



Full wwPDB X-ray Structure Validation Report

Oct 5, 2023 – 09:34 PM EDT

PDB ID : 6PL0
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP from Xanthomonas campestris in the Pr state bound to BV chromophore
Authors : Otero, L.H.; Sirigu, S.; Klinke, S.; Goldbaum, F.; Chavas, L.; Rinaldi, J.; Bonomi, H.R.
Deposited on : 2019-06-30
Resolution : 2.96 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

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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

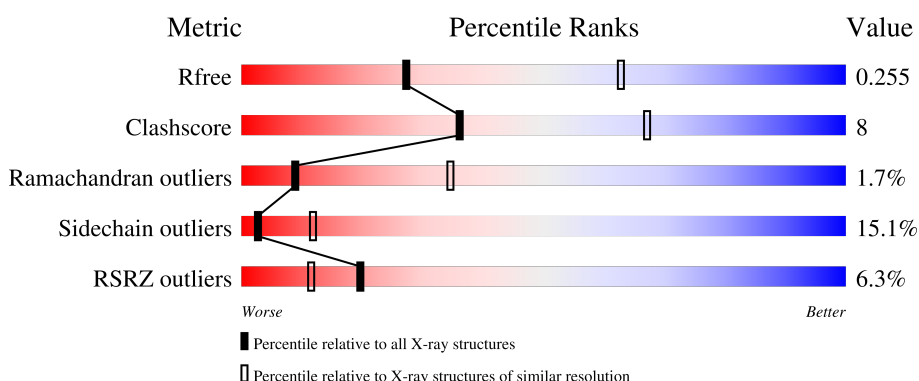
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	 4% 66% 26% • 5%
1	B	640	 8% 68% 25% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9597 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.

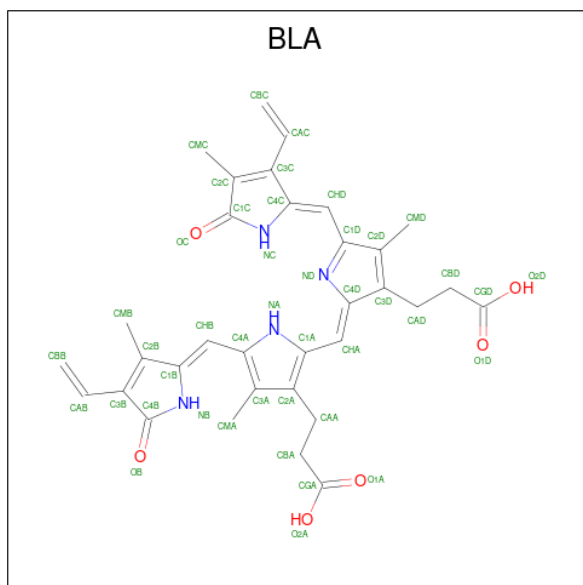
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	606	4748	3004	862	866	16	0	0	0
1	B	608	4761	3011	864	870	16	0	0	0

There are 14 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
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

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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		

