



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:52 pm BST

PDB ID : 3C2W  
Title : Crystal structure of the photosensory core domain of *P. aeruginosa* bacterio-  
phytochrome PaBphP in the Pfr state  
Authors : Yang, X.; Kuk, J.; Moffat, K.  
Deposited on : 2008-01-25  
Resolution : 2.90 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](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	:	2.11
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)	:	2.11

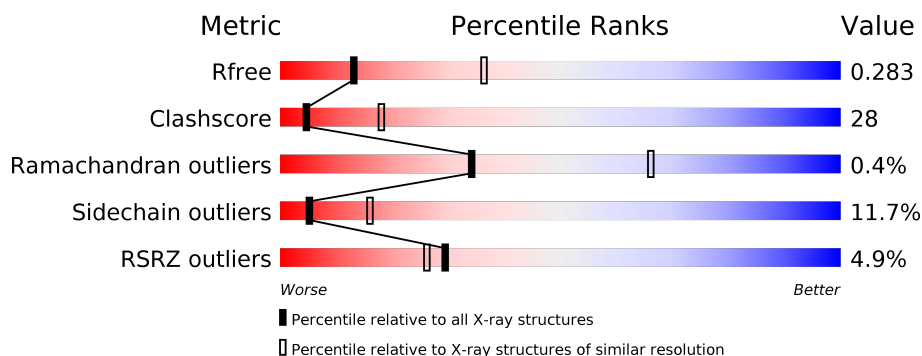
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	505	<div> <div>%</div> <div> <div>48%</div> <div>41%</div> <div>6%</div> <div>5%</div> </div> </div>
1	B	505	<div> <div>6%</div> <div>46%</div> <div>41%</div> <div>6%</div> <div>7%</div> </div>
1	C	505	<div> <div>%</div> <div>48%</div> <div>41%</div> <div>7%</div> <div>5%</div> </div>
1	D	505	<div> <div>5%</div> <div>49%</div> <div>41%</div> <div>5%</div> <div>5%</div> </div>
1	E	505	<div> <div>6%</div> <div>47%</div> <div>41%</div> <div>6%</div> <div>7%</div> </div>
1	F	505	<div> <div>6%</div> <div>48%</div> <div>39%</div> <div>6%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	505	<div><div></div><div>2%</div><div>44%</div><div>43%</div><div>8%</div><div>5%</div></div>
1	H	505	<div><div></div><div>10%</div><div>50%</div><div>39%</div><div>6%</div><div>5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30494 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 Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3782	2382	681	700	19			
1	B	468	Total	C	N	O	S	0	0	0
			3693	2322	663	689	19			
1	C	482	Total	C	N	O	S	0	0	0
			3812	2398	688	707	19			
1	D	478	Total	C	N	O	S	0	0	0
			3788	2383	683	703	19			
1	E	471	Total	C	N	O	S	0	0	0
			3725	2344	673	689	19			
1	F	469	Total	C	N	O	S	0	0	0
			3704	2331	664	690	19			
1	G	482	Total	C	N	O	S	0	1	0
			3816	2401	688	707	20			
1	H	480	Total	C	N	O	S	0	0	0
			3800	2392	686	703	19			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	498	LEU	-	expression tag	UNP Q9HWR3
A	499	GLU	-	expression tag	UNP Q9HWR3
A	500	HIS	-	expression tag	UNP Q9HWR3
A	501	HIS	-	expression tag	UNP Q9HWR3
A	502	HIS	-	expression tag	UNP Q9HWR3
A	503	HIS	-	expression tag	UNP Q9HWR3
A	504	HIS	-	expression tag	UNP Q9HWR3
A	505	HIS	-	expression tag	UNP Q9HWR3
B	498	LEU	-	expression tag	UNP Q9HWR3
B	499	GLU	-	expression tag	UNP Q9HWR3
B	500	HIS	-	expression tag	UNP Q9HWR3
B	501	HIS	-	expression tag	UNP Q9HWR3
B	502	HIS	-	expression tag	UNP Q9HWR3

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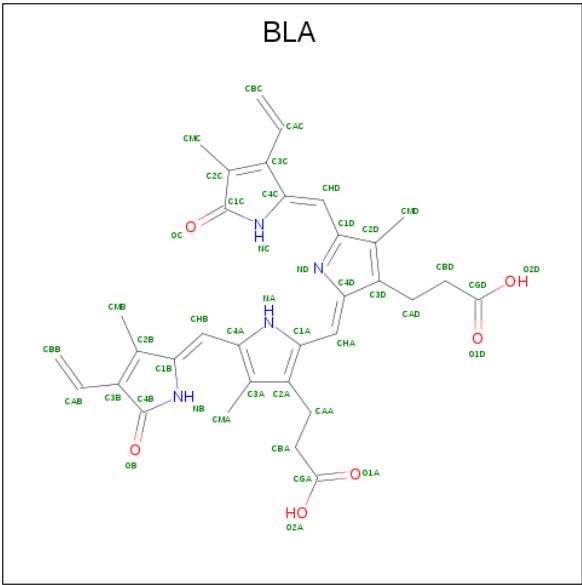
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3
C	498	LEU	-	expression tag	UNP Q9HWR3
C	499	GLU	-	expression tag	UNP Q9HWR3
C	500	HIS	-	expression tag	UNP Q9HWR3
C	501	HIS	-	expression tag	UNP Q9HWR3
C	502	HIS	-	expression tag	UNP Q9HWR3
C	503	HIS	-	expression tag	UNP Q9HWR3
C	504	HIS	-	expression tag	UNP Q9HWR3
C	505	HIS	-	expression tag	UNP Q9HWR3
D	498	LEU	-	expression tag	UNP Q9HWR3
D	499	GLU	-	expression tag	UNP Q9HWR3
D	500	HIS	-	expression tag	UNP Q9HWR3
D	501	HIS	-	expression tag	UNP Q9HWR3
D	502	HIS	-	expression tag	UNP Q9HWR3
D	503	HIS	-	expression tag	UNP Q9HWR3
D	504	HIS	-	expression tag	UNP Q9HWR3
D	505	HIS	-	expression tag	UNP Q9HWR3
E	498	LEU	-	expression tag	UNP Q9HWR3
E	499	GLU	-	expression tag	UNP Q9HWR3
E	500	HIS	-	expression tag	UNP Q9HWR3
E	501	HIS	-	expression tag	UNP Q9HWR3
E	502	HIS	-	expression tag	UNP Q9HWR3
E	503	HIS	-	expression tag	UNP Q9HWR3
E	504	HIS	-	expression tag	UNP Q9HWR3
E	505	HIS	-	expression tag	UNP Q9HWR3
F	498	LEU	-	expression tag	UNP Q9HWR3
F	499	GLU	-	expression tag	UNP Q9HWR3
F	500	HIS	-	expression tag	UNP Q9HWR3
F	501	HIS	-	expression tag	UNP Q9HWR3
F	502	HIS	-	expression tag	UNP Q9HWR3
F	503	HIS	-	expression tag	UNP Q9HWR3
F	504	HIS	-	expression tag	UNP Q9HWR3
F	505	HIS	-	expression tag	UNP Q9HWR3
G	498	LEU	-	expression tag	UNP Q9HWR3
G	499	GLU	-	expression tag	UNP Q9HWR3
G	500	HIS	-	expression tag	UNP Q9HWR3
G	501	HIS	-	expression tag	UNP Q9HWR3
G	502	HIS	-	expression tag	UNP Q9HWR3
G	503	HIS	-	expression tag	UNP Q9HWR3
G	504	HIS	-	expression tag	UNP Q9HWR3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	505	HIS	-	expression tag	UNP Q9HWR3
H	498	LEU	-	expression tag	UNP Q9HWR3
H	499	GLU	-	expression tag	UNP Q9HWR3
H	500	HIS	-	expression tag	UNP Q9HWR3
H	501	HIS	-	expression tag	UNP Q9HWR3
H	502	HIS	-	expression tag	UNP Q9HWR3
H	503	HIS	-	expression tag	UNP Q9HWR3
H	504	HIS	-	expression tag	UNP Q9HWR3
H	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C<sub>33</sub>H<sub>34</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		
2	E	1	Total	C	N	O	0	0
			43	33	4	6		
2	F	1	Total	C	N	O	0	0
			43	33	4	6		
2	G	1	Total	C	N	O	0	0
			43	33	4	6		

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

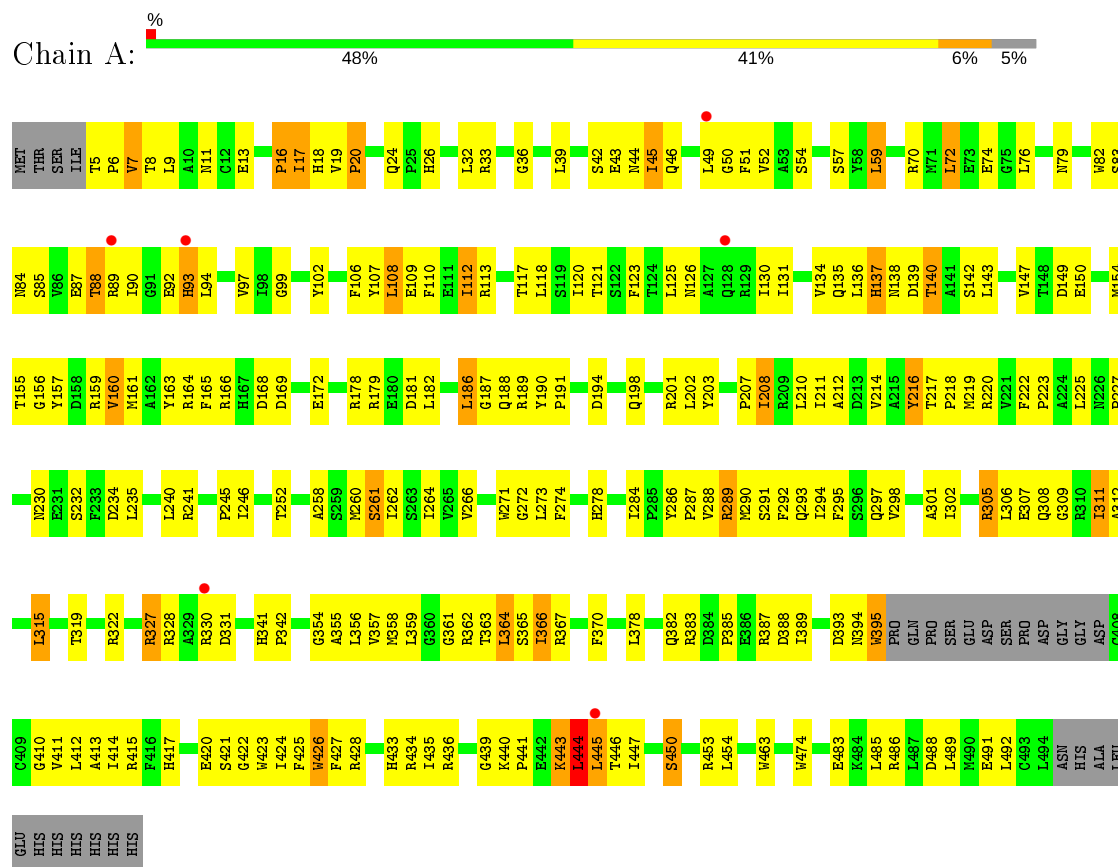
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		
3	B	2	Total	O	0	0
			2	2		
3	C	6	Total	O	0	0
			6	6		
3	D	3	Total	O	0	0
			3	3		
3	E	1	Total	O	0	0
			1	1		
3	F	2	Total	O	0	0
			2	2		
3	G	7	Total	O	0	0
			7	7		
3	H	2	Total	O	0	0
			2	2		

