



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2019 – 09:11 AM EST

PDB ID : 5C5K  
Title : Structure of the Pfr form of a canonical phytochrome  
Authors : Burgie, E.S.; Vierstra, R.D.  
Deposited on : 2015-06-20  
Resolution : 3.31 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.4  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.4

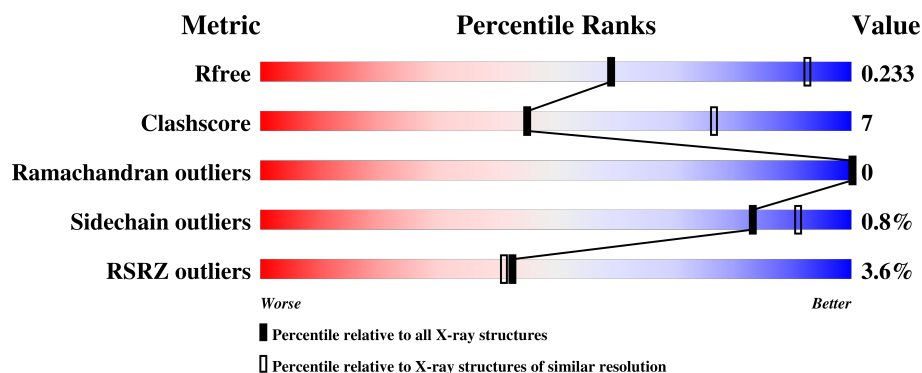
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.31 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))
$R_{free}$	111664	1128 (3.38-3.26)
Clashscore	122126	1187 (3.38-3.26)
Ramachandran outliers	120053	1167 (3.38-3.26)
Sidechain outliers	120020	1166 (3.38-3.26)
RSRZ outliers	108989	1094 (3.38-3.26)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	524	<div> <div>2%</div> <div>76% 17% 6%</div> </div>
1	B	524	<div> <div>3%</div> <div>78% 14% 7%</div> </div>
1	C	524	<div> <div>3%</div> <div>75% 15% 9%</div> </div>
1	D	524	<div> <div>5%</div> <div>76% 14% 10%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14949 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	490	Total	C	N	O	S	0	0	0
			3738	2379	660	688	11			
1	B	486	Total	C	N	O	S	0	0	0
			3716	2366	656	683	11			
1	C	476	Total	C	N	O	S	0	1	0
			3649	2324	644	670	11			
1	D	474	Total	C	N	O	S	0	1	0
			3636	2318	641	666	11			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP Q9RZA4
A	-13	ALA	-	expression tag	UNP Q9RZA4
A	-12	LEU	-	expression tag	UNP Q9RZA4
A	-11	SER	-	expression tag	UNP Q9RZA4
A	-10	MET	-	expression tag	UNP Q9RZA4
A	-9	THR	-	expression tag	UNP Q9RZA4
A	-8	GLY	-	expression tag	UNP Q9RZA4
A	-7	GLY	-	expression tag	UNP Q9RZA4
A	-6	GLN	-	expression tag	UNP Q9RZA4
A	-5	GLN	-	expression tag	UNP Q9RZA4
A	-4	MET	-	expression tag	UNP Q9RZA4
A	-3	GLY	-	expression tag	UNP Q9RZA4
A	-2	ARG	-	expression tag	UNP Q9RZA4
A	-1	GLY	-	expression tag	UNP Q9RZA4
A	0	SER	-	expression tag	UNP Q9RZA4
A	469	TRP	PHE	engineered mutation	UNP Q9RZA4
A	503	GLU	-	expression tag	UNP Q9RZA4
A	504	HIS	-	expression tag	UNP Q9RZA4
A	505	HIS	-	expression tag	UNP Q9RZA4
A	506	HIS	-	expression tag	UNP Q9RZA4
A	507	HIS	-	expression tag	UNP Q9RZA4

*Continued on next page...*

*Continued from previous page...*

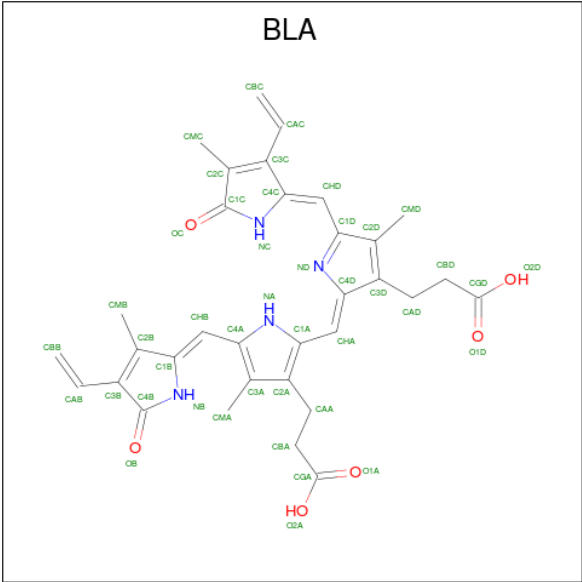
Chain	Residue	Modelled	Actual	Comment	Reference
A	508	HIS	-	expression tag	UNP Q9RZA4
A	509	HIS	-	expression tag	UNP Q9RZA4
B	-14	MET	-	initiating methionine	UNP Q9RZA4
B	-13	ALA	-	expression tag	UNP Q9RZA4
B	-12	LEU	-	expression tag	UNP Q9RZA4
B	-11	SER	-	expression tag	UNP Q9RZA4
B	-10	MET	-	expression tag	UNP Q9RZA4
B	-9	THR	-	expression tag	UNP Q9RZA4
B	-8	GLY	-	expression tag	UNP Q9RZA4
B	-7	GLY	-	expression tag	UNP Q9RZA4
B	-6	GLN	-	expression tag	UNP Q9RZA4
B	-5	GLN	-	expression tag	UNP Q9RZA4
B	-4	MET	-	expression tag	UNP Q9RZA4
B	-3	GLY	-	expression tag	UNP Q9RZA4
B	-2	ARG	-	expression tag	UNP Q9RZA4
B	-1	GLY	-	expression tag	UNP Q9RZA4
B	0	SER	-	expression tag	UNP Q9RZA4
B	469	TRP	PHE	engineered mutation	UNP Q9RZA4
B	503	GLU	-	expression tag	UNP Q9RZA4
B	504	HIS	-	expression tag	UNP Q9RZA4
B	505	HIS	-	expression tag	UNP Q9RZA4
B	506	HIS	-	expression tag	UNP Q9RZA4
B	507	HIS	-	expression tag	UNP Q9RZA4
B	508	HIS	-	expression tag	UNP Q9RZA4
B	509	HIS	-	expression tag	UNP Q9RZA4
C	-14	MET	-	initiating methionine	UNP Q9RZA4
C	-13	ALA	-	expression tag	UNP Q9RZA4
C	-12	LEU	-	expression tag	UNP Q9RZA4
C	-11	SER	-	expression tag	UNP Q9RZA4
C	-10	MET	-	expression tag	UNP Q9RZA4
C	-9	THR	-	expression tag	UNP Q9RZA4
C	-8	GLY	-	expression tag	UNP Q9RZA4
C	-7	GLY	-	expression tag	UNP Q9RZA4
C	-6	GLN	-	expression tag	UNP Q9RZA4
C	-5	GLN	-	expression tag	UNP Q9RZA4
C	-4	MET	-	expression tag	UNP Q9RZA4
C	-3	GLY	-	expression tag	UNP Q9RZA4
C	-2	ARG	-	expression tag	UNP Q9RZA4
C	-1	GLY	-	expression tag	UNP Q9RZA4
C	0	SER	-	expression tag	UNP Q9RZA4
C	469	TRP	PHE	engineered mutation	UNP Q9RZA4
C	503	GLU	-	expression tag	UNP Q9RZA4

*Continued on next page...*

*Continued from previous page...*

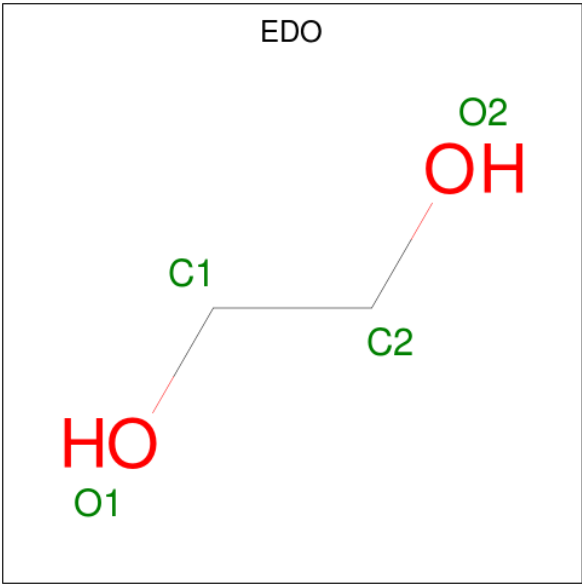
Chain	Residue	Modelled	Actual	Comment	Reference
C	504	HIS	-	expression tag	UNP Q9RZA4
C	505	HIS	-	expression tag	UNP Q9RZA4
C	506	HIS	-	expression tag	UNP Q9RZA4
C	507	HIS	-	expression tag	UNP Q9RZA4
C	508	HIS	-	expression tag	UNP Q9RZA4
C	509	HIS	-	expression tag	UNP Q9RZA4
D	-14	MET	-	initiating methionine	UNP Q9RZA4
D	-13	ALA	-	expression tag	UNP Q9RZA4
D	-12	LEU	-	expression tag	UNP Q9RZA4
D	-11	SER	-	expression tag	UNP Q9RZA4
D	-10	MET	-	expression tag	UNP Q9RZA4
D	-9	THR	-	expression tag	UNP Q9RZA4
D	-8	GLY	-	expression tag	UNP Q9RZA4
D	-7	GLY	-	expression tag	UNP Q9RZA4
D	-6	GLN	-	expression tag	UNP Q9RZA4
D	-5	GLN	-	expression tag	UNP Q9RZA4
D	-4	MET	-	expression tag	UNP Q9RZA4
D	-3	GLY	-	expression tag	UNP Q9RZA4
D	-2	ARG	-	expression tag	UNP Q9RZA4
D	-1	GLY	-	expression tag	UNP Q9RZA4
D	0	SER	-	expression tag	UNP Q9RZA4
D	469	TRP	PHE	engineered mutation	UNP Q9RZA4
D	503	GLU	-	expression tag	UNP Q9RZA4
D	504	HIS	-	expression tag	UNP Q9RZA4
D	505	HIS	-	expression tag	UNP Q9RZA4
D	506	HIS	-	expression tag	UNP Q9RZA4
D	507	HIS	-	expression tag	UNP Q9RZA4
D	508	HIS	-	expression tag	UNP Q9RZA4
D	509	HIS	-	expression tag	UNP Q9RZA4

