



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 02:15 AM BST

PDB ID : 6XWK  
Title : Crystal structure of Phormidium rubidum phycocyanin  
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Deposited on : 2020-01-23  
Resolution : 1.17 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

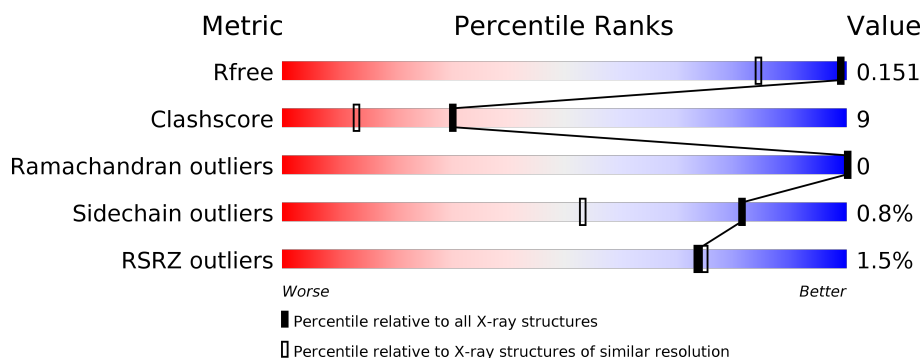
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1123 (1.20-1.16)
Clashscore	141614	1182 (1.20-1.16)
Ramachandran outliers	138981	1134 (1.20-1.16)
Sidechain outliers	138945	1134 (1.20-1.16)
RSRZ outliers	127900	1102 (1.20-1.16)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	AAA	162	
2	BBB	172	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	AAA	202	-	-	X	-
5	EDO	AAA	205	-	-	X	-
7	PGE	BBB	203	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 3359 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.

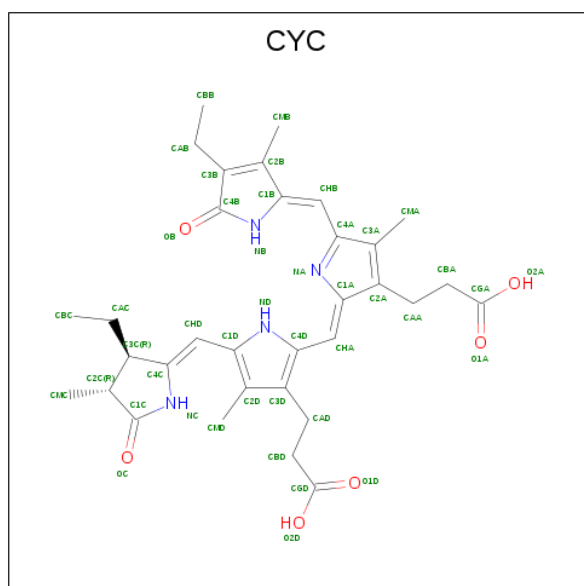
- Molecule 1 is a protein called Phycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	162	Total	C	N	O	S	0	18	0
			1330	838	217	265	10			

- Molecule 2 is a protein called Phycocyanin beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	172	Total	C	N	O	S	0	18	0
			1380	851	248	268	13			

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



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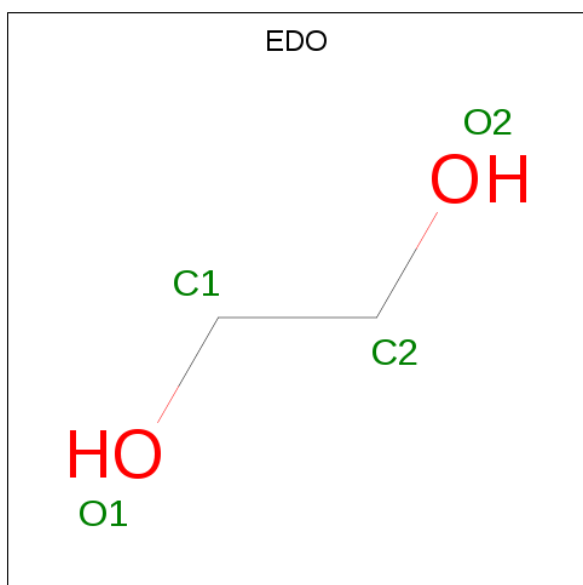
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	BBB	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



