



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:15 PM UTC

PDB ID : 6NDP / pdb_00006ndp
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP mutant L193Q from Xanthomonas campestris
Authors : Otero, L.H.; Sirigu, S.; Klinke, S.; Rinaldi, J.; Conforte, V.; Malamud, F.; Goldbaum, F.A.; Chavas, L.; Bonomi, H.R.
Deposited on : 2018-12-14
Resolution : 3.89 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

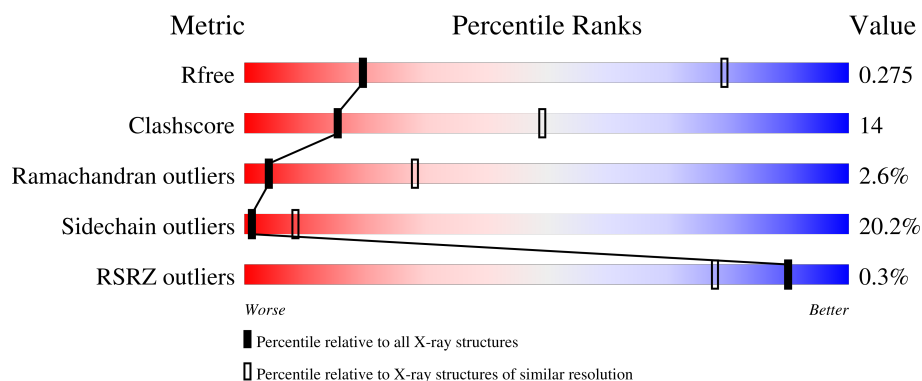
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.89 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}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	640	
1	B	640	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9407 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.

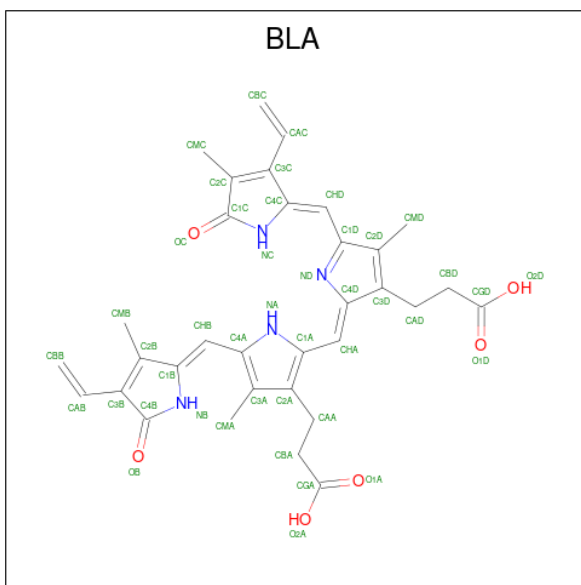
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4605	2913	838	838	16			
1	B	602	Total	C	N	O	S	0	0	0
			4716	2982	859	859	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0H2XCS3
A	-4	HIS	-	expression tag	UNP A0A0H2XCS3
A	-3	HIS	-	expression tag	UNP A0A0H2XCS3
A	-2	HIS	-	expression tag	UNP A0A0H2XCS3
A	-1	HIS	-	expression tag	UNP A0A0H2XCS3
A	0	HIS	-	expression tag	UNP A0A0H2XCS3
A	1	HIS	-	expression tag	UNP A0A0H2XCS3
A	193	GLN	LEU	engineered mutation	UNP A0A0H2XCS3
B	-5	MET	-	initiating methionine	UNP A0A0H2XCS3
B	-4	HIS	-	expression tag	UNP A0A0H2XCS3
B	-3	HIS	-	expression tag	UNP A0A0H2XCS3
B	-2	HIS	-	expression tag	UNP A0A0H2XCS3
B	-1	HIS	-	expression tag	UNP A0A0H2XCS3
B	0	HIS	-	expression tag	UNP A0A0H2XCS3
B	1	HIS	-	expression tag	UNP A0A0H2XCS3
B	193	GLN	LEU	engineered mutation	UNP A0A0H2XCS3

