



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 10:49 pm BST

PDB ID : 4R6L
Title : Crystal structure of bacteriophytochrome RpBphP2 from photosynthetic bacterium *R. palustris*
Authors : Yang, X.; Stojkovic, E.; Ozarowski, W.; Kuk, J.; Davydova, E.; Moffat, K.
Deposited on : 2014-08-25
Resolution : 3.40 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 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

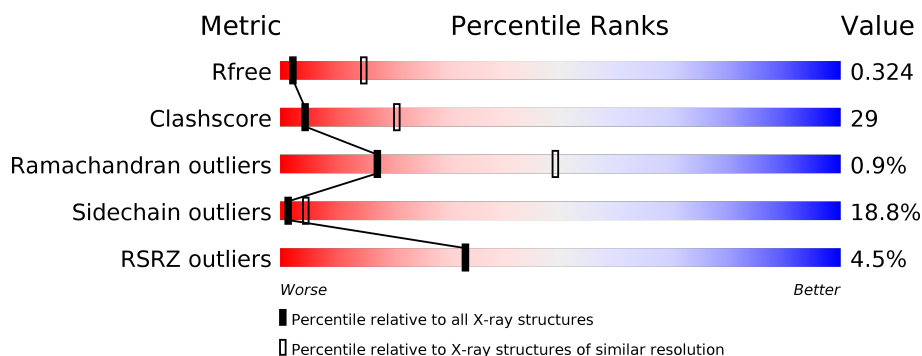
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 ≥ 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	519	<div> <div>2%</div> <div>42%</div> <div>39%</div> <div>10%</div> <div>9%</div> </div>
1	B	519	<div> <div>6%</div> <div>37%</div> <div>38%</div> <div>11%</div> <div>14%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7198 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 (Light-regulated signal transduction histidine kinase), PhyB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3639	2295	659	671	14			
1	B	448	Total	C	N	O	S	0	0	0
			3473	2191	627	641	14			

There are 26 discrepancies between the modelled and reference sequences:

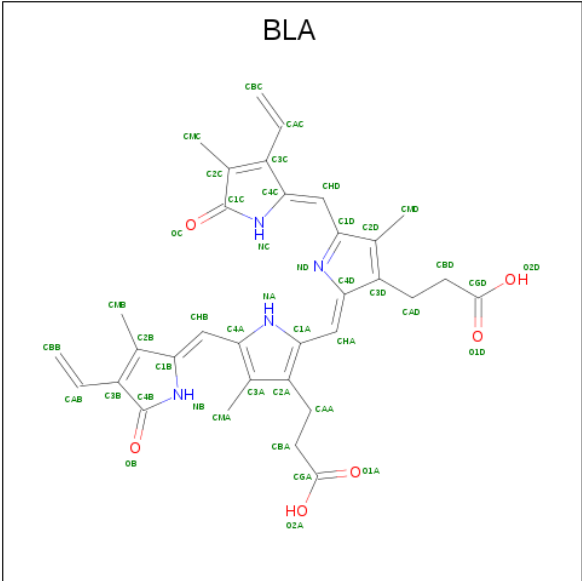
Chain	Residue	Modelled	Actual	Comment	Reference
A	507	LYS	-	EXPRESSION TAG	UNP Q6N5G3
A	508	LEU	-	EXPRESSION TAG	UNP Q6N5G3
A	509	ALA	-	EXPRESSION TAG	UNP Q6N5G3
A	510	ALA	-	EXPRESSION TAG	UNP Q6N5G3
A	511	ALA	-	EXPRESSION TAG	UNP Q6N5G3
A	512	LEU	-	EXPRESSION TAG	UNP Q6N5G3
A	513	GLU	-	EXPRESSION TAG	UNP Q6N5G3
A	514	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	515	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	516	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	517	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	518	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	519	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	507	LYS	-	EXPRESSION TAG	UNP Q6N5G3
B	508	LEU	-	EXPRESSION TAG	UNP Q6N5G3
B	509	ALA	-	EXPRESSION TAG	UNP Q6N5G3
B	510	ALA	-	EXPRESSION TAG	UNP Q6N5G3
B	511	ALA	-	EXPRESSION TAG	UNP Q6N5G3
B	512	LEU	-	EXPRESSION TAG	UNP Q6N5G3
B	513	GLU	-	EXPRESSION TAG	UNP Q6N5G3
B	514	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	515	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	516	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	517	HIS	-	EXPRESSION TAG	UNP Q6N5G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	518	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	519	HIS	-	EXPRESSION TAG	UNP Q6N5G3

