

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 1, 2023 – 04:45 PM JST

PDB ID	:	5TOU
Title	:	STRUCTURE OF C-PHYCOCYANIN FROM ARCTIC PSEUDAN-
		ABAENA SP. LW0831
Authors	:	Wang, Q.M.; Li, C.Y.; Su, H.N.; Zhang, Y.Z.; Xie, B.B.
Deposited on	:	2016-10-18
Resolution	:	2.04  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 (1)) were used in the production of this report:

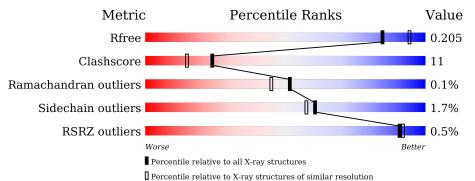
MolProbity Mogul Xtriage (Phenix) EDS	:	4.02b-467 1.8.5 (274361), CSD as541be (2020) 1.13 2.36
buster-report Percentile statistics Refmac	: : :	1.1.7 (2018) 20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)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

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.04 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	$\begin{array}{l} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1692(2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672(2.04-2.04)

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	А	162	92%	7% •
1	С	162	88%	12% ·
1	Е	162	90%	10%
1	G	162	93%	7%
1	Ι	162	88%	10% •
1	Κ	162	89%	11%



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Mol	Chain	Length	Quality of chain	
2	В	172	2% 94%	6%
2	D	172	2% <b>88</b> %	10% •
2	F	172	87%	12% •
2	Н	172	% 92%	8% •
2	J	172	88%	12%
2	L	172	92%	8%



# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17226 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	1 C	162	Total	С	Ν	0	$\mathbf{S}$	0	1	0
		102	1215	760	202	246	7	0	1	0
1	А	162	Total	С	Ν	Ο	S	0	1	0
1	Л	102	1215	760	202	246	7	0	1	0
1	Е	162	Total	С	Ν	0	S	0	0	0
L		102	1209	757	201	244	7	0	0	0
1	т	162	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
L	L	102	1209	757	201	244	7	0	0	0
1	G	162	Total	С	Ν	Ο	$\mathbf{S}$	0	2	0
1	G	102	1222	764	203	248	7	0	Δ.	0
1	K	162	Total	С	Ν	Ο	S	0	0	0
	IX	102	1209	757	201	244	7			0

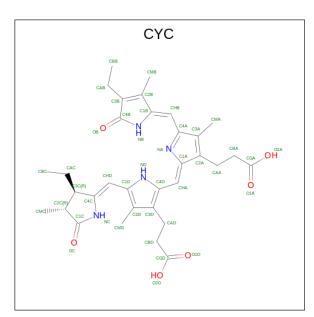
• Molecule 1 is a protein called Phycocyanin alpha-1 subunit.

• Molecule 2 is a protein called Phycocyanin beta-1 subunit.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	D	172	Total	С	Ν	0	S	0	1	0
2	D	112	1253	776	219	249	9	0	1	0
2	В	172	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2	D	112	1248	773	218	248	9		0	0
2	F	172	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2	Ľ	112	1247	773	218	247	9			
2	J	172	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2	5	112	1247	773	218	247	9	0	0	
2	Н	172	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2	11	112	1247	773	218	247	9	0	0	0
2	T.	172	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
2		112	1248	773	218	248	9	0	0	0

• Molecule 3 is PHYCOCYANOBILIN (three-letter code: CYC) (formula:  $C_{33}H_{40}N_4O_6$ ).





Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf
3	С	1	Total	С	Ν	0	0	0
5	U	1	43	33	4	6	0	0
3	D	1	Total	С	Ν	0	0	0
0	D	1	43	33	4	6	0	0
3	D	1	Total	С	Ν	Ο	0	0
		Ĩ	43	33	4	6		
3	А	1	Total	С	Ν	0	0	0
		-	43	33	4	6		<u> </u>
3	В	1	Total	С	Ν	O	0	0
			43	33	4	6	-	_
3	В	1	Total	С	Ν	0	0	0
			43	33	4	6		
3	Е	1	Total	C	N	0	0	0
			43	33 C	$\frac{4}{N}$	6 0		
3	F	1	Total 43	33	N 4	6	0	0
			Total	<u> </u>	4 N	$\frac{0}{0}$		
3	F	1	43	33	4	6	0	0
			Total	<u> </u>	N	0		
3	Ι	1	43	33	4	6	0	0
			Total	<u>C</u>	N	0		
3	J	1	43	33	4	6	0	0
-	-		Total	C	N	<del>0</del>	-	
3	J	1	43	33	4	6	0	0
0	G	1	Total	С	Ν	0	0	0
3	G	1	43	33	4	6	0	0
2	тт	1	Total	С	Ν	0	0	0
3	Η	1	43	33	4	6	0	0



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Mol	Chain	Residues	A	ton	ns		ZeroOcc	AltConf	
3	Н	1	Total	С	Ν	0	0	Ο	
0	11	1	43	33	4	6	0	0	
3	K	1	Total	С	Ν	Ο	0	0	
0	a n	T	43	33	4	6	0	0	
3	Т	1	Total	С	Ν	Ο	0	0	
0	L	1	43	33	4	6	0	0	
3	т	1	Total	С	Ν	0	0	0	
5		T	43	33	4	6	0	0	

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	144	Total O 144 144	0	0
4	D	171	Total O 171 171	0	0
4	А	160	Total O 160 160	0	0
4	В	138	Total O 138 138	0	0
4	Е	128	Total         O           128         128	0	0
4	F	113	Total O 113 113	0	0
4	Ι	119	Total O 119 119	0	0
4	J	123	Total         O           123         123	0	0
4	G	156	Total O 156 156	0	0
4	Н	150	Total O 150 150	0	0
4	K	122	Total         O           122         122	0	0
4	L	159	Total O 159 159	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: Phycocyanin alpha-1 subunit

Chain C:	88%	12% •
M1 K2 E7 R17 R30 S36 E49 F63	166 170 084 084 1111 1111 1118 1118 1118 1118	
• Molecule 1: Phycocy	anin alpha-1 subunit	
Chain A:	92%	7% •
M1 E7 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3 F3	1123 1123 1128 1136 1142 1142 1142 1142 1142	
• Molecule 1: Phycocy	anin alpha-1 subunit	
Chain E:	90%	10%
M1 K2 810 810 815 817 817 817 815 830 830 830 855 855 855 855 855 855	C84 188 790 790 107 1128 1128 1128 1128 1128 1128 1128 112	
• Molecule 1: Phycocy	anin alpha-1 subunit	
Chain I:	88%	10% •
M1 K2 L19 C119 R30 R30 R30 R31 R31 R31 R32 R32 R48 R48 R48 R32 R32 R32 R32 R32 R32 R32 R32 R32 R32	Y65 M69 C34 C34 C34 M107 M107 M107 M111 C114 C114 C114 C114 C114 C114 C118 M128 C141 C141 C141 C141 C141 C141 C142 C144 C144	
• Molecule 1: Phycocy	anin alpha-1 subunit	
Chain G:	93%	7%
M1 E7 Q15 721 721 721 721 725 730 730 730 730 7100	81.27 11.28 51.62	
• Molecule 1: Phycocy	anin alpha-1 subunit	
Chain K:	89%	11%





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	67.58Å 175.72Å 194.82Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	43.93 - 2.04	Depositor
Resolution (A)	43.93 - 2.04	EDS
% Data completeness	95.3 (43.93-2.04)	Depositor
(in resolution range)	96.6(43.93-2.04)	EDS
R <sub>merge</sub>	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$5.52 (at 2.05 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
D D.	0.172 , $0.207$	Depositor
$R, R_{free}$	0.170 , $0.205$	DCC
$R_{free}$ test set	7142 reflections $(5.00\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	25.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , $45.4$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.49, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17226	wwPDB-VP
Average B, all atoms $(Å^2)$	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MEN, 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
IVIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.40	0/1237	0.52	0/1676
1	С	0.40	0/1237	0.48	0/1676
1	Ε	0.36	0/1231	0.48	0/1668
1	G	0.39	0/1244	0.51	0/1686
1	Ι	0.37	0/1231	0.49	0/1668
1	Κ	0.36	0/1231	0.49	0/1668
2	В	0.37	0/1252	0.48	0/1691
2	D	0.38	0/1257	0.50	0/1699
2	F	0.34	0/1251	0.48	0/1691
2	Н	0.35	0/1251	0.47	0/1691
2	J	0.37	0/1251	0.49	0/1691
2	L	0.38	0/1252	0.48	0/1691
All	All	0.37	0/14925	0.49	0/20196

