Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 08:44 PM EDT

PDB ID	:	7T89
Title	:	Light harvesting complex Phycocyanin PC577 from the cryptophyte Hemiselmis pacifica CCMP 706
Authors	:	Michie, K.A.; Curmi, P.C.; Harrop, S.; Rathbone, H.W.
Deposited on	:	2021-12-16
Resolution	:	1.00 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:

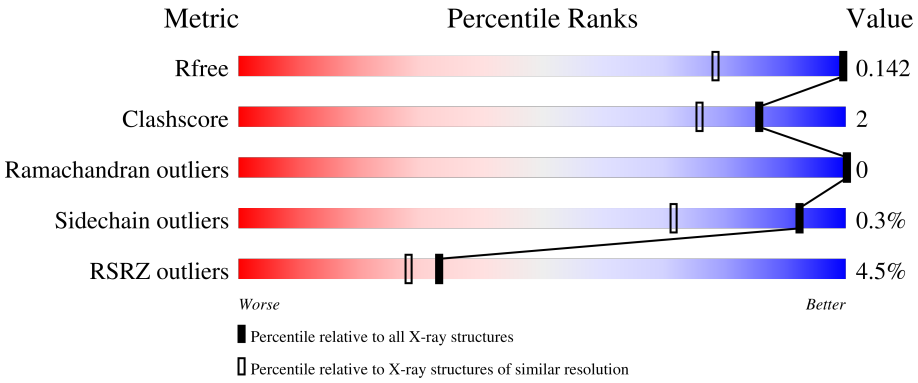
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.00 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	1050 (1.06-0.94)
Clashscore	141614	1117 (1.06-0.94)
Ramachandran outliers	138981	1043 (1.06-0.94)
Sidechain outliers	138945	1045 (1.06-0.94)
RSRZ outliers	127900	1023 (1.06-0.94)

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	63	3% 100%
1	C	63	2% 95%
2	B	177	5% 97%
2	D	177	5% 93%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10255 atoms, of which 4721 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.

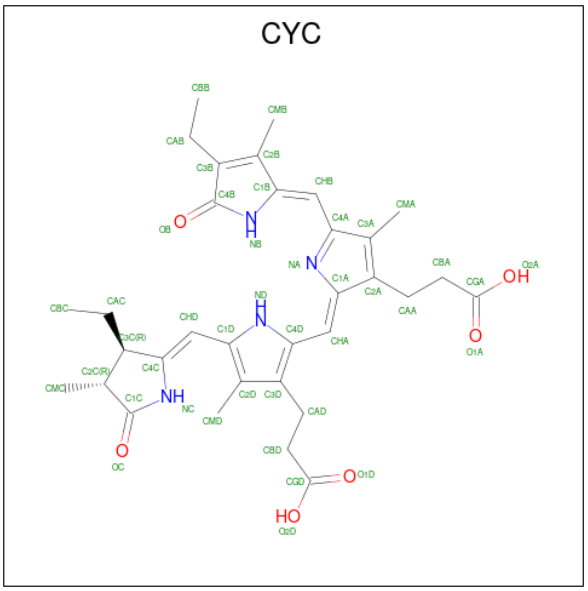
- Molecule 1 is a protein called Phycoerythrin alpha subunit 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	63	Total	C	H	N	O	S	0	14	0
			1104	337	559	93	109	6			
1	C	62	Total	C	H	N	O	S	0	15	0
			1077	328	543	91	109	6			

- Molecule 2 is a protein called Phycoerythrin beta subunit.

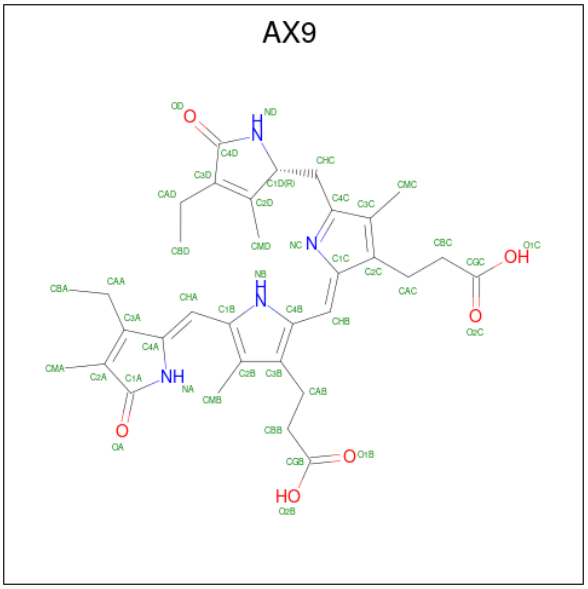
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	174	Total	C	H	N	O	S	0	48	0
			3153	963	1584	272	321	13			
2	D	171	Total	C	H	N	O	S	0	33	0
			2884	880	1447	249	296	12			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	B	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	B	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	C	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	D	1	Total	C	H	N	O	0	1
			160	66	74	8	12		
3	D	1	Total	C	H	N	O	0	1
			160	66	74	8	12		

- Molecule 4 is DiCys-(15,16)-Dihydrobiliverdin (three-letter code: AX9) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	1
			158	66	72	8	12		
4	D	1	Total	C	H	N	O	0	1
			158	66	72	8	12		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total	O	0	2
			111	111		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	279	Total O 281 281	0	8
5	C	120	Total O 121 121	0	1
5	D	248	Total O 248 248	0	12

3 Residue-property plots (i)

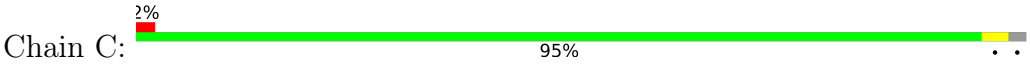
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

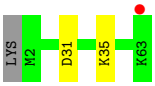
• Molecule 1: Phycoerythrin alpha subunit 1

Chain A:

• Molecule 1: Phycoerythrin alpha subunit 1

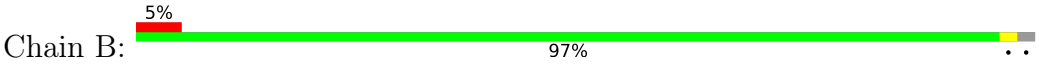
Chain C:

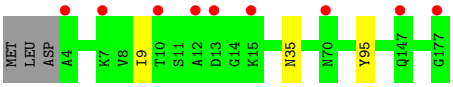




• Molecule 2: Phycoerythrin beta subunit

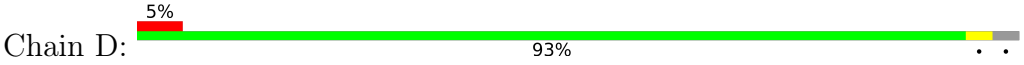
Chain B:

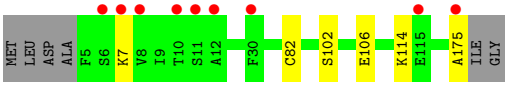




• Molecule 2: Phycoerythrin beta subunit

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	42.12Å 95.32Å 125.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.28 – 1.00 22.28 – 1.00	Depositor EDS
% Data completeness (in resolution range)	93.0 (22.28-1.00) 93.0 (22.28-1.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.133 , 0.143 0.133 , 0.142	Depositor DCC
R_{free} test set	12707 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	8.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.4	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	0.98	EDS
Total number of atoms	10255	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6073e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AX9, CYC

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	0.37	0/575	0.71	0/756
1	C	0.37	0/573	0.68	0/759
2	B	0.33	0/1639	0.59	0/2198
2	D	0.34	0/1501	0.58	0/2019
All	All	0.34	0/4288	0.62	0/5732

There are no bond length outliers.

There are no bond angle outliers.

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	545	559	539	0	0
1	C	534	543	515	2	0
2	B	1569	1584	1517	2	0
2	D	1437	1447	1391	3	0
3	A	86	74	74	1	0
3	B	172	148	147	7	0
3	C	86	74	74	2	0
3	D	172	148	148	7	0
4	B	86	72	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	86	72	0	0	0
5	A	111	0	0	1	0
5	B	281	0	0	0	0
5	C	121	0	0	1	0
5	D	248	0	0	0	0
All	All	5534	4721	4405	21	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 2.

All (21) 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)
3:D:203[A]:CYC:HMD2	3:D:203[A]:CYC:HC	1.61	0.65
1:C:35[B]:LYS:NZ	5:C:201:HOH:O	2.31	0.62
3:B:203[A]:CYC:HC	3:B:203[A]:CYC:HMD2	1.66	0.61
3:D:203[B]:CYC:HMD2	3:D:203[B]:CYC:HC	1.65	0.61
3:B:203[B]:CYC:NB	3:B:203[B]:CYC:HMA1	2.19	0.57
3:B:203[B]:CYC:HC	3:B:203[B]:CYC:HMD2	1.70	0.56
3:A:101[B]:CYC:O2D	5:A:201:HOH:O	2.08	0.55
1:C:31:ASP:HB3	3:C:101[B]:CYC:HBB1	1.94	0.48
3:D:202[B]:CYC:NB	3:D:202[B]:CYC:HMA1	2.27	0.48
2:B:9[A]:ILE:HD11	2:B:95:TYR:CZ	2.50	0.47
3:C:101[A]:CYC:HC	3:C:101[A]:CYC:HMD2	1.80	0.46
2:D:82:CYS:HA	3:D:203[B]:CYC:HHD	1.98	0.45
3:B:202[A]:CYC:HHD	3:B:202[A]:CYC:HBC3	2.00	0.44
2:D:114:LYS:HE2	2:D:175[B]:ALA:O	2.18	0.44
3:D:203[A]:CYC:HMA1	3:D:203[A]:CYC:NB	2.33	0.43
3:B:202[B]:CYC:HHA	3:B:202[B]:CYC:HBA1	2.00	0.43
3:D:203[B]:CYC:NB	3:D:203[B]:CYC:HMA1	2.34	0.42
3:D:202[A]:CYC:HBC3	3:D:202[A]:CYC:HHD	2.03	0.41
2:B:35:ASN:HB3	3:B:202[B]:CYC:C1A	2.51	0.41
2:D:102:SER:O	2:D:106:GLU:HG3	2.21	0.40
3:B:202[B]:CYC:HMA1	3:B:202[B]:CYC:NB	2.35	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	73/63 (116%)	72 (99%)	1 (1%)	0	100	100
1	C	75/63 (119%)	73 (97%)	2 (3%)	0	100	100
2	B	222/177 (125%)	218 (98%)	4 (2%)	0	100	100
2	D	203/177 (115%)	201 (99%)	2 (1%)	0	100	100
All	All	573/480 (119%)	564 (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	60/48 (125%)	60 (100%)	0	100	100
1	C	60/48 (125%)	60 (100%)	0	100	100
2	B	181/137 (132%)	181 (100%)	0	100	100
2	D	165/137 (120%)	164 (99%)	1 (1%)	86	61
All	All	466/370 (126%)	465 (100%)	1 (0%)	92	72

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	7	LYS

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)

16 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	$\#\|Z\| > 2$
3	CYC	A	101[A]	1	42,46,46	2.16	12 (28%)	50,67,67	1.58	8 (16%)
3	CYC	B	203[B]	2	42,46,46	2.67	13 (30%)	50,67,67	1.99	6 (12%)
3	CYC	C	101[B]	1	42,46,46	2.63	13 (30%)	50,67,67	1.96	6 (12%)
3	CYC	D	202[A]	2	42,46,46	2.44	12 (28%)	50,67,67	1.71	8 (16%)
3	CYC	D	203[B]	2	42,46,46	2.55	12 (28%)	50,67,67	1.70	10 (20%)
4	AX9	D	201[B]	2	41,46,46	1.64	9 (21%)	41,67,67	1.30	4 (9%)
3	CYC	C	101[A]	1	42,46,46	2.25	13 (30%)	50,67,67	1.84	5 (10%)
3	CYC	B	202[A]	2	42,46,46	2.39	12 (28%)	50,67,67	1.69	9 (18%)
4	AX9	B	201[A]	2	41,46,46	1.49	10 (24%)	41,67,67	1.04	2 (4%)
3	CYC	A	101[B]	1	42,46,46	2.79	12 (28%)	50,67,67	1.78	9 (18%)
3	CYC	D	203[A]	2	42,46,46	2.50	12 (28%)	50,67,67	1.80	9 (18%)
3	CYC	B	202[B]	2	42,46,46	2.88	13 (30%)	50,67,67	1.80	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	CYC	D	202[B]	2	42,46,46	2.80	14 (33%)	50,67,67	1.68	7 (14%)
4	AX9	D	201[A]	2	41,46,46	1.53	8 (19%)	41,67,67	1.11	3 (7%)
3	CYC	B	203[A]	2	42,46,46	2.15	13 (30%)	50,67,67	1.91	9 (18%)
4	AX9	B	201[B]	2	41,46,46	1.53	9 (21%)	41,67,67	1.22	4 (9%)

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
3	CYC	A	101[A]	1	-	6/25/74/74	0/4/4/4
3	CYC	B	203[B]	2	-	9/25/74/74	0/4/4/4
3	CYC	C	101[B]	1	-	7/25/74/74	0/4/4/4
3	CYC	D	202[A]	2	-	7/25/74/74	0/4/4/4
3	CYC	D	203[B]	2	-	6/25/74/74	0/4/4/4
4	AX9	D	201[B]	2	-	7/26/74/74	0/4/4/4
3	CYC	C	101[A]	1	-	5/25/74/74	0/4/4/4
3	CYC	B	202[A]	2	-	10/25/74/74	0/4/4/4
4	AX9	B	201[A]	2	-	9/26/74/74	0/4/4/4
3	CYC	A	101[B]	1	-	7/25/74/74	0/4/4/4
3	CYC	D	203[A]	2	-	10/25/74/74	0/4/4/4
3	CYC	B	202[B]	2	-	9/25/74/74	0/4/4/4
3	CYC	D	202[B]	2	-	12/25/74/74	0/4/4/4
4	AX9	D	201[A]	2	-	9/26/74/74	0/4/4/4
3	CYC	B	203[A]	2	-	8/25/74/74	0/4/4/4
4	AX9	B	201[B]	2	-	5/26/74/74	0/4/4/4

