wwPDB X-ray Structure Validation Summary Report (i)

Nov 21, 2023 – 02:49 AM JST

PDB ID	:	7EFW
Title	:	Crystal structure of hexameric state of C-phycocyanin from Thermoleptolyngbya sp. O-77
Authors	:	Minato, T.; Teramoto, T.; Hung, N.K.; Yamada, K.; Ogo, S.; Kakuta, Y.; Yoon, K.S.
Deposited on	:	2021-03-23
Resolution	:	1.65 Å(reported)

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

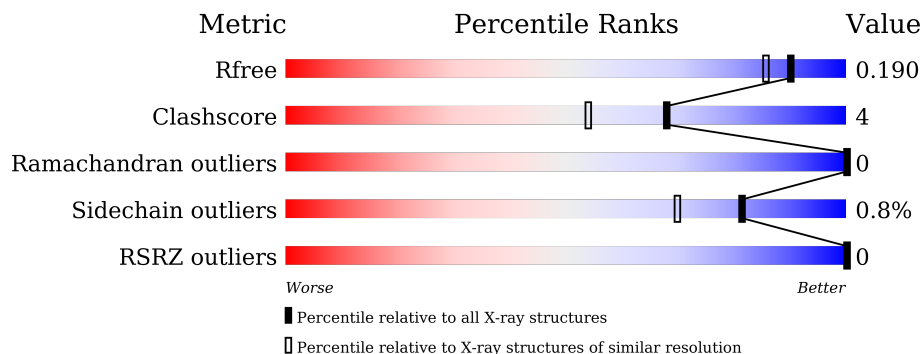|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.65 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	Percentile Ranks	Value
Rfree		0.190
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		0.8%
RSRZ outliers		0

Worse　　　　　　　　　　　　　　　　　　　　Better

▌Percentile relative to all X-ray structures

❙Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

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	162	94% 　　　　　　　　　　6%
1	C	162	93% 　　　　　　　　　　7%
1	E	162	92% 　　　　　　　　　　8%
1	G	162	93% 　　　　　　　　　　6% ·
1	I	162	93% 　　　　　　　　　　7% ·

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Mol	Chain	Length	Quality of chain
1	K	162	97%
2	B	172	94% · 6%
2	D	172	93% · 7%
2	F	172	97%
2	H	172	94% · 5%
2	J	172	94% · 5%
2	L	172	94% · 6%

2   Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 18822 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called C-phycocyanin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	7	0
			1272	797	217	254	4			
1	C	162	Total	C	N	O	S	0	8	0
			1283	804	221	254	4			
1	E	162	Total	C	N	O	S	0	6	0
			1271	796	219	252	4			
1	G	162	Total	C	N	O	S	0	9	0
			1287	807	222	254	4			
1	I	162	Total	C	N	O	S	0	6	0
			1264	792	216	252	4			
1	K	162	Total	C	N	O	S	0	5	0
			1260	789	215	252	4			

- Molecule 2 is a protein called C-phycocyanin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	172	Total	C	N	O	S	0	5	0
			1282	793	225	256	8			
2	D	172	Total	C	N	O	S	0	3	0
			1274	786	225	255	8			
2	F	172	Total	C	N	O	S	0	8	0
			1294	800	225	260	9			
2	H	172	Total	C	N	O	S	0	5	0
			1286	794	227	257	8			
2	J	172	Total	C	N	O	S	0	6	0
			1292	801	226	257	8			
2	L	172	Total	C	N	O	S	0	5	0
			1289	797	229	255	8			

- Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).
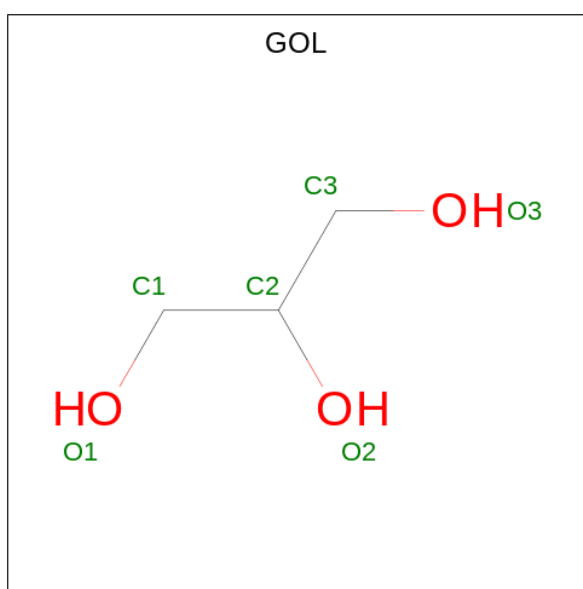
CYC
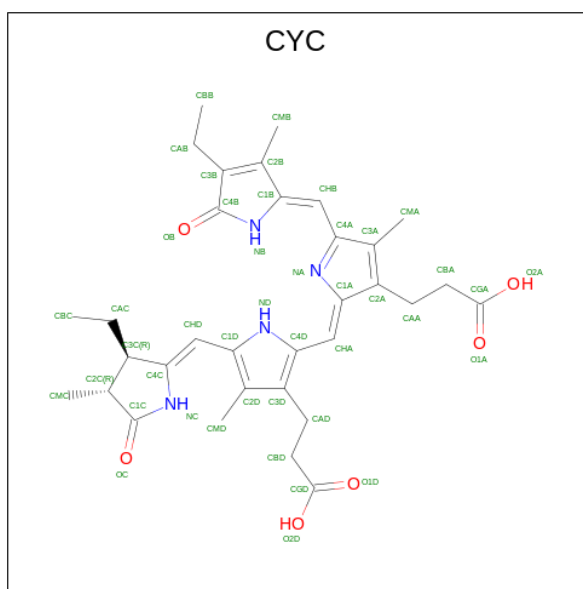
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	B	1	Total	C	N	O	0	0
			43	33	4	6		
3	C	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	D	1	Total	C	N	O	0	0
			43	33	4	6		
3	E	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	F	1	Total	C	N	O	0	0
			43	33	4	6		
3	G	1	Total	C	N	O	0	0
			43	33	4	6		
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	H	1	Total	C	N	O	0	0
			43	33	4	6		
3	I	1	Total	C	N	O	0	0
			43	33	4	6		
3	J	1	Total	C	N	O	0	0
			43	33	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	J	1	Total 43	C 33	N 4	O 6	0	0
3	K	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0
3	L	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 6	C 3	O 3	0	0
4	E	1	Total 6	C 3	O 3	0	0
4	J	1	Total 6	C 3	O 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total 194	O 194	0	0
5	B	265	Total 265	O 265	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	222	Total 222	O 222	0	0
5	D	215	Total 215	O 215	0	0
5	E	232	Total 232	O 232	0	0
5	F	243	Total 243	O 243	0	0
5	G	228	Total 228	O 228	0	0
5	H	244	Total 244	O 244	0	0
5	I	212	Total 212	O 212	0	0
5	J	234	Total 234	O 234	0	0
5	K	193	Total 193	O 193	0	0
5	L	194	Total 194	O 194	0	0

3 Residue-property plots ⓘ

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: C-phycocyanin alpha chain

Chain A:

- Molecule 1: C-phycocyanin alpha chain

Chain C:

- Molecule 1: C-phycocyanin alpha chain

Chain E:

- Molecule 1: C-phycocyanin alpha chain

Chain G:
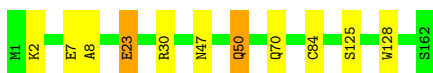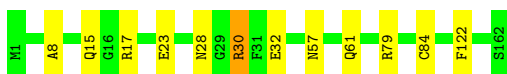
- Molecule 1: C-phycocyanin alpha chain

Chain I:

- Molecule 1: C-phycocyanin alpha chain

Chain K:

M1 P4 R30 M38 Q50 E117 S162

• Molecule 2: C-phycocyanin beta chain

Chain B: 94% 6%

M1 K32 K36 E62 N72 R77 R84 L113 V127 I139 V157 A161 A172

• Molecule 2: C-phycocyanin beta chain

Chain D: 93% 7%

M1 K7 Q23 L24 K36 N72 D101 L113 R114 L120 I139 V157 A172

• Molecule 2: C-phycocyanin beta chain

Chain F: 97%

M1 N72 V104 L113 V127 A172

• Molecule 2: C-phycocyanin beta chain

Chain H: 94% 5%

M1 K7 R37 N72 R84 D101 L113 V127 I139 L156 V157 A172

• Molecule 2: C-phycocyanin beta chain

Chain J: 94% 5%

M1 Q23 K32 Q68 N72 L113 R114 V127 I139 V157 A172

• Molecule 2: C-phycocyanin beta chain

Chain L: 94% 6%

M1 K15 R37 N72 R84 L113 R114 V127 K135 I139 L156 A172

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.09Å 187.44Å 210.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 1.65 49.18 – 1.65	Depositor EDS
% Data completeness (in resolution range)	92.6 (49.18-1.65) 92.6 (49.18-1.65)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.65Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.171 , 0.190 0.171 , 0.190	Depositor DCC
R_{free} test set	1999 reflections (0.76%)	wwPDB-VP
Wilson B-factor (Å^2)	13.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18822	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 43.39 % 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 1.7763e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CYC, MEN

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	0/1314	0.52	2/1780 (0.1%)
1	C	0.38	0/1331	0.51	1/1802 (0.1%)
1	E	0.34	0/1310	0.52	2/1774 (0.1%)
1	G	0.46	1/1335 (0.1%)	0.55	0/1806
1	I	0.42	0/1303	0.51	0/1766
1	K	0.34	0/1296	0.50	2/1756 (0.1%)
2	B	0.25	0/1299	0.41	0/1756
2	D	0.25	0/1285	0.42	0/1737
2	F	0.26	0/1320	0.42	0/1783
2	H	0.26	0/1303	0.46	1/1760 (0.1%)
2	J	0.26	0/1312	0.42	0/1773
2	L	0.25	0/1306	0.42	0/1764
All	All	0.33	1/15714 (0.0%)	0.47	8/21257 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	23	GLU	CD-OE2	-5.05	1.20	1.25

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	117[A]	GLU	CA-C-O	6.04	132.79	120.10
1	A	117[B]	GLU	CA-C-O	6.04	132.79	120.10
1	E	117[A]	GLU	CA-C-O	5.94	132.58	120.10
1	E	117[B]	GLU	CA-C-O	5.94	132.58	120.10
1	C	117	GLU	CA-C-O	5.62	131.90	120.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1272	0	1251	4	0
1	C	1283	0	1271	7	0
1	E	1271	0	1249	10	0
1	G	1287	0	1276	8	0
1	I	1264	0	1242	9	0
1	K	1260	0	1233	2	0
2	B	1282	0	1299	9	0
2	D	1274	0	1283	8	0
2	F	1294	0	1313	4	0
2	H	1286	0	1301	6	0
2	J	1292	0	1315	8	0
2	L	1289	0	1311	7	0
3	A	43	0	37	2	0
3	B	86	0	74	11	0
3	C	43	0	37	5	0
3	D	86	0	74	8	0
3	E	43	0	37	4	0
3	F	86	0	74	7	0
3	G	43	0	37	3	0
3	H	86	0	74	8	0
3	I	43	0	37	5	0
3	J	86	0	74	7	0
3	K	43	0	37	3	0
3	L	86	0	74	8	0
4	E	12	0	16	0	0
4	J	6	0	8	1	0
5	A	194	0	0	0	0
5	B	265	0	0	1	0
5	C	222	0	0	0	0
5	D	215	0	0	1	0
5	E	232	0	0	3	0
5	F	243	0	0	0	0
5	G	228	0	0	1	0
5	H	244	0	0	0	0
5	I	212	0	0	0	0
5	J	234	0	0	0	0
5	K	193	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	194	0	0	0	0
All	All	18822	0	16034	122	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 4.