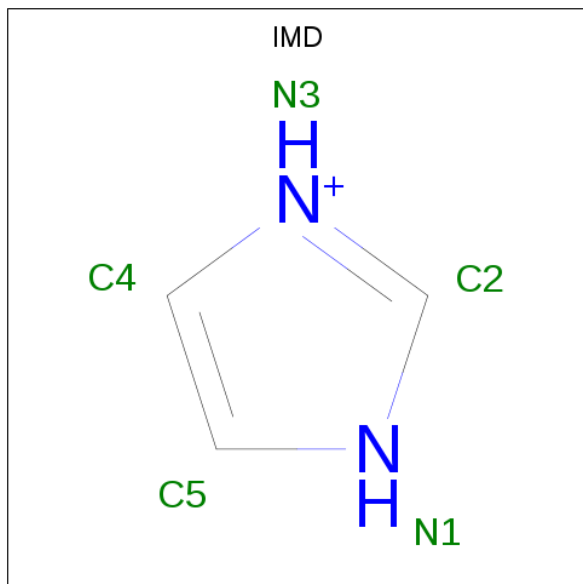
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AAA	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0
5	AAA	1	Total C O 4 2 2	0	0

- Molecule 6 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	AAA	1	Total C N 5 3 2	0	0
6	AAA	1	Total C N 5 3 2	0	0
6	BBB	1	Total C N 5 3 2	0	0
6	BBB	1	Total C N 5 3 2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	BBB	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	AAA	236	Total	O	0	0
			236	236		
8	BBB	223	Total	O	0	0
			223	223		

### 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: Phycocyanin alpha subunit

Chain AAA: 



- Molecule 2: Phycocyanin beta subunit

Chain BBB: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.32Å 106.32Å 58.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.39 – 1.17 46.04 – 1.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.39-1.17) 100.0 (46.04-1.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.17Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.119 , 0.145 0.124 , 0.151	Depositor DCC
$R_{free}$ test set	6165 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.2	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: PGE, IMD, MEN, EDO, CYC, PEG

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	AAA	0.66	0/1378	0.78	1/1862 (0.1%)
2	BBB	0.69	0/1413	0.80	1/1900 (0.1%)
All	All	0.67	0/2791	0.79	2/3762 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	95	TYR	CB-CG-CD1	5.72	124.43	121.00
1	AAA	90	TYR	CB-CG-CD1	5.08	124.05	121.00

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	AAA	1330	0	1307	21	0
2	BBB	1380	0	1403	26	0
3	AAA	43	0	37	2	0
3	BBB	86	0	74	4	0
4	AAA	7	0	10	6	0
5	AAA	24	0	36	12	0
6	AAA	10	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BBB	10	0	10	0	0
7	BBB	10	0	13	16	0
8	AAA	236	0	0	6	0
8	BBB	223	0	0	6	0
All	All	3359	0	2900	54	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 9.