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 (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	А	1215	0	1180	21	0	



5	Т	$\cap$	ΤT
υ	т	$\mathbf{U}$	U

Mol	Chain	n previous Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1215	0	1179	22	0
1	E	1219	0	1176	30	0
1	G	1203	0	1185	24	0
1	I	1209	0	1176	24	0
1	K	1209	0	1176	20	0
$\frac{1}{2}$	B	1248	0	1249	12	0
$\frac{2}{2}$	D	1253	0	1252	25	1
2	F	1233	0	1202	20	0
2	H	1247	0	1248	15	0
2	J	1247	0	1248	23	1
2	L	1248	0	1248	11	0
3	A	43	0	38	12	0
3	B	86	0	74	18	0
3	C	43	0	37	10	0
3	D	86	0	74	16	0
3	Е	43	0	38	15	0
3	F	86	0	75	25	0
3	G	43	0	37	9	0
3	Н	86	0	74	24	0
3	Ι	43	0	38	16	0
3	J	86	0	73	26	0
3	K	43	0	38	13	0
3	L	86	0	73	23	0
4	А	160	0	0	2	0
4	В	138	0	0	1	0
4	С	144	0	0	1	0
4	D	171	0	0	7	0
4	Е	128	0	0	0	0
4	F	113	0	0	2	0
4	G	156	0	0	1	0
4	Н	150	0	0	3	0
4	Ι	119	0	0	3	0
4	J	123	0	0	3	0
4	K	122	0	0	2	0
4	L	159	0	0	2	0
All	All	17226	0	15235	342	1

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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 11.

The worst 5 of 342 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:F:82:CYS:SG	3:F:201:CYC:HAC2	1.19	1.73
2:F:82:CYS:SG	3:F:201:CYC:CAC	2.10	1.40
2:B:82:CYS:SG	3:B:201:CYC:HAC2	1.66	1.34
1:K:84:CYS:SG	3:K:200:CYC:HAC2	1.68	1.32
1:I:84:CYS:SG	3:I:200:CYC:HAC2	1.76	1.26

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125[A]:SER:OG	$2:J:165:ASP:OD2[1_455]$	2.17	0.03

### 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	Perce	ntiles
1	А	161/162~(99%)	157~(98%)	4 (2%)	0	100	100
1	С	161/162~(99%)	159 (99%)	2 (1%)	0	100	100
1	Е	160/162~(99%)	157 (98%)	3 (2%)	0	100	100
1	G	162/162~(100%)	159 (98%)	3 (2%)	0	100	100
1	Ι	160/162~(99%)	158 (99%)	2 (1%)	0	100	100
1	Κ	160/162~(99%)	157 (98%)	3 (2%)	0	100	100
2	В	169/172~(98%)	165 (98%)	4 (2%)	0	100	100
2	D	170/172~(99%)	164 (96%)	5 (3%)	1 (1%)	25	15
2	F	169/172~(98%)	166 (98%)	3 (2%)	0	100	100
2	Н	169/172~(98%)	166 (98%)	3 (2%)	0	100	100
2	J	169/172~(98%)	166 (98%)	3 (2%)	0	100	100
2	L	169/172~(98%)	166 (98%)	3 (2%)	0	100	100
All	All	1979/2004~(99%)	1940 (98%)	38 (2%)	1 (0%)	51	45



All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	25	ASP

#### 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	Perce	ntiles
1	А	126/125~(101%)	122~(97%)	4(3%)	39	32
1	$\mathbf{C}$	126/125~(101%)	123~(98%)	3~(2%)	49	42
1	Ε	125/125~(100%)	123~(98%)	2(2%)	62	59
1	G	127/125~(102%)	126~(99%)	1 (1%)	81	82
1	Ι	125/125~(100%)	119~(95%)	6~(5%)	25	18
1	Κ	125/125~(100%)	125~(100%)	0	100	100
2	В	124/124~(100%)	124 (100%)	0	100	100
2	D	125/124~(101%)	123~(98%)	2(2%)	62	59
2	F	124/124~(100%)	120~(97%)	4 (3%)	39	32
2	Н	124/124~(100%)	122~(98%)	2(2%)	62	59
2	J	124/124~(100%)	124 (100%)	0	100	100
2	L	124/124~(100%)	123 (99%)	1 (1%)	81	82
All	All	1499/1494~(100%)	1474~(98%)	25~(2%)	60	57

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	120	LEU
1	Ι	49	GLU
2	L	118	LEU
1	Ι	32	ARG
1	Ι	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:



Mol	Chain	Res	Type
1	G	57	ASN
1	Κ	159	ASN
1	Κ	33	GLN
1	Е	159	ASN
1	G	33	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)

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	Turne	Chain	Res Link		Bond lengths			Bond angles		
	Type	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
2	MEN	J	72	2	7,8,9	0.64	0	6,9,11	0.71	0
2	MEN	L	72	2	7,8,9	0.63	0	6,9,11	0.79	0
2	MEN	Н	72	2	7,8,9	0.63	0	6,9,11	0.82	0
2	MEN	F	72	2	7,8,9	0.63	0	6,9,11	0.76	0
2	MEN	В	72	2	7,8,9	0.64	0	6,9,11	0.80	0
2	MEN	D	72	2	7,8,9	0.63	0	6,9,11	0.84	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	J	72	2	-	5/7/8/10	-
2	MEN	L	72	2	-	7/7/8/10	-
2	MEN	Н	72	2	-	2/7/8/10	-
2	MEN	F	72	2	-	2/7/8/10	-
2	MEN	В	72	2	-	4/7/8/10	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	D	72	2	-	3/7/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	72	MEN	CB-CG-ND2-CE2
2	J	72	MEN	CB-CG-ND2-CE2
2	L	72	MEN	O-C-CA-CB
2	L	72	MEN	C-CA-CB-CG
2	L	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	L	72	MEN	1	0
2	D	72	MEN	1	0

# 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

18 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	B	ond leng	gths	Bond angles		
WIOI	Type	Ullalli	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
3	CYC	D	202	2	42,46,46	<mark>3.30</mark>	13 (30%)	50,67,67	2.82	17 (34%)



Mol	Type	Chain	Res	Link	В	ond leng	gths	B	ond ang	gles
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	CYC	В	202	2	42,46,46	3.25	11 (26%)	50,67,67	2.75	17 (34%)
3	CYC	L	202	2	42,46,46	<mark>3.25</mark>	12 (28%)	50,67,67	2.78	16 (32%)
3	CYC	А	200	-	42,46,46	5.01	19 (45%)	50,67,67	3.17	17 (34%)
3	CYC	Ι	200	-	42,46,46	<mark>4.93</mark>	18 (42%)	50,67,67	3.47	21 (42%)
3	CYC	Е	200	-	42,46,46	4.93	21 (50%)	50,67,67	3.50	20 (40%)
3	CYC	F	202	2	42,46,46	<mark>3.28</mark>	12 (28%)	50,67,67	2.78	17 (34%)
3	CYC	J	201	2	42,46,46	<mark>3.26</mark>	12 (28%)	50,67,67	2.77	16 (32%)
3	CYC	G	200	1	42,46,46	<mark>3.23</mark>	12 (28%)	50,67,67	2.84	18 (36%)
3	CYC	С	200	1	42,46,46	<b>3.27</b>	12 (28%)	50,67,67	2.78	19 (38%)
3	CYC	Н	201	2	42,46,46	<mark>3.29</mark>	13 (30%)	50,67,67	2.85	18 (36%)
3	CYC	K	200	-	42,46,46	<mark>5.12</mark>	19 (45%)	50,67,67	3.42	20 (40%)
3	CYC	F	201	-	42,46,46	<mark>3.26</mark>	12 (28%)	50,67,67	2.86	18 (36%)
3	CYC	В	201	-	42,46,46	5.02	19 (45%)	50,67,67	3.29	19 (38%)
3	CYC	J	202	2	42,46,46	<mark>3.28</mark>	13 (30%)	50,67,67	2.82	17 (34%)
3	CYC	D	201	2	42,46,46	<mark>3.25</mark>	10 (23%)	50,67,67	2.79	16 (32%)
3	CYC	L	201	2	42,46,46	<mark>3.27</mark>	13 (30%)	50,67,67	2.84	17 (34%)
3	CYC	Н	202	2	42,46,46	3.31	12 (28%)	50,67,67	2.75	17 (34%)