The worst 5 of 122 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)
2:J:23:GLN:HG2	4:J:203:GOL:H2	1.56	0.87
1:C:15:GLN:NE2	1:C:17[A]:ARG:HE	1.81	0.78
1:E:79[A]:ARG:NH2	3:E:201:CYC:O2D	2.23	0.70
2:L:114:ARG:NH1	2:L:172:ALA:O	2.24	0.70
1:E:61[B]:GLN:NE2	5:E:304:HOH:O	2.27	0.68

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	167/162 (103%)	165 (99%)	2 (1%)	0	100	100
1	C	169/162 (104%)	166 (98%)	3 (2%)	0	100	100
1	E	166/162 (102%)	163 (98%)	3 (2%)	0	100	100
1	G	169/162 (104%)	167 (99%)	2 (1%)	0	100	100
1	I	166/162 (102%)	163 (98%)	3 (2%)	0	100	100
1	K	165/162 (102%)	163 (99%)	2 (1%)	0	100	100
2	B	174/172 (101%)	171 (98%)	3 (2%)	0	100	100
2	D	172/172 (100%)	169 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	177/172 (103%)	174 (98%)	3 (2%)	0	100	100
2	H	174/172 (101%)	171 (98%)	3 (2%)	0	100	100
2	J	175/172 (102%)	172 (98%)	3 (2%)	0	100	100
2	L	174/172 (101%)	171 (98%)	3 (2%)	0	100	100
All	All	2048/2004 (102%)	2015 (98%)	33 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2   Protein sidechains ⓘ

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	130/123 (106%)	128 (98%)	2 (2%)	65	44
1	C	132/123 (107%)	129 (98%)	3 (2%)	50	25
1	E	129/123 (105%)	128 (99%)	1 (1%)	81	70
1	G	132/123 (107%)	129 (98%)	3 (2%)	50	25
1	I	129/123 (105%)	128 (99%)	1 (1%)	81	70
1	K	128/123 (104%)	125 (98%)	3 (2%)	50	25
2	B	135/130 (104%)	135 (100%)	0	100	100
2	D	133/130 (102%)	133 (100%)	0	100	100
2	F	138/130 (106%)	138 (100%)	0	100	100
2	H	135/130 (104%)	135 (100%)	0	100	100
2	J	136/130 (105%)	134 (98%)	2 (2%)	65	44
2	L	135/130 (104%)	133 (98%)	2 (2%)	65	44
All	All	1592/1518 (105%)	1575 (99%)	17 (1%)	81	57

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	50[B]	GLN

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Res	Type
2	L	15[B]	LYS
1	G	50[A]	GLN
1	G	50[B]	GLN
1	I	30	ARG

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

Mol	Chain	Res	Type
1	A	49	GLN
1	C	15	GLN
2	F	68	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\#|Z| > 2$
2	MEN	H	72	2	7,8,9	0.92	0	6,9,11	1.38	1 (16%)
2	MEN	F	72	2	7,8,9	0.87	0	6,9,11	1.46	2 (33%)
2	MEN	J	72	2	7,8,9	0.91	0	6,9,11	1.39	1 (16%)
2	MEN	B	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	L	72	2	7,8,9	0.91	0	6,9,11	1.36	1 (16%)
2	MEN	D	72	2	7,8,9	0.92	0	6,9,11	1.45	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
2	MEN	H	72	2	-	2/7/8/10	-
2	MEN	F	72	2	-	2/7/8/10	-
2	MEN	J	72	2	-	2/7/8/10	-
2	MEN	B	72	2	-	2/7/8/10	-
2	MEN	L	72	2	-	2/7/8/10	-
2	MEN	D	72	2	-	2/7/8/10	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	72	MEN	CB-CA-C	-2.67	106.45	111.47
2	F	72	MEN	CB-CA-C	-2.58	106.63	111.47
2	B	72	MEN	CB-CA-C	-2.52	106.74	111.47
2	L	72	MEN	CB-CA-C	-2.43	106.90	111.47
2	H	72	MEN	CB-CA-C	-2.42	106.93	111.47

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

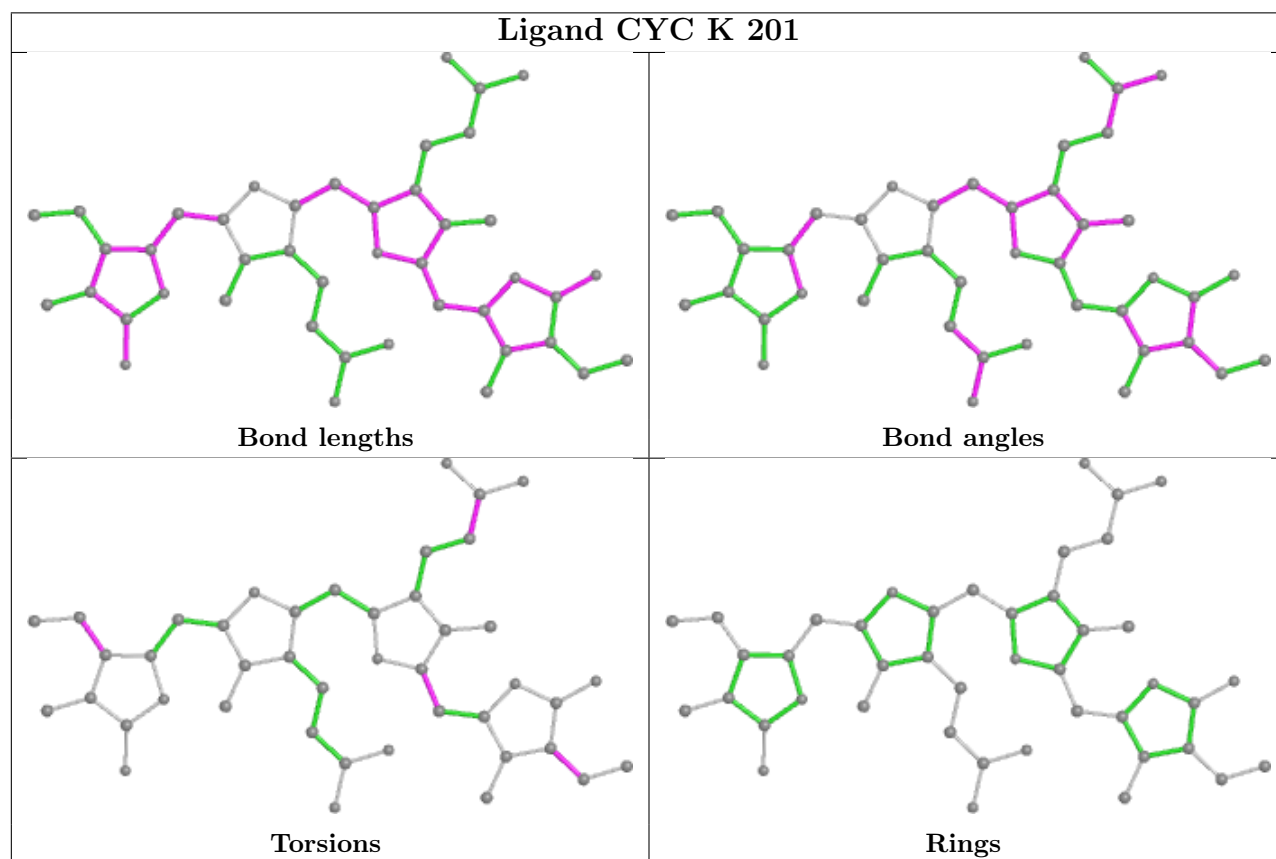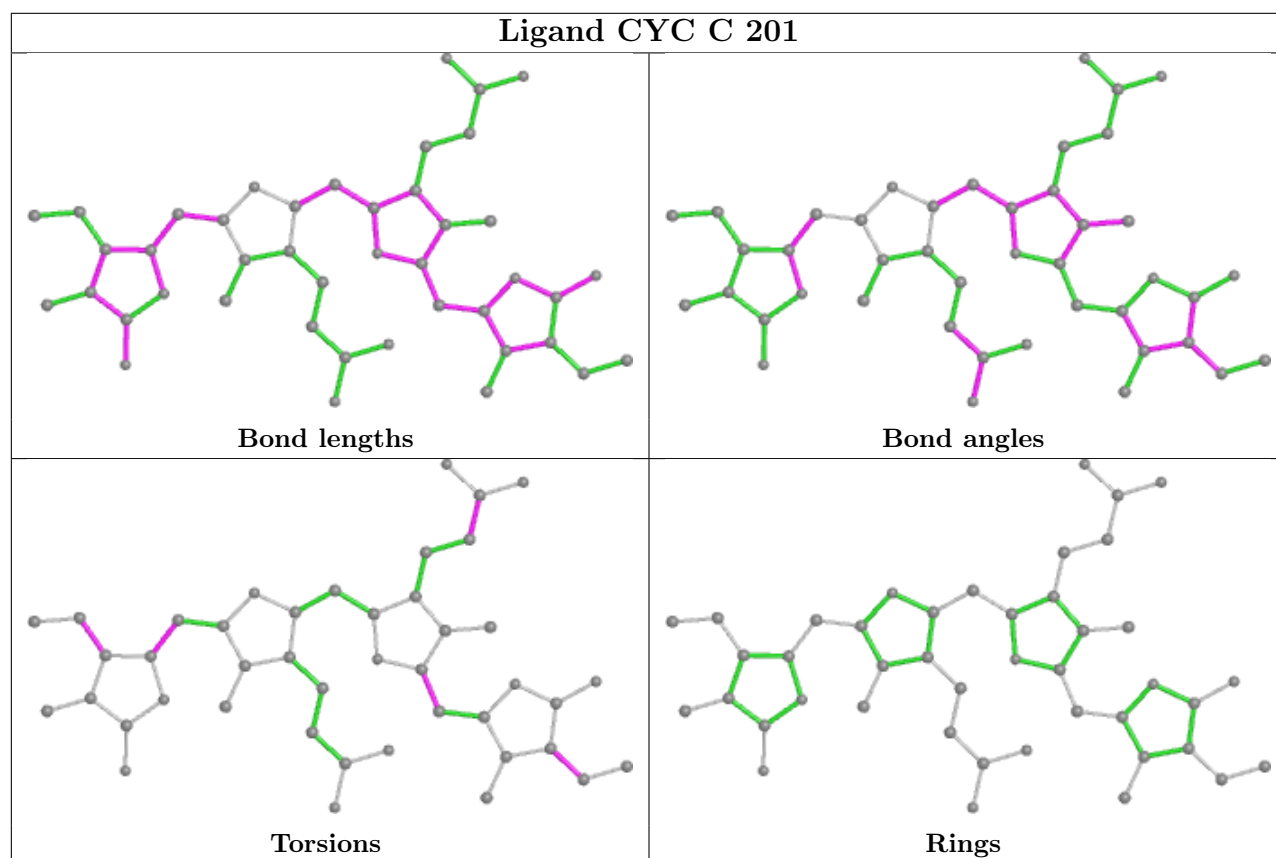| Mol	Chain	Res	Type	Atoms
2	D	72	MEN	CA-CB-CG-OD1
2	H	72	MEN	CA-CB-CG-OD1
2	L	72	MEN	CA-CB-CG-OD1
2	B	72	MEN	CA-CB-CG-OD1
2	F	72	MEN	CA-CB-CG-OD1