- 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		

V488	A489	A490	A491	V492	E493	I494	R495	D496	L497	I498	I499	D500	V501	I502	LEU	ARG	ASN	THR	LYS	ALA	ALA	ALA	LEU	ALA	ALA	LEU	GLU	HIS	HIS	HIS	HIS	VAL	THR	ALA	GLU	SER	GLY	ARG	LEU	ARG	PRO	R466	T467	S468	P469	W472	T473	E474	Q475	T476	H477	G478	R479	A480	I481	A482	W483	Q484	P485	H486	L487	E487																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
E352	A353	L281	E285	R286	K288	S361	G362	L363	C364	L365	H366	S367	R368	Q298	A308	W309	Q310	Q376	T377	P378	P379	I382	L383	D384	Q385	Q388	L389	A390	G391	R392	S396	E397	L398	F399	Q400	T401	D402	R403	L404	S405	T406	I407	L408	P409	E410	A415	A418	S419	G420	V421	L422	A423	E351	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L347	A348	R349	N350	S351	D342	H343	R344	A345	G346	L34

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	174.40 Å 174.40 Å 95.67 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.02 – 3.40 49.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.3 (49.02-3.40) 95.5 (49.02-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.40 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.268 , 0.322 0.273 , 0.324	Depositor DCC
R_{free} test set	1121 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	114.4	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 91.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.105 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7198	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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	0.40	0/3716	0.83	3/5057 (0.1%)
1	B	0.43	0/3546	0.87	6/4825 (0.1%)
All	All	0.41	0/7262	0.85	9/9882 (0.1%)

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	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	355	LEU	CA-CB-CG	6.93	131.24	115.30
1	B	333	LEU	CB-CG-CD1	6.18	121.51	111.00
1	A	89	ALA	C-N-CD	-5.63	108.21	120.60
1	B	354	LEU	CA-CB-CG	5.58	128.13	115.30
1	A	273	LEU	CA-CB-CG	5.28	127.44	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	341	HIS	Peptide

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Mol	Chain	Res	Type	Group
1	B	38	ASP	Peptide
1	B	426	LEU	Peptide
1	B	68	PHE	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	3639	0	3625	197	0
1	B	3473	0	3453	220	0
2	A	43	0	31	5	0
2	B	43	0	31	7	0
All	All	7198	0	7140	412	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 29.

The worst 5 of 412 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:202:ASP:OD1	1:B:466:ARG:NH2	1.95	1.00
1:B:274:ARG:NH1	1:B:308:ALA:O	1.99	0.94
1:A:75:ARG:NH2	1:A:92:ALA:O	2.01	0.94
1:B:330:GLN:NE2	1:B:493:GLU:OE2	2.01	0.93
1:B:451:ASN:OD1	1:B:453:ASP:N	2.05	0.90

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	463/519 (89%)	429 (93%)	30 (6%)	4 (1%)	17	49
1	B	436/519 (84%)	398 (91%)	34 (8%)	4 (1%)	17	49
All	All	899/1038 (87%)	827 (92%)	64 (7%)	8 (1%)	17	49

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	379	PRO
1	A	430	PRO
1	B	111	ASP
1	B	379	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	382/418 (91%)	313 (82%)	69 (18%)	1	6
1	B	368/418 (88%)	296 (80%)	72 (20%)	1	4
All	All	750/836 (90%)	609 (81%)	141 (19%)	1	4

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	472	TRP
1	B	91	ILE
1	B	451	ASN
1	A	479	ARG
1	B	35	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	305	GLN
1	A	330	GLN
1	B	29	HIS
1	B	143	GLN
1	B	255	HIS

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 carbohydrates 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	36,46,46	3.00	18 (50%)	47,67,67	2.24	14 (29%)
2	BLA	B	900	1	36,46,46	3.13	14 (38%)	47,67,67	2.24	14 (29%)

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	-	3/22/74/74	0/4/4/4
2	BLA	B	900	1	-	8/22/74/74	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	CHB-C1B	9.18	1.53	1.34
2	B	900	BLA	CHB-C1B	9.12	1.53	1.34
2	A	900	BLA	CHD-C4C	6.80	1.54	1.38
2	B	900	BLA	CHD-C4C	6.65	1.53	1.38
2	A	900	BLA	CHD-C1D	6.20	1.54	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C1A-CHA-C4D	-9.02	118.03	128.81
2	A	900	BLA	C1A-CHA-C4D	-8.74	118.37	128.81
2	A	900	BLA	CHA-C4D-ND	5.02	135.79	128.83
2	B	900	BLA	CHD-C1D-ND	4.81	134.99	124.93
2	A	900	BLA	C4C-CHD-C1D	-4.23	117.75	128.08

There are no chirality outliers.