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	D	202	2	-	8/25/74/74	0/4/4/4
3	CYC	В	202	2	-	10/25/74/74	0/4/4/4
3	CYC	L	202	2	-	10/25/74/74	0/4/4/4
3	CYC	А	200	-	-	9/25/74/74	0/4/4/4
3	CYC	Ι	200	-	-	12/25/74/74	0/4/4/4
3	CYC	Е	200	-	-	9/25/74/74	0/4/4/4
3	CYC	F	202	2	-	11/25/74/74	0/4/4/4
3	CYC	J	201	2	-	10/25/74/74	0/4/4/4
3	CYC	G	200	1	-	11/25/74/74	0/4/4/4
3	CYC	С	200	1	-	11/25/74/74	0/4/4/4
3	CYC	Н	201	2	-	8/25/74/74	0/4/4/4
3	CYC	K	200	-	-	10/25/74/74	0/4/4/4



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CYC	F	201	-	-	8/25/74/74	0/4/4/4
3	CYC	В	201	-	-	10/25/74/74	0/4/4/4
3	CYC	J	202	2	-	8/25/74/74	0/4/4/4
3	CYC	D	201	2	-	10/25/74/74	0/4/4/4
3	CYC	L	201	2	-	6/25/74/74	0/4/4/4
3	CYC	Н	202	2	-	10/25/74/74	0/4/4/4

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The worst 5 of 253 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Κ	200	CYC	CHA-C1A	20.80	1.52	1.35
3	В	201	CYC	CHA-C1A	20.22	1.52	1.35
3	А	200	CYC	CHA-C1A	19.64	1.51	1.35
3	Ι	200	CYC	CHA-C1A	18.66	1.50	1.35
3	Ε	200	CYC	CHA-C1A	18.55	1.50	1.35

The worst 5 of 320 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
3	В	201	CYC	C2C-C1C-NC	11.39	118.09	108.27
3	J	202	CYC	C3B-C4B-NB	11.15	115.78	106.78
3	Н	201	CYC	C3B-C4B-NB	11.13	115.77	106.78
3	D	202	CYC	C3B-C4B-NB	11.11	115.76	106.78
3	L	201	CYC	C3B-C4B-NB	11.11	115.75	106.78

There are no chirality outliers.

5 of 171 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	С	200	CYC	NA-C4A-CHB-C1B
3	С	200	CYC	C2C-C3C-CAC-CBC
3	С	200	CYC	C4C-C3C-CAC-CBC
3	С	200	CYC	ND-C1D-CHD-C4C
3	С	200	CYC	C2D-C1D-CHD-C4C

There are no ring outliers.

18 monomers are involved in 207 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	202	CYC	9	0

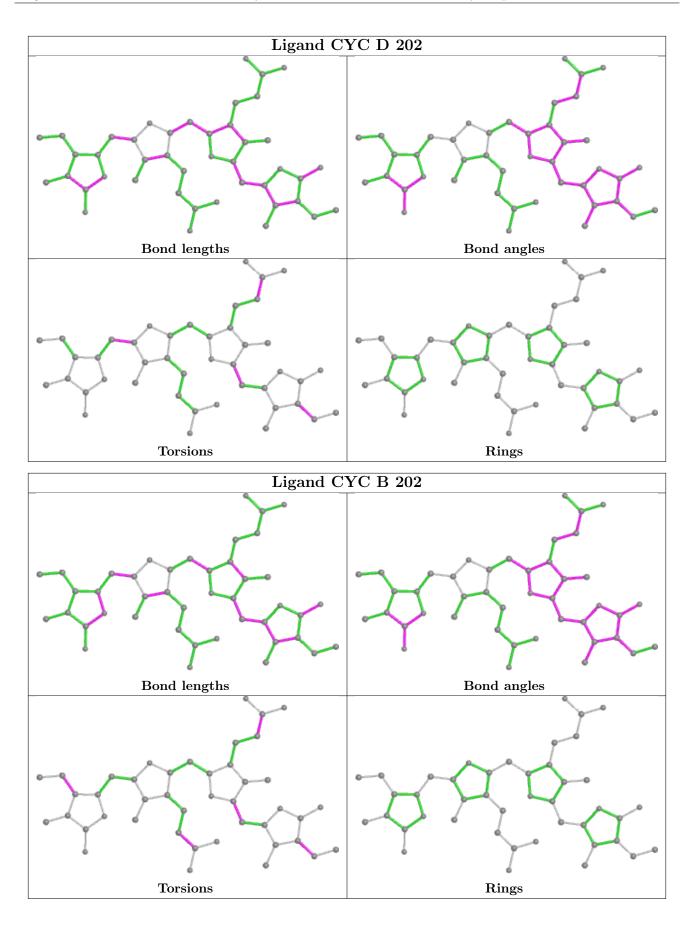


Mol	nuea fron Chain	Res	Type	Clashes	Symm-Clashes
3	В	202	CYC	8	0
3	L	202	CYC	14	0
3	А	200	CYC	12	0
3	Ι	200	CYC	16	0
3	Е	200	CYC	15	0
3	F	202	CYC	11	0
3	J	201	CYC	9	0
3	G	200	CYC	9	0
3	С	200	CYC	10	0
3	Н	201	CYC	9	0
3	Κ	200	CYC	13	0
3	F	201	CYC	14	0
3	В	201	CYC	10	0
3	J	202	CYC	17	0
3	D	201	CYC	7	0
3	L	201	CYC	9	0
3	Н	202	CYC	15	0

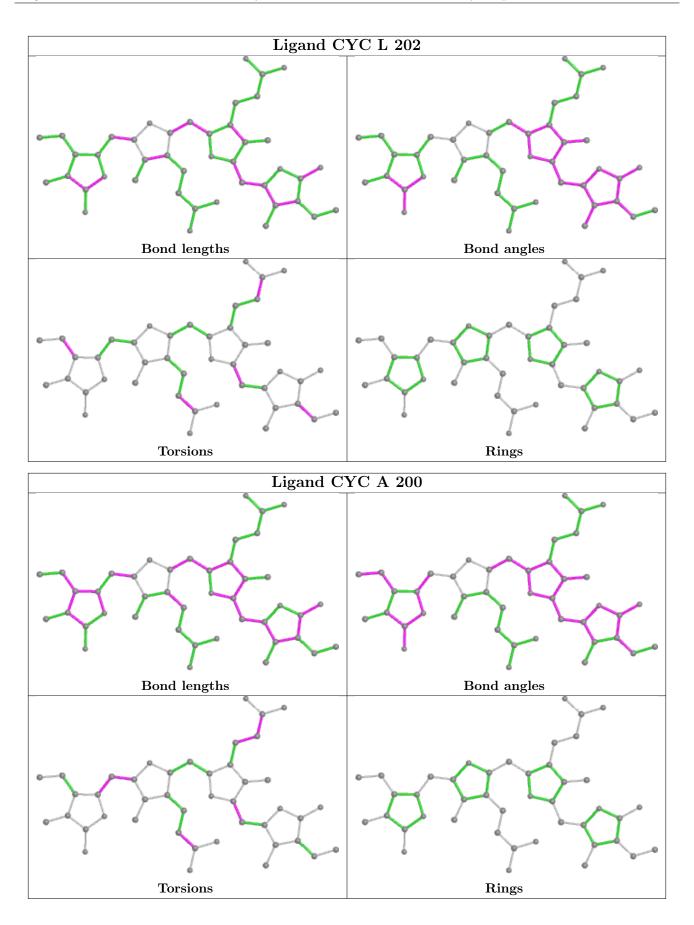
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The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers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