There are no ring outliers.
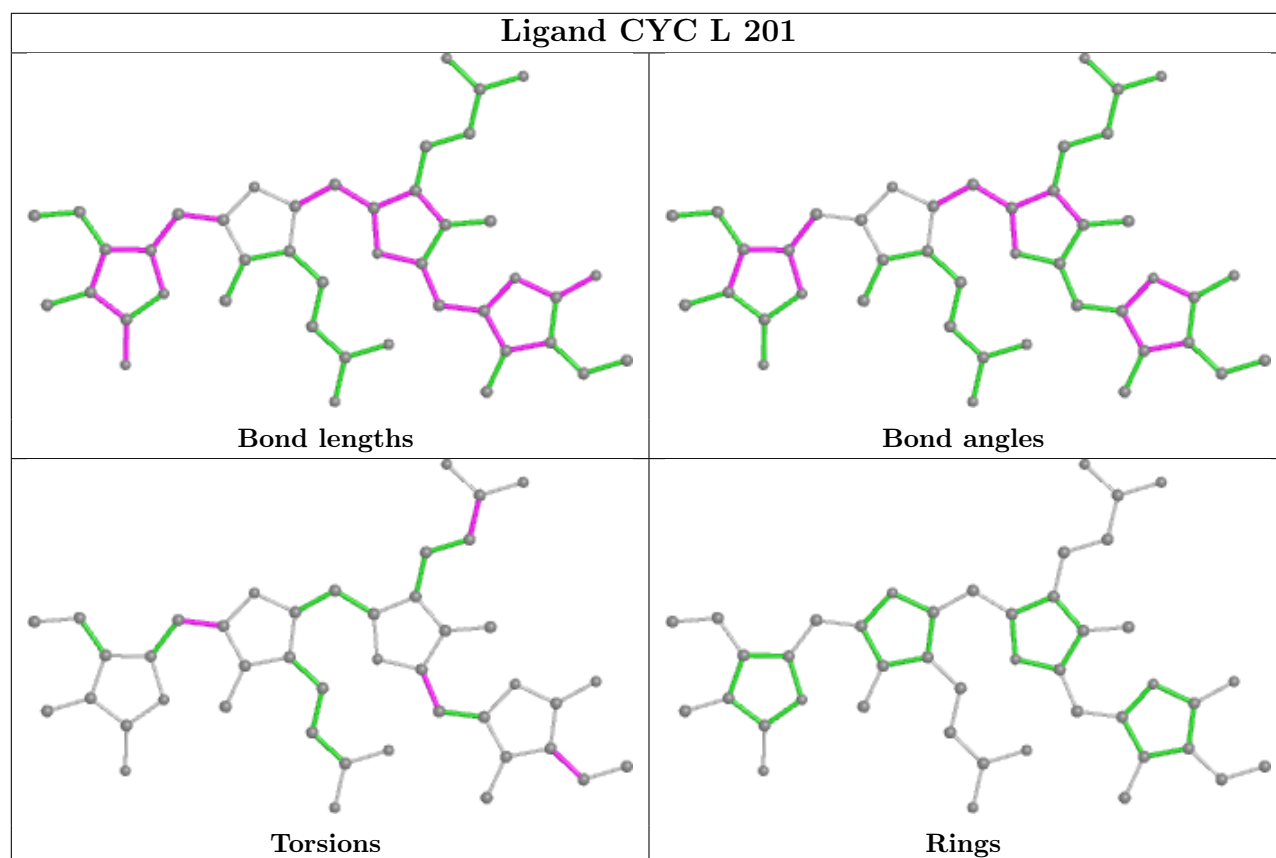
2 monomers are involved in 2 short contacts:
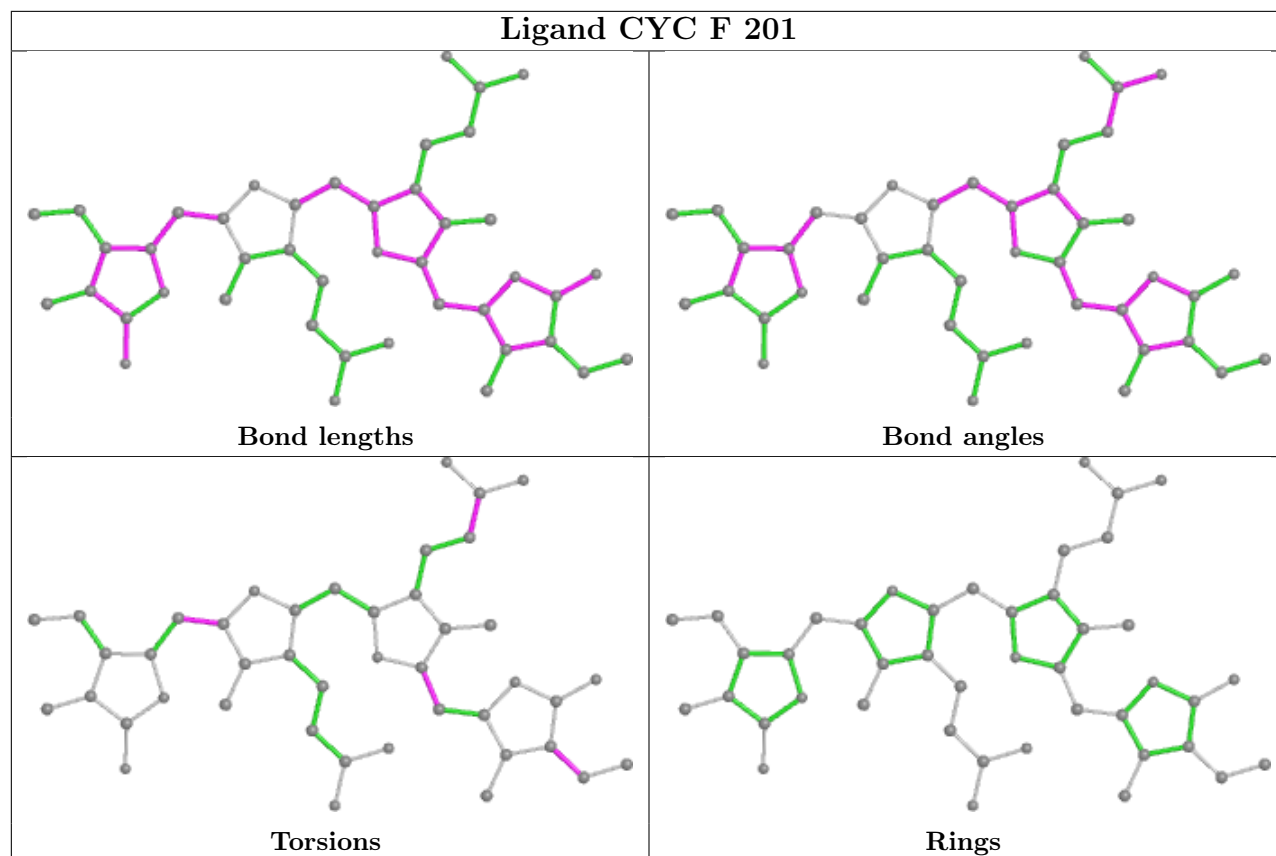
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	72	MEN	1	0
2	J	72	MEN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