5 of 11 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	B	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	NB-C1B-CHB-C4A

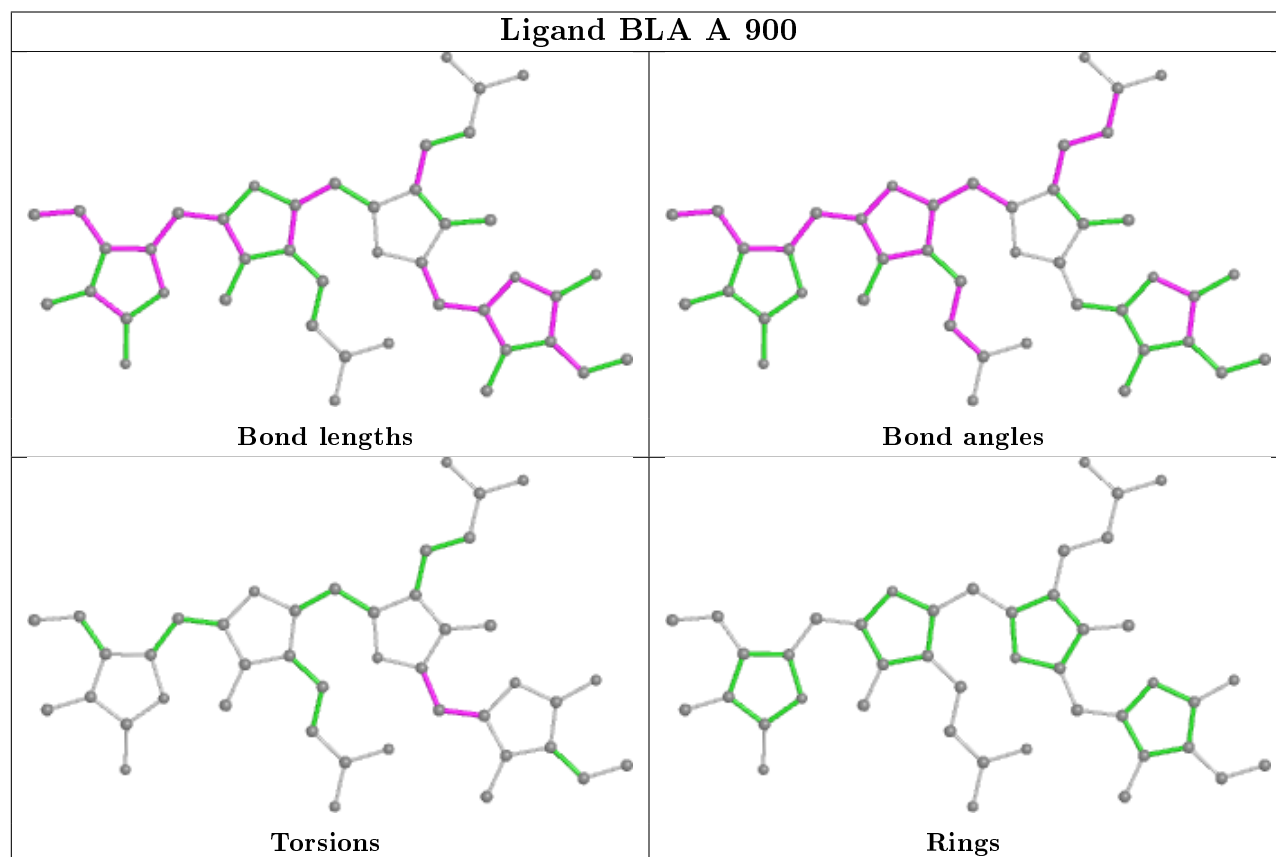
There are no ring outliers.