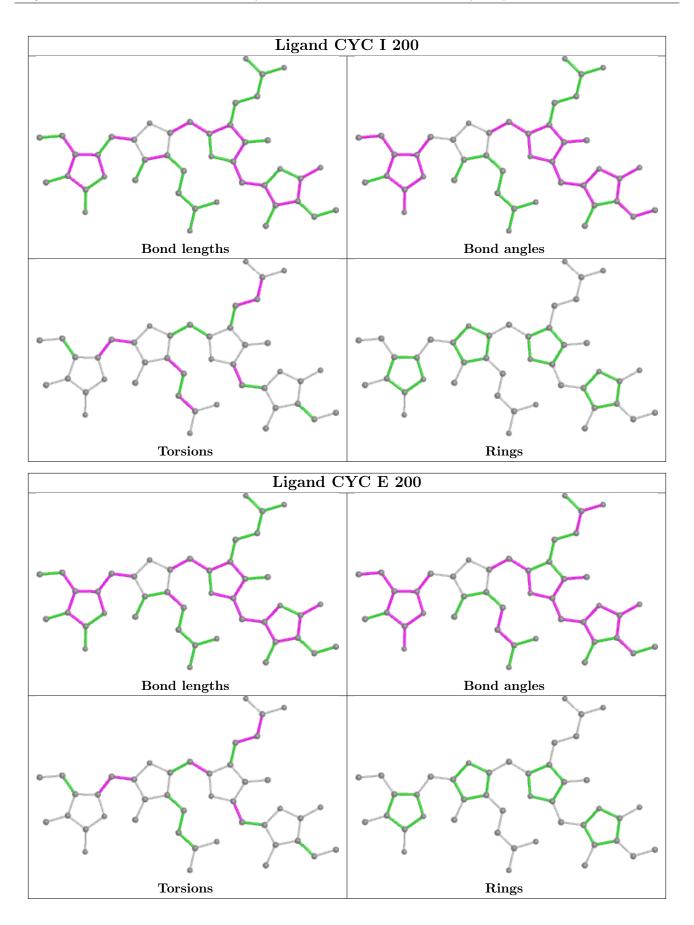




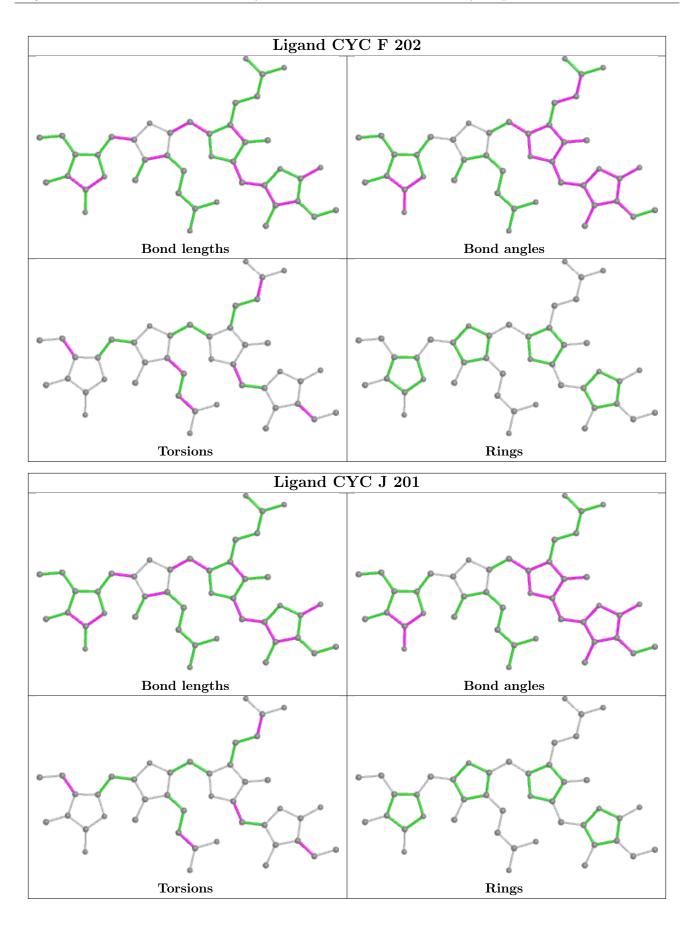




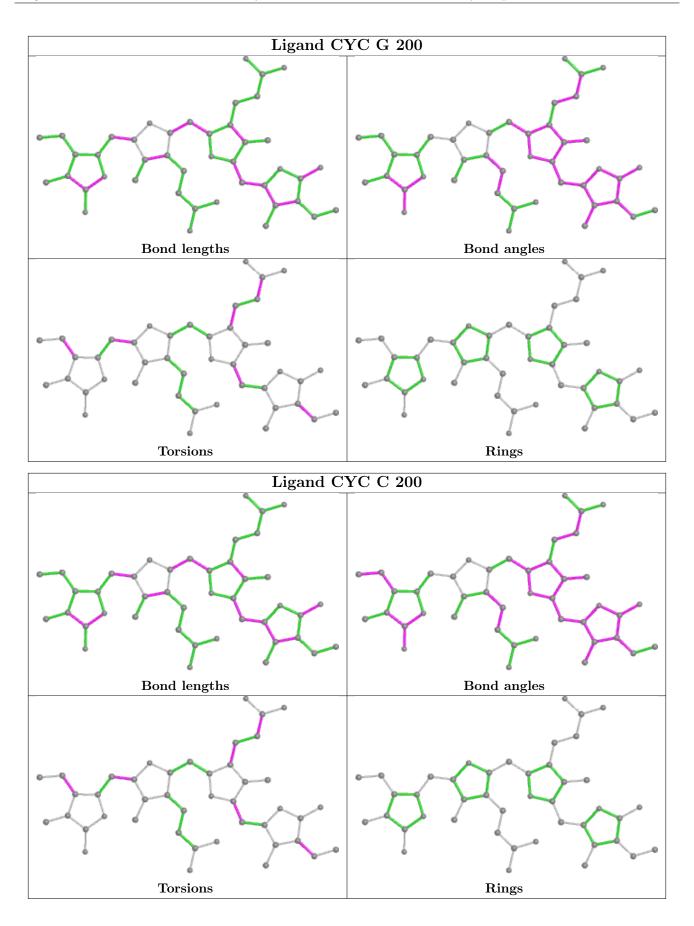




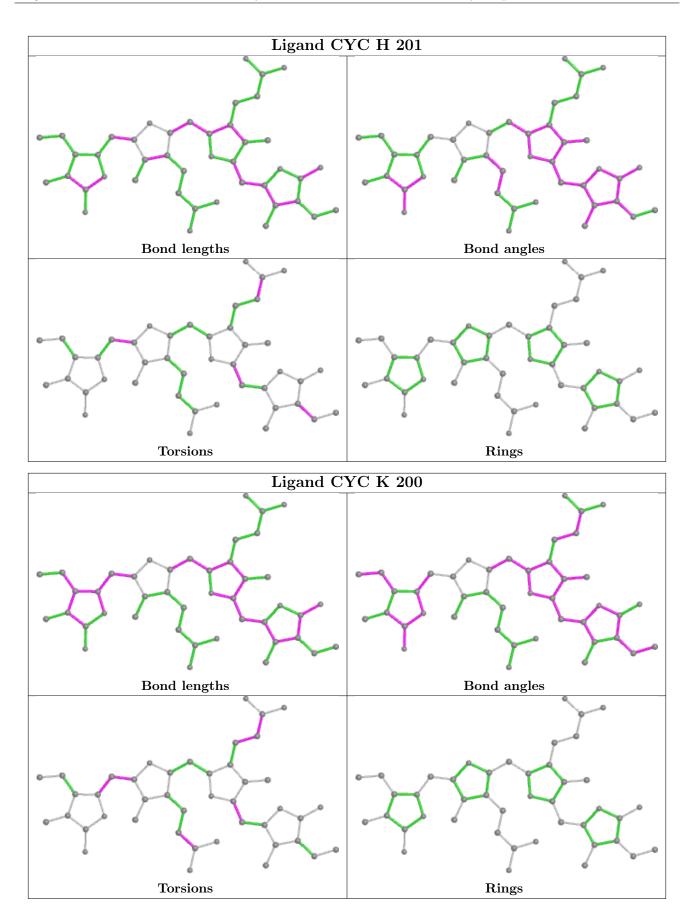




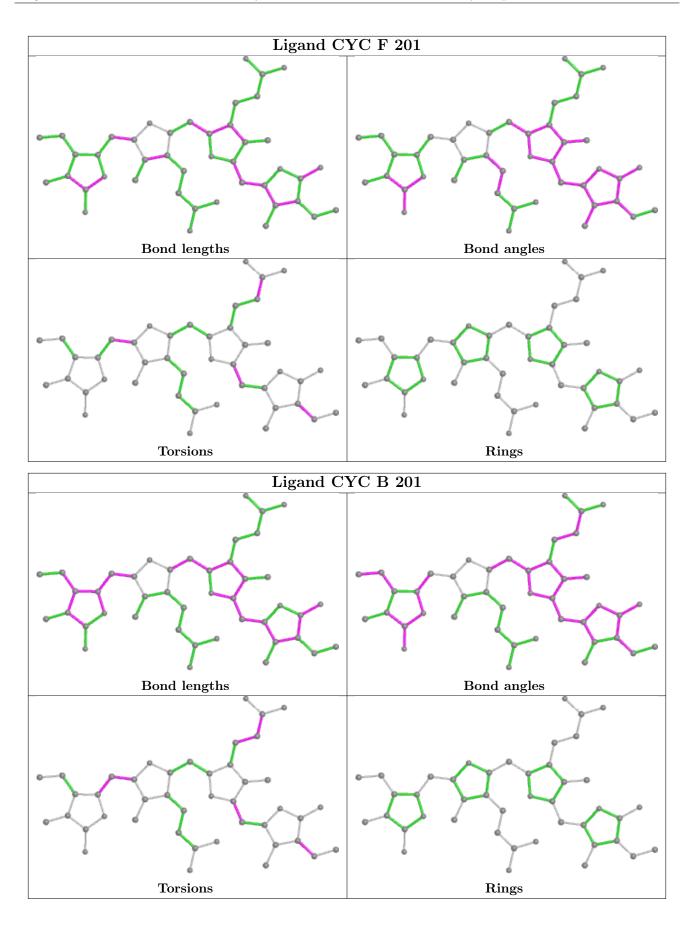




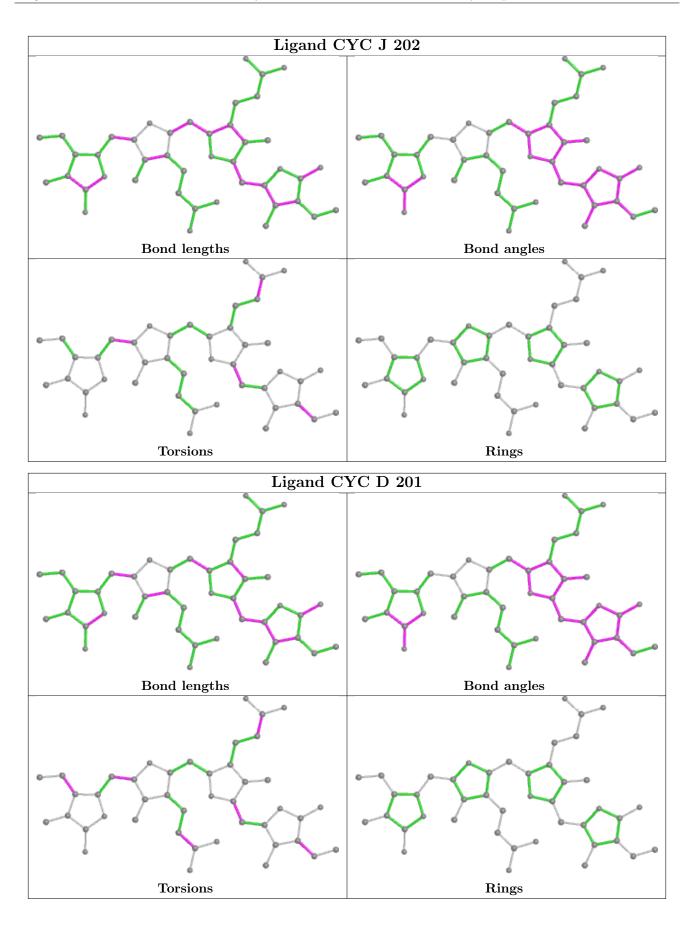




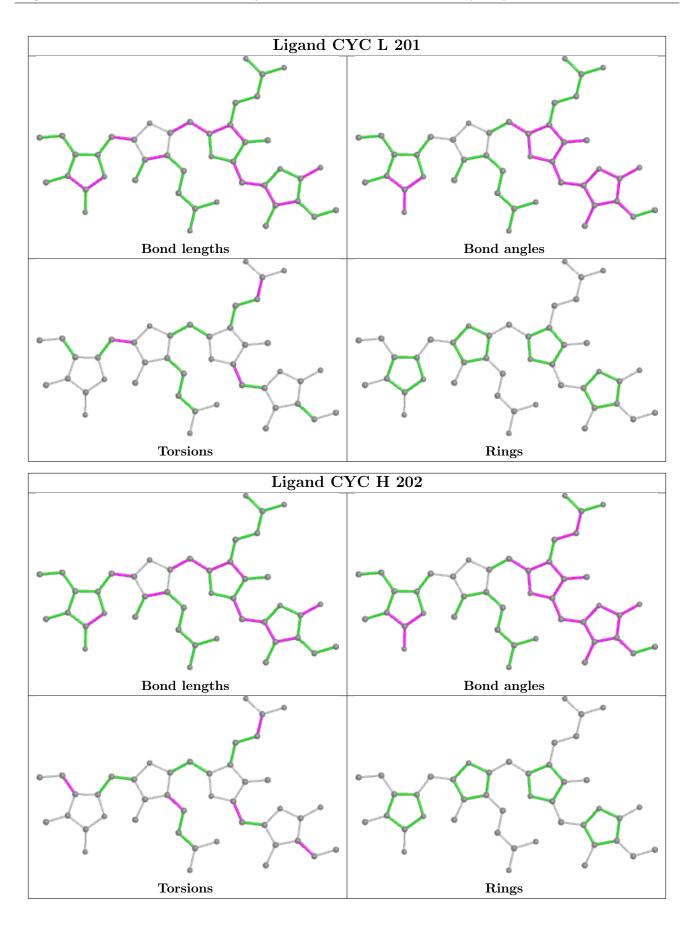














### 5.7 Other polymers (i)

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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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		Z>2	$OWAB(Å^2)$	Q < 0.9
1	А	162/162~(100%)	-0.52	0	100	100	18, 22, 35, 41	0
1	С	162/162~(100%)	-0.42	0	100	100	16, 24, 39, 48	0
1	Ε	162/162~(100%)	-0.30	0	100	100	18, 24, 38, 47	0
1	G	162/162~(100%)	-0.50	0	100	100	18, 23, 35, 52	0
1	Ι	162/162~(100%)	-0.17	0	100	100	20, 27, 44, 54	0
1	K	162/162~(100%)	-0.44	0	100	100	20, 26, 37, 53	0
2	В	171/172~(99%)	-0.30	3 (1	%) 6	8 71	17, 25, 40, 81	0