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202[B]	CYC	C1C-NC	-10.99	1.23	1.37
3	D	202[B]	CYC	C1C-NC	-10.52	1.24	1.37
3	A	101[B]	CYC	C1C-NC	-10.38	1.24	1.37
3	B	203[B]	CYC	C1C-NC	-9.72	1.25	1.37
3	C	101[B]	CYC	C1C-NC	-9.31	1.25	1.37
3	D	202[A]	CYC	C1C-NC	-9.30	1.25	1.37
3	D	203[B]	CYC	C1C-NC	-9.14	1.25	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	203[A]	CYC	C1C-NC	-9.11	1.25	1.37
3	B	202[A]	CYC	C1C-NC	-8.69	1.26	1.37
3	C	101[A]	CYC	C1C-NC	-7.42	1.28	1.37
3	B	202[B]	CYC	C4C-NC	-6.99	1.22	1.37
3	B	203[A]	CYC	C1C-NC	-6.82	1.28	1.37
3	A	101[A]	CYC	C1C-NC	-6.64	1.29	1.37
3	D	202[B]	CYC	C4C-NC	-6.62	1.23	1.37
3	A	101[B]	CYC	C4C-NC	-6.48	1.23	1.37
3	B	203[B]	CYC	C4C-NC	-6.08	1.24	1.37
3	C	101[B]	CYC	C4C-NC	-5.94	1.24	1.37
3	D	203[B]	CYC	C4C-NC	-5.84	1.25	1.37
3	B	202[B]	CYC	CHB-C4A	5.78	1.54	1.40
3	B	203[B]	CYC	CHB-C4A	5.64	1.53	1.40
3	D	202[B]	CYC	CHB-C4A	5.57	1.53	1.40
3	B	202[A]	CYC	C4C-NC	-5.41	1.26	1.37
3	C	101[B]	CYC	CHB-C4A	5.32	1.52	1.40
3	A	101[B]	CYC	CHB-C4A	5.31	1.52	1.40
3	D	203[B]	CYC	CHB-C4A	5.19	1.52	1.40
3	A	101[B]	CYC	C4B-C3B	-5.08	1.38	1.48
3	D	203[A]	CYC	C4C-NC	-5.06	1.26	1.37
3	C	101[B]	CYC	C4B-C3B	-5.05	1.38	1.48
3	D	203[A]	CYC	CHB-C4A	5.05	1.52	1.40
3	D	202[A]	CYC	CHB-C4A	4.97	1.52	1.40
3	B	202[A]	CYC	CHB-C4A	4.93	1.52	1.40
3	B	202[B]	CYC	C4B-C3B	-4.88	1.38	1.48
3	B	203[B]	CYC	C4B-C3B	-4.83	1.39	1.48
3	D	202[A]	CYC	C4C-NC	-4.82	1.27	1.37
3	A	101[A]	CYC	C4B-C3B	-4.78	1.39	1.48
3	C	101[A]	CYC	CHB-C4A	4.75	1.51	1.40
3	D	203[B]	CYC	C4B-C3B	-4.66	1.39	1.48
3	D	203[A]	CYC	C4B-C3B	-4.64	1.39	1.48
3	B	202[B]	CYC	CAC-C3C	-4.61	1.44	1.54
3	C	101[A]	CYC	C4B-C3B	-4.58	1.39	1.48
3	B	203[A]	CYC	CHA-C1A	4.58	1.38	1.35
3	C	101[A]	CYC	C4C-NC	-4.56	1.27	1.37
3	D	202[B]	CYC	C4B-C3B	-4.53	1.39	1.48
3	B	203[B]	CYC	CAC-C3C	-4.50	1.45	1.54
4	D	201[B]	AX9	C1C-C2C	-4.47	1.38	1.45
3	D	202[B]	CYC	CAC-C3C	-4.46	1.45	1.54
3	A	101[B]	CYC	CAC-C3C	-4.38	1.45	1.54
3	C	101[B]	CYC	CAC-C3C	-4.37	1.45	1.54
3	B	202[A]	CYC	C4B-C3B	-4.37	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	203[A]	CYC	C4B-C3B	-4.34	1.40	1.48
3	A	101[A]	CYC	CHB-C4A	4.18	1.50	1.40
3	B	203[A]	CYC	CHB-C4A	4.14	1.50	1.40
3	D	202[A]	CYC	CHA-C1A	4.08	1.38	1.35
3	D	202[A]	CYC	C4B-C3B	-4.05	1.40	1.48
3	C	101[B]	CYC	CHA-C1A	4.03	1.38	1.35
3	A	101[A]	CYC	C4C-NC	-4.02	1.28	1.37
3	D	202[B]	CYC	CHA-C1A	4.02	1.38	1.35
4	B	201[B]	AX9	C1C-C2C	-3.90	1.39	1.45
3	A	101[A]	CYC	CHA-C1A	3.85	1.38	1.35
3	D	203[A]	CYC	CHA-C1A	3.83	1.38	1.35
3	B	203[A]	CYC	C4C-NC	-3.80	1.29	1.37
3	A	101[A]	CYC	CAC-C3C	-3.77	1.46	1.54
3	B	202[A]	CYC	C2C-C3C	3.76	1.64	1.54
3	D	203[B]	CYC	CAC-C3C	-3.73	1.46	1.54
3	D	202[B]	CYC	C2C-C3C	3.73	1.64	1.54
3	B	203[B]	CYC	C1A-C2A	-3.67	1.39	1.45
3	A	101[B]	CYC	C1A-C2A	-3.66	1.39	1.45
4	D	201[A]	AX9	C1C-C2C	-3.65	1.39	1.45
3	D	203[B]	CYC	CHA-C1A	3.64	1.38	1.35
3	B	202[B]	CYC	C2C-C3C	3.63	1.64	1.54
3	B	202[B]	CYC	C1A-C2A	-3.63	1.39	1.45
3	A	101[B]	CYC	CHA-C1A	3.60	1.38	1.35
4	B	201[A]	AX9	C1C-C2C	-3.59	1.40	1.45
3	A	101[B]	CYC	C4D-CHA	3.59	1.55	1.41
3	A	101[B]	CYC	C2C-C3C	3.55	1.64	1.54
3	B	202[B]	CYC	C4D-CHA	3.54	1.54	1.41
3	D	202[A]	CYC	C2C-C3C	3.52	1.64	1.54
3	D	202[B]	CYC	C4D-CHA	3.50	1.54	1.41
3	D	202[B]	CYC	C1D-CHD	3.48	1.54	1.41
3	C	101[A]	CYC	CAC-C3C	-3.48	1.47	1.54
3	D	203[B]	CYC	C1D-CHD	3.48	1.54	1.41
3	D	203[A]	CYC	C2C-C3C	3.45	1.64	1.54
3	D	203[A]	CYC	CAC-C3C	-3.45	1.47	1.54
3	D	203[A]	CYC	C4D-CHA	3.45	1.54	1.41
3	A	101[B]	CYC	C1D-CHD	3.43	1.54	1.41
3	B	202[B]	CYC	C1D-CHD	3.42	1.54	1.41
3	D	203[B]	CYC	C1B-C2B	-3.39	1.39	1.45
4	D	201[B]	AX9	C1A-C2A	-3.37	1.38	1.47
3	A	101[A]	CYC	C1B-C2B	-3.37	1.39	1.45
3	A	101[B]	CYC	C1B-C2B	-3.37	1.39	1.45
3	B	203[B]	CYC	C4D-CHA	3.36	1.54	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	101[A]	CYC	CHA-C1A	3.35	1.37	1.35
3	C	101[A]	CYC	C1B-C2B	-3.35	1.39	1.45
3	D	203[A]	CYC	C1A-C2A	-3.33	1.40	1.45
4	D	201[B]	AX9	C4A-C3A	-3.33	1.38	1.45
4	D	201[A]	AX9	C4D-ND	3.33	1.39	1.35
3	D	203[B]	CYC	C2C-C3C	3.32	1.63	1.54
3	D	202[A]	CYC	CAC-C3C	-3.31	1.47	1.54
3	D	202[B]	CYC	C1A-C2A	-3.30	1.40	1.45
3	B	202[B]	CYC	CHA-C1A	3.30	1.37	1.35
3	B	203[B]	CYC	C1D-CHD	3.29	1.53	1.41
3	D	203[B]	CYC	C4D-CHA	3.28	1.53	1.41
3	C	101[B]	CYC	C4D-CHA	3.26	1.53	1.41
3	D	203[A]	CYC	C1B-C2B	-3.26	1.39	1.45
3	A	101[A]	CYC	C1A-C2A	-3.25	1.40	1.45
3	B	202[A]	CYC	C1A-C2A	-3.25	1.40	1.45
3	B	203[B]	CYC	C1B-C2B	-3.24	1.39	1.45
3	B	203[A]	CYC	C1B-C2B	-3.23	1.39	1.45
3	C	101[B]	CYC	C1A-C2A	-3.22	1.40	1.45
4	B	201[B]	AX9	C1A-C2A	-3.21	1.39	1.47
3	B	202[A]	CYC	CAC-C3C	-3.21	1.47	1.54
4	D	201[B]	AX9	CHC-C1D	-3.21	1.46	1.53
3	B	203[B]	CYC	CHA-C1A	3.21	1.37	1.35
3	D	202[A]	CYC	C1A-C2A	-3.21	1.40	1.45
3	B	203[B]	CYC	C2C-C3C	3.20	1.63	1.54
3	C	101[B]	CYC	C2C-C3C	3.20	1.63	1.54
3	A	101[A]	CYC	C4A-C3A	-3.17	1.39	1.45
4	D	201[B]	AX9	C4D-ND	3.16	1.39	1.35
3	B	202[A]	CYC	C1D-CHD	3.12	1.53	1.41
3	C	101[A]	CYC	C1A-C2A	-3.10	1.40	1.45
3	D	202[A]	CYC	C1D-CHD	3.09	1.53	1.41
3	D	203[A]	CYC	C1D-CHD	3.09	1.53	1.41
3	D	202[A]	CYC	C4D-CHA	3.07	1.53	1.41
4	D	201[A]	AX9	CHB-C1C	3.07	1.37	1.35
3	B	202[A]	CYC	C4D-CHA	3.06	1.53	1.41
3	D	203[B]	CYC	C1A-C2A	-3.06	1.40	1.45
3	B	202[B]	CYC	C1B-C2B	-3.05	1.39	1.45
4	B	201[B]	AX9	CHC-C1D	-3.05	1.47	1.53
3	B	203[A]	CYC	C2C-C3C	3.03	1.62	1.54
3	C	101[B]	CYC	C1D-CHD	3.02	1.52	1.41
4	B	201[B]	AX9	C4A-C3A	-3.00	1.39	1.45
4	B	201[A]	AX9	C1A-C2A	-2.95	1.39	1.47
3	D	202[B]	CYC	C1B-C2B	-2.94	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	101[A]	CYC	C4D-CHA	2.93	1.52	1.41
3	C	101[B]	CYC	C1B-C2B	-2.92	1.39	1.45
4	D	201[B]	AX9	C4B-CHB	2.87	1.52	1.41
3	B	203[A]	CYC	CAC-C3C	-2.87	1.48	1.54
4	B	201[B]	AX9	C4D-ND	2.85	1.38	1.35
3	A	101[A]	CYC	C2C-C3C	2.84	1.62	1.54
4	D	201[A]	AX9	C1A-C2A	-2.83	1.40	1.47
3	C	101[B]	CYC	C2C-C1C	-2.83	1.49	1.52
3	B	203[A]	CYC	C1A-C2A	-2.82	1.41	1.45
4	B	201[A]	AX9	C4B-CHB	2.82	1.52	1.41
4	B	201[A]	AX9	C4D-ND	2.82	1.38	1.35
3	C	101[A]	CYC	C1D-CHD	2.82	1.52	1.41
3	A	101[B]	CYC	C4A-C3A	-2.79	1.39	1.45
4	B	201[B]	AX9	C4B-CHB	2.79	1.51	1.41
4	D	201[A]	AX9	CHC-C1D	-2.77	1.47	1.53
4	B	201[A]	AX9	CHC-C1D	-2.77	1.47	1.53
4	B	201[A]	AX9	CHB-C1C	2.77	1.37	1.35
3	B	203[A]	CYC	C4A-C3A	-2.75	1.39	1.45
3	C	101[B]	CYC	C4A-C3A	-2.74	1.39	1.45
4	D	201[B]	AX9	C1B-CHA	2.73	1.51	1.41
3	B	203[A]	CYC	C1D-CHD	2.72	1.51	1.41
4	D	201[A]	AX9	C4A-C3A	-2.71	1.39	1.45
3	B	202[A]	CYC	CHA-C1A	2.69	1.37	1.35
4	D	201[A]	AX9	C4B-CHB	2.69	1.51	1.41
3	C	101[A]	CYC	C4A-C3A	-2.69	1.40	1.45
3	A	101[A]	CYC	C4D-CHA	2.69	1.51	1.41
3	C	101[A]	CYC	C2C-C3C	2.68	1.61	1.54
3	B	203[A]	CYC	C4D-CHA	2.65	1.51	1.41
3	D	202[A]	CYC	C1B-C2B	-2.64	1.40	1.45
4	B	201[B]	AX9	C1B-CHA	2.60	1.51	1.41
3	D	202[B]	CYC	C4A-C3A	-2.60	1.40	1.45
3	D	202[A]	CYC	C4A-C3A	-2.51	1.40	1.45
3	B	202[A]	CYC	C4A-C3A	-2.48	1.40	1.45
4	B	201[A]	AX9	C4A-C3A	-2.48	1.40	1.45
3	B	202[A]	CYC	C1B-C2B	-2.45	1.40	1.45
4	D	201[A]	AX9	C1B-CHA	2.44	1.50	1.41
3	B	202[B]	CYC	C4A-C3A	-2.41	1.40	1.45
4	D	201[B]	AX9	C4D-C3D	-2.41	1.43	1.48
3	A	101[A]	CYC	C1D-CHD	2.41	1.50	1.41
3	D	203[A]	CYC	C4A-C3A	-2.38	1.40	1.45
3	B	203[B]	CYC	C2C-C1C	-2.38	1.50	1.52
4	B	201[B]	AX9	C1D-ND	-2.35	1.42	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	201[A]	AX9	C1B-CHA	2.35	1.50	1.41
3	D	203[B]	CYC	C4A-C3A	-2.34	1.40	1.45
3	B	203[B]	CYC	C4A-C3A	-2.34	1.40	1.45
4	B	201[A]	AX9	C4D-C3D	-2.30	1.43	1.48
3	B	203[A]	CYC	C2C-C1C	-2.30	1.50	1.52
4	B	201[B]	AX9	C4D-C3D	-2.25	1.44	1.48
3	C	101[A]	CYC	C2C-C1C	-2.23	1.50	1.52
3	B	202[B]	CYC	C2C-C1C	-2.14	1.50	1.52
4	D	201[B]	AX9	C1D-ND	-2.14	1.42	1.45
3	D	202[B]	CYC	C2C-C1C	-2.13	1.50	1.52
4	B	201[A]	AX9	C1D-ND	-2.05	1.42	1.45
3	D	202[B]	CYC	CMC-C2C	-2.05	1.48	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	101[B]	CYC	OC-C1C-C2C	-7.86	119.92	126.17
3	C	101[A]	CYC	OC-C1C-C2C	-7.85	119.93	126.17
3	C	101[B]	CYC	C2C-C1C-NC	7.76	114.96	108.27
3	B	203[A]	CYC	OC-C1C-C2C	-7.55	120.17	126.17
3	B	203[B]	CYC	C2C-C1C-NC	7.42	114.67	108.27
3	B	202[B]	CYC	C2C-C1C-NC	7.23	114.51	108.27
3	B	203[B]	CYC	OC-C1C-C2C	-6.88	120.70	126.17
3	A	101[B]	CYC	C2C-C1C-NC	6.40	113.79	108.27
3	B	202[A]	CYC	OC-C1C-C2C	-6.39	121.10	126.17
3	D	203[A]	CYC	OC-C1C-C2C	-6.03	121.38	126.17
3	A	101[A]	CYC	OC-C1C-C2C	-5.78	121.57	126.17
3	D	202[A]	CYC	OC-C1C-C2C	-5.78	121.58	126.17
3	B	203[A]	CYC	C2C-C1C-NC	5.73	113.22	108.27
3	A	101[B]	CYC	OC-C1C-C2C	-5.61	121.71	126.17
3	D	203[B]	CYC	OC-C1C-C2C	-5.59	121.73	126.17
3	D	202[B]	CYC	C2C-C1C-NC	5.47	112.99	108.27
3	B	202[B]	CYC	OC-C1C-C2C	-5.42	121.86	126.17
3	C	101[A]	CYC	C2C-C1C-NC	5.26	112.81	108.27
3	D	202[A]	CYC	C2C-C1C-NC	4.82	112.43	108.27
3	D	202[B]	CYC	OC-C1C-C2C	-4.81	122.35	126.17
4	D	201[B]	AX9	C4B-CHB-C1C	-4.38	123.58	128.81
3	D	203[B]	CYC	C2C-C1C-NC	4.34	112.02	108.27
3	D	203[A]	CYC	C2C-C1C-NC	4.26	111.94	108.27
3	B	203[B]	CYC	C4D-CHA-C1A	-4.20	123.79	128.81
3	B	202[A]	CYC	C2C-C1C-NC	3.99	111.71	108.27
3	D	203[B]	CYC	CAB-C3B-C4B	3.88	127.50	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	202[A]	CYC	CAC-C3C-C4C	3.83	122.50	112.67
3	A	101[A]	CYC	C2C-C1C-NC	3.80	111.55	108.27
3	D	203[A]	CYC	CAB-C3B-C4B	3.72	127.26	121.38
3	B	203[A]	CYC	CHD-C4C-NC	3.48	129.35	125.20
3	D	202[B]	CYC	C2C-C3C-C4C	-3.48	96.12	101.34
3	D	203[A]	CYC	CBD-CAD-C3D	-3.46	106.72	112.62
3	D	202[B]	CYC	C4D-CHA-C1A	-3.45	124.69	128.81
3	A	101[A]	CYC	CHD-C4C-NC	3.44	129.30	125.20
3	C	101[A]	CYC	CHD-C4C-NC	3.26	129.08	125.20
3	B	202[B]	CYC	C4D-CHA-C1A	-3.25	124.92	128.81
3	D	203[B]	CYC	CBD-CAD-C3D	-3.23	107.11	112.62
3	B	203[A]	CYC	CAB-C3B-C4B	3.22	126.46	121.38
3	B	203[B]	CYC	CHD-C4C-NC	3.12	128.91	125.20
4	B	201[B]	AX9	C4B-CHB-C1C	-3.11	125.09	128.81
3	A	101[B]	CYC	CAB-C3B-C4B	3.06	126.21	121.38
3	B	203[B]	CYC	CBD-CAD-C3D	-3.03	107.45	112.62
3	D	203[A]	CYC	CAC-C3C-C4C	3.00	120.38	112.67
3	B	202[A]	CYC	CAC-C3C-C4C	2.94	120.23	112.67
3	C	101[B]	CYC	CAA-CBA-CGA	-2.92	107.32	113.60
3	B	202[A]	CYC	C2C-C3C-C4C	-2.91	96.98	101.34
3	A	101[B]	CYC	C4D-CHA-C1A	-2.90	125.35	128.81
3	B	203[A]	CYC	CAC-C3C-C4C	2.88	120.07	112.67
3	A	101[A]	CYC	CAB-C3B-C4B	2.88	125.92	121.38
3	B	203[A]	CYC	CHB-C4A-C3A	2.85	132.22	124.90
3	B	202[A]	CYC	O2A-CGA-CBA	2.80	123.02	114.03
3	B	203[A]	CYC	CHB-C4A-NA	-2.79	119.11	124.93
3	D	203[A]	CYC	CHD-C4C-NC	2.77	128.49	125.20
3	D	202[B]	CYC	CAB-C3B-C4B	2.76	125.74	121.38
3	D	202[A]	CYC	C2C-C3C-C4C	-2.76	97.21	101.34
3	A	101[B]	CYC	CAC-C3C-C4C	2.74	119.71	112.67
4	D	201[A]	AX9	C2C-C1C-NC	-2.71	106.11	110.05
3	B	202[B]	CYC	C2C-C3C-C4C	-2.68	97.32	101.34
3	D	202[A]	CYC	CAB-C3B-C4B	2.66	125.58	121.38
3	D	202[A]	CYC	CAA-CBA-CGA	-2.62	107.97	113.60
3	D	202[A]	CYC	CHB-C4A-NA	-2.62	119.46	124.93
3	B	202[B]	CYC	CAB-C3B-C4B	2.60	125.48	121.38
3	D	203[B]	CYC	CAC-C3C-C4C	2.56	119.24	112.67
3	C	101[A]	CYC	CAB-C3B-C4B	2.55	125.41	121.38
3	D	202[B]	CYC	CAC-C3C-C4C	2.55	119.22	112.67
3	B	203[A]	CYC	CBD-CAD-C3D	-2.53	108.30	112.62
3	B	202[A]	CYC	O2D-CGD-CBD	2.53	122.17	114.03
3	B	202[A]	CYC	CHB-C4A-NA	-2.52	119.67	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	101[A]	CYC	O2A-CGA-CBA	2.47	121.97	114.03
4	B	201[A]	AX9	C2C-C1C-NC	-2.45	106.49	110.05
3	D	202[B]	CYC	O2A-CGA-CBA	2.44	121.87	114.03
3	D	202[A]	CYC	CHB-C4A-C3A	2.42	131.12	124.90
3	C	101[B]	CYC	C2A-C1A-NA	-2.40	106.56	110.05
3	B	202[B]	CYC	CAA-CBA-CGA	-2.36	108.53	113.60
3	B	203[B]	CYC	CAB-C3B-C4B	2.35	125.10	121.38
3	D	203[A]	CYC	CHB-C4A-C3A	2.34	130.92	124.90
3	A	101[A]	CYC	C1B-NB-C4B	-2.34	107.69	110.67
3	A	101[B]	CYC	CAA-CBA-CGA	-2.31	108.63	113.60
3	B	202[A]	CYC	C3B-C4B-NB	2.30	108.63	106.78
3	A	101[A]	CYC	C3B-C4B-NB	2.30	108.63	106.78
4	D	201[B]	AX9	CAD-C3D-C4D	2.26	124.95	121.38
3	A	101[A]	CYC	O2A-CGA-CBA	2.25	121.26	114.03
3	B	202[A]	CYC	CHB-C4A-C3A	2.25	130.68	124.90
3	D	203[B]	CYC	C2C-C3C-C4C	-2.23	97.99	101.34
4	B	201[B]	AX9	CAD-C3D-C4D	2.22	124.89	121.38
4	B	201[B]	AX9	CHC-C1D-ND	-2.21	110.93	113.72
3	A	101[B]	CYC	CAC-C3C-C2C	-2.20	108.75	114.26
4	D	201[A]	AX9	CHC-C1D-ND	-2.20	110.94	113.72
4	D	201[B]	AX9	CMA-C2A-C1A	2.20	126.56	121.39
3	A	101[B]	CYC	OB-C4B-C3B	-2.18	125.68	128.04
3	B	202[B]	CYC	CAC-C3C-C4C	2.13	118.14	112.67
3	B	203[A]	CYC	C2A-C1A-NA	-2.12	106.96	110.05
4	D	201[A]	AX9	O1C-CGC-CBC	2.11	120.82	114.03
3	D	203[B]	CYC	CHB-C4A-C3A	2.10	130.31	124.90
3	C	101[B]	CYC	CAB-C3B-C4B	2.10	124.70	121.38
3	C	101[B]	CYC	C1A-C2A-C3A	2.10	109.11	106.78
4	B	201[A]	AX9	CHC-C1D-ND	-2.09	111.08	113.72
3	D	203[A]	CYC	C2C-C3C-C4C	-2.07	98.24	101.34
3	D	203[B]	CYC	C2A-C1A-NA	-2.07	107.04	110.05
3	D	203[A]	CYC	C1B-NB-C4B	-2.06	108.04	110.67
4	D	201[B]	AX9	C2C-C1C-NC	-2.05	107.06	110.05
4	B	201[B]	AX9	C2C-C1C-NC	-2.05	107.07	110.05
3	A	101[B]	CYC	C3B-C4B-NB	2.03	108.42	106.78
3	D	203[B]	CYC	CHD-C4C-NC	2.00	127.59	125.20
3	D	203[B]	CYC	O2D-CGD-CBD	2.00	120.46	114.03
3	A	101[A]	CYC	C2A-C1A-NA	-2.00	107.14	110.05

There are no chirality outliers.

