



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2020 – 06:48 am BST

PDB ID : 4S21
Title : Crystal structure of the photosensory core module of bacteriophytochrome RPA3015 from *R. palustris*
Authors : Yang, X.; Stojkovi, E.A.; Ozarowski, W.B.; Moffat, K.
Deposited on : 2015-01-17
Resolution : 3.25 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

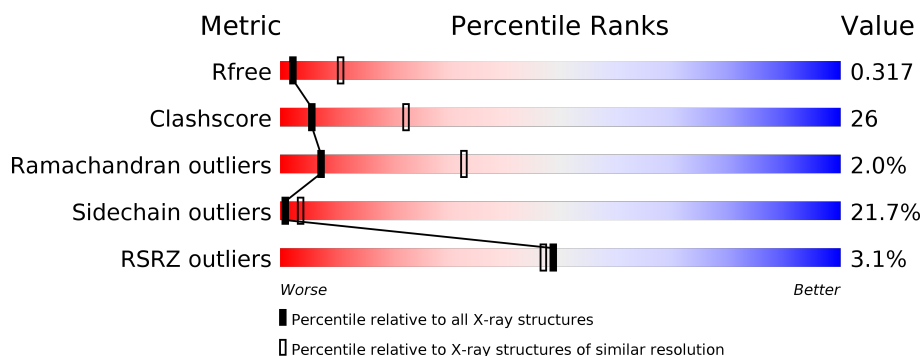
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	525	<div> <div> <div></div> <div>42%</div> <div>34%</div> <div>12%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	525	<div> <div>5%</div> <div>39%</div> <div>38%</div> <div>9%</div> <div>13%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7251 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	455	Total	C	N	O	S	0	0	0
			3525	2221	638	651	15			

There are 40 discrepancies between the modelled and reference sequences:

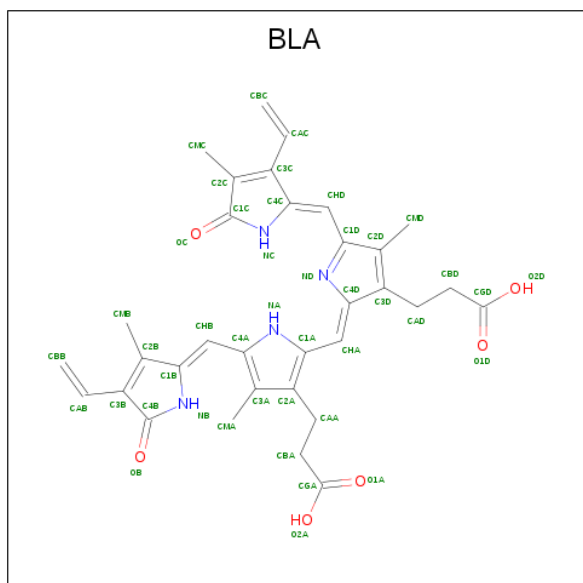
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q6N5G3
A	-18	GLY	-	EXPRESSION TAG	UNP Q6N5G3
A	-17	SER	-	EXPRESSION TAG	UNP Q6N5G3
A	-16	SER	-	EXPRESSION TAG	UNP Q6N5G3
A	-15	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-14	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-13	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-12	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-11	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-10	HIS	-	EXPRESSION TAG	UNP Q6N5G3
A	-9	SER	-	EXPRESSION TAG	UNP Q6N5G3
A	-8	SER	-	EXPRESSION TAG	UNP Q6N5G3
A	-7	GLY	-	EXPRESSION TAG	UNP Q6N5G3
A	-6	LEU	-	EXPRESSION TAG	UNP Q6N5G3
A	-5	VAL	-	EXPRESSION TAG	UNP Q6N5G3
A	-4	PRO	-	EXPRESSION TAG	UNP Q6N5G3
A	-3	ARG	-	EXPRESSION TAG	UNP Q6N5G3
A	-2	GLY	-	EXPRESSION TAG	UNP Q6N5G3
A	-1	SER	-	EXPRESSION TAG	UNP Q6N5G3
A	0	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-19	MET	-	EXPRESSION TAG	UNP Q6N5G3
B	-18	GLY	-	EXPRESSION TAG	UNP Q6N5G3
B	-17	SER	-	EXPRESSION TAG	UNP Q6N5G3
B	-16	SER	-	EXPRESSION TAG	UNP Q6N5G3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-14	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-13	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-12	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-11	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-10	HIS	-	EXPRESSION TAG	UNP Q6N5G3
B	-9	SER	-	EXPRESSION TAG	UNP Q6N5G3
B	-8	SER	-	EXPRESSION TAG	UNP Q6N5G3
B	-7	GLY	-	EXPRESSION TAG	UNP Q6N5G3
B	-6	LEU	-	EXPRESSION TAG	UNP Q6N5G3
B	-5	VAL	-	EXPRESSION TAG	UNP Q6N5G3
B	-4	PRO	-	EXPRESSION TAG	UNP Q6N5G3
B	-3	ARG	-	EXPRESSION TAG	UNP Q6N5G3
B	-2	GLY	-	EXPRESSION TAG	UNP Q6N5G3
B	-1	SER	-	EXPRESSION TAG	UNP Q6N5G3
B	0	HIS	-	EXPRESSION TAG	UNP Q6N5G3