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

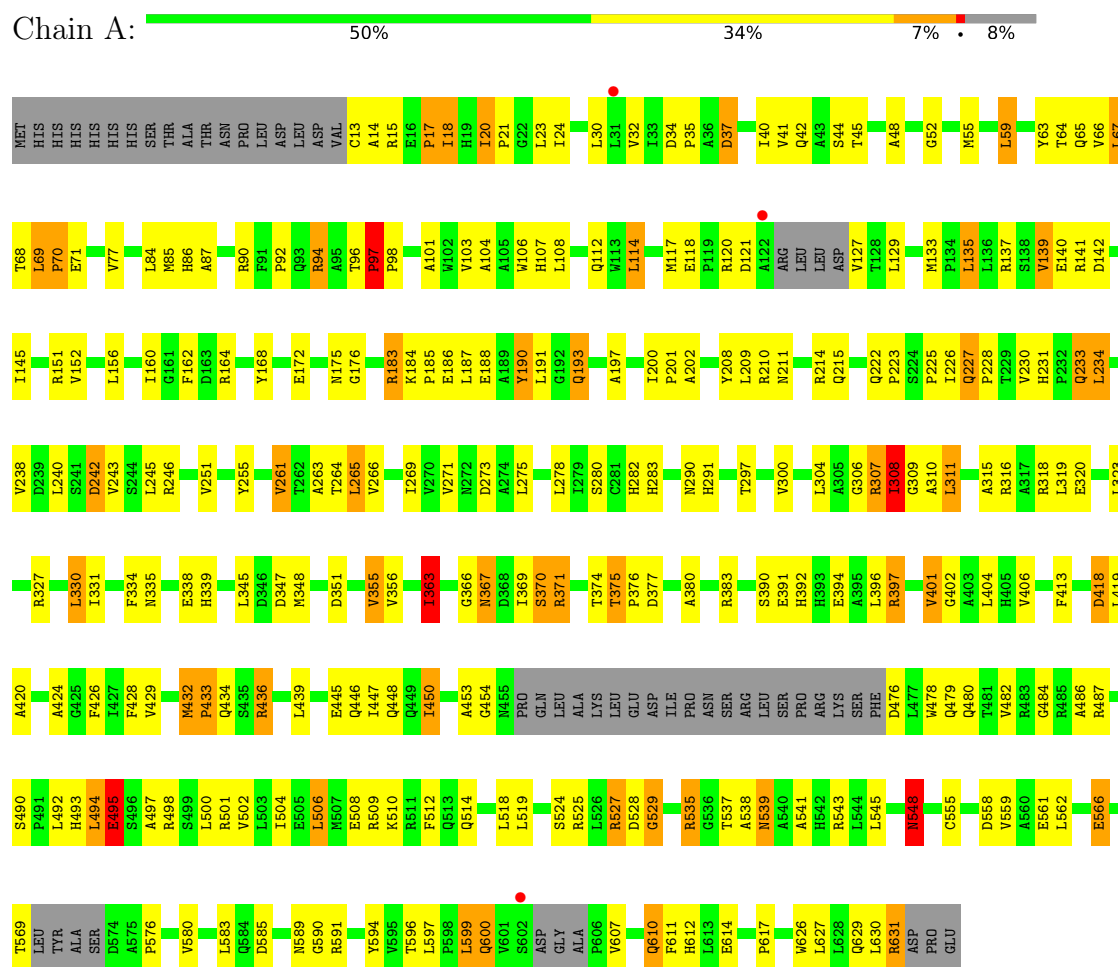


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0

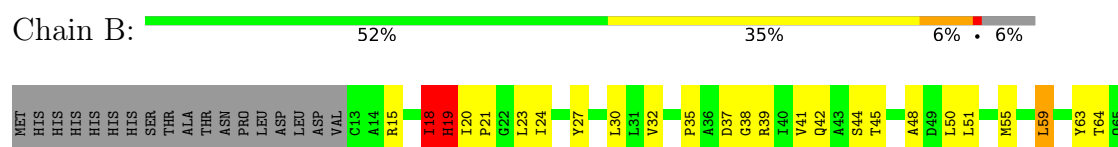
3 Residue-property plots

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: Bacteriophytochrome



• Molecule 1: Bacteriophytochrome



R577	R578	N579	V580	F581	L582	L583		L597	F598	L599	Q600	V601	A605	Y608	R609	Q610	F611	H612	L613	E614	P615	L616	P617	W626	L627	L628	Q629	L630	R631	D632	PRO	GLU																					
V482	A486	R487	L492	R493	L494	E495	R498	S499	L500	R501	V502	L503	I504	F505	L506	R507	E508	R509	K510	Q513	Q514	L518	L519	L523	S524	R525	L526	R527	D528	I533	L545	N548	F551	C555	D558	V559	R565	E566	L567	Q568	T569	L570	Y571	P576									
H405	V406	E411	V412	F413	D418	L419	A420	A424	G425	F426	V429	P430	L431	M432	P433	Q434	L344	L345	R436	L439	Q446	I447	Q448	Q449	I480	K451	W452	A453	G454	W455	PRO	GLN	LEU	ALA	LYS	LEU	GLU	ASP	ILE	PRO	ASN	SER	ARG	LEU	SER	R472	K473	S474	F475	D476	L477	W478	Q479
R316	A317	R318	L319	E320	L323	R327	L330	I331	F334	E338	H339	M340	E343	L344	L345	D346	D347	M348	D351	Q446	I447	Q448	Q449	I480	K451	W452	A453	G454	W455	PRO	GLN	LEU	ALA	LYS	LEU	GLU	ASP	ILE	PRO	ASN	SER	ARG	LEU	SER	R472	K473	S474	F475	D476	L477	W478	Q479	
Q222	P223	S224	P225	I226	Q227	P228	T229	V230	H231	P232	Q233	L234	V238	D239	L240	S241	D242	V243	S244	R246	V251	H252	V261	T262	A263	T264	L265	V266	V271	N272	D273	S280	C281	H282	H283	N290	M293	R294	D295	V296	T297	V300	T303	I308	Q312	A315							
R141	D142	G143	E147	R151	V152	L156	L159	I160	R164	Y168	R169	F170	D171	E172	E173	W174	W175	G176	I179	R183	K184	P185	E186	L187	E188	A189	Y190	L191	G192	Q193	H194	Y195	P196	A197	I200	Q203	A204	Y208	L209	R210	N211	V212	V213	R214	Q215	I216							