All (126) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	101[A]	CYC	NA-C4A-CHB-C1B
3	A	101[A]	CYC	C3A-C4A-CHB-C1B
3	A	101[B]	CYC	NA-C4A-CHB-C1B
3	A	101[B]	CYC	C3A-C4A-CHB-C1B
3	A	101[B]	CYC	C4C-C3C-CAC-CBC
3	B	202[A]	CYC	NA-C4A-CHB-C1B
3	B	202[A]	CYC	C3A-C4A-CHB-C1B
3	B	202[A]	CYC	C4C-C3C-CAC-CBC
3	B	202[A]	CYC	ND-C1D-CHD-C4C
3	B	202[B]	CYC	NA-C4A-CHB-C1B
3	B	202[B]	CYC	C3A-C4A-CHB-C1B
3	B	202[B]	CYC	C4C-C3C-CAC-CBC
3	B	203[A]	CYC	NA-C4A-CHB-C1B
3	B	203[A]	CYC	C3A-C4A-CHB-C1B
3	B	203[A]	CYC	C4B-C3B-CAB-CBB
3	B	203[A]	CYC	ND-C1D-CHD-C4C
3	B	203[A]	CYC	C2D-C1D-CHD-C4C
3	B	203[B]	CYC	NA-C4A-CHB-C1B
3	B	203[B]	CYC	C3A-C4A-CHB-C1B
3	B	203[B]	CYC	C4B-C3B-CAB-CBB
3	B	203[B]	CYC	ND-C1D-CHD-C4C
3	B	203[B]	CYC	C2D-C1D-CHD-C4C
3	C	101[A]	CYC	NA-C4A-CHB-C1B
3	C	101[A]	CYC	C3A-C4A-CHB-C1B
3	C	101[A]	CYC	ND-C1D-CHD-C4C
3	C	101[B]	CYC	NA-C4A-CHB-C1B
3	C	101[B]	CYC	C3A-C4A-CHB-C1B
3	C	101[B]	CYC	C2D-C1D-CHD-C4C
3	D	202[A]	CYC	NA-C4A-CHB-C1B
3	D	202[A]	CYC	C3A-C4A-CHB-C1B
3	D	202[A]	CYC	ND-C1D-CHD-C4C
3	D	202[B]	CYC	NA-C4A-CHB-C1B
3	D	202[B]	CYC	C3A-C4A-CHB-C1B
3	D	202[B]	CYC	C2C-C3C-CAC-CBC
3	D	202[B]	CYC	C4C-C3C-CAC-CBC
3	D	202[B]	CYC	ND-C1D-CHD-C4C
3	D	202[B]	CYC	C2D-C1D-CHD-C4C
3	D	203[A]	CYC	NA-C4A-CHB-C1B
3	D	203[A]	CYC	C3A-C4A-CHB-C1B
3	D	203[A]	CYC	ND-C1D-CHD-C4C
3	D	203[A]	CYC	C2D-C1D-CHD-C4C
3	D	203[B]	CYC	NA-C4A-CHB-C1B
3	D	203[B]	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
4	B	201[A]	AX9	NB-C1B-CHA-C4A
4	B	201[A]	AX9	NC-C4C-CHC-C1D
4	B	201[B]	AX9	NB-C1B-CHA-C4A
4	B	201[B]	AX9	C2B-C1B-CHA-C4A
4	B	201[B]	AX9	NC-C4C-CHC-C1D
4	D	201[A]	AX9	NB-C1B-CHA-C4A
4	D	201[A]	AX9	NC-C4C-CHC-C1D
4	D	201[B]	AX9	NB-C1B-CHA-C4A
4	D	201[B]	AX9	NC-C4C-CHC-C1D
3	B	203[A]	CYC	C2B-C3B-CAB-CBB
3	D	203[A]	CYC	C2B-C3B-CAB-CBB
3	B	203[B]	CYC	C2B-C3B-CAB-CBB
3	D	203[B]	CYC	C2B-C3B-CAB-CBB
4	D	201[A]	AX9	C4A-C3A-CAA-CBA
4	D	201[A]	AX9	C2A-C3A-CAA-CBA
4	B	201[A]	AX9	C2A-C3A-CAA-CBA
3	D	203[A]	CYC	C4B-C3B-CAB-CBB
3	D	203[B]	CYC	C4B-C3B-CAB-CBB
4	B	201[A]	AX9	C4A-C3A-CAA-CBA
3	D	202[B]	CYC	NC-C4C-CHD-C1D
3	B	202[B]	CYC	C2C-C3C-CAC-CBC
4	D	201[B]	AX9	C3B-CAB-CBB-CGB
4	B	201[A]	AX9	C2D-C3D-CAD-CBD
3	D	202[A]	CYC	C4C-C3C-CAC-CBC
3	B	202[A]	CYC	C2C-C3C-CAC-CBC
3	B	203[B]	CYC	NA-C1A-CHA-C4D
4	D	201[A]	AX9	C2D-C3D-CAD-CBD
3	D	202[B]	CYC	C2B-C3B-CAB-CBB
3	B	202[A]	CYC	CAA-CBA-CGA-O1A
3	B	202[B]	CYC	CAD-CBD-CGD-O1D
4	D	201[B]	AX9	CAB-CBB-CGB-O2B
3	D	203[A]	CYC	CAA-CBA-CGA-O2A
3	D	203[A]	CYC	CAD-CBD-CGD-O1D
3	B	203[B]	CYC	CAD-CBD-CGD-O1D
3	C	101[A]	CYC	CAD-CBD-CGD-O1D
3	D	203[B]	CYC	CAA-CBA-CGA-O1A
3	C	101[B]	CYC	CAA-CBA-CGA-O1A
3	D	202[B]	CYC	CAA-CBA-CGA-O1A
3	D	203[A]	CYC	CAA-CBA-CGA-O1A
3	A	101[A]	CYC	CAD-CBD-CGD-O1D
3	B	203[B]	CYC	CAD-CBD-CGD-O2D
3	D	202[A]	CYC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	203[B]	CYC	CAA-CBA-CGA-O2A
3	A	101[B]	CYC	CAA-CBA-CGA-O1A
3	C	101[B]	CYC	CAD-CBD-CGD-O1D
4	D	201[A]	AX9	CAB-CBB-CGB-O2B
3	A	101[A]	CYC	CAD-CBD-CGD-O2D
3	A	101[B]	CYC	CAD-CBD-CGD-O1D
4	D	201[A]	AX9	CAC-CBC-CGC-O2C
3	C	101[A]	CYC	CAD-CBD-CGD-O2D
4	D	201[A]	AX9	CAB-CBB-CGB-O1B
3	A	101[B]	CYC	CAA-CBA-CGA-O2A
3	A	101[B]	CYC	CAD-CBD-CGD-O2D
3	B	202[A]	CYC	CAA-CBA-CGA-O2A
3	B	202[B]	CYC	CAD-CBD-CGD-O2D
3	D	202[A]	CYC	CAA-CBA-CGA-O2A
3	B	202[B]	CYC	C2B-C3B-CAB-CBB
4	B	201[A]	AX9	CAB-CBB-CGB-O2B
3	D	203[A]	CYC	CAD-CBD-CGD-O2D
3	C	101[B]	CYC	CAA-CBA-CGA-O2A
4	B	201[A]	AX9	CAB-CBB-CGB-O1B
3	B	202[B]	CYC	CAA-CBA-CGA-O2A
4	D	201[A]	AX9	CAC-CBC-CGC-O1C
4	D	201[B]	AX9	CAB-CBB-CGB-O1B
3	B	203[A]	CYC	CAA-CBA-CGA-O2A
4	D	201[B]	AX9	CAC-CBC-CGC-O2C
3	C	101[B]	CYC	CAD-CBD-CGD-O2D
3	B	202[B]	CYC	CAA-CBA-CGA-O1A
3	D	202[B]	CYC	CAA-CBA-CGA-O2A
4	B	201[B]	AX9	CAB-CBB-CGB-O2B
3	B	203[A]	CYC	CAA-CBA-CGA-O1A
4	B	201[A]	AX9	CAC-CBC-CGC-O1C
3	A	101[A]	CYC	CAA-CBA-CGA-O1A
4	B	201[B]	AX9	CAB-CBB-CGB-O1B
4	B	201[A]	AX9	CAC-CBC-CGC-O2C
3	A	101[A]	CYC	CAA-CBA-CGA-O2A
3	D	202[B]	CYC	CAD-CBD-CGD-O2D
4	D	201[B]	AX9	CAC-CBC-CGC-O1C
3	B	202[A]	CYC	CAD-CBD-CGD-O1D
3	D	202[B]	CYC	CAD-CBD-CGD-O1D
3	B	202[A]	CYC	CAD-CBD-CGD-O2D
3	D	202[A]	CYC	C2C-C3C-CAC-CBC
3	B	202[A]	CYC	C2B-C3B-CAB-CBB

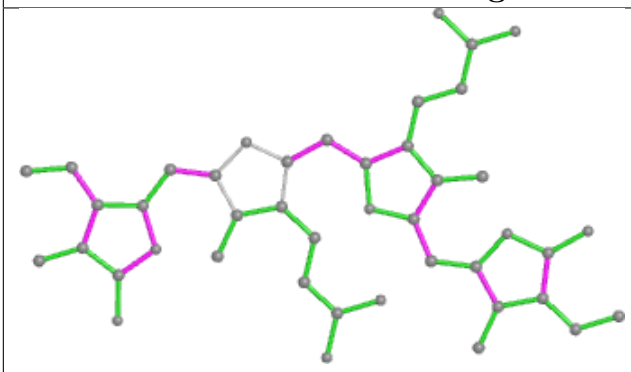
There are no ring outliers.

11 monomers are involved in 17 short contacts:

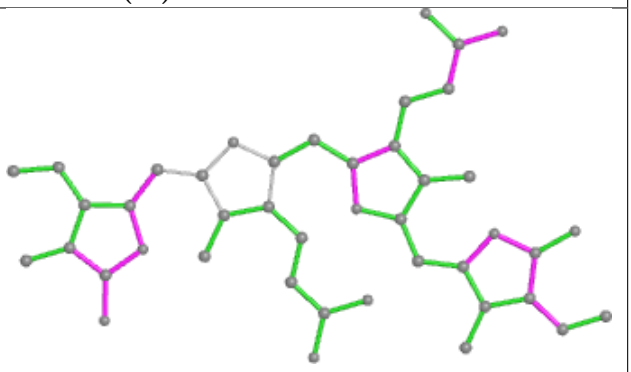
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203[B]	CYC	2	0
3	C	101[B]	CYC	1	0
3	D	202[A]	CYC	1	0
3	D	203[B]	CYC	3	0
3	C	101[A]	CYC	1	0
3	B	202[A]	CYC	1	0
3	A	101[B]	CYC	1	0
3	D	203[A]	CYC	2	0
3	B	202[B]	CYC	3	0
3	D	202[B]	CYC	1	0
3	B	203[A]	CYC	1	0

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.

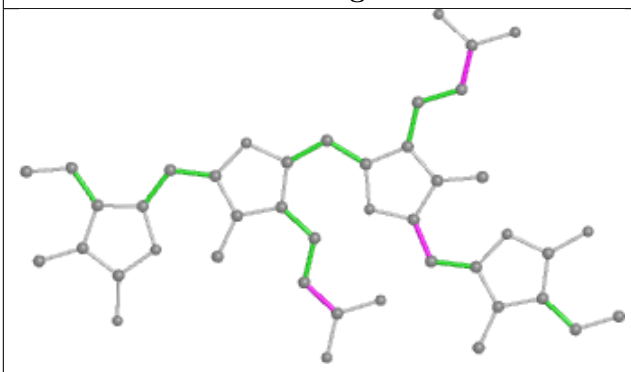
Ligand CYC A 101 (A)



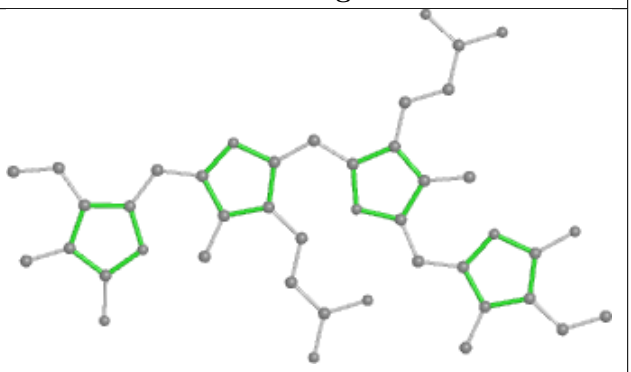
Bond lengths



Bond angles

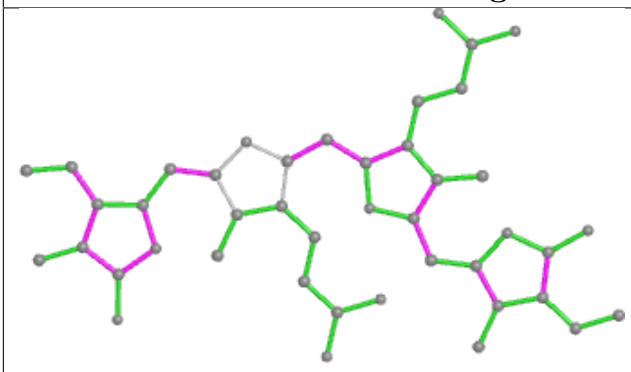


Torsions

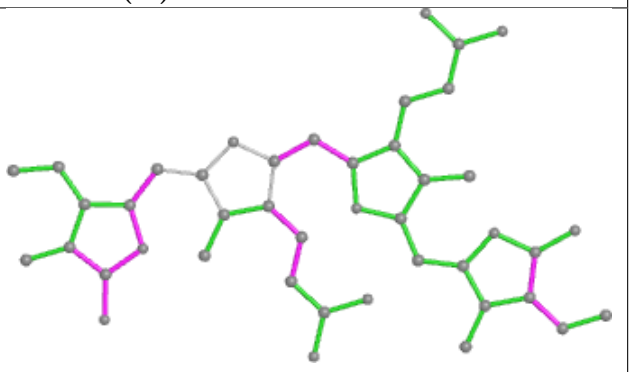


Rings

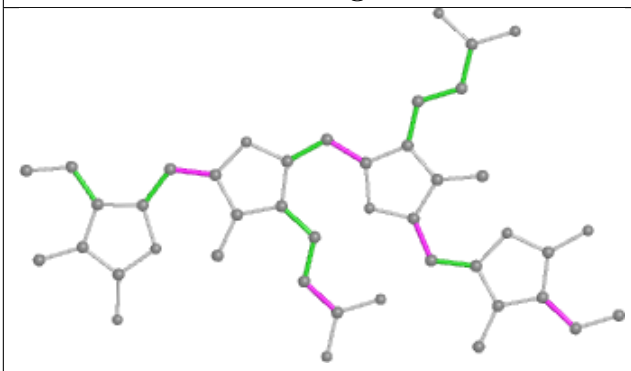
Ligand CYC B 203 (B)



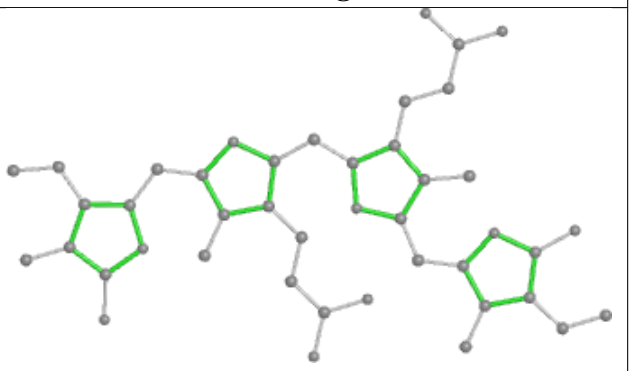
Bond lengths



Bond angles

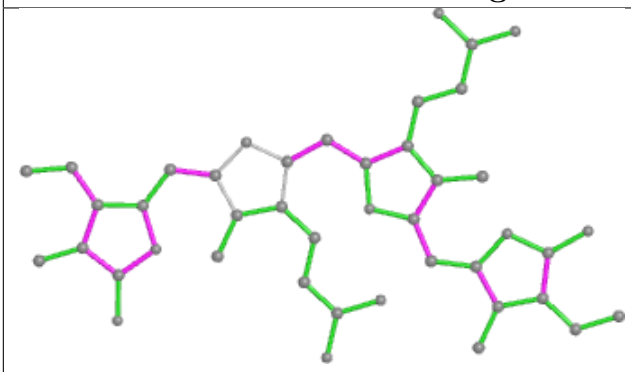


Torsions

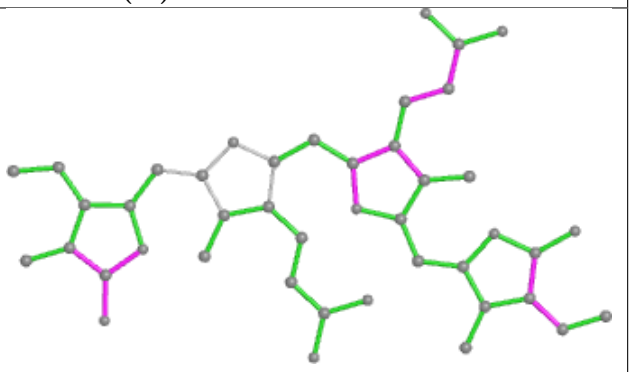


Rings

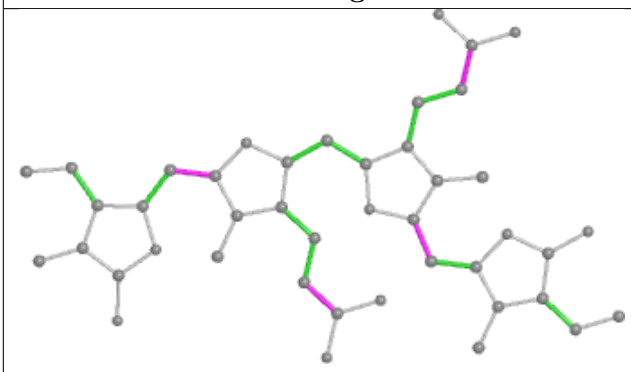
Ligand CYC C 101 (B)



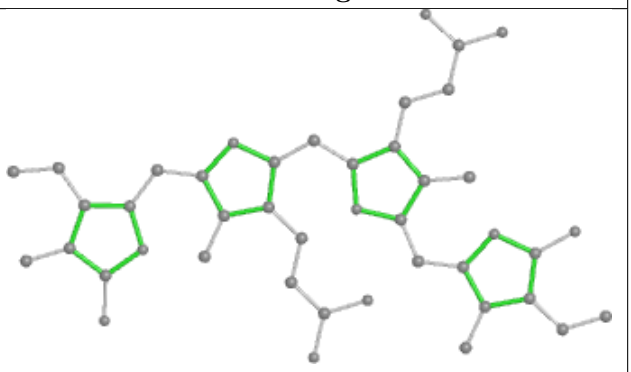
Bond lengths



Bond angles

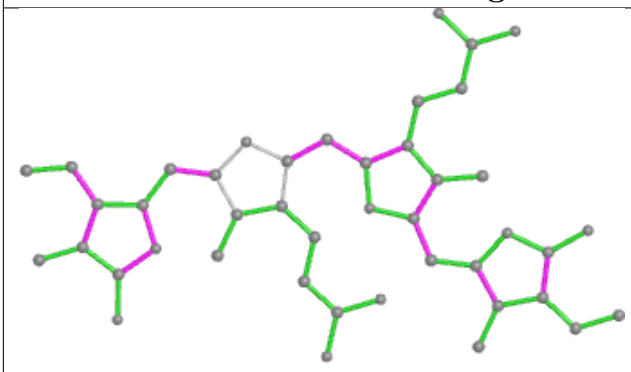


Torsions

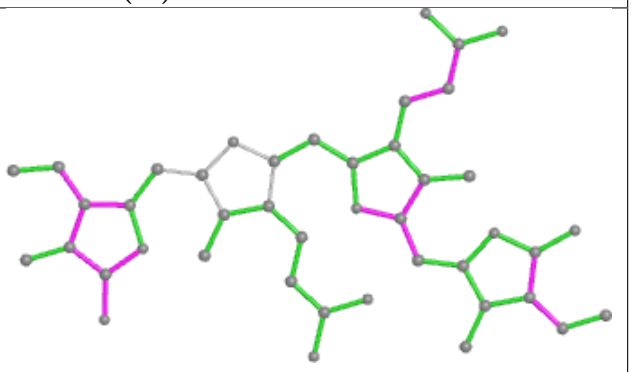


Rings

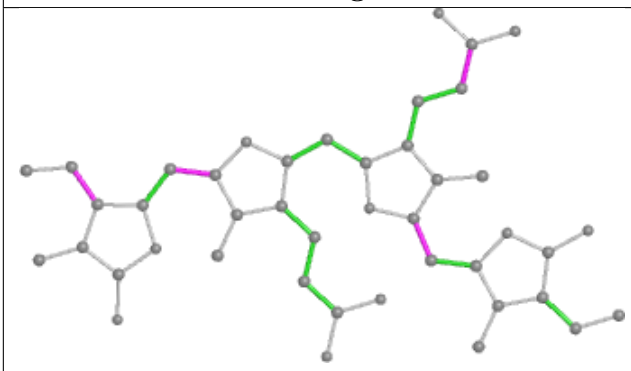
Ligand CYC D 202 (A)



