wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2021 – 01:59 PM EDT

PDB ID	:	3G6O
Title	:	Crystal structure of P. aeruginosa bacteriophytochrome PaBphP photosensory core domain mutant Q188L
Authors	:	Yang, X.; Kuk, J.; Moffat, K.
Deposited on	:	2009-02-07
Resolution	:	2.85 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

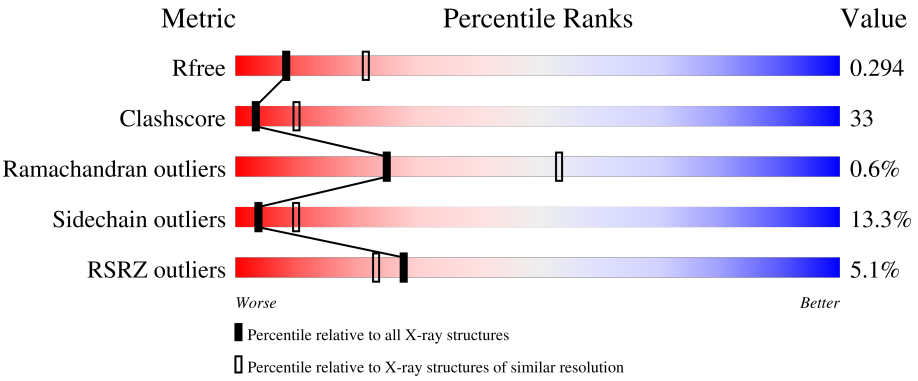
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	505	5% 45% 38% 7% 10%
1	B	505	5% 46% 38% 6% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7512 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.

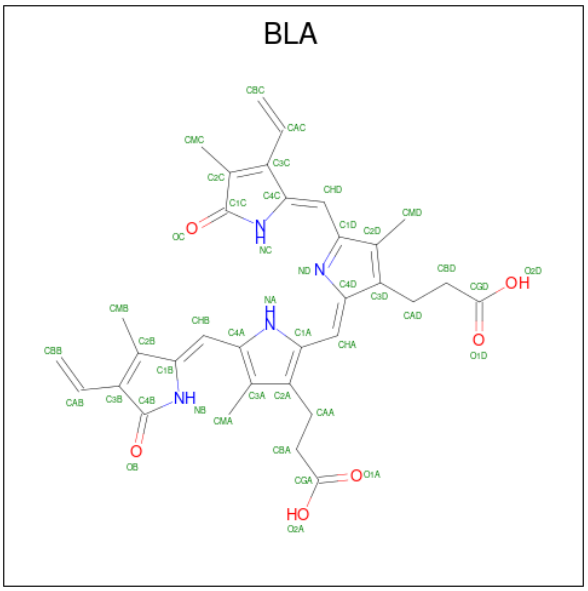
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	6	0
			3666	2313	653	680	20			
1	B	457	Total	C	N	O	S	0	7	0
			3672	2316	654	682	20			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	LEU	GLN	engineered mutation	UNP Q9HWR3
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	188	LEU	GLN	engineered mutation	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
B	503	HIS	-	expression tag	UNP Q9HWR3
B	504	HIS	-	expression tag	UNP Q9HWR3
B	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 86 66 8 12	0	1
2	B	1	Total C N O 86 66 8 12	0	1

- Molecule 3 is water.

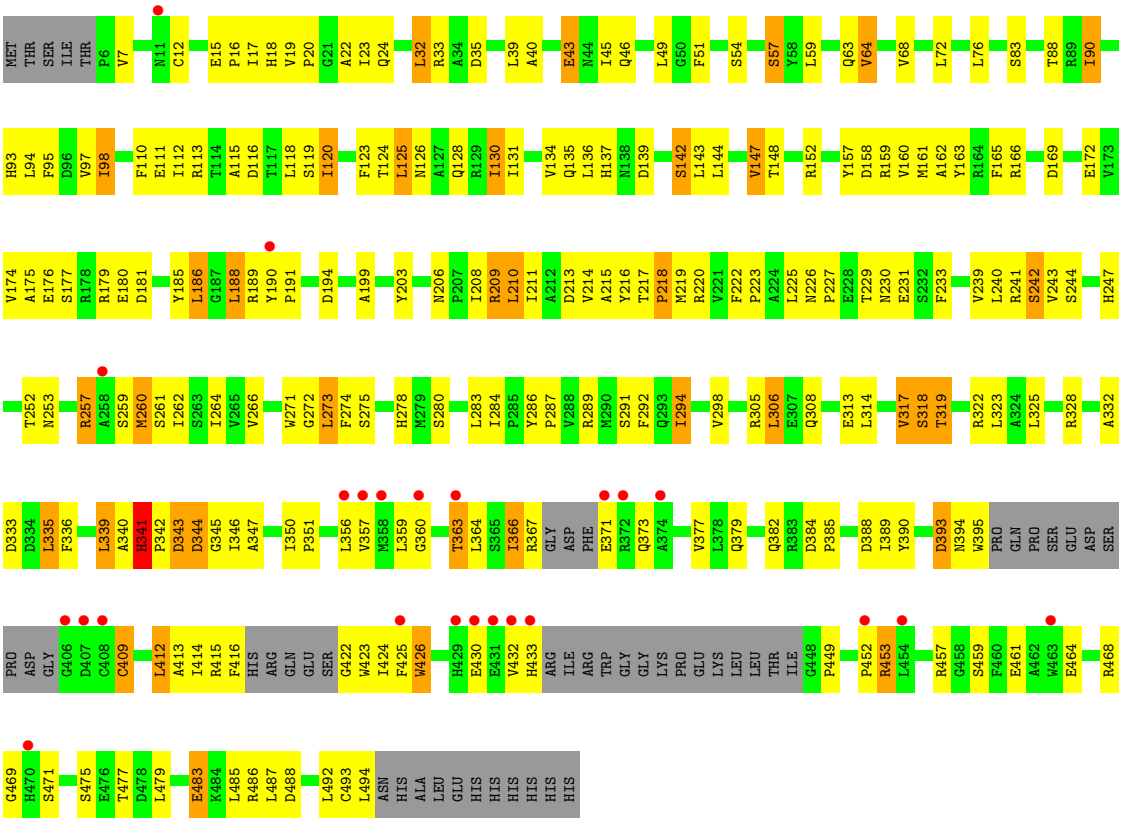
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

