wwPDB X-ray Structure Validation Summary Report (i)

Oct 14, 2023 – 09:05 PM EDT

PDB ID	:	7T7U
Title	:	Light Harvesting complex phycocyanin PC 630, from the cryptophyte Chroomonas sp. M1627
Authors	:	Michie, K.A.; Harrop, S.J.; Rathbone, H.W.; Wilk, K.E.; Curmi, P.M.G.
Deposited on	:	2021-12-15
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

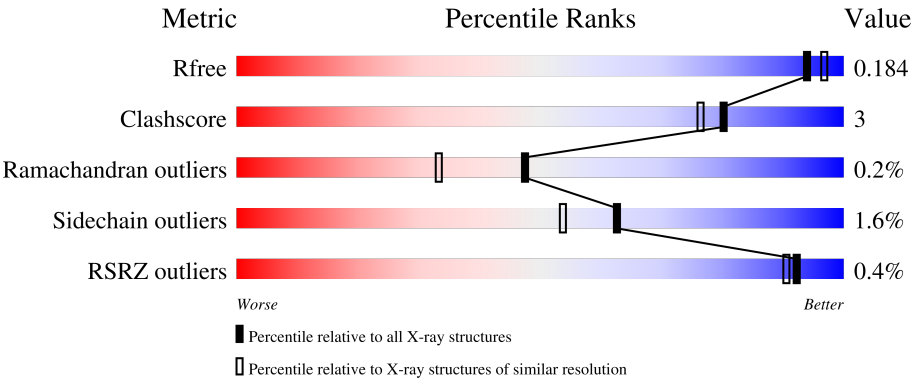
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	81	95% 5%
2	B	173	90% 6%
2	D	173	92% 5%
3	C	70	99%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8530 atoms, of which 4048 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 L1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	81	Total	C	H	N	O	S	0	6	0
			1349	414	694	109	127	5			

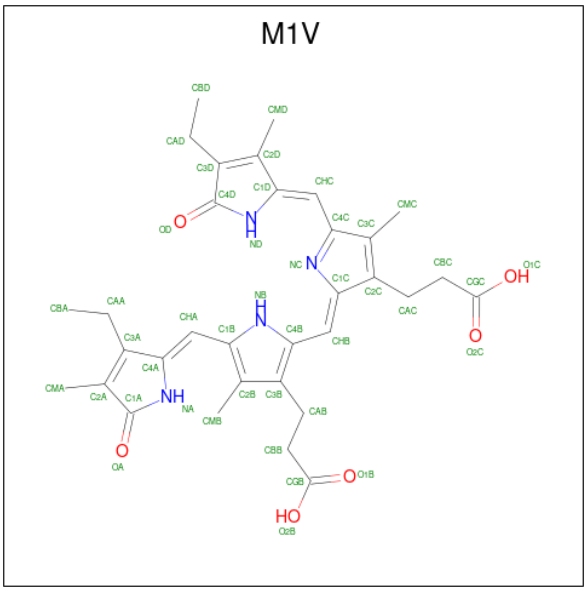
- Molecule 2 is a protein called Phycoerythrin beta subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	162	Total	C	H	N	O	S	0	7	0
			2415	744	1210	206	245	10			
2	D	168	Total	C	H	N	O	S	0	6	0
			2526	780	1267	217	252	10			

- Molecule 3 is a protein called Phycoerythrin alpha subunit S1.

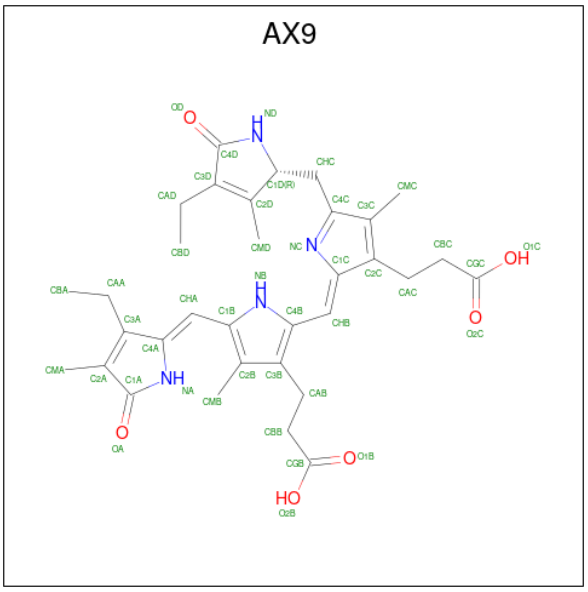
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	70	Total	C	H	N	O	S	0	5	0
			1140	345	579	96	113	7			

- Molecule 4 is mesobiliverdin IX(alpha) (three-letter code: M1V) (formula: $C_{33}H_{38}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			78	33	35	4	6		
4	C	1	Total	C	H	N	O	0	0
			78	33	35	4	6		

- Molecule 5 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
5	B	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

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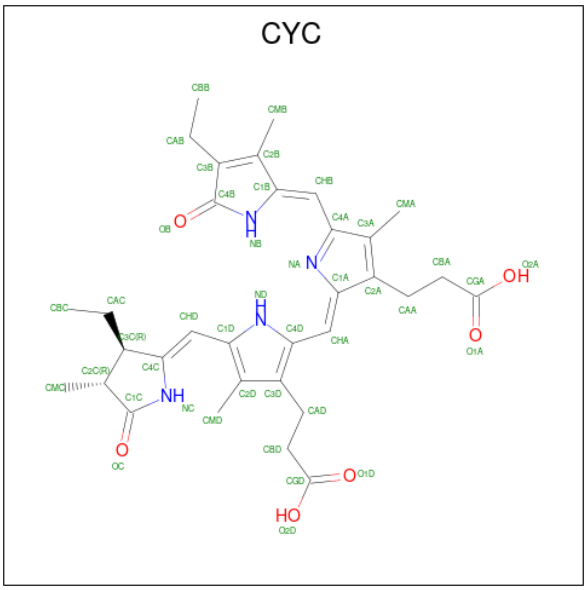
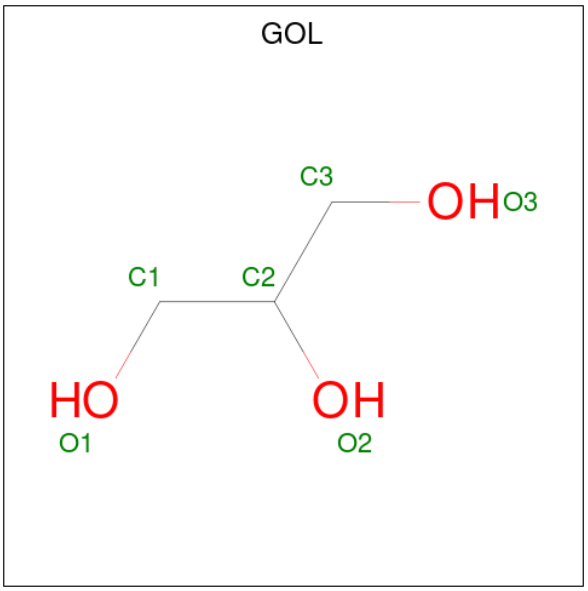
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	D	1	Total	C	H	N	O	0	0
			79	33	36	4	6		

- Molecule 6 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
6	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
6	B	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
6	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		
6	D	1	Total	C	H	N	O	0	0
			80	33	37	4	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C H O 14 3 8 3	0	0

- Molecule 8 is water.

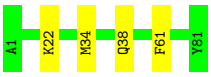
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	98	Total O 98 98	0	0
8	B	122	Total O 122 122	0	0
8	C	85	Total O 85 85	0	0
8	D	147	Total O 147 147	0	0

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.

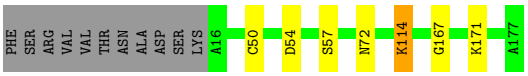
• Molecule 1: Phycoerythrin alpha subunit L1

Chain A:



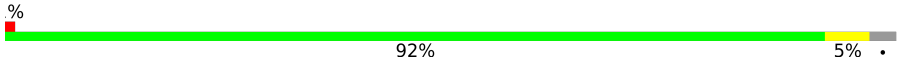
• Molecule 2: Phycoerythrin beta subunit

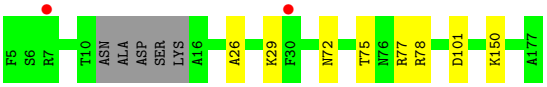
Chain B:



• Molecule 2: Phycoerythrin beta subunit

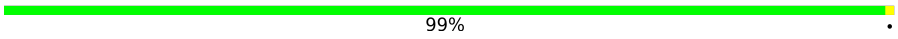
Chain D:

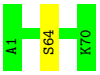




• Molecule 3: Phycoerythrin alpha subunit S1

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	90.29Å 93.41Å 132.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 1.80 39.58 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.58-1.80) 98.5 (39.58-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.158 , 0.185 0.158 , 0.184	Depositor DCC
R_{free} test set	2622 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.014 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.017 for k,h,-l 0.013 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.013 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8530	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.52% 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: LYZ, MEN, AX9, CYC, GOL, M1V

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/663	0.61	0/883
2	B	0.56	0/1224	0.63	0/1652
2	D	0.59	0/1273	0.63	0/1716
3	C	0.61	0/559	0.64	0/740
All	All	0.57	0/3719	0.63	0/4991

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	655	694	703	3	0
2	B	1205	1210	1205	5	0
2	D	1259	1267	1271	3	0
3	C	561	579	579	0	0
4	A	43	35	35	1	0
4	C	43	35	35	2	0
5	B	43	36	0	0	0
5	D	43	36	0	0	0
6	B	86	74	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	86	74	74	4	0
7	B	6	8	8	0	0
8	A	98	0	0	2	0
8	B	122	0	0	0	0
8	C	85	0	0	0	0
8	D	147	0	0	0	0
All	All	4482	4048	3984	22	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 3.

