



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 08:24 PM EDT

PDB ID : 3NHQ
Title : The dark Pfr structure of the photosensory core module of *P. aeruginosa* Bacteriophytochrome
Authors : Yang, X.; Ren, Z.; Kuk, J.; Moffat, K.
Deposited on : 2010-06-14
Resolution : 2.55 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 ⓘ 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 ⓘ](#)) 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 : 2.35
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) : 2.35

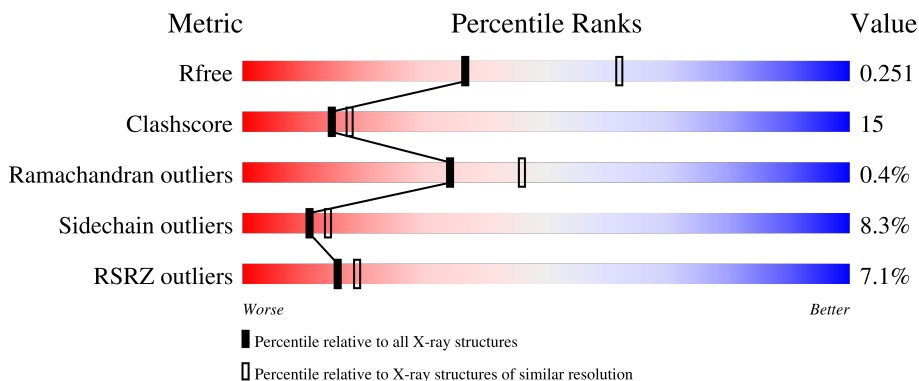
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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.



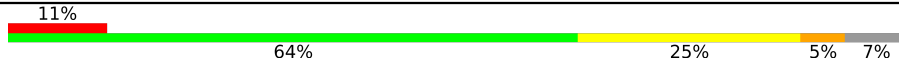

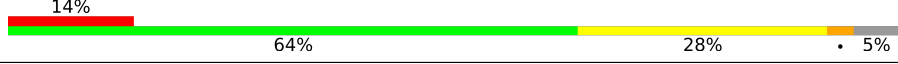
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 $\leq 5\%$. 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	
1	B	505	
1	C	505	
1	D	505	
1	E	505	

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Mol	Chain	Length	Quality of chain
1	F	505	 11% 64% 25% 5% 7%
1	G	505	 % 65% 26% 5%
1	H	505	 14% 64% 28% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 30788 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
			Total	C	N	O	S			
1	A	479	3790	2386	682	703	19	0	0	0
1	B	470	3709	2332	665	693	19	0	0	0
1	C	482	3812	2398	688	707	19	0	0	0
1	D	480	3801	2391	686	705	19	0	0	0
1	E	479	3790	2386	683	702	19	0	0	0
1	F	471	3717	2338	666	694	19	0	0	0
1	G	482	3816	2401	688	708	19	0	1	0
1	H	481	3808	2396	687	706	19	0	0	0

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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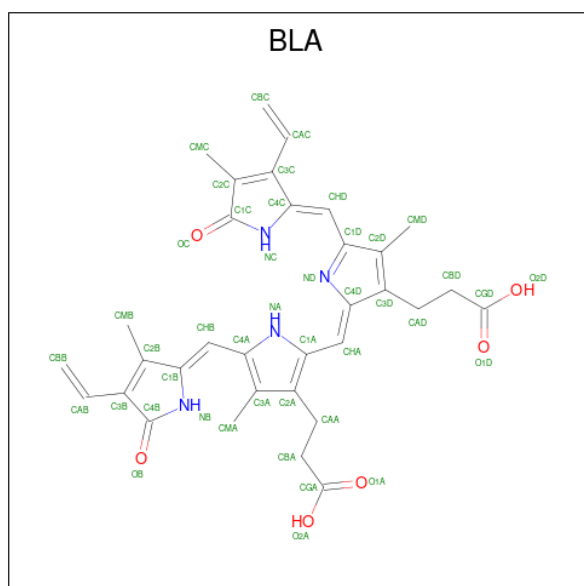
Chain	Residue	Modelled	Actual	Comment	Reference
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3
C	498	LEU	-	expression tag	UNP Q9HWR3
C	499	GLU	-	expression tag	UNP Q9HWR3
C	500	HIS	-	expression tag	UNP Q9HWR3
C	501	HIS	-	expression tag	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: C₃₃H₃₄N₄O₆).



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		

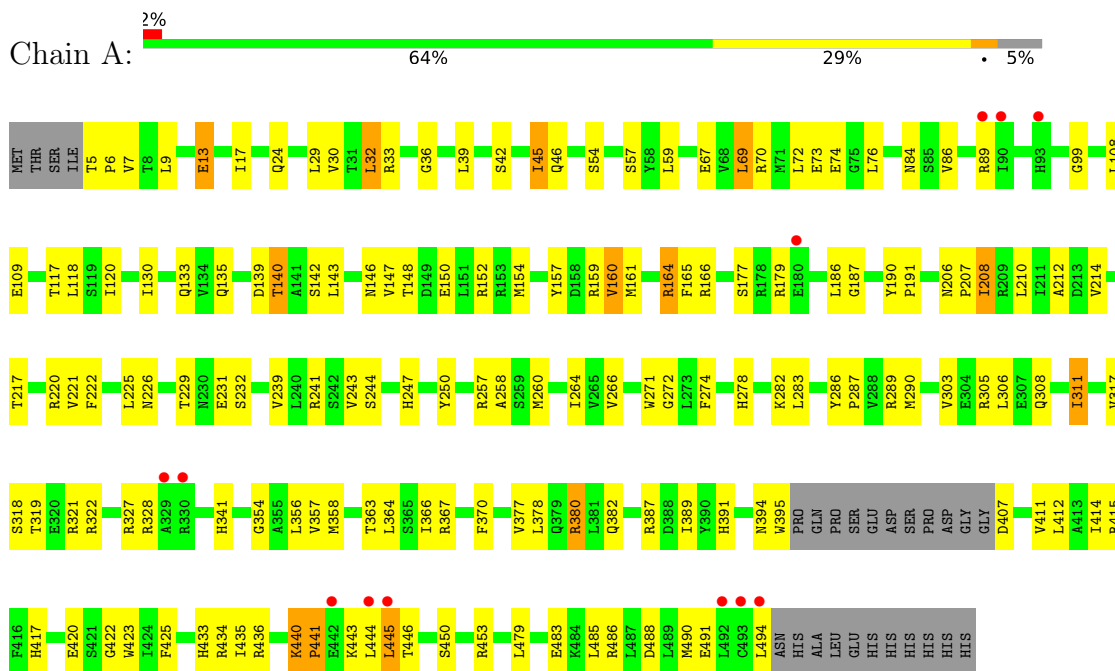
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	61	Total	O	0	0
			61	61		
3	B	16	Total	O	0	0
			16	16		
3	C	44	Total	O	0	0
			44	44		
3	D	14	Total	O	0	0
			14	14		
3	E	15	Total	O	0	0
			15	15		
3	F	7	Total	O	0	0
			7	7		
3	G	37	Total	O	0	0
			37	37		
3	H	7	Total	O	0	0
			7	7		

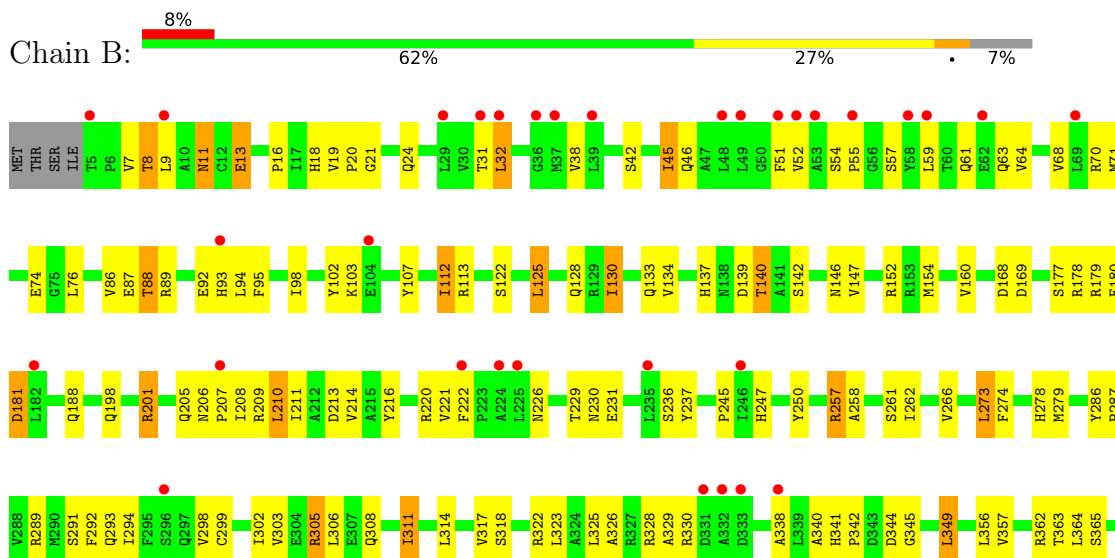
3 Residue-property plots [i](#)

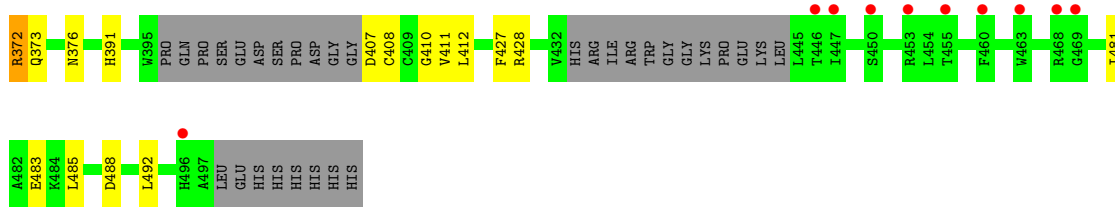
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bacteriophytochrome