All (54) 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)
5:AAA:210:EDO:H21	8:AAA:317:HOH:O	1.32	1.24
2:BBB:7[A]:LYS:NZ	8:BBB:301:HOH:O	1.81	1.13
2:BBB:123:PRO:HB2	7:BBB:203:PGE:H62	1.14	1.07
5:AAA:210:EDO:C2	8:AAA:317:HOH:O	2.01	0.93
1:AAA:7[A]:GLU:OE1	8:AAA:301:HOH:O	1.88	0.91
1:AAA:81[B]:LYS:HZ1	4:AAA:202:PEG:H22	1.36	0.89
2:BBB:65:GLN:HE21	7:BBB:203:PGE:H4	1.37	0.88
1:AAA:81[B]:LYS:HZ1	4:AAA:202:PEG:H41	1.44	0.83
2:BBB:126:SER:OG	7:BBB:203:PGE:H52	1.81	0.79
1:AAA:159[B]:ASN:OD1	5:AAA:206:EDO:O2	2.01	0.78
2:BBB:15:ARG:NH1	8:BBB:302:HOH:O	2.09	0.77
1:AAA:7[A]:GLU:OE1	5:AAA:205:EDO:O1	2.06	0.74
2:BBB:77:ARG:HH22	2:BBB:78[B]:ARG:HH11	1.35	0.74
1:AAA:81[B]:LYS:NZ	4:AAA:202:PEG:H41	2.04	0.73
2:BBB:50[B]:THR:HG22	8:BBB:348:HOH:O	1.89	0.73
1:AAA:81[B]:LYS:NZ	4:AAA:202:PEG:H22	2.06	0.71
1:AAA:81[B]:LYS:HZ1	4:AAA:202:PEG:C2	2.05	0.70
2:BBB:123:PRO:HB2	7:BBB:203:PGE:C6	2.09	0.69
2:BBB:66:LEU:HD23	7:BBB:203:PGE:H3	1.76	0.68
2:BBB:77:ARG:NH2	2:BBB:78[B]:ARG:HH11	1.94	0.65
3:BBB:201:CYC:HMD2	3:BBB:201:CYC:HC	1.62	0.65
2:BBB:84[A]:ARG:NH2	3:BBB:201:CYC:O2A	2.30	0.65
2:BBB:78[B]:ARG:CZ	3:BBB:201:CYC:O1D	2.46	0.63
2:BBB:50[B]:THR:CG2	8:BBB:348:HOH:O	2.44	0.61
2:BBB:123:PRO:CB	7:BBB:203:PGE:H62	2.09	0.61
2:BBB:65:GLN:HE21	7:BBB:203:PGE:C4	2.11	0.60
1:AAA:2[A]:LYS:HB3	5:AAA:205:EDO:H21	1.84	0.59
2:BBB:7[B]:LYS:NZ	8:BBB:304:HOH:O	2.37	0.58
2:BBB:65:GLN:NE2	7:BBB:203:PGE:H4	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BBB:203:PGE:H1	8:BBB:323:HOH:O	2.05	0.56
1:AAA:70:GLN:NE2	8:AAA:306:HOH:O	2.39	0.55
1:AAA:158:VAL:HG11	5:AAA:206:EDO:H12	1.88	0.55
2:BBB:66:LEU:CD2	7:BBB:203:PGE:H3	2.35	0.55
1:AAA:114:GLY:H	5:AAA:207:EDO:C2	2.20	0.54
3:AAA:201:CYC:HMD2	3:AAA:201:CYC:HC	1.72	0.54
2:BBB:125:ALA:HB3	7:BBB:203:PGE:H6	1.90	0.54
2:BBB:65:GLN:HG2	7:BBB:203:PGE:H32	1.89	0.53
1:AAA:67:THR:HB	4:AAA:202:PEG:H21	1.92	0.52
5:AAA:210:EDO:C1	8:AAA:317:HOH:O	2.47	0.51
2:BBB:126:SER:OG	7:BBB:203:PGE:C5	2.55	0.51
1:AAA:2[B]:LYS:HB3	5:AAA:205:EDO:H21	1.94	0.50
1:AAA:162:SER:O	8:AAA:302:HOH:O	2.19	0.50
1:AAA:6:THR:HB	5:AAA:205:EDO:H11	1.96	0.48
2:BBB:126:SER:HG	7:BBB:203:PGE:H52	1.76	0.47
1:AAA:114:GLY:C	5:AAA:207:EDO:H12	2.35	0.47
1:AAA:107[B]:MET:HG3	1:AAA:112[B]:ILE:HG12	1.96	0.46
2:BBB:65:GLN:CG	7:BBB:203:PGE:H32	2.47	0.45
2:BBB:145[A]:ARG:HG3	2:BBB:145[A]:ARG:HH11	1.82	0.45
2:BBB:123:PRO:HG3	7:BBB:203:PGE:H22	1.99	0.43
1:AAA:125[B]:SER:HB2	1:AAA:128:TRP:CE2	2.55	0.42
1:AAA:116:ALA:HB3	5:AAA:207:EDO:H11	2.02	0.42
3:AAA:201:CYC:NB	3:AAA:201:CYC:HMA1	2.36	0.41
1:AAA:114:GLY:O	1:AAA:118[B]:ILE:HD13	2.21	0.41
2:BBB:78[B]:ARG:NH1	3:BBB:201:CYC:O1D	2.53	0.41

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	AAA	177/162 (109%)	175 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BBB	186/172 (108%)	184 (99%)	2 (1%)	0	100	100
All	All	363/334 (109%)	359 (99%)	4 (1%)	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	AAA	140/122 (115%)	138 (99%)	2 (1%)	67	31
2	BBB	147/129 (114%)	145 (99%)	2 (1%)	67	31
All	All	287/251 (114%)	283 (99%)	4 (1%)	81	31

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	2[A]	LYS
1	AAA	2[B]	LYS
2	BBB	145[A]	ARG
2	BBB	145[B]	ARG