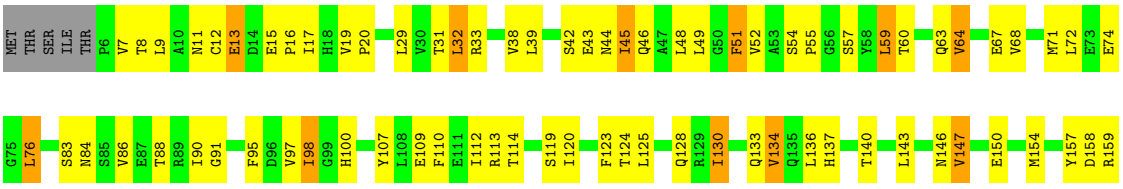
• Molecule 1: Bacteriophytochrome

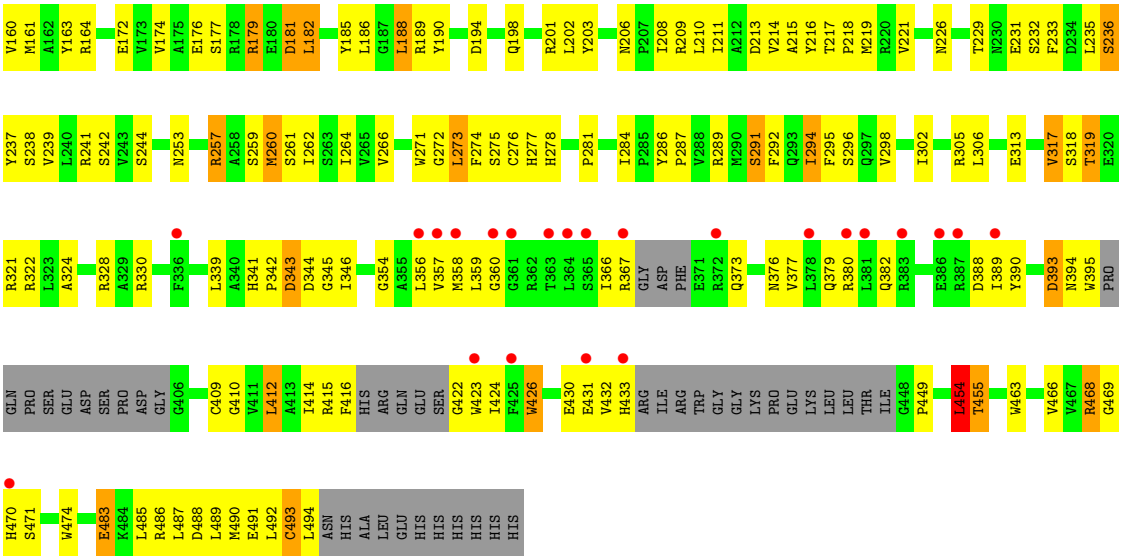
Chain A:



• Molecule 1: Bacteriophytochrome

Chain B:




V160 M161 A162 Y163 R164
E172 V173 V174 A175 E176 S177 R178 R179 E180 D181 L182
Y185 L186 G187 L188 R189 Y190
D194
Q198
R201 L202 Y203
N206 P207 I208 R209 L210 I211 A212
D213 V214 A215 Y216 T217 P218 M219 R220 V221
N226
T229 N230 E231 S232 F233 D234 L235 S236
Y237 S238 V239 L240 R241 S242 V243 S244
N253
R257 A258 S259 M260 S261 I262 S263 I264 V265 V266
W271 G272 L273 F274 S275 C276 H277 H278
P281
I284 P285 Y286 P287 V288 R289 M290 S291 F292 Q293 I294 F295 S296 Q297 V298
I302
R305 L306
E313
V317 S318 T319 E320
R321 R322 L323 A324
R328 A329 R330
F336
L339 A340 H341 P342 D343 D344 G345 I346
G354 A355 L356 V357 M358 L359 G360 G361 R362 T363 L364 S365 I366 R367
GLY ASP PHE E371 R372 Q373
N376 V377 L378 Q379 R380 L381 Q382 R383
E386 R387 D388 I389 Y390
D393 N394 W395 PRO
GLN PRO SER GLU ASP SER PRO ASP GLY G406
C409 G410 V411 L412 A413 I414 R415 F416 HIS ARG GLN GLU SER G422 W423 I424 F425 W426
E430 E431 V432 H433 ARG ILE ARG TRP GLY GLY LYS PRO GLU LYS LEU LEU THR ILE G448 P449
L454 T455
W463
V466 V467 R468 G469
H470 S471
W474
E483 K484 L485 R486 L487 D488 L489 M490 E491 L492 C493 L494 ASN HIS ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	109.79Å 109.79Å 189.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.47 – 2.85 42.47 – 2.62	Depositor EDS
% Data completeness (in resolution range)	82.8 (42.47-2.85) 67.1 (42.47-2.62)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.229 , 0.298 0.223 , 0.294	Depositor DCC
R_{free} test set	1331 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.488 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.33	0/3746	0.58	0/5083
1	B	0.31	0/3752	0.56	0/5091
All	All	0.32	0/7498	0.57	0/10174

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	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	LEU	Peptide
1	A	341	HIS	Peptide
1	A	90	ILE	Peptide

5.2 Too-close contacts

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	3666	0	3592	240	0
1	B	3672	0	3596	233	0
2	A	86	0	62	18	0
2	B	86	0	62	31	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
All	All	7512	0	7312	486	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 33.

The worst 5 of 486 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:A:209[A]:ARG:HH11	1:A:209[A]:ARG:HG2	1.21	1.04
2:A:900[A]:BLA:HMC1	2:A:900[A]:BLA:HBC1	1.38	1.01
1:A:194:ASP:HB3	2:A:900[A]:BLA:HHB	1.45	0.97
1:A:33:ARG:HB3	1:A:39:LEU:HD11	1.48	0.95
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.34	0.93

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	453/505 (90%)	415 (92%)	35 (8%)	3 (1%)	22 50
1	B	454/505 (90%)	411 (90%)	41 (9%)	2 (0%)	34 62
All	All	907/1010 (90%)	826 (91%)	76 (8%)	5 (1%)	25 53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	454	LEU
1	A	341	HIS
1	A	218	PRO
1	A	452	PRO
1	B	342	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	394/431 (91%)	339 (86%)	55 (14%)	3 9
1	B	395/431 (92%)	346 (88%)	49 (12%)	4 12
All	All	789/862 (92%)	685 (87%)	104 (13%)	4 10

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	45	ILE
1	B	160	VAL
1	B	483	GLU
1	B	59	LEU
1	B	119	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
1	B	308	GLN
1	B	373	GLN
1	A	26	HIS
1	A	24	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)

4 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	B	900[B]	1	36,46,46	3.02	18 (50%)	47,67,67	1.42	8 (17%)
2	BLA	B	900[A]	1	36,46,46	3.01	18 (50%)	47,67,67	1.70	9 (19%)
2	BLA	A	900[B]	1	36,46,46	2.99	18 (50%)	47,67,67	1.64	10 (21%)
2	BLA	A	900[A]	1	36,46,46	3.03	18 (50%)	47,67,67	1.64	7 (14%)

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	B	900[B]	1	-	2/22/74/74	0/4/4/4
2	BLA	B	900[A]	1	-	8/22/74/74	0/4/4/4
2	BLA	A	900[B]	1	-	1/22/74/74	0/4/4/4
2	BLA	A	900[A]	1	-	5/22/74/74	0/4/4/4

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900[A]	BLA	CHB-C1B	9.11	1.53	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900[A]	BLA	CHB-C1B	8.76	1.52	1.34
2	B	900[B]	BLA	CHB-C1B	8.37	1.51	1.34
2	A	900[B]	BLA	CHB-C1B	8.21	1.51	1.34
2	B	900[A]	BLA	CHD-C4C	6.55	1.53	1.38

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	900[A]	BLA	C1A-CHA-C4D	-6.22	121.38	128.81
2	B	900[A]	BLA	C1A-CHA-C4D	-5.45	122.30	128.81
2	A	900[B]	BLA	C4C-CHD-C1D	-5.12	115.57	128.08
2	A	900[A]	BLA	CMB-C2B-C1B	3.48	128.51	124.17
2	B	900[A]	BLA	C4C-CHD-C1D	-3.41	119.75	128.08

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

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

There are no ring outliers.