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C<sub>33</sub>H<sub>34</sub>N<sub>4</sub>O<sub>6</sub>).



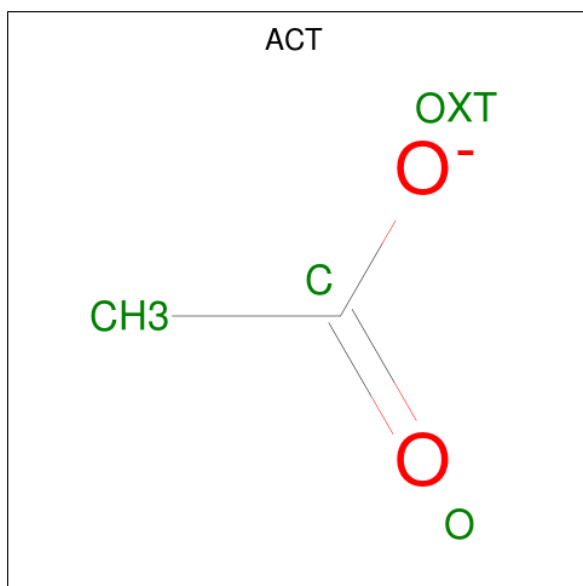
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	33	4	6		
2	B	1	Total	C	N	O	0	0
			43	33	4	6		
2	C	1	Total	C	N	O	0	0
			43	33	4	6		
2	D	1	Total	C	N	O	0	0
			43	33	4	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



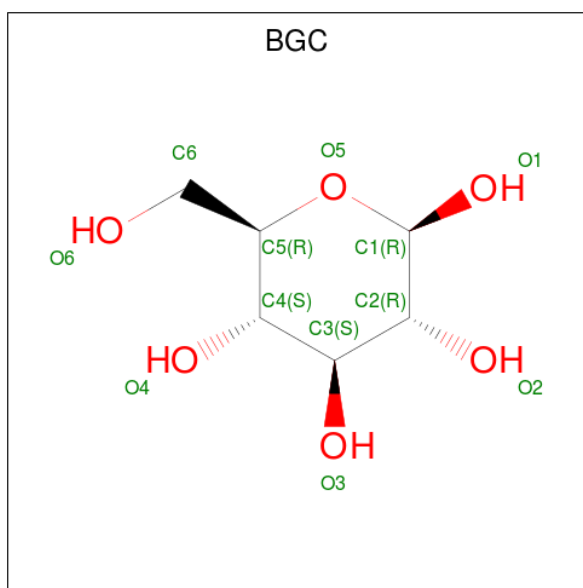
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is BETA-D-GLUCOSE (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is water.

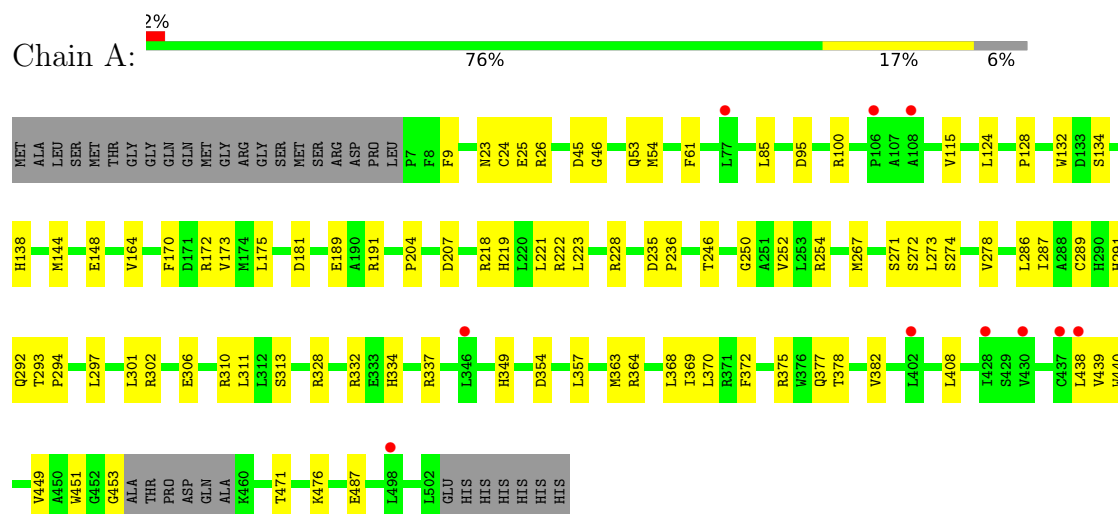
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	6	Total	O	0	0
			6	6		
6	C	1	Total	O	0	0
			1	1		
6	D	1	Total	O	0	0
			1	1		



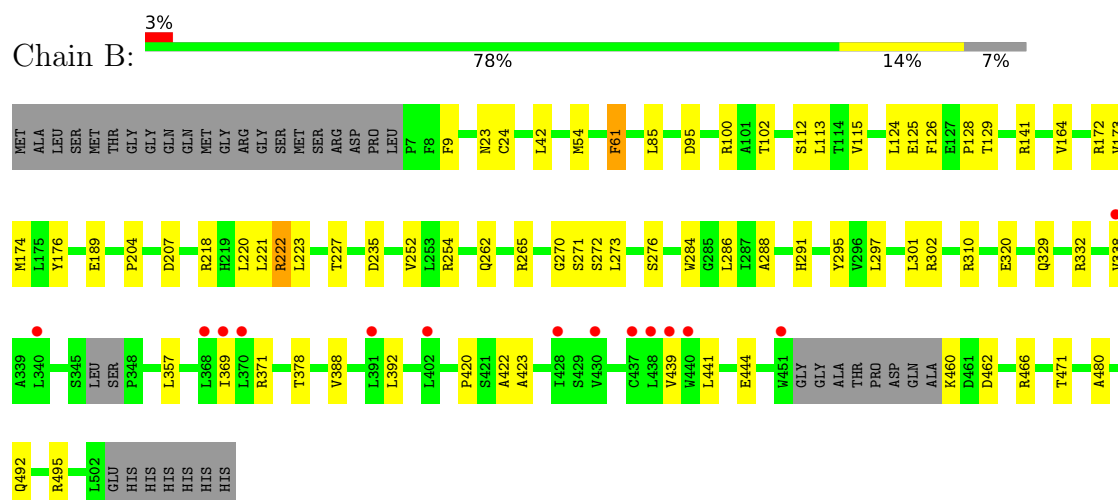
### 3 Residue-property plots [i](#)

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.