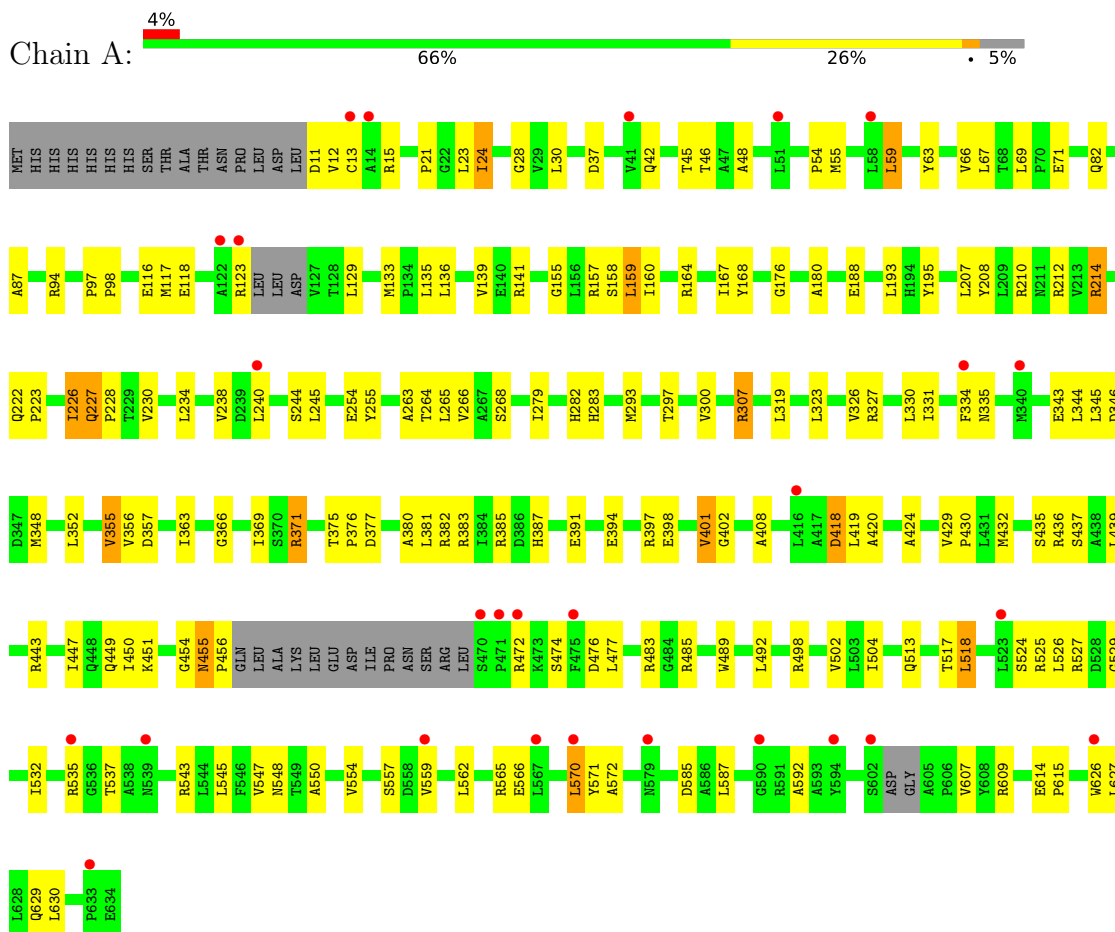
- Molecule 3 is water.

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

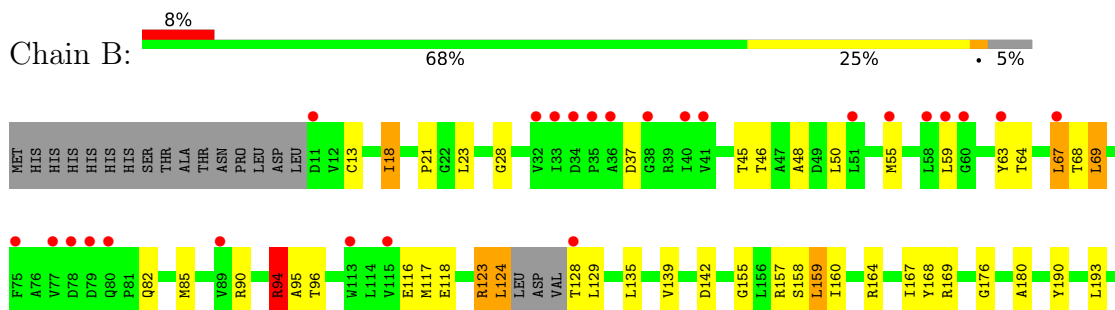
3 Residue-property plots i

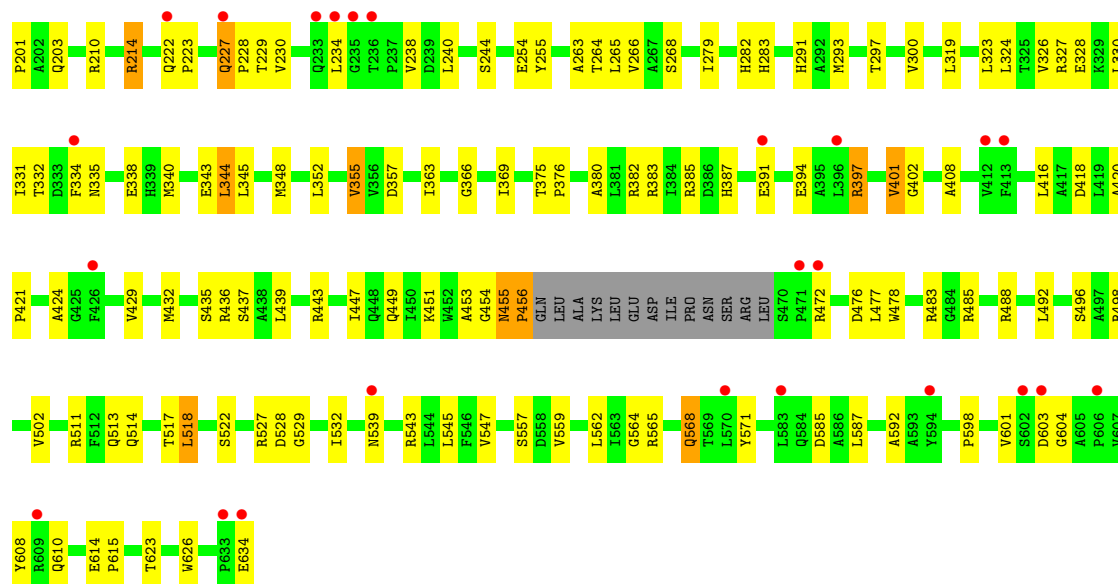
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Bacteriophytochrome