The worst 5 of 22 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:101:M1V:H41	4:A:101:M1V:H13	1.58	0.68
4:C:101:M1V:H13	4:C:101:M1V:H41	1.58	0.67
6:B:203:CYC:NB	6:B:203:CYC:HMA1	2.23	0.54
6:D:302:CYC:HMD2	6:D:302:CYC:HC	1.73	0.54
6:B:203:CYC:HMA1	6:B:203:CYC:HB	1.72	0.53

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	84/81 (104%)	79 (94%)	5 (6%)	0	100 100
2	B	166/173 (96%)	164 (99%)	2 (1%)	0	100 100
2	D	169/173 (98%)	167 (99%)	1 (1%)	1 (1%)	25 12
3	C	72/70 (103%)	71 (99%)	1 (1%)	0	100 100
All	All	491/497 (99%)	481 (98%)	9 (2%)	1 (0%)	47 33

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	75	THR

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	73/67 (109%)	72 (99%)	1 (1%)	67	59
2	B	133/136 (98%)	130 (98%)	3 (2%)	50	37
2	D	138/136 (102%)	137 (99%)	1 (1%)	84	81
3	C	61/56 (109%)	60 (98%)	1 (2%)	62	54
All	All	405/395 (102%)	399 (98%)	6 (2%)	62	56

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	114	LYS
3	C	64	SER
2	D	101	ASP
2	B	50	CYS
1	A	22	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
2	B	148	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	LYZ	A	4	1	7,9,10	0.65	0	4,10,12	0.79	0
2	MEN	B	72	2	7,8,9	0.94	0	6,9,11	1.75	2 (33%)
3	LYZ	C	4	3	7,9,10	0.76	0	4,10,12	0.75	0
2	MEN	D	72	2	7,8,9	0.67	0	6,9,11	1.83	2 (33%)

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
1	LYZ	A	4	1	-	1/8/9/11	-
2	MEN	B	72	2	-	4/7/8/10	-
3	LYZ	C	4	3	-	0/8/9/11	-
2	MEN	D	72	2	-	2/7/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	72	MEN	CB-CG-ND2	3.61	120.33	115.48
2	B	72	MEN	CB-CA-C	-3.12	105.62	111.47
2	B	72	MEN	CB-CG-ND2	2.53	118.88	115.48
2	D	72	MEN	CB-CA-C	-2.39	106.98	111.47

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	4	LYZ	CG-CD-CE-NZ
2	B	72	MEN	C-CA-CB-CG
2	B	72	MEN	N-CA-CB-CG
2	B	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-ND2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
4	M1V	A	101	1	42,46,46	1.94	10 (23%)	53,67,67	1.37	8 (15%)
5	AX9	B	201	2	41,46,46	1.57	9 (21%)	41,67,67	1.10	3 (7%)
5	AX9	D	303	2	41,46,46	1.56	7 (17%)	41,67,67	1.41	6 (14%)
6	CYC	B	203	2	42,46,46	2.74	14 (33%)	50,67,67	2.05	11 (22%)
4	M1V	C	101	3	42,46,46	2.16	11 (26%)	53,67,67	1.25	6 (11%)
6	CYC	D	302	2	42,46,46	2.40	13 (30%)	50,67,67	2.15	11 (22%)
7	GOL	B	204	-	5,5,5	0.62	0	5,5,5	1.13	0
6	CYC	D	301	2	42,46,46	2.63	11 (26%)	50,67,67	2.35	13 (26%)
6	CYC	B	202	2	42,46,46	2.66	12 (28%)	50,67,67	1.95	8 (16%)

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
4	M1V	A	101	1	-	10/26/74/74	0/4/4/4
5	AX9	B	201	2	-	5/26/74/74	0/4/4/4
5	AX9	D	303	2	-	8/26/74/74	0/4/4/4
6	CYC	B	203	2	-	7/25/74/74	0/4/4/4
4	M1V	C	101	3	-	7/26/74/74	0/4/4/4
6	CYC	D	302	2	-	8/25/74/74	0/4/4/4
7	GOL	B	204	-	-	2/4/4/4	-
6	CYC	D	301	2	-	10/25/74/74	0/4/4/4
6	CYC	B	202	2	-	6/25/74/74	0/4/4/4

The worst 5 of 87 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	301	CYC	C1C-NC	-10.97	1.23	1.37
6	B	203	CYC	C1C-NC	-9.39	1.25	1.37
6	B	202	CYC	C1C-NC	-9.19	1.25	1.37
6	D	302	CYC	C1C-NC	-7.96	1.27	1.37
6	B	202	CYC	C4C-NC	-7.04	1.22	1.37

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	301	CYC	OC-C1C-C2C	-9.03	118.99	126.17
6	D	302	CYC	OC-C1C-C2C	-8.16	119.69	126.17
6	D	301	CYC	C2C-C1C-NC	7.92	115.10	108.27
6	B	202	CYC	C2C-C1C-NC	7.39	114.64	108.27
6	B	203	CYC	C2C-C1C-NC	7.32	114.58	108.27

There are no chirality outliers.

5 of 63 torsion outliers are listed below:

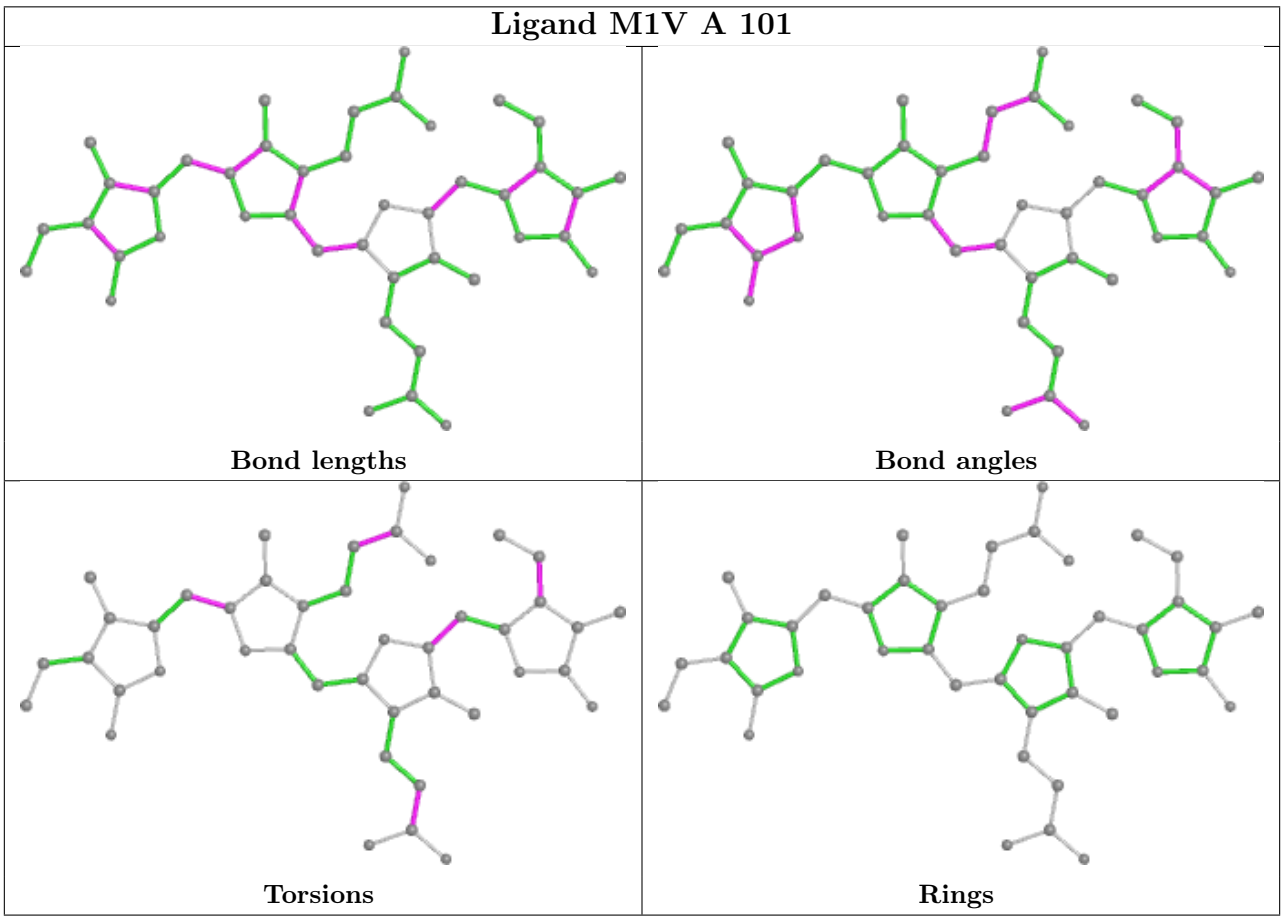
Mol	Chain	Res	Type	Atoms
4	A	101	M1V	C2B-C1B-CHA-C4A
4	A	101	M1V	NB-C1B-CHA-C4A
4	A	101	M1V	C3C-C4C-CHC-C1D
4	A	101	M1V	NC-C4C-CHC-C1D
4	C	101	M1V	C2B-C1B-CHA-C4A

There are no ring outliers.