V66	L67	T68	L69	P70	E71	A72	Q73	V77	Q80	L84	M85	H86	A87	R90	F91	T96	P97	P98	A99	S100	A101	W102	V103	A104	A105	W106	H107	L108	Q112	W113	L114	M117	E118	P119	R120	D121	A122	R123	LEU	LEU	ASP	W127	T128	L129	M133	P134	L135	L136	R137	E140			

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.22Å 103.22Å 344.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.89 49.43 – 3.89	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.43-3.89) 99.7 (49.43-3.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.33	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.88Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.213 , 0.270 (Not available) , 0.275	Depositor DCC
R_{free} test set	895 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	187.1	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 191.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å ²)	212.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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	0.88	3/4708 (0.1%)	1.46	45/6420 (0.7%)
1	B	0.89	1/4824 (0.0%)	1.45	42/6579 (0.6%)
All	All	0.89	4/9532 (0.0%)	1.45	87/12999 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	VAL	CA-C	5.17	1.59	1.52
1	A	97	PRO	CA-C	5.16	1.56	1.52
1	A	600	GLN	CA-C	5.07	1.59	1.53
1	A	121	ASP	CA-C	5.03	1.57	1.52

The worst 5 of 87 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ASP	CA-CB-CG	9.76	122.36	112.60
1	A	142	ASP	CA-CB-CG	9.43	122.03	112.60
1	B	419	LEU	CA-C-N	7.31	129.22	120.09
1	B	419	LEU	C-N-CA	7.31	129.22	120.09
1	A	308	ILE	N-CA-CB	7.05	120.67	110.52

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	A	4605	0	4594	132	0
1	B	4716	0	4702	125	0
2	A	43	0	31	10	0
2	B	43	0	31	11	0
All	All	9407	0	9358	254	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 14.