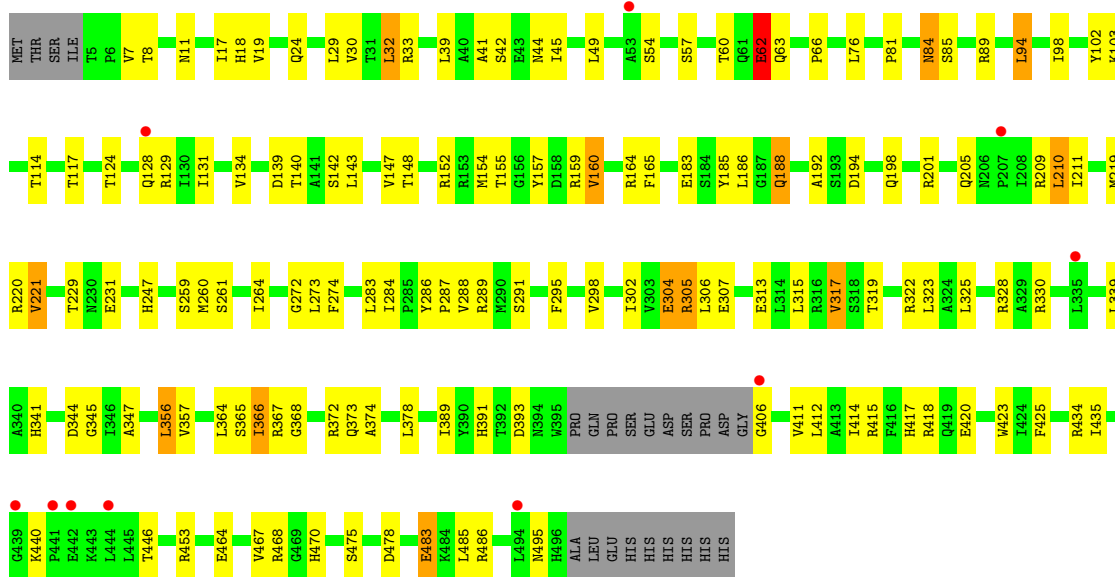


- Molecule 1: Bacteriophytochrome

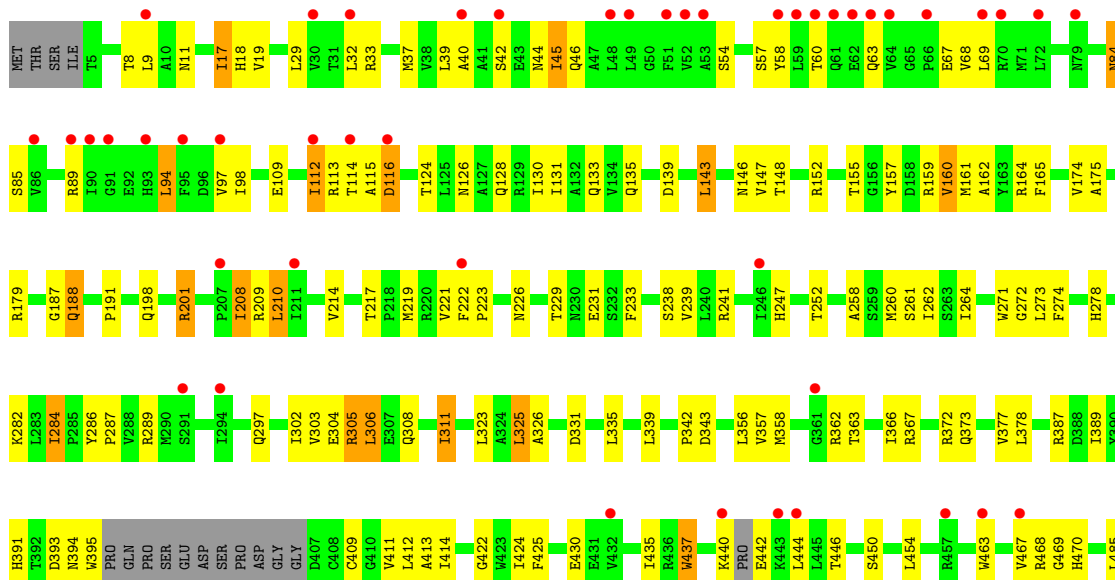


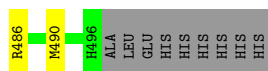


• Molecule 1: Bacteriophytochrome

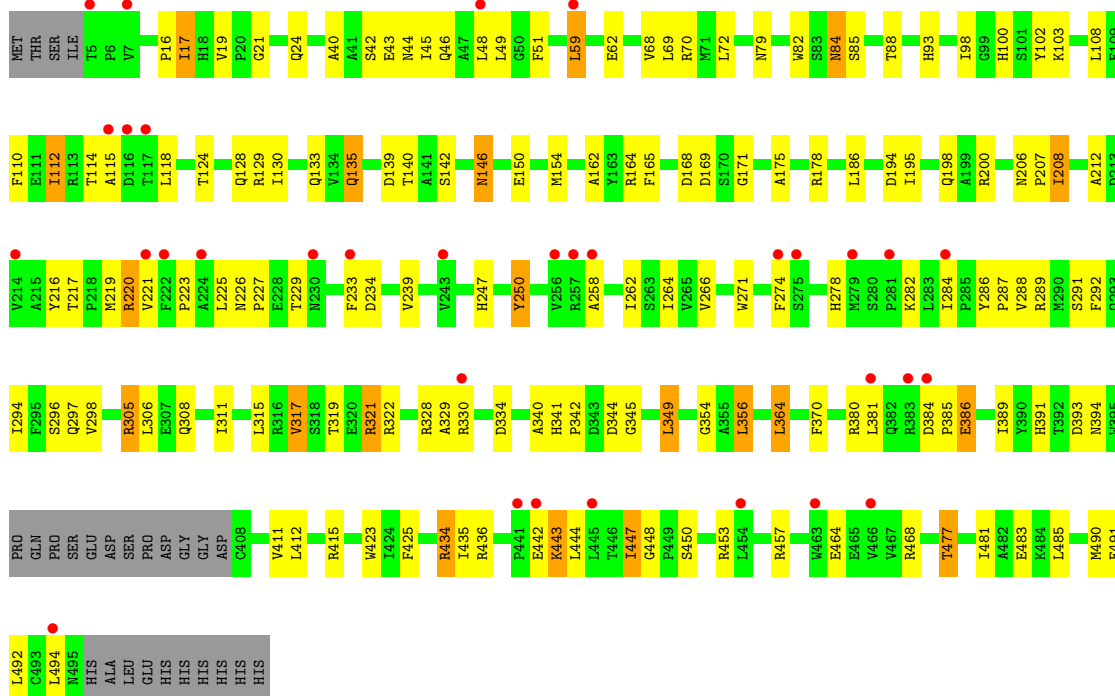


• Molecule 1: Bacteriophytochrome

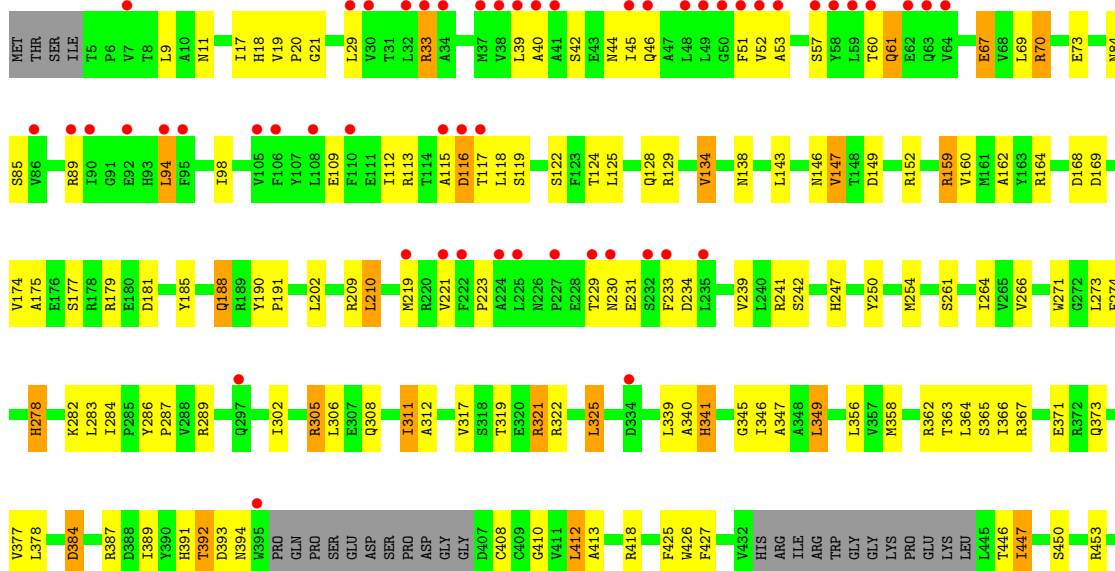




• Molecule 1: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 162.98Å 436.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.48 – 2.55 49.49 – 2.53	Depositor EDS
% Data completeness (in resolution range)	82.9 (48.48-2.55) 81.3 (49.49-2.53)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.215 , 0.258 0.209 , 0.251	Depositor DCC
R_{free} test set	7437 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtrriage
Anisotropy	0.538	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30788	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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	0.26	0/3874	0.48	0/5258
1	B	0.24	0/3789	0.45	0/5144
1	C	0.25	0/3897	0.46	0/5289
1	D	0.24	0/3884	0.45	0/5269
1	E	0.23	0/3874	0.45	0/5258
1	F	0.23	0/3797	0.45	0/5155
1	G	0.25	0/3904	0.47	0/5299
1	H	0.24	0/3893	0.44	0/5284
All	All	0.24	0/30912	0.46	0/41956

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	0	2
1	B	0	1
1	C	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	407	ASP	Peptide
1	A	441	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	92	GLU	Peptide
1	C	62	GLU	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	3790	0	3734	104	0
1	B	3709	0	3641	119	0
1	C	3812	0	3750	108	0
1	D	3801	0	3739	122	0
1	E	3790	0	3736	124	0
1	F	3717	0	3652	125	0
1	G	3816	0	3757	116	0
1	H	3808	0	3747	115	0
2	A	43	0	30	4	0
2	B	43	0	31	8	0
2	C	43	0	31	14	0
2	D	43	0	31	5	0
2	E	43	0	30	7	0
2	F	43	0	31	9	0
2	G	43	0	30	5	0
2	H	43	0	31	6	0
3	A	61	0	0	4	0
3	B	16	0	0	1	0
3	C	44	0	0	4	0
3	D	14	0	0	6	0
3	E	15	0	0	4	0
3	F	7	0	0	1	0
3	G	37	0	0	0	0
3	H	7	0	0	0	0
All	All	30788	0	30001	925	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 15.