- Molecule 1: Bacteriophytochrome





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.53Å 103.53Å 346.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 2.96 49.60 – 2.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.60-2.96) 100.0 (49.60-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.206 , 0.248 0.223 , 0.255	Depositor DCC
R_{free} test set	2021 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	112.6	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9597	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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	0.51	0/4857	0.74	0/6625
1	B	0.50	0/4871	0.73	0/6645
All	All	0.51	0/9728	0.74	0/13270

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	4748	0	4734	73	0
1	B	4761	0	4744	70	0
2	A	43	0	30	11	0
2	B	43	0	31	11	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9597	0	9539	153	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 8.

All (153) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASN:HB3	1:A:456:PRO:HD3	1.47	0.96
1:B:455:ASN:HB3	1:B:456:PRO:HD3	1.51	0.89
1:A:524:SER:HA	1:A:548:ASN:HB2	1.59	0.85
2:A:900:BLA:HHD	2:A:900:BLA:HBC1	1.58	0.83
2:A:900:BLA:NB	2:A:900:BLA:HMA1	1.97	0.79
1:B:164:ARG:HG2	1:B:282:HIS:HB2	1.64	0.79
1:A:394:GLU:HG2	1:A:397:ARG:HH22	1.49	0.77
1:B:63:TYR:HE2	1:B:67:LEU:HD13	1.48	0.77
2:A:900:BLA:OB	2:A:900:BLA:HBB1	1.87	0.74
1:A:455:ASN:HB3	1:A:456:PRO:CD	2.17	0.74
2:B:900:BLA:NB	2:B:900:BLA:HMA1	2.02	0.74
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.53	0.72
1:B:63:TYR:CE2	1:B:67:LEU:HD13	2.26	0.71
1:B:123:ARG:HG2	1:B:124:LEU:HG	1.71	0.70
1:B:455:ASN:HB3	1:B:456:PRO:CD	2.21	0.69
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.75	0.68
1:B:227:GLN:HB3	1:B:228:PRO:HD3	1.78	0.65
2:A:900:BLA:HMA1	2:A:900:BLA:HB	1.62	0.64
2:B:900:BLA:HBB1	2:B:900:BLA:OB	1.98	0.63
2:A:900:BLA:HHD	2:A:900:BLA:CBC	2.28	0.63
1:A:447:ILE:HG12	1:A:483:ARG:HG2	1.80	0.63
1:B:326:VAL:HG12	1:B:355:VAL:HG13	1.79	0.63
2:A:900:BLA:HB	2:A:900:BLA:CMA	2.12	0.62
1:B:282:HIS:CE1	2:B:900:BLA:OB	2.52	0.62
1:B:401:VAL:HG13	1:B:402:GLY:H	1.65	0.61
1:A:455:ASN:CB	1:A:456:PRO:HD3	2.24	0.61
1:A:371:ARG:HG3	1:A:381:LEU:HD11	1.83	0.61
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.82	0.61
1:B:455:ASN:CB	1:B:456:PRO:HD3	2.26	0.60
1:A:164:ARG:HG2	1:A:282:HIS:HB2	1.83	0.60
1:A:327:ARG:O	1:A:331:ILE:HG12	2.02	0.60
1:A:451:LYS:HB3	1:A:477:LEU:HD11	1.82	0.60
2:B:900:BLA:CMA	2:B:900:BLA:HB	2.15	0.60
1:A:345:LEU:HD22	1:A:363:ILE:HD13	1.84	0.59