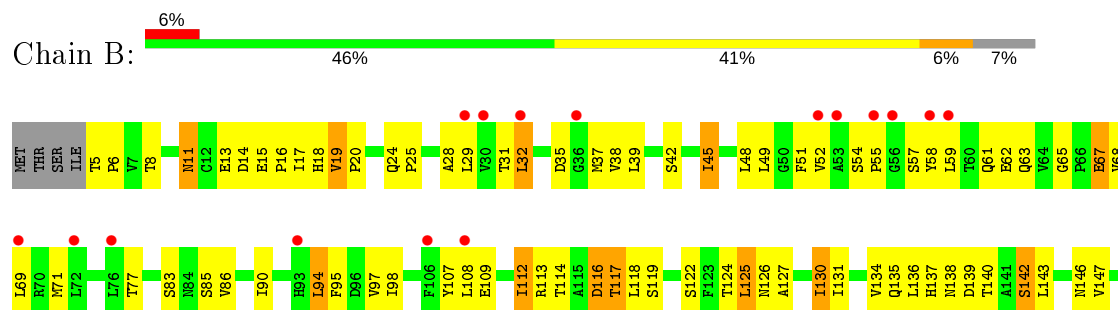
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

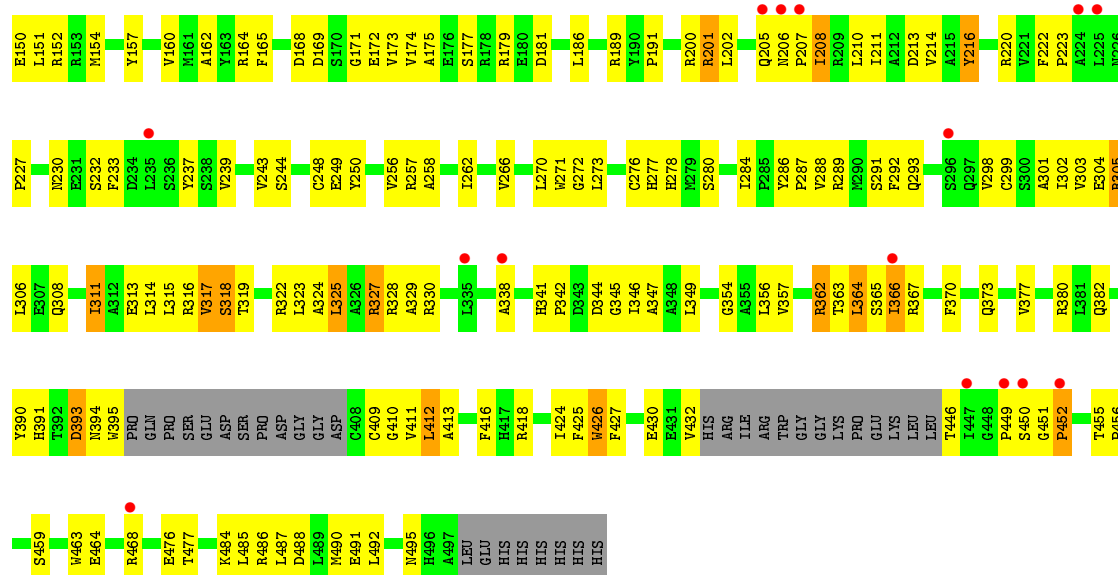
#### • Molecule 1: Bacteriophytochrome



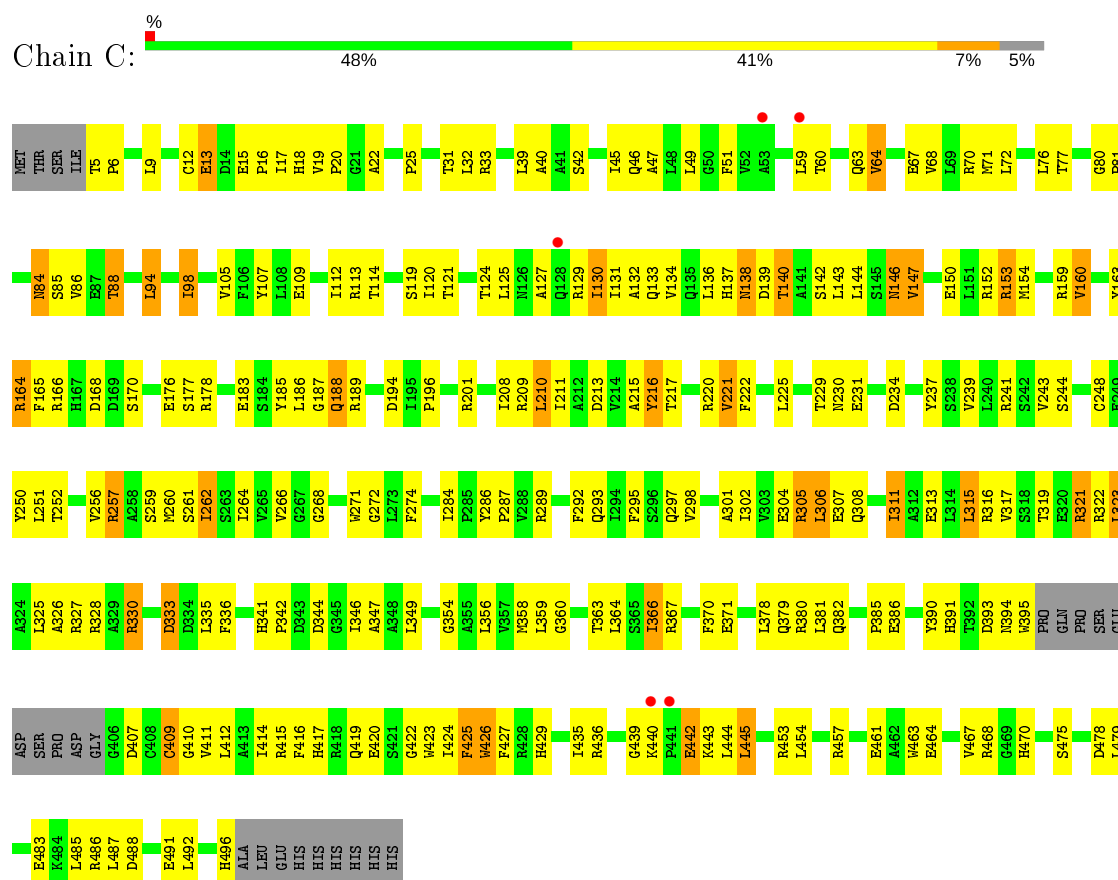
#### • Molecule 1: Bacteriophytochrome





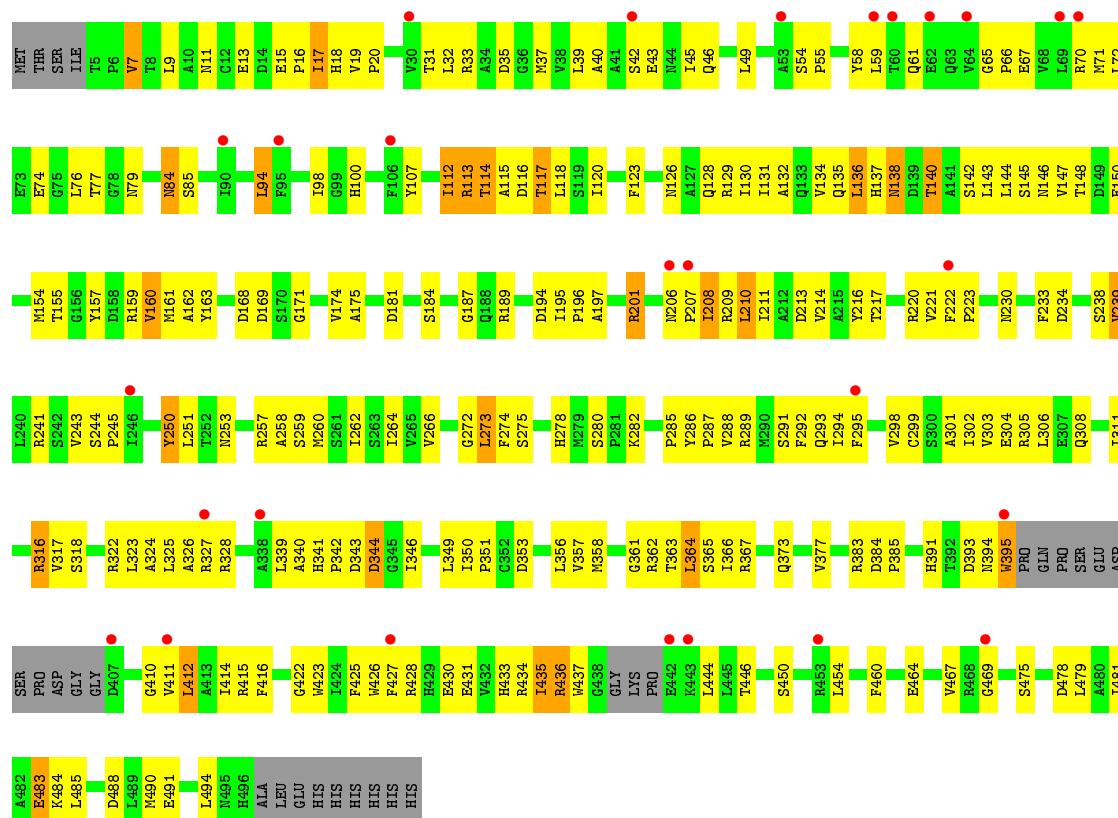


• Molecule 1: Bacteriophytochrome

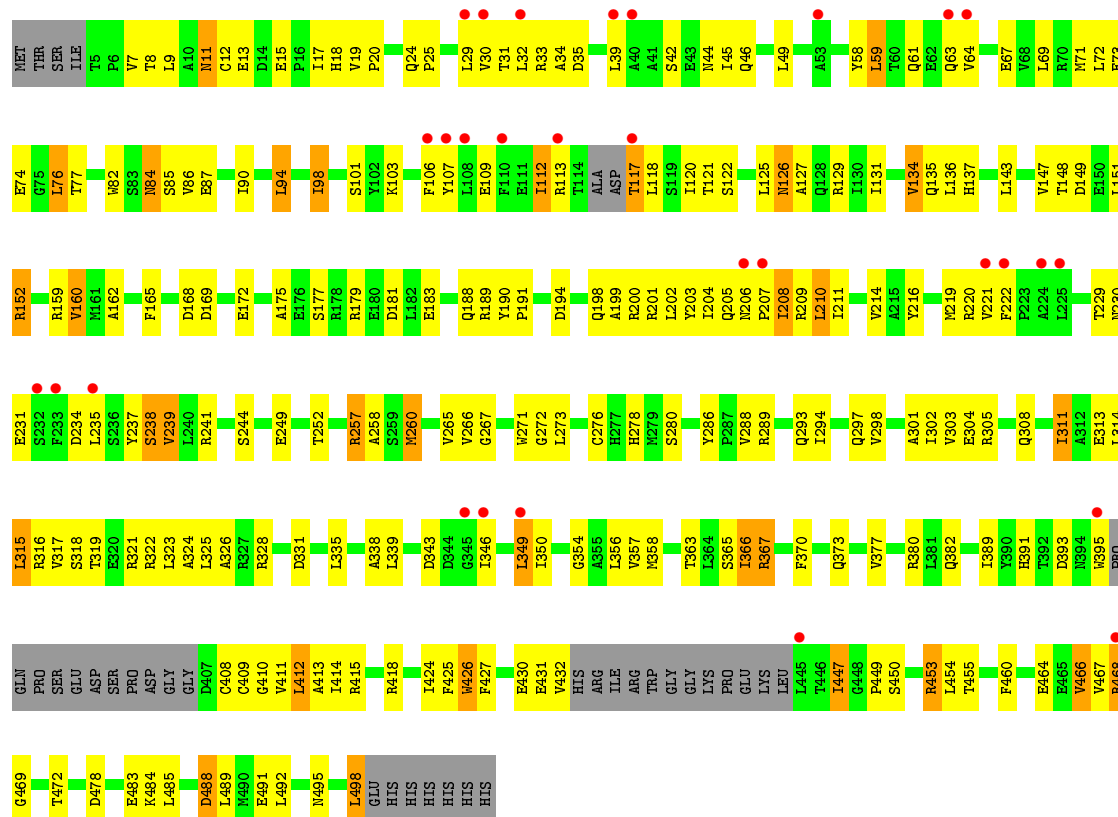


• Molecule 1: Bacteriophytochrome

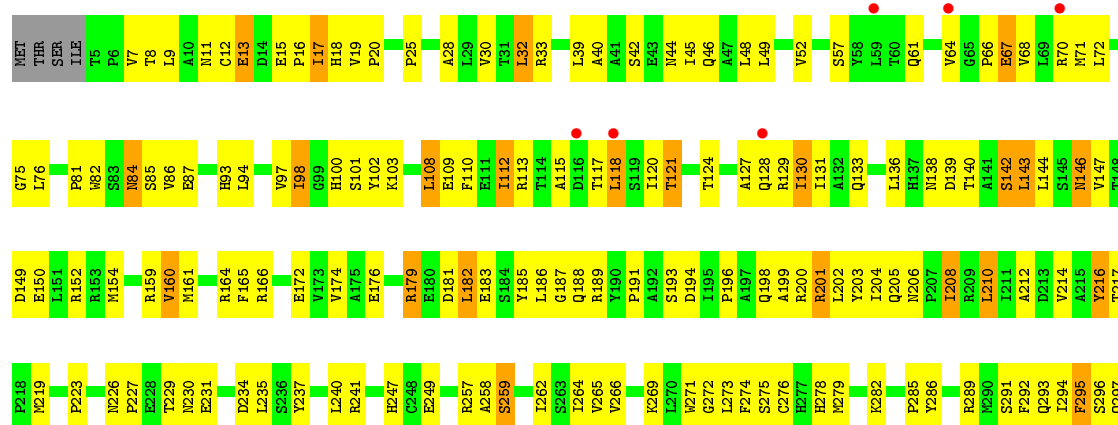
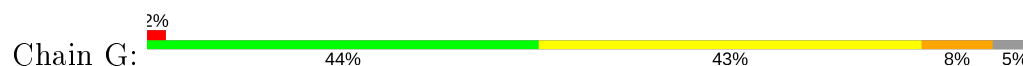


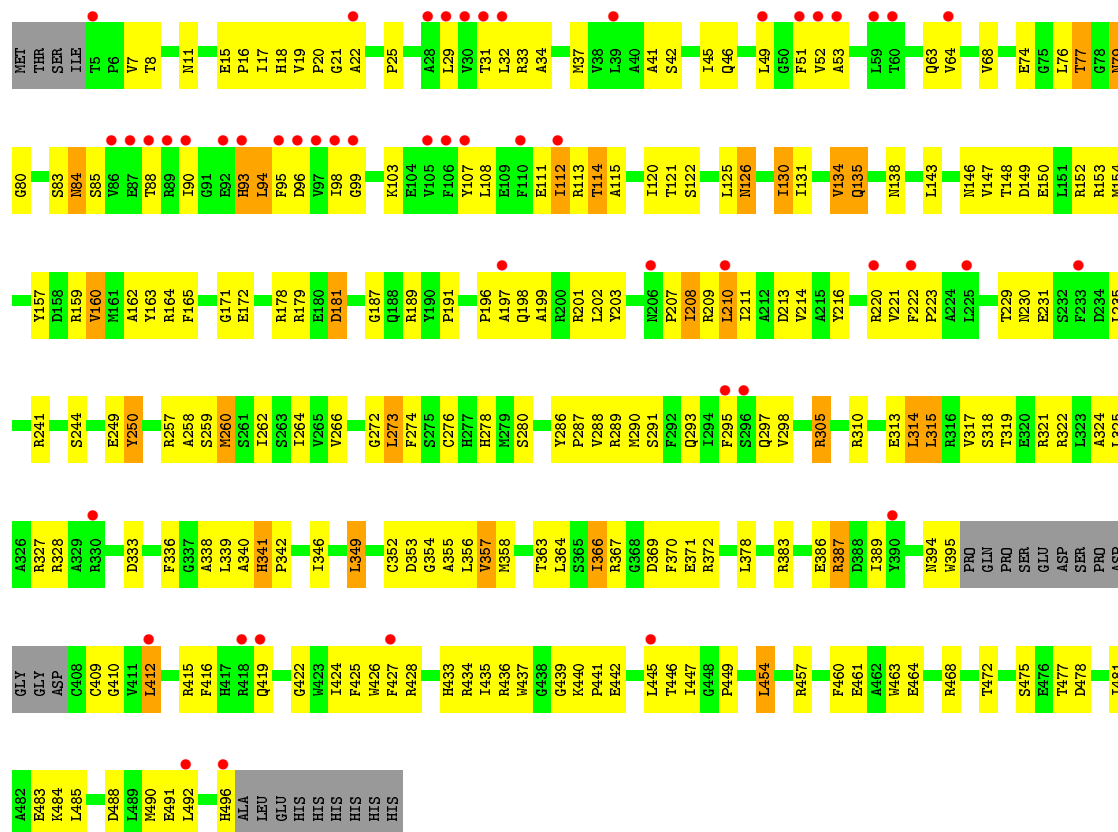


- Molecule 1: Bacteriophytochrome



- Molecule 1: Bacteriophytochrome





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.42Å 164.25Å 434.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90 49.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	72.1 (15.00-2.90) 60.1 (49.96-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.69Å)	Xtriage
Refinement program	PHENIX ?	Depositor
R, $R_{free}$	0.219 , 0.283 0.216 , 0.283	Depositor DCC
$R_{free}$ test set	4546 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 61.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	30494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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: BLA

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	0.31	0/3866	0.59	4/5247 (0.1%)
1	B	0.26	0/3773	0.50	0/5122
1	C	0.33	1/3897 (0.0%)	0.58	2/5289 (0.0%)
1	D	0.26	0/3871	0.49	0/5253