2	D	171/172~(99%)	-0.38	4 (2	2%) 6	0 64	17, 23, 41, 66	0
2	F	171/172~(99%)	-0.45	0	100	100	18, 28, 41, 56	0
2	Н	171/172~(99%)	-0.34	2 (1	%) 7	9 81	17, 26, 39, 54	0
2	J	171/172~(99%)	-0.39	0	100	100	18, 26, 43, 57	0
2	L	171/172~(99%)	-0.38	0	100	100	18, 25, 42, 60	0
All	All	1998/2004 (99%)	-0.38	9 (0	9%) 9	1 92	16, 25, 40, 81	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	21	ALA	4.7
2	D	24	ILE	3.1
2	Н	172	ALA	3.0
2	В	172	ALA	2.9
2	D	22	SER	2.8

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



Mol	Type	Chain	Res	Atoms	RSCC	$\mathbf{RSR}$	$\operatorname{B-factors}(\operatorname{\AA}^2)$	Q < 0.9
2	MEN	J	72	9/10	0.93	0.10	$26,\!30,\!33,\!35$	0
2	MEN	F	72	9/10	0.95	0.09	24,28,31,33	0
2	MEN	D	72	9/10	0.95	0.09	$21,\!25,\!28,\!30$	0
2	MEN	В	72	9/10	0.96	0.12	21,24,27,29	0
2	MEN	Н	72	9/10	0.96	0.11	28,31,35,36	0
2	MEN	L	72	9/10	0.97	0.15	21,24,28,30	0

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.

### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 6.4 Ligands (i)

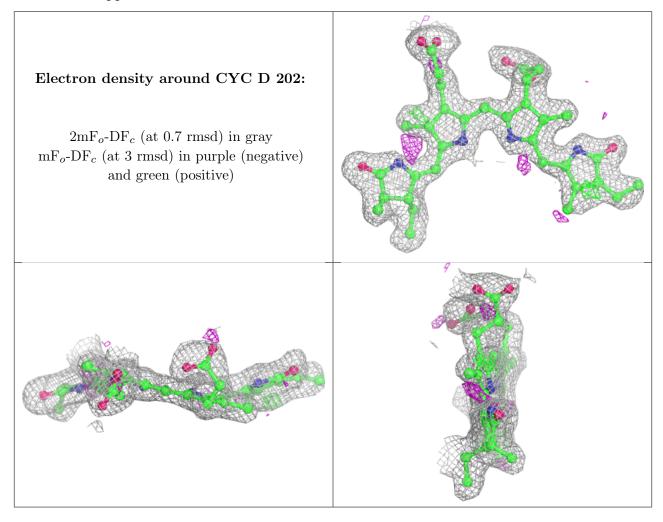
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	D	202	43/43	0.87	0.17	$22,\!29,\!43,\!55$	0
3	CYC	Ι	200	43/43	0.88	0.16	22,27,31,37	0
3	CYC	В	201	43/43	0.89	0.20	$19,\!29,\!45,\!55$	0
3	CYC	Н	201	43/43	0.89	0.20	23,31,42,56	0
3	CYC	K	200	43/43	0.89	0.16	19,24,31,34	0
3	CYC	Е	200	43/43	0.90	0.15	17,24,32,33	0
3	CYC	J	202	43/43	0.91	0.17	$26,\!33,\!43,\!55$	0
3	CYC	F	202	43/43	0.91	0.14	$23,\!33,\!44,\!53$	0
3	CYC	А	200	43/43	0.91	0.14	17,22,27,33	0
3	CYC	L	201	43/43	0.91	0.19	20,27,43,58	0
3	CYC	L	202	43/43	0.91	0.13	20,27,34,40	0
3	CYC	В	202	43/43	0.92	0.14	23,30,36,44	0
3	CYC	D	201	43/43	0.92	0.14	21,27,44,55	0
3	CYC	J	201	43/43	0.92	0.13	20,30,38,45	0
3	CYC	F	201	43/43	0.92	0.16	$23,\!31,\!45,\!60$	0
3	CYC	G	200	43/43	0.93	0.12	15,21,27,35	0
3	CYC	С	200	43/43	0.93	0.14	16,24,31,41	0
3	CYC	Н	202	43/43	0.93	0.14	20,24,36,39	0

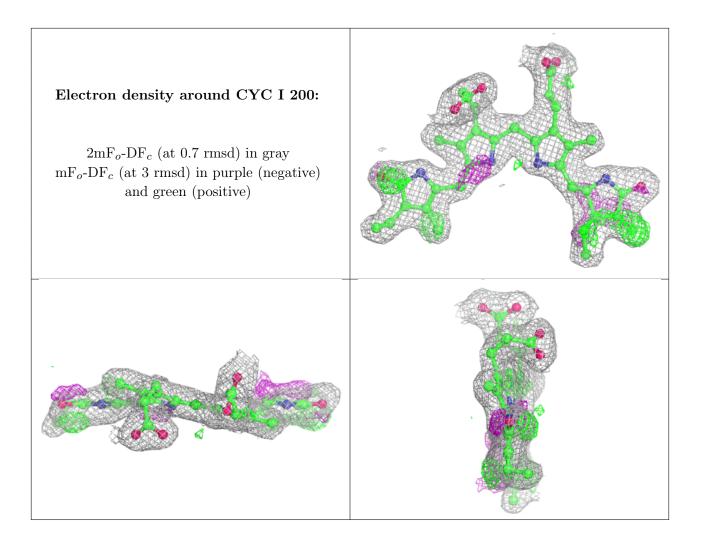
The following is a graphical depiction of the model fit to experimental electron density of all



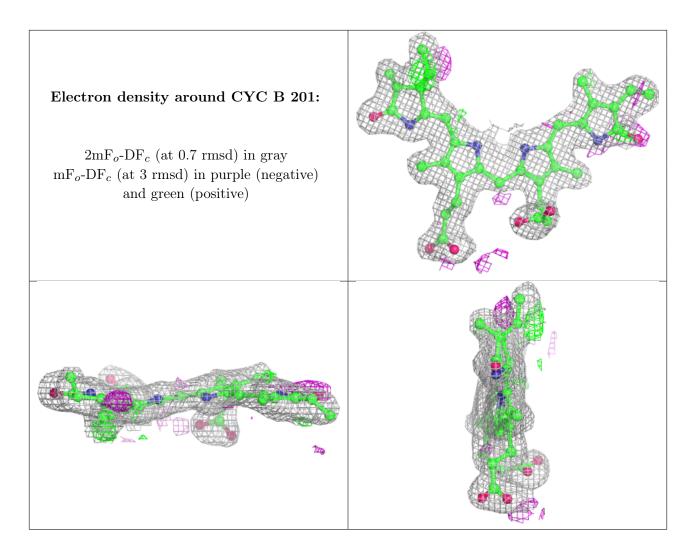
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