The worst 5 of 925 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:F:70:ARG:HG3	1:F:70:ARG:HH11	1.00	1.10
1:H:444:LEU:HD23	1:H:444:LEU:H	1.26	0.96
1:F:70:ARG:HG3	1:F:70:ARG:NH1	1.76	0.93
1:G:84:ASN:HD22	1:G:85:SER:H	1.02	0.92
1:D:112:ILE:HD13	1:D:112:ILE:H	1.36	0.91

There are no symmetry-related clashes.

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	475/505 (94%)	442 (93%)	30 (6%)	3 (1%)	25	34
1	B	464/505 (92%)	436 (94%)	28 (6%)	0	100	100
1	C	478/505 (95%)	455 (95%)	20 (4%)	3 (1%)	25	34
1	D	474/505 (94%)	451 (95%)	23 (5%)	0	100	100
1	E	475/505 (94%)	452 (95%)	22 (5%)	1 (0%)	47	60
1	F	465/505 (92%)	436 (94%)	27 (6%)	2 (0%)	34	46
1	G	479/505 (95%)	460 (96%)	18 (4%)	1 (0%)	47	60
1	H	477/505 (94%)	444 (93%)	28 (6%)	5 (1%)	15	22
All	All	3787/4040 (94%)	3576 (94%)	196 (5%)	15 (0%)	34	46

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	LEU
1	H	444	LEU
1	H	445	LEU
1	E	443	LYS
1	A	441	PRO

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	Percentiles	
1	A	408/431 (95%)	377 (92%)	31 (8%)	13	17
1	B	400/431 (93%)	365 (91%)	35 (9%)	10	12
1	C	410/431 (95%)	376 (92%)	34 (8%)	11	14
1	D	409/431 (95%)	384 (94%)	25 (6%)	18	24
1	E	408/431 (95%)	369 (90%)	39 (10%)	8	9
1	F	401/431 (93%)	366 (91%)	35 (9%)	10	12
1	G	411/431 (95%)	380 (92%)	31 (8%)	13	17
1	H	410/431 (95%)	370 (90%)	40 (10%)	8	9
All	All	3257/3448 (94%)	2987 (92%)	270 (8%)	11	14

5 of 270 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	63	GLN
1	H	134	VAL
1	H	431	GLU
1	C	412	LEU
1	C	366	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	247	HIS
1	G	419	GLN
1	F	394	ASN
1	G	198	GLN
1	H	46	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	42,46,46	2.82	16 (38%)	53,67,67	2.18	8 (15%)
2	BLA	H	900	1	42,46,46	2.79	15 (35%)	53,67,67	1.64	8 (15%)
2	BLA	C	900	1	42,46,46	2.78	18 (42%)	53,67,67	1.86	9 (16%)
2	BLA	B	900	1	42,46,46	2.85	17 (40%)	53,67,67	1.77	9 (16%)
2	BLA	E	900	1	42,46,46	2.86	17 (40%)	53,67,67	1.67	7 (13%)
2	BLA	G	900	1	42,46,46	2.82	17 (40%)	53,67,67	1.67	9 (16%)
2	BLA	A	900	1	42,46,46	2.76	18 (42%)	53,67,67	1.94	9 (16%)
2	BLA	F	900	1	42,46,46	2.77	17 (40%)	53,67,67	1.74	8 (15%)

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	-	6/26/74/74	0/4/4/4
2	BLA	H	900	1	-	10/26/74/74	0/4/4/4
2	BLA	C	900	1	-	10/26/74/74	0/4/4/4
2	BLA	B	900	1	-	11/26/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	E	900	1	-	14/26/74/74	0/4/4/4
2	BLA	G	900	1	-	12/26/74/74	0/4/4/4
2	BLA	A	900	1	-	11/26/74/74	0/4/4/4
2	BLA	F	900	1	-	10/26/74/74	0/4/4/4

The worst 5 of 135 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	BLA	CHB-C1B	8.86	1.52	1.34
2	G	900	BLA	CHB-C1B	8.82	1.52	1.34
2	H	900	BLA	CHB-C1B	8.81	1.52	1.34
2	B	900	BLA	CHB-C1B	8.81	1.52	1.34
2	A	900	BLA	CHB-C1B	8.66	1.52	1.34

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	BLA	C1A-CHA-C4D	-11.32	115.29	128.81
2	A	900	BLA	C1A-CHA-C4D	-9.92	116.95	128.81
2	C	900	BLA	C1A-CHA-C4D	-8.97	118.09	128.81
2	F	900	BLA	C1A-CHA-C4D	-7.65	119.67	128.81
2	B	900	BLA	C1A-CHA-C4D	-6.74	120.76	128.81

There are no chirality outliers.

5 of 84 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	A	900	BLA	NB-C1B-CHB-C4A
2	A	900	BLA	C2B-C1B-CHB-C4A
2	B	900	BLA	NA-C4A-CHB-C1B

There are no ring outliers.

8 monomers are involved in 58 short contacts:

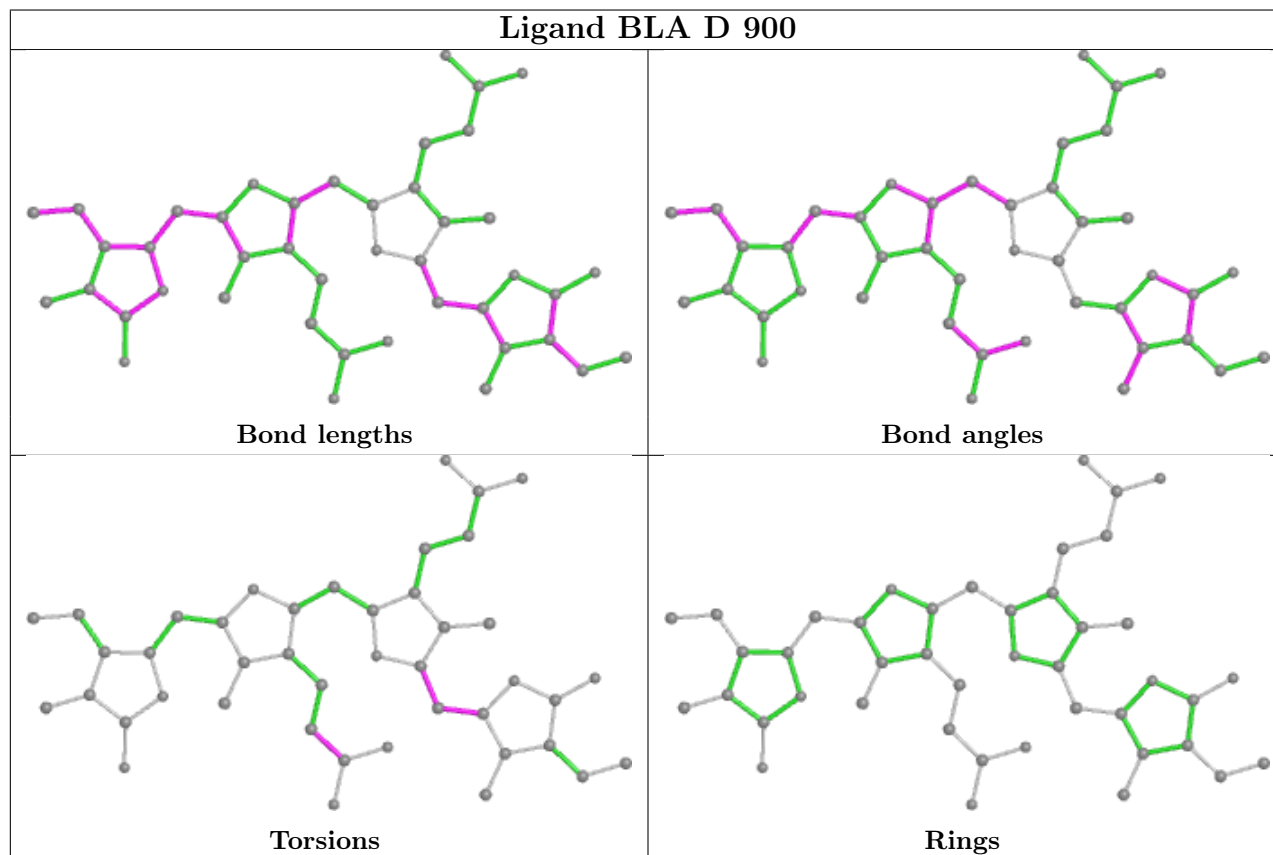
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	900	BLA	5	0
2	H	900	BLA	6	0
2	C	900	BLA	14	0