1	E	0.26	0/3806	0.49	0/5163
1	F	0.26	0/3783	0.52	1/5134 (0.0%)
1	G	0.36	2/3904 (0.1%)	0.57	3/5299 (0.1%)
1	H	0.26	0/3885	0.49	0/5273
All	All	0.29	3/30785 (0.0%)	0.53	10/41780 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	G	0	1
All	All	1	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	333	ASP	CB-CG	5.53	1.63	1.51
1	C	442	GLU	CB-CG	5.28	1.62	1.52
1	G	334	ASP	CA-CB	5.21	1.65	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	498	LEU	CB-CG-CD2	-12.96	88.97	111.00
1	A	444	LEU	CB-CA-C	10.35	129.87	110.20
1	G	333	ASP	CB-CG-OD2	7.60	125.14	118.30
1	C	153	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	G	333	ASP	N-CA-C	7.13	130.25	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	444	LEU	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	443	LYS	Peptide
1	A	444	LEU	Mainchain,Peptide
1	G	333	ASP	Peptide

## 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	3782	0	3730	236	1
1	B	3693	0	3626	211	0
1	C	3812	0	3750	209	1
1	D	3788	0	3723	219	0
1	E	3725	0	3662	231	0
1	F	3704	0	3642	215	0
1	G	3816	0	3757	247	0
1	H	3800	0	3743	201	0
2	A	43	0	31	6	0
2	B	43	0	31	6	0
2	C	43	0	30	11	0
2	D	43	0	30	11	0
2	E	43	0	31	8	0
2	F	43	0	31	7	0
2	G	43	0	31	10	0
2	H	43	0	30	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	7	0	0	0	0
3	B	2	0	0	0	0
3	C	6	0	0	0	0
3	D	3	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	G	7	0	0	2	0
3	H	2	0	0	0	0
All	All	30494	0	29878	1694	1

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 28.