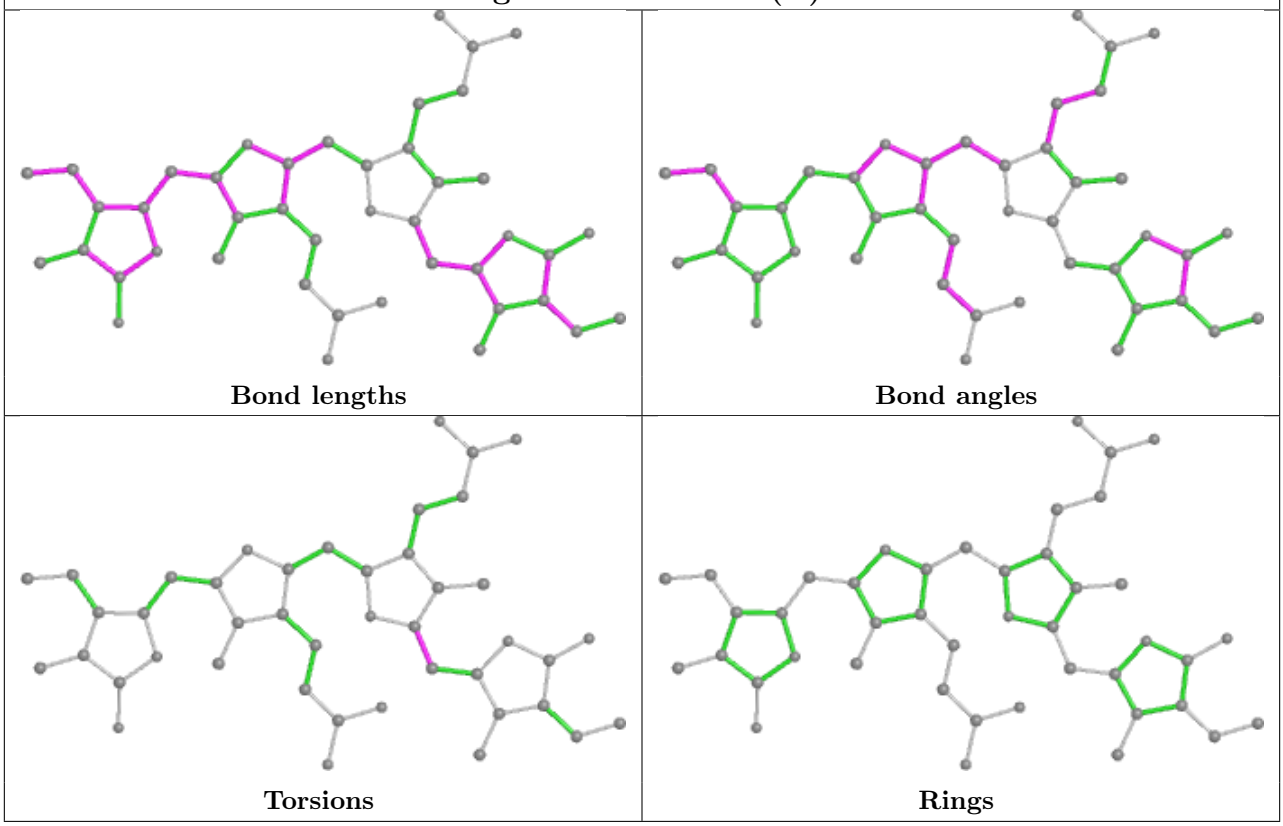
4 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900[B]	BLA	20	0
2	B	900[A]	BLA	11	0
2	A	900[B]	BLA	9	0
2	A	900[A]	BLA	9	0

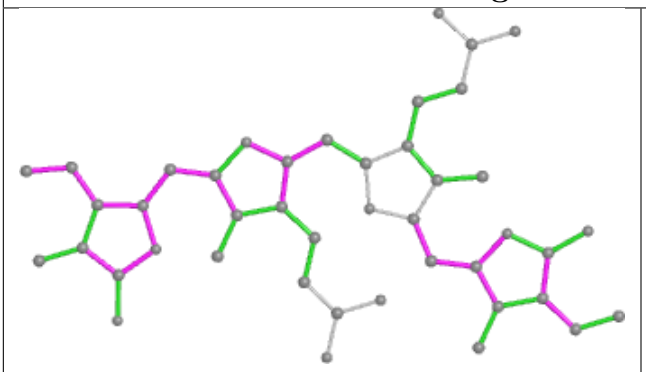
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

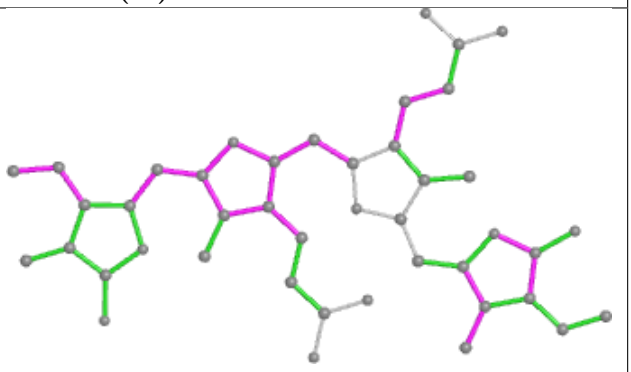
Ligand BLA B 900 (B)