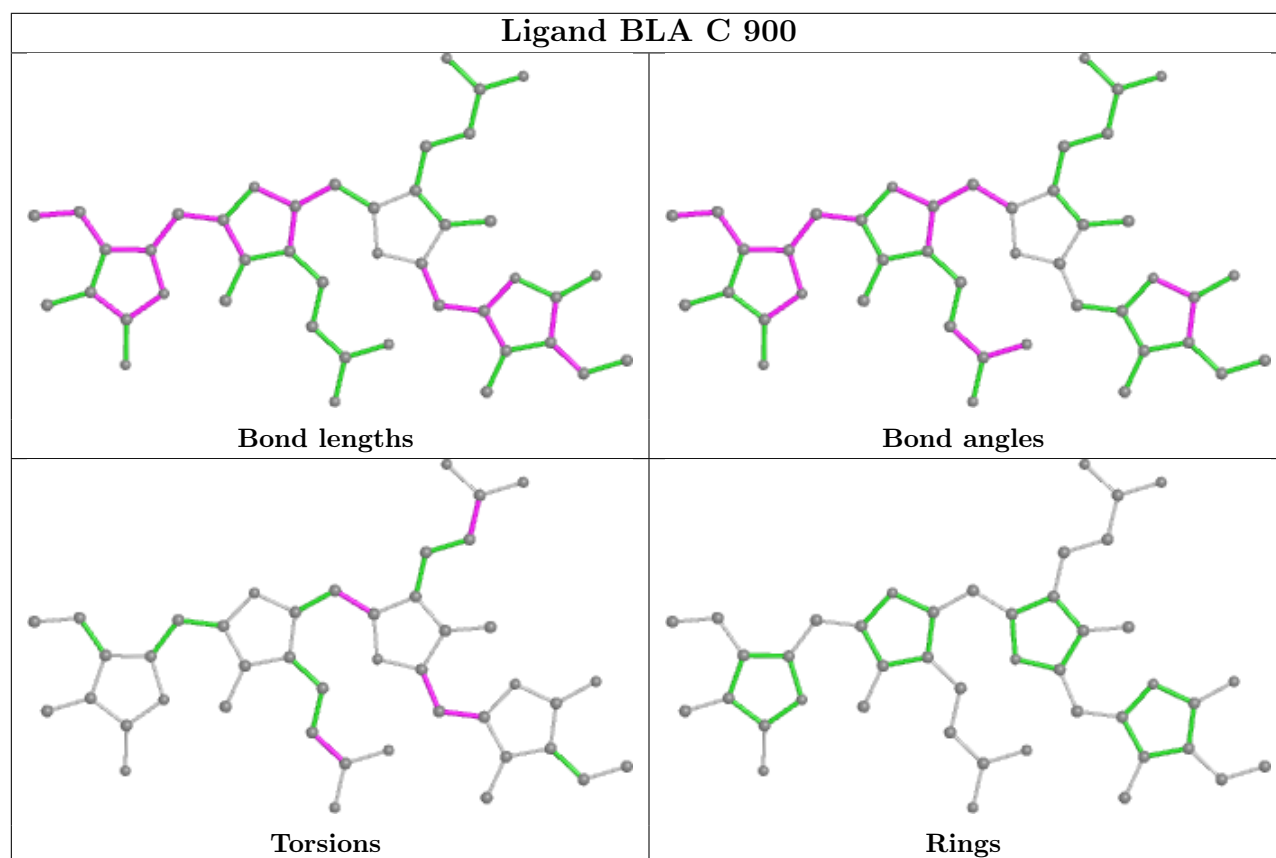
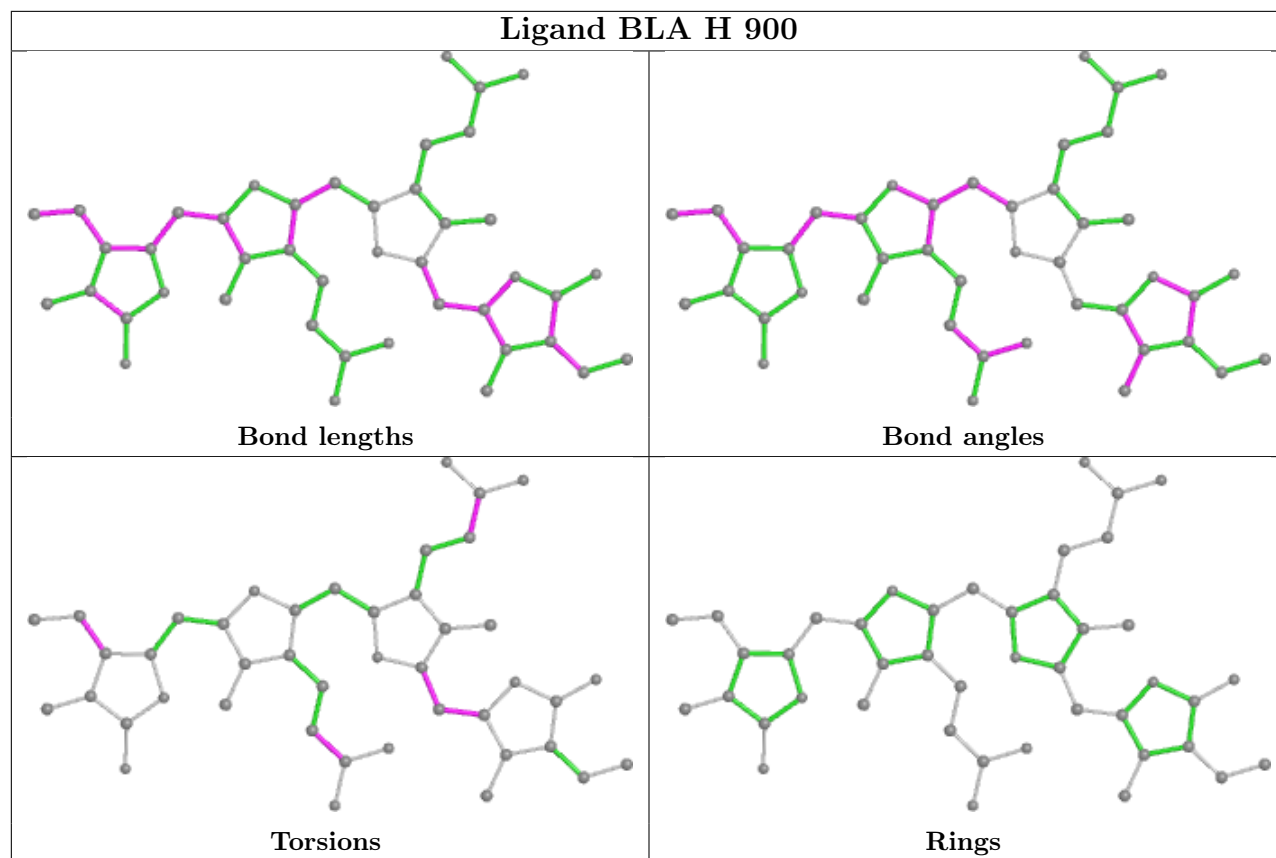
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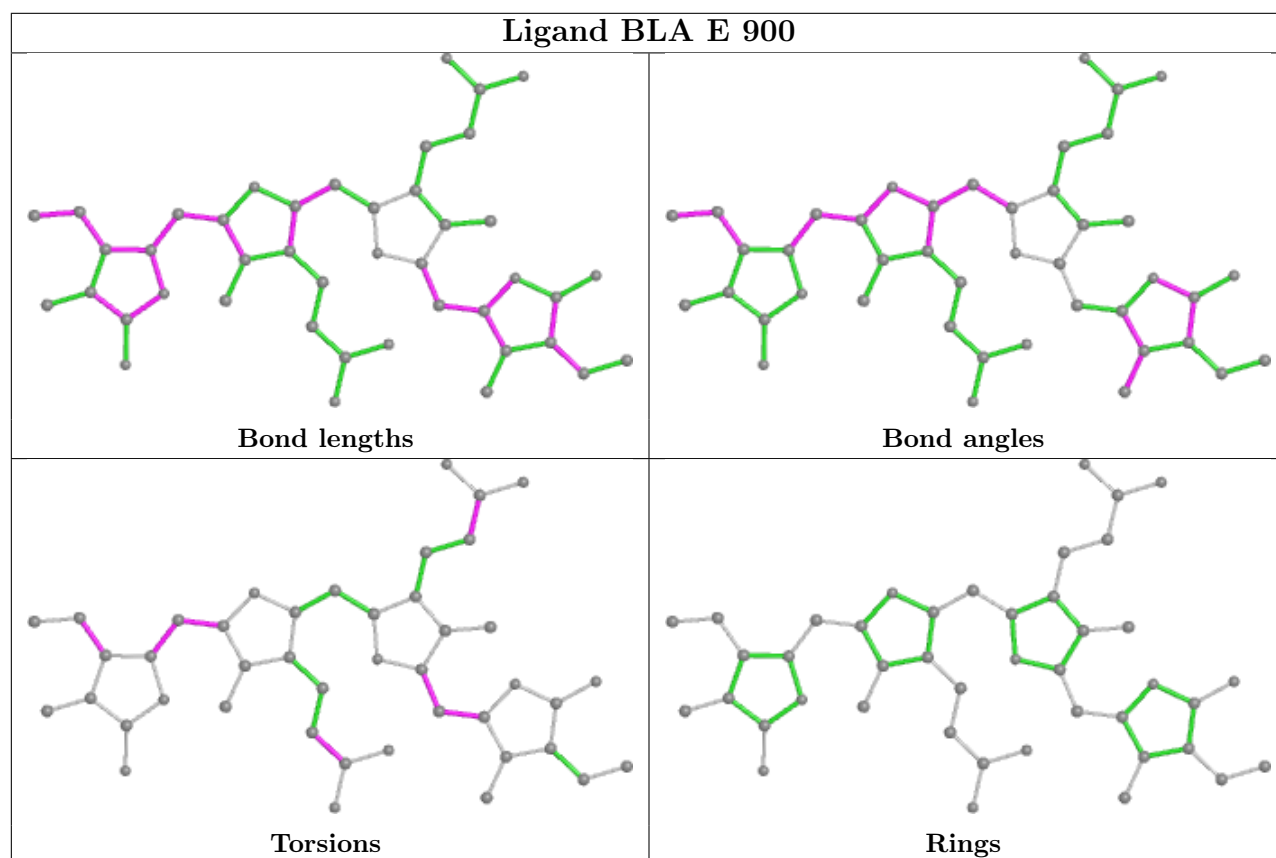
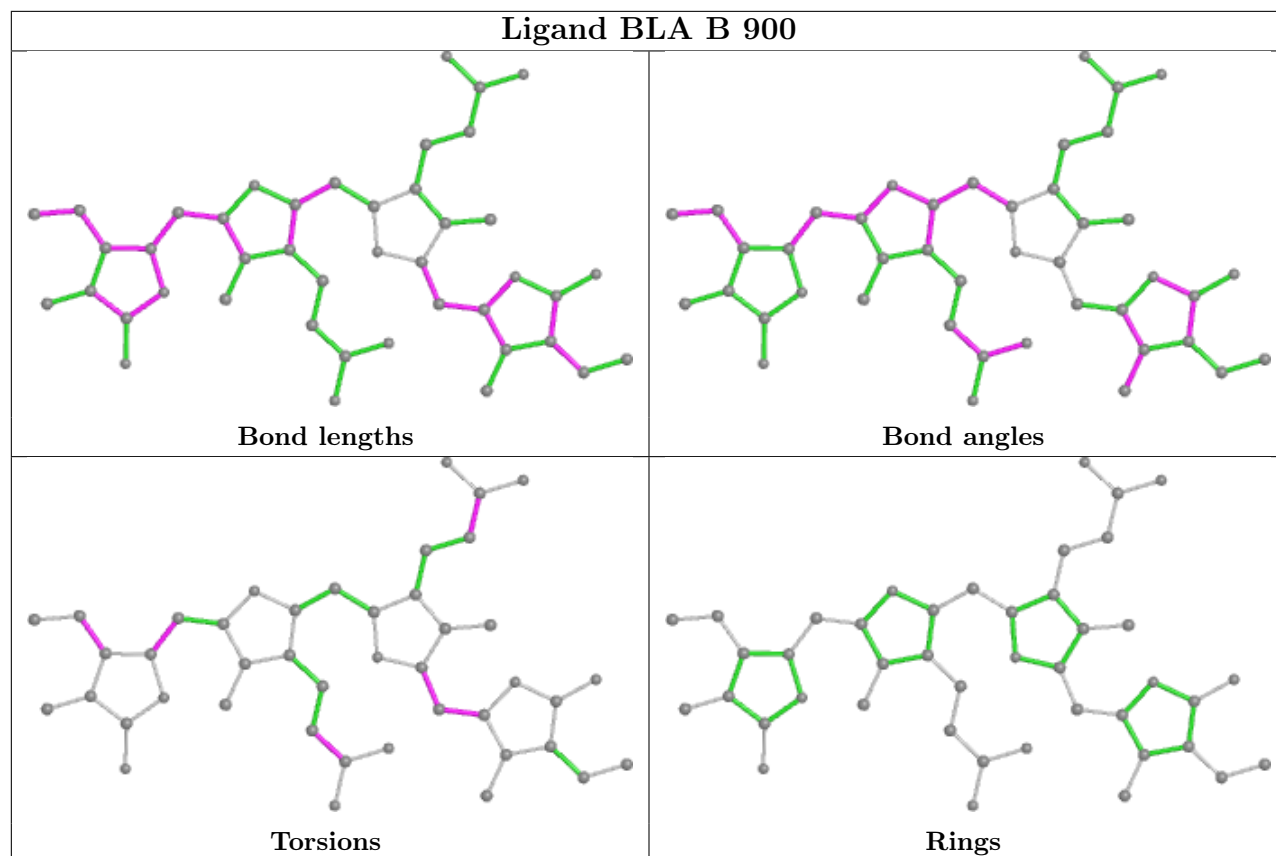
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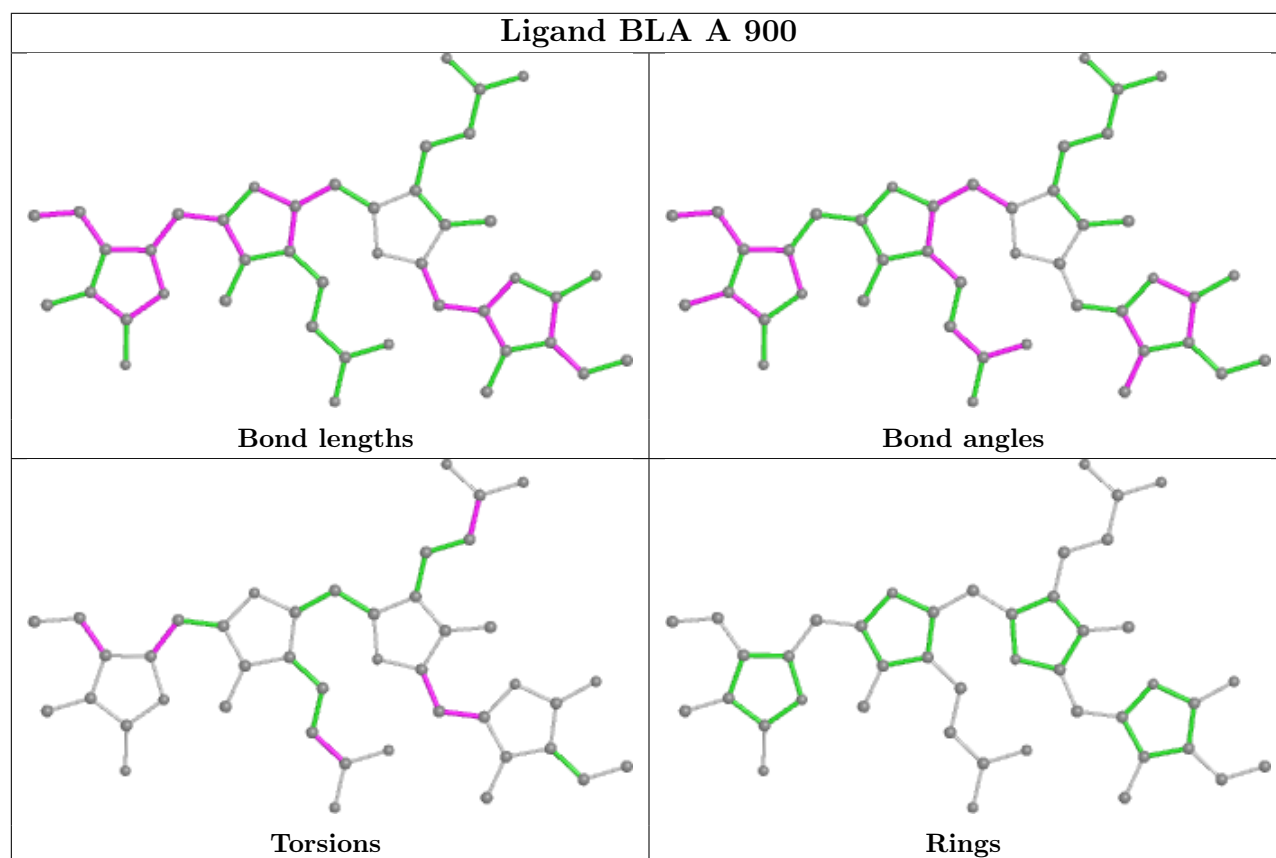
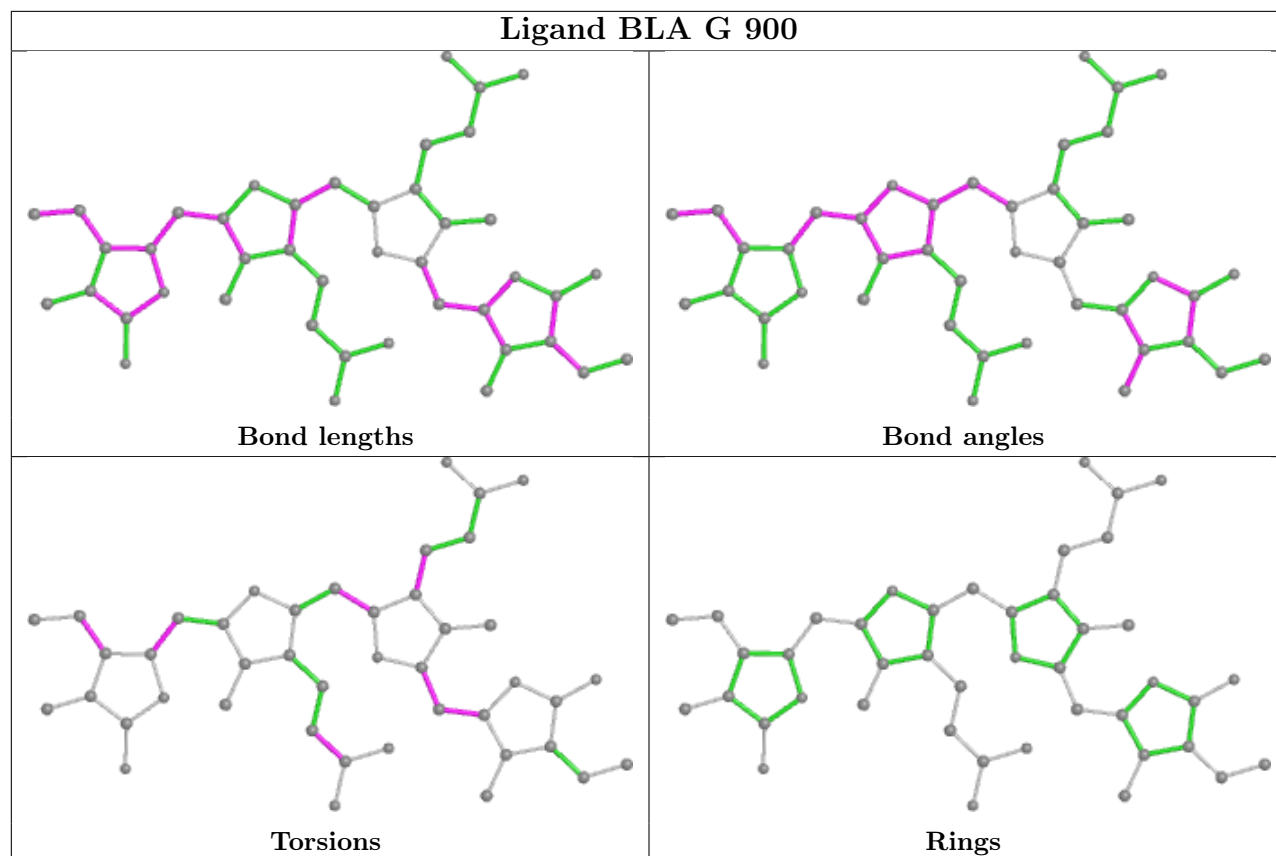
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	8	0
2	E	900	BLA	7	0
2	G	900	BLA	5	0
2	A	900	BLA	4	0
2	F	900	BLA	9	0