- 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	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		

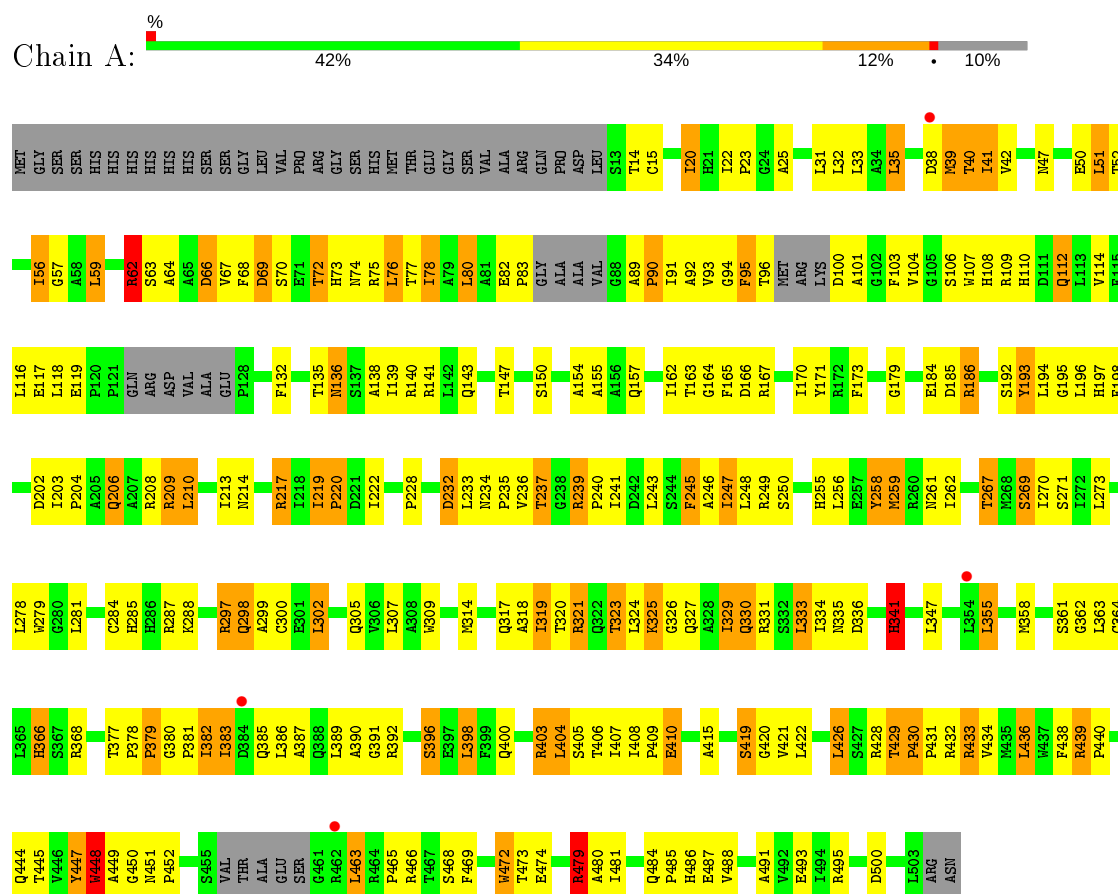
- Molecule 3 is water.