The worst 5 of 254 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:B:208:TYR:OH	2:B:900:BLA:HAA1	1.52	1.09
1:A:599:LEU:HG	1:A:600:GLN:H	1.25	0.98
1:B:21:PRO:HD2	1:B:240:LEU:HD23	1.55	0.89
1:A:599:LEU:HG	1:A:600:GLN:N	1.90	0.86
1:B:42:GLN:HA	1:B:228:PRO:HG2	1.56	0.86

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	578/640 (90%)	496 (86%)	68 (12%)	14 (2%)	4	29
1	B	596/640 (93%)	519 (87%)	60 (10%)	17 (3%)	3	26
All	All	1174/1280 (92%)	1015 (86%)	128 (11%)	31 (3%)	4	28

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	VAL
1	B	19	HIS
1	B	401	VAL
1	A	140	GLU
1	A	366	GLY

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	485/532 (91%)	388 (80%)	97 (20%)	1	9
1	B	496/532 (93%)	395 (80%)	101 (20%)	1	8
All	All	981/1064 (92%)	783 (80%)	198 (20%)	1	8

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	123	ARG
1	B	264	THR
1	B	141	ARG
1	B	200	ILE
1	B	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	405	HIS
1	B	455	ASN
1	A	455	ASN
1	A	405	HIS
1	B	479	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	A	900	1	46,46,46	1.82	10 (21%)	66,67,67	2.18	17 (25%)
2	BLA	B	900	1	46,46,46	1.57	10 (21%)	66,67,67	2.56	20 (30%)

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	A	900	1	-	8/26/74/74	0/4/4/4
2	BLA	B	900	1	-	8/26/74/74	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	C3B-C2B	5.75	1.48	1.37
2	A	900	BLA	CHB-C1B	4.68	1.49	1.37
2	B	900	BLA	CHA-C4D	4.28	1.46	1.38
2	B	900	BLA	C3B-C2B	4.18	1.45	1.37
2	A	900	BLA	CHB-C4A	4.09	1.49	1.40

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3B-C4B-NB	8.19	116.42	106.13
2	B	900	BLA	C2A-C1A-NA	6.57	115.81	107.57
2	B	900	BLA	C1B-NB-C4B	-6.50	102.68	110.66
2	B	900	BLA	C3A-C4A-NA	6.36	116.11	107.43
2	B	900	BLA	C2B-C1B-NB	5.96	115.66	106.97