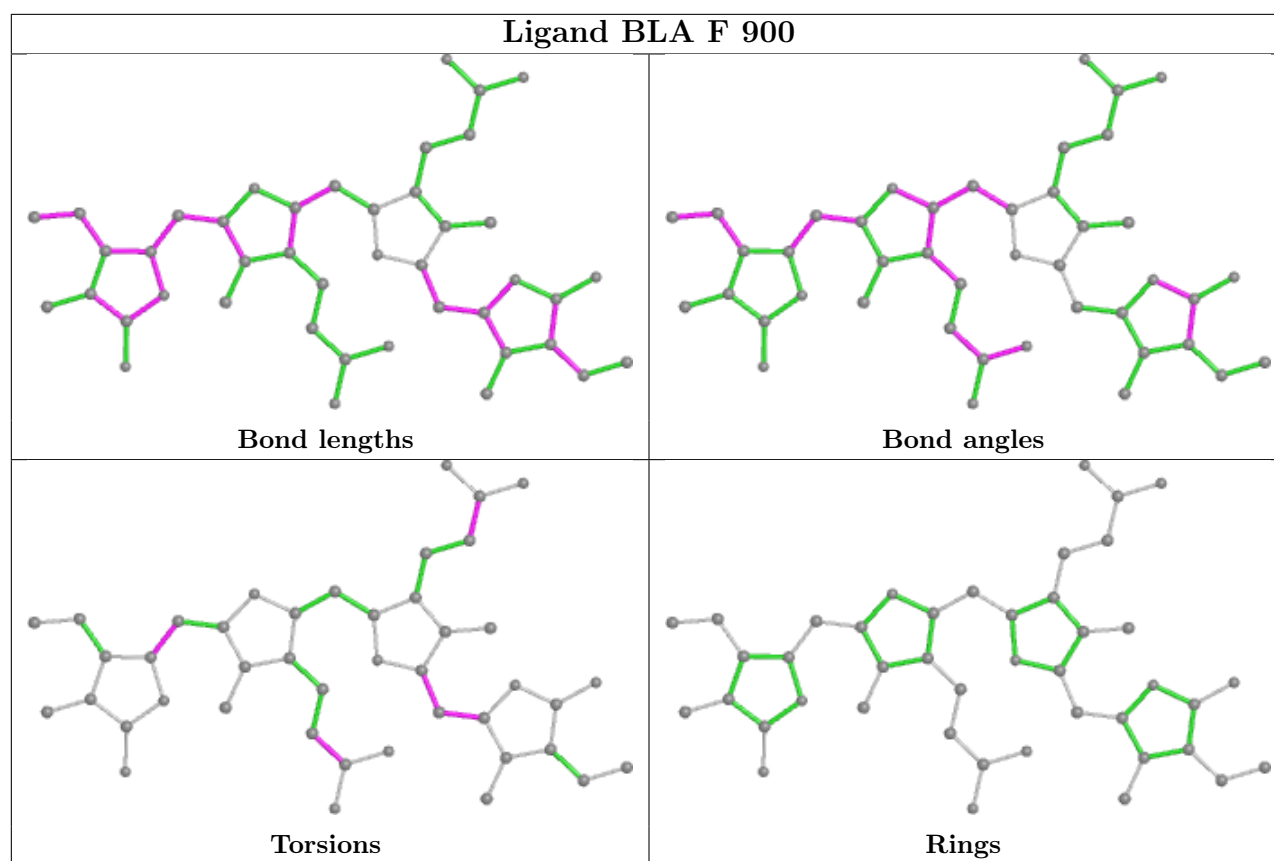
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	479/505 (94%)	0.12	12 (2%) 57 63	37, 58, 109, 160	0
1	B	470/505 (93%)	0.68	42 (8%) 9 11	48, 88, 136, 183	0
1	C	482/505 (95%)	0.19	10 (2%) 63 70	39, 61, 102, 147	0
1	D	480/505 (95%)	0.62	46 (9%) 8 10	55, 92, 144, 191	0
1	E	479/505 (94%)	0.52	33 (6%) 16 20	49, 92, 134, 191	0
1	F	471/505 (93%)	0.58	54 (11%) 4 6	41, 81, 144, 171	0
1	G	482/505 (95%)	0.06	6 (1%) 79 84	37, 63, 105, 165	1 (0%)
1	H	481/505 (95%)	0.84	70 (14%) 2 3	55, 95, 158, 207	0
All	All	3824/4040 (94%)	0.45	273 (7%) 16 19	37, 79, 138, 207	1 (0%)