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

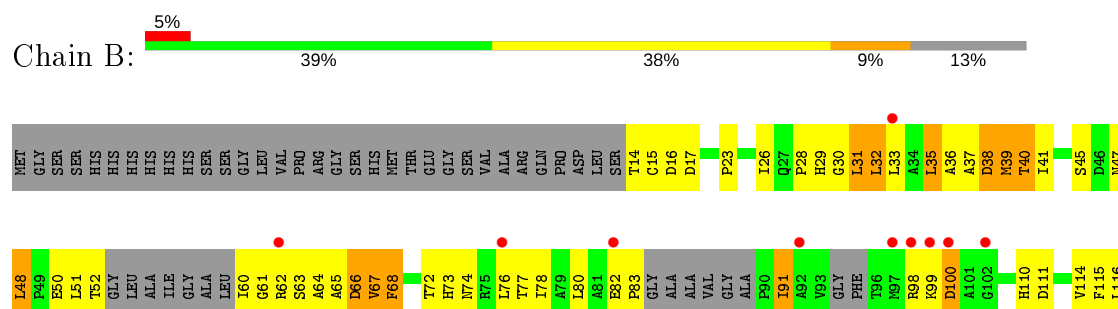
3 Residue-property plots

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

- Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB1



- Molecule 1: Bacteriophytochrome (Light-regulated signal transduction histidine kinase), PhyB1



A489	S419	A348	R274	S201	E117
A490	G420		G275	D202	L118
A491	V421	S351	E276	I203	E119
V492	L422	E352	R277	P204	P120
E493	A423	A353	L278	A205	P121
I494	V424	L354	L279	Q206	GLN
R495	P425	L355	G280	A207	ARG
D496	L426	E356	L281	R208	ASP
L497	S427	L357		R209	VAL
I498	R428	K358	H285	L210	ALA
I499	T429		H286	Y211	GLU
D500	P430		R287		PRO
V501	P431		K288	N214	GLN
I502	R432		P289	P215	ALA
LEU	R433	C364	H290	V216	F132
ARG	V434	L365	Y291	R217	F131
ASN				I218	R133
	V437	H366	E301	I219	R134
	F438	G362	L302	P220	T135
	R439	L363		E221	M136
	P440	C364		I222	S137
	E441			N223	A138
				Y224	I139
					R140
	V448	T373	A308	V227	R141
	A449	I374	K309		L142
	G450	G375	G310		
	M451	Q376	I311	T230	
	P452	T377	G312	P231	E146
	D453	P378	V313	D232	
	K454	P379		L233	G152
	S455			N234	
	VAL	I382	E316	P235	V159
	THR	L383	Q317		R160
	ALA	D384	A318	R239	E161
	GLU	Q385	T320	P240	I162
	SER	L386	R321	I241	
	GLY	A387	Q322	D242	F165
	ARG	Q388	T323	L243	D166
	LEU	L389	L324		R167
	ARG	A390	K325	T247	V168
	ARG	G391	G326	L248	M169
	PRO	R392		R249	I170
	R466	S393	I329		Y171
			Q330	S252	R172
	F469	L398	R331	P253	F173
	V472	F399	S332		
		Q400	L333	L256	D176
	T476	T401	I334		G179
	H477	D402	N335	M259	
	G478	R403	D336	R260	
	R479	L404	I337	N261	C187
	A480	S405	E338	I262	
	I481	T406	Q339	G263	V190
	V483	I407	L340	N264	
	Q484	P409			Y193
	P485	E410	H343	T267	L196
	H486		R344	M268	H197
	E487	A415	A345	S269	F198
	V488		G346	I270	

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	175.36 Å 175.36 Å 96.19 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.89 – 3.25 42.17 – 3.05	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.89-3.25) 61.9 (42.17-3.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 3.06 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.262 , 0.316 0.270 , 0.317	Depositor DCC
R_{free} test set	997 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	108.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.107 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7251	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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	0.34	0/3716	0.64	4/5057 (0.1%)
1	B	0.32	0/3598	0.69	1/4893 (0.0%)
All	All	0.33	0/7314	0.66	5/9950 (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	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	89	ALA	C-N-CD	-5.66	108.14	120.60
1	A	62	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	355	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	100	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (5) 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	A	448	TRP	Peptide
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	186	0
1	B	3525	0	3507	181	0
2	A	43	0	31	10	0
2	B	43	0	31	10	0
3	A	1	0	0	1	0
All	All	7251	0	7194	370	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 26.