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

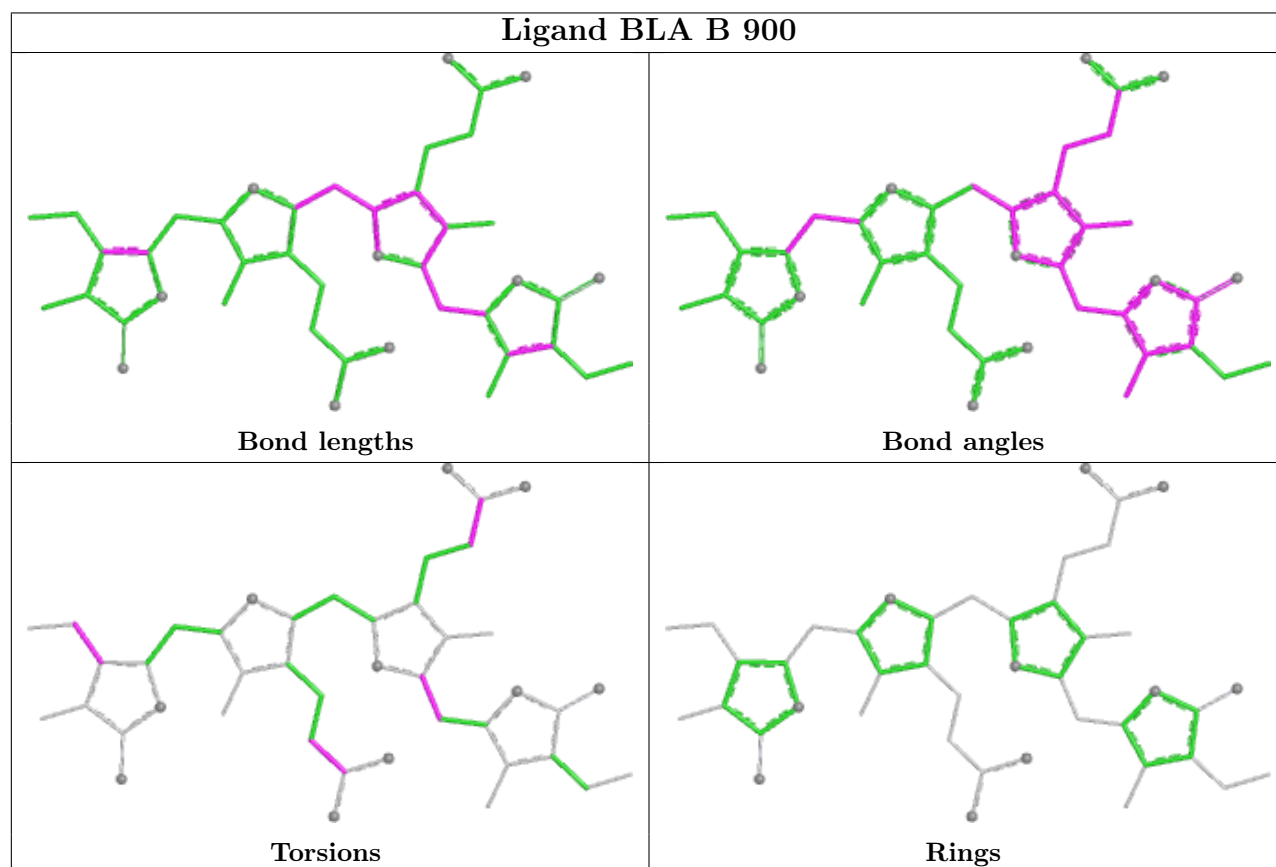