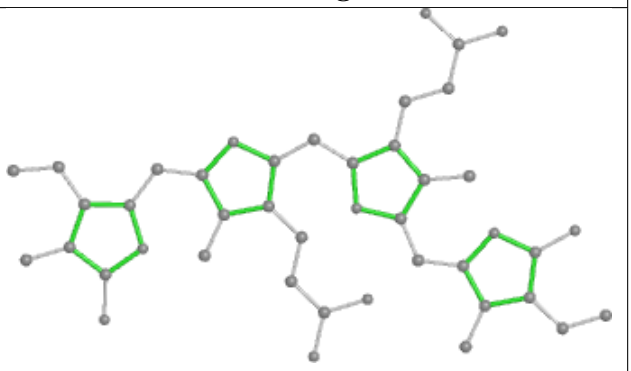
Bond lengths



Bond angles

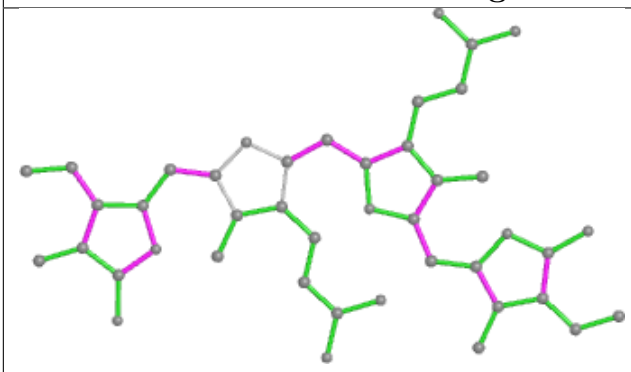


Torsions

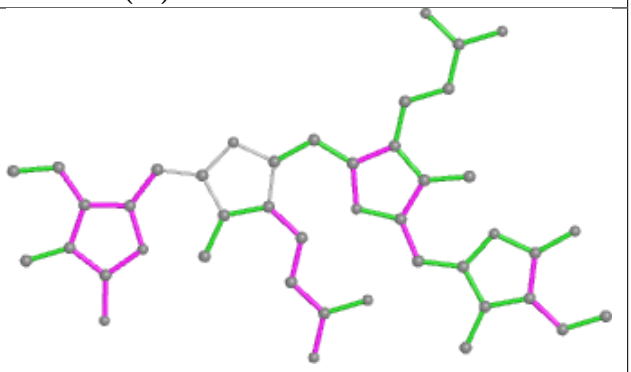


Rings

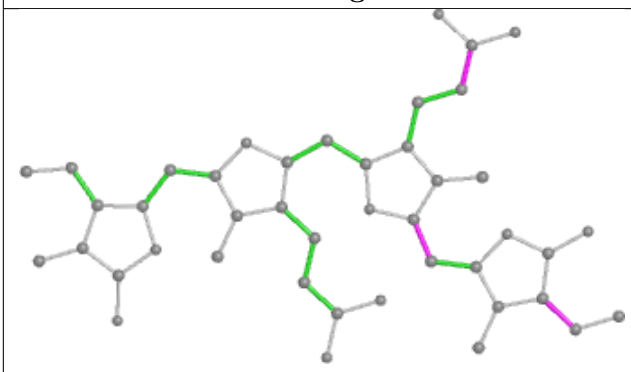
Ligand CYC D 203 (B)



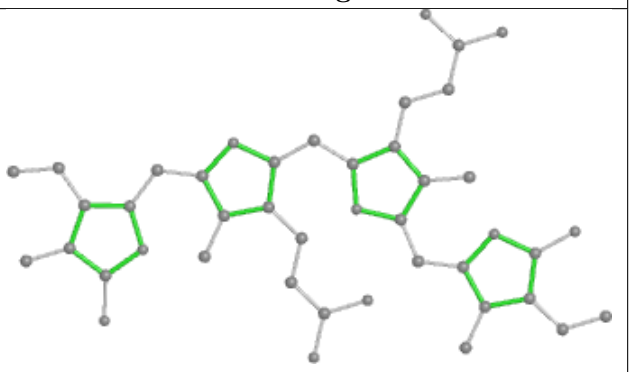
Bond lengths



Bond angles

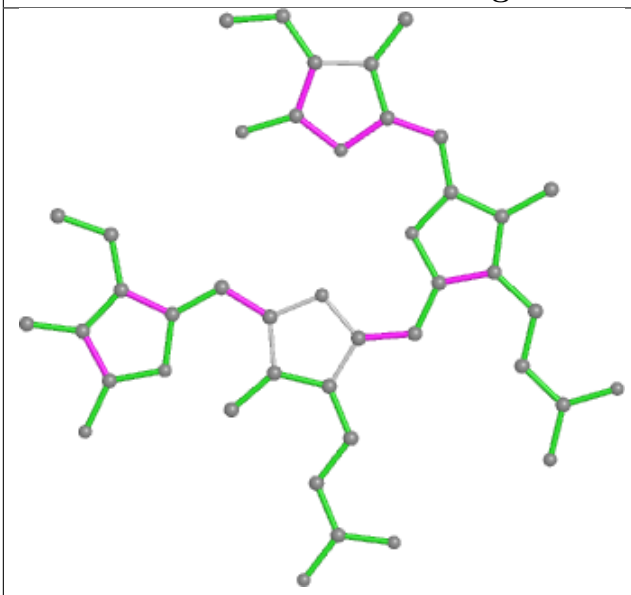


Torsions

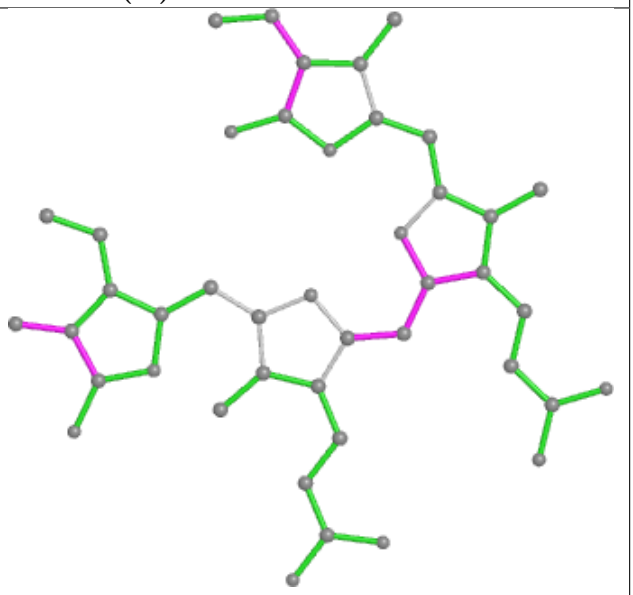


Rings

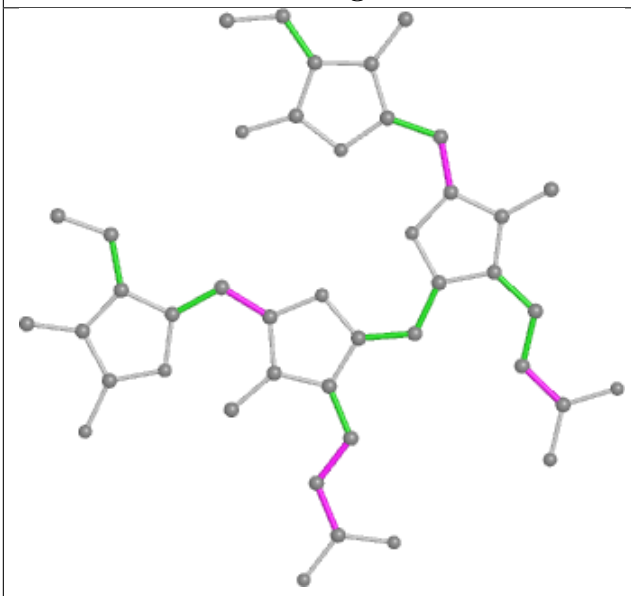
Ligand AX9 D 201 (B)



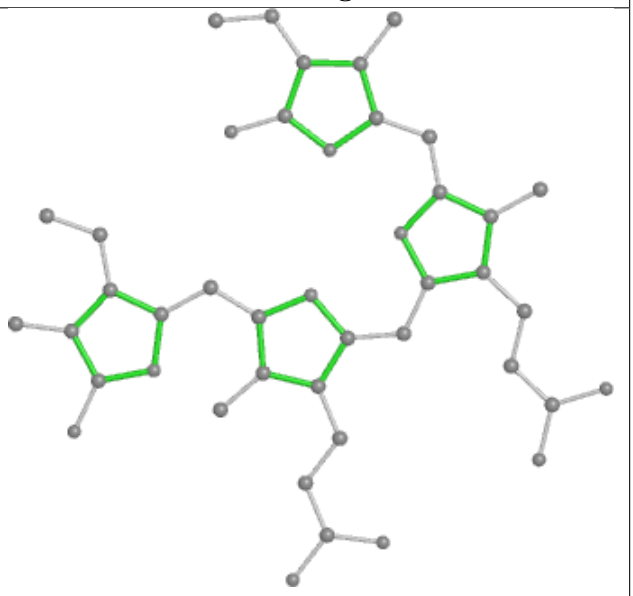
Bond lengths



Bond angles

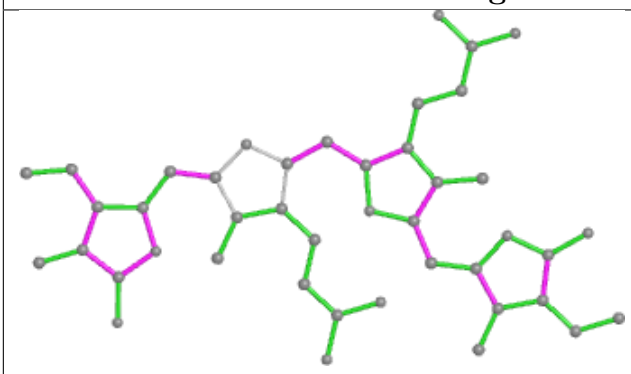


Torsions

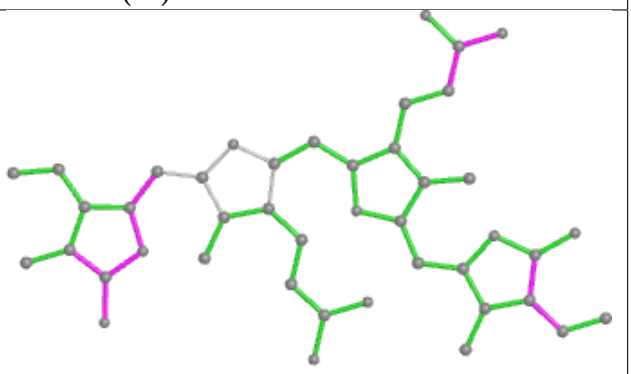


Rings

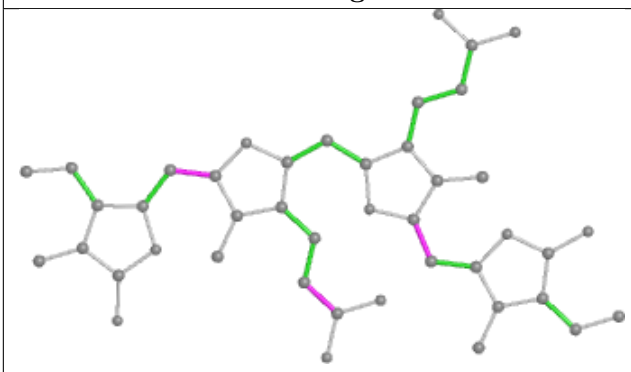
Ligand CYC C 101 (A)



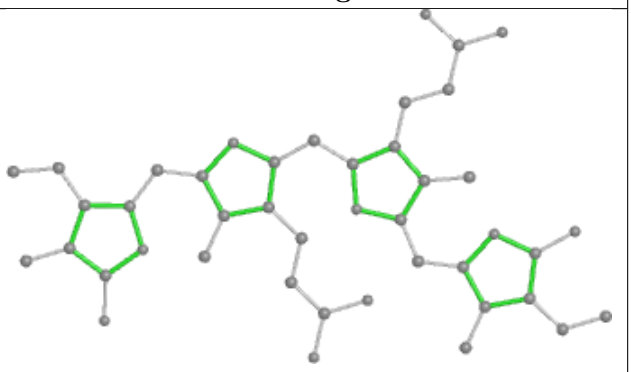
Bond lengths



Bond angles

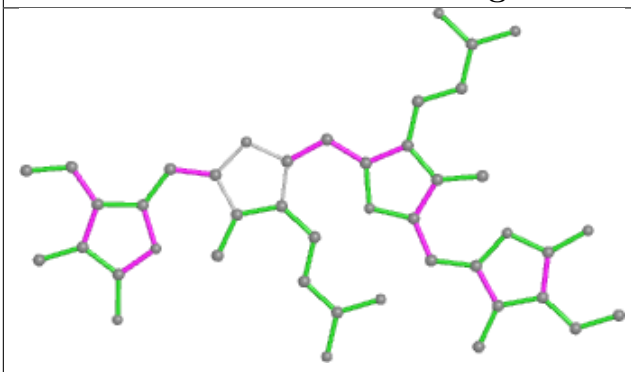


Torsions

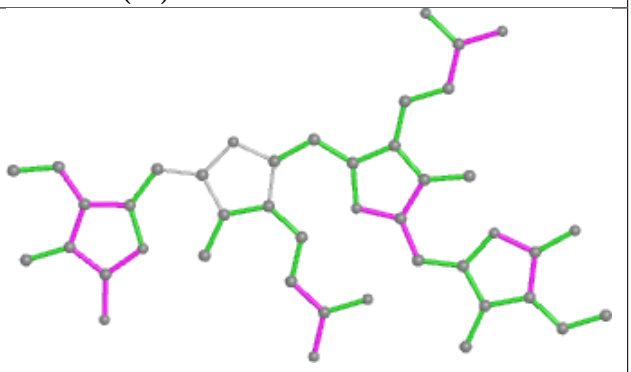


Rings

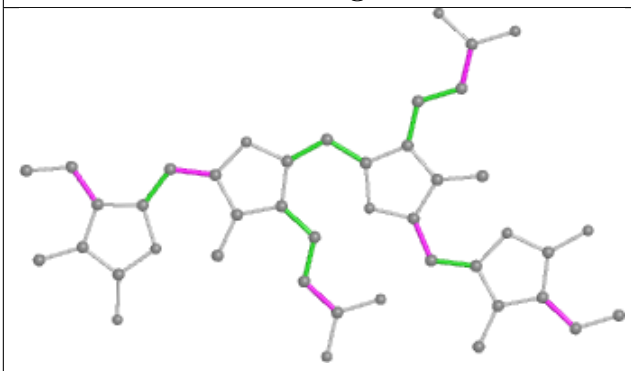
Ligand CYC B 202 (A)



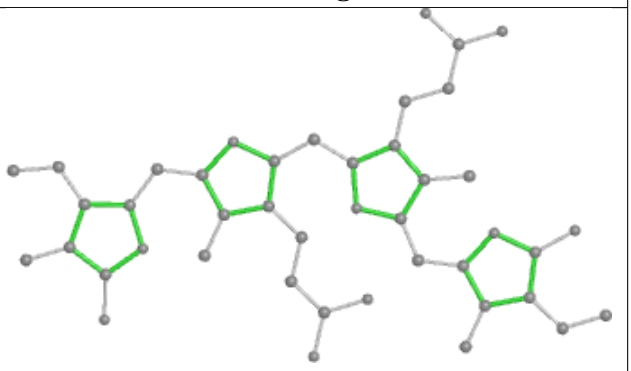
Bond lengths



Bond angles

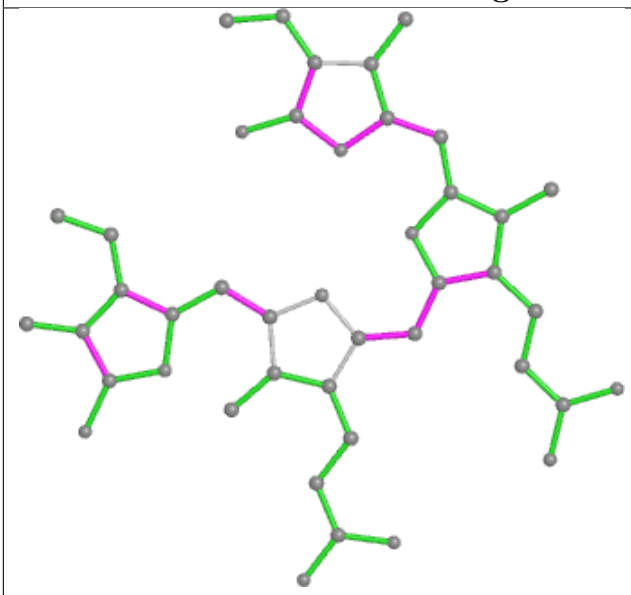


Torsions

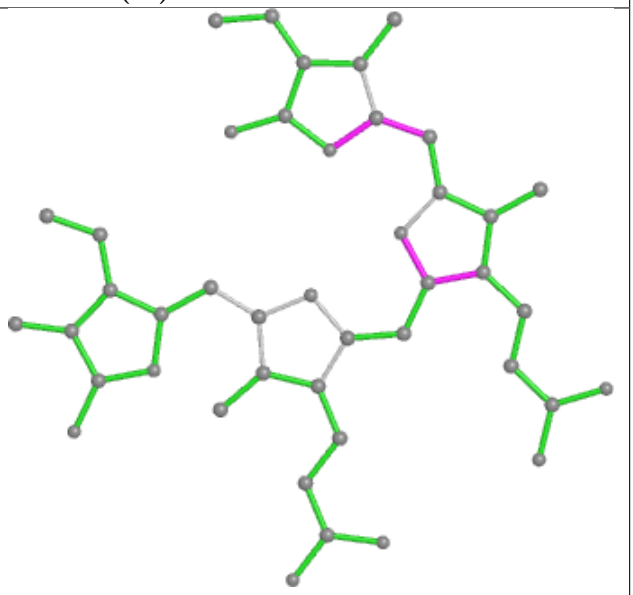


Rings

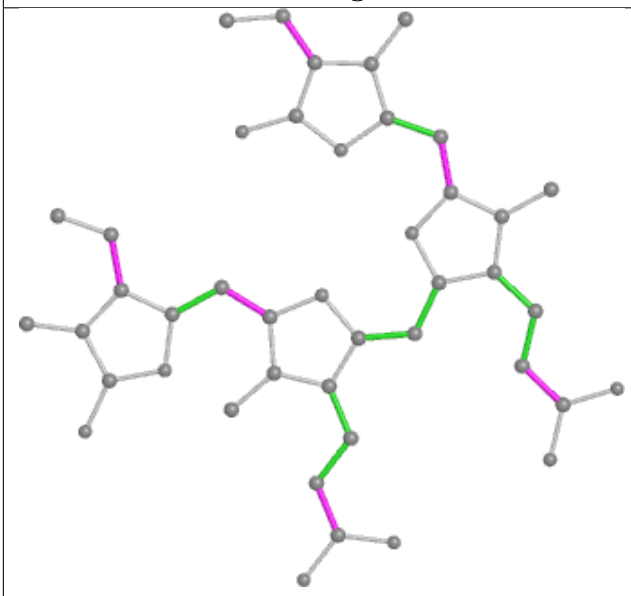
Ligand AX9 B 201 (A)



