

wwPDB X-ray Structure Validation Summary Report (i)

Jan 7, 2024 - 11:52 am GMT

PDB ID	:	5MJP
Title	:	Multi-bunch pink beam serial crystallography: Phycocyanin (One chip)
Authors	:	Meents, A.; Oberthuer, D.; Lieske, J.; Srajer, V.; Sarrou, I.
Deposited on		
Resolution	:	2.11 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:

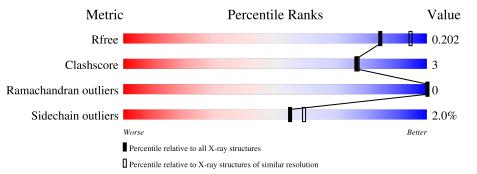
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.11 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)

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%

Mol	Chain	Length	Quality of chain	
1	А	162	94%	6% •
2	В	172	94%	6%



$5 \mathrm{MJP}$

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5431 atoms, of which 2604 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.

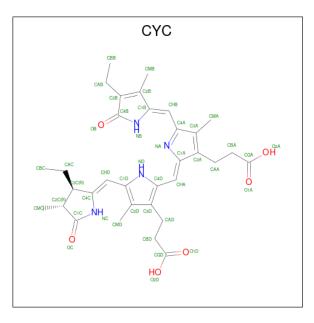
• Molecule 1 is a protein called C-phycocyanin alpha chain.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	А	162	Total 2452	С 777	Н 1216	N 209	0 243	${f S} 7$	0	2	0

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

Mol	Chain	Residues			Atom	IS			ZeroOcc	AltConf	Trace
2	В	172	Total 2559	C 794	Н 1277	N 229	0 251	S 8	0	2	0

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	۸	1	Total	С	Η	Ν	Ο	0	0	
Ð	3 A	1	80	33	37	4	6	0	0	
9	D	1	Total	С	Η	Ν	0	0	0	
0	D	1	80	33	37	4	6	0	0	

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
2	В	1	Total	С	Η	Ν	Ο	0	0
0	D	1	80	33	37	4	6	0	0

• Molecule 4 is water.

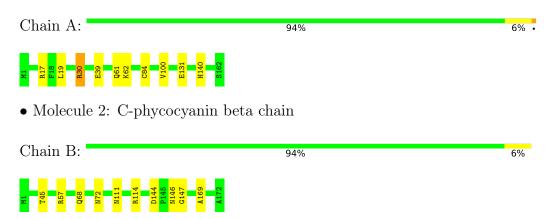
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	91	Total O 91 91	0	0
4	В	89	Total O 89 89	0	0



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. 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. 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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants	187.80Å 187.80Å 60.70Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.90 - 2.11	Depositor
Resolution (A)	36.21 - 2.11	EDS
% Data completeness	65.3 (14.90-2.11)	Depositor
(in resolution range)	65.4(36.21-2.11)	EDS
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$7.98 (at 2.10 \text{\AA})$	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
D D.	0.169 , 0.200	Depositor
R, R_{free}	0.170 , 0.202	DCC
R_{free} test set	1533 reflections (9.89%)	wwPDB-VP
Wilson B-factor $(Å^2)$	33.6	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 46.2	EDS
L-test for twinning ²	$ < L >=0.46, < L^2>=0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.35	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms $(Å^2)$	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.60% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: 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		lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.28	0/1270	0.41	0/1721	
2	В	0.26	0/1292	0.40	0/1748	
All	All	0.27	0/2562	0.41	0/3469	

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	1236	1216	1206	7	0
2	В	1282	1277	1282	6	0
3	А	43	37	37	3	0
3	В	86	74	73	2	0
4	А	91	0	0	3	2
4	В	89	0	0	4	1
All	All	2827	2604	2598	16	2

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 16 close contacts within the same asymmetric unit are listed below, sorted by their



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:NE2	4:A:601:HOH:O	2.06	0.87
2:B:68[B]:GLN:OE1	4:B:601:HOH:O	2.05	0.74
1:A:39:GLU:OE1	4:A:602:HOH:O	2.12	0.67
2:B:144:ASP:OD1	4:B:602:HOH:O	2.14	0.66
1:A:131:GLU:OE1	4:A:603:HOH:O	2.18	0.56

clash magnitude.