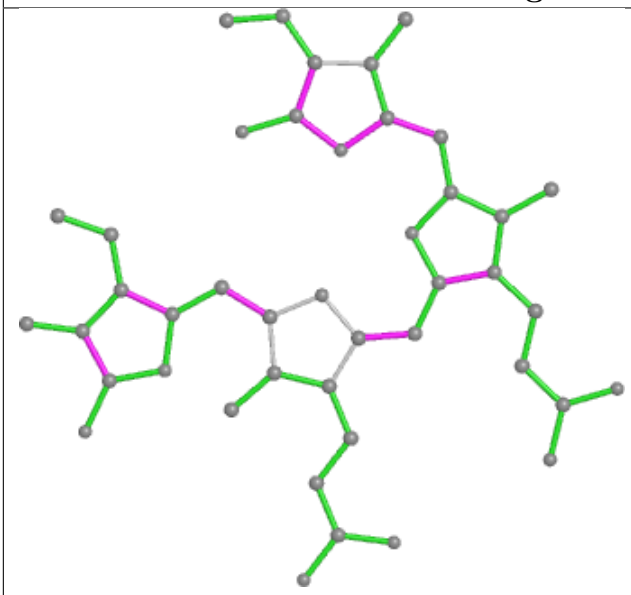
6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	101	M1V	1	0
6	B	203	CYC	3	0
4	C	101	M1V	2	0
6	D	302	CYC	3	0
6	D	301	CYC	1	0
6	B	202	CYC	2	0

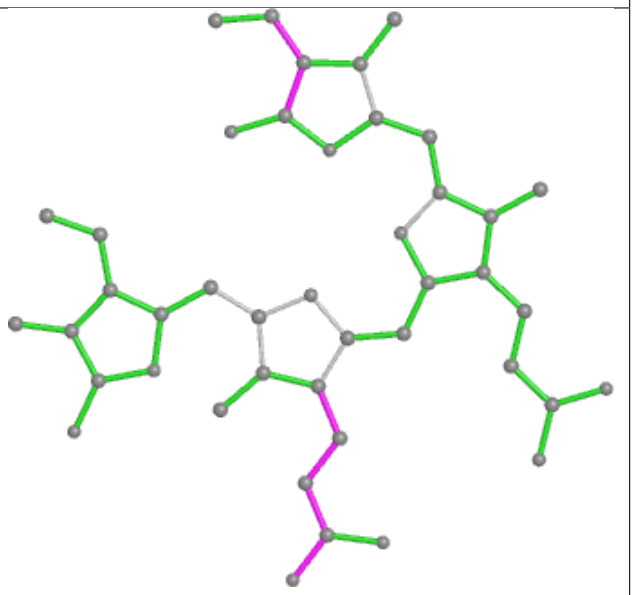
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