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	MEN	BBB	72	2	7,8,9	1.04	1 (14%)	6,9,11	1.02	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	BBB	72	2	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	72	MEN	CE2-ND2	2.13	1.49	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	72	MEN	CA-CB-CG-OD1
2	BBB	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](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	IMD	AAA	208	-	3,5,5	0.28	0	4,5,5	0.62	0
7	PGE	BBB	203	-	9,9,9	0.60	0	8,8,8	0.74	0
6	IMD	BBB	205	-	3,5,5	0.36	0	4,5,5	0.71	0
5	EDO	AAA	205	-	3,3,3	0.53	0	2,2,2	0.17	0
3	CYC	BBB	202	2	36,46,46	1.17	1 (2%)	44,67,67	1.05	4 (9%)
6	IMD	AAA	209	-	3,5,5	0.27	0	4,5,5	0.69	0
4	PEG	AAA	202	-	6,6,6	0.35	0	5,5,5	0.35	0
5	EDO	AAA	206	-	3,3,3	0.22	0	2,2,2	0.65	0
6	IMD	BBB	204	-	3,5,5	0.47	0	4,5,5	0.66	0
5	EDO	AAA	210	-	3,3,3	0.05	0	2,2,2	0.06	0
5	EDO	AAA	203	-	3,3,3	0.09	0	2,2,2	0.21	0
3	CYC	AAA	201	1	36,46,46	1.16	2 (5%)	44,67,67	1.14	3 (6%)
5	EDO	AAA	207	-	3,3,3	0.47	0	2,2,2	1.31	0
5	EDO	AAA	204	-	3,3,3	0.39	0	2,2,2	0.73	0
3	CYC	BBB	201	2	36,46,46	1.37	2 (5%)	44,67,67	1.11	4 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IMD	AAA	208	-	-	-	0/1/1/1
6	IMD	BBB	205	-	-	-	0/1/1/1
7	PGE	BBB	203	-	-	4/7/7/7	-
5	EDO	AAA	205	-	-	1/1/1/1	-
3	CYC	BBB	202	2	-	4/21/74/74	0/4/4/4
6	IMD	AAA	209	-	-	-	0/1/1/1
4	PEG	AAA	202	-	-	1/4/4/4	-
5	EDO	AAA	206	-	-	1/1/1/1	-
6	IMD	BBB	204	-	-	-	0/1/1/1
5	EDO	AAA	210	-	-	1/1/1/1	-
5	EDO	AAA	203	-	-	0/1/1/1	-
3	CYC	AAA	201	1	-	7/21/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	AAA	207	-	-	1/1/1/1	-
5	EDO	AAA	204	-	-	0/1/1/1	-
3	CYC	BBB	201	2	-	4/21/74/74	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	BBB	201	CYC	CHA-C1A	7.18	1.41	1.35
3	BBB	202	CYC	CHA-C1A	6.11	1.40	1.35
3	AAA	201	CYC	CHA-C1A	5.82	1.40	1.35
3	BBB	201	CYC	C2C-C1C	-2.31	1.50	1.52
3	AAA	201	CYC	C1B-C2B	-2.08	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AAA	201	CYC	C4D-CHA-C1A	3.27	132.72	128.81
3	BBB	201	CYC	C4D-CHA-C1A	3.03	132.43	128.81
3	BBB	202	CYC	CMB-C2B-C1B	2.73	127.57	124.17
3	BBB	201	CYC	CAB-C3B-C2B	2.61	132.00	127.53
3	BBB	202	CYC	CMA-C3A-C4A	2.49	128.90	125.06
3	AAA	201	CYC	CAC-C3C-C4C	2.43	118.92	112.67
3	BBB	201	CYC	CHD-C4C-NC	2.42	128.08	125.20
3	BBB	202	CYC	C4D-CHA-C1A	2.42	131.70	128.81
3	BBB	201	CYC	C2C-C3C-C4C	2.27	104.73	101.34
3	BBB	202	CYC	CHD-C4C-NC	-2.26	122.52	125.20
3	AAA	201	CYC	C3B-C4B-NB	-2.26	104.95	106.78

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	BBB	202	CYC	NA-C4A-CHB-C1B
3	BBB	202	CYC	C3A-C4A-CHB-C1B
3	AAA	201	CYC	NA-C4A-CHB-C1B
3	AAA	201	CYC	C3A-C4A-CHB-C1B
3	AAA	201	CYC	C4C-C3C-CAC-CBC
3	AAA	201	CYC	ND-C1D-CHD-C4C
3	AAA	201	CYC	C2D-C1D-CHD-C4C
3	BBB	201	CYC	NA-C4A-CHB-C1B
3	BBB	201	CYC	C3A-C4A-CHB-C1B

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Mol	Chain	Res	Type	Atoms
3	BBB	201	CYC	ND-C1D-CHD-C4C
3	BBB	201	CYC	C2D-C1D-CHD-C4C
7	BBB	203	PGE	O2-C3-C4-O3
5	AAA	205	EDO	O1-C1-C2-O2
3	BBB	202	CYC	C2C-C3C-CAC-CBC
3	AAA	201	CYC	C2C-C3C-CAC-CBC
3	AAA	201	CYC	C2B-C3B-CAB-CBB
5	AAA	210	EDO	O1-C1-C2-O2
3	BBB	202	CYC	C4C-C3C-CAC-CBC
7	BBB	203	PGE	O3-C5-C6-O4
5	AAA	207	EDO	O1-C1-C2-O2
5	AAA	206	EDO	O1-C1-C2-O2
7	BBB	203	PGE	C6-C5-O3-C4
7	BBB	203	PGE	C4-C3-O2-C2
4	AAA	202	PEG	C4-C3-O2-C2