The worst 5 of 370 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:322:GLN:HG3	1:B:486:HIS:HA	1.50	0.94
1:A:75:ARG:NH2	1:A:92:ALA:O	2.06	0.88
1:B:202:ASP:OD1	1:B:466:ARG:NH2	2.10	0.83
1:A:141:ARG:HH21	1:A:154:ALA:HA	1.48	0.79
2:A:900:BLA:ND	3:A:1001:HOH:O	2.16	0.79

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	463/525 (88%)	418 (90%)	38 (8%)	7 (2%)	10	39
1	B	443/525 (84%)	398 (90%)	34 (8%)	11 (2%)	5	28
All	All	906/1050 (86%)	816 (90%)	72 (8%)	18 (2%)	7	33

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	430	PRO
1	B	66	ASP
1	A	164	GLY
1	A	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	382/424 (90%)	291 (76%)	91 (24%)	0	2
1	B	373/424 (88%)	300 (80%)	73 (20%)	1	5
All	All	755/848 (89%)	591 (78%)	164 (22%)	1	4

5 of 164 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	419	SER
1	B	31	LEU
1	B	402	ASP
1	A	429	THR
1	A	448	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	285	HIS
1	A	330	GLN
1	B	29	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	B	900	1	36,46,46	3.05	15 (41%)	47,67,67	2.23	14 (29%)
2	BLA	A	900	1	36,46,46	3.11	19 (52%)	47,67,67	2.12	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	B	900	1	-	7/22/74/74	0/4/4/4
2	BLA	A	900	1	-	3/22/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHB-C1B	9.17	1.53	1.34
2	A	900	BLA	CHB-C1B	8.37	1.51	1.34
2	A	900	BLA	CHD-C4C	6.87	1.54	1.38
2	A	900	BLA	CHD-C1D	6.47	1.55	1.40
2	B	900	BLA	CHD-C4C	6.23	1.52	1.38

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	-8.16	119.06	128.81
2	A	900	BLA	CHA-C4D-ND	5.83	136.91	128.83
2	B	900	BLA	CAD-C3D-C4D	4.85	133.59	125.01
2	A	900	BLA	CHA-C4D-C3D	-4.76	114.32	125.32
2	A	900	BLA	C1A-CHA-C4D	-4.73	123.16	128.81

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

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

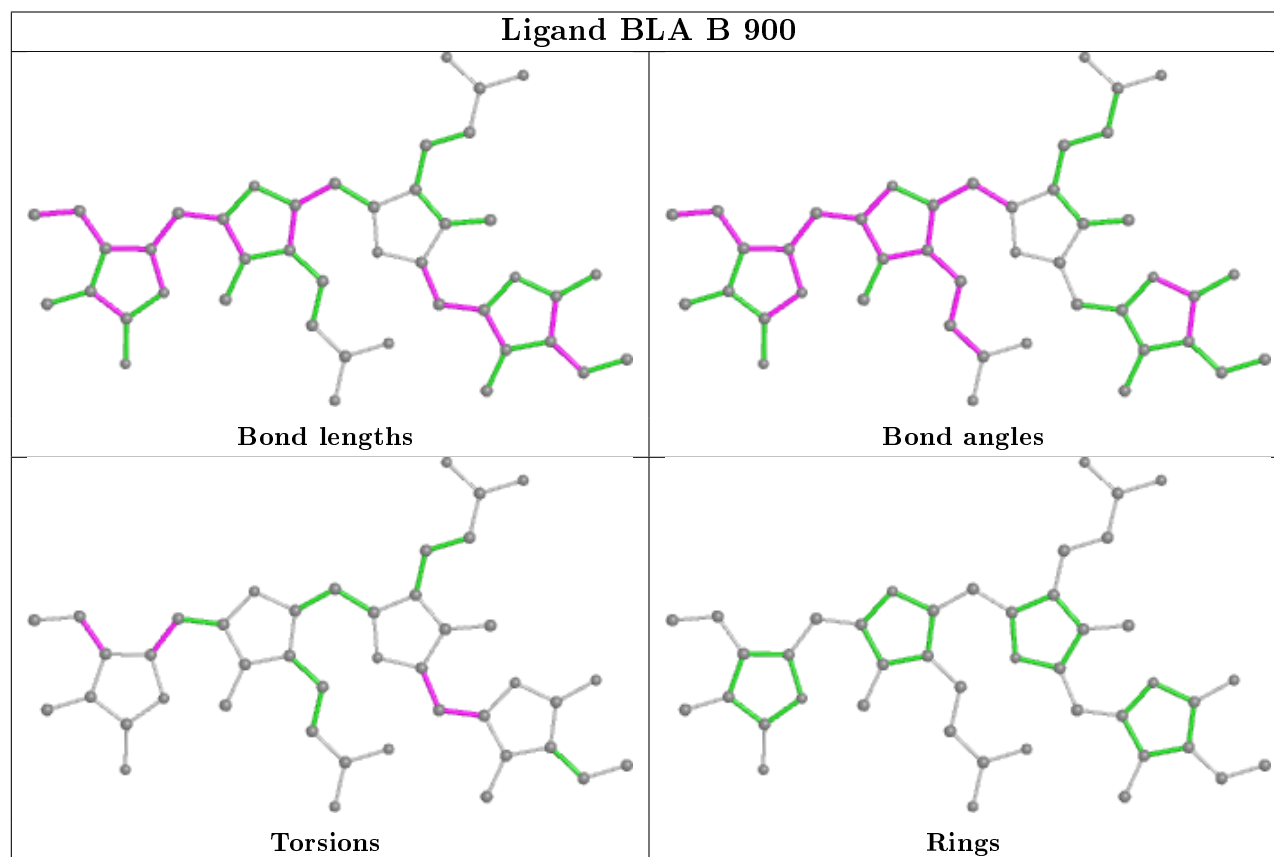
There are no ring outliers.