21 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 Counts	Bond lengths RMSZ	Bond lengths #$|Z| > 2$	Bond angles Counts	Bond angles RMSZ	Bond angles #$|Z| > 2$
3	CYC	K	201	1	42,46,46	3.73	21 (50%)	50,67,67	1.84	9 (18%)
3	CYC	L	202	2	42,46,46	3.80	21 (50%)	50,67,67	1.78	9 (18%)
3	CYC	C	201	1	42,46,46	3.73	21 (50%)	50,67,67	1.83	8 (16%)
4	GOL	J	203	-	5,5,5	0.89	0	5,5,5	0.99	0
3	CYC	F	201	2	42,46,46	3.75	21 (50%)	50,67,67	1.87	9 (18%)
3	CYC	L	201	2	42,46,46	3.77	20 (47%)	50,67,67	1.85	7 (14%)
3	CYC	A	201	1	42,46,46	3.74	21 (50%)	50,67,67	1.82	12 (24%)
3	CYC	J	201	2	42,46,46	3.76	20 (47%)	50,67,67	1.83	10 (20%)
4	GOL	E	203	-	5,5,5	0.88	0	5,5,5	1.00	0
3	CYC	B	201	2	42,46,46	3.73	20 (47%)	50,67,67	2.02	11 (22%)
3	CYC	F	202	2	42,46,46	3.70	21 (50%)	50,67,67	1.80	9 (18%)
4	GOL	E	202	-	5,5,5	0.90	0	5,5,5	1.00	0
3	CYC	D	202	2	42,46,46	3.72	21 (50%)	50,67,67	1.73	11 (22%)
3	CYC	G	201	1	42,46,46	3.73	21 (50%)	50,67,67	1.74	8 (16%)
3	CYC	I	201	1	42,46,46	3.72	21 (50%)	50,67,67	1.79	9 (18%)
3	CYC	H	201	2	42,46,46	3.75	21 (50%)	50,67,67	1.97	11 (22%)
3	CYC	B	202	2	42,46,46	3.76	20 (47%)	50,67,67	1.77	9 (18%)
3	CYC	D	201	2	42,46,46	3.78	20 (47%)	50,67,67	2.05	10 (20%)
3	CYC	H	202	2	42,46,46	3.72	21 (50%)	50,67,67	1.79	8 (16%)
3	CYC	E	201	1	42,46,46	3.70	21 (50%)	50,67,67	1.85	9 (18%)
3	CYC	J	202	2	42,46,46	3.76	21 (50%)	50,67,67	1.79	9 (18%)

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	K	201	1	-	8/25/74/74	0/4/4/4
3	CYC	L	202	2	-	9/25/74/74	0/4/4/4
3	CYC	C	201	1	-	9/25/74/74	0/4/4/4
4	GOL	J	203	-	-	2/4/4/4	-
3	CYC	F	201	2	-	7/25/74/74	0/4/4/4
3	CYC	L	201	2	-	7/25/74/74	0/4/4/4
3	CYC	A	201	1	-	9/25/74/74	0/4/4/4
3	CYC	J	201	2	-	8/25/74/74	0/4/4/4
4	GOL	E	203	-	-	0/4/4/4	-
3	CYC	B	201	2	-	8/25/74/74	0/4/4/4
3	CYC	F	202	2	-	8/25/74/74	0/4/4/4
4	GOL	E	202	-	-	0/4/4/4	-
3	CYC	D	202	2	-	9/25/74/74	0/4/4/4
3	CYC	G	201	1	-	8/25/74/74	0/4/4/4
3	CYC	I	201	1	-	8/25/74/74	0/4/4/4
3	CYC	H	201	2	-	8/25/74/74	0/4/4/4
3	CYC	B	202	2	-	8/25/74/74	0/4/4/4
3	CYC	D	201	2	-	7/25/74/74	0/4/4/4
3	CYC	H	202	2	-	8/25/74/74	0/4/4/4
3	CYC	E	201	1	-	9/25/74/74	0/4/4/4
3	CYC	J	202	2	-	10/25/74/74	0/4/4/4

The worst 5 of 373 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	201	CYC	C1B-NB	9.76	1.54	1.37
3	L	202	CYC	C2C-C1C	9.68	1.60	1.52
3	L	201	CYC	C1B-NB	9.65	1.54	1.37
3	F	201	CYC	C1B-NB	9.65	1.53	1.37
3	L	202	CYC	C1B-NB	9.57	1.53	1.37

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	CYC	C4D-CHA-C1A	-7.97	119.29	128.81
3	K	201	CYC	C4D-CHA-C1A	-7.93	119.34	128.81
3	E	201	CYC	C4D-CHA-C1A	-7.82	119.47	128.81
3	A	201	CYC	C4D-CHA-C1A	-7.67	119.65	128.81
3	H	202	CYC	C4D-CHA-C1A	-7.56	119.78	128.81

There are no chirality outliers.

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	201	CYC	NA-C4A-CHB-C1B
3	A	201	CYC	C3A-C4A-CHB-C1B
3	A	201	CYC	C2C-C3C-CAC-CBC
3	A	201	CYC	C4C-C3C-CAC-CBC
3	B	201	CYC	NA-C4A-CHB-C1B

There are no ring outliers.

19 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	201	CYC	3	0
3	L	202	CYC	4	0
3	C	201	CYC	5	0
4	J	203	GOL	1	0
3	F	201	CYC	4	0
3	L	201	CYC	4	0
3	A	201	CYC	2	0
3	J	201	CYC	4	0
3	B	201	CYC	5	0
3	F	202	CYC	3	0
3	D	202	CYC	4	0
3	G	201	CYC	3	0
3	I	201	CYC	5	0
3	H	201	CYC	4	0
3	B	202	CYC	6	0
3	D	201	CYC	4	0
3	H	202	CYC	4	0
3	E	201	CYC	4	0
3	J	202	CYC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 K 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC L 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC C 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC L 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC J 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC F 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC D 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC G 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC I 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC H 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC B 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC H 202

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC J 202

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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(Å²)	Q<0.9
1	A	162/162 (100%)	-0.42	0	100	100	11, 13, 21, 31	0
1	C	162/162 (100%)	-0.35	0	100	100	10, 13, 22, 31	0
1	E	162/162 (100%)	-0.36	0	100	100	9, 12, 21, 29	0
1	G	162/162 (100%)	-0.36	0	100	100	10, 12, 22, 34	0
1	I	162/162 (100%)	-0.39	0	100	100	12, 16, 25, 33	0
1	K	162/162 (100%)	-0.31	0	100	100	11, 15, 25, 34	0
2	B	171/172 (99%)	-0.49	0	100	100	10, 14, 25, 30	0
2	D	171/172 (99%)	-0.41	0	100	100	11, 18, 29, 37	0
2	F	171/172 (99%)	-0.50	0	100	100	10, 14, 25, 31	0
2	H	171/172 (99%)	-0.50	0	100	100	9, 14, 24, 30	0
2	J	171/172 (99%)	-0.38	0	100	100	12, 18, 30, 34	0
2	L	171/172 (99%)	-0.37	0	100	100	12, 19, 30, 42	0
All	All	1998/2004 (99%)	-0.41	0	100	100	9, 15, 26, 42	0

There are no RSRZ outliers to report.

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, 95th 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(Å²)	Q<0.9
2	MEN	D	72	9/10	0.96	0.07	15,17,19,20	0
2	MEN	B	72	9/10	0.97	0.06	11,12,16,16	0
2	MEN	H	72	9/10	0.97	0.07	12,14,15,15	0

Continued on next page...