All (2) 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)
4:A:677:HOH:O	4:A:677:HOH:O[6_556]	1.77	0.43
4:A:647:HOH:O	4:B:672:HOH:O[5_556]	2.04	0.16

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	А	162/162~(100%)	160 (99%)	2(1%)	0	100	100	
2	В	171/172~(99%)	169~(99%)	2(1%)	0	100	100	
All	All	333/334~(100%)	329~(99%)	4 (1%)	0	100	100	

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	125/123~(102%)	122~(98%)	3~(2%)	49 52		
2	В	129/127~(102%)	127~(98%)	2(2%)	62 68		
All	All	254/250~(102%)	249~(98%)	5(2%)	55 59		

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	30	ARG
1	А	62	LYS
1	А	140	HIS
2	В	111	ASN
2	В	146	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	Mol Type Chain Res		Type	Chain	Res	Bos	Bos	Bos	Bos	Bos	Bos	Bos	Bos	Link	B	ond leng	gths	В	ond ang	gles
	Type	Ullaili	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2										
2	MEN	В	72	2	7,8,9	0.93	0	6, 9, 11	1.19	1 (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
2	MEN	В	72	2	-	2/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	72	MEN	CB-CA-C	-2.33	107.10	111.47

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	72	MEN	CA-CB-CG-OD1
2	В	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)

3 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	Trune	Chain	Dec	Link	В	ond leng	gths	B	ond ang	gles
	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	CYC	В	202	2	42,46,46	3.54	19 (45%)	50,67,67	1.55	11 (22%)
3	CYC	А	501	1	42,46,46	3.57	18 (42%)	50,67,67	1.54	12 (24%)
3	CYC	В	201	2	42,46,46	3.60	18 (42%)	50,67,67	1.74	12 (24%)



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	В	202	2	-	7/25/74/74	0/4/4/4
3	CYC	А	501	1	-	11/25/74/74	0/4/4/4
3	CYC	В	201	2	-	8/25/74/74	0/4/4/4

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	В	201	CYC	C1B-NB	9.59	1.53	1.37
3	В	202	CYC	C1B-NB	9.49	1.53	1.37
3	А	501	CYC	C1B-NB	9.41	1.53	1.37
3	В	202	CYC	C1C-NC	9.29	1.49	1.37
3	В	201	CYC	C1C-NC	9.15	1.49	1.37

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	В	201	CYC	C2C-C3C-C4C	4.52	108.12	101.34
3	В	201	CYC	CHD-C4C-NC	3.86	129.80	125.20
3	В	202	CYC	C2C-C3C-C4C	3.68	106.86	101.34
3	В	202	CYC	C2A-C1A-NA	-3.27	105.29	110.05
3	В	201	CYC	C2A-C1A-NA	-3.27	105.30	110.05

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	501	CYC	NA-C4A-CHB-C1B
3	А	501	CYC	C3A-C4A-CHB-C1B
3	А	501	CYC	C4C-C3C-CAC-CBC
3	А	501	CYC	ND-C1D-CHD-C4C
3	А	501	CYC	C2D-C1D-CHD-C4C

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	202	CYC	1	0

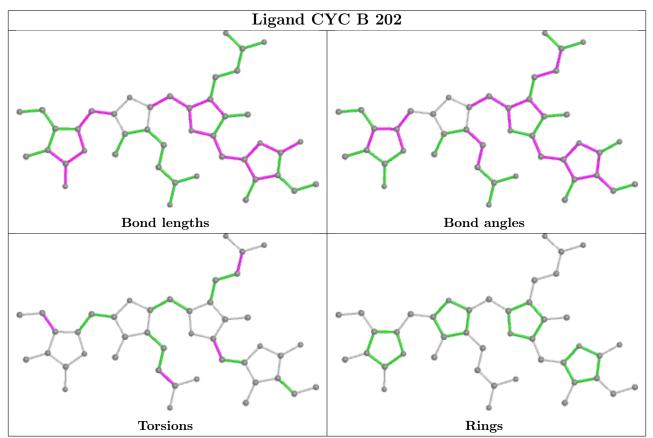
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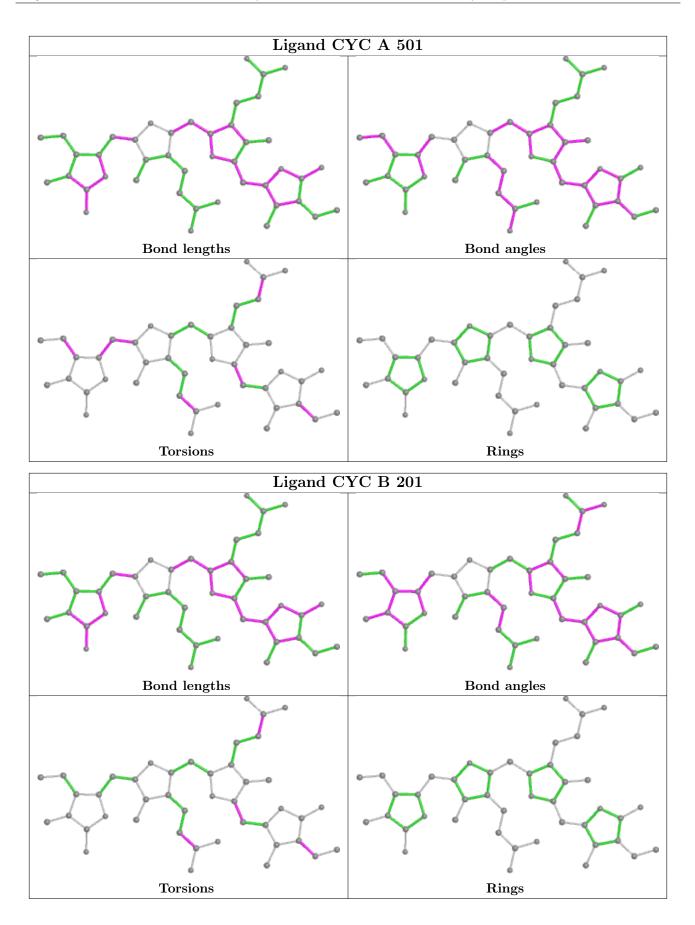
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	501	CYC	3	0
3	В	201	CYC	1	0