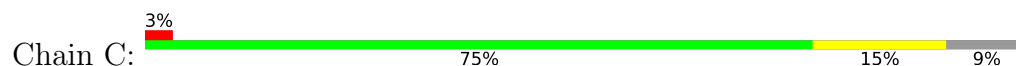
#### • Molecule 1: Bacteriophytochrome

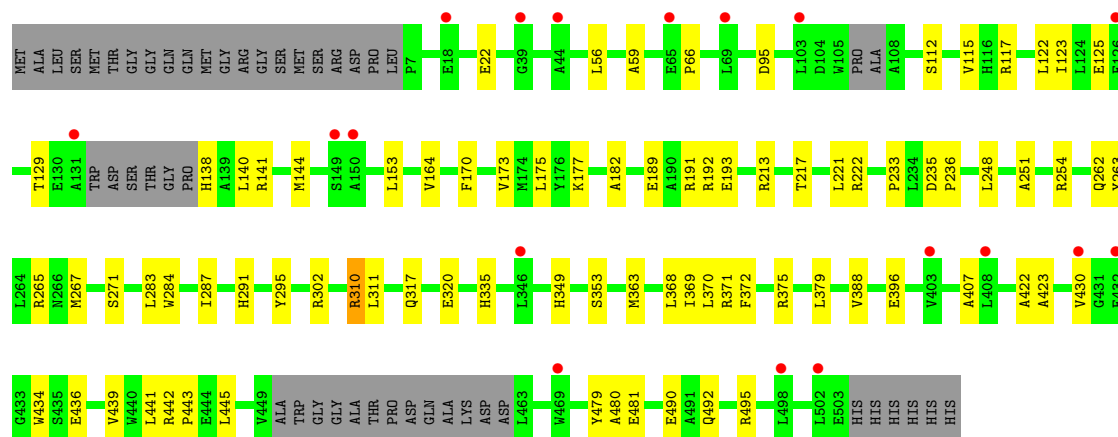


#### • Molecule 1: Bacteriophytochrome

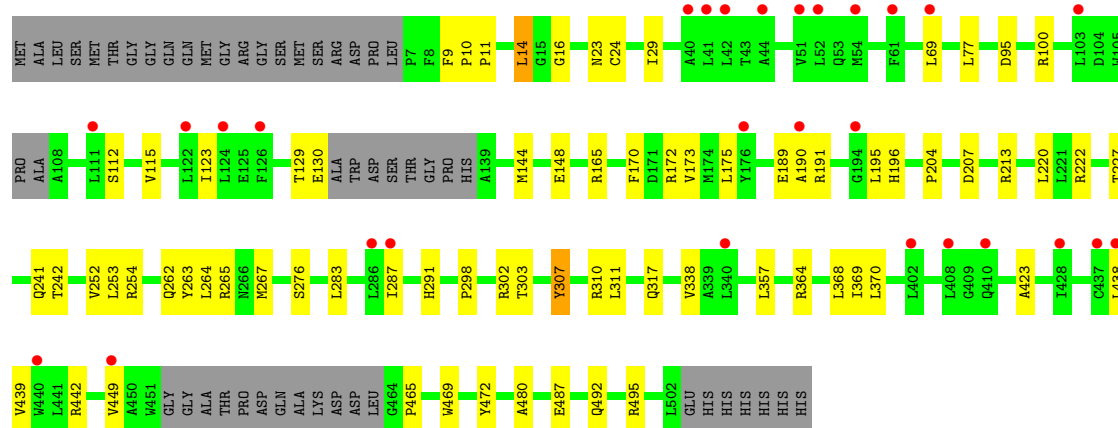
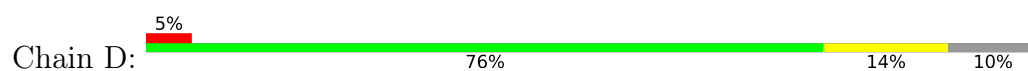


#### • Molecule 1: Bacteriophytochrome





● Molecule 1: Bacteriophytochrome



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.40Å 192.75Å 225.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 3.31 48.80 – 3.31	Depositor EDS
% Data completeness (in resolution range)	87.9 (48.80-3.31) 87.9 (48.80-3.31)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, $R_{free}$	0.196 , 0.232 0.197 , 0.233	Depositor DCC
$R_{free}$ test set	1885 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.7	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 90.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	153.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: BGC, BLA, EDO, ACT

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	0.25	0/3839	0.42	0/5257
1	B	0.25	0/3816	0.44	0/5224
1	C	0.24	0/3743	0.42	0/5120
1	D	0.25	0/3731	0.43	0/5105
All	All	0.25	0/15129	0.43	0/20706

There are no bond length outliers.

There are no bond angle outliers.

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	3738	0	3695	58	1
1	B	3716	0	3673	51	1
1	C	3649	0	3616	54	0
1	D	3636	0	3602	51	0
2	A	43	0	31	4	0
2	B	43	0	31	6	0
2	C	43	0	31	2	0
2	D	43	0	31	4	0
3	A	4	0	6	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	3	0	0
5	C	12	0	12	0	0
6	A	10	0	0	1	0
6	B	6	0	0	2	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
All	All	14949	0	14731	208	1

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 7.