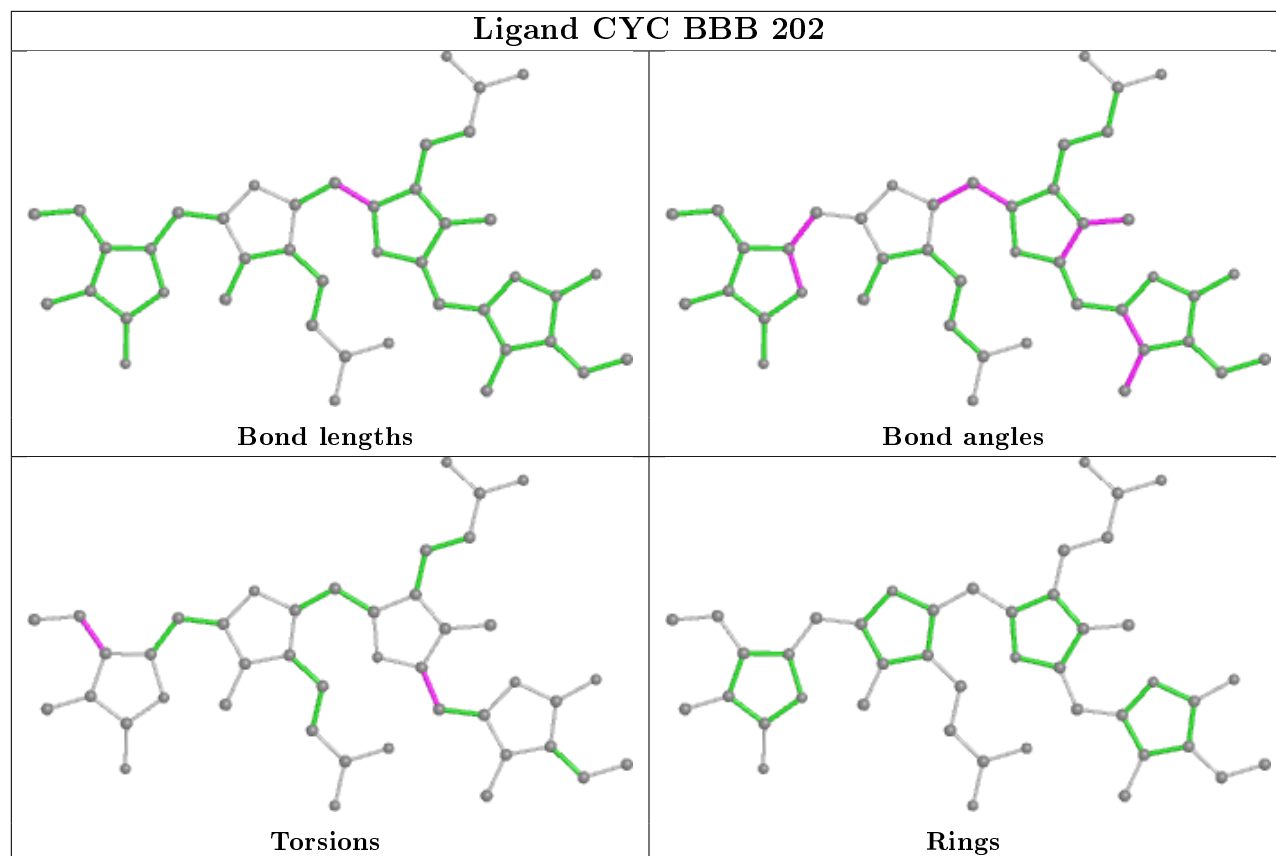
There are no ring outliers.

8 monomers are involved in 40 short contacts:

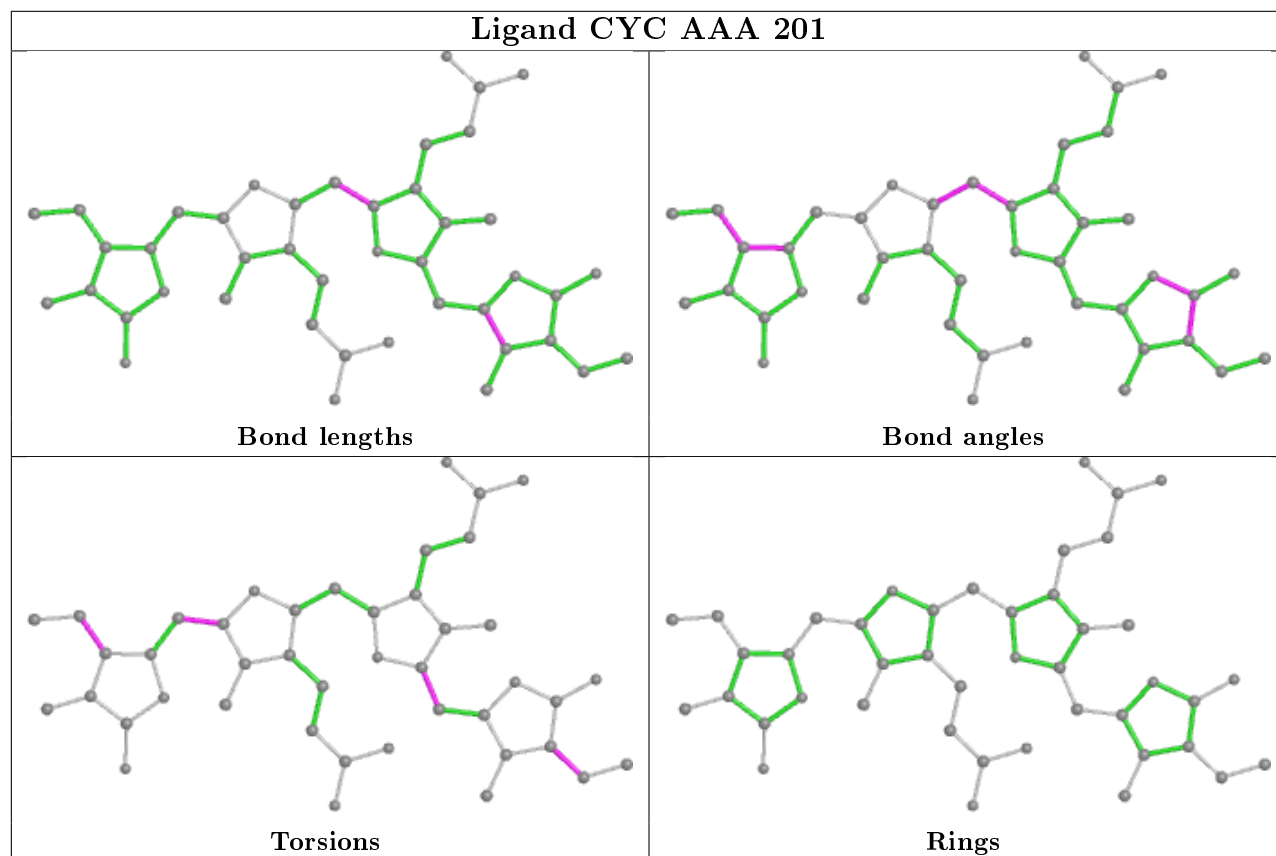
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	BBB	203	PGE	16	0
5	AAA	205	EDO	4	0
4	AAA	202	PEG	6	0
5	AAA	206	EDO	2	0
5	AAA	210	EDO	3	0
3	AAA	201	CYC	2	0
5	AAA	207	EDO	3	0
3	BBB	201	CYC	4	0