The worst 5 of 1694 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)
1:C:153:ARG:CD	1:F:498:LEU:HD21	1.25	1.57
1:C:153:ARG:HD3	1:F:498:LEU:CD2	1.13	1.56
1:C:153:ARG:NH1	1:F:498:LEU:HD11	1.41	1.35
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.04	1.13
1:E:48:LEU:HD11	1:E:93:HIS:HD2	1.16	1.05

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)
1:A:79:ASN:O	1:C:47:ALA:O[7_445]	2.14	0.06

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/505 (94%)	428 (90%)	42 (9%)	4 (1%)	19	51
1	B	462/505 (92%)	434 (94%)	25 (5%)	3 (1%)	25	58
1	C	478/505 (95%)	439 (92%)	37 (8%)	2 (0%)	34	66
1	D	472/505 (94%)	443 (94%)	29 (6%)	0	100	100
1	E	463/505 (92%)	425 (92%)	36 (8%)	2 (0%)	34	66
1	F	461/505 (91%)	433 (94%)	28 (6%)	0	100	100
1	G	479/505 (95%)	443 (92%)	33 (7%)	3 (1%)	25	58
1	H	476/505 (94%)	427 (90%)	47 (10%)	2 (0%)	34	66
All	All	3765/4040 (93%)	3472 (92%)	277 (7%)	16 (0%)	34	66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	333	ASP
1	C	442	GLU
1	A	289	ARG
1	E	333	ASP
1	H	196	PRO

### 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	407/431 (94%)	366 (90%)	41 (10%)	7	23
1	B	398/431 (92%)	351 (88%)	47 (12%)	5	16
1	C	410/431 (95%)	353 (86%)	57 (14%)	3	10
1	D	408/431 (95%)	367 (90%)	41 (10%)	7	23
1	E	400/431 (93%)	357 (89%)	43 (11%)	6	20
1	F	400/431 (93%)	351 (88%)	49 (12%)	4	14
1	G	411/431 (95%)	353 (86%)	58 (14%)	3	10
1	H	409/431 (95%)	367 (90%)	42 (10%)	7	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3243/3448 (94%)	2865 (88%)	378 (12%)	5 16

5 of 378 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	273	LEU
1	E	311	ILE
1	H	160	VAL
1	D	384	ASP
1	E	84	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	205	GLN
1	E	394	ASN
1	H	137	HIS
1	D	293	GLN
1	E	128	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	$\# Z  > 2$
2	BLA	D	900	1	36,46,46	3.19	17 (47%)	47,67,67	2.18	12 (25%)
2	BLA	G	900	1	36,46,46	3.10	15 (41%)	47,67,67	2.12	13 (27%)
2	BLA	A	900	1	36,46,46	3.11	16 (44%)	47,67,67	2.14	12 (25%)
2	BLA	C	900	1	36,46,46	3.38	18 (50%)	47,67,67	2.32	13 (27%)
2	BLA	H	900	1	36,46,46	3.00	17 (47%)	47,67,67	2.15	12 (25%)
2	BLA	F	900	1	36,46,46	3.06	16 (44%)	47,67,67	2.10	11 (23%)
2	BLA	B	900	1	36,46,46	3.26	19 (52%)	47,67,67	2.08	13 (27%)
2	BLA	E	900	1	36,46,46	3.38	19 (52%)	47,67,67	2.07	12 (25%)

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	BLA	D	900	1	-	6/22/74/74	0/4/4/4
2	BLA	G	900	1	-	6/22/74/74	0/4/4/4
2	BLA	A	900	1	-	4/22/74/74	0/4/4/4
2	BLA	C	900	1	-	6/22/74/74	0/4/4/4
2	BLA	H	900	1	-	5/22/74/74	0/4/4/4
2	BLA	F	900	1	-	5/22/74/74	0/4/4/4
2	BLA	B	900	1	-	4/22/74/74	0/4/4/4
2	BLA	E	900	1	-	7/22/74/74	0/4/4/4

The worst 5 of 137 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	900	BLA	CHB-C1B	9.75	1.54	1.34
2	G	900	BLA	CHB-C1B	9.69	1.54	1.34
2	D	900	BLA	CHB-C1B	9.61	1.54	1.34
2	E	900	BLA	CHB-C1B	9.54	1.54	1.34
2	B	900	BLA	CHB-C1B	9.52	1.54	1.34

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	BLA	C1A-CHA-C4D	-9.79	117.12	128.81
2	G	900	BLA	C1A-CHA-C4D	-9.02	118.04	128.81
2	D	900	BLA	C1A-CHA-C4D	-8.90	118.17	128.81
2	A	900	BLA	C1A-CHA-C4D	-8.79	118.31	128.81
2	E	900	BLA	C1A-CHA-C4D	-8.56	118.58	128.81

There are no chirality outliers.

5 of 43 torsion outliers are listed below:

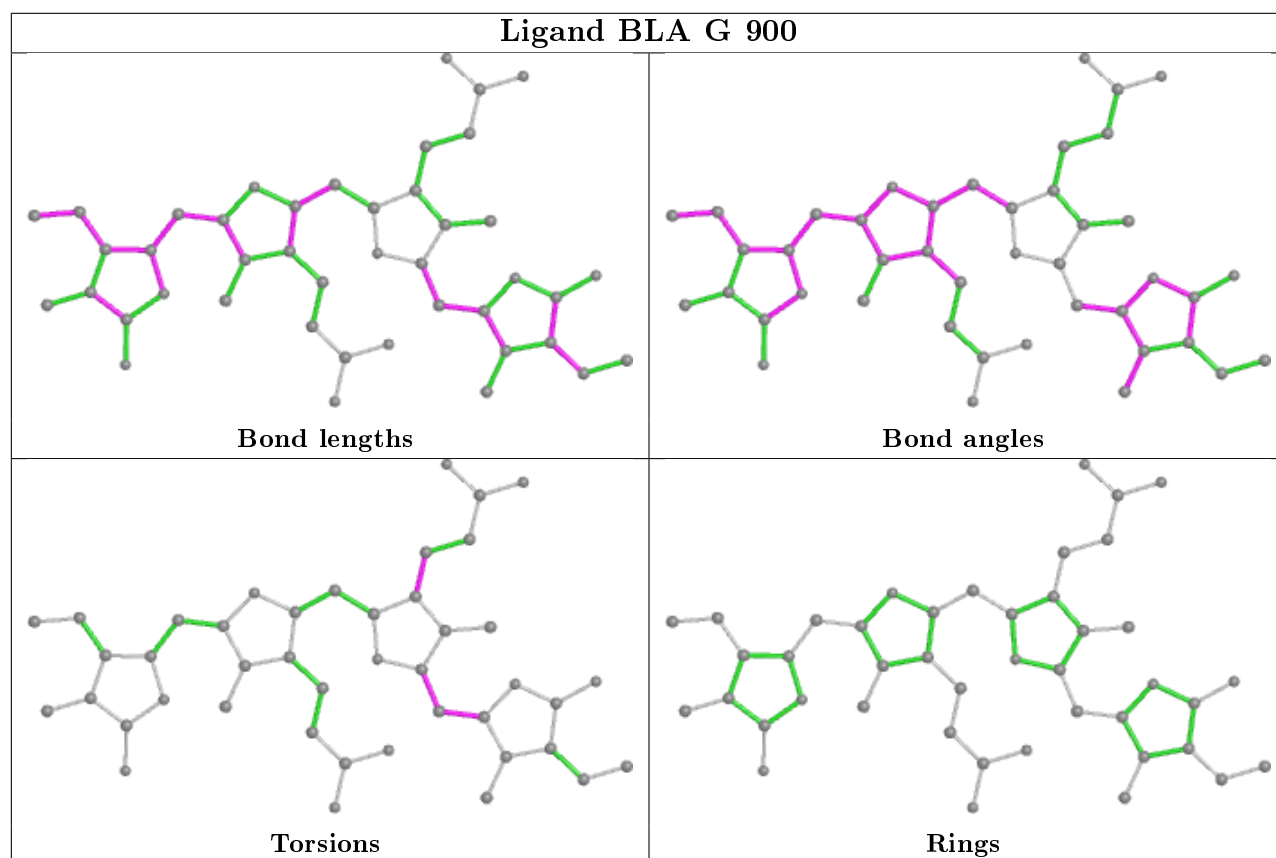
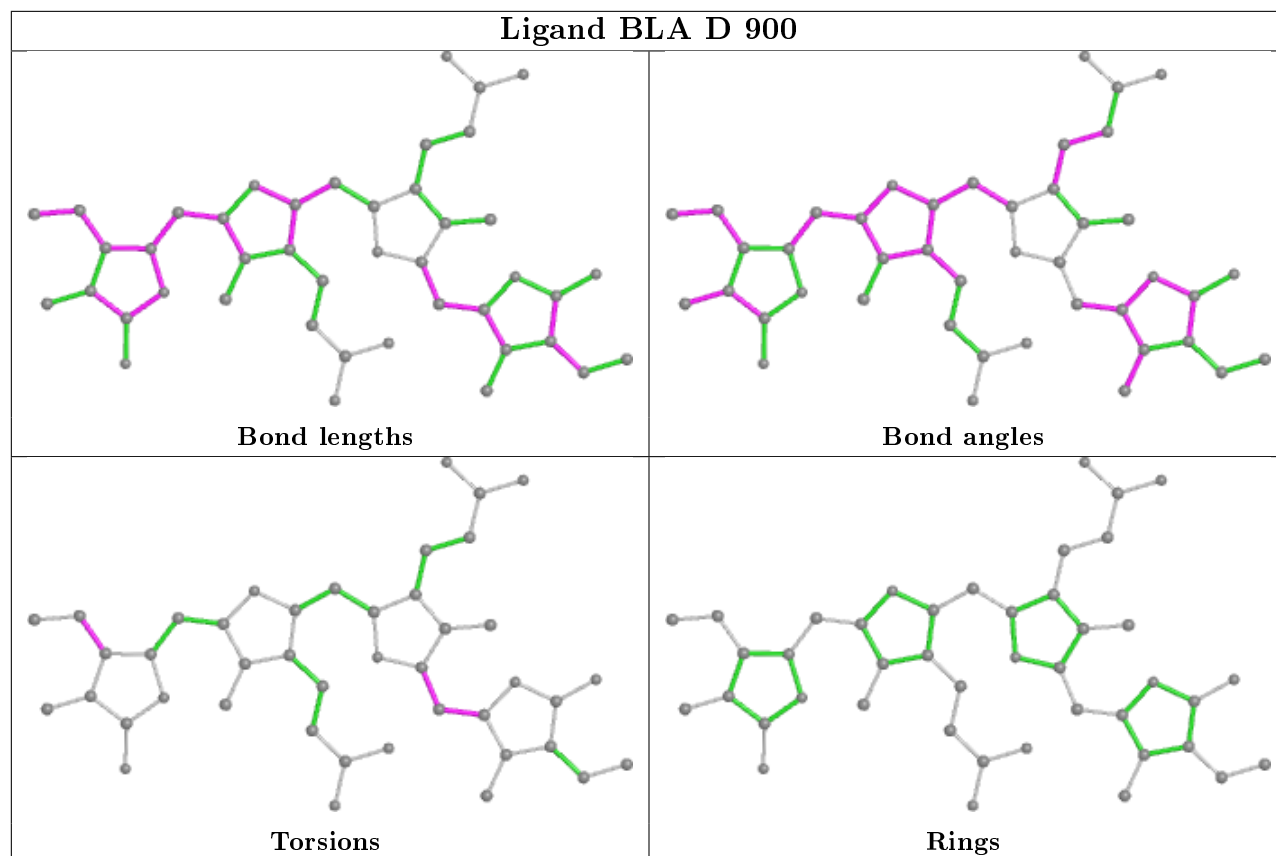
Mol	Chain	Res	Type	Atoms
2	D	900	BLA	NA-C4A-CHB-C1B
2	D	900	BLA	C3A-C4A-CHB-C1B
2	D	900	BLA	NB-C1B-CHB-C4A
2	D	900	BLA	C2B-C1B-CHB-C4A
2	G	900	BLA	C1A-C2A-CAA-CBA

There are no ring outliers.