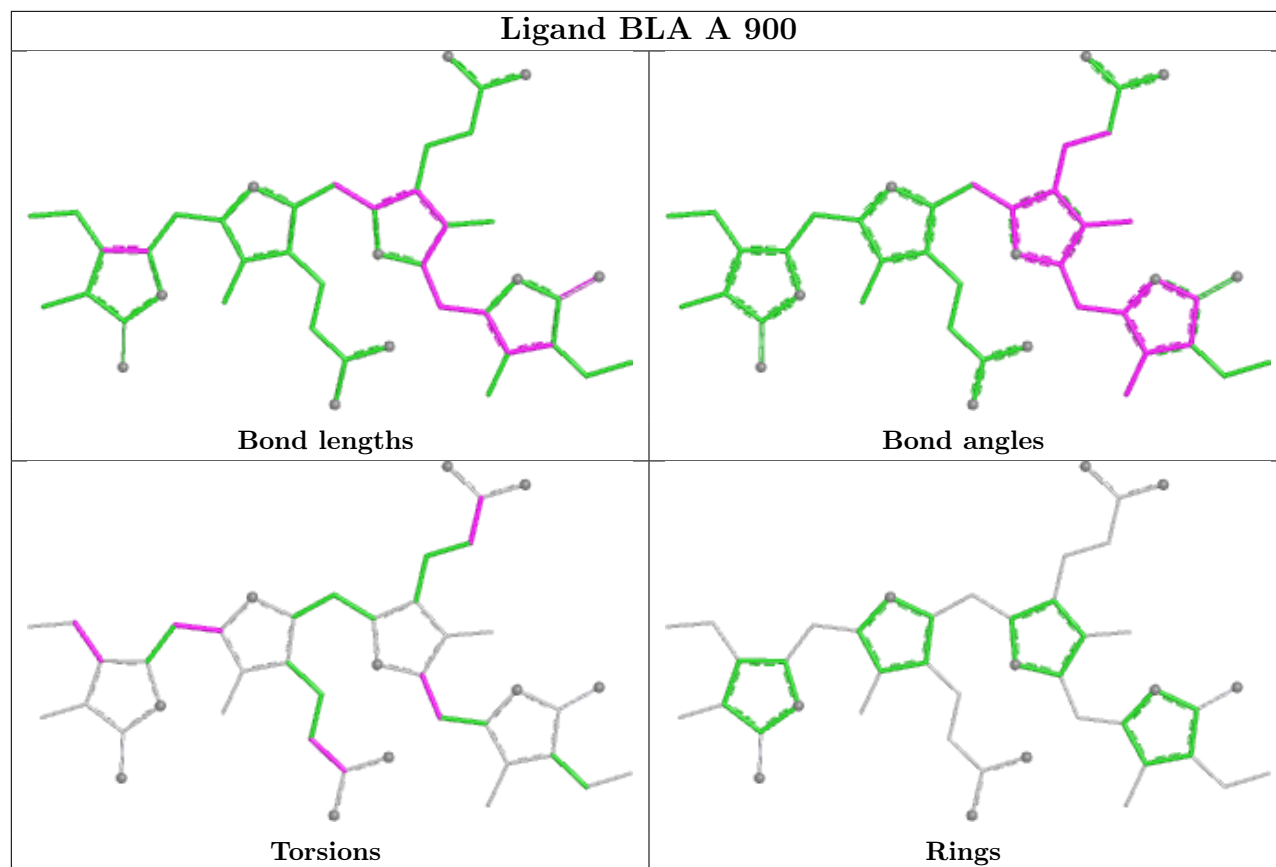
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C2C-C3C-CAC-CBC