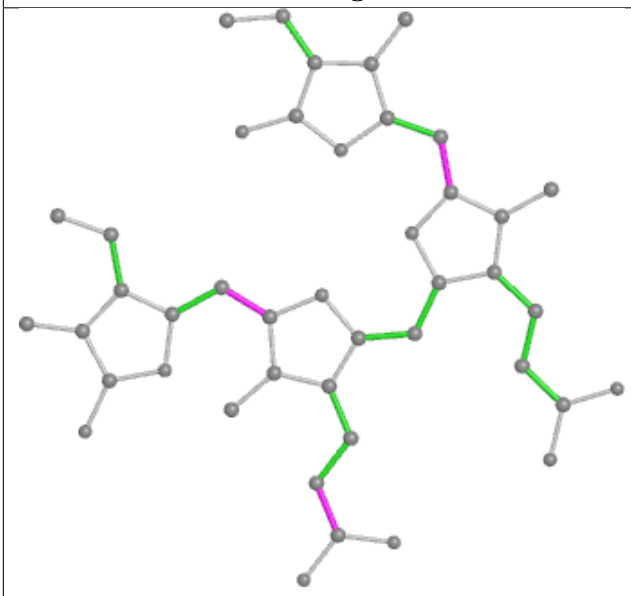
Ligand AX9 B 201



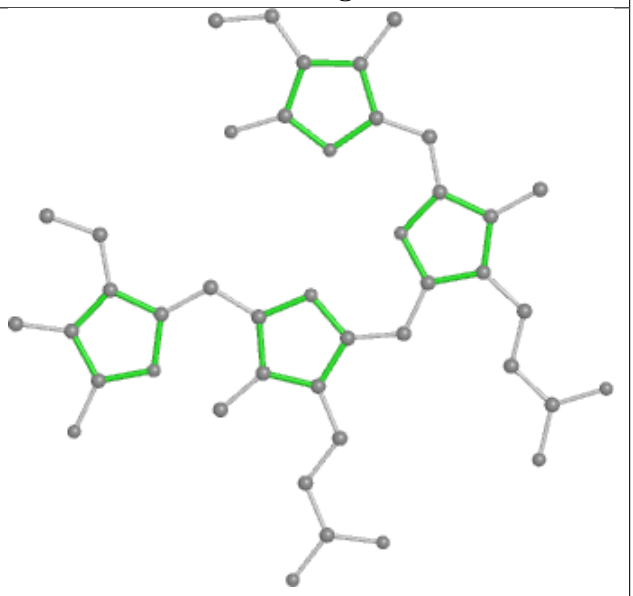
Bond lengths



Bond angles

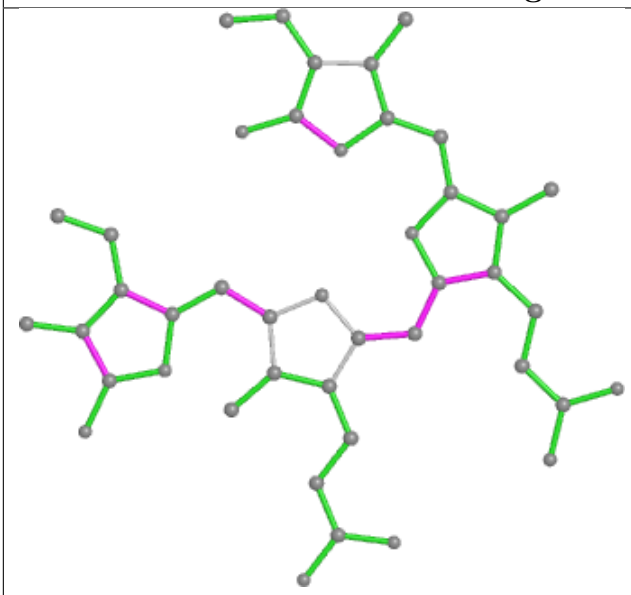


Torsions

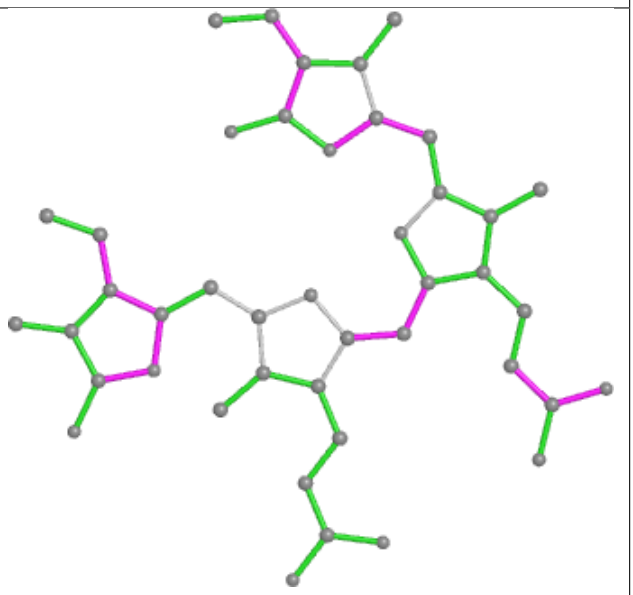


Rings

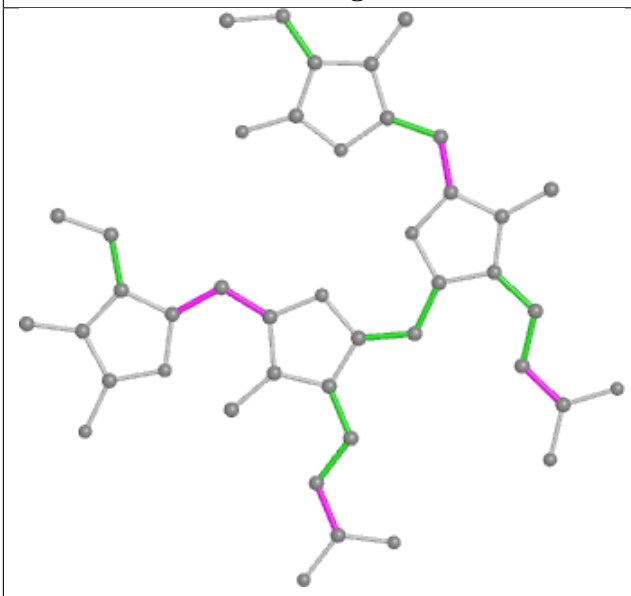
Ligand AX9 D 303



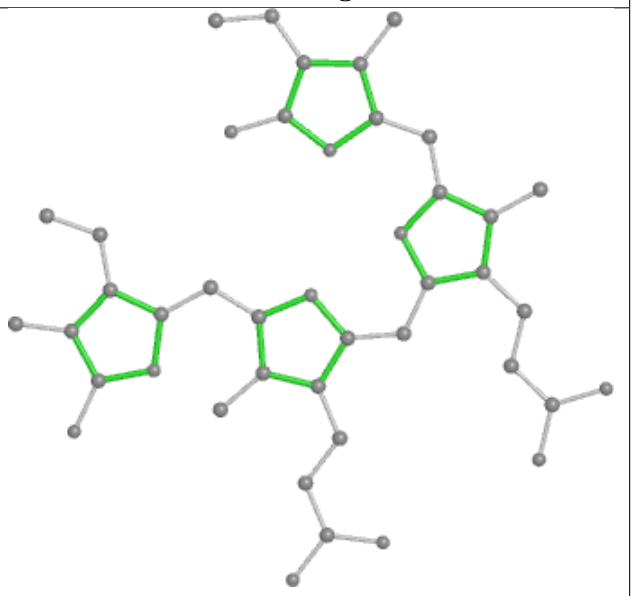
Bond lengths



Bond angles

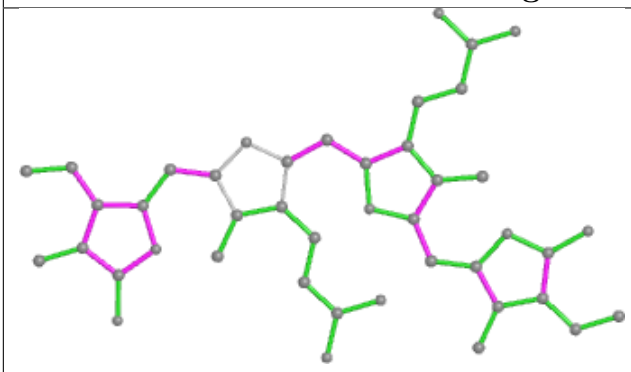


Torsions

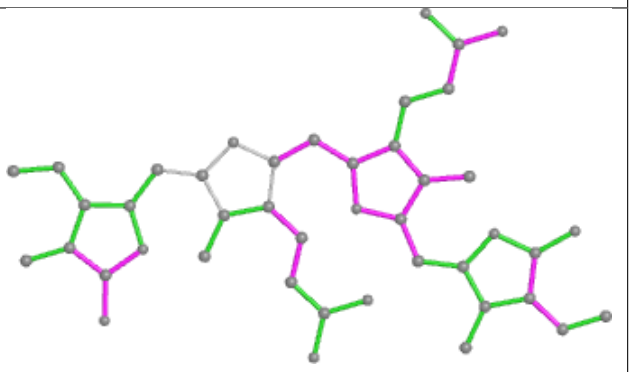


Rings

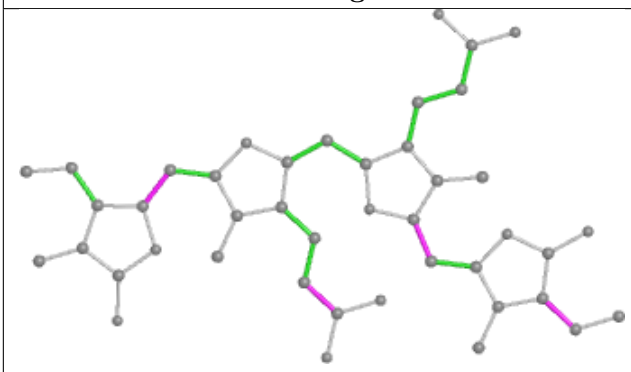
Ligand CYC B 203



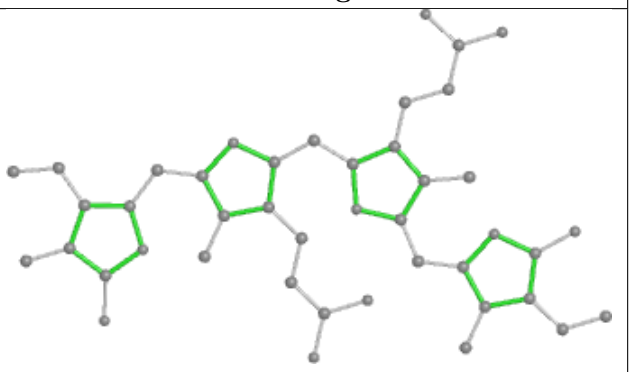
Bond lengths



Bond angles

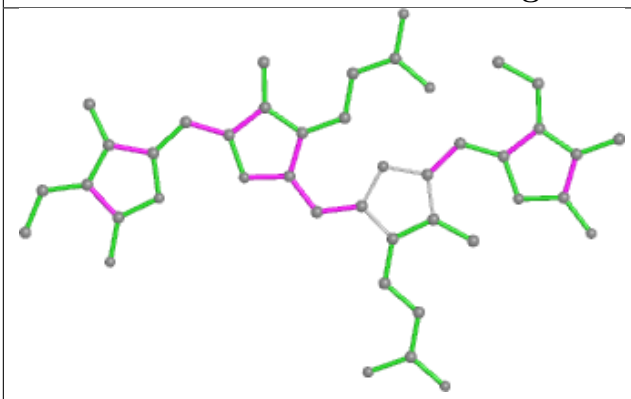


Torsions

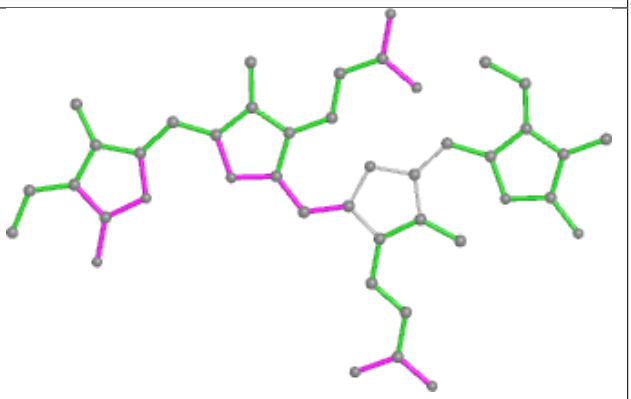


Rings

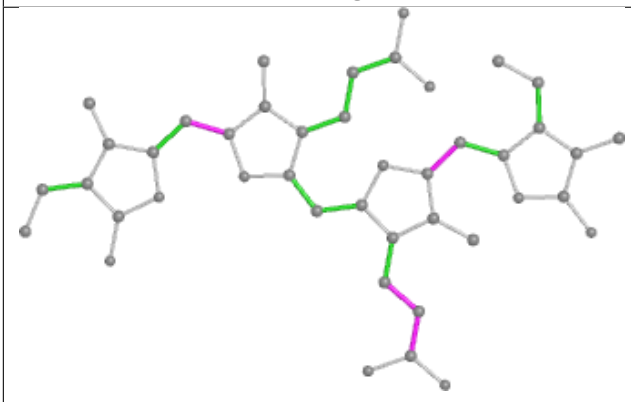
Ligand M1V C 101



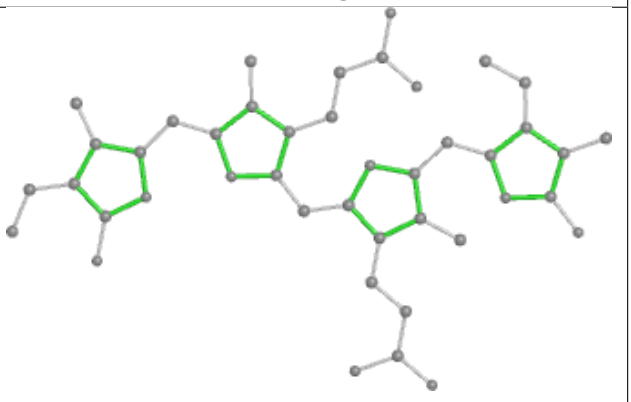
Bond lengths



Bond angles

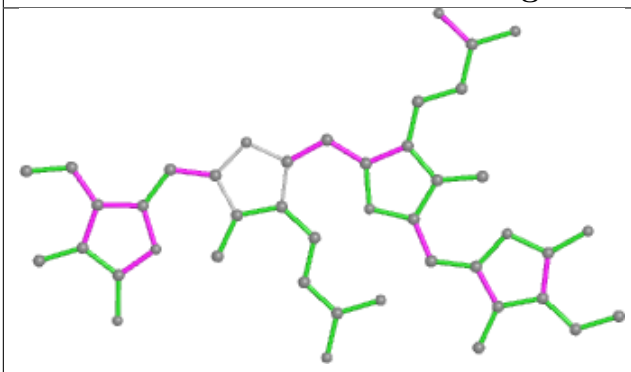


Torsions