The worst 5 of 273 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	LEU	9.7
1	H	51	PHE	8.8
1	B	453	ARG	8.6
1	H	442	GLU	8.5
1	H	110	PHE	7.5

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

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

6.3 Carbohydrates [i](#)

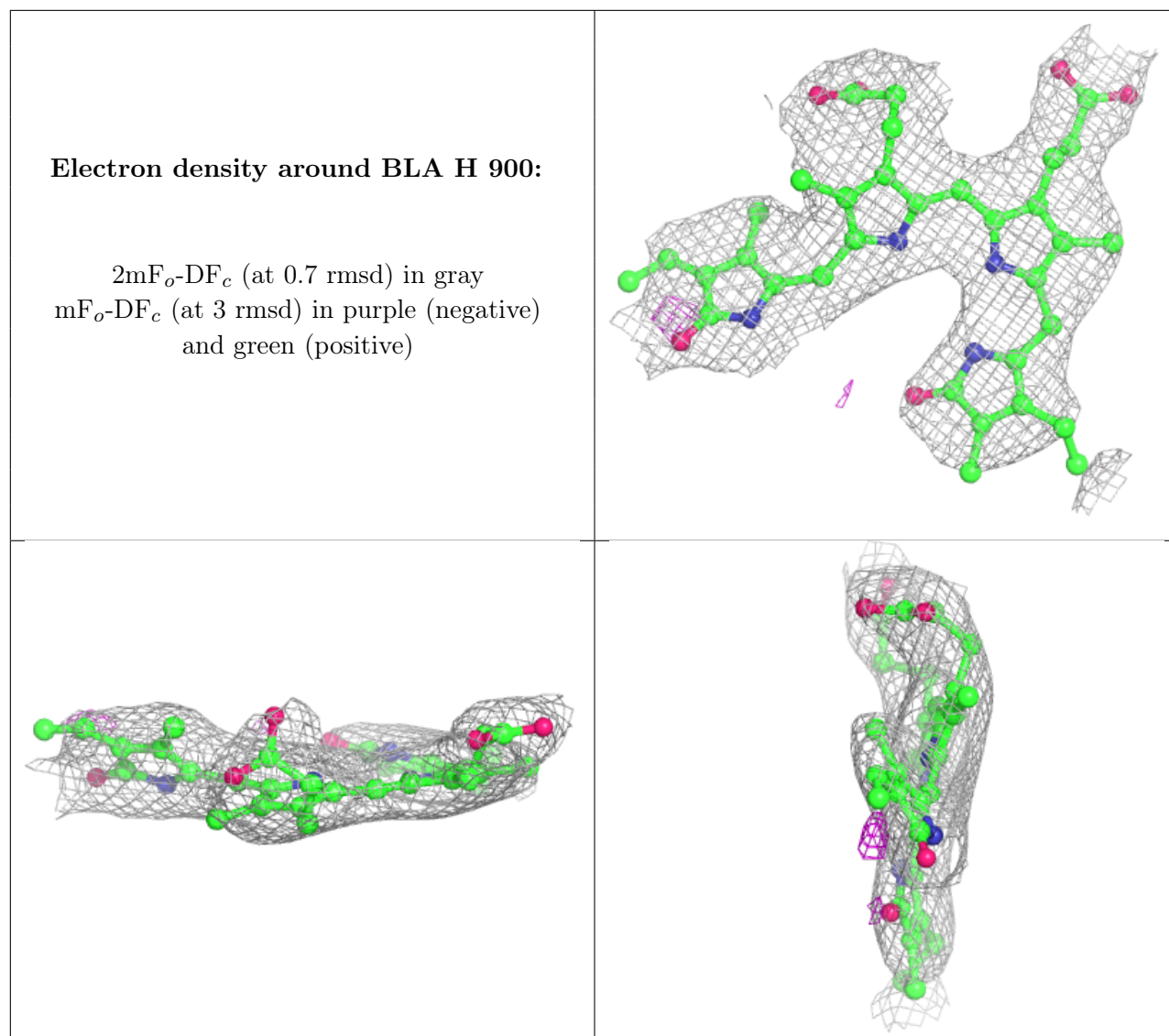
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