All (208) 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:95:ASP:OD1	1:B:218:ARG:NH1	1.92	1.03
1:C:112:SER:HB2	1:C:129:THR:HB	1.67	0.75
1:B:273:LEU:HD13	1:B:297:LEU:HD12	1.71	0.72
1:A:207:ASP:HB3	2:A:601:BLA:HHB	1.73	0.70
1:C:144:MET:HG3	1:C:311:LEU:HD21	1.73	0.68
1:C:353:SER:HA	1:C:379:LEU:HD11	1.74	0.68
1:C:222:ARG:HE	1:C:254:ARG:NH1	1.92	0.67
1:D:112:SER:HB2	1:D:129:THR:HB	1.75	0.67
1:B:271:SER:HB2	1:B:295:TYR:H	1.59	0.67
1:B:460:LYS:HE2	1:B:462:ASP:HB3	1.78	0.66
1:D:29:ILE:HD12	2:D:601:BLA:HMD1	1.78	0.66
1:A:144:MET:HG3	1:A:311:LEU:HD11	1.78	0.65
1:B:371:ARG:HH11	1:B:392:LEU:HD13	1.60	0.65
1:D:220:LEU:HD12	1:D:310:ARG:NH1	2.11	0.65
1:A:9:PHE:HE2	1:A:23:ASN:HB2	1.62	0.64
1:A:274:SER:HB2	1:A:286:LEU:HD21	1.79	0.64
1:A:271:SER:HB2	1:A:294:PRO:HA	1.80	0.64
1:A:100:ARG:O	1:B:141:ARG:NH1	2.30	0.64
1:D:252:VAL:HG11	1:D:302:ARG:HH21	1.61	0.63
1:B:220:LEU:HD12	1:B:310:ARG:NH1	2.15	0.62
1:A:297:LEU:HD13	1:A:302:ARG:HB2	1.80	0.62
1:B:423:ALA:HB3	1:B:480:ALA:HB2	1.80	0.62
1:A:95:ASP:OD1	1:A:218:ARG:NH2	2.29	0.62
1:B:9:PHE:HE2	1:B:23:ASN:HB2	1.65	0.61
1:B:284:TRP:NE1	1:B:320:GLU:OE2	2.35	0.60
1:C:317:GLN:OE1	1:D:317:GLN:NE2	2.32	0.60
1:A:85:LEU:HD11	1:A:115:VAL:HG11	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ARG:NH2	1:D:254:ARG:O	2.32	0.59
1:A:334:HIS:CD2	1:A:337:ARG:HH22	2.21	0.59
1:C:217:THR:HG22	1:C:283:LEU:HB2	1.85	0.58
1:A:292:GLN:HG3	1:A:293:THR:HG23	1.85	0.58
1:C:310:ARG:NH1	1:D:144:MET:SD	2.77	0.58
1:D:369:ILE:HB	1:D:439:VAL:HB	1.86	0.58
1:A:369:ILE:HB	1:A:439:VAL:HB	1.85	0.58
1:B:272:SER:OG	2:B:601:BLA:O1A	2.19	0.57
1:B:276:SER:HA	1:B:286:LEU:HD12	1.85	0.57
1:D:252:VAL:HG23	1:D:253:LEU:HD12	1.84	0.57
1:B:125:GLU:OE2	1:B:252:VAL:N	2.37	0.57
1:B:297:LEU:HD22	1:B:301:LEU:HD22	1.87	0.57
1:A:310:ARG:NH1	3:A:602:EDO:H12	2.19	0.57
1:A:170:PHE:CD1	1:A:291:HIS:HB2	2.40	0.57
1:C:222:ARG:HE	1:C:254:ARG:HH11	1.51	0.56
1:B:112:SER:HB2	1:B:129:THR:HB	1.86	0.56
1:C:153:LEU:HD11	1:C:320:GLU:HG2	1.87	0.56
1:A:354:ASP:HB3	1:A:357:LEU:HD13	1.88	0.56
1:C:423:ALA:HB3	1:C:480:ALA:HB2	1.87	0.55
1:C:140:LEU:HD21	1:D:307[A]:TYR:HE2	1.71	0.55
1:A:25:GLU:HG3	1:A:26:ARG:HG3	1.88	0.55
1:D:172:ARG:NH2	1:D:196:HIS:O	2.39	0.55
1:C:271:SER:HB2	1:C:295:TYR:H	1.71	0.55
1:B:338:VAL:HA	1:B:357:LEU:HD11	1.88	0.55
1:D:175:LEU:HD13	1:D:287:ILE:HG12	1.89	0.55
1:C:125:GLU:OE2	1:C:251:ALA:HA	2.07	0.54
1:A:451:TRP:HD1	1:A:453:GLY:H	1.55	0.54
1:A:278:VAL:O	1:A:313:SER:OG	2.13	0.54
1:A:115:VAL:HG12	1:A:124:LEU:HA	1.89	0.54
1:C:22:GLU:N	1:C:22:GLU:OE2	2.41	0.54
1:A:221:LEU:HD13	1:A:306:GLU:HG2	1.91	0.53
1:D:492:GLN:HG3	1:D:495:ARG:HH21	1.73	0.53
1:B:420:PRO:HA	1:B:444:GLU:HB2	1.91	0.53
1:A:164:VAL:HB	1:A:173:VAL:HG11	1.92	0.52
1:A:189:GLU:OE2	1:A:191:ARG:HD3	2.09	0.52
1:D:227:THR:HG21	1:D:264:LEU:HB2	1.91	0.52
1:A:375:ARG:NH2	1:A:377:GLN:OE1	2.42	0.52
1:B:174:MET:HG2	1:B:189:GLU:HG3	1.92	0.52
1:A:53:GLN:OE1	1:A:246:THR:OG1	2.23	0.52
2:B:601:BLA:NC	6:B:701:HOH:O	2.33	0.52
1:A:252:VAL:HG11	1:A:302:ARG:HH12	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ASP:HB3	2:B:601:BLA:HHB	1.92	0.51
1:B:95:ASP:OD1	1:B:95:ASP:N	2.44	0.51
1:D:267:MET:SD	2:D:601:BLA:HAB	2.50	0.51
1:C:221:LEU:HD21	1:C:302:ARG:HD2	1.91	0.51
1:C:492:GLN:HA	1:C:495:ARG:HG2	1.92	0.51
1:D:241:GLN:HG3	1:D:242:THR:HG23	1.91	0.51
2:B:601:BLA:HMB3	2:B:601:BLA:CMA	2.40	0.51
1:B:221:LEU:HD21	1:B:302:ARG:HD2	1.93	0.50
1:B:222:ARG:HG3	1:B:254:ARG:HH12	1.77	0.50
1:D:172:ARG:HD2	1:D:195:LEU:HD13	1.93	0.50
1:D:165:ARG:HB2	1:D:173:VAL:HG11	1.93	0.50
1:D:222:ARG:HE	1:D:254:ARG:NH1	2.08	0.50
1:C:189:GLU:OE2	1:C:191:ARG:HD3	2.11	0.50
1:C:170:PHE:CD1	1:C:291:HIS:HB2	2.47	0.50
1:C:164:VAL:HB	1:C:173:VAL:HG11	1.94	0.49
1:B:460:LYS:N	1:B:466:ARG:HH11	2.11	0.49
1:B:85:LEU:HD11	1:B:115:VAL:HG21	1.95	0.49
1:C:141:ARG:NH1	1:D:100:ARG:HD3	2.28	0.49
1:A:222:ARG:HB3	1:A:274:SER:OG	2.13	0.49
1:B:254:ARG:NH1	6:B:702:HOH:O	2.45	0.48
2:B:601:BLA:HMB3	2:B:601:BLA:HMA1	1.95	0.48
1:A:223:LEU:HD13	1:A:273:LEU:HD13	1.95	0.48
1:B:262:GLN:OE1	1:B:265:ARG:NH1	2.39	0.48
1:D:10:PRO:HG2	1:D:16:GLY:HA2	1.96	0.48
1:C:445:LEU:HD13	1:C:481:GLU:HG2	1.96	0.48
1:D:267:MET:HG2	1:D:465:PRO:HG3	1.95	0.48
1:A:370:LEU:HD23	1:A:438:LEU:HD22	1.96	0.48
1:C:117:ARG:HH11	1:C:122:LEU:HD21	1.78	0.48
1:B:460:LYS:HG2	1:B:462:ASP:H	1.79	0.47
1:B:338:VAL:HG22	1:B:357:LEU:HG	1.95	0.47
1:B:371:ARG:NH1	1:B:392:LEU:HD13	2.28	0.47
1:B:113:LEU:HD11	1:B:124:LEU:HD23	1.97	0.47
1:D:364:ARG:NE	1:D:487:GLU:OE2	2.46	0.47
1:A:222:ARG:NE	1:A:254:ARG:NH1	2.62	0.47
2:A:601:BLA:O2A	2:A:601:BLA:HMA2	2.15	0.47
1:D:207:ASP:HB3	2:D:601:BLA:HHB	1.96	0.47
1:B:329:GLN:HA	1:B:332:ARG:HE	1.79	0.47
1:B:369:ILE:HD13	1:B:388:VAL:HG13	1.97	0.46
1:C:175:LEU:HD12	1:C:287:ILE:HG12	1.97	0.46
1:C:369:ILE:HB	1:C:439:VAL:HB	1.96	0.46
1:C:59:ALA:HB2	1:C:66:PRO:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ASP:OD1	1:D:95:ASP:N	2.48	0.46
1:D:204:PRO:HD3	1:D:472:TYR:HB2	1.97	0.46
1:A:172:ARG:NH1	6:A:701:HOH:O	2.38	0.46
1:C:371:ARG:O	1:C:436:GLU:HA	2.15	0.46
1:C:422:ALA:HB1	1:C:441:LEU:HD22	1.98	0.46
1:C:372:PHE:HA	1:C:436:GLU:HG2	1.97	0.46
1:A:138:HIS:NE2	1:B:102:THR:OG1	2.46	0.46
1:C:95:ASP:OD1	1:C:95:ASP:N	2.48	0.46
1:A:252:VAL:HG11	1:A:302:ARG:HH22	1.81	0.46
1:C:349:HIS:HE1	1:C:375:ARG:HG3	1.80	0.46
1:A:132:TRP:CZ2	1:A:134:SER:HB3	2.51	0.45
1:D:170:PHE:CD1	1:D:291:HIS:HB2	2.50	0.45
1:A:378:THR:HG21	1:A:382:VAL:HG11	1.97	0.45
1:C:335:HIS:HB2	1:C:490:GLU:OE2	2.16	0.45
1:A:181:ASP:OD2	1:A:476:LYS:NZ	2.42	0.45
1:D:213:ARG:HG3	1:D:283:LEU:HD23	1.97	0.45
1:B:54:MET:HE3	1:B:54:MET:HB2	1.67	0.45
1:C:369:ILE:HD13	1:C:388:VAL:HG13	1.98	0.45
1:C:396:GLU:HG2	1:C:434:TRP:HB2	1.98	0.45
1:D:130:GLU:OE2	1:D:298:PRO:HB3	2.16	0.45
1:D:222:ARG:NE	1:D:254:ARG:NH1	2.64	0.45
1:C:222:ARG:NE	1:C:254:ARG:HH11	2.13	0.45
1:C:368:LEU:HD21	1:C:370:LEU:HD21	1.99	0.45
1:A:61:PHE:HZ	1:A:128:PRO:HD3	1.82	0.45
1:A:95:ASP:OD1	1:A:95:ASP:N	2.48	0.45
1:D:449:VAL:HG22	1:D:469:TRP:NE1	2.32	0.45
1:D:173:VAL:HG13	1:D:190:ALA:HB3	1.98	0.45
1:A:267:MET:SD	2:A:601:BLA:HAB	2.57	0.45
1:C:138:HIS:ND1	1:C:138:HIS:O	2.50	0.44
1:D:338:VAL:HA	1:D:357:LEU:HD22	1.99	0.44
1:D:69:LEU:HD11	1:D:77:LEU:HD21	1.99	0.44
1:B:369:ILE:HB	1:B:439:VAL:HB	1.99	0.44
1:B:24:CYS:HB2	2:B:601:BLA:HAC	1.76	0.44
1:A:54:MET:O	1:A:235:ASP:N	2.33	0.44
1:B:172:ARG:HD3	1:B:174:MET:SD	2.57	0.44
1:D:423:ALA:HB3	1:D:480:ALA:HB2	1.99	0.44
1:A:364:ARG:HD3	1:A:487:GLU:OE2	2.18	0.44
1:C:56:LEU:HD12	1:C:233:PRO:HD2	2.00	0.44
1:D:115:VAL:HA	1:D:123:ILE:O	2.18	0.44
1:D:423:ALA:N	1:D:442:ARG:O	2.49	0.44
1:C:140:LEU:HD21	1:D:307[A]:TYR:CE2	2.52	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:LEU:HD11	1:D:438:LEU:HD11	2.00	0.43
1:C:310:ARG:HG2	1:D:148:GLU:OE2	2.18	0.43
1:D:189:GLU:OE2	1:D:191:ARG:HD3	2.19	0.43
1:A:204:PRO:HG3	1:A:471:THR:HG23	1.99	0.43
1:D:144:MET:HG3	1:D:311:LEU:HD21	2.00	0.43
1:A:222:ARG:HE	1:A:254:ARG:NH1	2.17	0.43
1:C:267:MET:HE1	2:C:601:BLA:HAB	2.01	0.43
1:B:54:MET:O	1:B:235:ASP:N	2.37	0.42
1:C:213:ARG:O	1:C:217:THR:HG23	2.19	0.42
1:A:132:TRP:CZ2	1:A:301:LEU:HD13	2.54	0.42
1:A:223:LEU:HD12	1:A:272:SER:O	2.19	0.42
1:D:220:LEU:HD12	1:D:310:ARG:HH11	1.82	0.42
1:D:9:PHE:HE2	1:D:23:ASN:HB2	1.85	0.42
1:A:363:MET:HG3	1:A:440:TRP:CD2	2.55	0.42
1:B:270:GLY:N	1:B:291:HIS:O	2.44	0.42
1:A:349:HIS:NE2	1:A:372:PHE:HB2	2.34	0.42
1:A:219:HIS:NE2	1:A:250:GLY:HA2	2.35	0.42
1:D:220:LEU:HA	1:D:276:SER:HB2	2.02	0.42
1:B:42:LEU:HD13	1:B:126:PHE:CE1	2.55	0.42
1:D:11:PRO:HD2	1:D:14:LEU:HD21	2.02	0.42
1:A:45:ASP:OD1	1:A:46:GLY:N	2.53	0.41
1:B:61:PHE:HE2	1:B:128:PRO:HD3	1.85	0.41
1:B:204:PRO:HG3	1:B:471:THR:HG23	2.02	0.41
1:D:24:CYS:HB2	2:D:601:BLA:HAC	1.89	0.41
1:A:148:GLU:OE2	1:B:310:ARG:NE	2.50	0.41
1:B:176:TYR:CE2	1:B:288:ALA:HB2	2.54	0.41
1:C:363:MET:O	1:C:442:ARG:NH2	2.38	0.41
1:D:370:LEU:HD23	1:D:438:LEU:CD1	2.50	0.41
1:A:175:LEU:HD13	1:A:287:ILE:HG12	2.01	0.41
1:C:235:ASP:HA	1:C:236:PRO:HA	1.93	0.41
1:C:177:LYS:HD3	1:C:284:TRP:CZ2	2.55	0.41
1:A:170:PHE:CG	1:A:289:CYS:HB3	2.56	0.41
1:A:328:ARG:O	1:A:332:ARG:HG2	2.20	0.41
1:C:222:ARG:NH2	1:C:254:ARG:O	2.52	0.41
1:C:267:MET:HE1	2:C:601:BLA:HMB1	2.01	0.41
1:A:24:CYS:HB2	2:A:601:BLA:HAC	1.59	0.41
1:B:492:GLN:HG3	1:B:495:ARG:HH21	1.85	0.41
1:A:53:GLN:HA	1:A:236:PRO:HD2	2.02	0.41
1:B:222:ARG:HD3	1:B:223:LEU:N	2.36	0.41
1:C:248:LEU:O	1:C:254:ARG:HD3	2.21	0.41
1:C:407:ALA:HB2	1:C:479:TYR:HA	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:HB	1:B:173:VAL:HG11	2.02	0.41
1:B:329:GLN:HG3	1:B:332:ARG:HH21	1.86	0.41
1:C:115:VAL:HA	1:C:123:ILE:O	2.20	0.41
1:C:262:GLN:HG2	1:C:265:ARG:NH1	2.36	0.41
1:B:100:ARG:HA	1:B:113:LEU:O	2.21	0.41
1:B:422:ALA:HB2	1:B:441:LEU:HD23	2.02	0.41
1:C:442:ARG:HA	1:C:443:PRO:HD3	1.95	0.41
1:C:141:ARG:HD3	1:D:100:ARG:HE	1.83	0.41
1:D:262:GLN:HG2	1:D:265:ARG:NH1	2.35	0.41
1:A:297:LEU:HD12	1:A:297:LEU:O	2.21	0.40
1:A:368:LEU:HD21	1:A:370:LEU:HD21	2.04	0.40
1:C:192:ARG:HD2	1:C:193:GLU:O	2.21	0.40
1:D:303:THR:HG22	1:D:307[B]:TYR:CZ	2.55	0.40
1:A:363:MET:HG3	1:A:440:TRP:CE2	2.56	0.40
1:C:182:ALA:O	1:C:213:ARG:NH2	2.54	0.40
1:A:310:ARG:HH12	3:A:602:EDO:H12	1.83	0.40
1:B:460:LYS:HB3	1:B:460:LYS:NZ	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ARG:NH1	1:B:128:PRO:O[4_445]	2.09	0.11