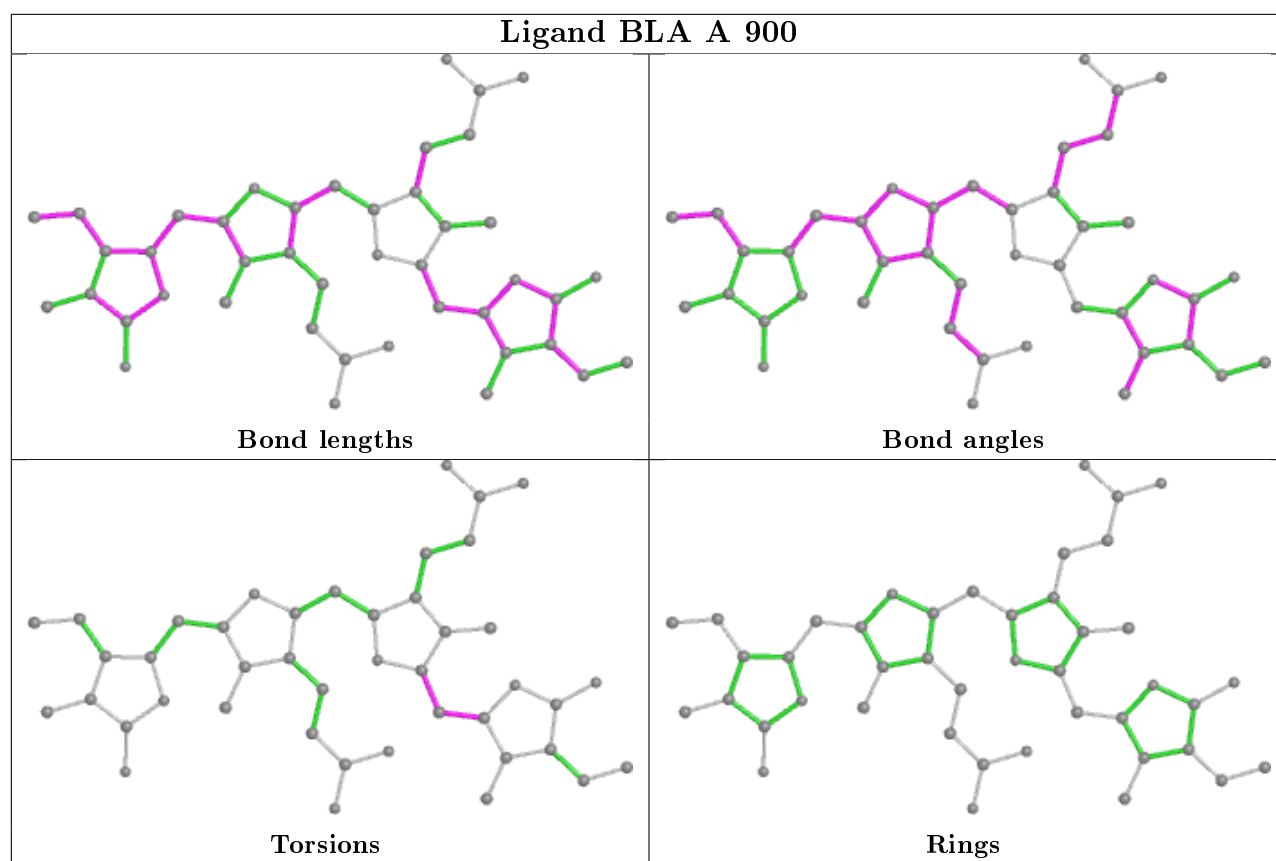
2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	10	0
2	A	900	BLA	10	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	473/525 (90%)	-0.20	4 (0%) 86 86	79, 125, 206, 294	0
1	B	455/525 (86%)	0.10	25 (5%) 25 23	106, 174, 272, 340	0
All	All	928/1050 (88%)	-0.05	29 (3%) 49 47	79, 149, 250, 340	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	ALA	10.9
1	B	393	SER	6.1
1	B	384	ASP	4.9
1	B	82	GLU	4.7
1	B	97	MET	4.2