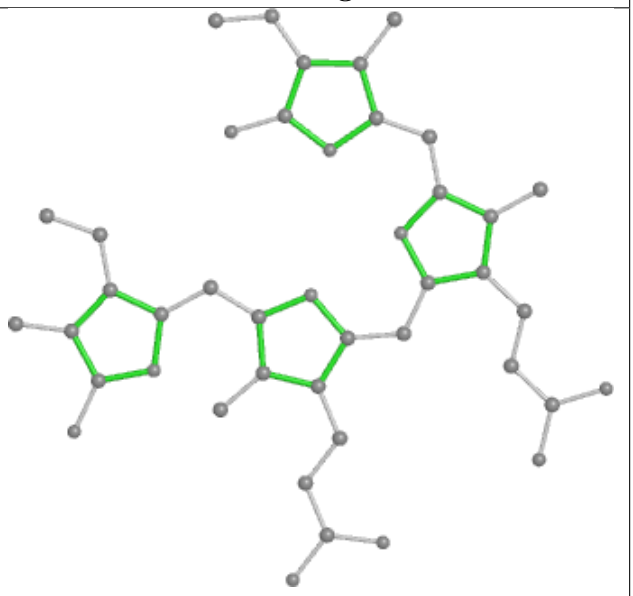
Bond lengths



Bond angles

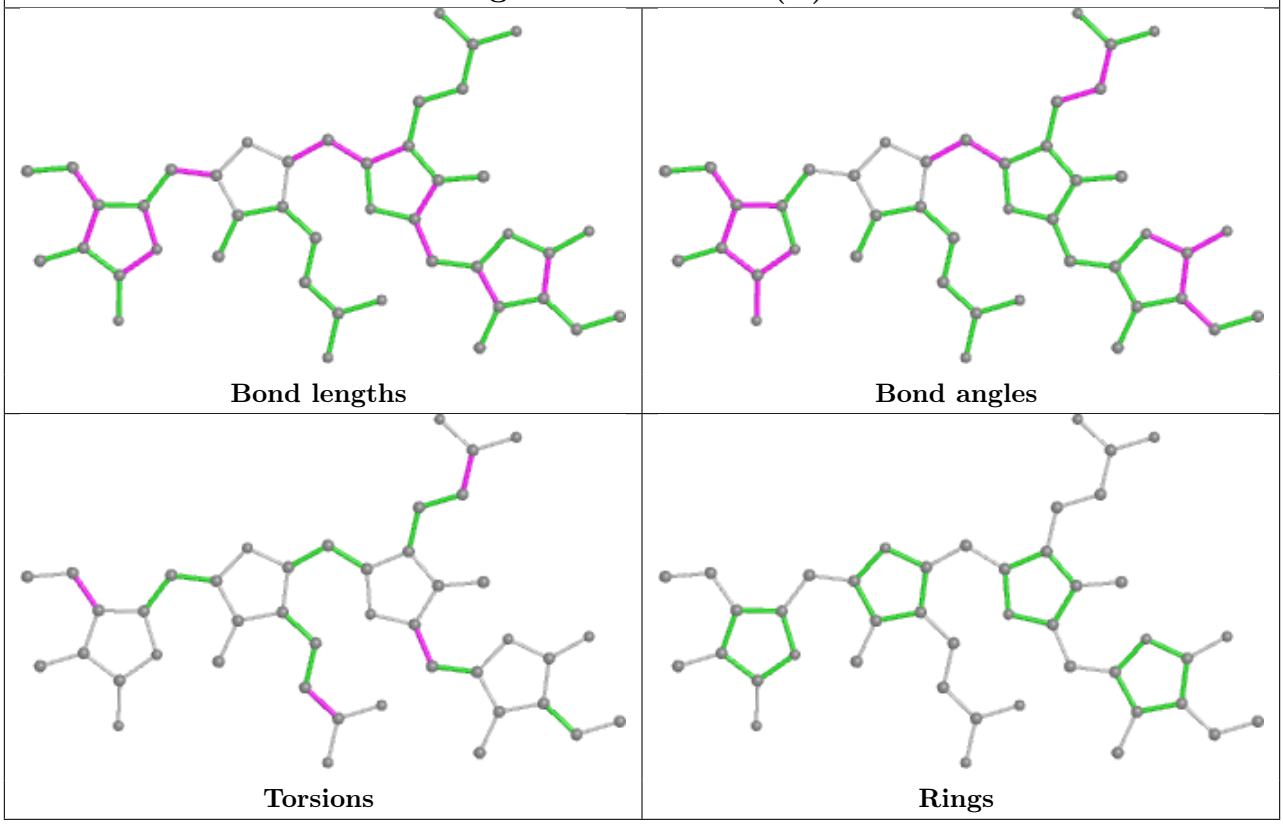


Torsions

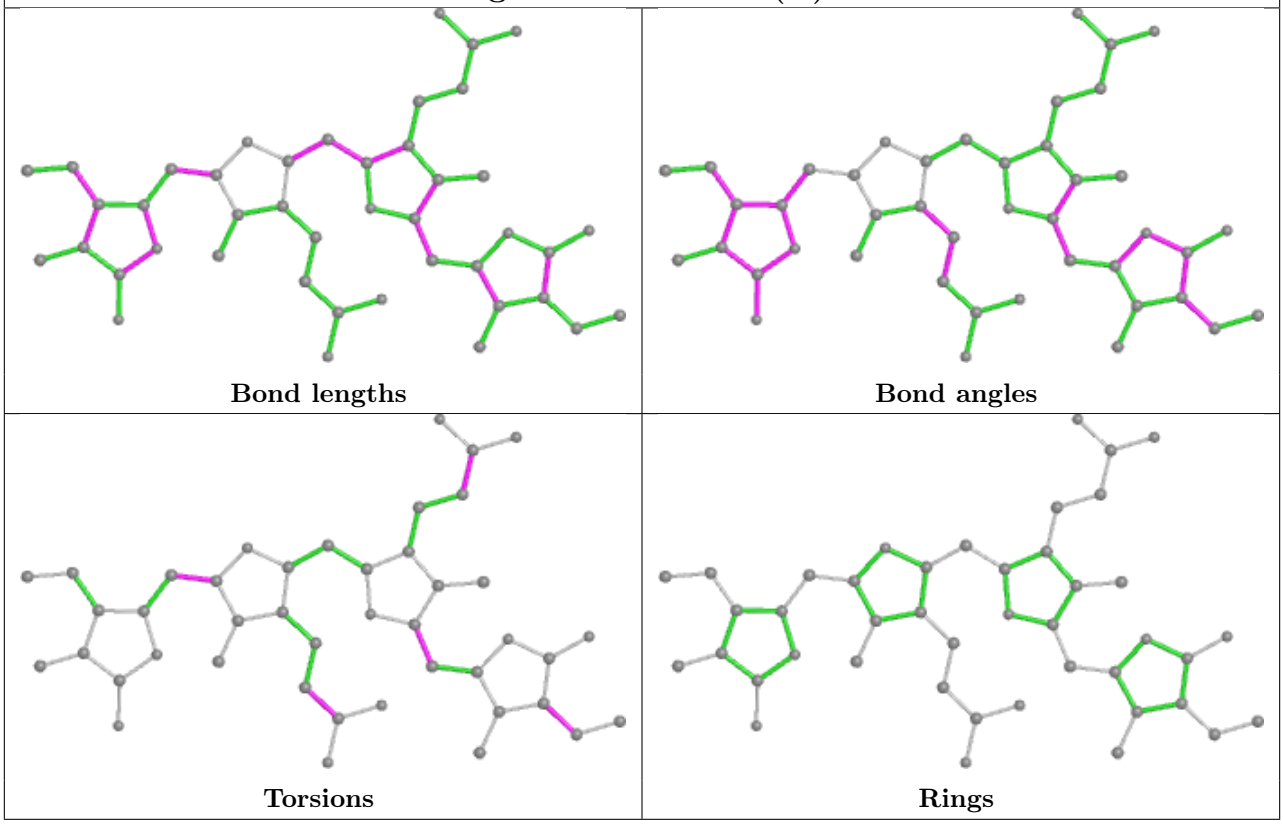


Rings

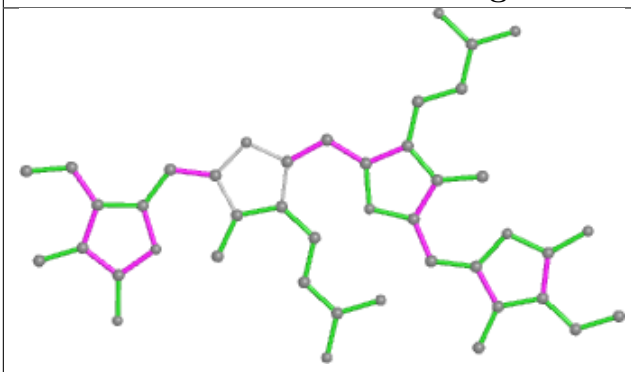
Ligand CYC A 101 (B)



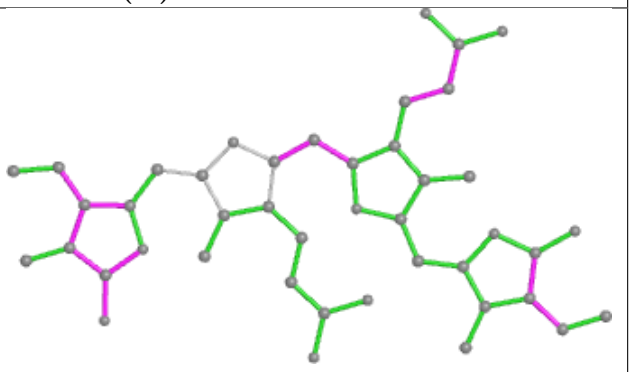
Ligand CYC D 203 (A)



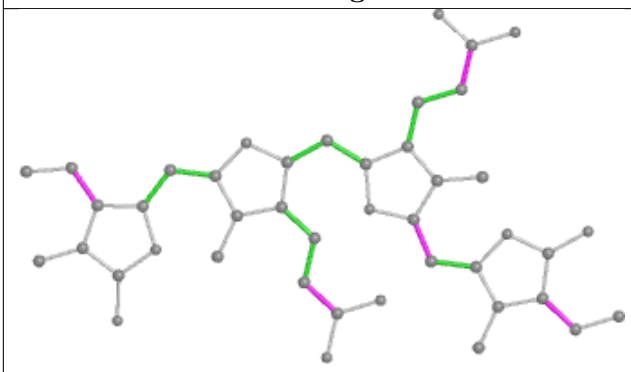
Ligand CYC B 202 (B)



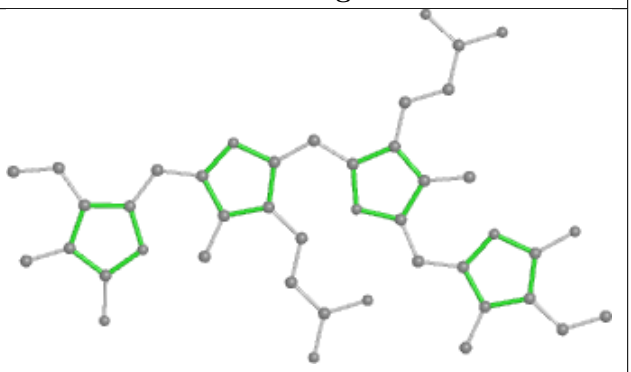
Bond lengths



Bond angles

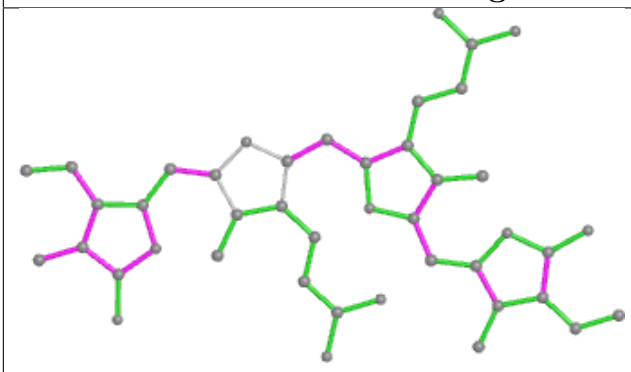


Torsions

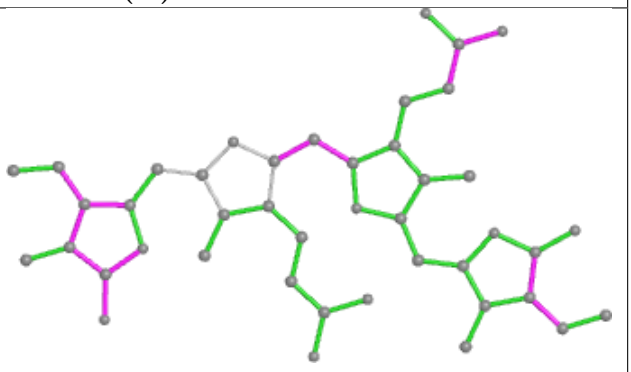


Rings

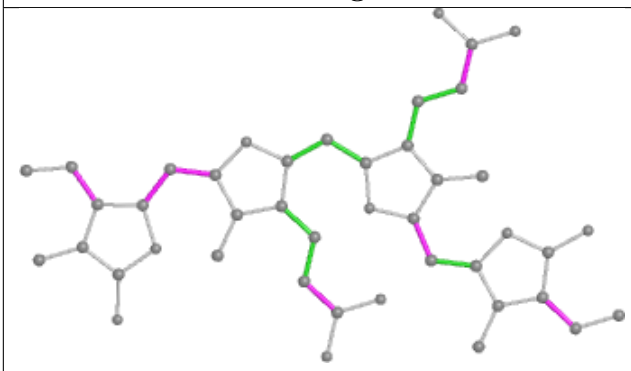
Ligand CYC D 202 (B)



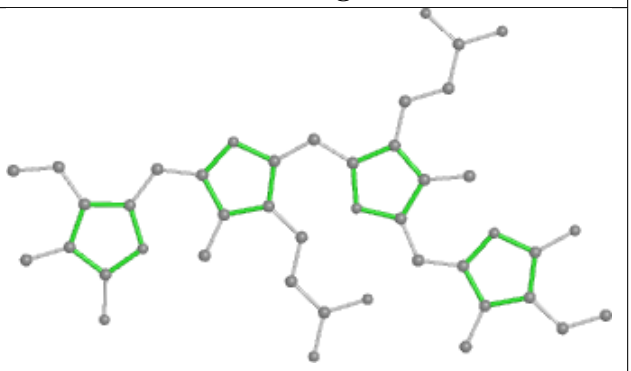
Bond lengths



Bond angles

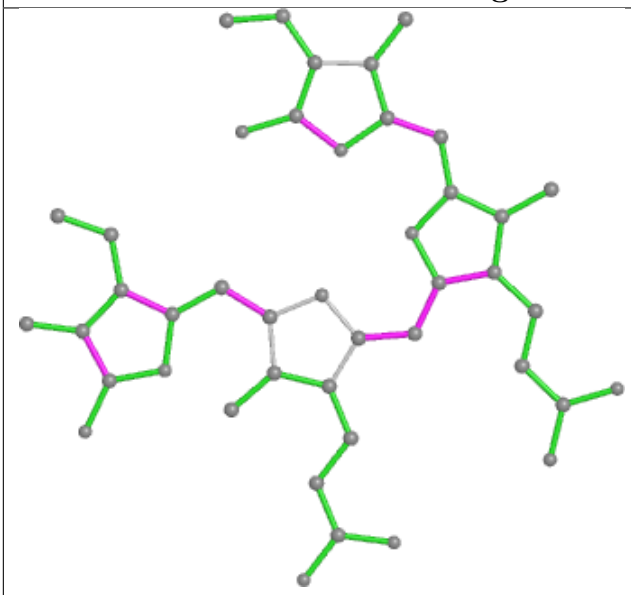


Torsions

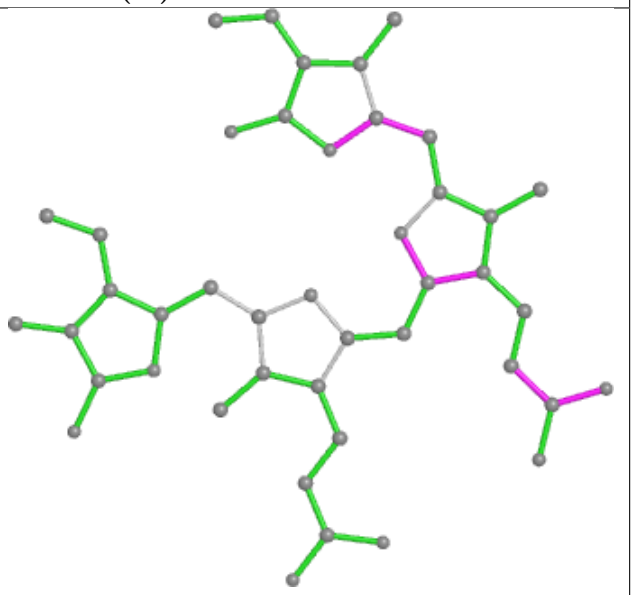


Rings

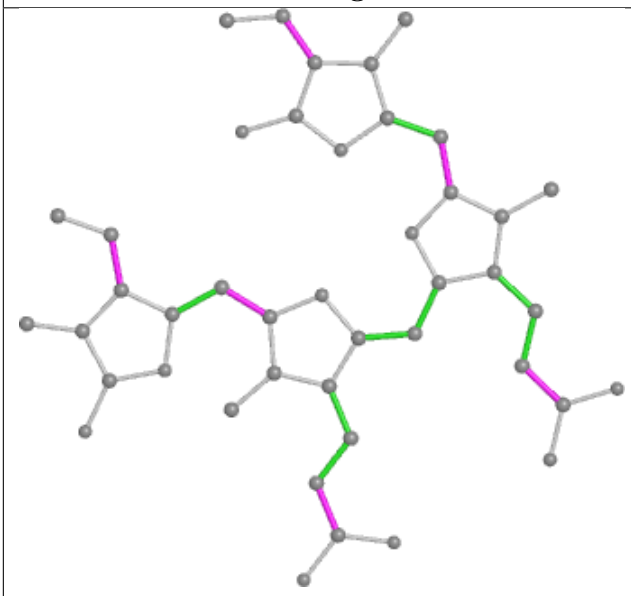
Ligand AX9 D 201 (A)