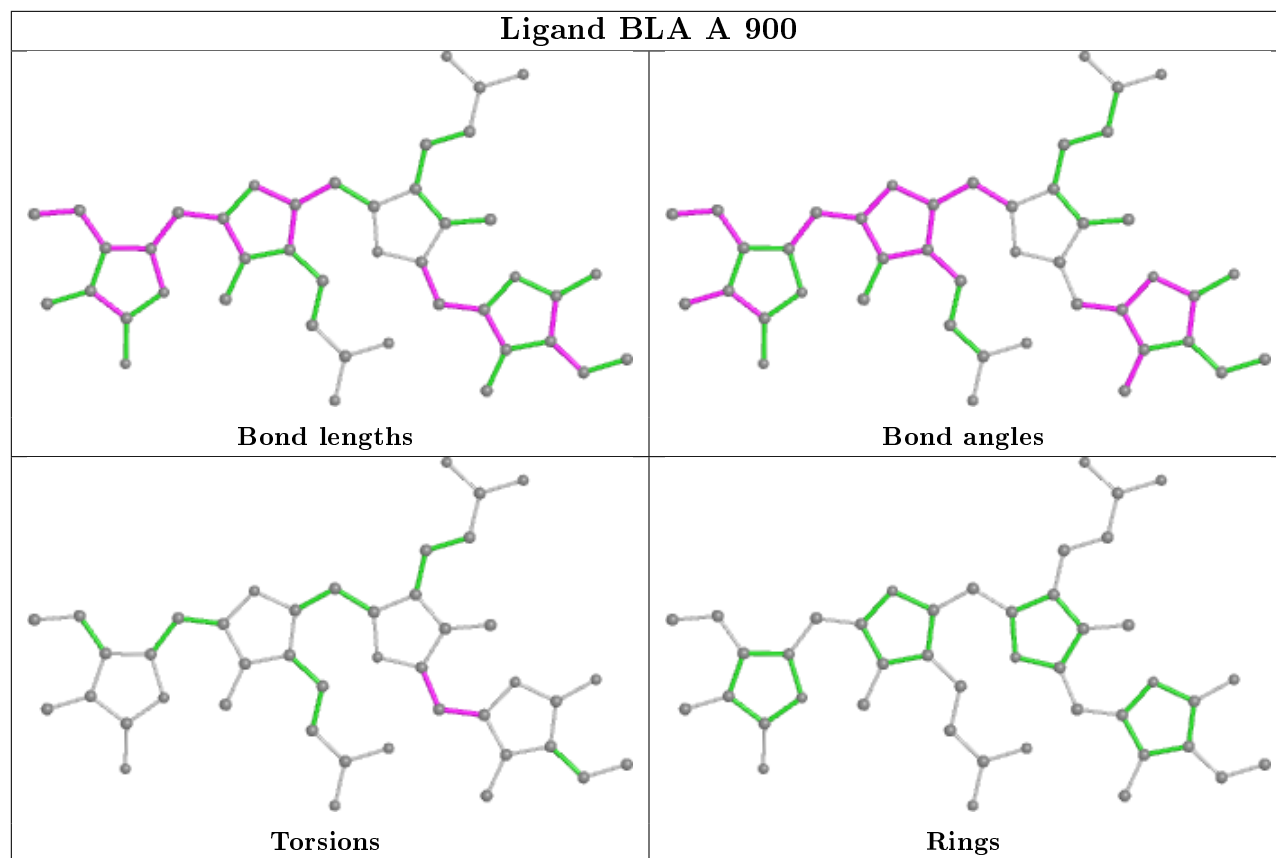
8 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	BLA	11	0
2	G	900	BLA	10	0
2	A	900	BLA	6	0
2	C	900	BLA	11	0
2	H	900	BLA	10	0
2	F	900	BLA	7	0
2	B	900	BLA	6	0
2	E	900	BLA	8	0

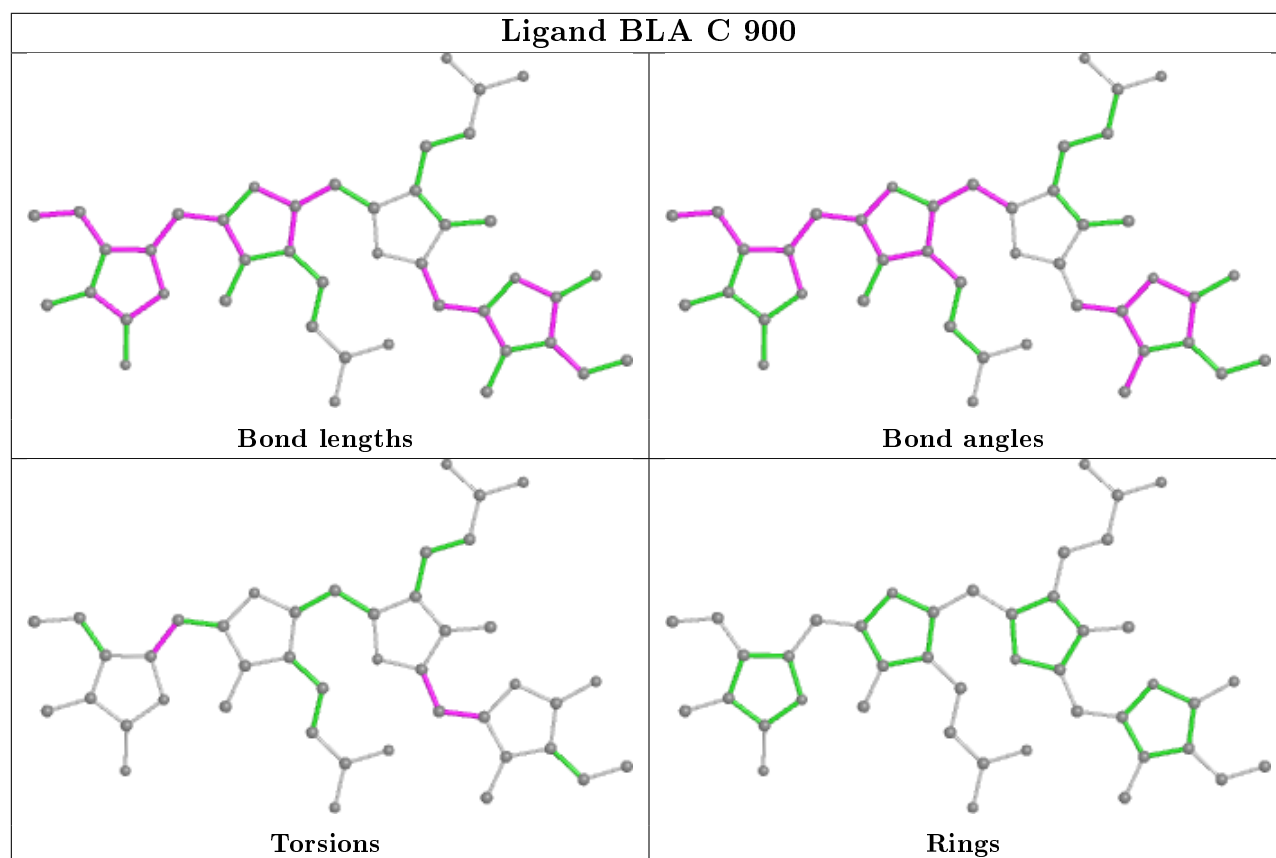
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