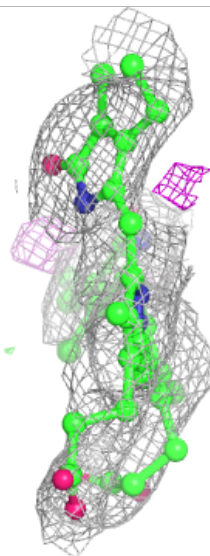
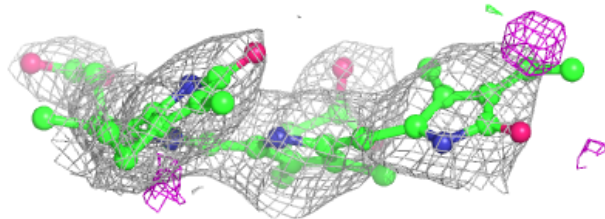
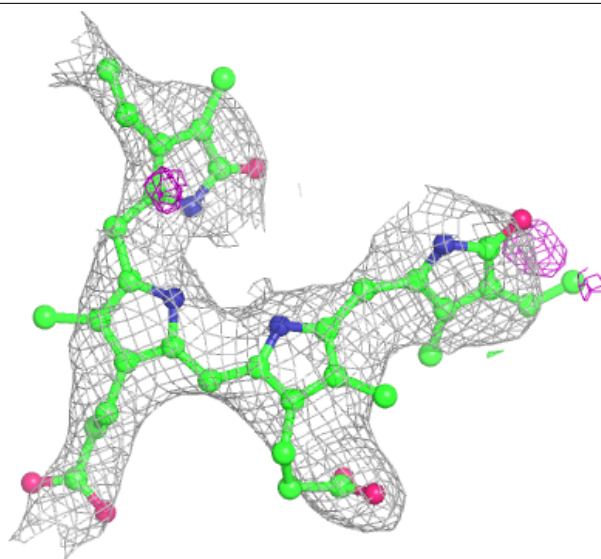
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	H	900	43/43	0.92	0.21	64,83,93,105	0
2	BLA	E	900	43/43	0.93	0.31	72,92,104,113	0
2	BLA	B	900	43/43	0.93	0.21	60,76,95,107	0
2	BLA	D	900	43/43	0.94	0.17	62,81,95,101	0
2	BLA	G	900	43/43	0.95	0.18	37,58,68,89	0
2	BLA	F	900	43/43	0.96	0.17	39,60,70,84	0
2	BLA	A	900	43/43	0.96	0.17	34,49,64,77	0
2	BLA	C	900	43/43	0.96	0.18	34,54,68,85	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.



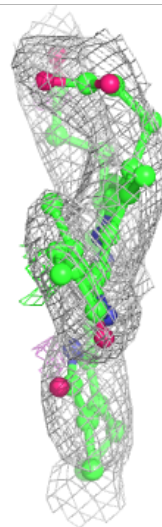
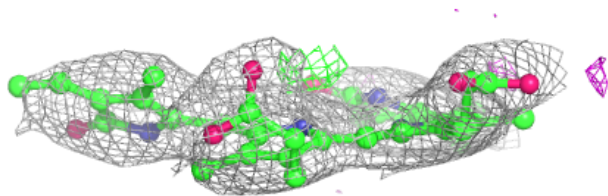
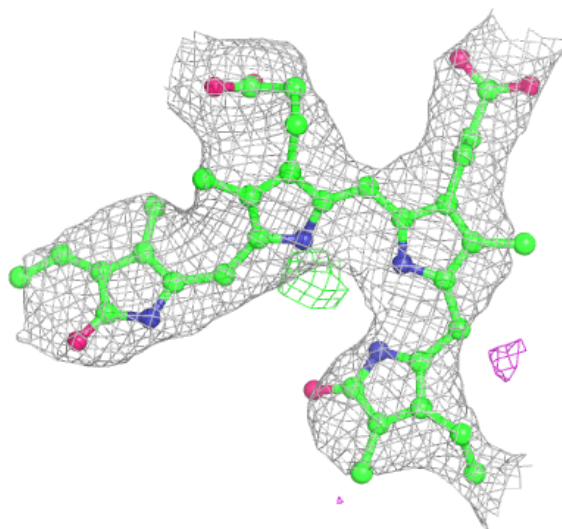
Electron density around BLA E 900:

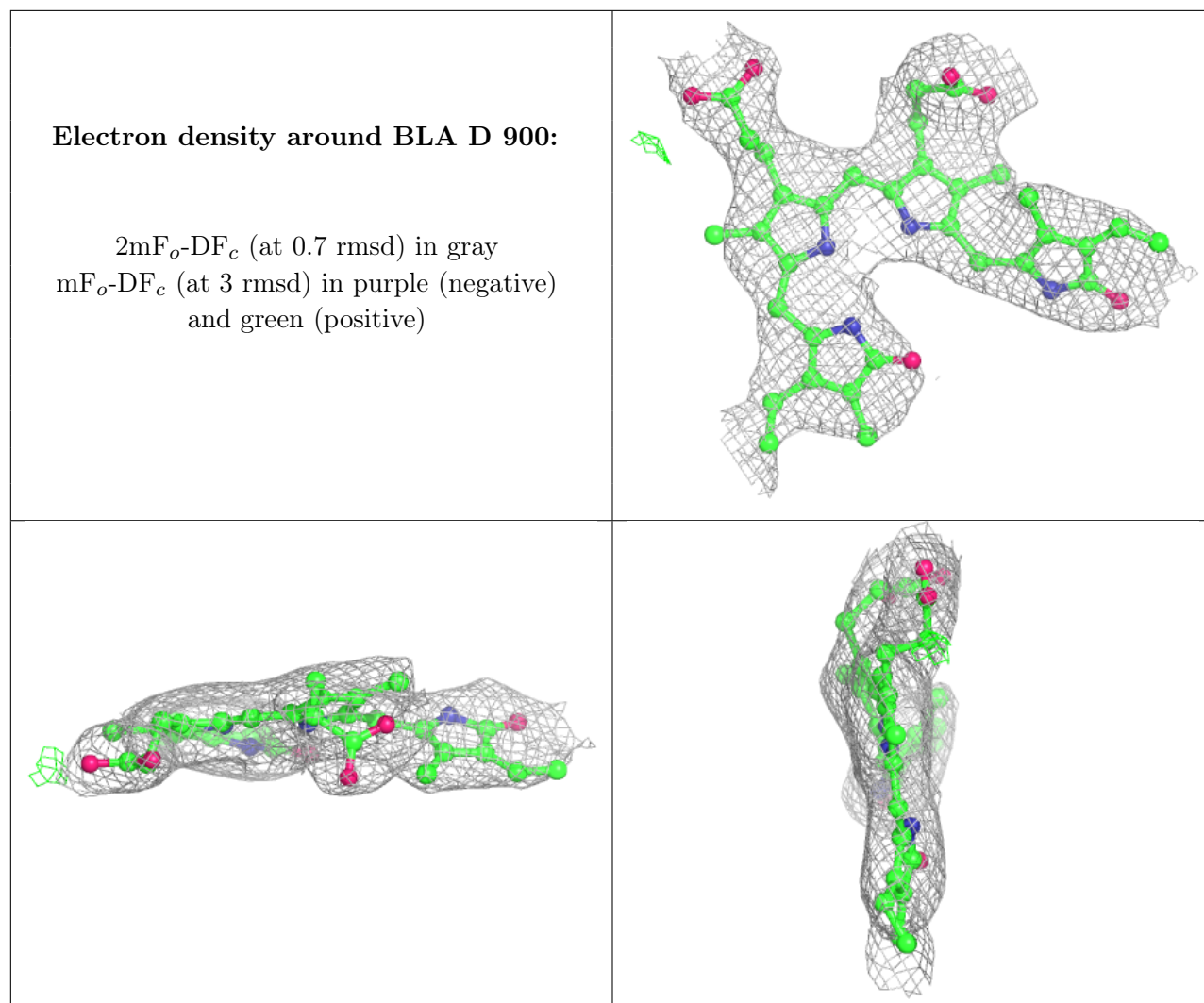
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