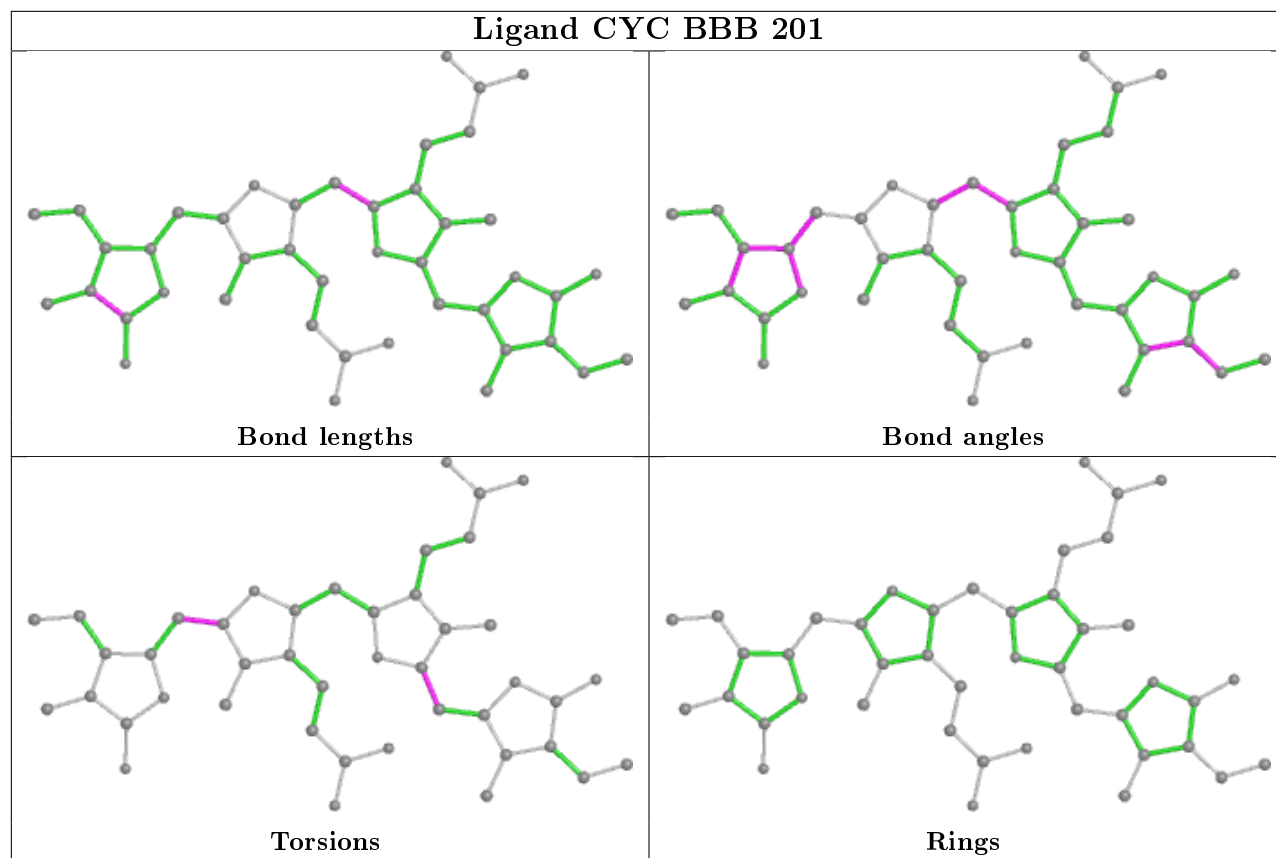
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 BBB 202



## Ligand CYC AAA 201





## 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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	162/162 (100%)	-0.13	0 <b>100</b> <b>100</b>	9, 13, 21, 39	0
2	BBB	171/172 (99%)	-0.10	5 (2%) 51 53	10, 13, 25, 41	0
All	All	333/334 (99%)	-0.12	5 (1%) <b>73</b> <b>75</b>	9, 13, 23, 41	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	145[A]	ARG	4.7
2	BBB	147	GLY	2.4
2	BBB	150	GLN	2.4
2	BBB	146	GLY	2.4
2	BBB	148	ILE	2.2

### 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, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	MEN	BBB	72	9/10	0.98	0.06	11,12,15,15	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

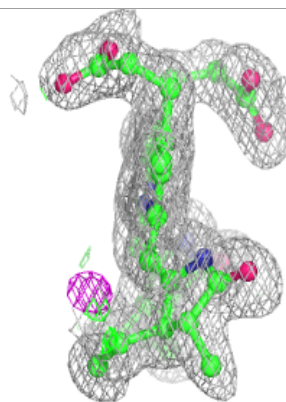
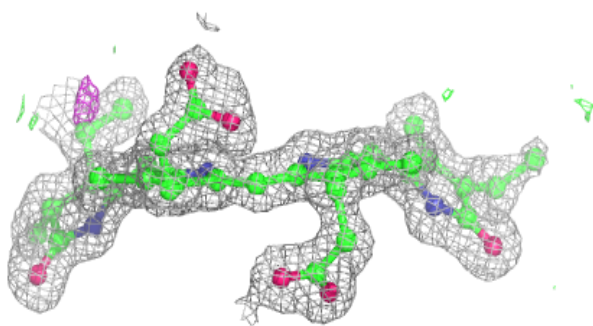
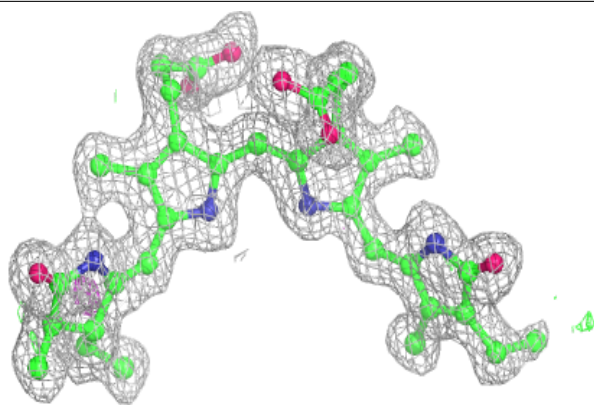
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	AAA	210	4/4	0.75	0.35	26,27,29,36	4
5	EDO	AAA	206	4/4	0.81	0.24	26,29,30,30	4
6	IMD	AAA	209	5/5	0.82	0.35	53,53,54,54	0
6	IMD	BBB	204	5/5	0.83	0.12	24,31,44,44	0
5	EDO	AAA	203	4/4	0.83	0.22	27,28,33,34	4
4	PEG	AAA	202	7/7	0.84	0.23	14,19,23,28	7
5	EDO	AAA	205	4/4	0.85	0.21	23,27,28,28	4
7	PGE	BBB	203	10/10	0.88	0.24	16,18,23,29	10
5	EDO	AAA	207	4/4	0.88	0.17	18,18,20,23	4
6	IMD	BBB	205	5/5	0.88	0.12	40,49,52,56	0
5	EDO	AAA	204	4/4	0.89	0.25	21,24,26,26	4
6	IMD	AAA	208	5/5	0.94	0.15	27,29,33,35	0
3	CYC	BBB	202	43/43	0.95	0.09	17,21,30,37	0
3	CYC	BBB	201	43/43	0.96	0.08	9,13,28,35	0
3	CYC	AAA	201	43/43	0.98	0.06	8,10,12,15	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.