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](#)

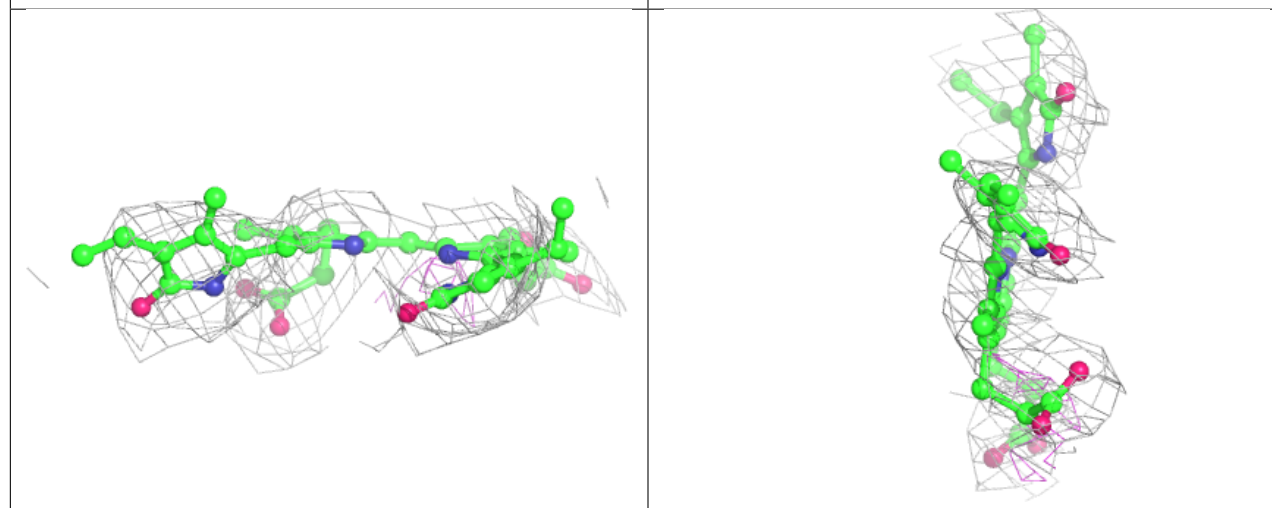
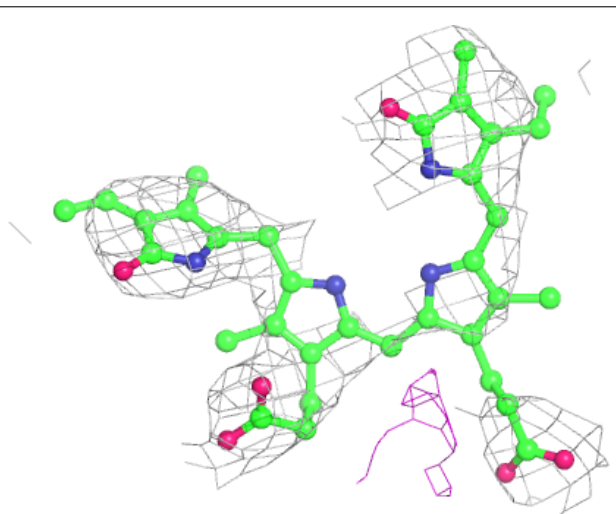
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