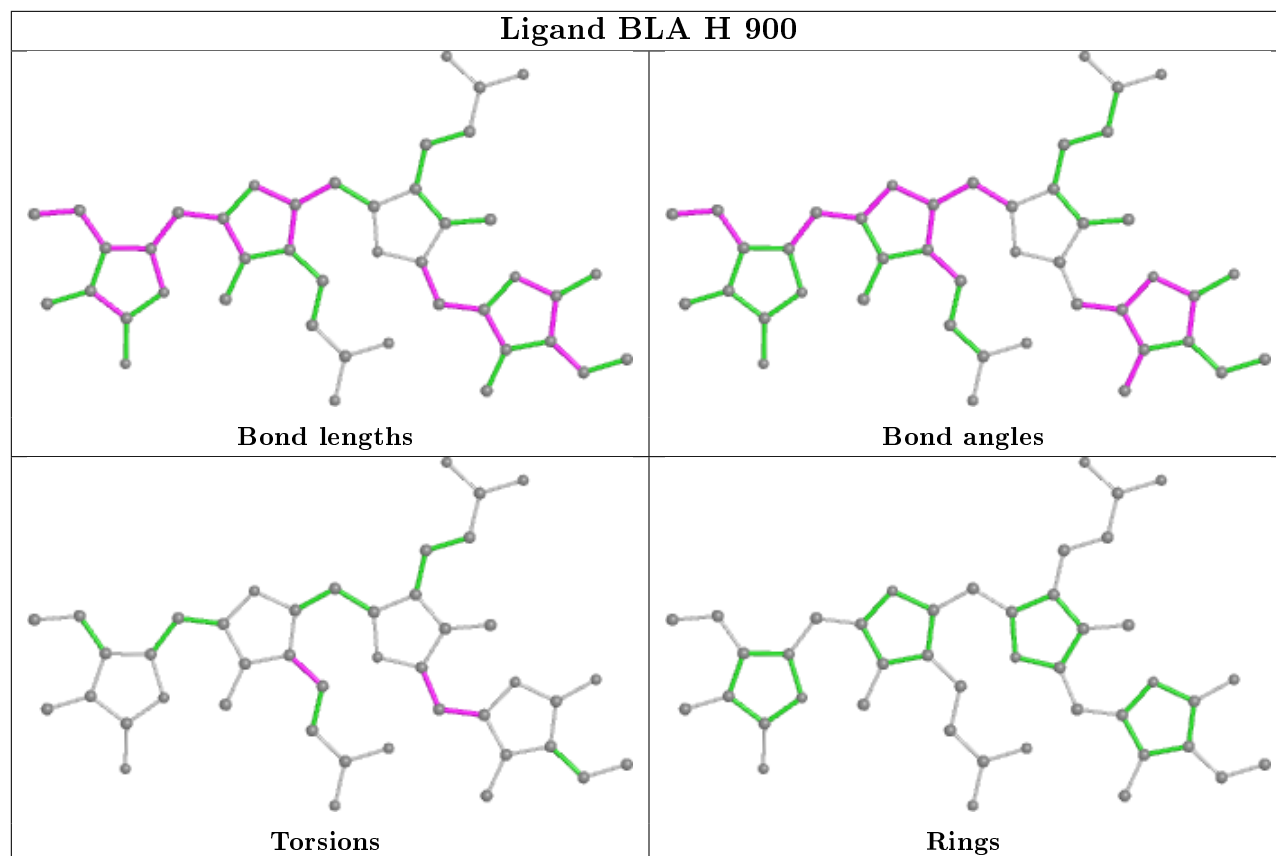
## Ligand BLA A 900



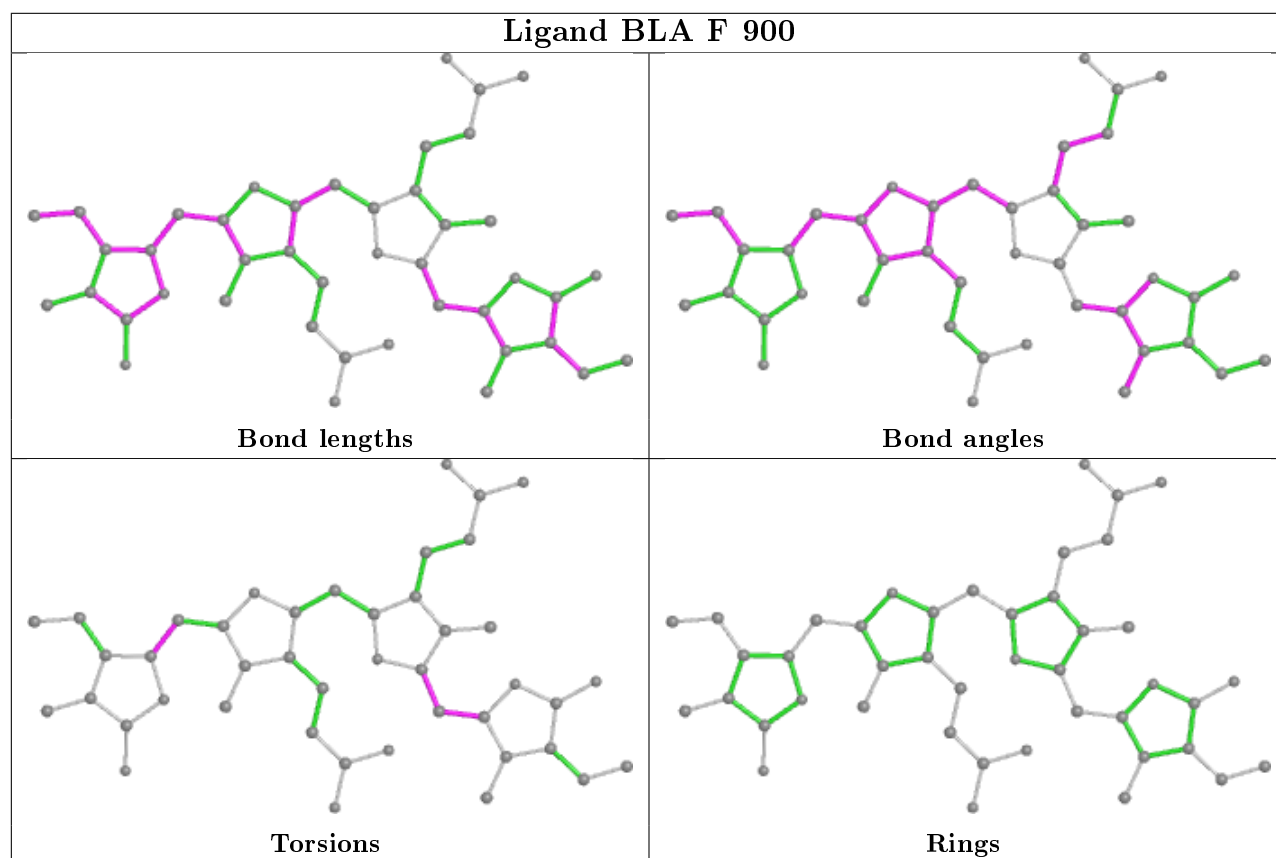
## Ligand BLA C 900



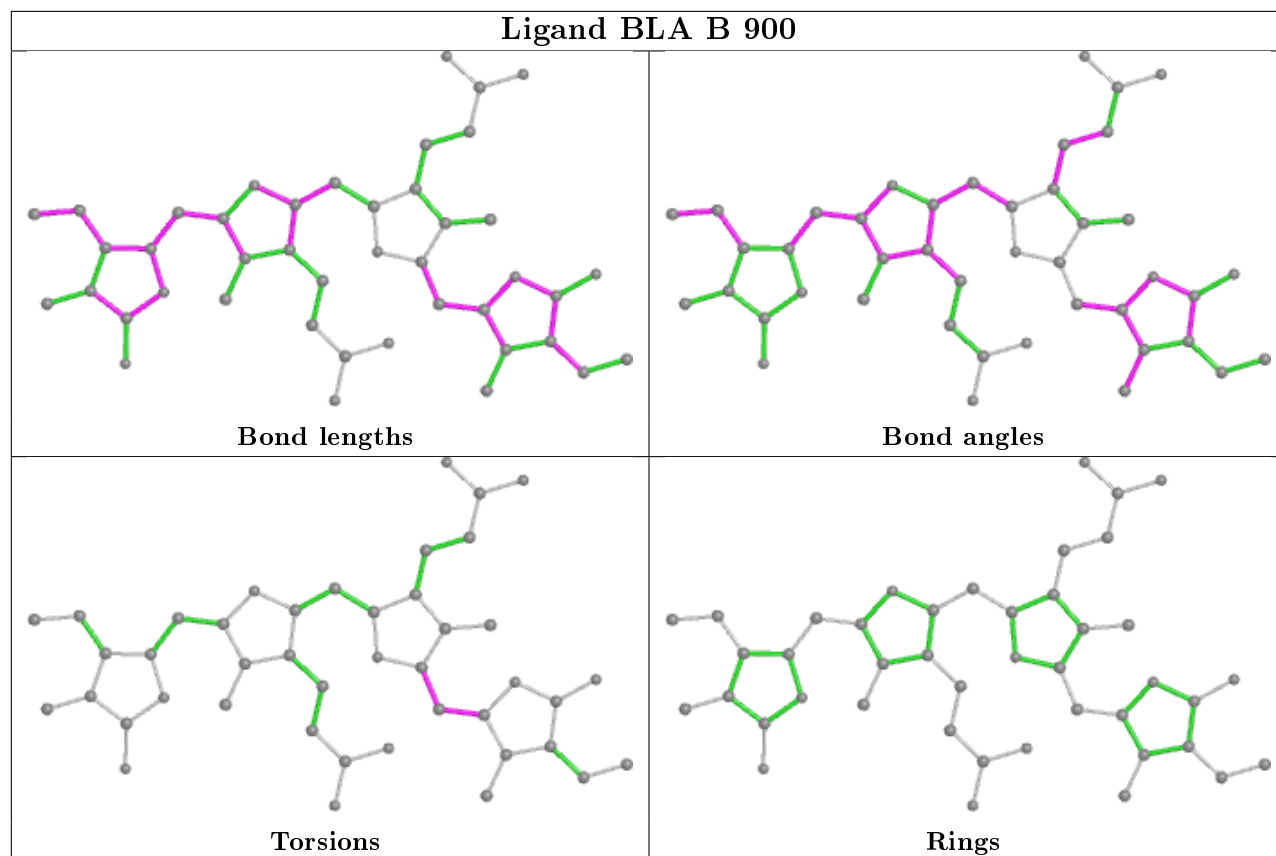
## Ligand BLA H 900



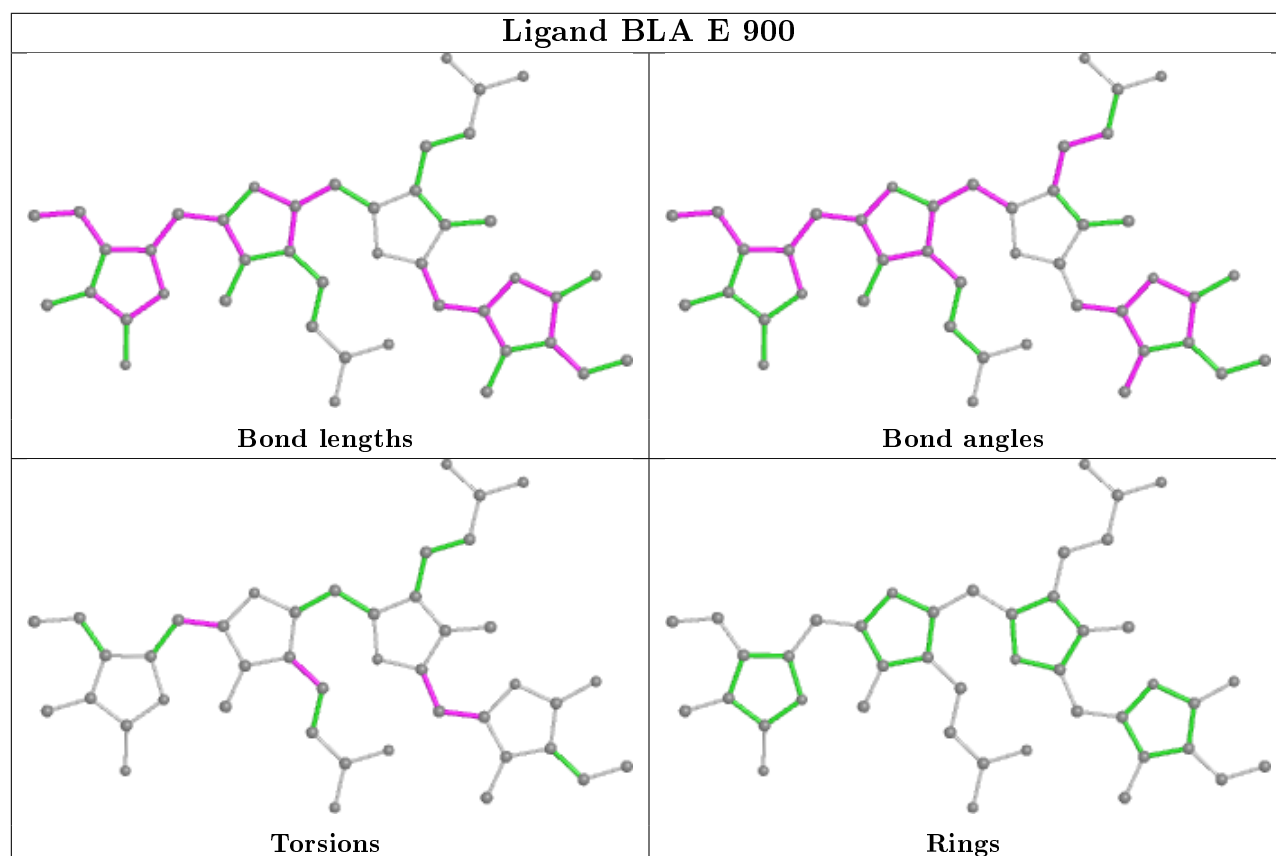
## Ligand BLA F 900



## Ligand BLA B 900



## Ligand BLA E 900





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	A	478/505 (94%)	-0.09	6 (1%) 77 77	67, 98, 155, 233	0
1	B	468/505 (92%)	0.33	31 (6%) 18 14	74, 129, 188, 243	0
1	C	482/505 (95%)	-0.10	5 (1%) 82 82	66, 99, 148, 206	0
1	D	478/505 (94%)	0.26	27 (5%) 24 20	83, 139, 194, 239	0
1	E	471/505 (93%)	0.27	31 (6%) 18 14	87, 139, 186, 225	0
1	F	469/505 (92%)	0.24	29 (6%) 20 16	80, 124, 203, 282	0
1	G	482/505 (95%)	-0.10	8 (1%) 70 69	66, 103, 152, 217	0
1	H	480/505 (95%)	0.50	50 (10%) 6 5	84, 139, 214, 274	0
All	All	3808/4040 (94%)	0.16	187 (4%) 29 26	66, 122, 191, 282	0

The worst 5 of 187 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	ALA	7.5
1	H	59	LEU	6.6
1	H	5	THR	5.8
1	F	222	PHE	5.2
1	H	29	LEU	5.2

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

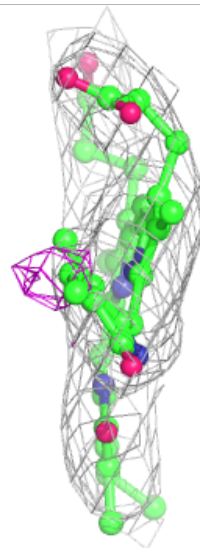