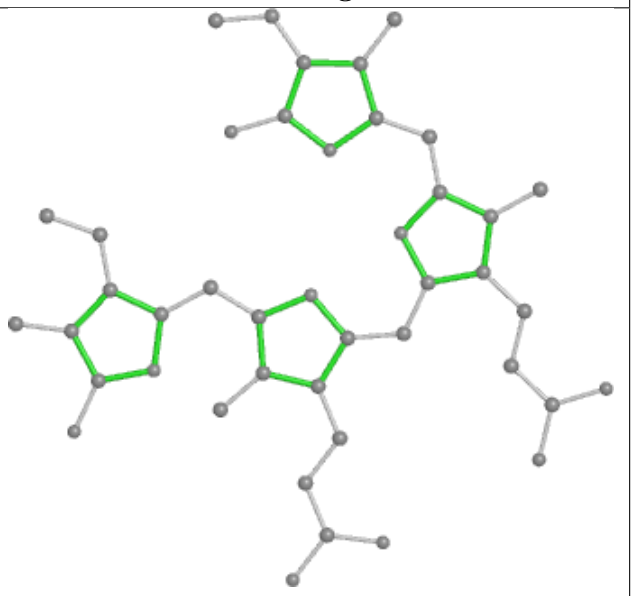
Bond lengths



Bond angles

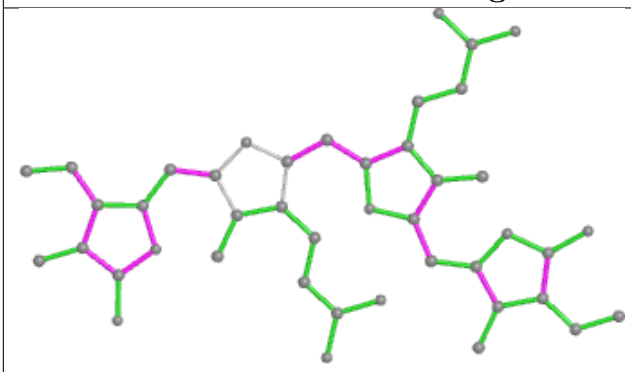


Torsions

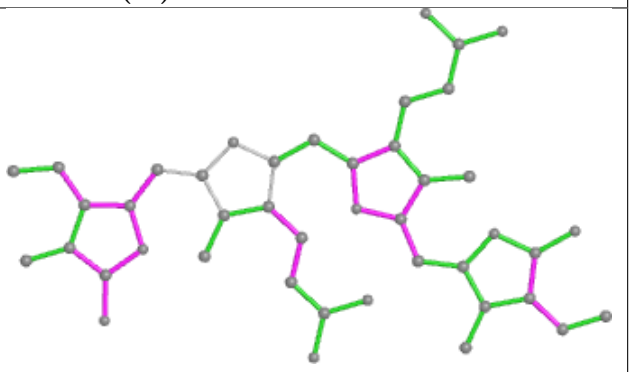


Rings

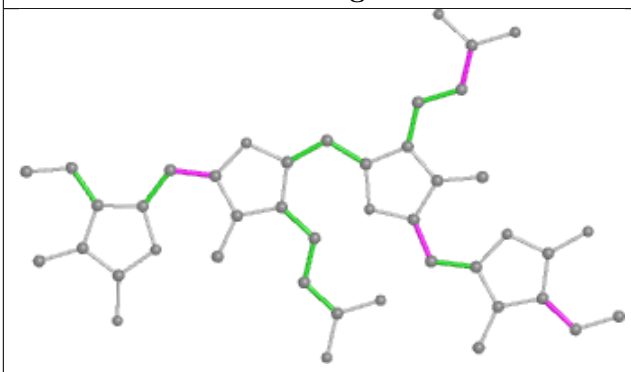
Ligand CYC B 203 (A)



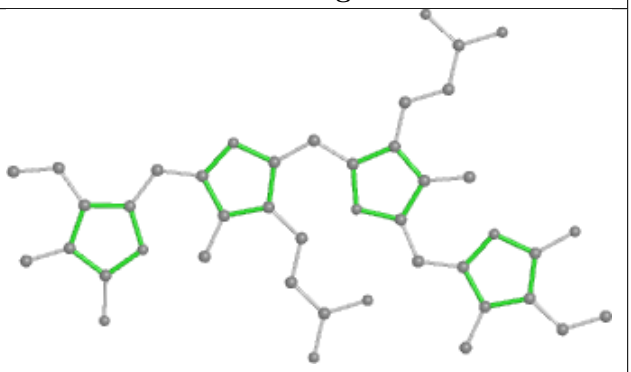
Bond lengths



Bond angles

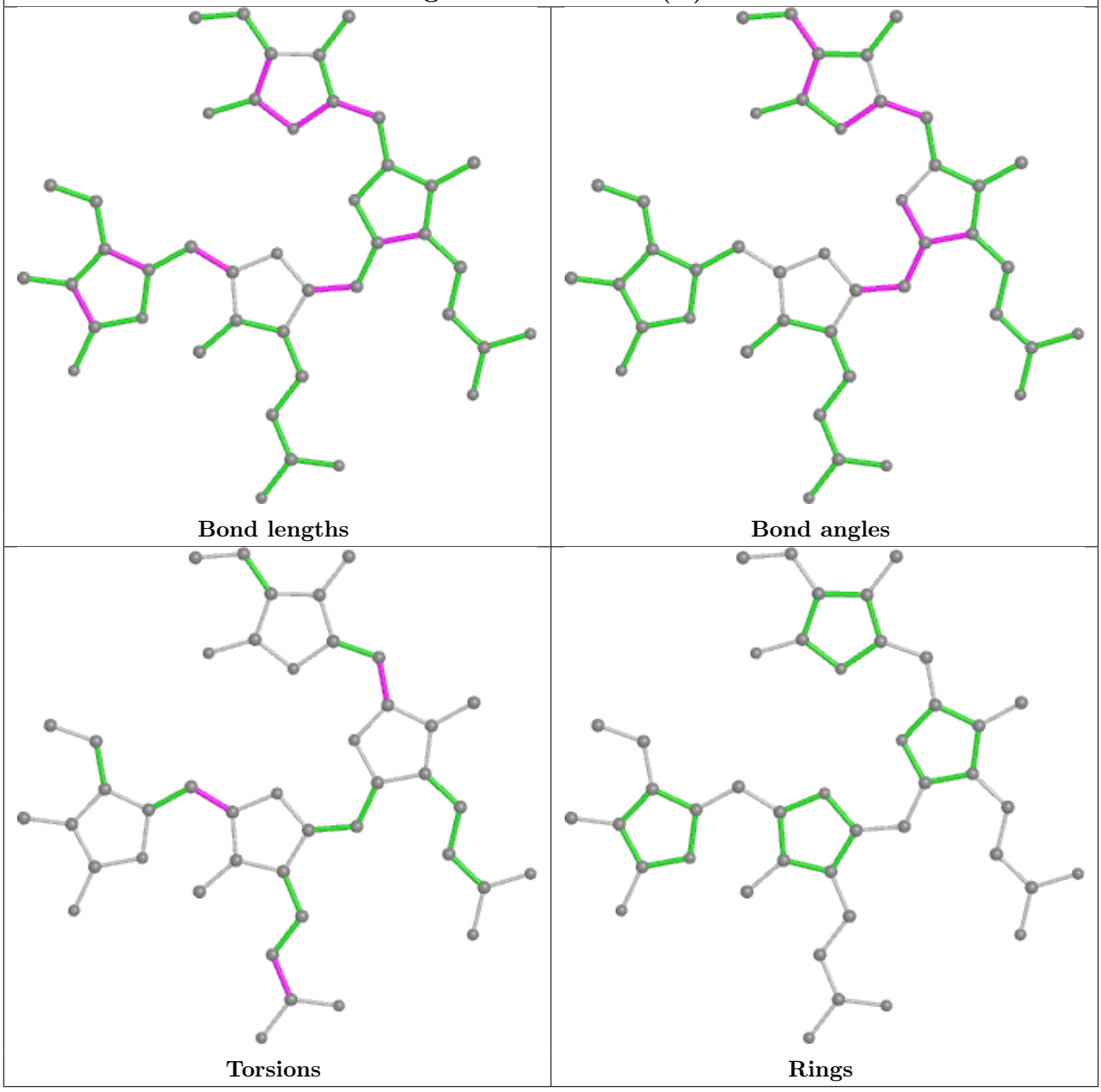


Torsions



Rings

Ligand AX9 B 201 (B)



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^{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	63/63 (100%)	-0.21	2 (3%)	47	39	6, 10, 17, 25	0
1	C	62/63 (98%)	-0.21	1 (1%)	72	62	7, 10, 17, 34	0
2	B	174/177 (98%)	-0.09	9 (5%)	27	23	5, 9, 21, 31	0
2	D	171/177 (96%)	-0.08	9 (5%)	26	23	6, 10, 24, 36	0
All	All	470/480 (97%)	-0.12	21 (4%)	33	28	5, 10, 21, 36	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	LYS	4.5
2	B	70[A]	ASN	4.1
1	A	63[A]	LYS	4.0
2	B	4	ALA	3.9
2	B	7[A]	LYS	3.8
1	A	1[A]	LYS	3.6
2	D	7	LYS	3.5
2	D	30	PHE	3.0
2	D	12	ALA	2.9
2	B	147[A]	GLN	2.7
2	B	15[A]	LYS	2.6
2	B	13	ASP	2.6
2	B	10[A]	THR	2.4
2	D	10	THR	2.3
2	D	11	SER	2.2
2	B	177[A]	GLY	2.2
2	D	8	VAL	2.2
2	D	115[A]	GLU	2.2
2	D	175[A]	ALA	2.1
2	B	12	ALA	2.1
2	D	6	SER	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)

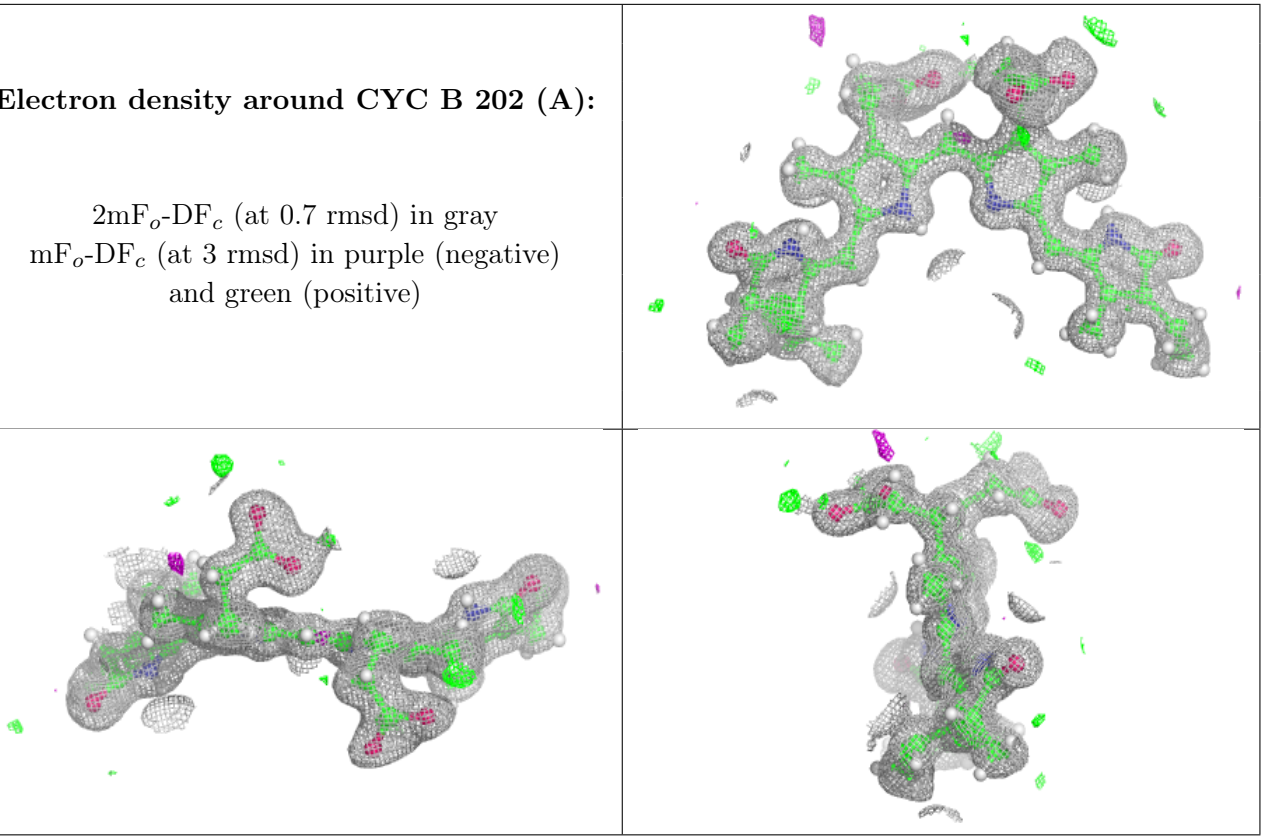
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	CYC	B	202[A]	43/43	0.97	0.08	7,9,14,16	80
3	CYC	B	202[B]	43/43	0.97	0.08	7,10,13,15	80
4	AX9	B	201[A]	43/43	0.97	0.07	7,10,15,16	79
4	AX9	B	201[B]	43/43	0.97	0.07	7,9,14,15	79
4	AX9	D	201[A]	43/43	0.97	0.09	7,11,16,19	79
4	AX9	D	201[B]	43/43	0.97	0.09	7,12,19,21	79
3	CYC	C	101[A]	43/43	0.98	0.07	4,8,12,13	80
3	CYC	C	101[B]	43/43	0.98	0.07	6,8,11,14	80
3	CYC	D	202[A]	43/43	0.98	0.07	7,9,14,16	80
3	CYC	D	202[B]	43/43	0.98	0.07	5,9,11,13	80
3	CYC	D	203[A]	43/43	0.98	0.08	5,8,13,14	80
3	CYC	D	203[B]	43/43	0.98	0.08	5,8,11,13	80
3	CYC	A	101[A]	43/43	0.98	0.07	6,8,17,20	80
3	CYC	A	101[B]	43/43	0.98	0.07	5,9,11,11	80
3	CYC	B	203[A]	43/43	0.98	0.09	5,7,13,15	80
3	CYC	B	203[B]	43/43	0.98	0.09	3,6,9,10	80

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.

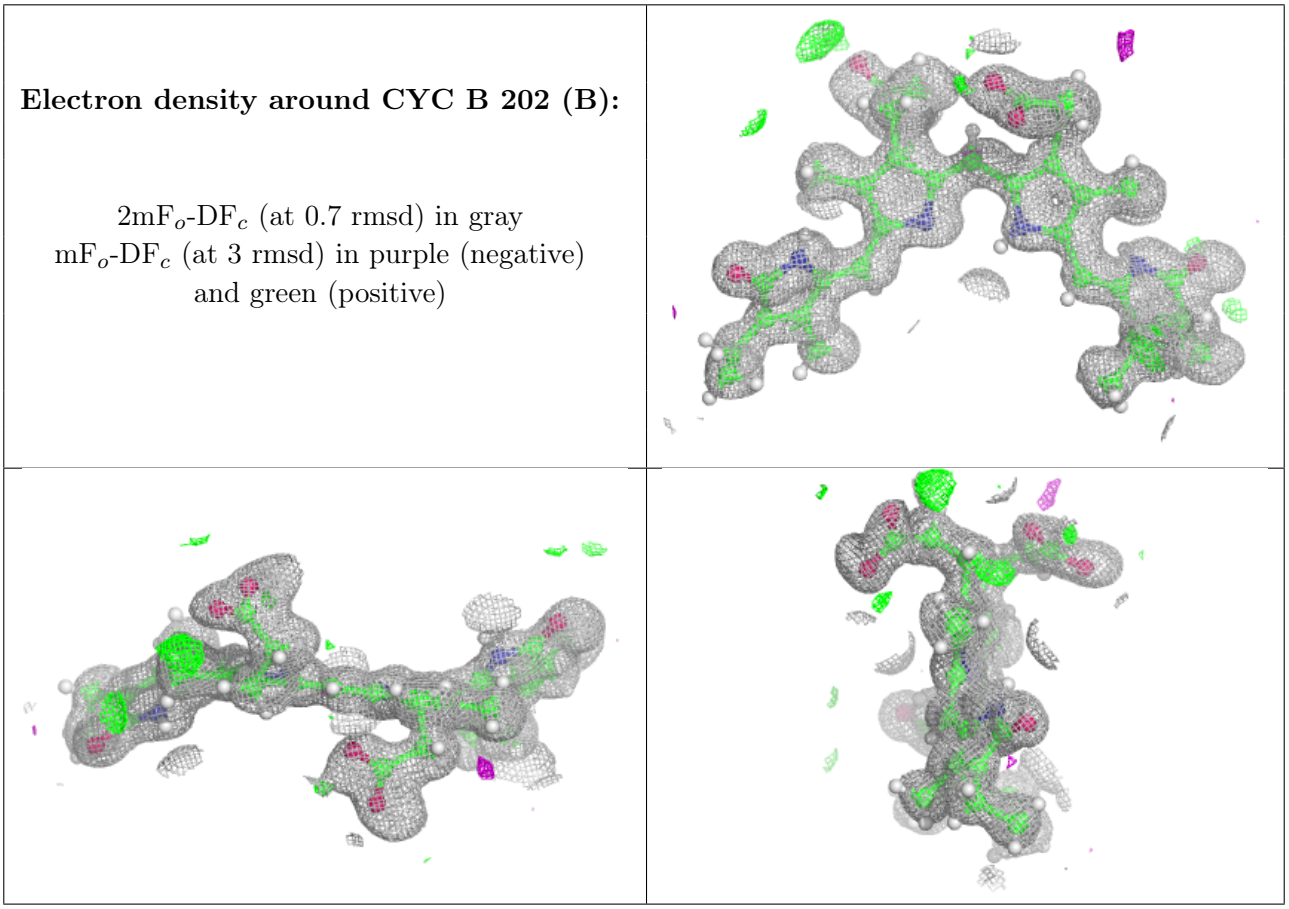
Electron density around CYC B 202 (A):

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



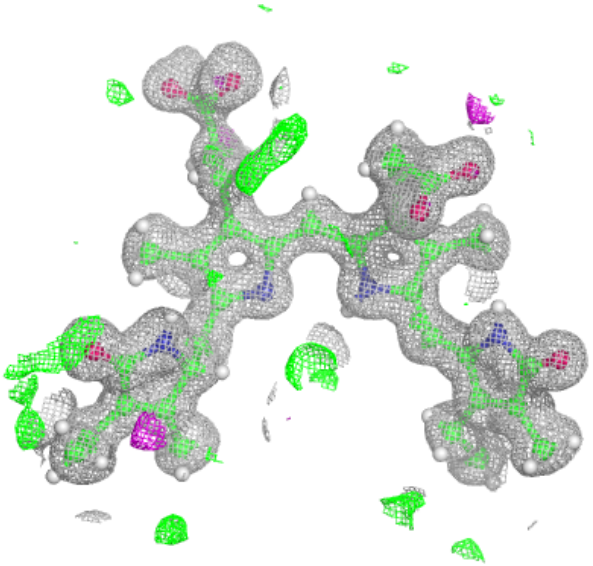
Electron density around CYC B 202 (B):

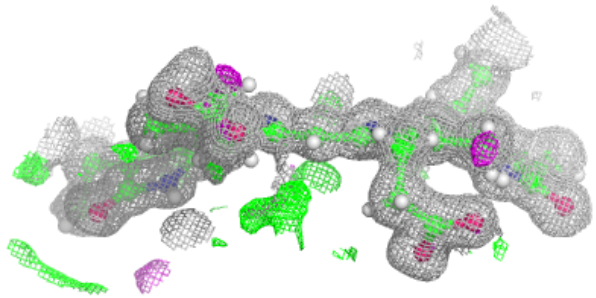
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

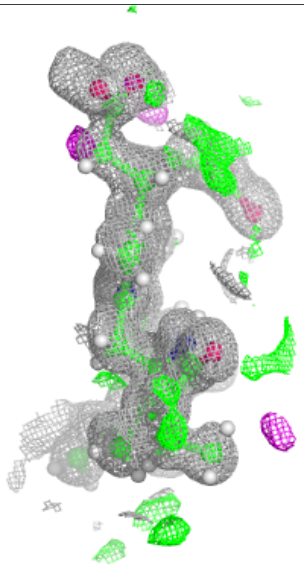


Electron density around AX9 B 201 (A):