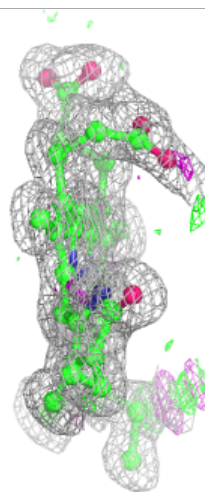
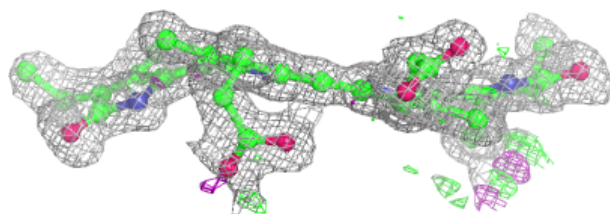
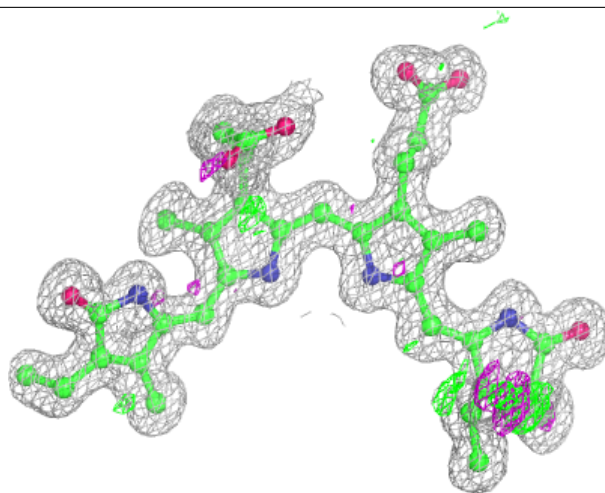
**Electron density around CYC BBB 202:**

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



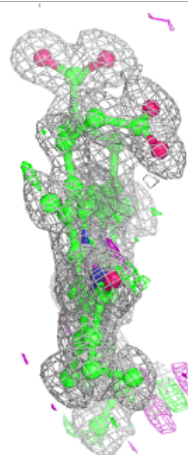
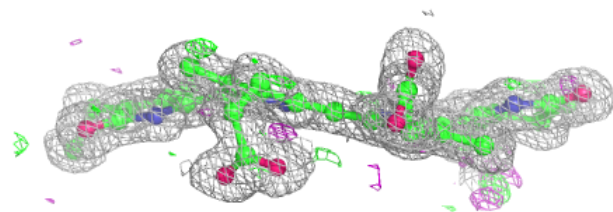
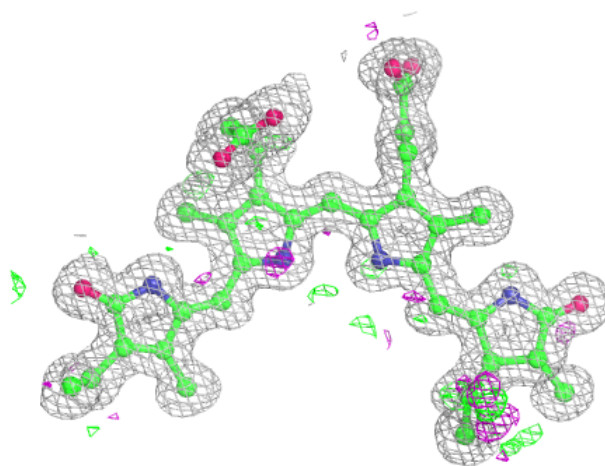
**Electron density around CYC BBB 201:**

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



**Electron density around CYC AAA 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 [i](#)

There are no such residues in this entry.