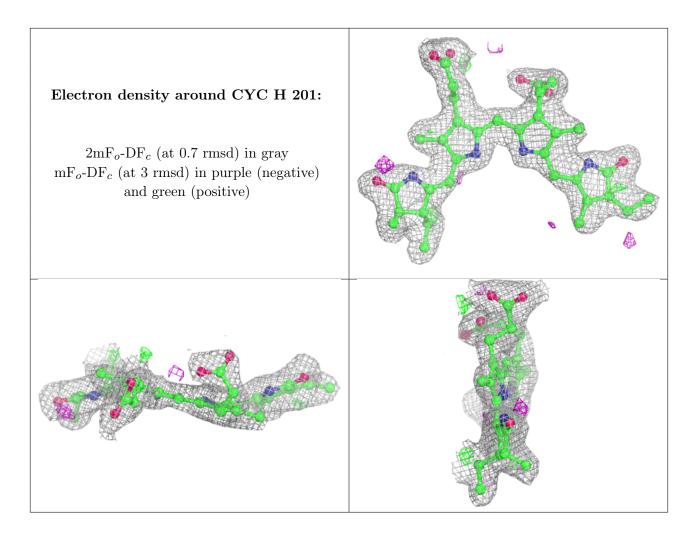




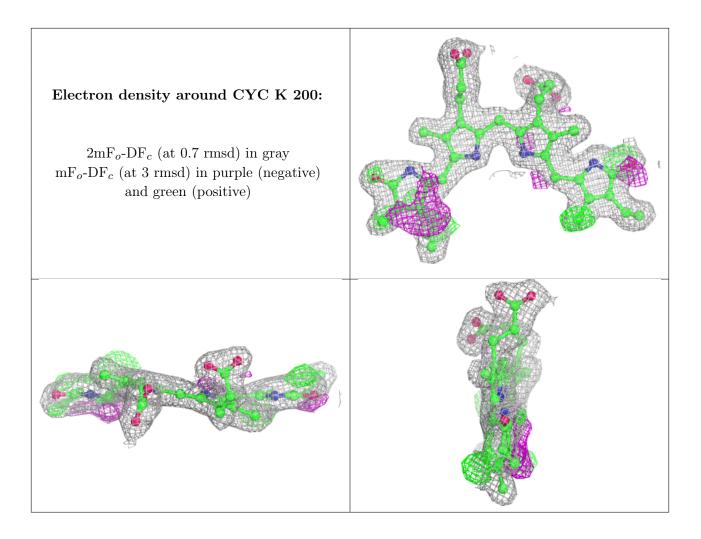




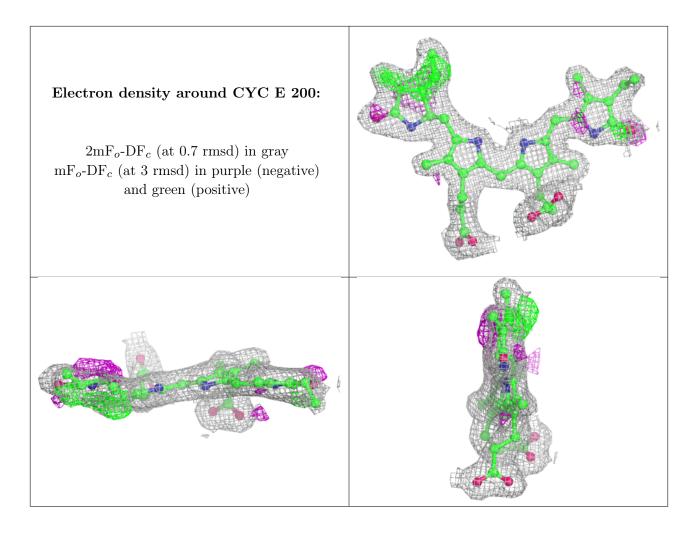




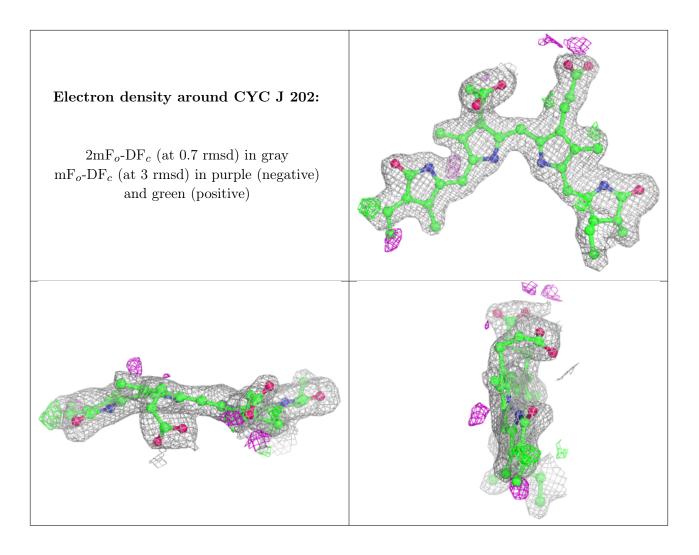




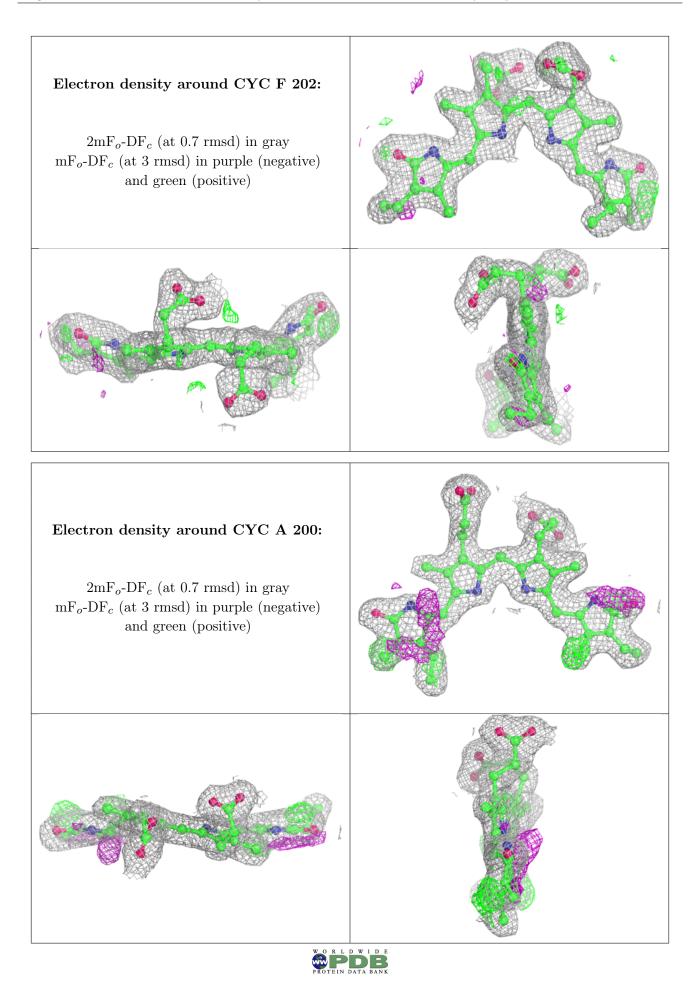


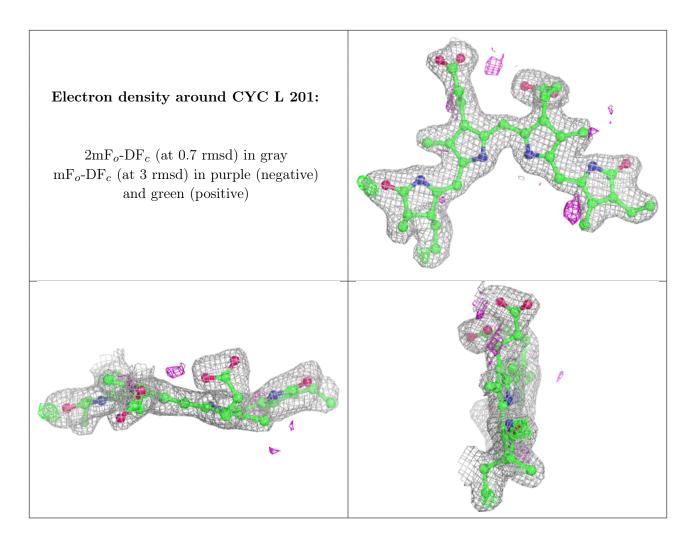




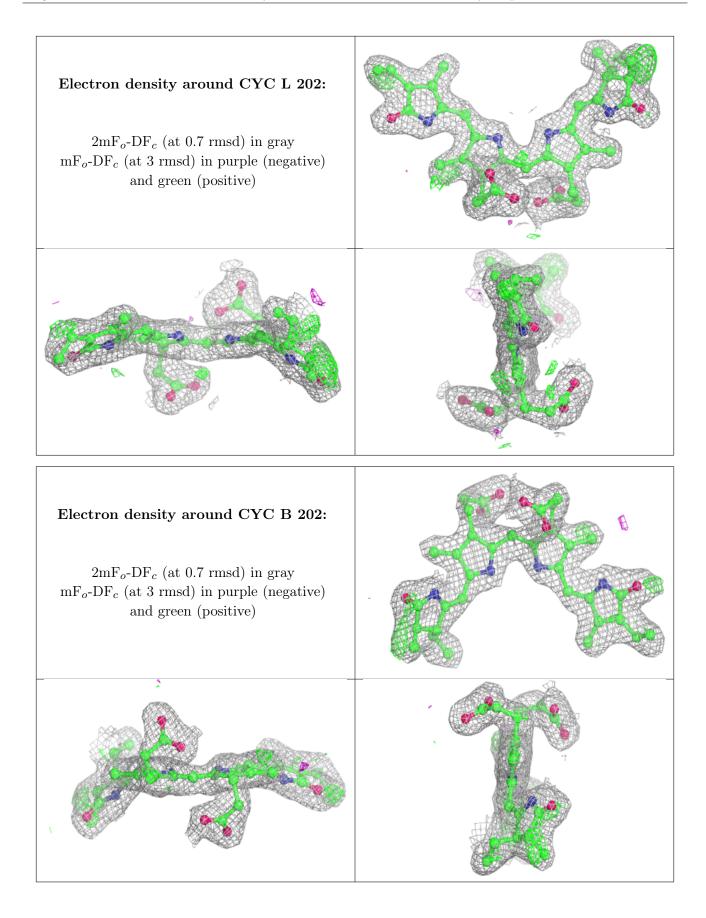