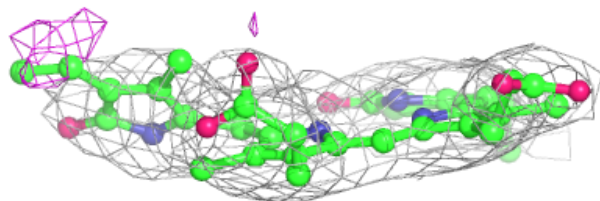
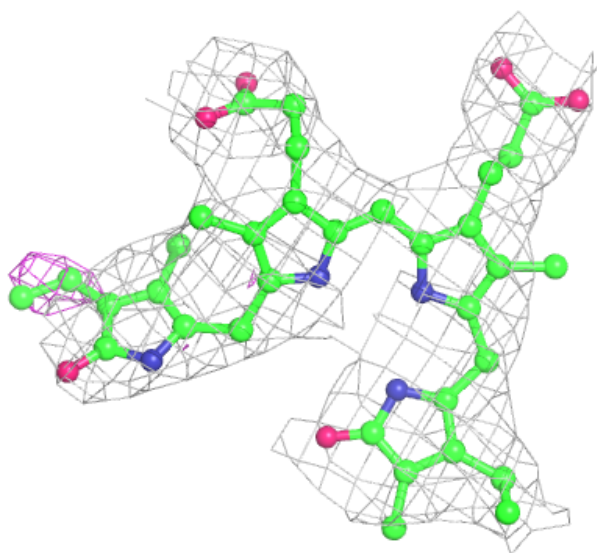
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	BLA	D	900	43/43	0.88	0.25	99,123,140,148	0
2	BLA	B	900	43/43	0.90	0.22	105,121,135,145	0
2	BLA	E	900	43/43	0.90	0.46	100,144,164,174	0
2	BLA	H	900	43/43	0.91	0.22	79,121,140,148	0
2	BLA	C	900	43/43	0.94	0.21	64,88,102,108	0
2	BLA	G	900	43/43	0.94	0.24	67,93,104,128	0
2	BLA	F	900	43/43	0.95	0.24	74,102,118,132	0
2	BLA	A	900	43/43	0.96	0.22	60,83,113,119	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.

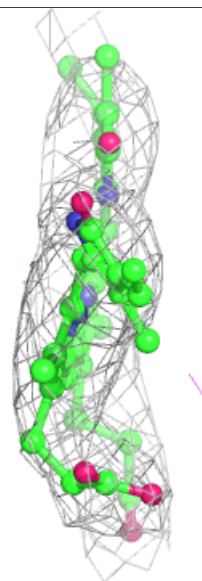
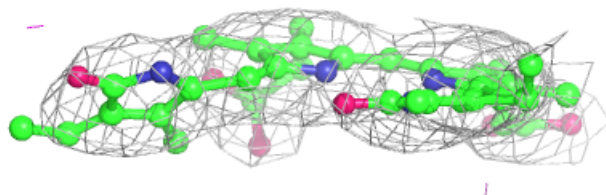
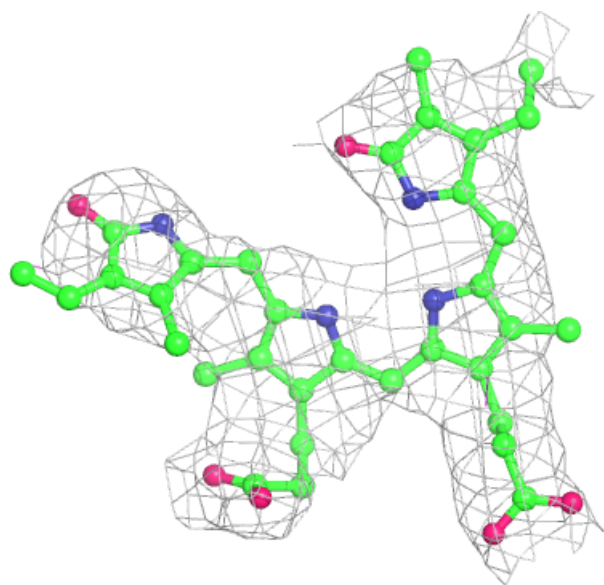
**Electron density around BLA D 900:**

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



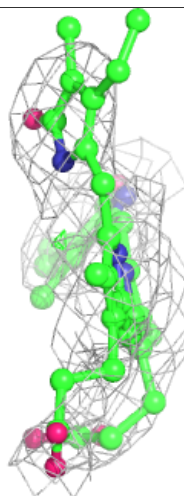
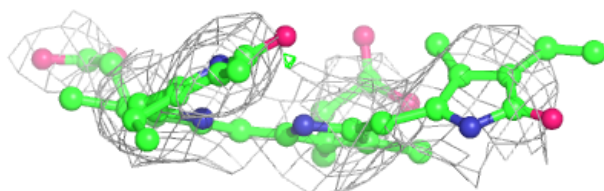
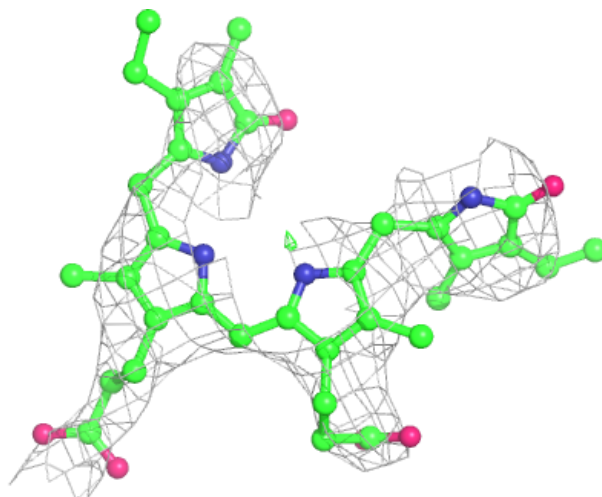
**Electron density around BLA B 900:**

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



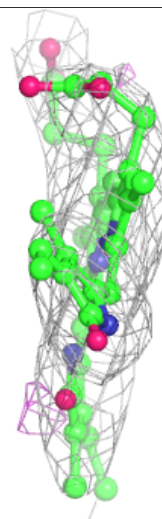
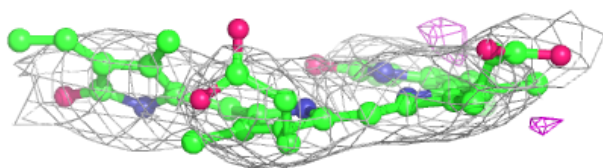
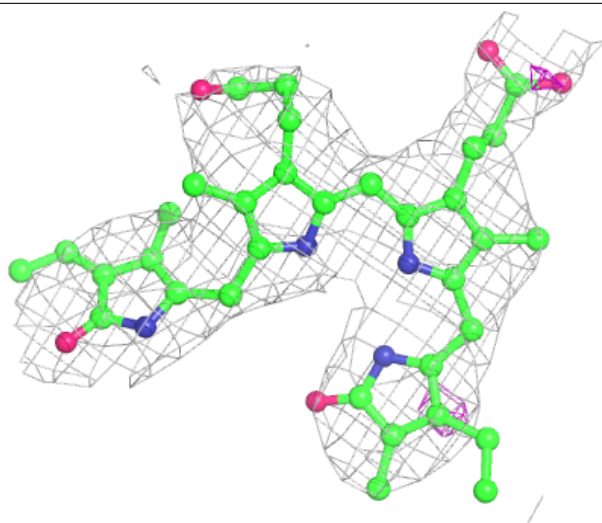
**Electron density around BLA E 900:**