## 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	486/524 (93%)	478 (98%)	8 (2%)	0	100	100
1	B	480/524 (92%)	473 (98%)	7 (2%)	0	100	100
1	C	469/524 (90%)	463 (99%)	6 (1%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	467/524 (89%)	460 (98%)	7 (2%)	0	100	100
All	All	1902/2096 (91%)	1874 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	384/411 (93%)	382 (100%)	2 (0%)	90	94
1	B	382/411 (93%)	378 (99%)	4 (1%)	78	88
1	C	376/411 (92%)	373 (99%)	3 (1%)	83	91
1	D	374/411 (91%)	370 (99%)	4 (1%)	76	87
All	All	1516/1644 (92%)	1503 (99%)	13 (1%)	83	89

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	LEU
1	A	449	VAL
1	B	61	PHE
1	B	222	ARG
1	B	227	THR
1	B	378	THR
1	C	263	TYR
1	C	310	ARG
1	C	430	VAL
1	D	14	LEU
1	D	263	TYR
1	D	307[A]	TYR
1	D	307[B]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	260	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](#)

7 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	601	1	36,46,46	3.92	11 (30%)	46,67,67	1.62	6 (13%)
3	EDO	A	602	-	3,3,3	0.48	0	2,2,2	0.34	0
4	ACT	A	603	-	1,3,3	1.31	0	0,3,3	0.00	-
2	BLA	B	601	1	36,46,46	4.09	11 (30%)	46,67,67	1.77	7 (15%)
2	BLA	C	601	1	36,46,46	3.90	11 (30%)	46,67,67	1.55	6 (13%)
5	BGC	C	602	-	12,12,12	0.54	0	17,17,17	0.67	0
2	BLA	D	601	1	36,46,46	3.92	11 (30%)	46,67,67	1.69	7 (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	A	601	1	-	5/22/74/74	0/4/4/4
3	EDO	A	602	-	-	0/1/1/1	-
2	BLA	B	601	1	-	10/22/74/74	0/4/4/4
2	BLA	C	601	1	-	6/22/74/74	0/4/4/4
5	BGC	C	602	-	-	2/2/22/22	0/1/1/1
2	BLA	D	601	1	-	4/22/74/74	0/4/4/4

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BLA	CHA-C4D	21.20	1.53	1.35
2	D	601	BLA	CHA-C4D	20.21	1.52	1.35
2	A	601	BLA	CHA-C4D	20.20	1.52	1.35
2	C	601	BLA	CHA-C4D	20.09	1.52	1.35
2	B	601	BLA	CHD-C1D	5.73	1.53	1.40
2	A	601	BLA	CHD-C1D	5.64	1.53	1.40
2	D	601	BLA	CHD-C1D	5.62	1.53	1.40
2	C	601	BLA	CHD-C1D	5.50	1.53	1.40
2	B	601	BLA	CBC-CAC	4.09	1.50	1.30
2	D	601	BLA	CBC-CAC	4.01	1.50	1.30
2	A	601	BLA	CBC-CAC	4.00	1.50	1.30
2	C	601	BLA	CBC-CAC	3.96	1.50	1.30
2	C	601	BLA	C3C-C4C	-3.69	1.40	1.45
2	A	601	BLA	C4D-C3D	-3.56	1.40	1.45
2	D	601	BLA	C4D-C3D	-3.44	1.40	1.45
2	B	601	BLA	C4A-CHB	3.43	1.54	1.41
2	C	601	BLA	C4D-C3D	-3.42	1.40	1.45
2	A	601	BLA	C3C-C4C	-3.42	1.40	1.45
2	D	601	BLA	C3C-C4C	-3.32	1.40	1.45
2	B	601	BLA	C4D-C3D	-3.32	1.40	1.45
2	B	601	BLA	C3C-C4C	-3.26	1.40	1.45
2	B	601	BLA	CHB-C1B	3.20	1.41	1.34
2	C	601	BLA	C4A-CHB	3.17	1.53	1.41
2	A	601	BLA	C4A-CHB	3.16	1.53	1.41
2	D	601	BLA	C4A-CHB	3.11	1.53	1.41
2	A	601	BLA	C1C-C2C	-3.06	1.39	1.47
2	C	601	BLA	C1C-C2C	-3.05	1.39	1.47
2	D	601	BLA	C1C-C2C	-3.03	1.39	1.47
2	B	601	BLA	C1C-C2C	-2.95	1.39	1.47
2	B	601	BLA	C3B-C4B	-2.92	1.39	1.47
2	A	601	BLA	C3B-C4B	-2.90	1.39	1.47
2	D	601	BLA	C3B-C4B	-2.84	1.39	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	BLA	C3B-C4B	-2.84	1.39	1.47
2	C	601	BLA	C1B-C2B	-2.74	1.40	1.45
2	D	601	BLA	C1B-C2B	-2.72	1.40	1.45
2	C	601	BLA	C1D-C2D	-2.71	1.39	1.45
2	D	601	BLA	C1D-C2D	-2.69	1.40	1.45
2	B	601	BLA	C1D-C2D	-2.64	1.40	1.45
2	A	601	BLA	C1B-C2B	-2.63	1.40	1.45
2	A	601	BLA	C1D-C2D	-2.62	1.40	1.45
2	A	601	BLA	CHB-C1B	2.57	1.39	1.34
2	D	601	BLA	CHB-C1B	2.53	1.39	1.34
2	C	601	BLA	CHB-C1B	2.50	1.39	1.34
2	B	601	BLA	C3D-C2D	2.03	1.41	1.36

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	BLA	C1A-CHA-C4D	-6.83	120.65	128.81
2	A	601	BLA	C1A-CHA-C4D	-5.82	121.86	128.81
2	C	601	BLA	C1A-CHA-C4D	-5.71	121.99	128.81
2	B	601	BLA	CMB-C2B-C1B	4.77	130.18	124.17
2	B	601	BLA	CHB-C1B-C2B	4.27	135.43	126.97
2	B	601	BLA	C1A-CHA-C4D	-4.21	123.78	128.81
2	B	601	BLA	CAA-CBA-CGA	3.94	119.40	112.66
2	B	601	BLA	CBA-CAA-C2A	3.87	119.88	112.48
2	A	601	BLA	CAA-CBA-CGA	3.68	118.94	112.66
2	B	601	BLA	CHB-C1B-NB	-3.58	118.13	130.33
2	A	601	BLA	CMB-C2B-C1B	3.45	128.52	124.17
2	A	601	BLA	CBA-CAA-C2A	3.40	118.99	112.48
2	D	601	BLA	CBA-CAA-C2A	3.39	118.96	112.48
2	D	601	BLA	CAA-CBA-CGA	3.20	118.12	112.66
2	D	601	BLA	CMB-C2B-C1B	2.95	127.90	124.17
2	C	601	BLA	CAA-CBA-CGA	2.94	117.68	112.66
2	C	601	BLA	CAD-CBD-CGD	2.93	117.67	112.66
2	C	601	BLA	CMB-C2B-C1B	2.78	127.67	124.17
2	D	601	BLA	CAD-CBD-CGD	2.77	117.39	112.66
2	A	601	BLA	CAD-CBD-CGD	2.64	117.18	112.66
2	C	601	BLA	CBA-CAA-C2A	2.61	117.47	112.48
2	B	601	BLA	CMB-C2B-C3B	-2.40	122.35	128.28
2	D	601	BLA	CHB-C1B-NB	-2.26	122.62	130.33
2	D	601	BLA	C4C-CHD-C1D	-2.24	122.59	128.09
2	A	601	BLA	CHB-C1B-NB	-2.21	122.79	130.33
2	C	601	BLA	CHB-C1B-NB	-2.08	123.25	130.33

