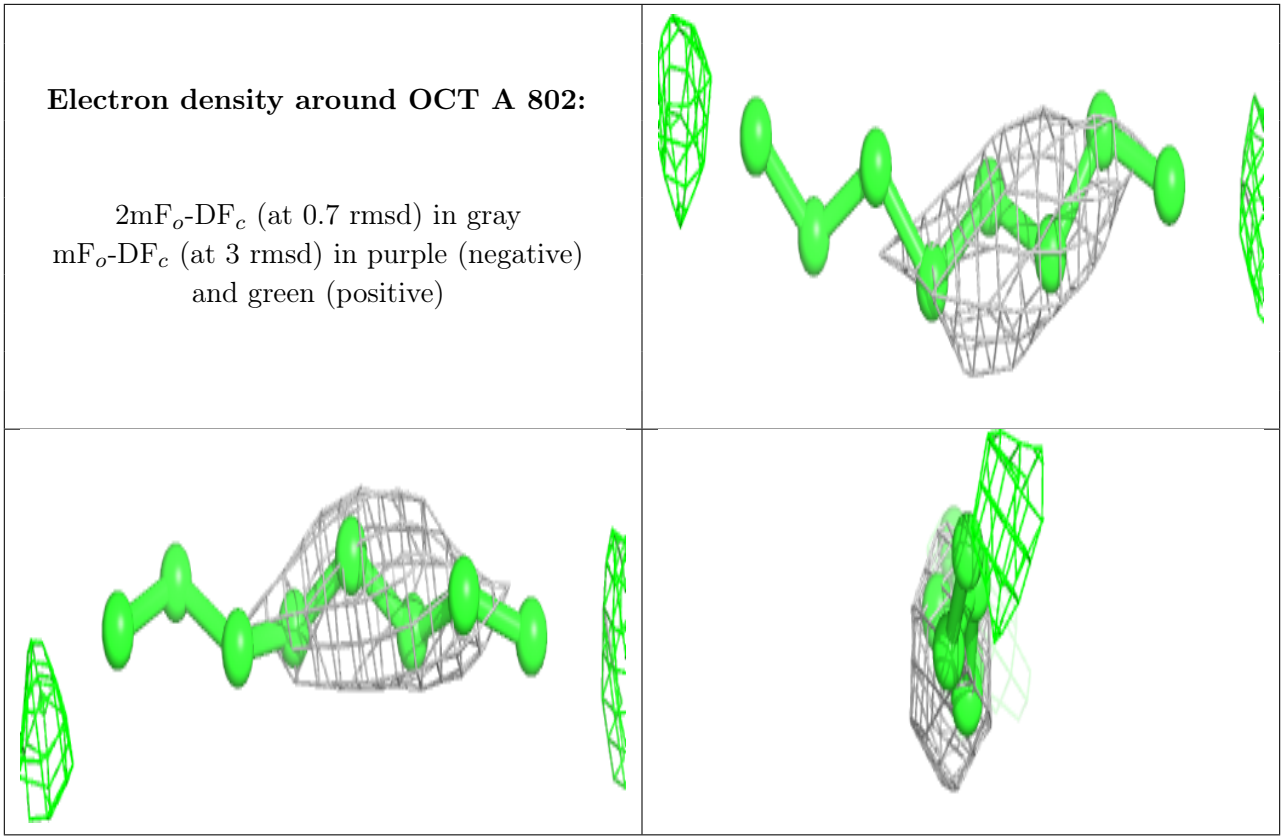
Electron density around 1PE A 811:

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



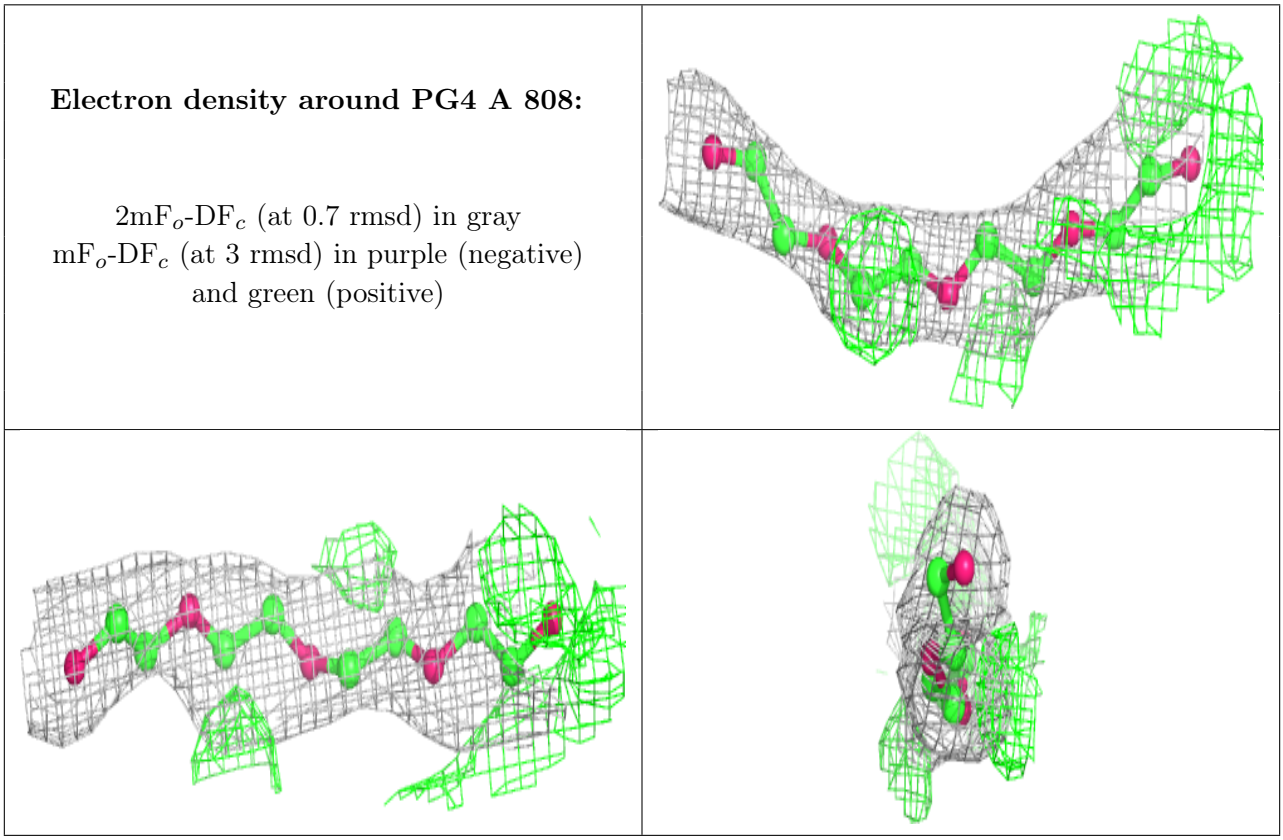
Electron density around OCT A 802:

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



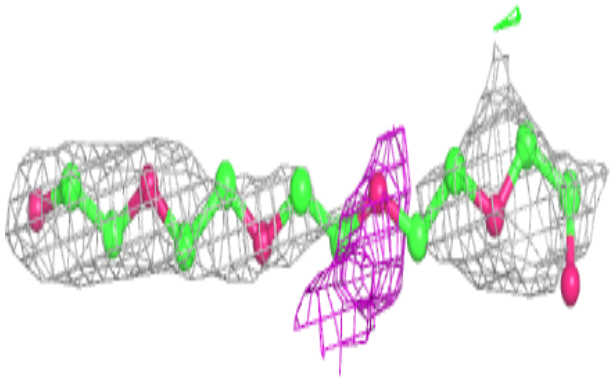
Electron density around PG4 A 808:

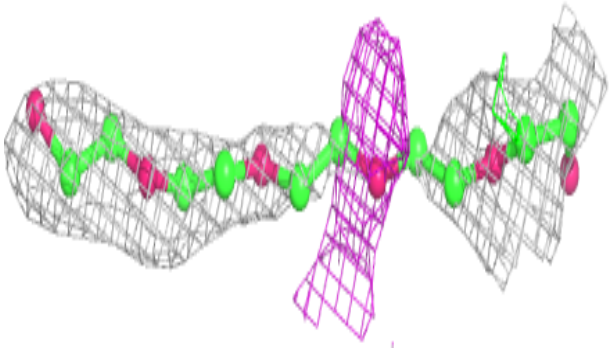
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

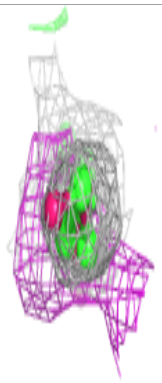


Electron density around 1PE A 804:

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

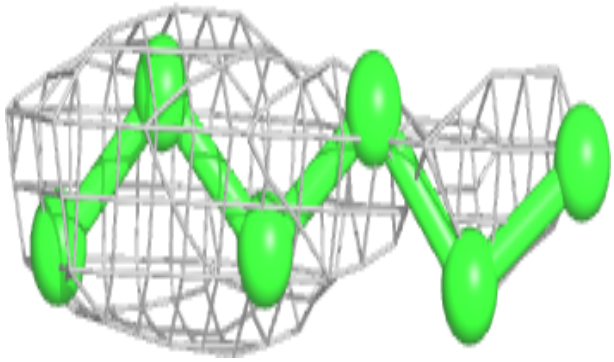


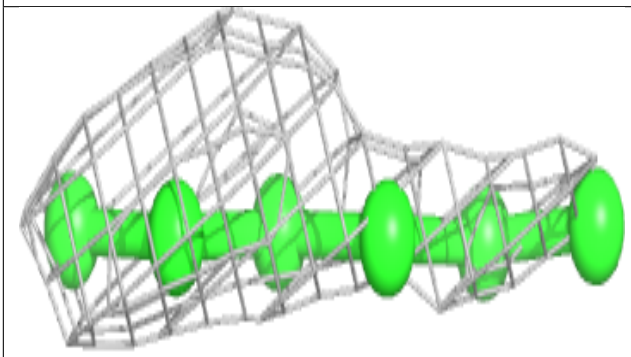


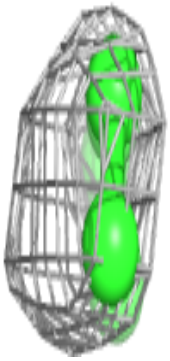


Electron density around HEX A 814:

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

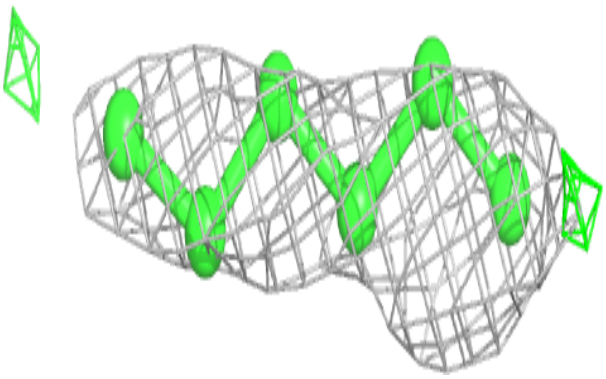


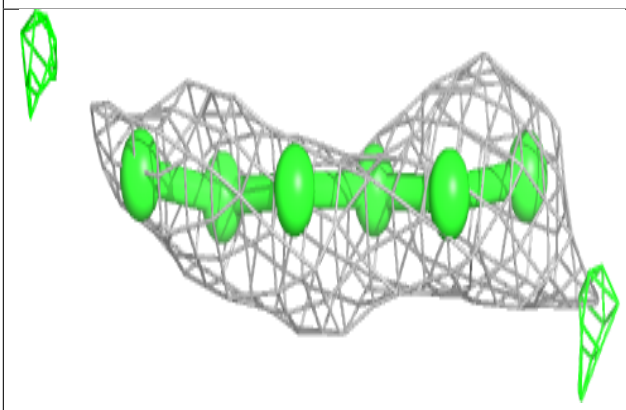


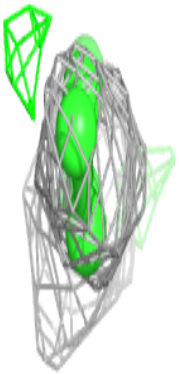


Electron density around HEX A 815:

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

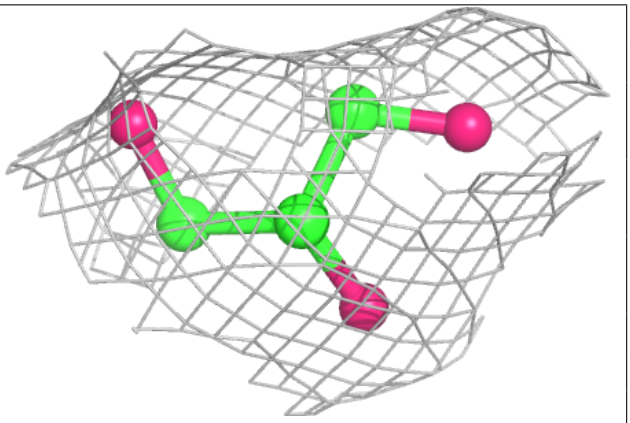


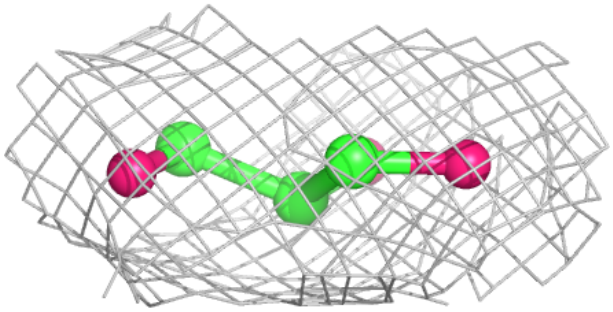


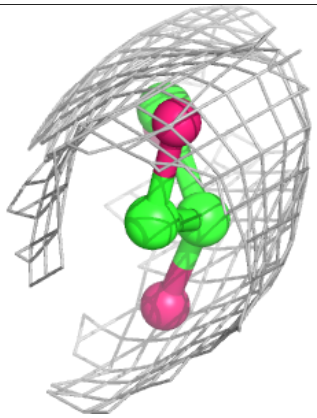


Electron density around GOL A 810:

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

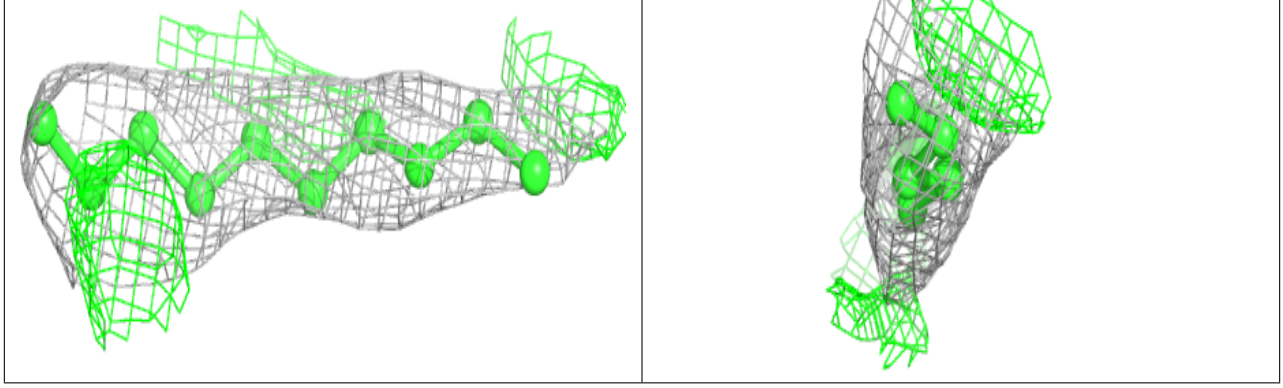






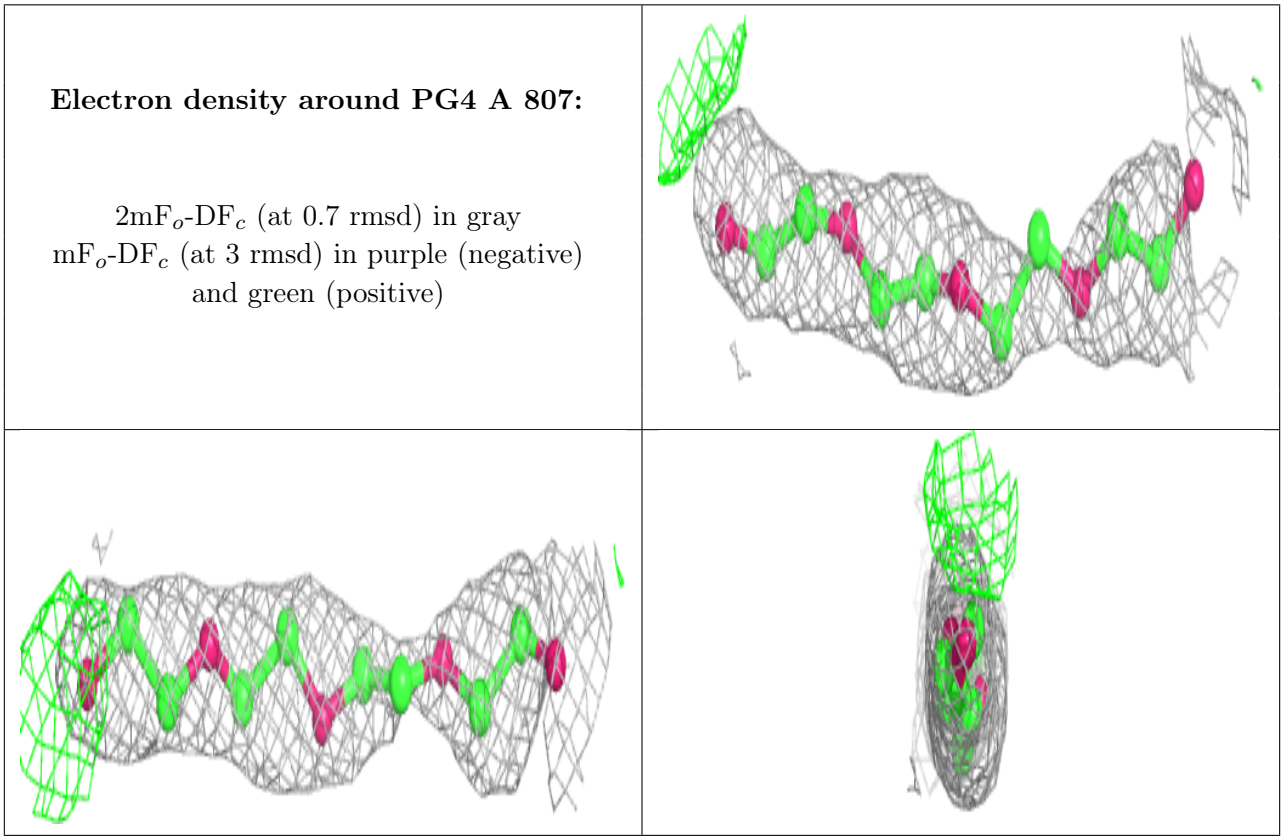
Electron density around D10 A 812:

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



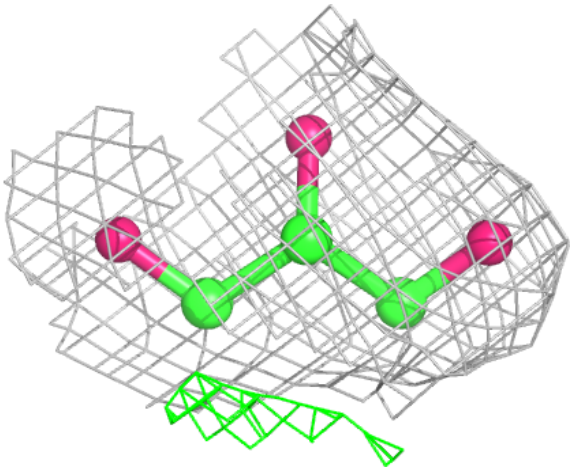
Electron density around PG4 A 807:

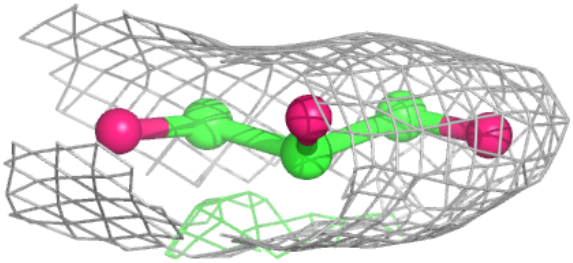
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

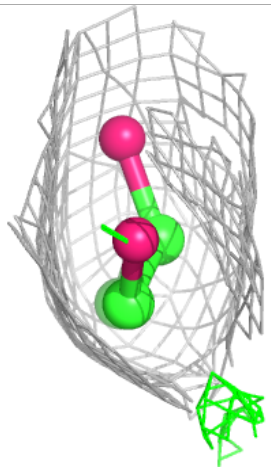


Electron density around GOL A 813:

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

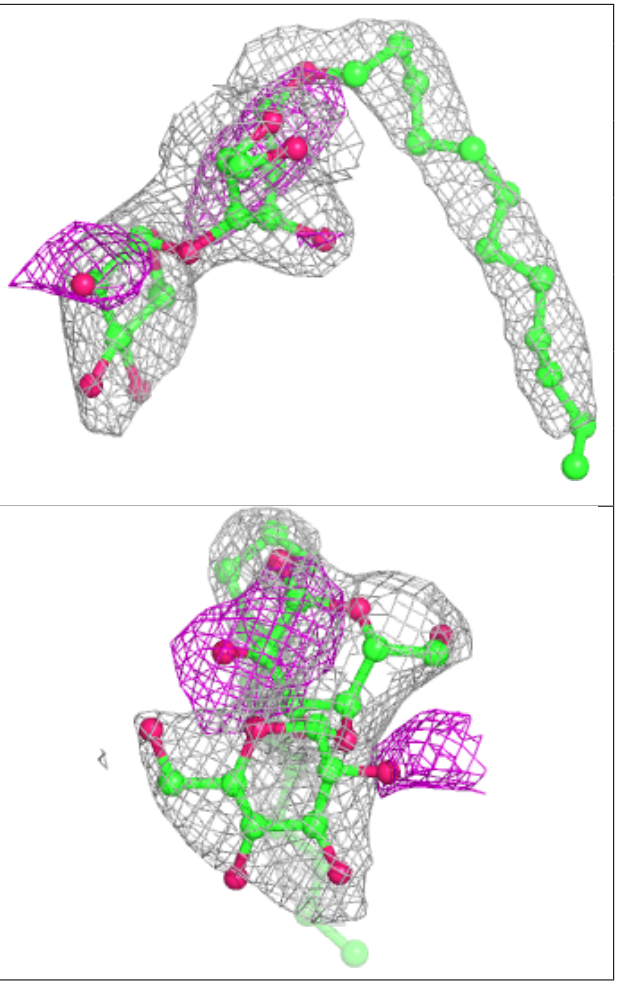


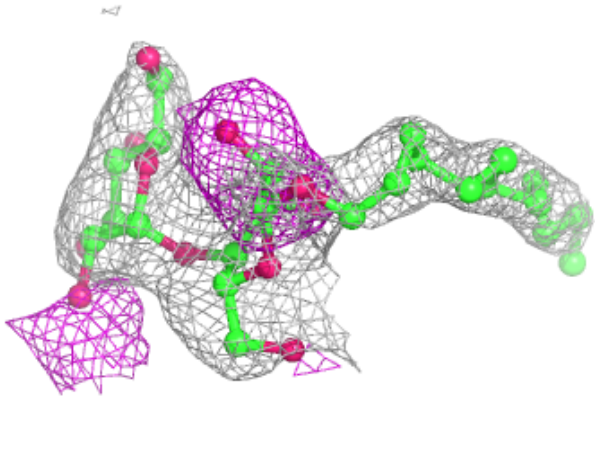




Electron density around LMT A 801:

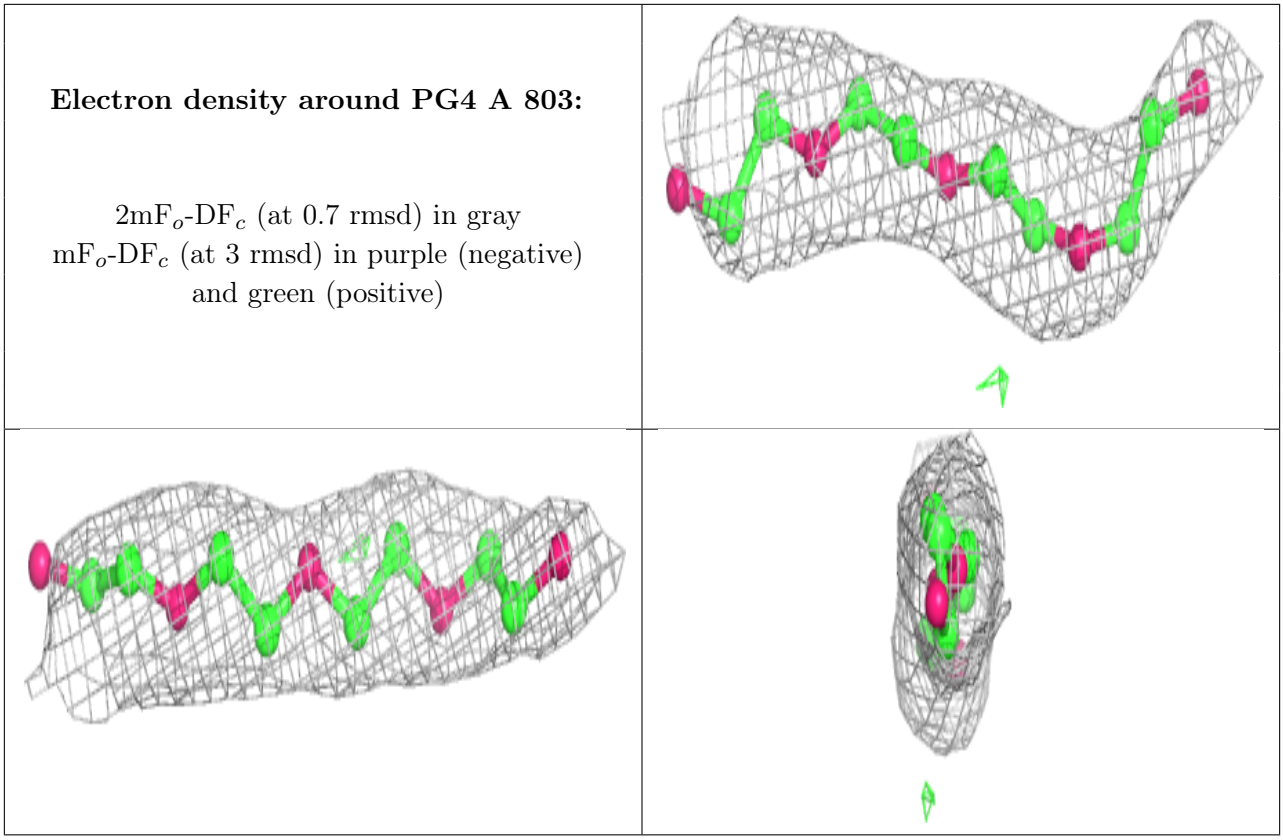
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around PG4 A 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.