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MEN	J	72	9/10	0.97	0.06	13,14,16,17	0
2	MEN	L	72	9/10	0.97	0.06	14,16,19,22	0
2	MEN	F	72	9/10	0.98	0.06	13,14,16,16	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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, 95th 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
4	GOL	E	202	6/6	0.81	0.18	31,35,36,37	0
4	GOL	E	203	6/6	0.84	0.20	21,23,27,30	0
4	GOL	J	203	6/6	0.86	0.36	42,44,48,55	0
3	CYC	F	201	43/43	0.90	0.12	10,18,35,45	0
3	CYC	D	201	43/43	0.91	0.11	11,21,36,41	0
3	CYC	L	201	43/43	0.92	0.12	12,22,34,42	0
3	CYC	J	201	43/43	0.92	0.11	11,18,33,43	0
3	CYC	L	202	43/43	0.93	0.08	15,20,30,36	0
3	CYC	H	202	43/43	0.93	0.11	9,13,21,34	0
3	CYC	B	201	43/43	0.93	0.11	10,17,31,39	0
3	CYC	H	201	43/43	0.93	0.11	10,16,29,37	0
3	CYC	J	202	43/43	0.94	0.08	12,18,26,34	0
3	CYC	K	201	43/43	0.95	0.10	11,11,14,16	0
3	CYC	F	202	43/43	0.95	0.08	9,12,19,28	0
3	CYC	A	201	43/43	0.95	0.09	10,11,14,14	0
3	CYC	D	202	43/43	0.95	0.09	11,15,28,49	0
3	CYC	E	201	43/43	0.95	0.09	9,10,11,13	0
3	CYC	B	202	43/43	0.95	0.07	12,15,22,29	0
3	CYC	I	201	43/43	0.96	0.08	11,12,15,17	0