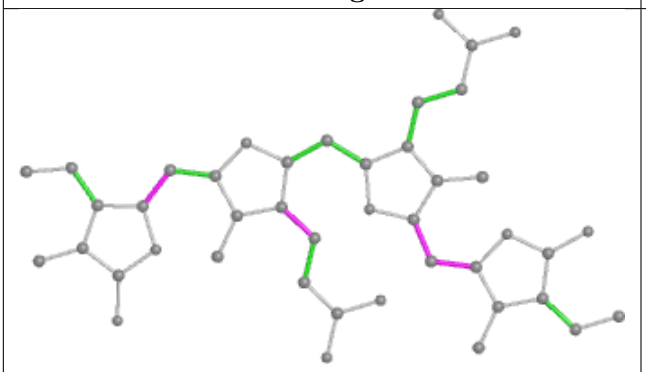
Ligand BLA B 900 (A)



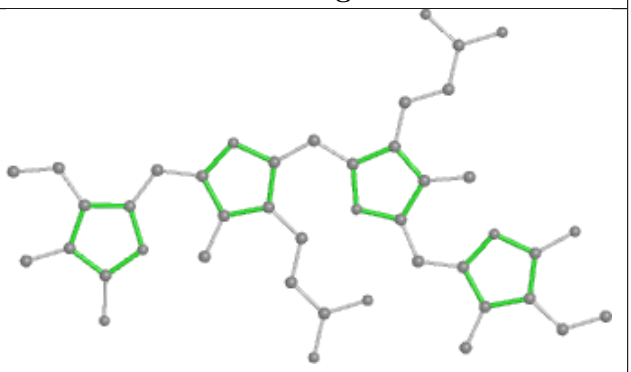
Bond lengths



Bond angles

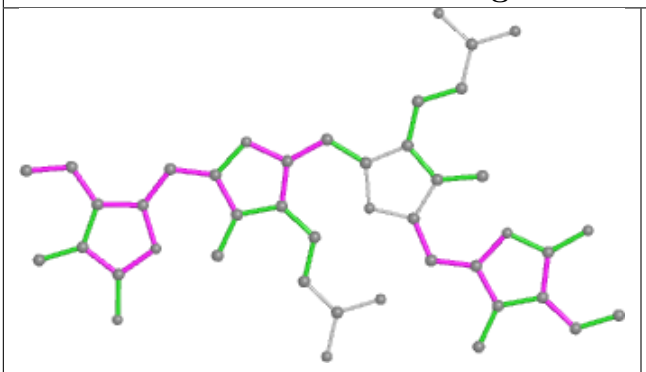


Torsions

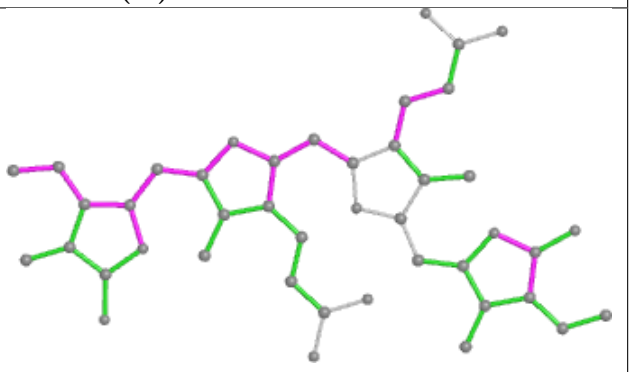


Rings

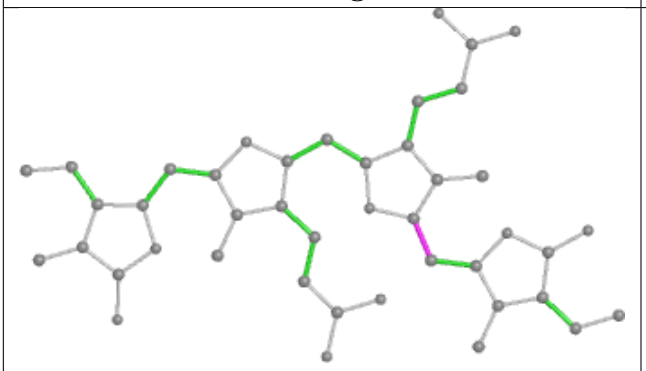
Ligand BLA A 900 (B)