There are no ring outliers.

2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	10	0
2	B	900	BLA	11	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	588/640 (91%)	-0.33	3 (0%) 87 72	141, 211, 257, 280	0
1	B	602/640 (94%)	-0.44	0 100 100	147, 213, 268, 280	0
All	All	1190/1280 (92%)	-0.38	3 (0%) 90 78	141, 212, 266, 280	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	2.3
1	A	31	LEU	2.2
1	A	602	SER	2.1

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](#)

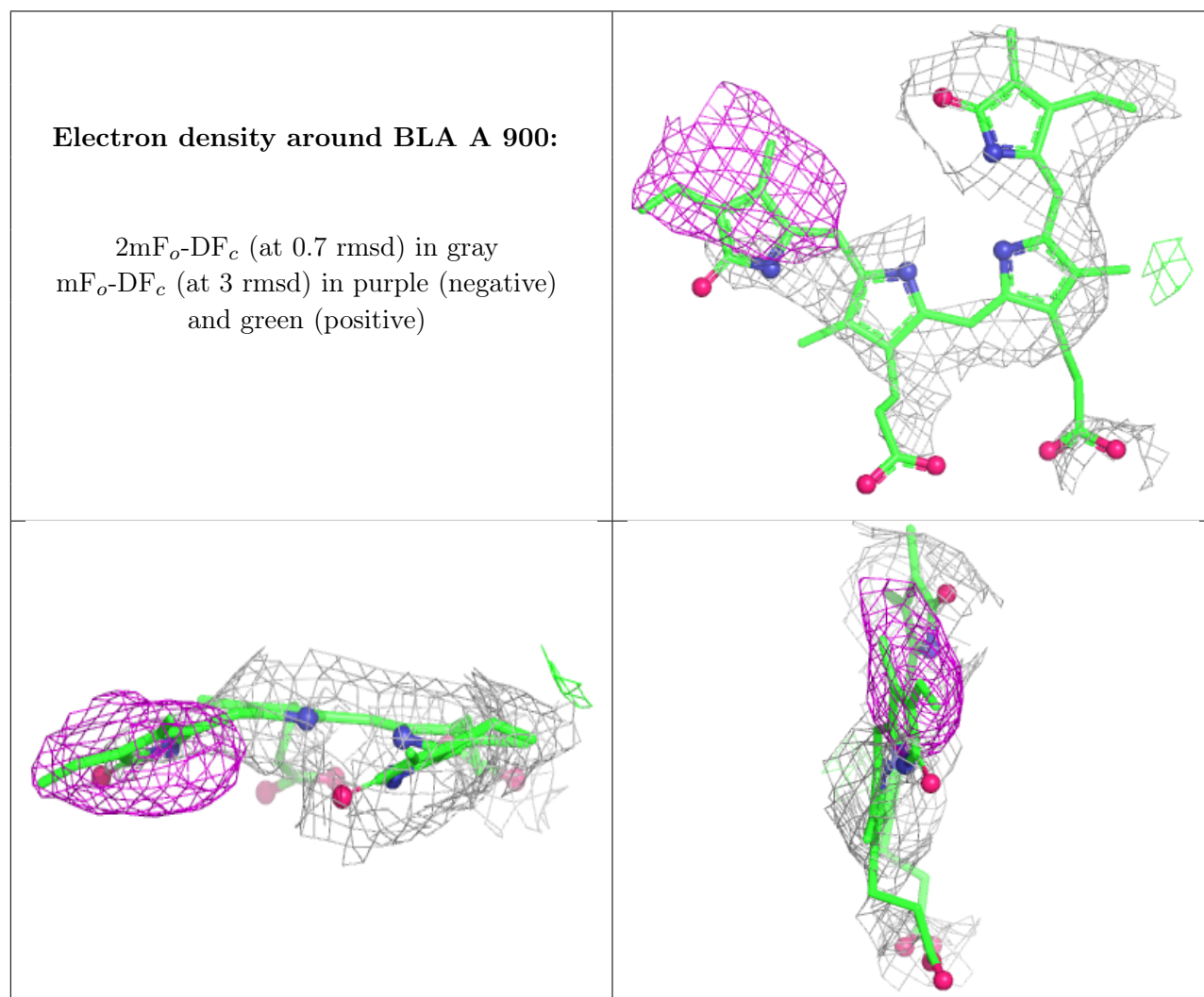
There are no oligosaccharides in this entry.

6.4 Ligands [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, 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.

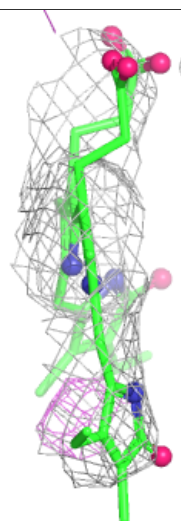
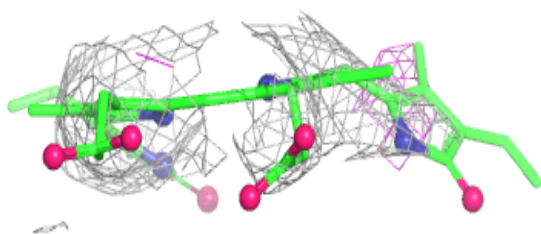
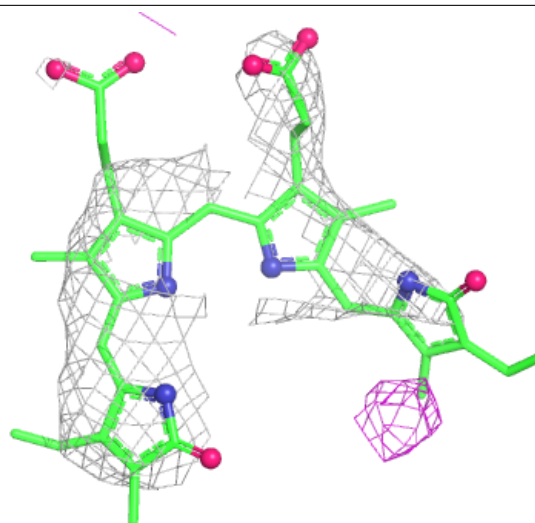
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	A	900	43/43	0.87	0.11	178,184,186,187	0
2	BLA	B	900	43/43	0.92	0.10	213,218,221,222	0

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 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.