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BLA	NA-C4A-CHB-C1B
2	A	601	BLA	NB-C1B-CHB-C4A
2	A	601	BLA	C2B-C1B-CHB-C4A
2	A	601	BLA	C2C-C3C-CAC-CBC
2	C	601	BLA	NA-C4A-CHB-C1B
2	C	601	BLA	C3A-C4A-CHB-C1B
2	C	601	BLA	NB-C1B-CHB-C4A
2	C	601	BLA	C2B-C1B-CHB-C4A
2	C	601	BLA	C2C-C3C-CAC-CBC
2	C	601	BLA	C4C-C3C-CAC-CBC
2	D	601	BLA	NB-C1B-CHB-C4A
2	D	601	BLA	C2B-C1B-CHB-C4A
2	D	601	BLA	C2C-C3C-CAC-CBC
2	B	601	BLA	NA-C4A-CHB-C1B
2	B	601	BLA	C3A-C4A-CHB-C1B
2	B	601	BLA	C2A-CAA-CBA-CGA
2	B	601	BLA	NB-C1B-CHB-C4A
2	B	601	BLA	C2C-C3C-CAC-CBC
5	C	602	BGC	O5-C5-C6-O6
2	A	601	BLA	C4C-C3C-CAC-CBC
2	D	601	BLA	C4C-C3C-CAC-CBC
2	B	601	BLA	C4C-C3C-CAC-CBC
2	B	601	BLA	C4D-C3D-CAD-CBD
2	B	601	BLA	C2B-C1B-CHB-C4A
2	B	601	BLA	C2D-C3D-CAD-CBD
2	B	601	BLA	C1A-C2A-CAA-CBA
5	C	602	BGC	C4-C5-C6-O6

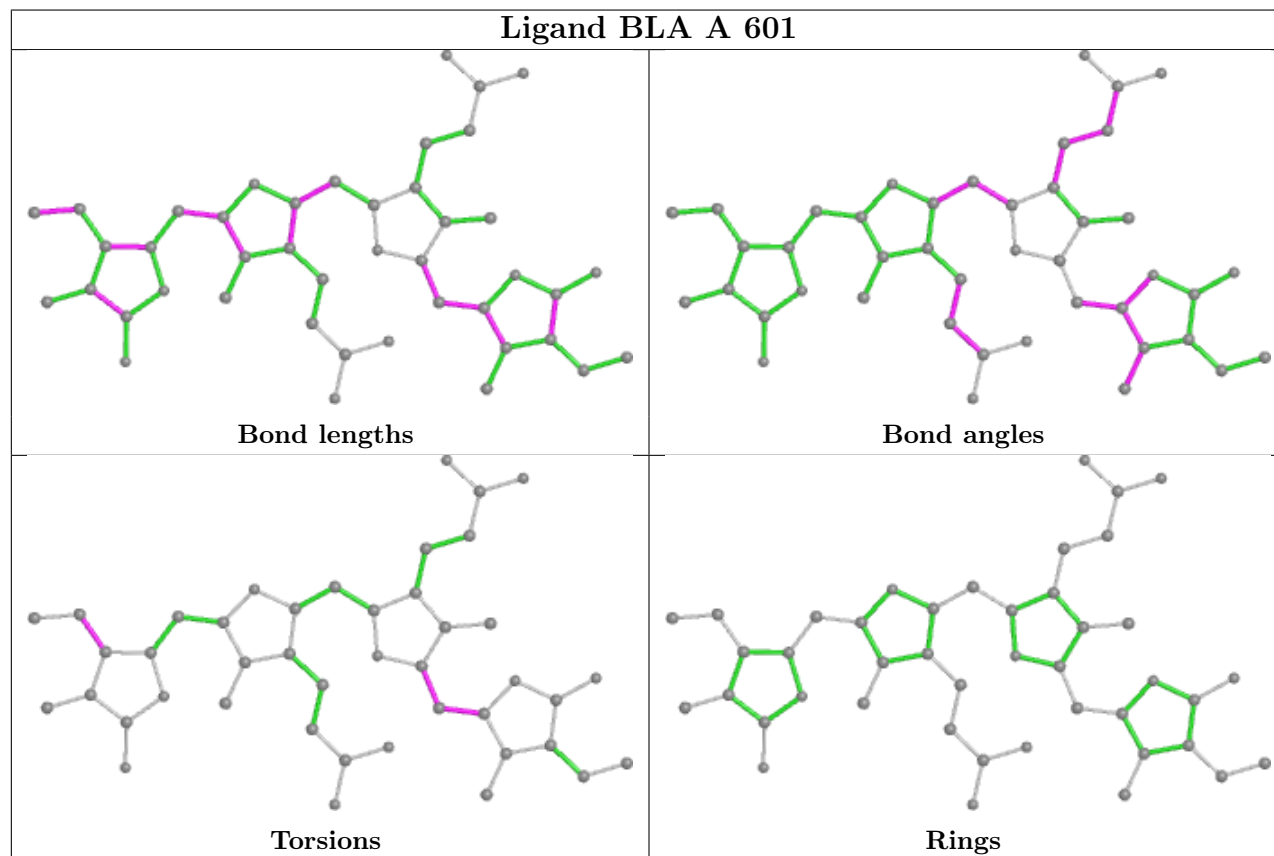
There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BLA	4	0
3	A	602	EDO	2	0
2	B	601	BLA	6	0
2	C	601	BLA	2	0
2	D	601	BLA	4	0

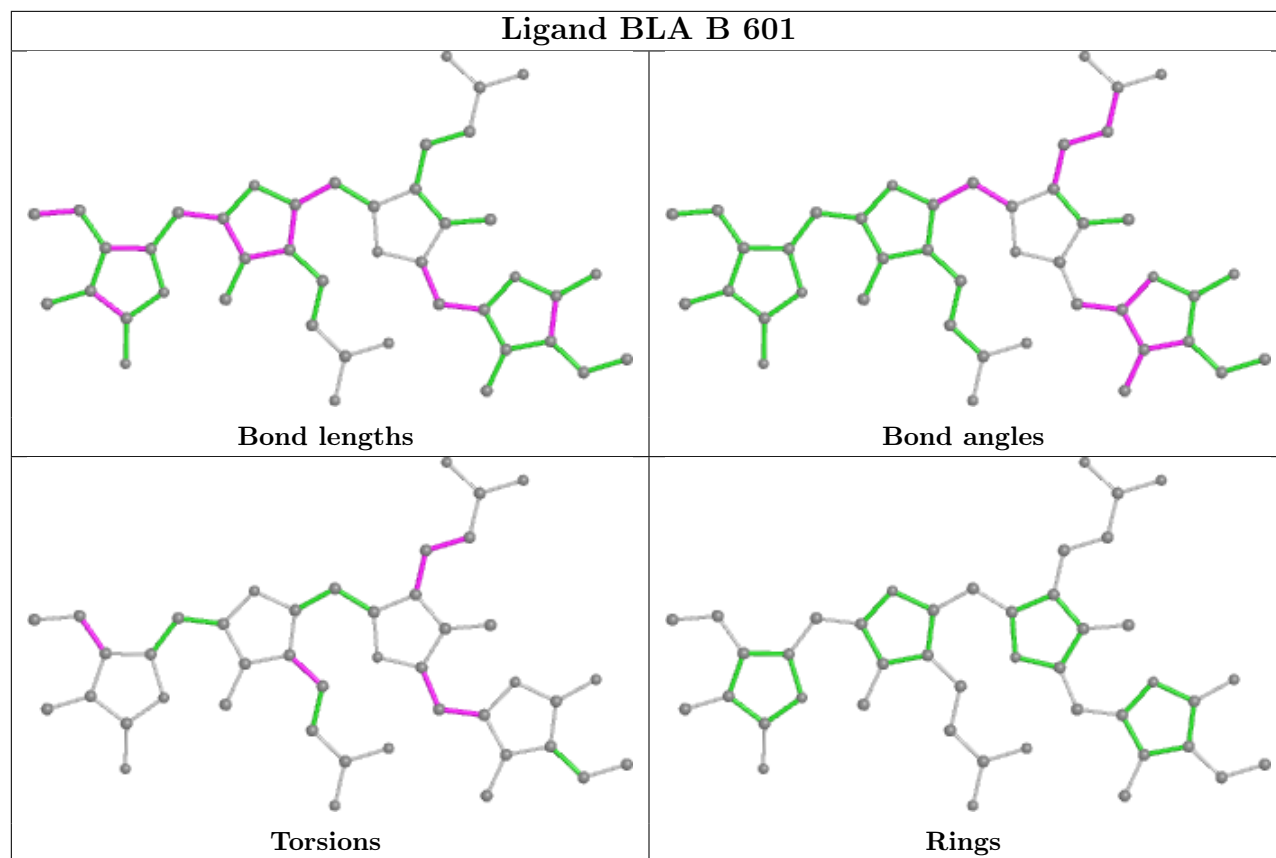
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