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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 sufficient must be 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

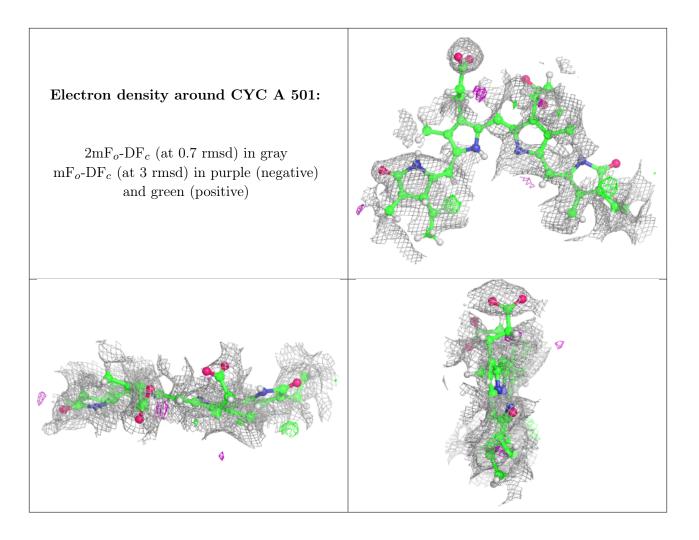
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6.4 Ligands (i)

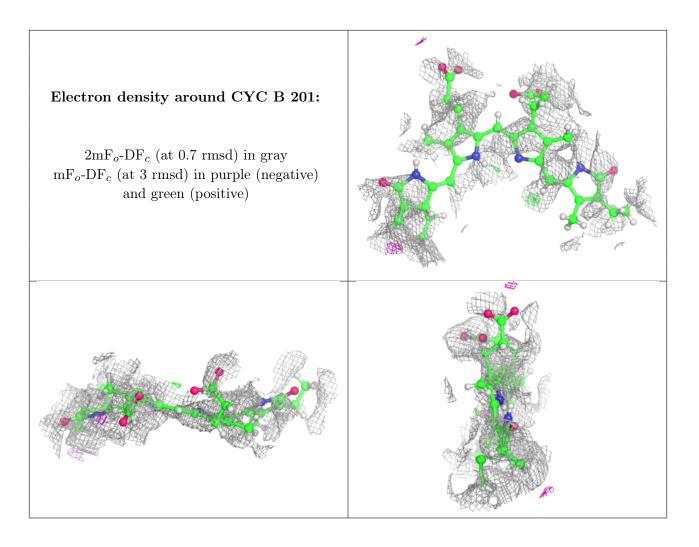
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

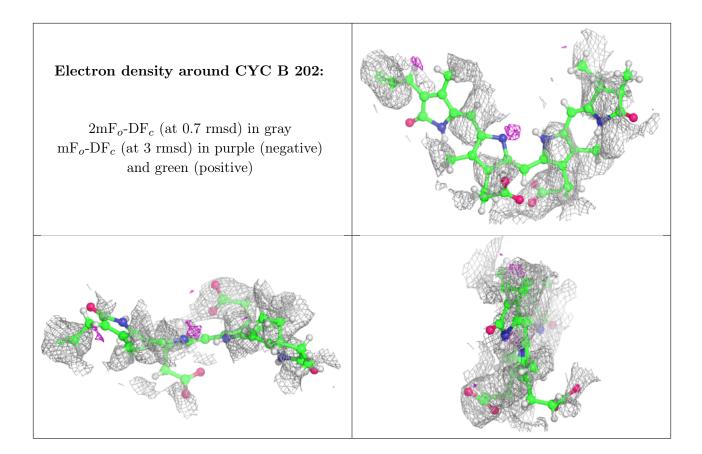












6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