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

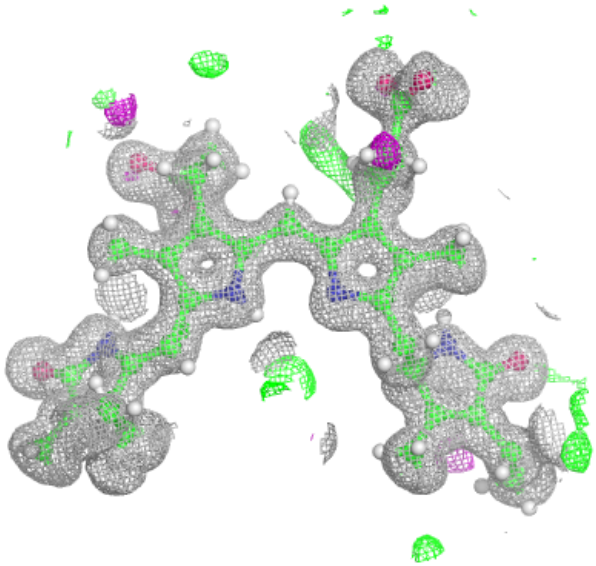


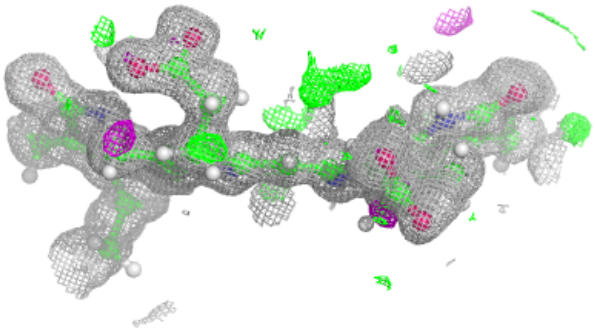


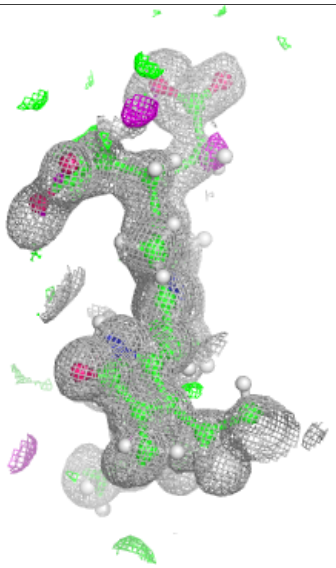


Electron density around AX9 B 201 (B):

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

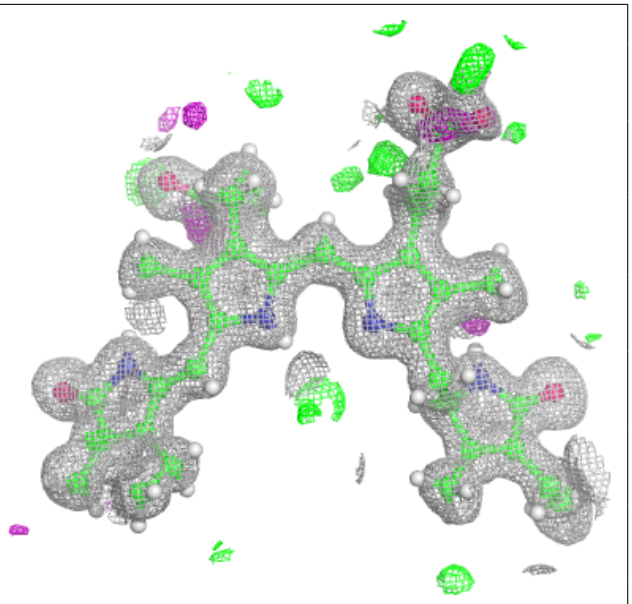


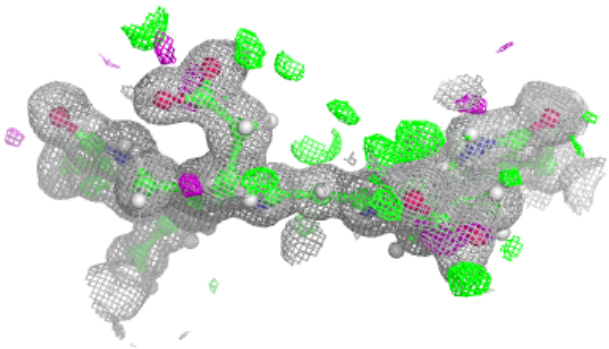


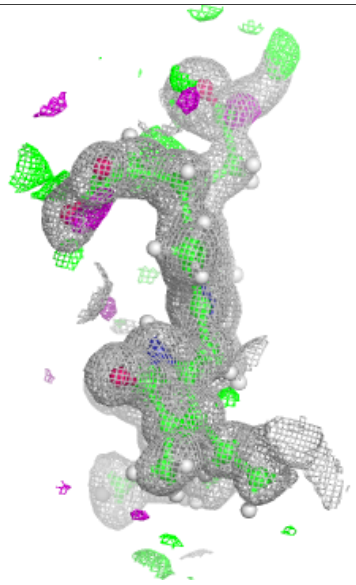


Electron density around AX9 D 201 (A):

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

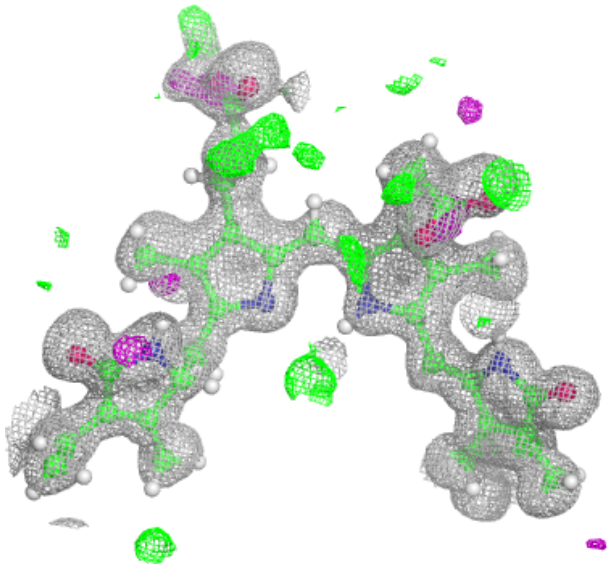


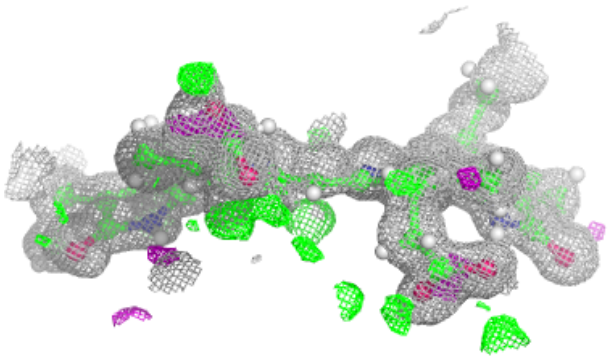


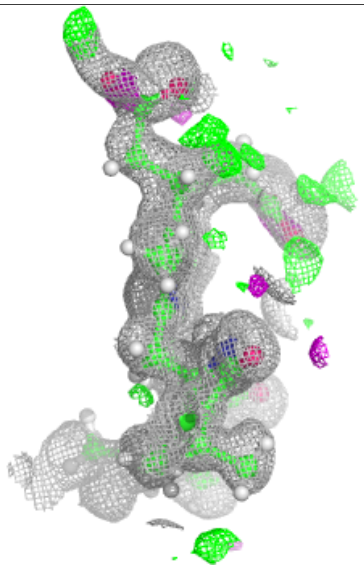


Electron density around AX9 D 201 (B):

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

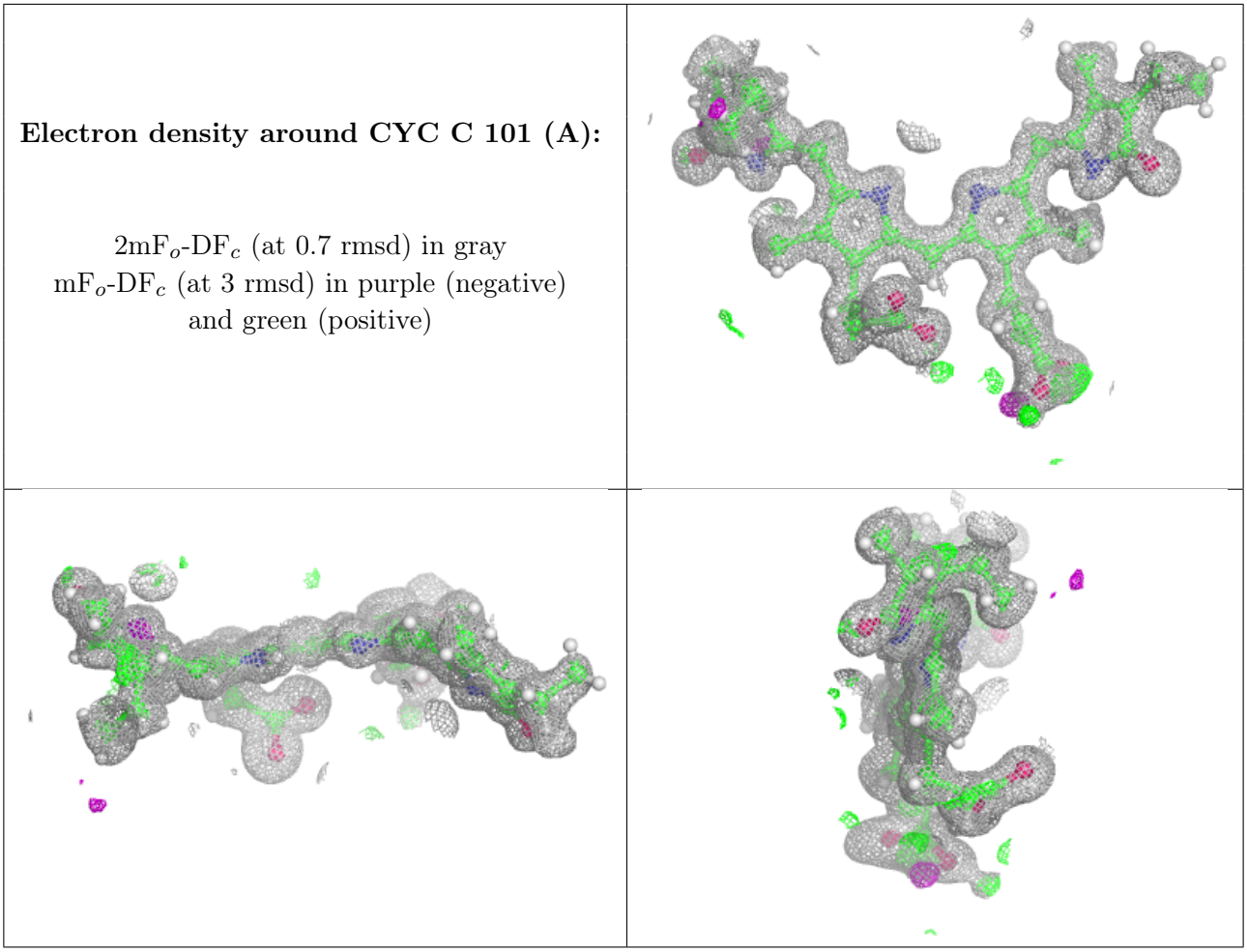






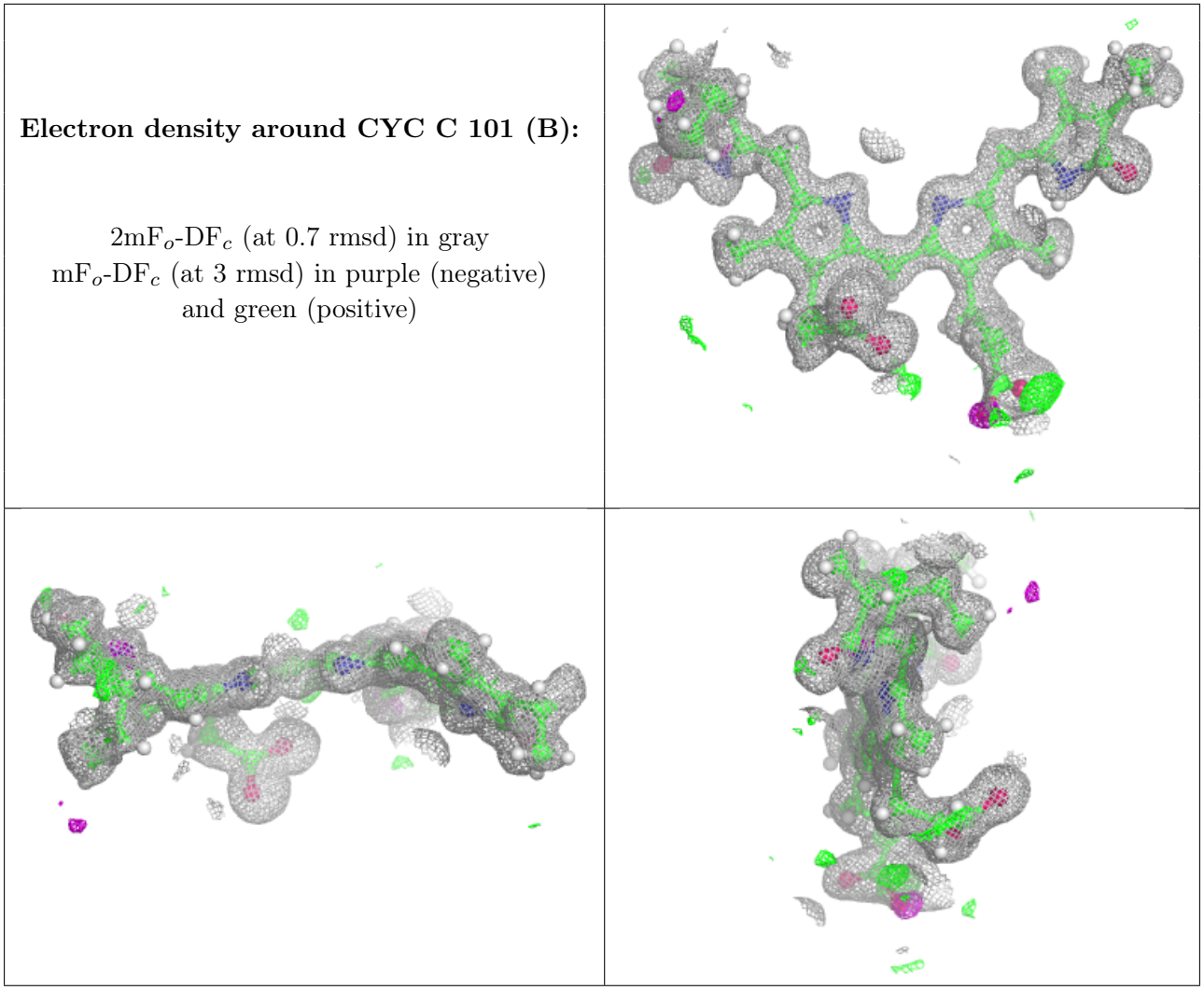
Electron density around CYC C 101 (A):

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



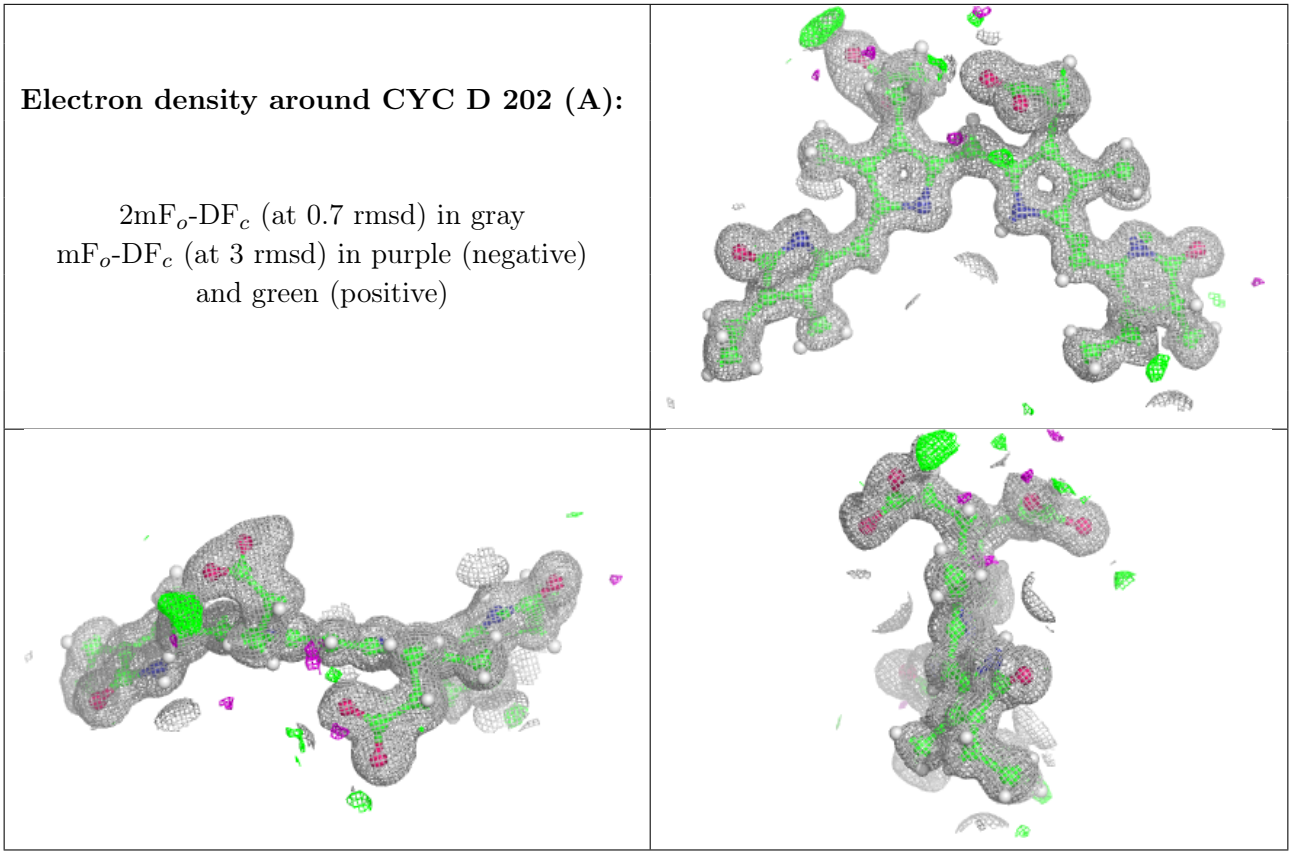
Electron density around CYC C 101 (B):