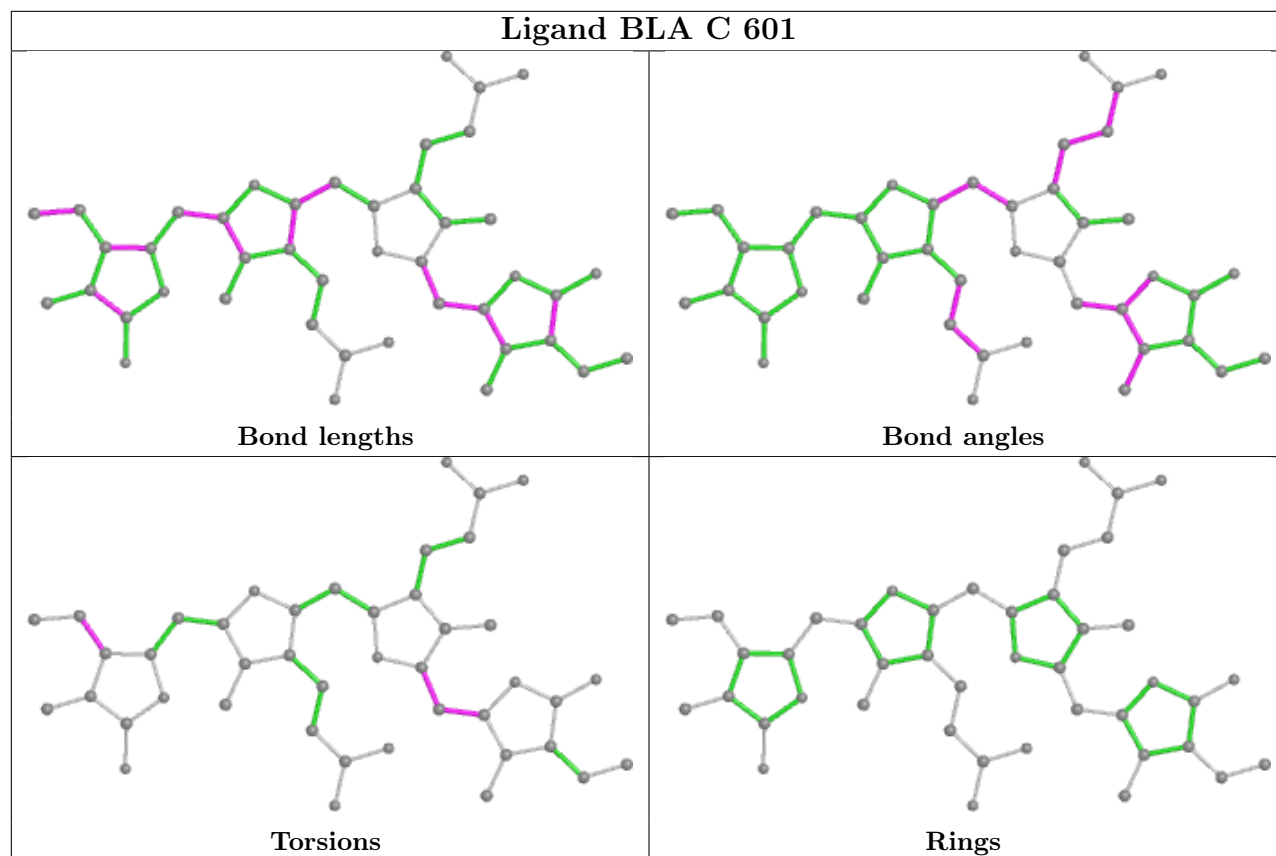


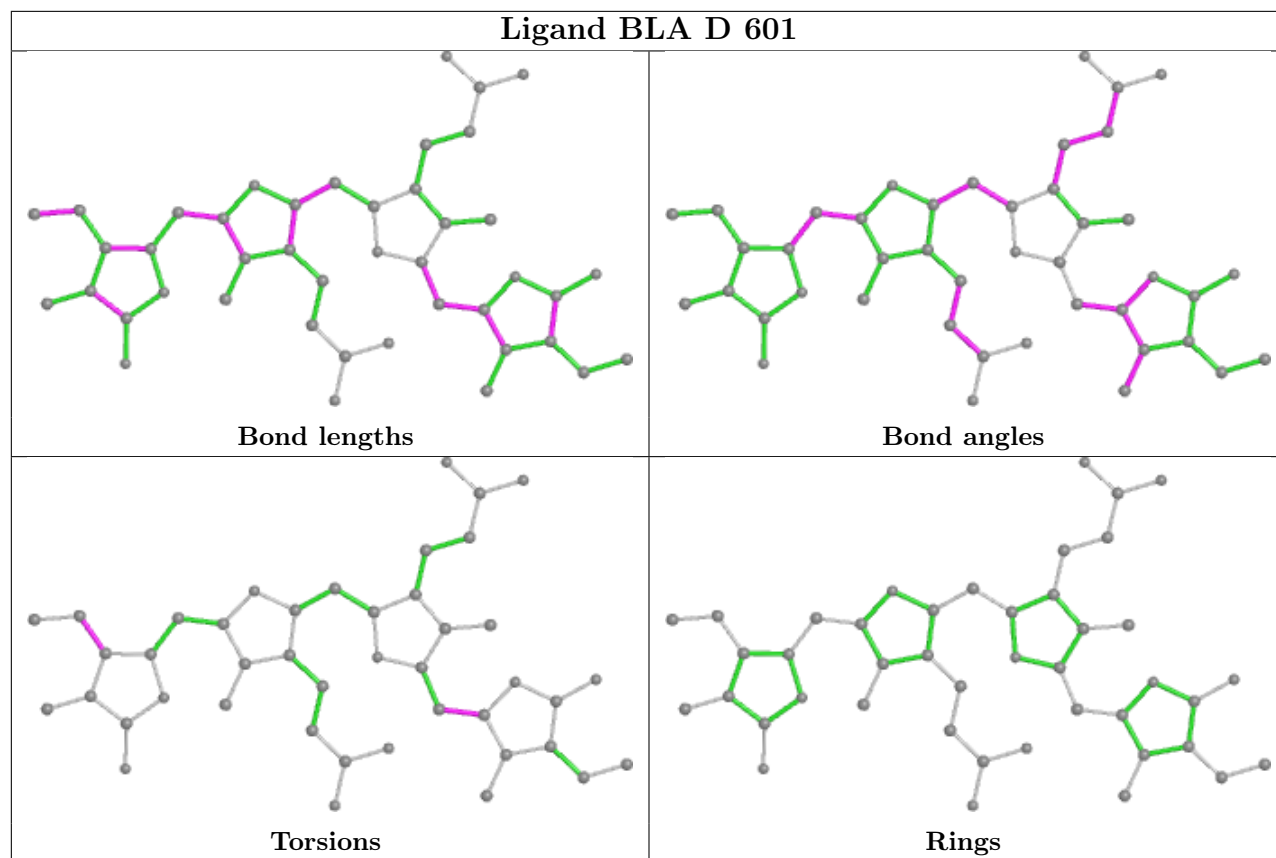


## Ligand BLA B 601



## Ligand BLA C 601





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	490/524 (93%)	0.16	10 (2%) 65 65	60, 121, 201, 257	0
1	B	486/524 (92%)	0.20	14 (2%) 51 51	66, 121, 213, 273	1 (0%)
1	C	476/524 (90%)	0.10	18 (3%) 40 38	102, 169, 231, 297	0
1	D	474/524 (90%)	0.33	28 (5%) 22 23	106, 182, 247, 313	0
All	All	1926/2096 (91%)	0.20	70 (3%) 42 41	60, 156, 228, 313	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	44	ALA	6.7
1	B	402	LEU	4.3
1	B	430	VAL	4.3
1	A	106	PRO	3.7
1	D	408	LEU	3.6
1	B	437	CYS	3.6
1	B	369	ILE	3.5
1	D	40	ALA	3.5
1	D	54	MET	3.4
1	D	103	LEU	3.3
1	B	438	LEU	3.2
1	C	65	GLU	3.1
1	C	126	PHE	3.0
1	D	69	LEU	3.0
1	D	124	LEU	2.9
1	D	126	PHE	2.9
1	B	440	TRP	2.9
1	B	368	LEU	2.9
1	C	149	SER	2.9
1	A	438	LEU	2.9
1	A	430	VAL	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	437	CYS	2.8
1	B	340	LEU	2.8
1	A	108	ALA	2.8
1	C	502	LEU	2.8
1	D	51	VAL	2.7
1	A	77	LEU	2.7
1	C	39	GLY	2.7
1	A	346	LEU	2.6
1	D	440	TRP	2.6
1	D	437	CYS	2.6
1	D	428	ILE	2.6
1	C	150	ALA	2.5
1	C	69	LEU	2.5
1	D	42	LEU	2.5
1	D	176	TYR	2.5
1	D	286	LEU	2.5
1	D	194	GLY	2.5
1	D	190	ALA	2.5
1	C	44	ALA	2.5
1	C	430	VAL	2.4
1	D	122	LEU	2.4
1	A	428	ILE	2.4
1	D	111	LEU	2.4
1	B	451	TRP	2.4
1	C	432	GLU	2.3
1	D	402	LEU	2.3
1	D	340	LEU	2.3
1	D	410	GLN	2.3
1	D	438	LEU	2.3
1	D	41	LEU	2.3
1	B	428	ILE	2.3
1	A	498	LEU	2.2
1	C	18	GLU	2.2
1	D	287	ILE	2.2
1	C	346	LEU	2.2
1	C	469	TRP	2.2
1	D	449	VAL	2.2
1	C	103	LEU	2.2
1	A	402	LEU	2.2
1	B	338	VAL	2.1
1	C	408	LEU	2.1
1	C	403	VAL	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	370	LEU	2.1
1	B	439	VAL	2.1
1	D	52	LEU	2.1
1	C	131	ALA	2.0
1	B	391	LEU	2.0
1	C	498	LEU	2.0
1	D	61	PHE	2.0