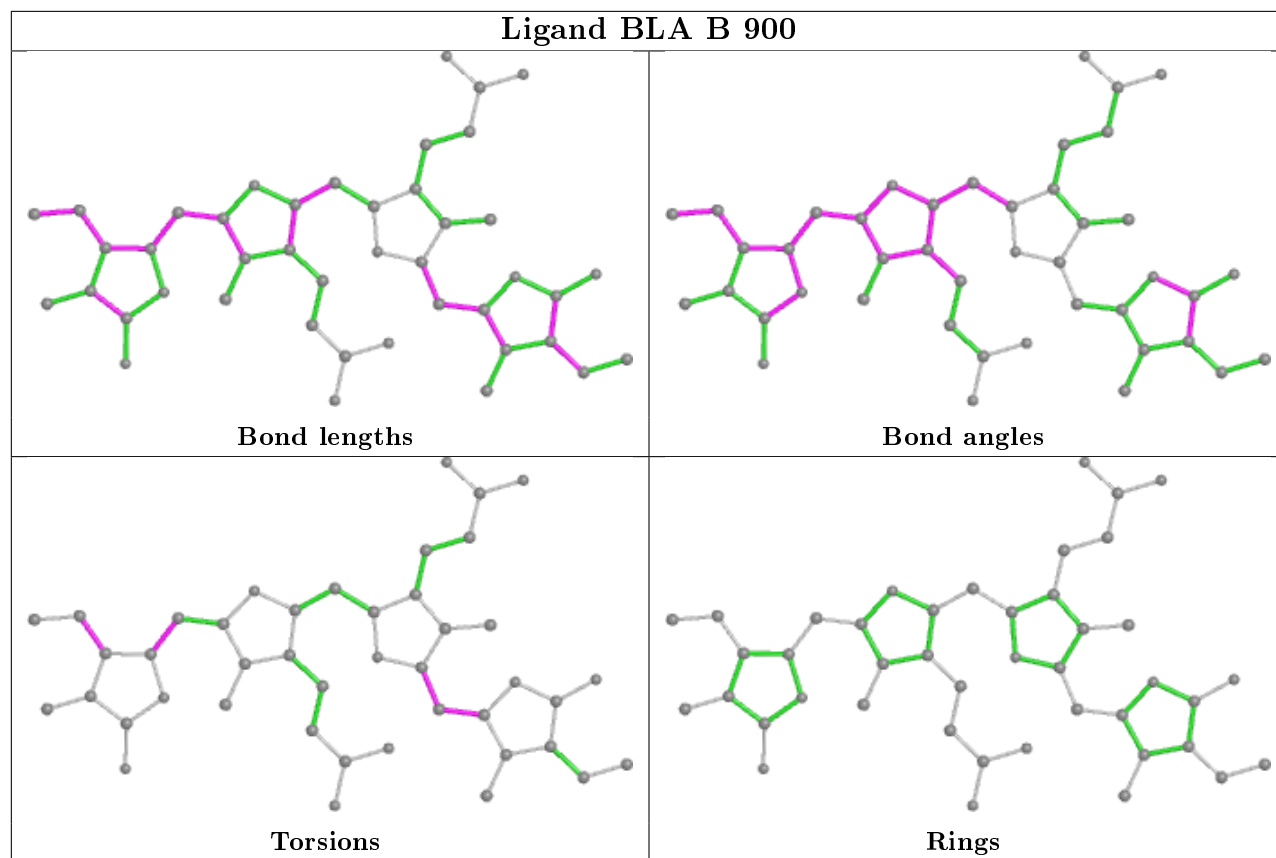
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	5	0
2	B	900	BLA	7	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	473/519 (91%)	0.13	9 (1%) 66 65	93, 131, 185, 270	0
1	B	448/519 (86%)	0.43	32 (7%) 16 18	119, 172, 245, 344	0
All	All	921/1038 (88%)	0.28	41 (4%) 33 33	93, 149, 232, 344	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	226	PRO	6.0
1	B	236	VAL	4.7
1	B	103	PHE	4.6
1	B	237	THR	4.6
1	B	191	GLU	3.7

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 carbohydrates in this entry.

6.4 Ligands [i](#)

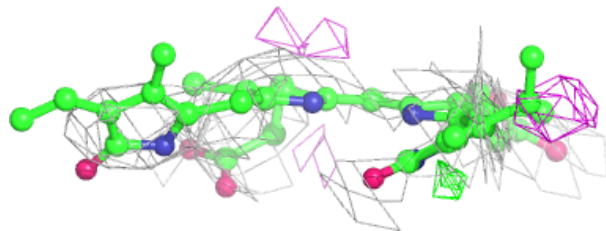
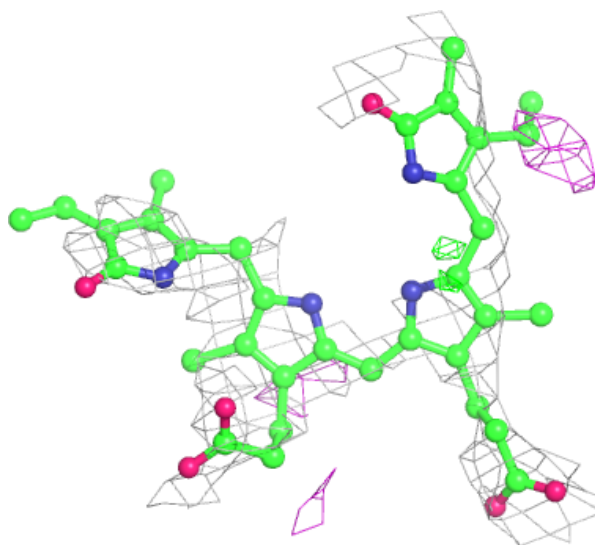
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