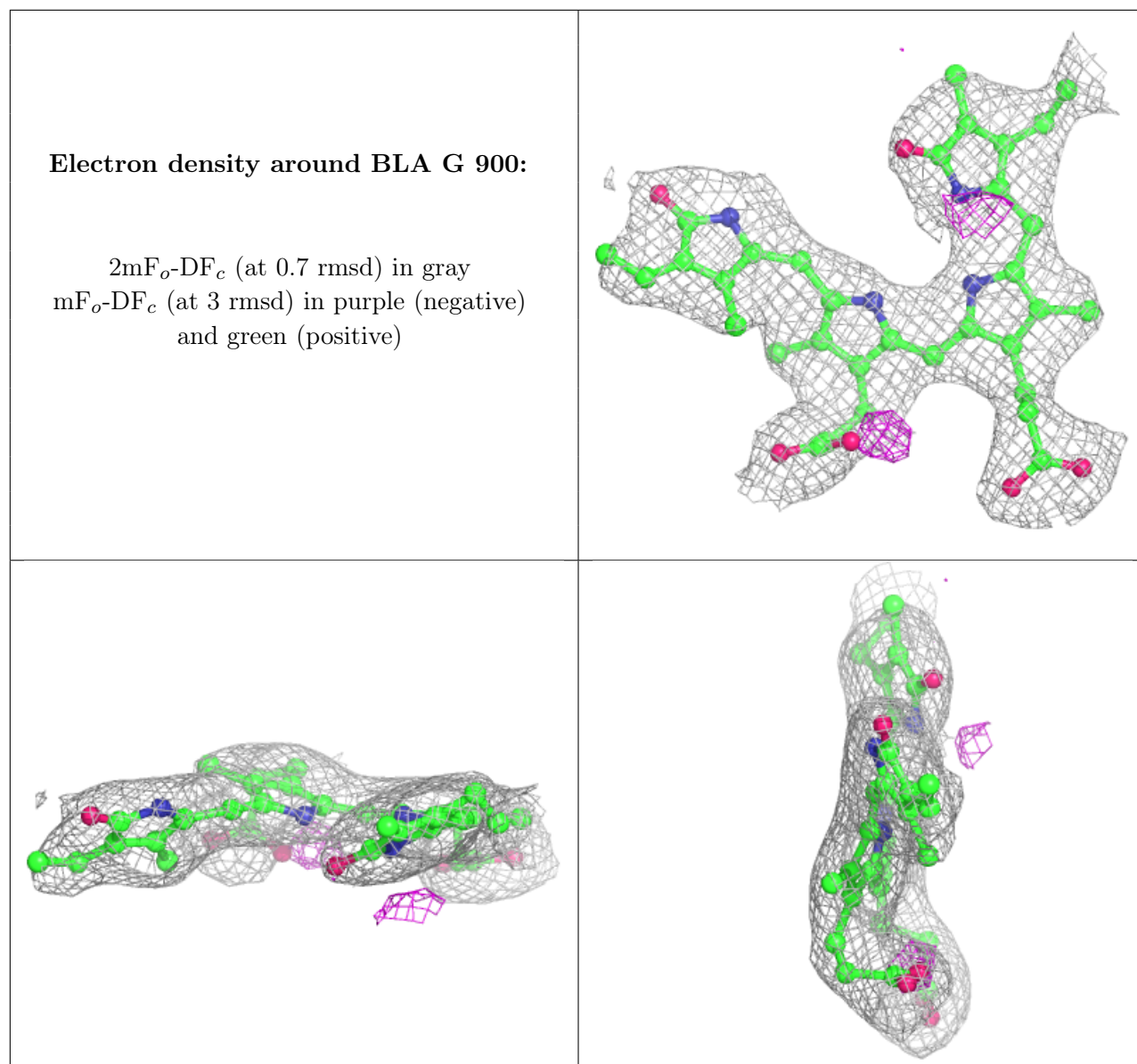


Electron density around BLA B 900:

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

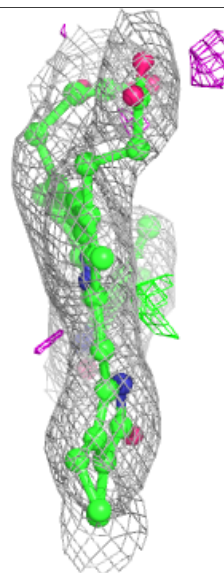
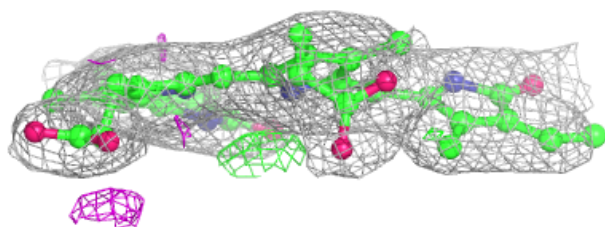
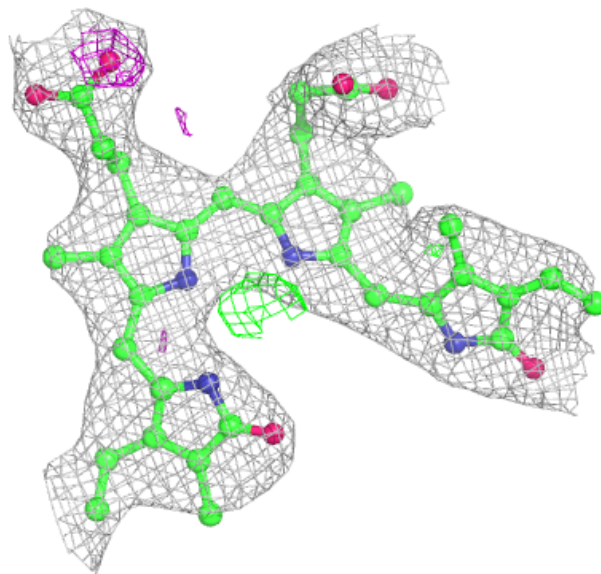






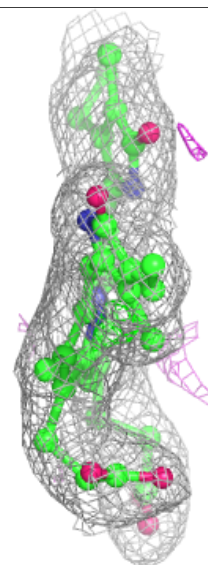
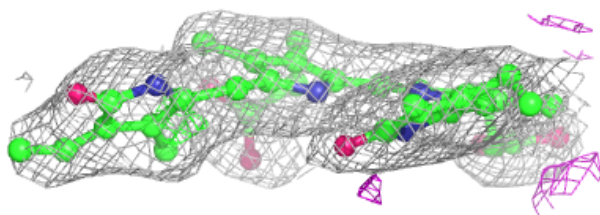
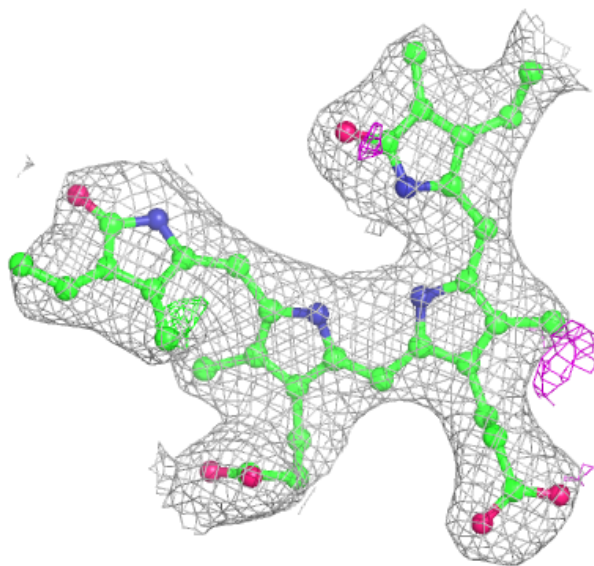
Electron density around BLA F 900:

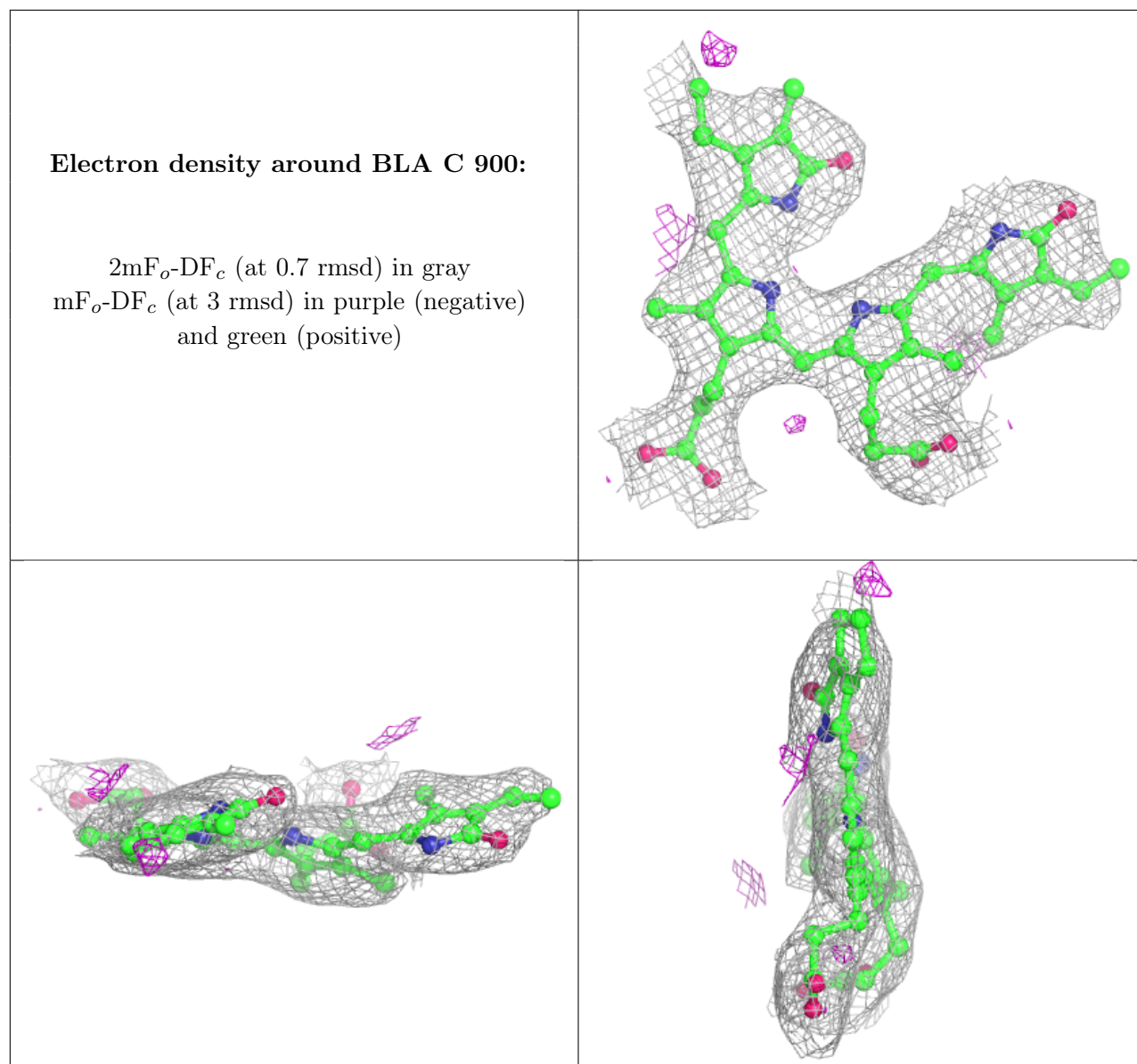
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BLA A 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 [i](#)

There are no such residues in this entry.