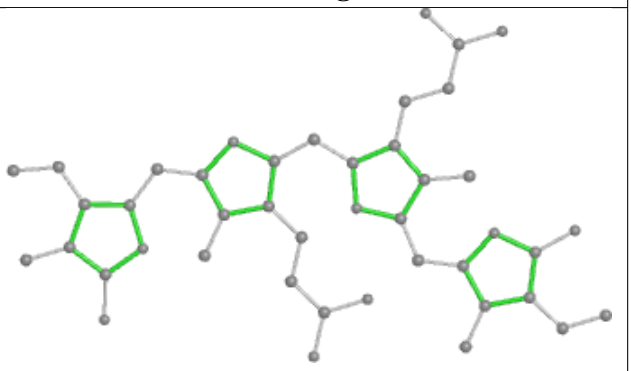
Bond lengths



Bond angles

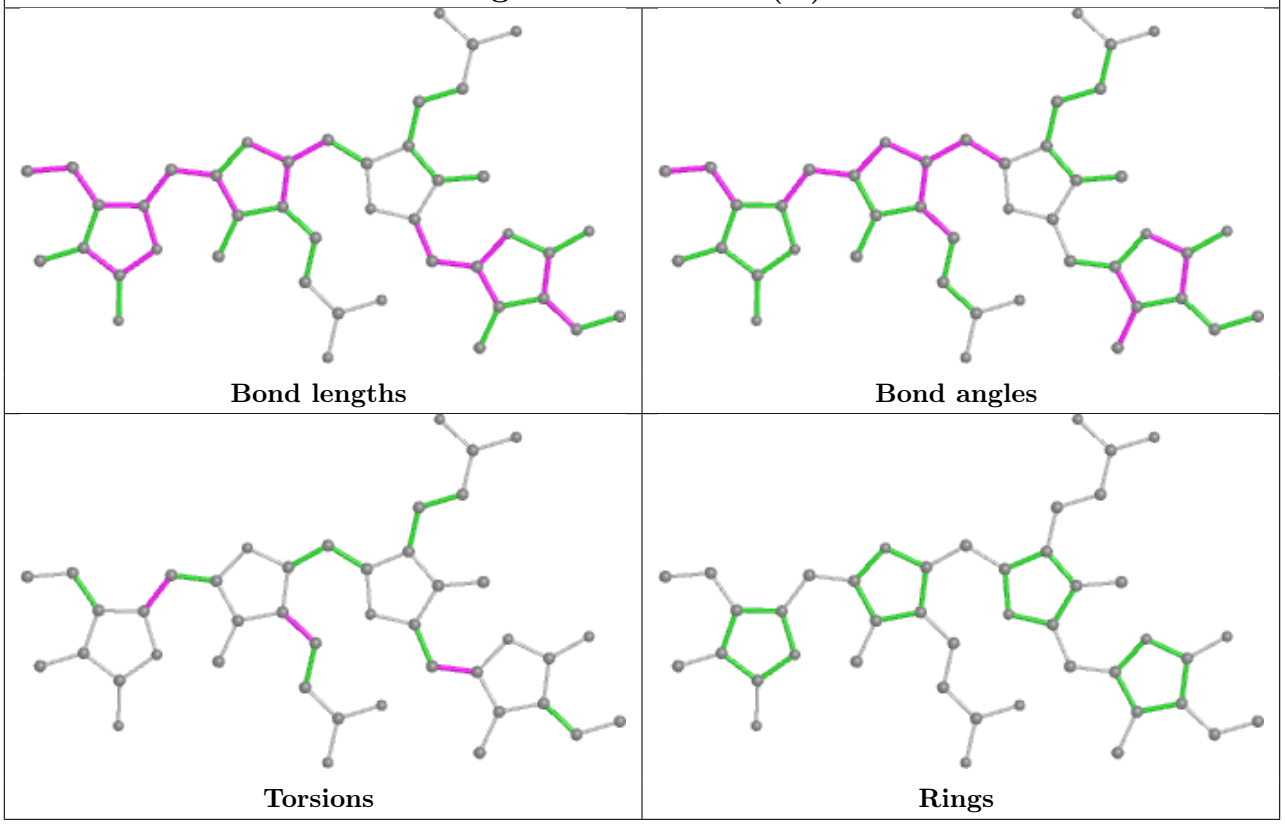


Torsions



Rings

Ligand BLA A 900 (A)



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	457/505 (90%)	-0.07	24 (5%)	26	22	63, 120, 219, 317	0
1	B	457/505 (90%)	-0.11	23 (5%)	28	24	62, 119, 230, 373	0
All	All	914/1010 (90%)	-0.09	47 (5%)	28	23	62, 119, 222, 373	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	372	ARG	10.0
1	A	431	GLU	8.0
1	A	452	PRO	7.9
1	A	433	HIS	6.9
1	B	360	GLY	6.5

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 monosaccharides in this entry.

6.4 Ligands

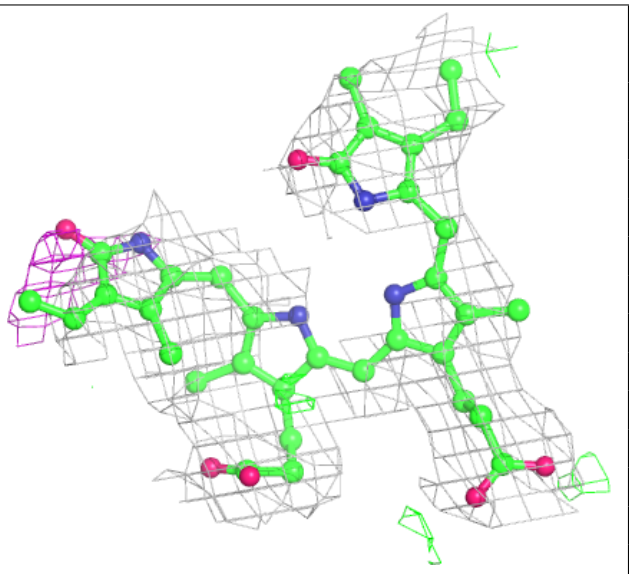
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