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



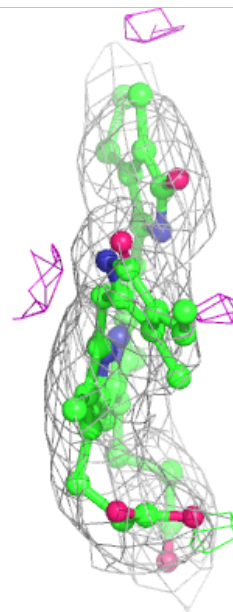
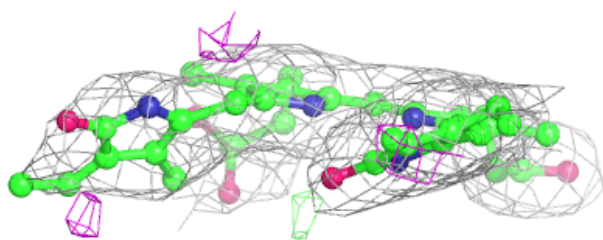
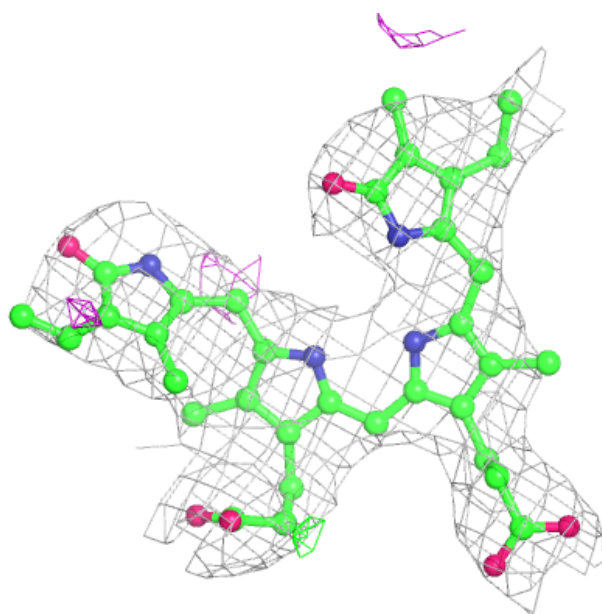
**Electron density around BLA H 900:**

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



**Electron density around BLA C 900:**

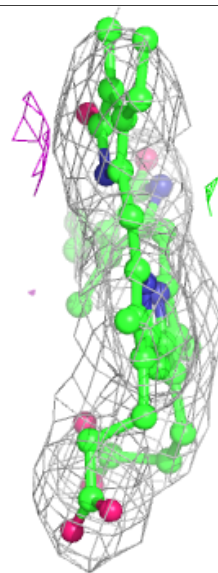
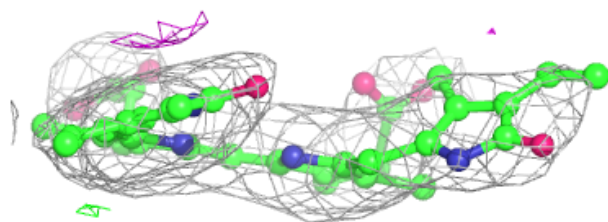
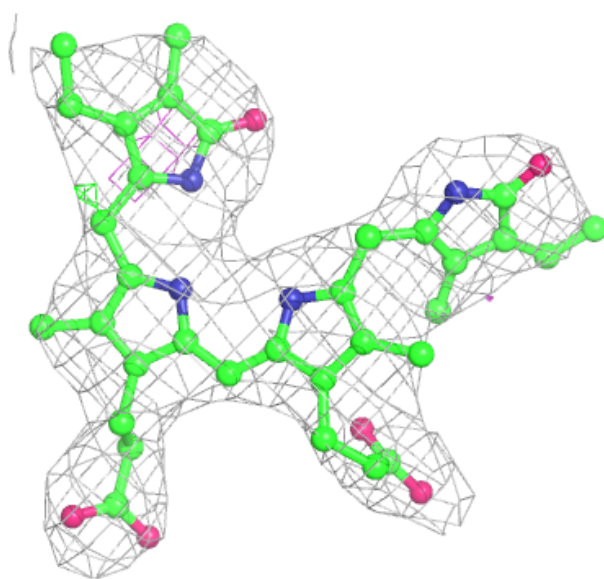
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





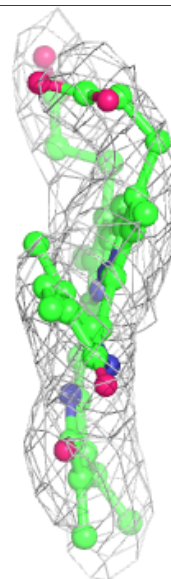
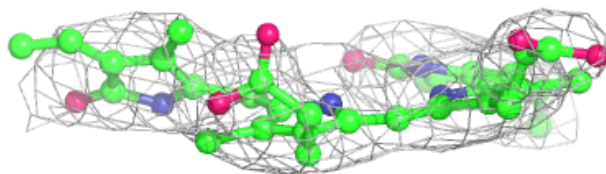
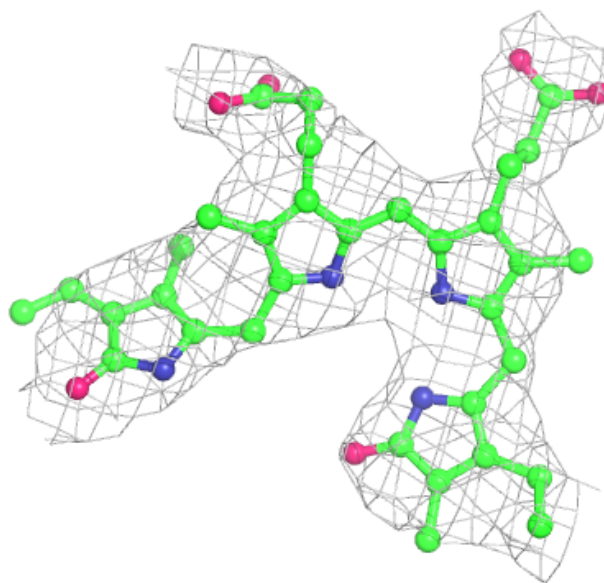
**Electron density around BLA G 900:**

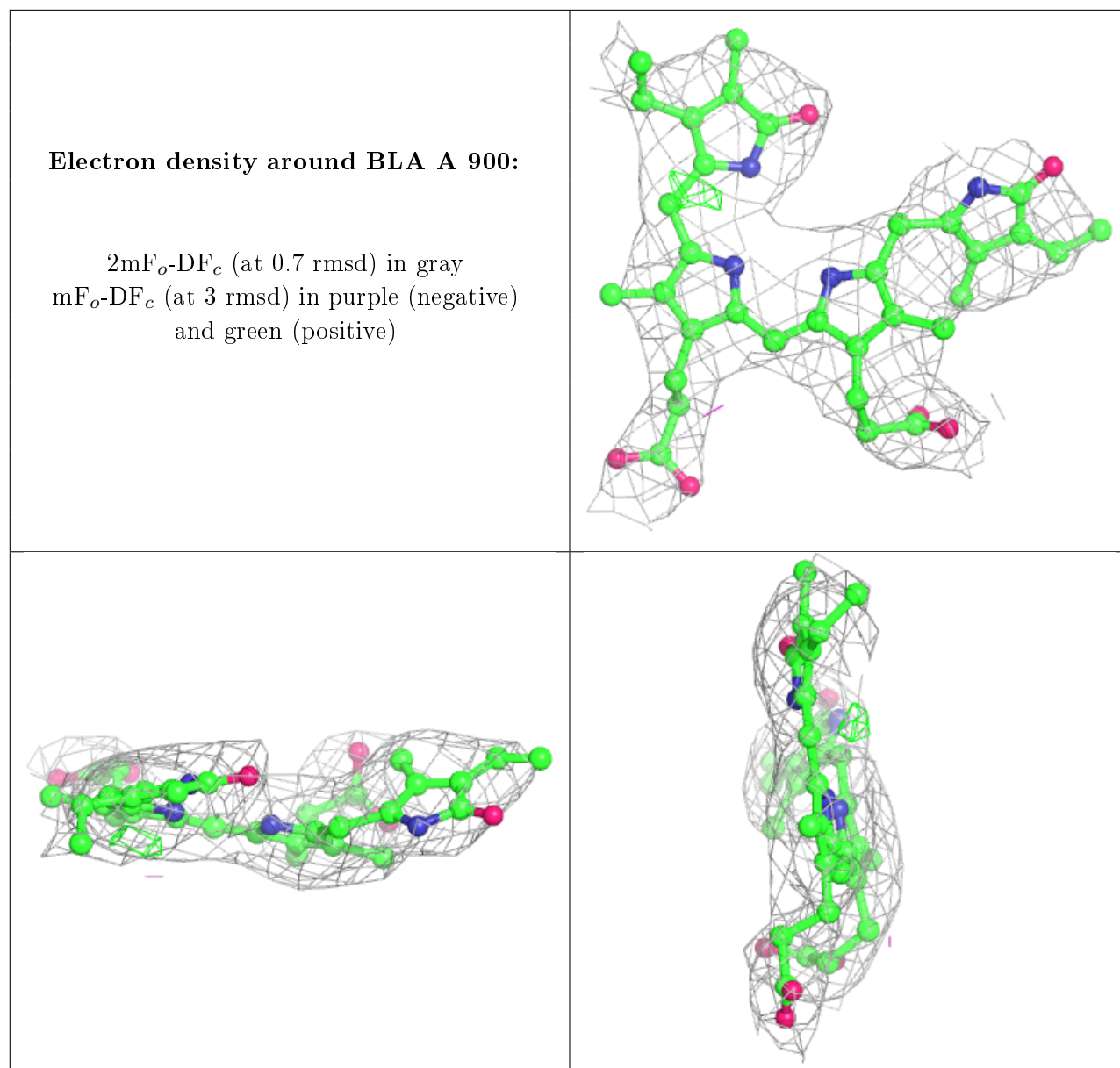
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BLA F 900:**

$2mF_o-DF_c$  (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.