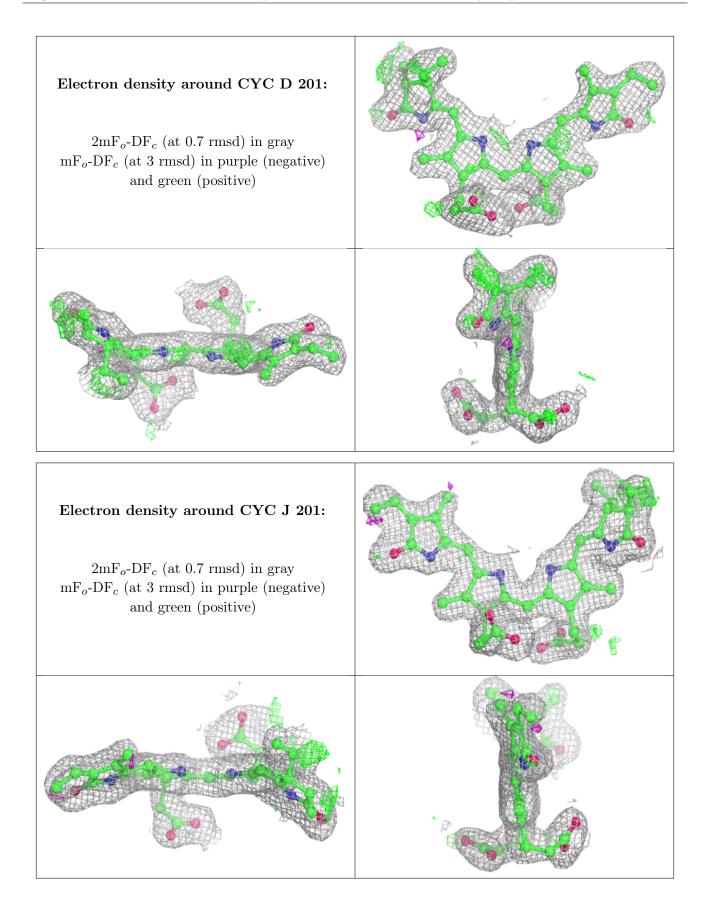




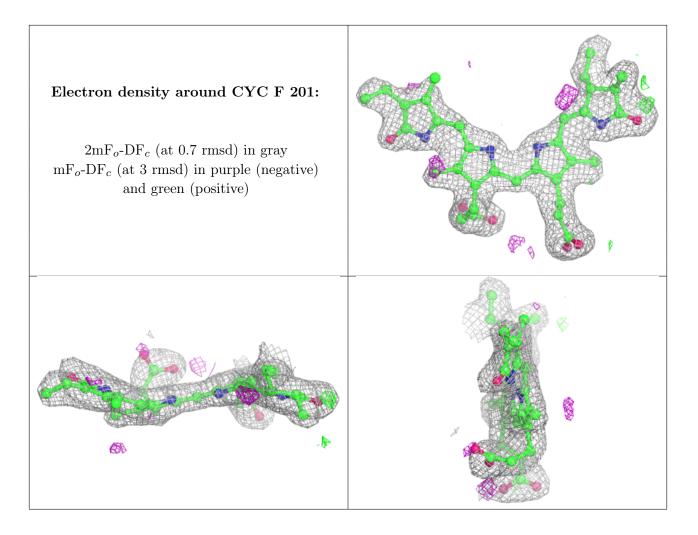




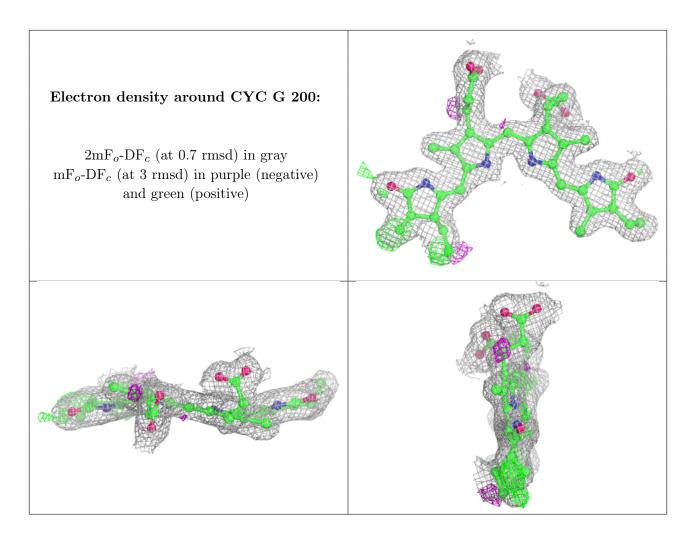




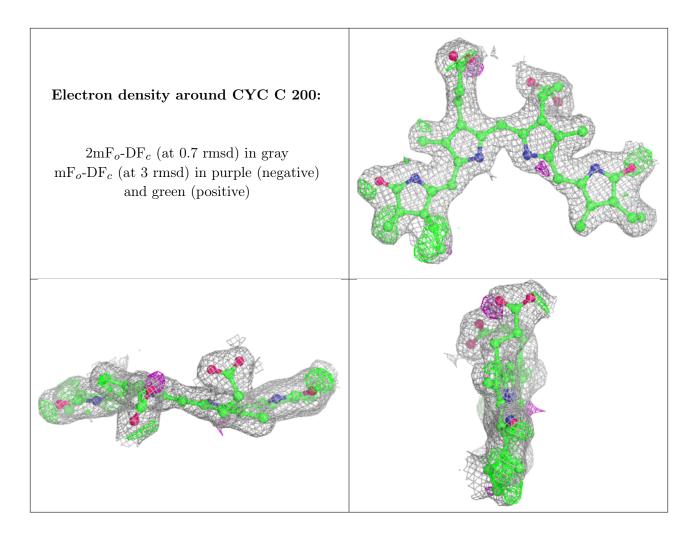




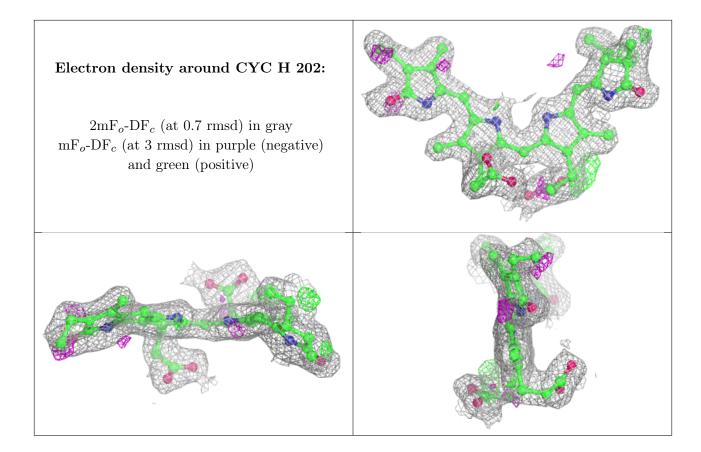












# 6.5 Other polymers (i)

There are no such residues in this entry.