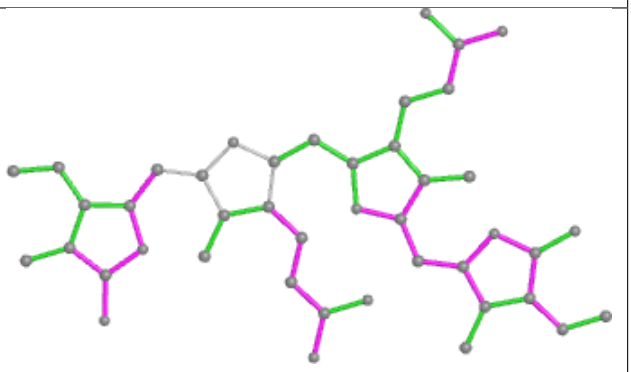


Rings

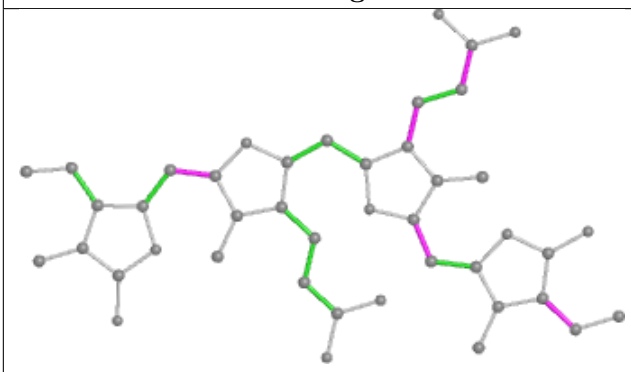
Ligand CYC D 302



Bond lengths



Bond angles



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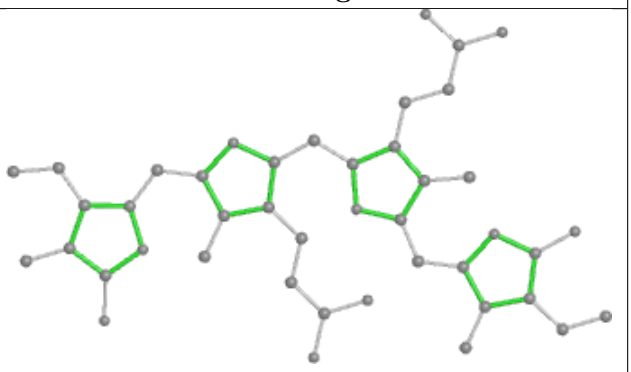
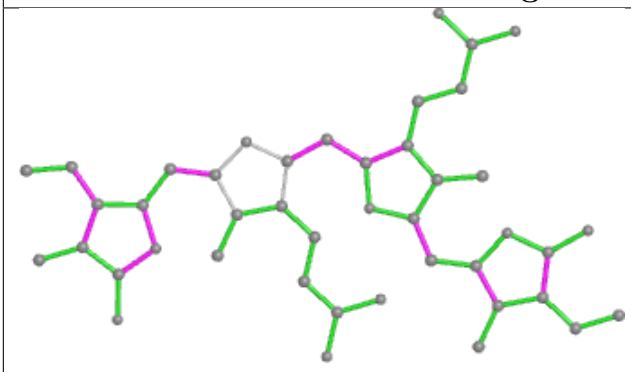
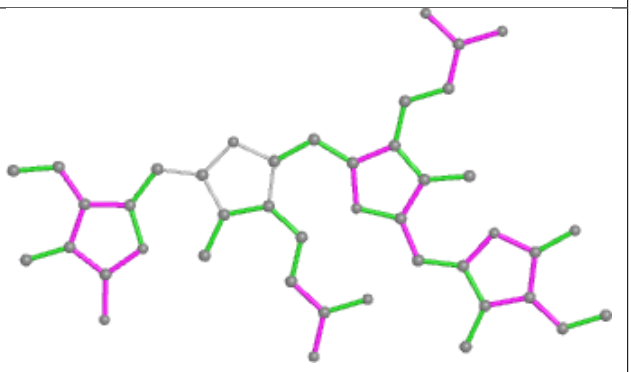


Rings

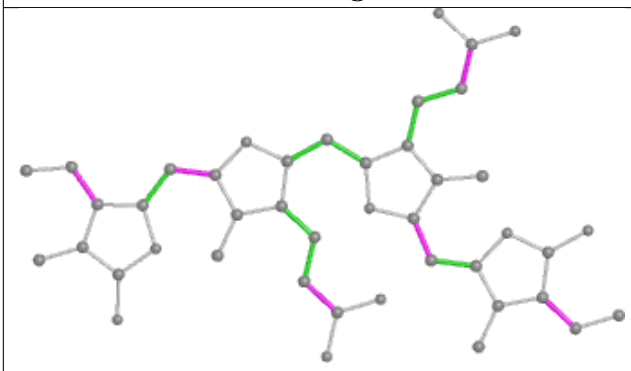
Ligand CYC D 301



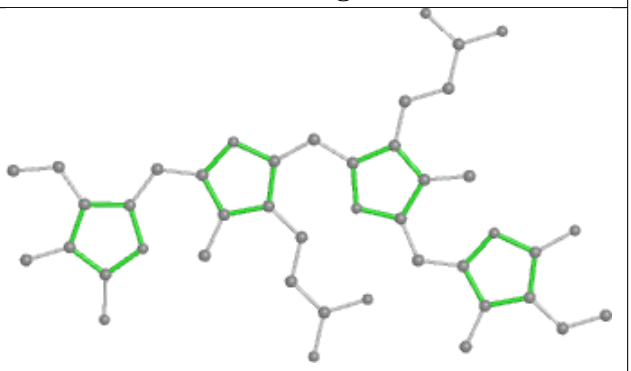
Bond lengths



Bond angles

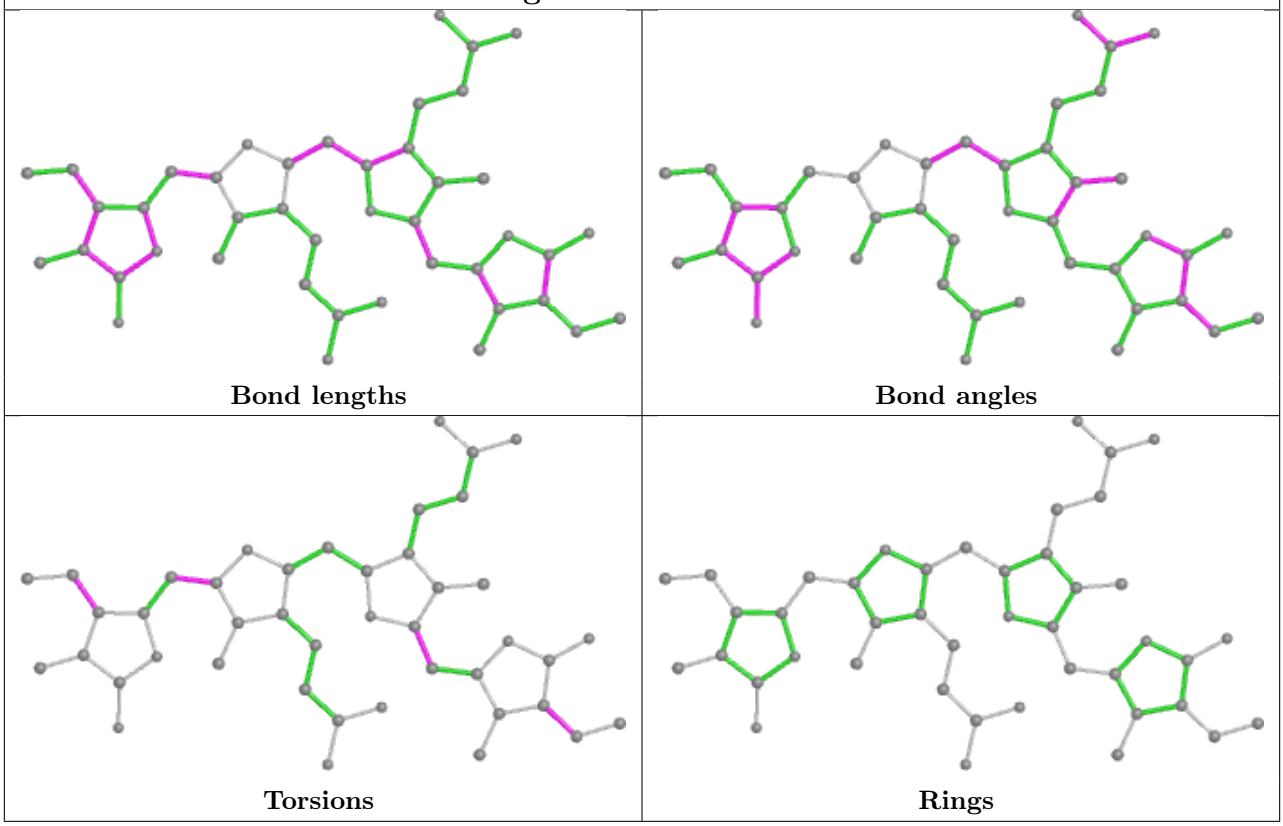


Torsions



Rings

Ligand CYC B 202



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	80/81 (98%)	-0.43	0 100 100	11, 15, 26, 31	0
2	B	161/173 (93%)	-0.30	0 100 100	11, 19, 29, 33	0
2	D	167/173 (96%)	-0.37	2 (1%) 79 76	10, 15, 27, 62	0
3	C	69/70 (98%)	-0.51	0 100 100	11, 16, 21, 24	0
All	All	477/497 (95%)	-0.38	2 (0%) 92 90	10, 16, 28, 62	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	30	PHE	2.6
2	D	7	ARG	2.3