3	CYC	C	201	43/43	0.96	0.10	10,10,11,13	0
3	CYC	G	201	43/43	0.96	0.10	10,11,13,15	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 F 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
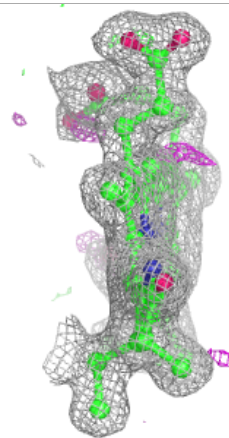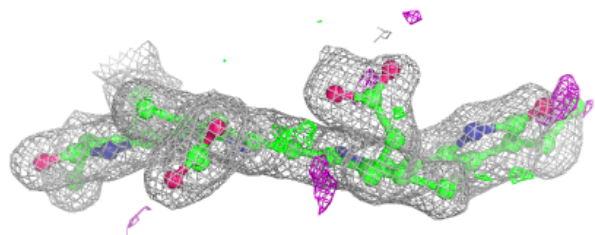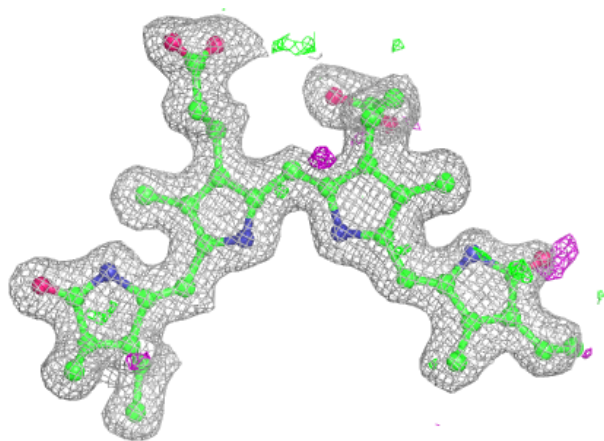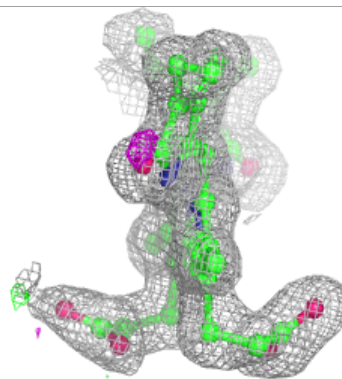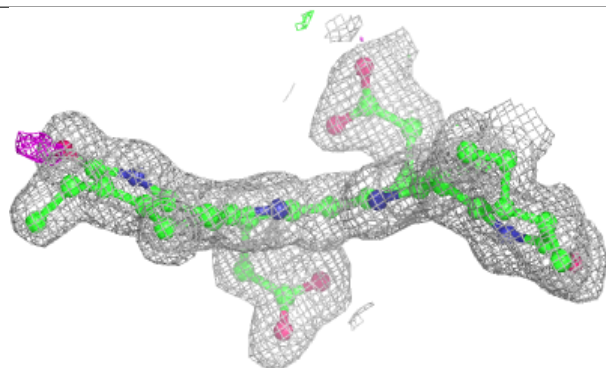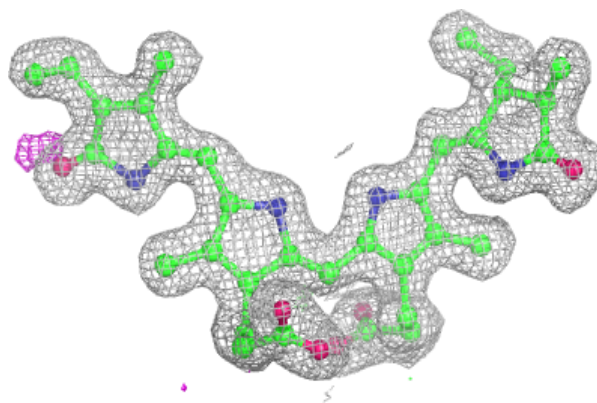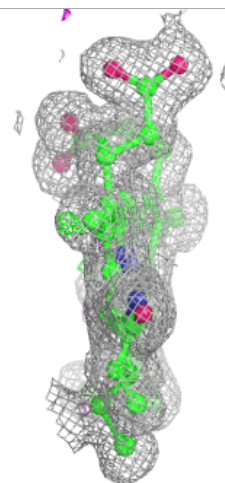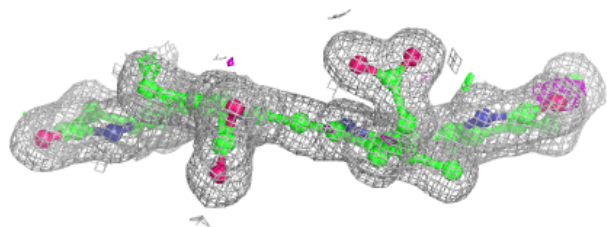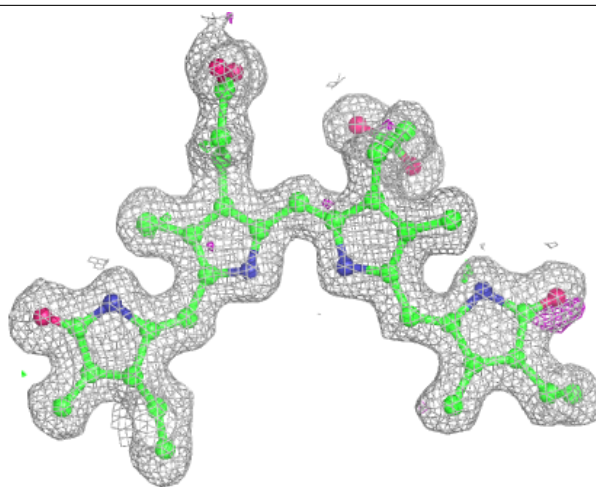mF_o-DF_c (at 3 rmsd) in purple (negative)
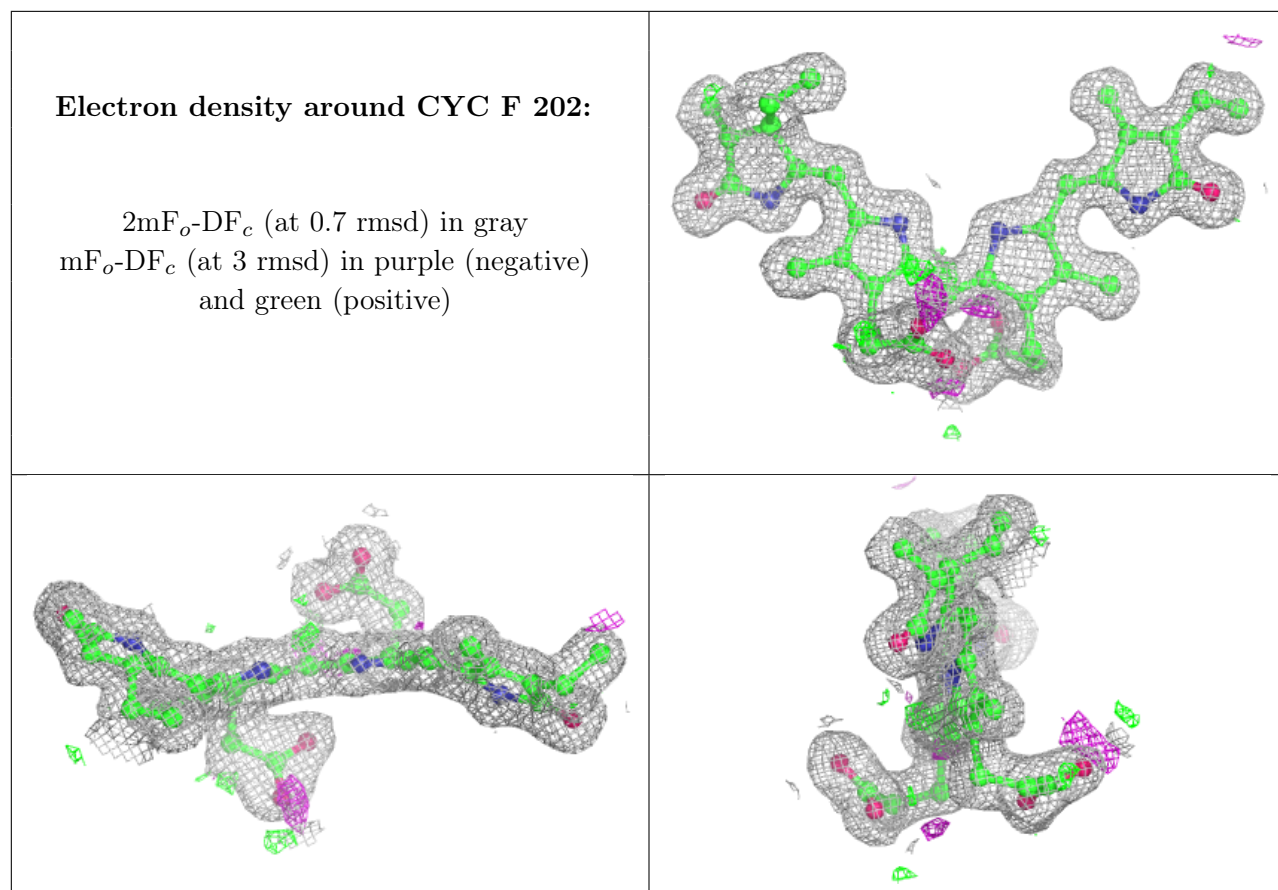and green (positive)
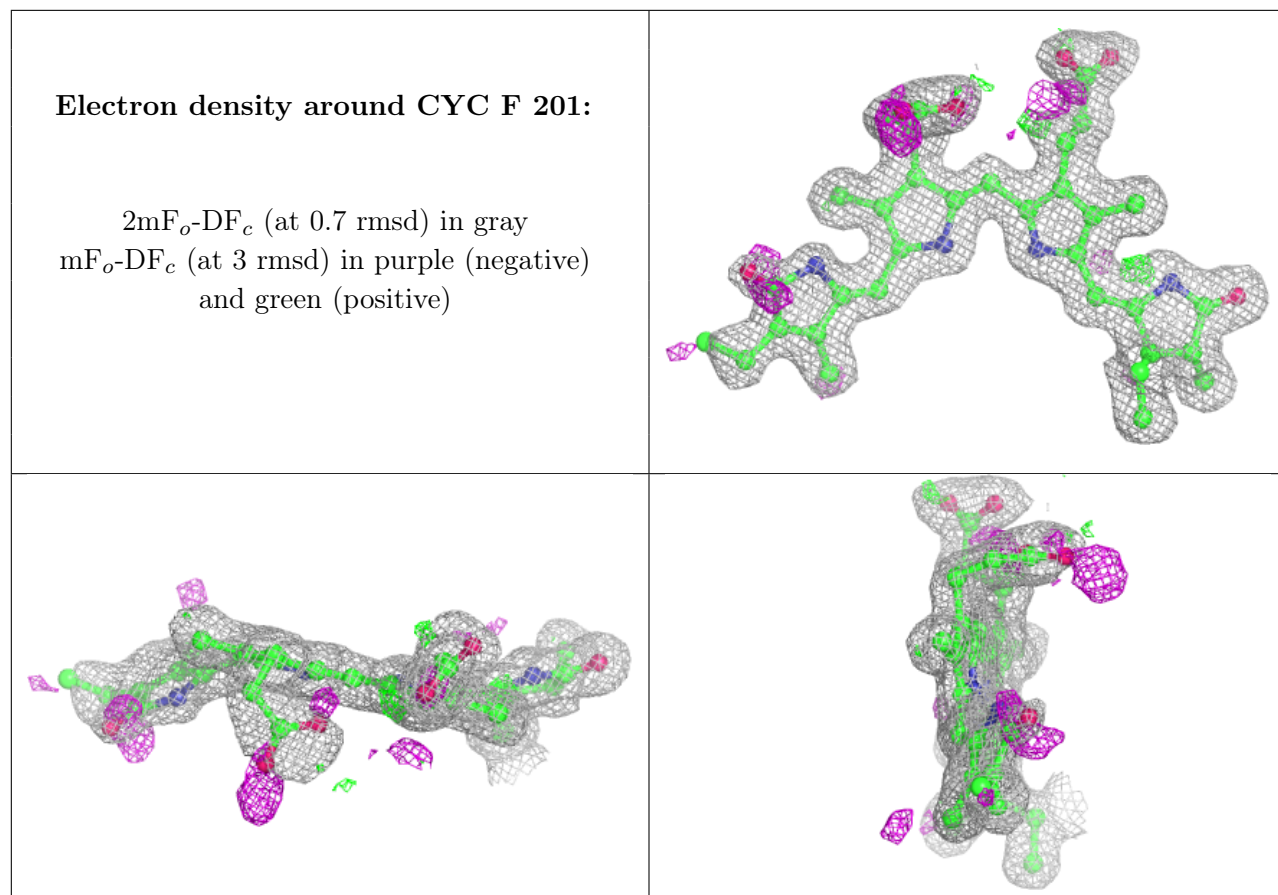
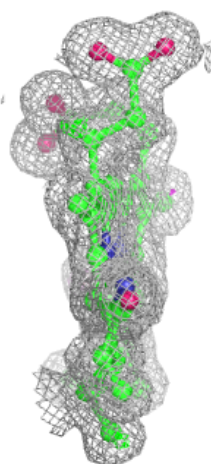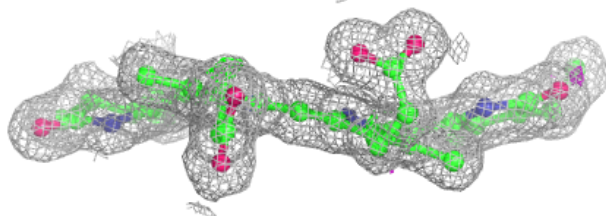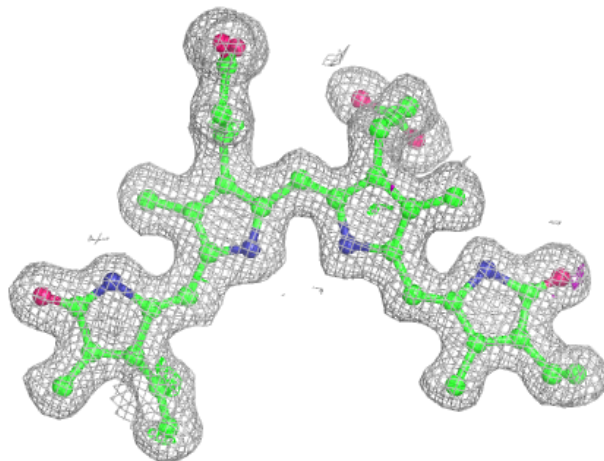**Electron density around CYC D 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
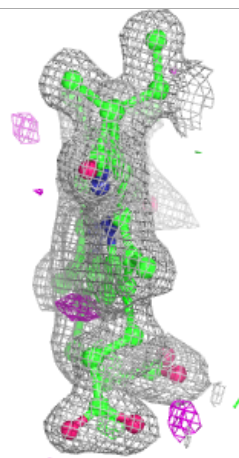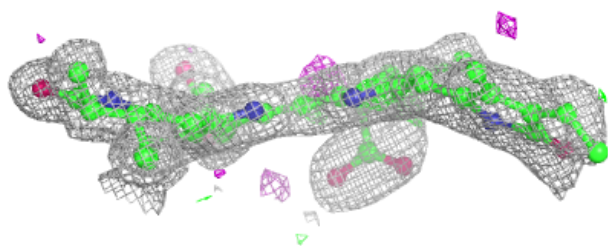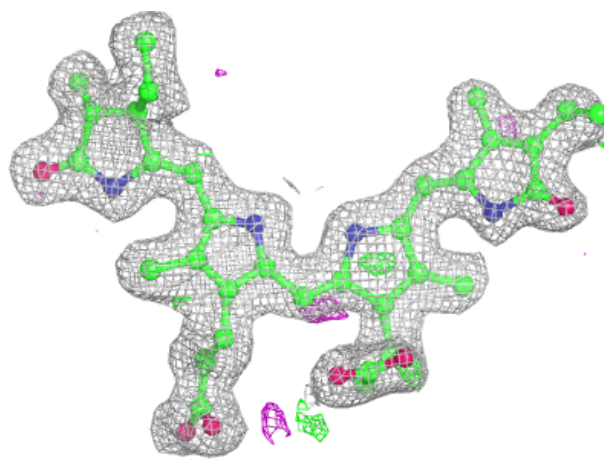
Electron density around CYC L 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