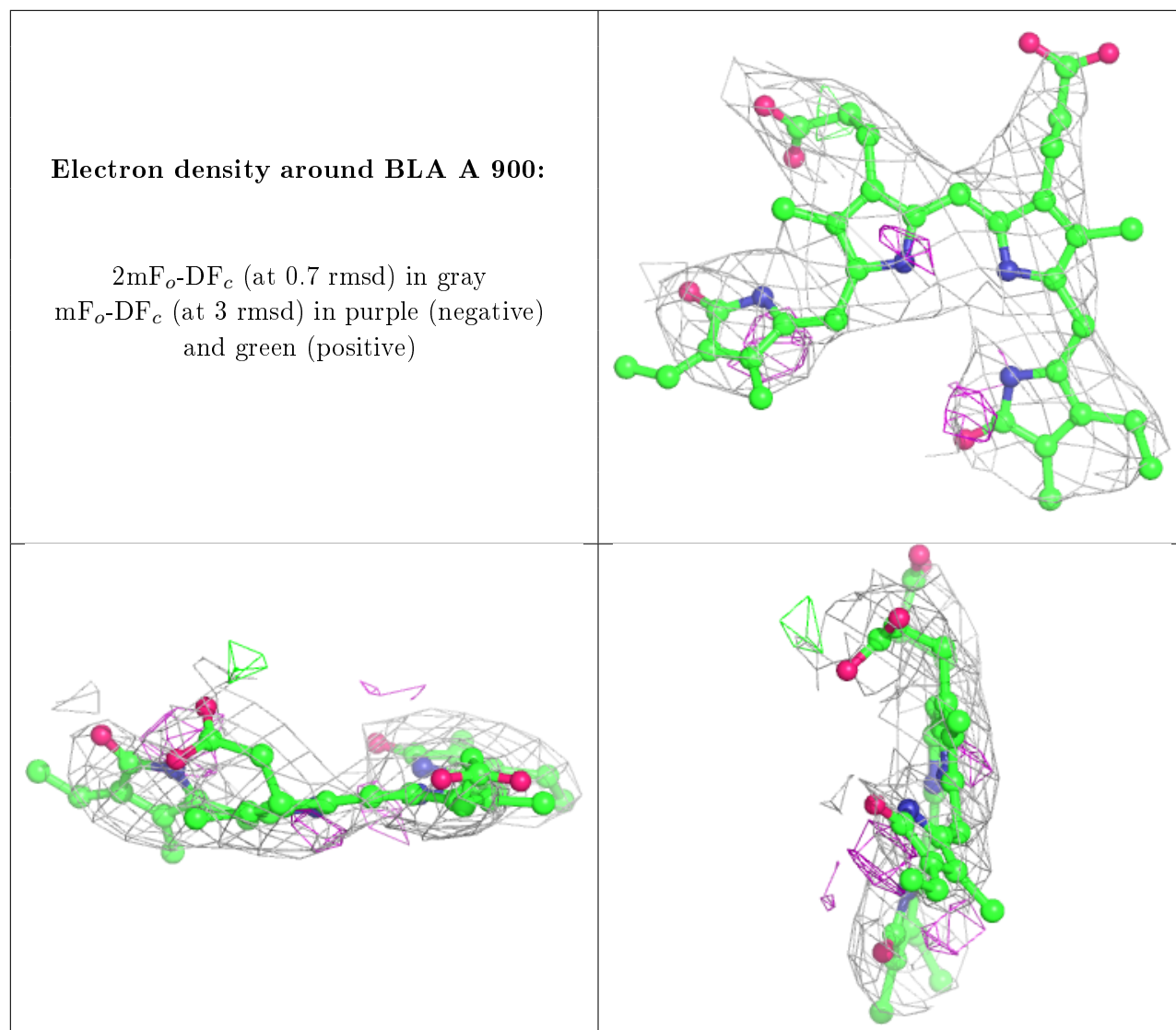
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BLA	B	900	43/43	0.89	0.56	140,153,180,212	0
2	BLA	A	900	43/43	0.90	0.50	90,114,146,153	0

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 ⓘ

There are no such residues in this entry.