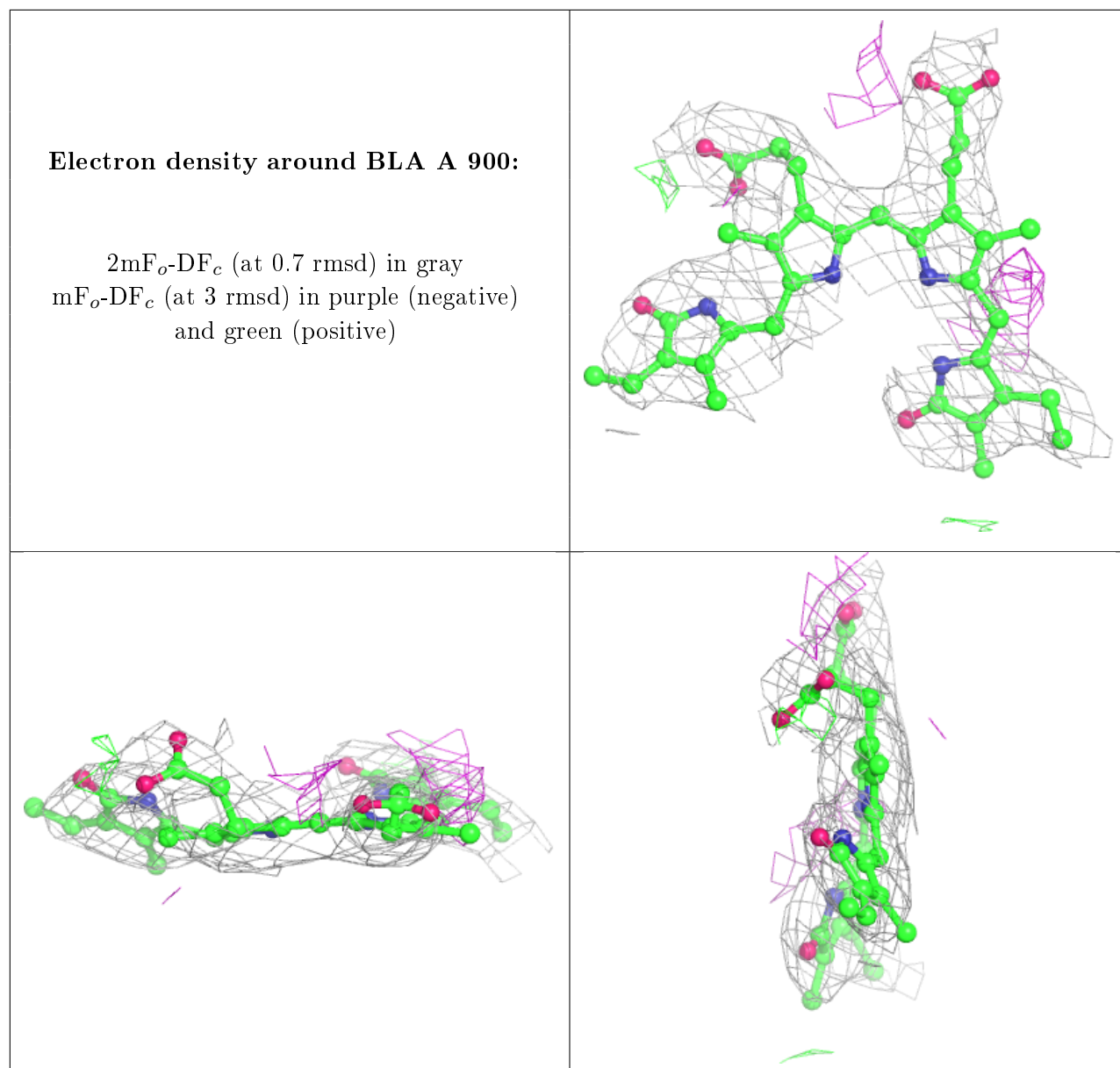
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BLA	B	900	43/43	0.90	0.35	134,144,172,183	0
2	BLA	A	900	43/43	0.92	0.30	80,115,135,145	0

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.