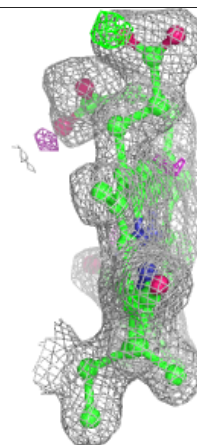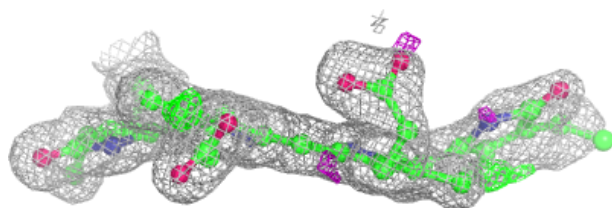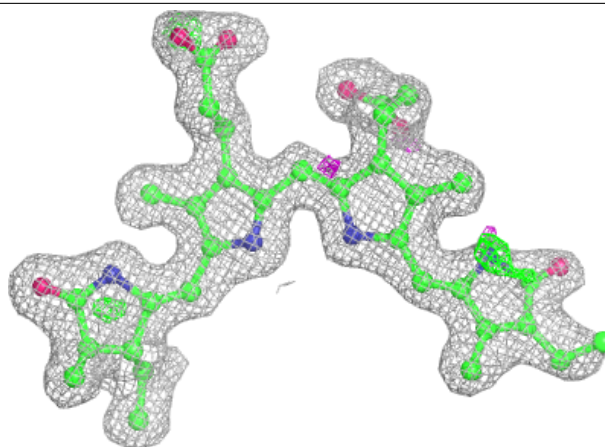
Electron density around CYC J 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
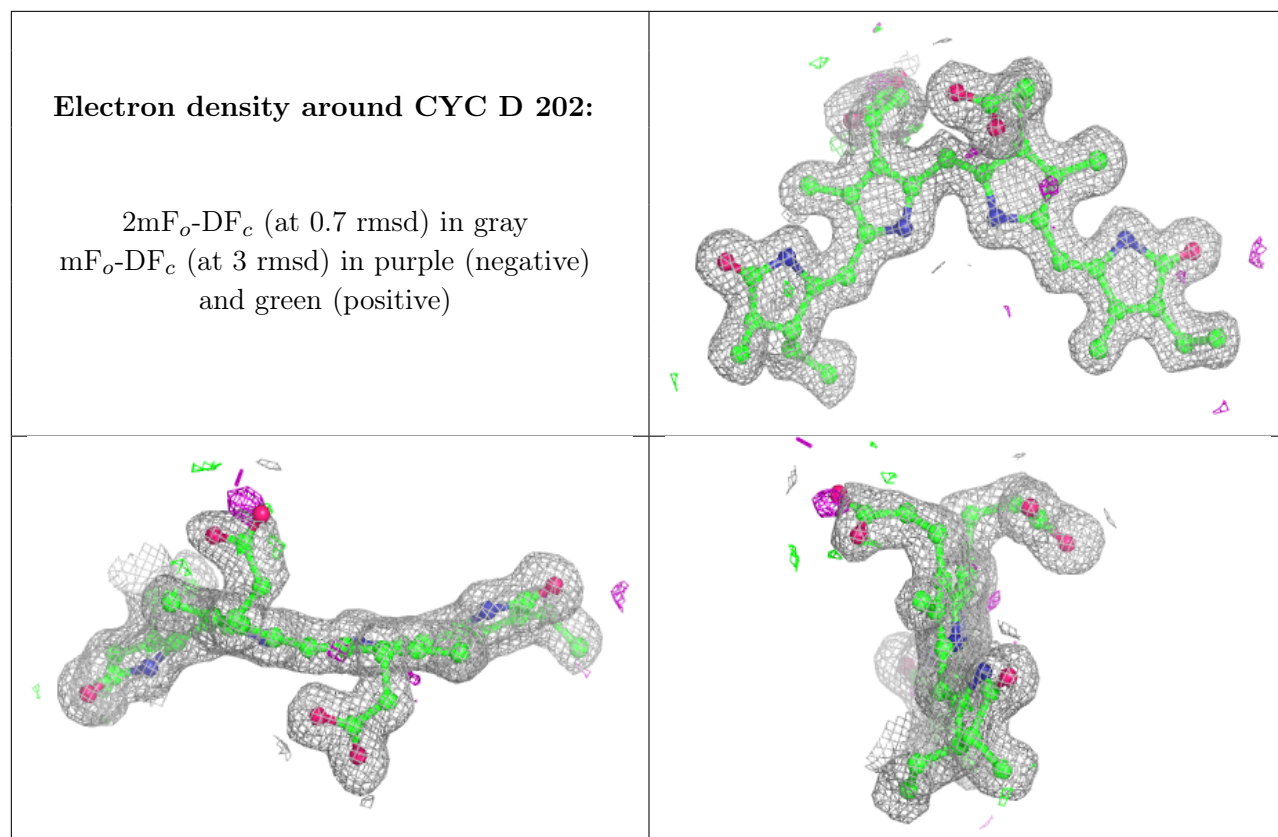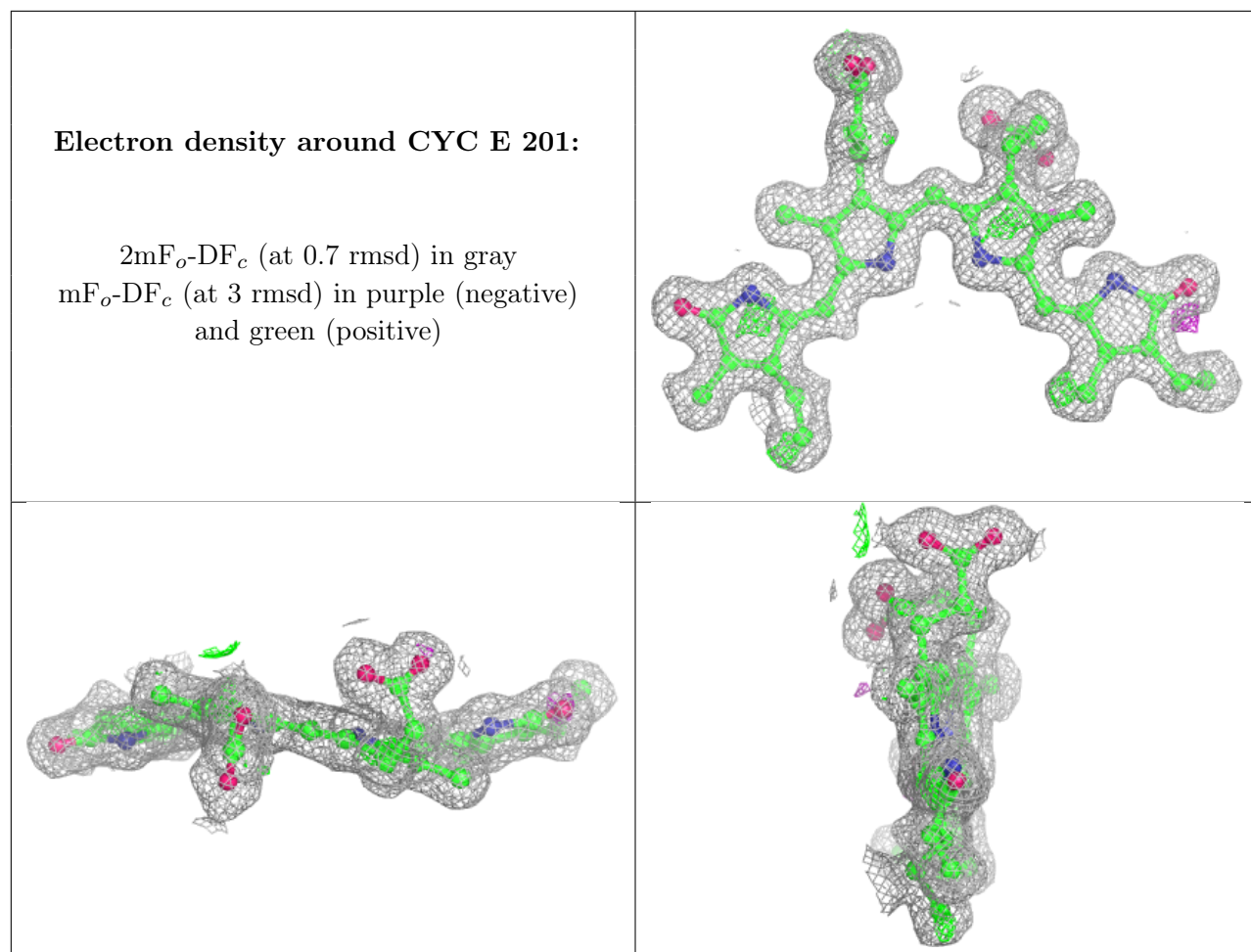and green (positive)
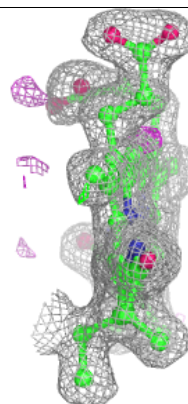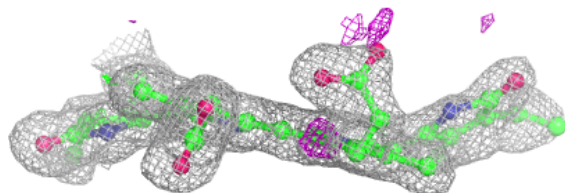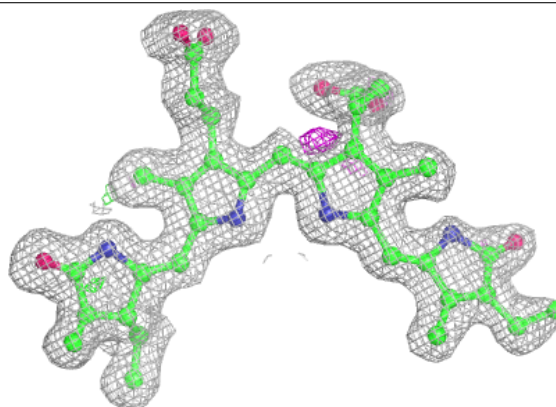
Electron density around CYC L 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
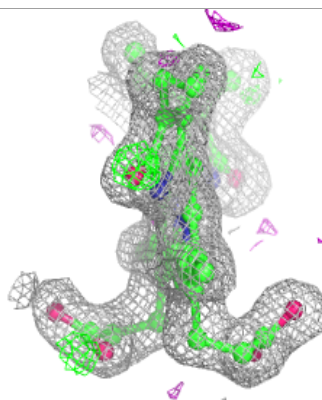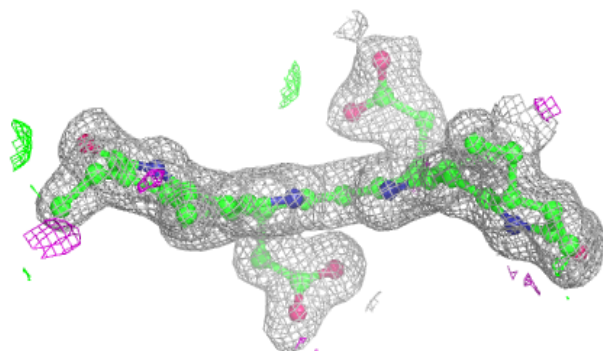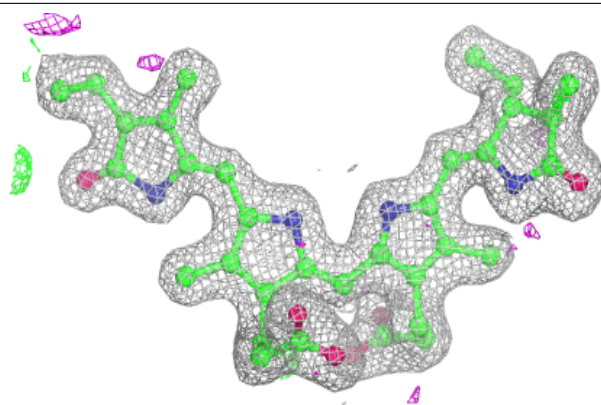
Electron density around CYC H 202:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
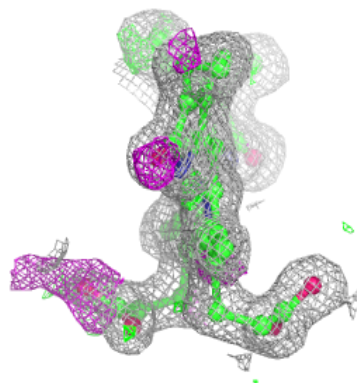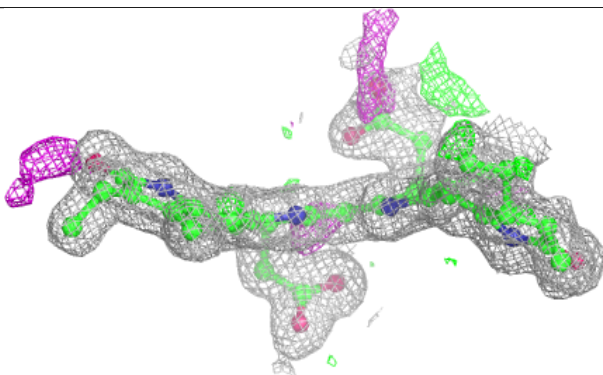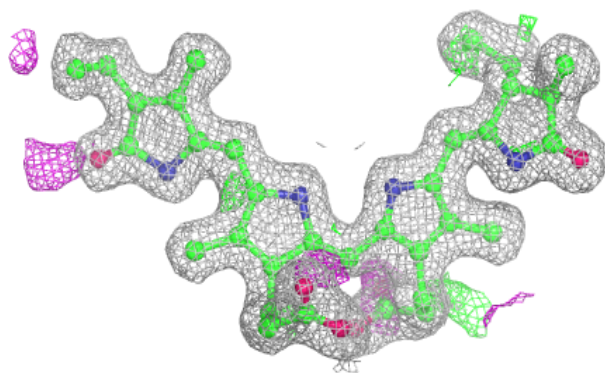
Electron density around CYC B 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
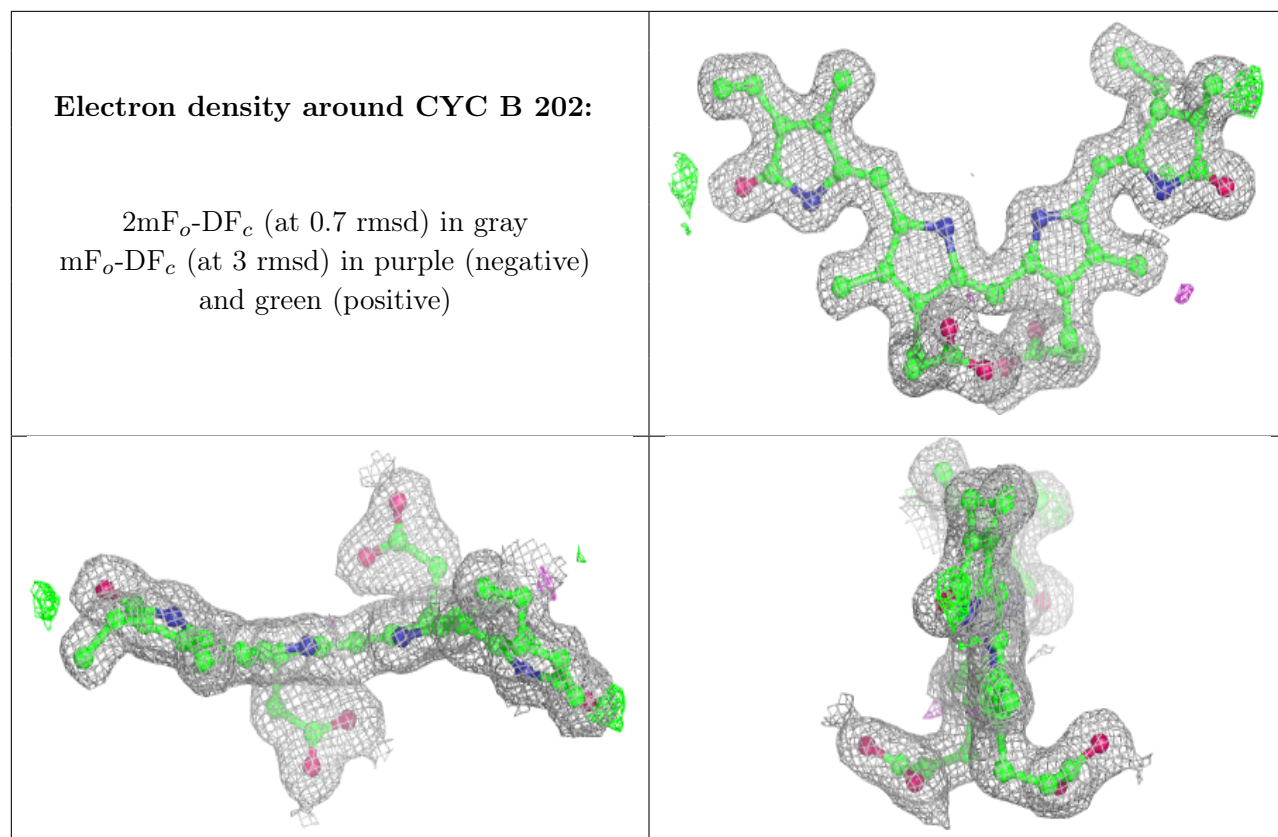and green (positive)
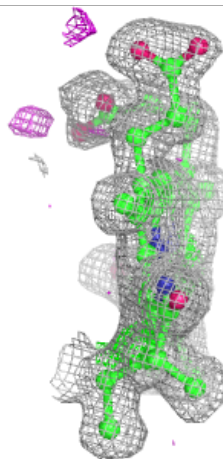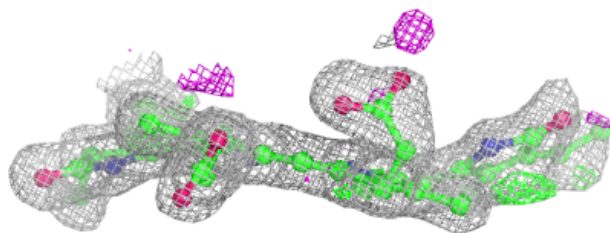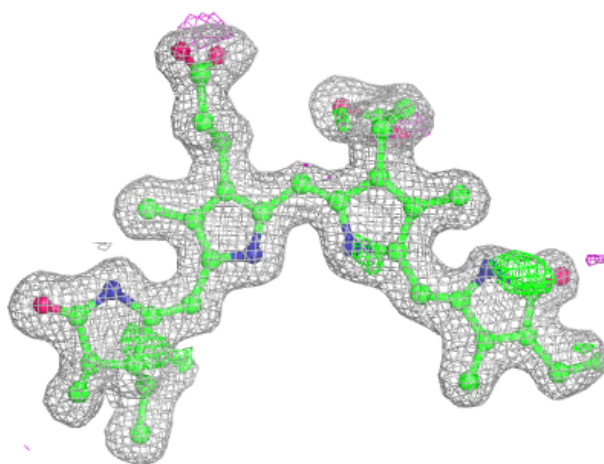
Electron density around CYC H 201:

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

Electron density around CYC J 202:

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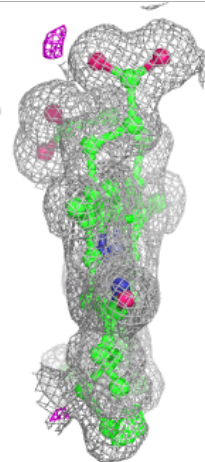mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CYC K 201:

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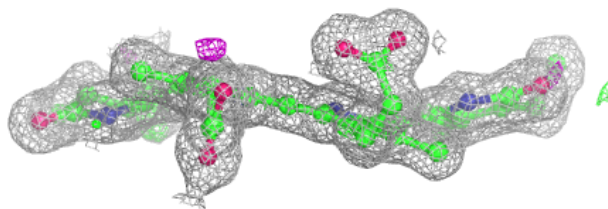and green (positive)

Electron density around CYC F 202:

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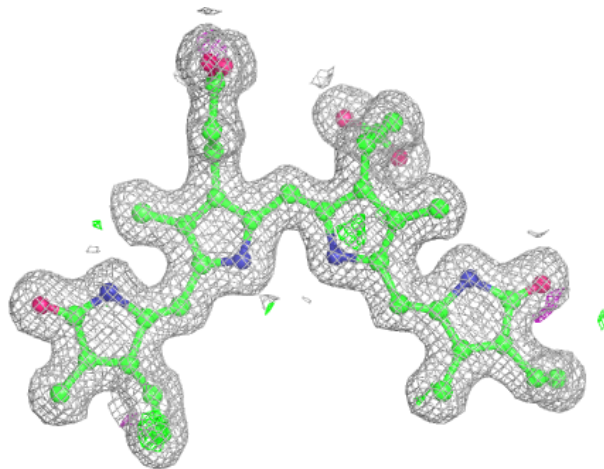$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around CYC A 201:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

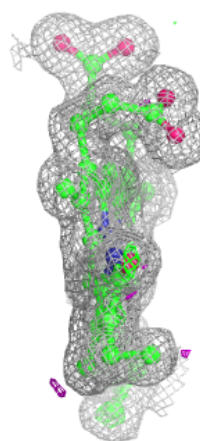**Electron density around CYC D 202:**

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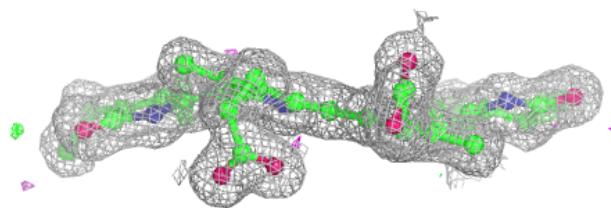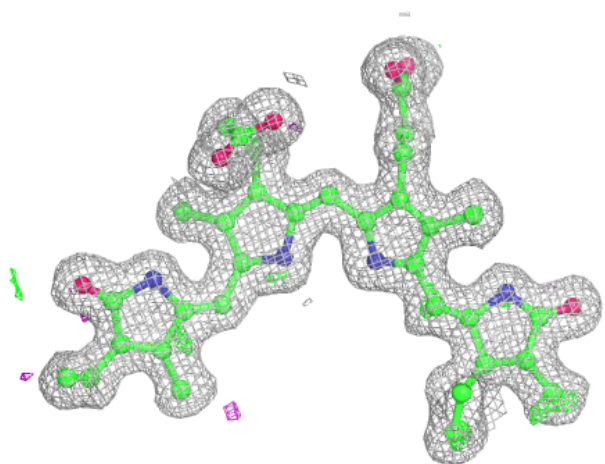and green (positive)

Electron density around CYC E 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 CYC B 202:

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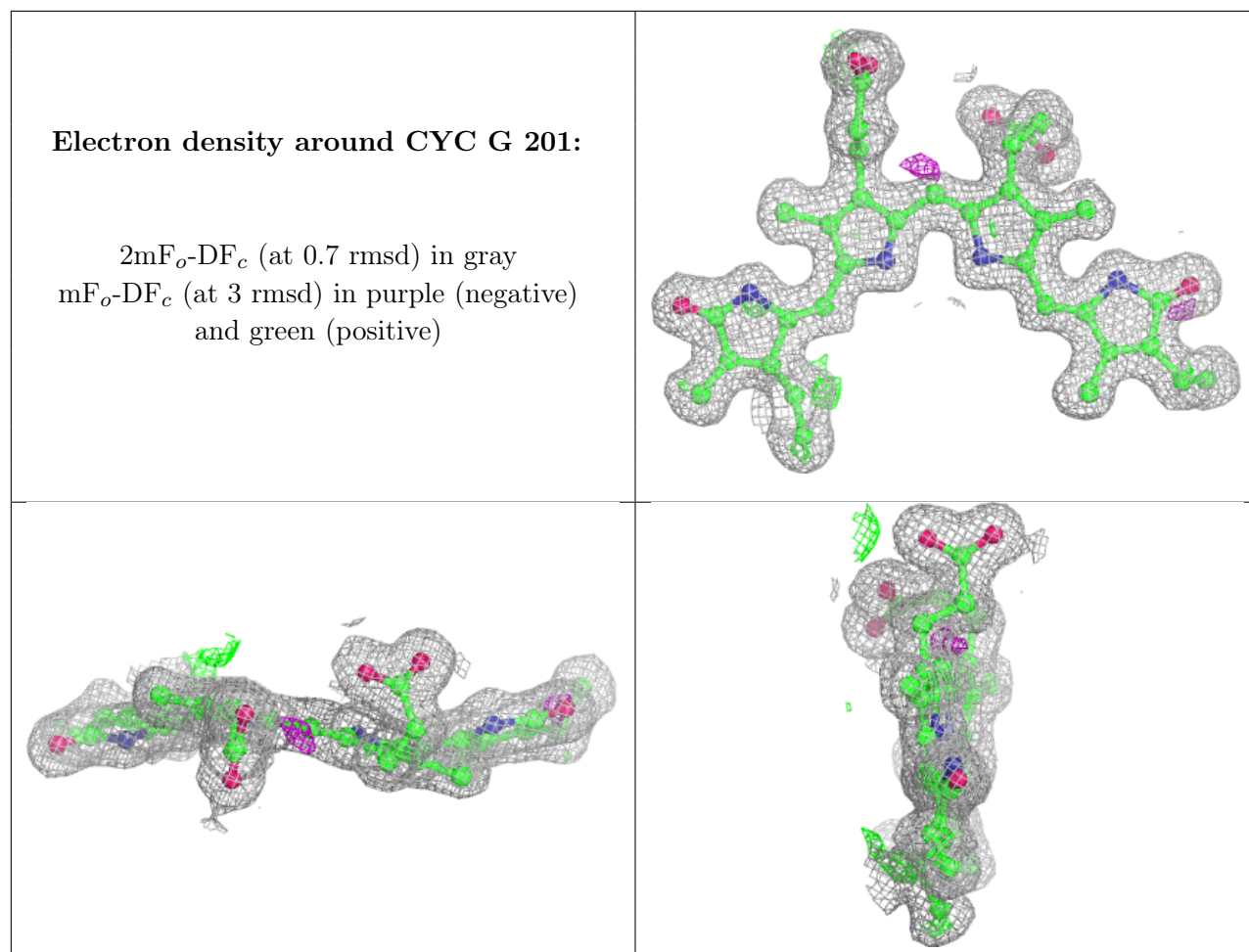and green (positive)

Electron density around CYC I 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 CYC C 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 CYC G 201:

$2mF_o$-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.