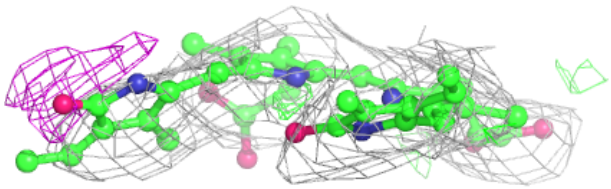
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BLA	A	900[A]	43/43	0.89	0.30	92,130,170,177	43
2	BLA	A	900[B]	43/43	0.89	0.30	85,127,170,173	43
2	BLA	B	900[A]	43/43	0.91	0.31	85,123,149,164	43
2	BLA	B	900[B]	43/43	0.91	0.31	79,114,146,176	43

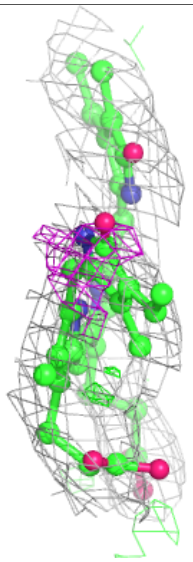
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BLA A 900 (A):

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

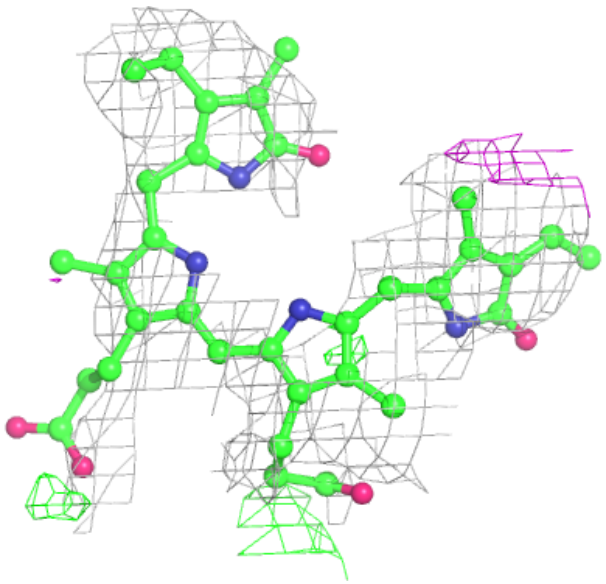


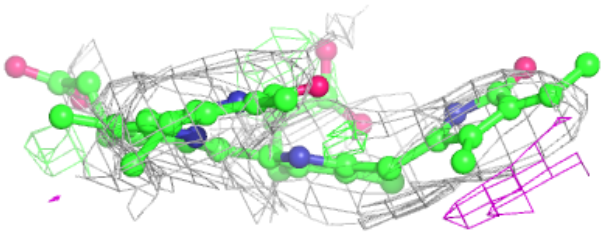


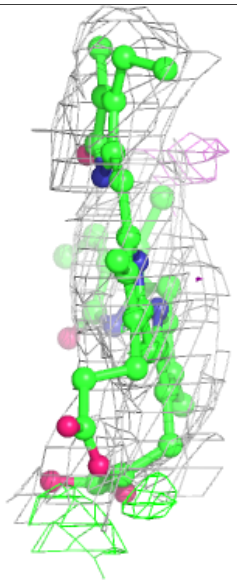


Electron density around BLA A 900 (B):