## 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](#)

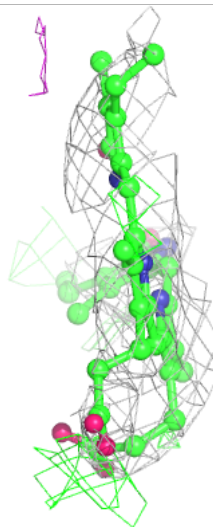
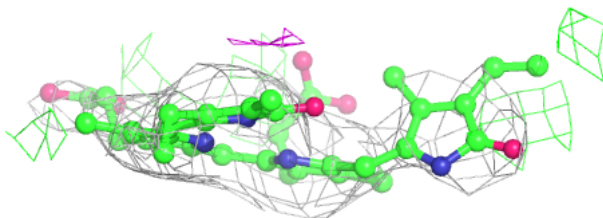
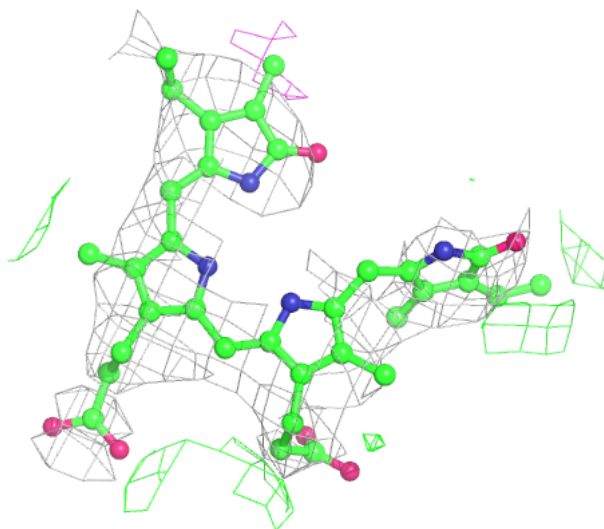
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	BGC	C	602	12/12	0.86	0.30	139,208,225,229	0
2	BLA	D	601	43/43	0.87	0.34	128,168,232,252	0
3	EDO	A	602	4/4	0.87	0.49	101,108,130,143	0
2	BLA	B	601	43/43	0.89	0.34	72,109,164,187	0
2	BLA	C	601	43/43	0.93	0.35	112,151,220,232	0
2	BLA	A	601	43/43	0.93	0.31	54,87,121,156	0
4	ACT	A	603	4/4	0.95	0.32	94,120,123,135	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.

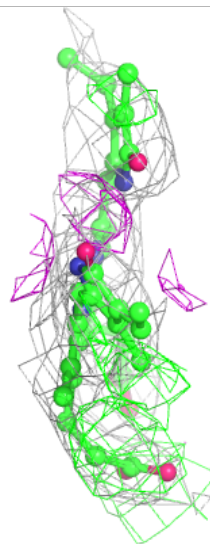
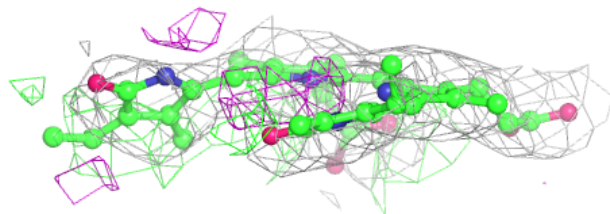
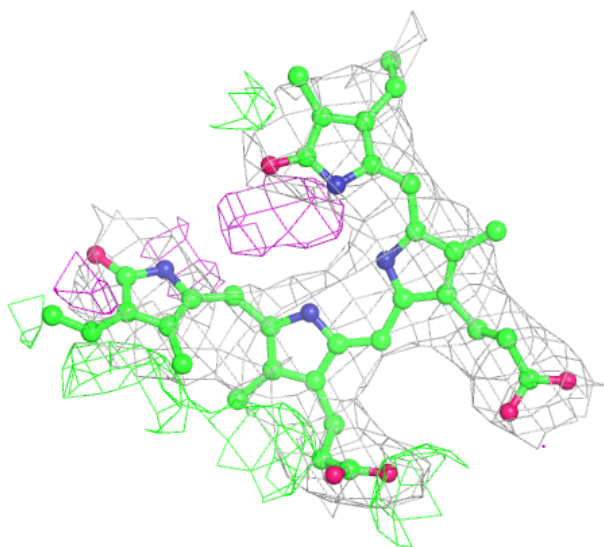
**Electron density around BLA D 601:**

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



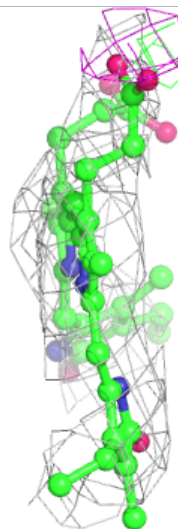
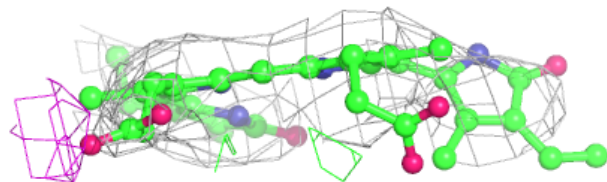
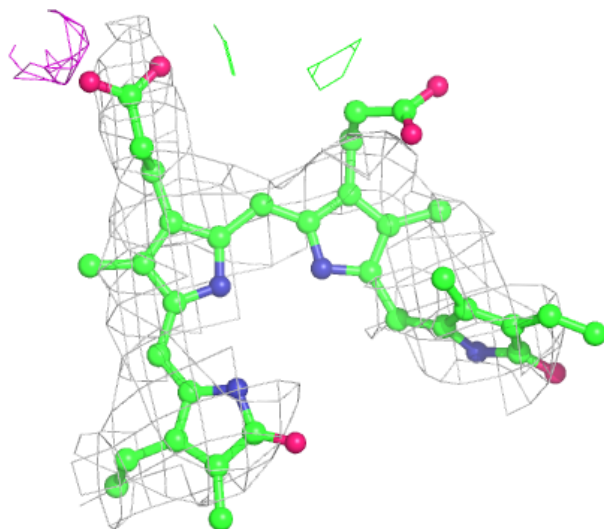
**Electron density around BLA B 601:**

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



**Electron density around BLA C 601:**

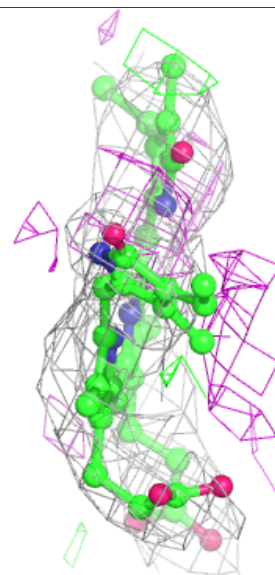
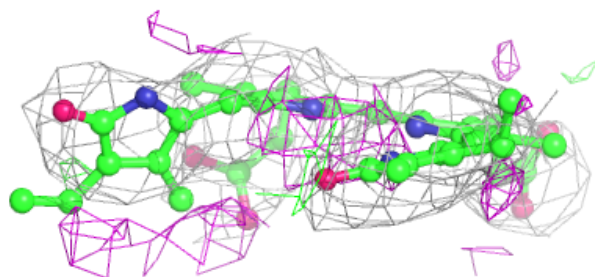
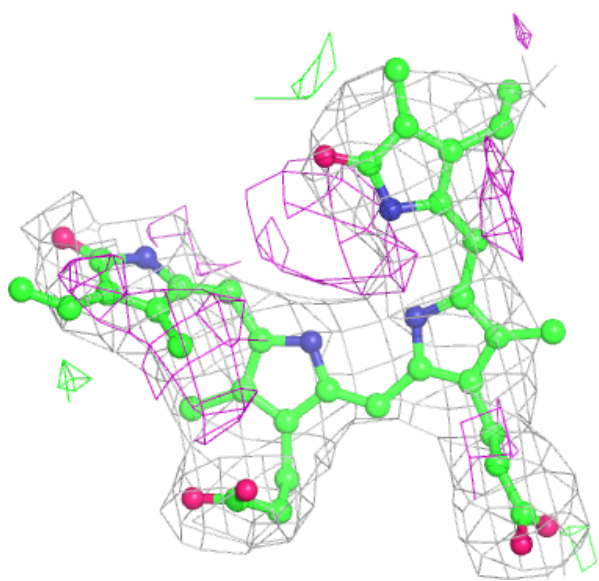
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around BLA A 601:**

$2mF_o-DF_c$  (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.