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

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
2	MEN	B	72	9/10	0.94	0.09	17,22,28,28	0
1	LYZ	A	4	10/11	0.96	0.12	23,31,39,43	0
3	LYZ	C	4	10/11	0.97	0.09	15,20,27,29	0
2	MEN	D	72	9/10	0.98	0.07	12,15,19,19	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

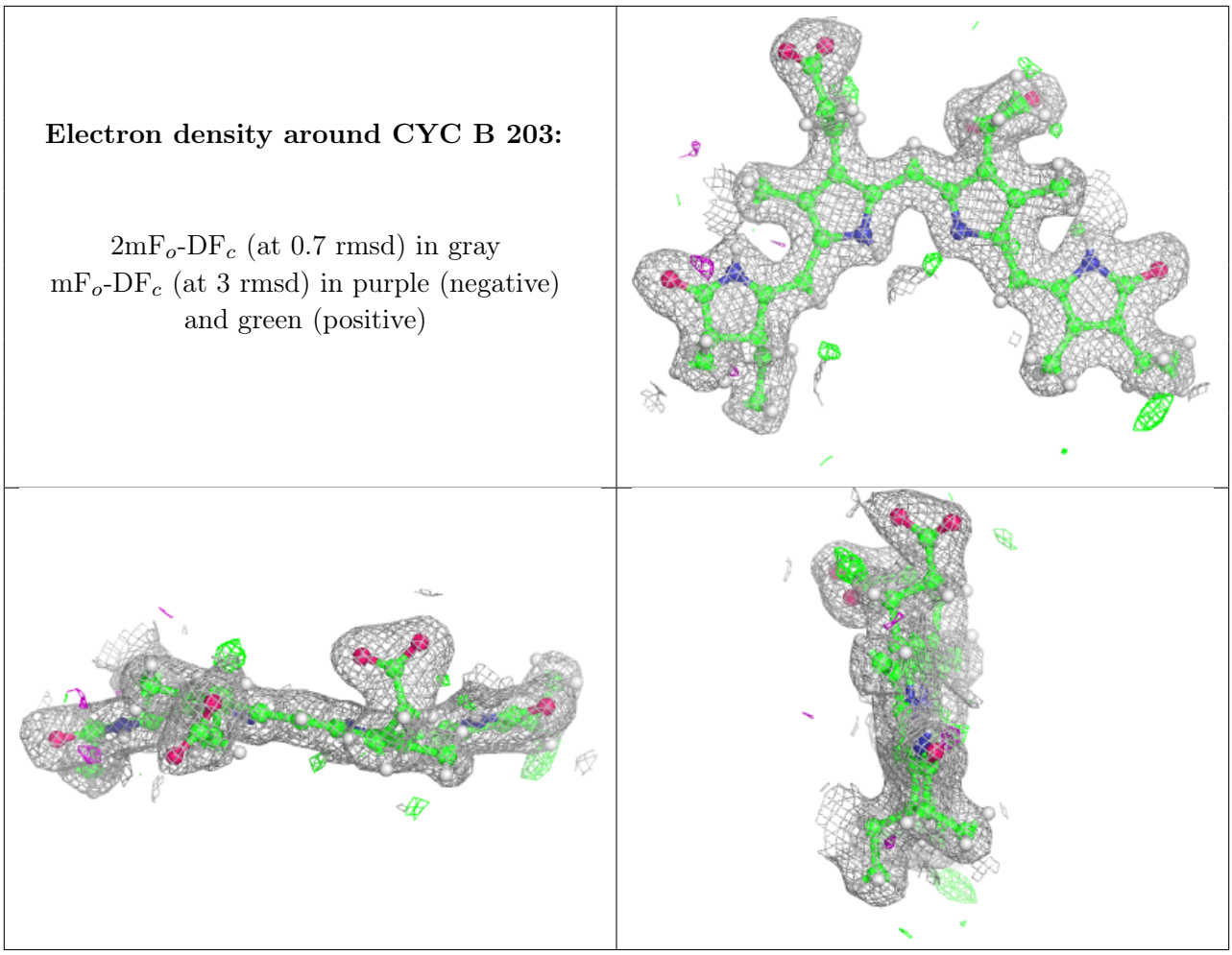
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
7	GOL	B	204	6/6	0.92	0.12	16,20,23,27	0
6	CYC	B	203	43/43	0.93	0.10	13,21,30,35	0
6	CYC	B	202	43/43	0.93	0.10	12,21,28,30	0
6	CYC	D	301	43/43	0.94	0.11	12,17,24,27	0
5	AX9	B	201	43/43	0.95	0.10	9,13,22,28	0
4	M1V	C	101	43/43	0.96	0.09	12,15,19,26	0
6	CYC	D	302	43/43	0.96	0.08	9,14,23,28	0
4	M1V	A	101	43/43	0.96	0.09	12,16,21,27	0
5	AX9	D	303	43/43	0.97	0.10	10,13,18,22	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.

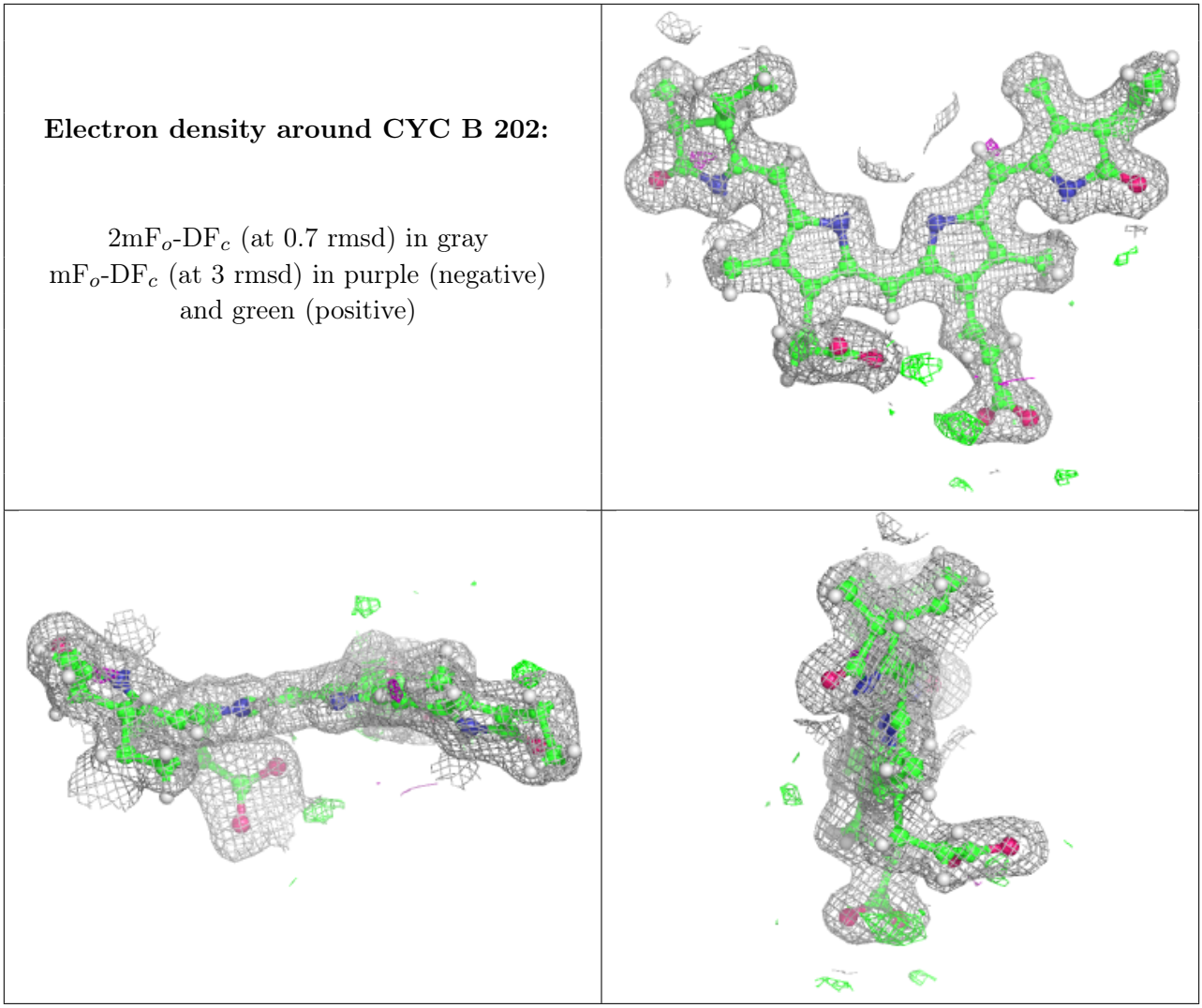
Electron density around CYC B 203:

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



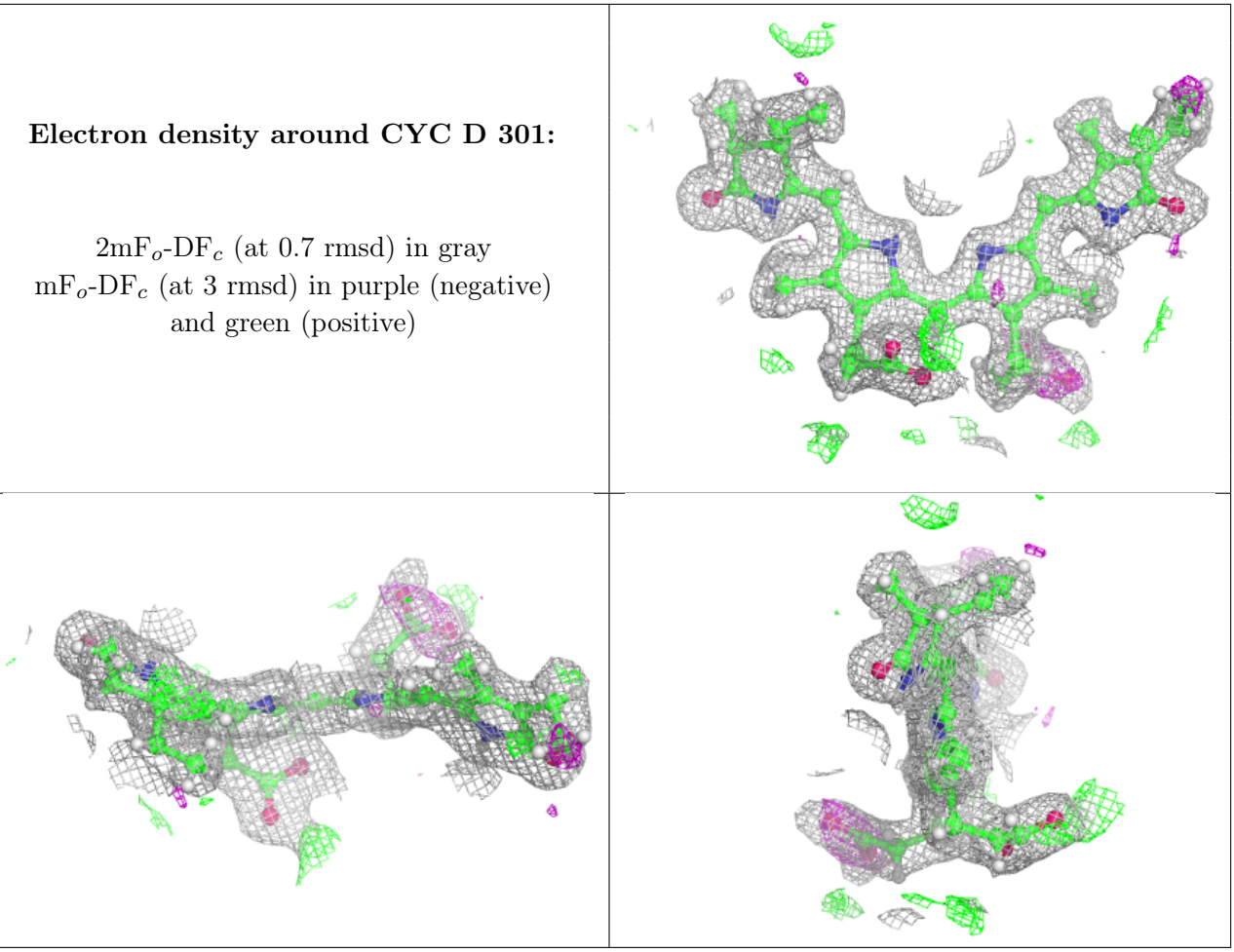
Electron density around CYC B 202:

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



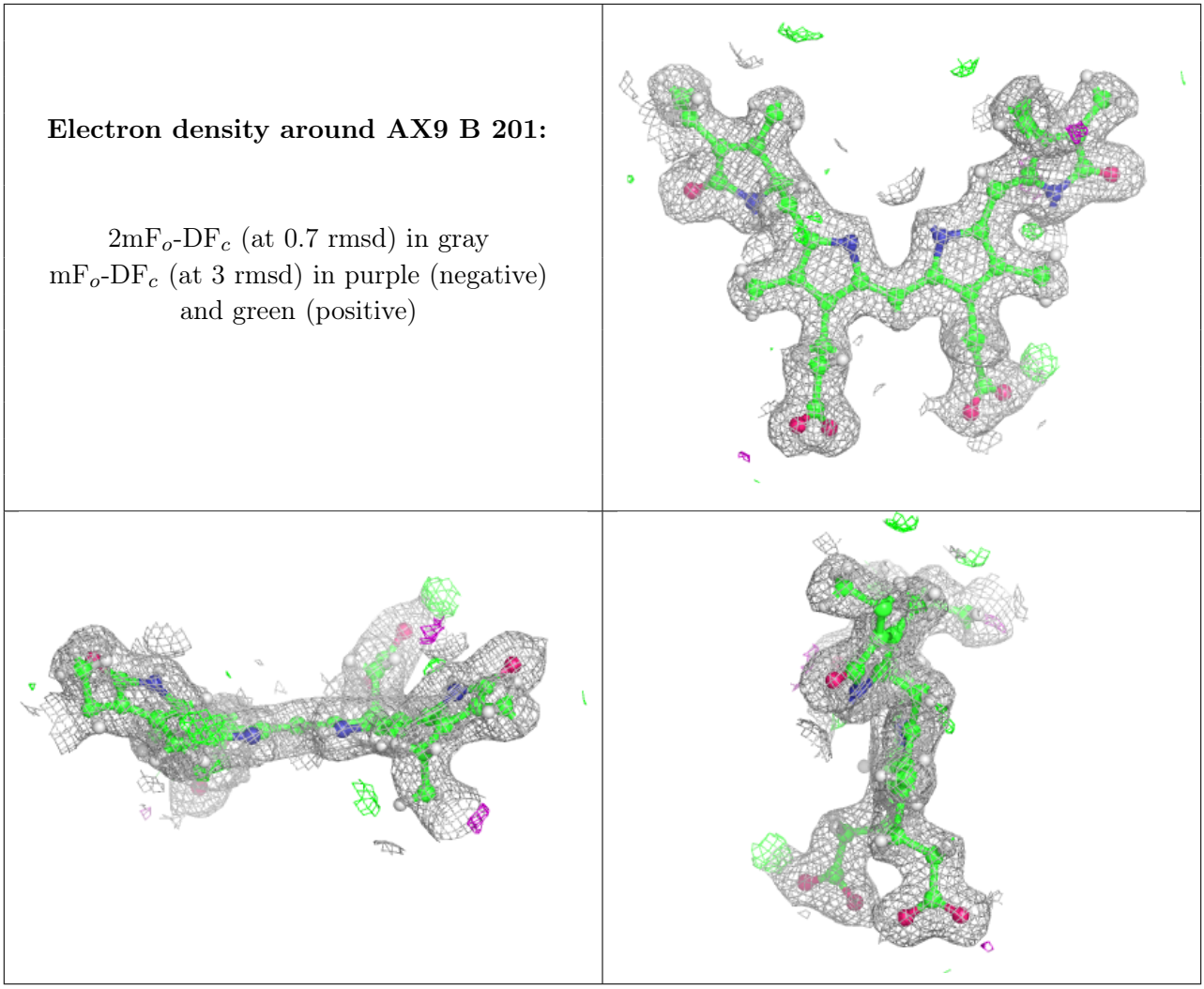
Electron density around CYC D 301:

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



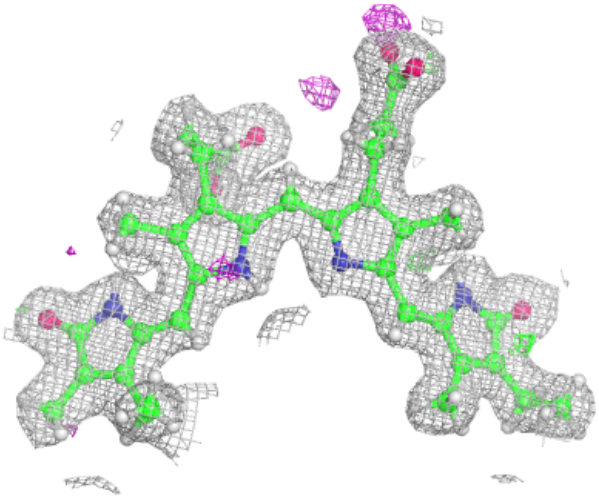
Electron density around AX9 B 201:

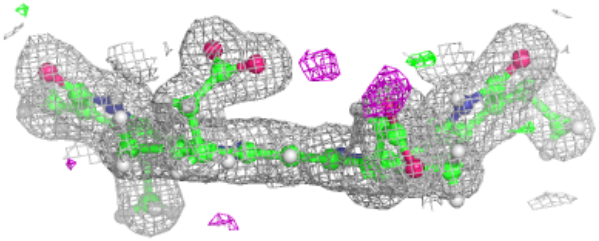
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

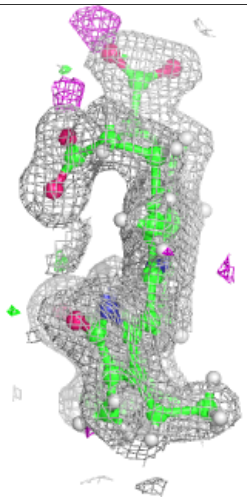


Electron density around M1V C 101:

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

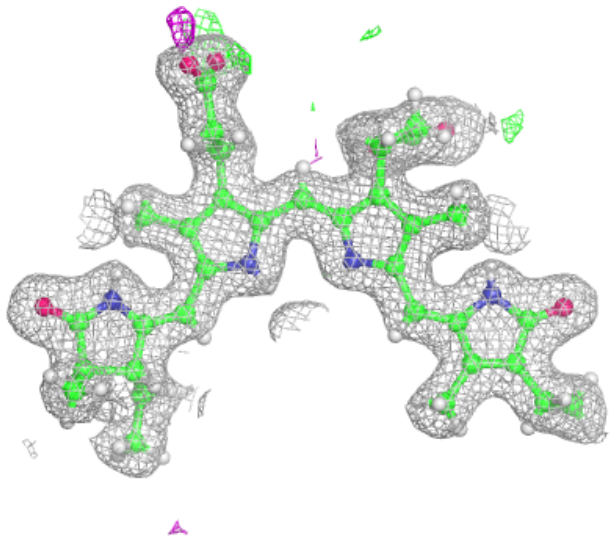


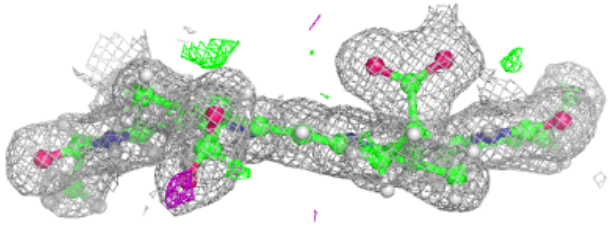


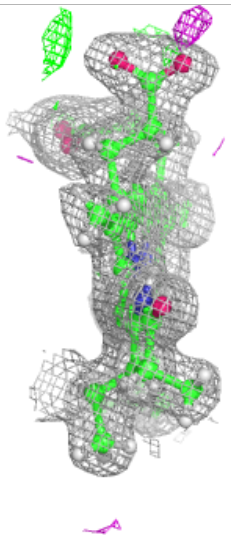


Electron density around CYC D 302:

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

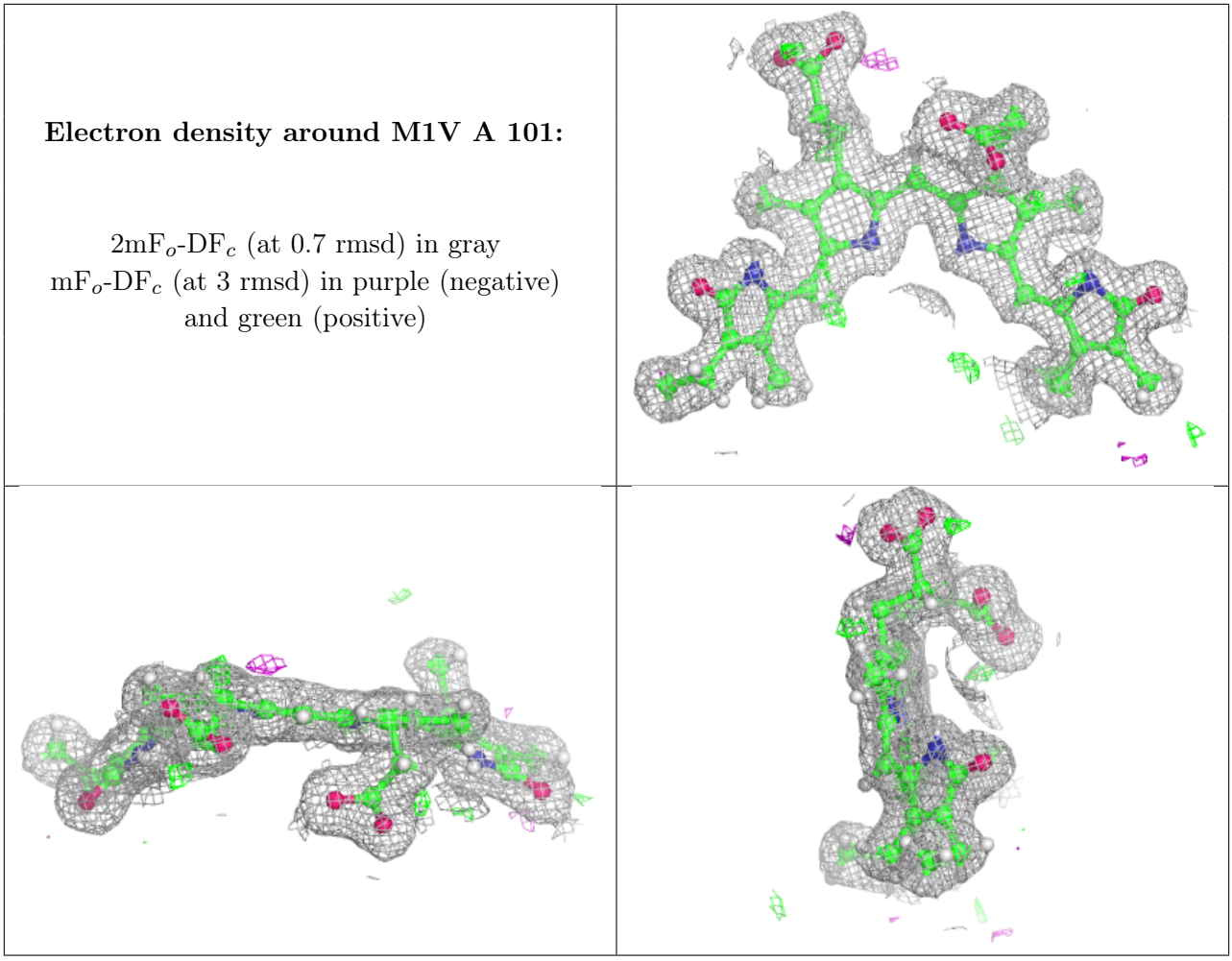






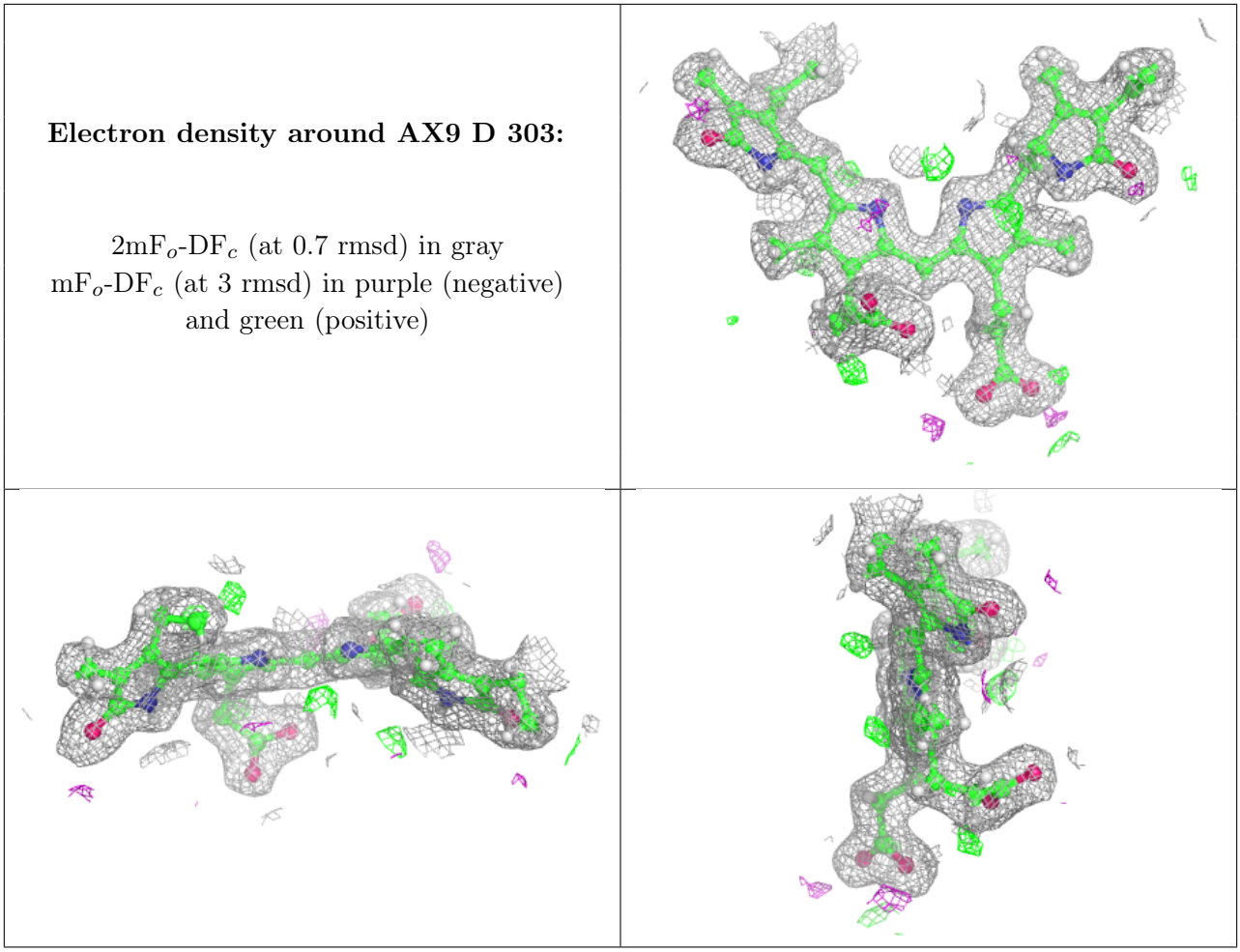
Electron density around M1V A 101:

$2mF_o$-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 303:

$2mF_o$-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.