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

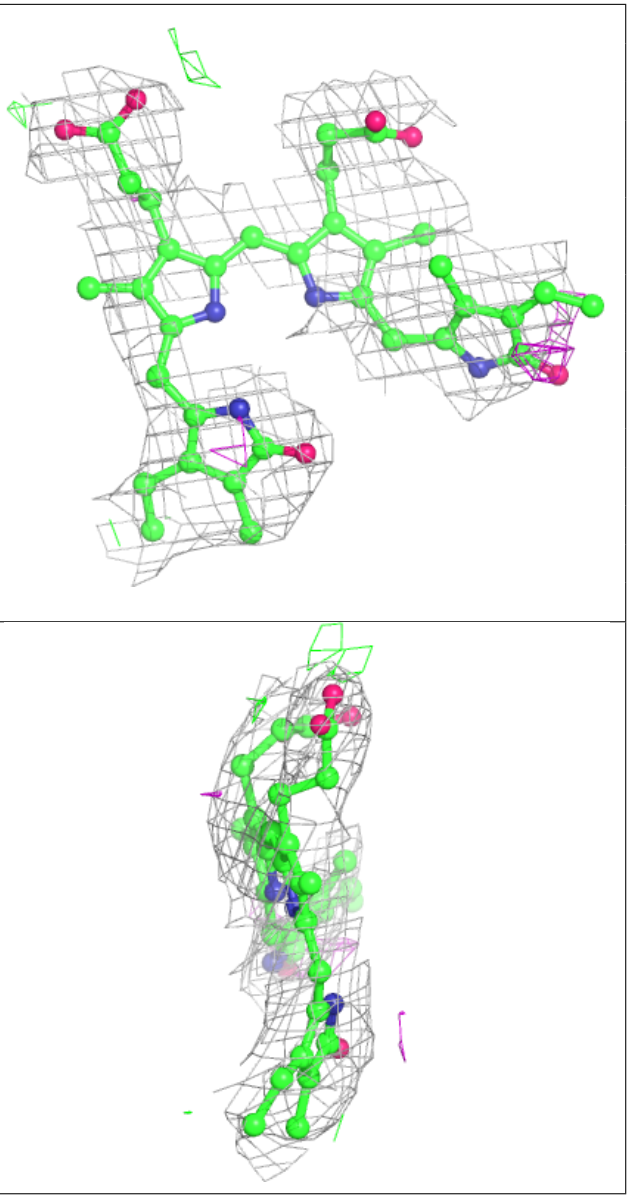


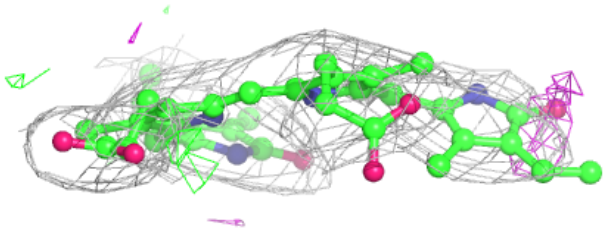




Electron density around BLA B 900 (A):

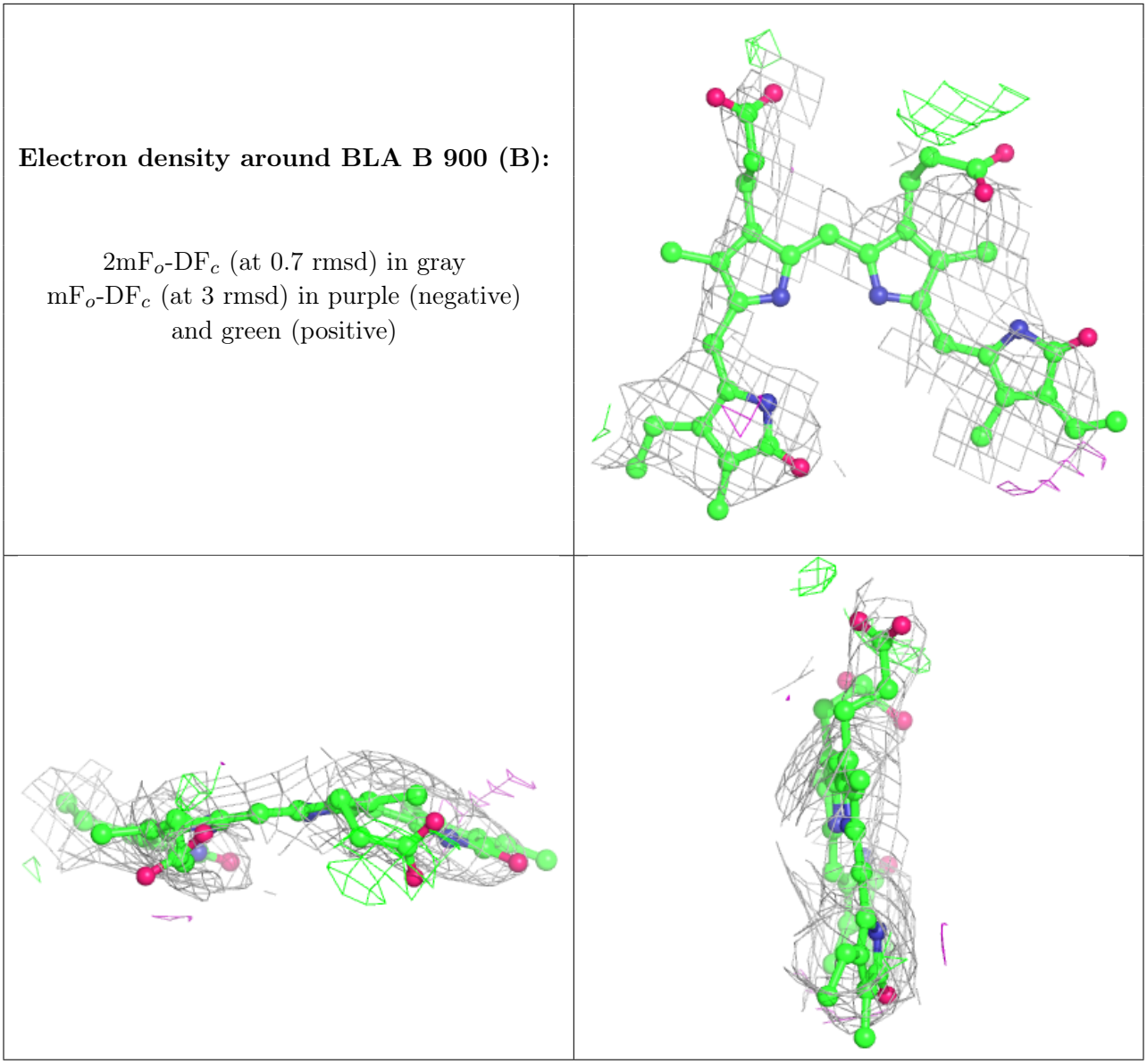
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around BLA B 900 (B):

$2mF_o$-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.