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



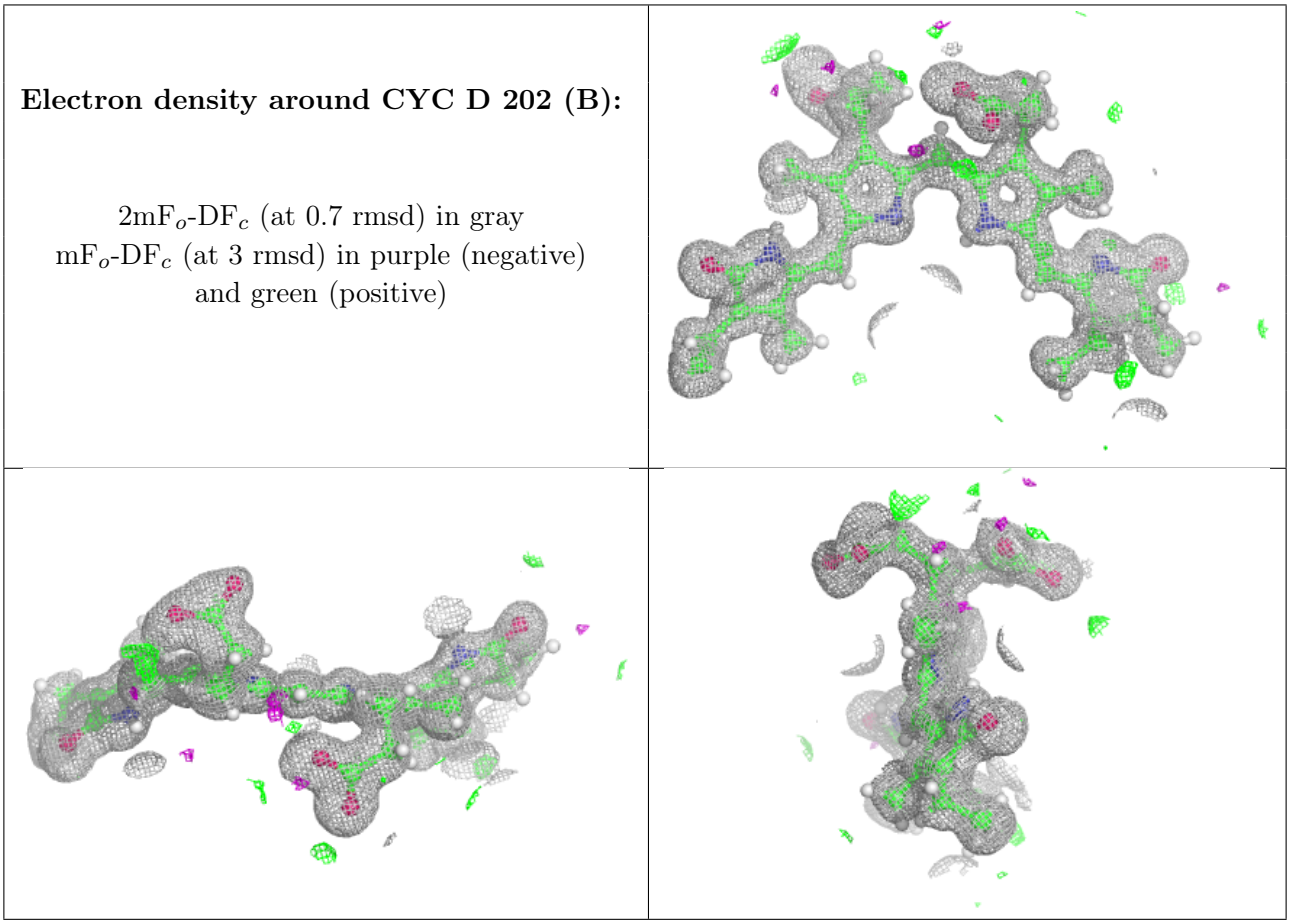
Electron density around CYC D 202 (A):

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



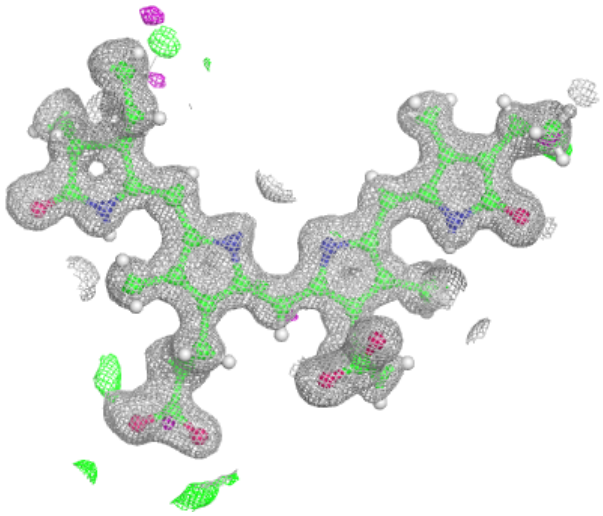
Electron density around CYC D 202 (B):

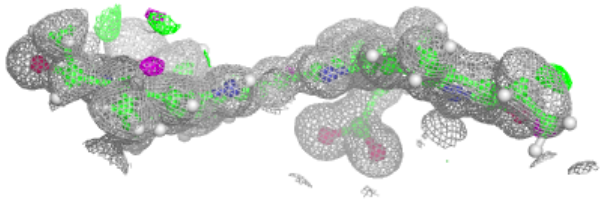
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

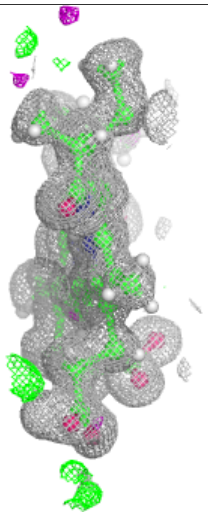


Electron density around CYC D 203 (A):

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

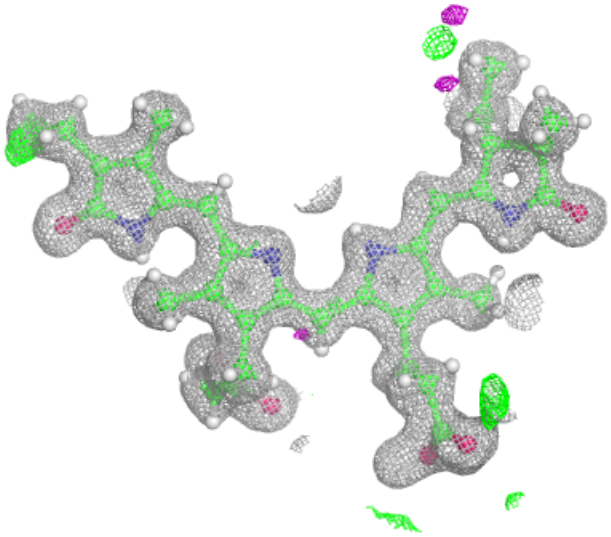


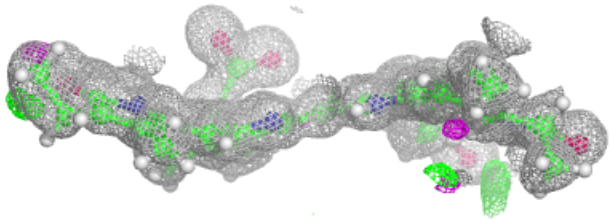


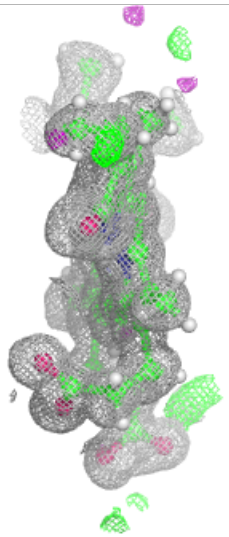


Electron density around CYC D 203 (B):

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

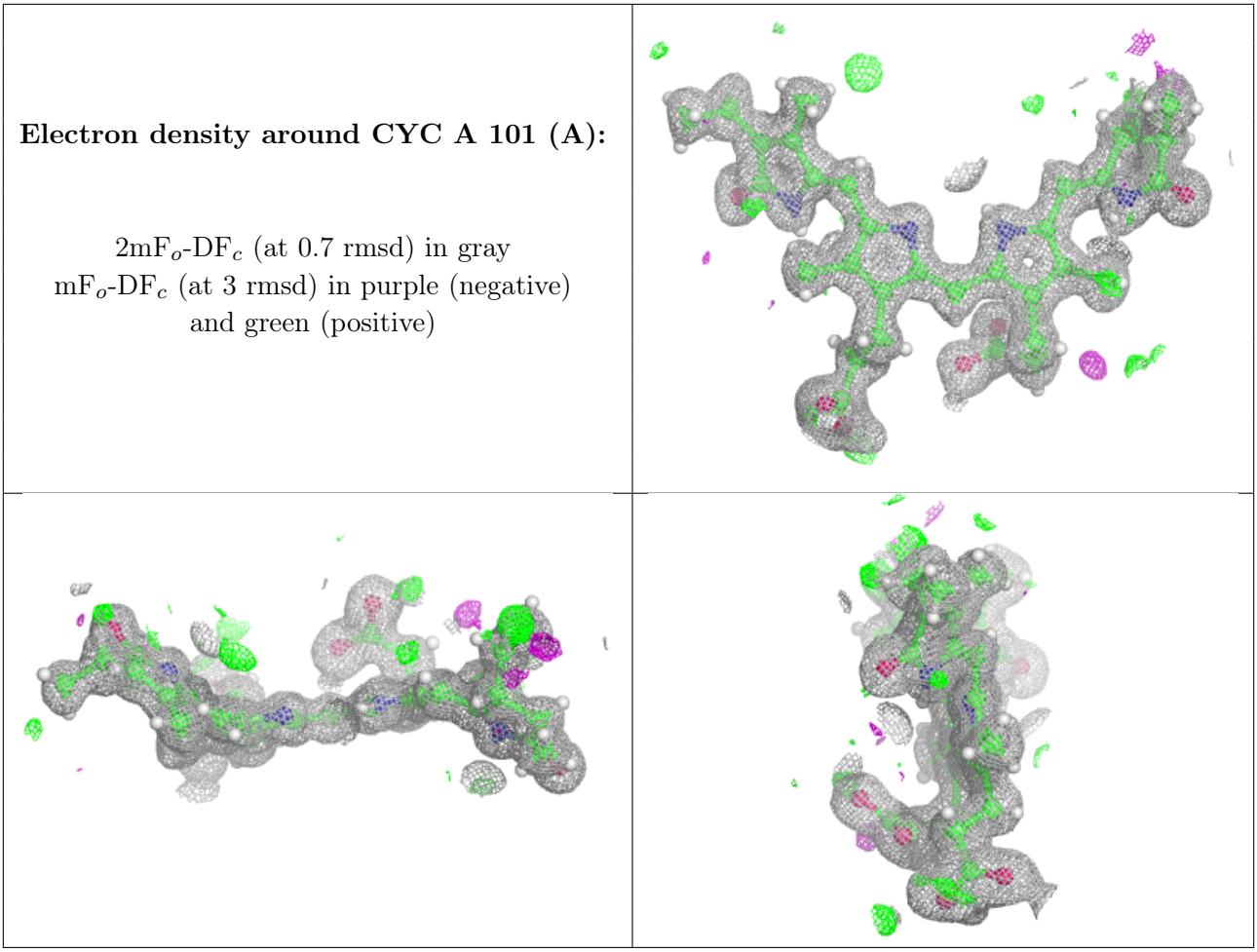






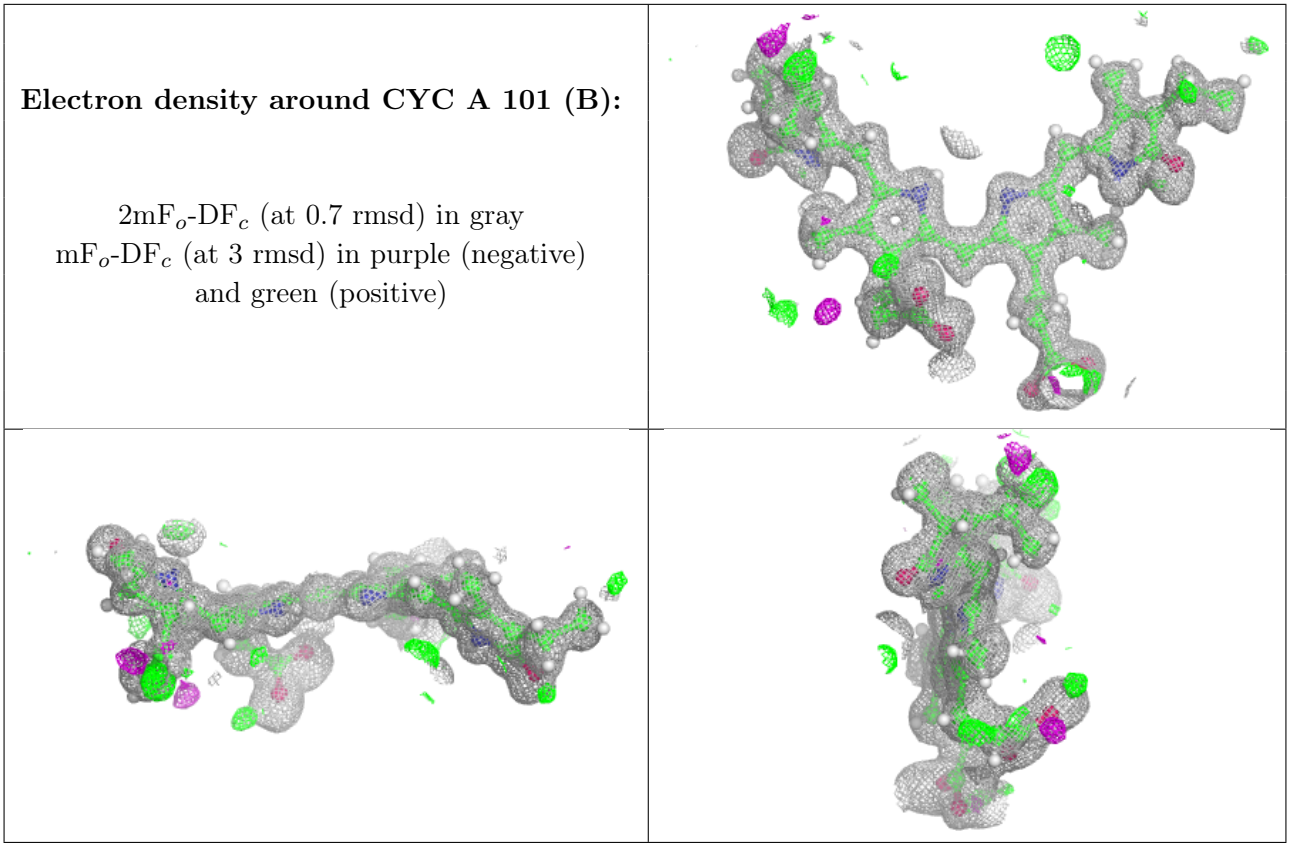
Electron density around CYC A 101 (A):

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



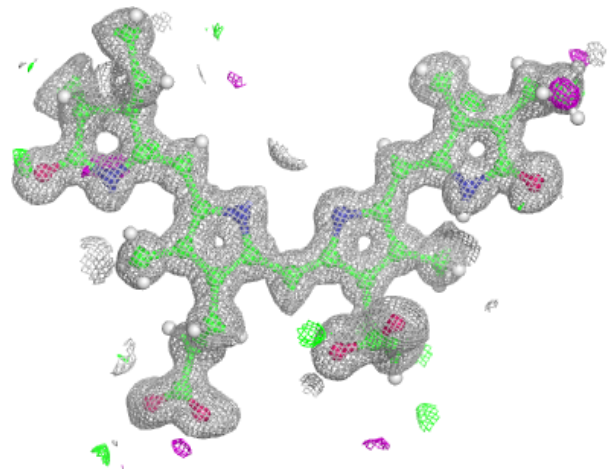
Electron density around CYC A 101 (B):

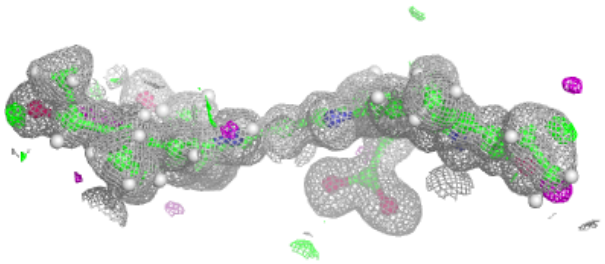
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

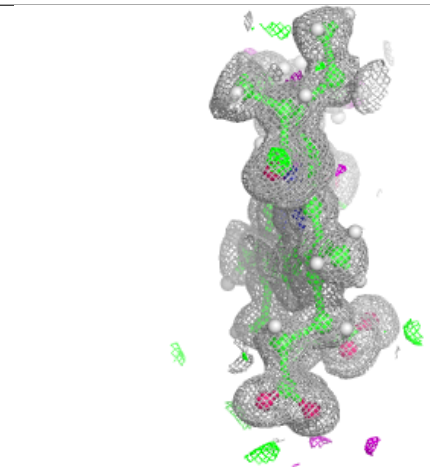


Electron density around CYC B 203 (A):

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

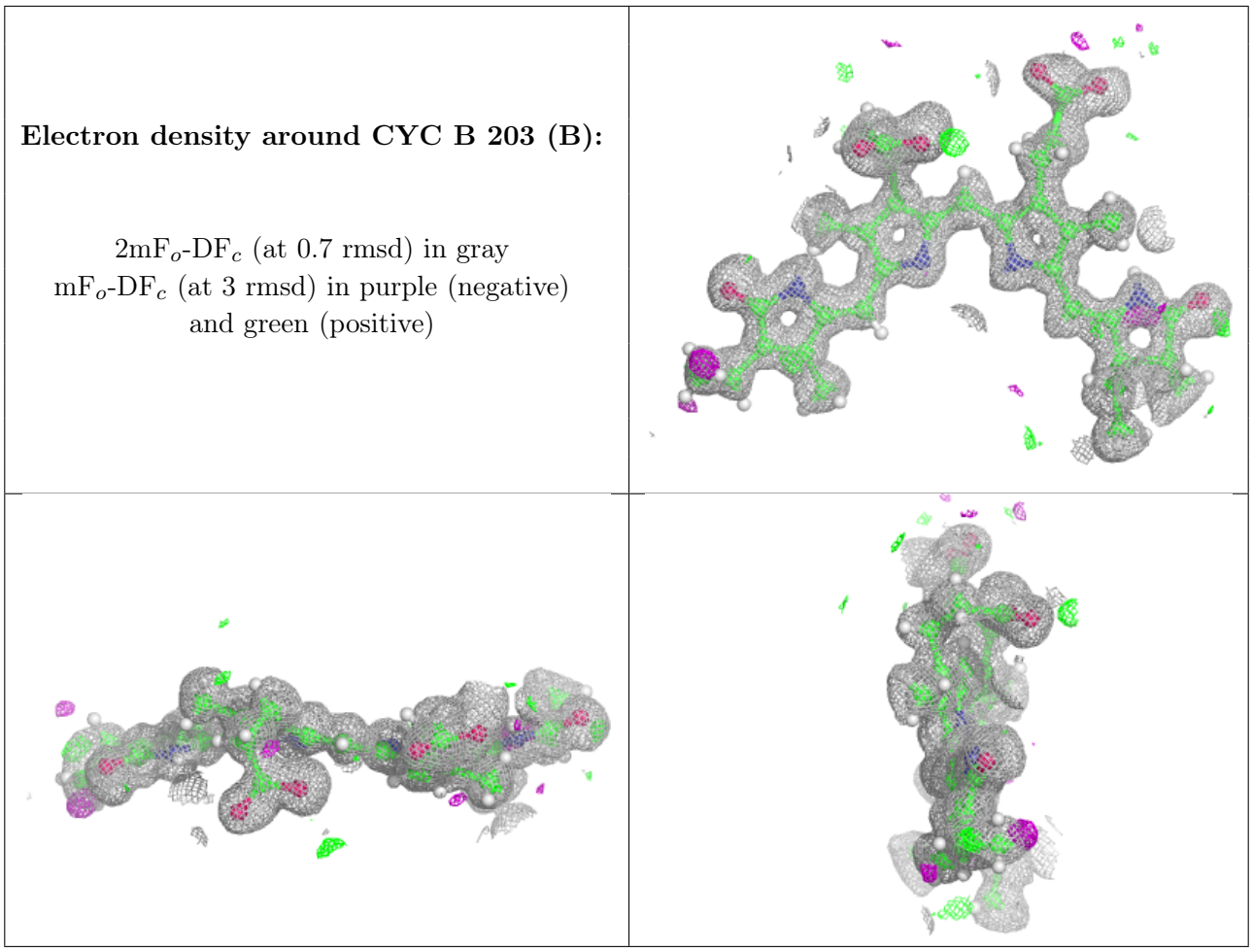






Electron density around CYC B 203 (B):

$2mF_o$-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

There are no such residues in this entry.