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.85	0.59
1:B:345:LEU:HD22	1:B:363:ILE:HD13	1.85	0.58
1:B:557:SER:HB3	1:B:562:LEU:HD13	1.84	0.58
1:A:24:ILE:HD12	1:A:245:LEU:HB2	1.84	0.58
1:A:326:VAL:HG12	1:A:355:VAL:HG13	1.85	0.58
1:A:565:ARG:HH12	1:A:570:LEU:HB3	1.68	0.57
1:A:265:LEU:HD21	1:A:297:THR:HG21	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:HG13	1:A:402:GLY:H	1.69	0.56
1:A:371:ARG:NH2	1:A:377:ASP:HA	2.19	0.56
1:B:401:VAL:HG11	1:B:498:ARG:HH21	1.70	0.56
1:A:557:SER:HB3	1:A:562:LEU:HD13	1.87	0.56
1:A:401:VAL:HG11	1:A:498:ARG:NH2	2.21	0.56
1:A:160:ILE:HD13	1:A:293:MET:HG3	1.88	0.56
2:B:900:BLA:HMA1	2:B:900:BLA:HB	1.71	0.56
1:A:21:PRO:HD2	1:A:240:LEU:HD12	1.89	0.55
1:B:394:GLU:HG2	1:B:397:ARG:HH21	1.71	0.54
1:B:447:ILE:HG22	1:B:483:ARG:HG2	1.89	0.54
2:B:900:BLA:HBC1	2:B:900:BLA:HHD	1.90	0.54
1:A:408:ALA:HB2	1:A:485:ARG:HG2	1.88	0.54
1:B:21:PRO:HD2	1:B:240:LEU:HD12	1.88	0.54
1:B:451:LYS:HB3	1:B:477:LEU:HD11	1.90	0.53
1:A:380:ALA:HB1	1:A:419:LEU:HD23	1.90	0.53
1:A:454:GLY:O	1:A:455:ASN:HB2	2.08	0.53
1:B:408:ALA:HB2	1:B:485:ARG:HG2	1.90	0.53
1:A:394:GLU:O	1:A:398:GLU:HG2	2.09	0.53
1:A:139:VAL:O	1:A:307:ARG:HD2	2.11	0.52
1:A:513:GLN:O	1:A:517:THR:HG23	2.10	0.52
2:A:900:BLA:NB	2:A:900:BLA:CMA	2.70	0.52
1:B:327:ARG:O	1:B:331:ILE:HG12	2.10	0.52
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.92	0.51
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.91	0.51
1:B:513:GLN:O	1:B:517:THR:HG23	2.10	0.51
1:B:357:ASP:HB3	1:B:443:ARG:HH21	1.75	0.51
2:B:900:BLA:HHD	2:B:900:BLA:CBC	2.41	0.51
1:A:293:MET:O	1:A:297:THR:HG23	2.11	0.51
1:A:30:LEU:HD23	1:A:226:ILE:HD12	1.93	0.51
1:B:293:MET:O	1:B:297:THR:HG23	2.11	0.51
1:A:71:GLU:HB2	1:A:87:ALA:HB1	1.92	0.50
1:A:401:VAL:HG11	1:A:498:ARG:HH21	1.76	0.50
1:A:547:VAL:HG13	1:A:559:VAL:HG13	1.94	0.49
1:A:42:GLN:HA	1:A:228:PRO:HD2	1.94	0.49
1:B:420:ALA:O	1:B:424:ALA:HB2	2.12	0.49
1:A:48:ALA:HB1	1:A:54:PRO:HA	1.94	0.49
1:B:547:VAL:HG13	1:B:559:VAL:HG13	1.93	0.49
1:A:263:ALA:HB3	1:A:283:HIS:HB3	1.93	0.49
1:B:587:LEU:HA	1:B:626:TRP:CZ2	2.48	0.48
1:B:68:THR:HB	1:B:90:ARG:HB2	1.94	0.48
1:A:587:LEU:HA	1:A:626:TRP:CZ2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HA	1:A:55:MET:CE	2.44	0.48
1:B:454:GLY:O	1:B:478:TRP:CD1	2.67	0.48
1:A:208:TYR:OH	2:A:900:BLA:HAA1	2.14	0.47
1:B:420:ALA:N	1:B:421:PRO:HD2	2.28	0.47
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.96	0.47
1:B:592:ALA:HB2	1:B:615:PRO:HD3	1.96	0.47
1:B:376:PRO:HB2	1:B:380:ALA:HB3	1.96	0.47
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.49	0.47
1:B:45:THR:HA	1:B:55:MET:CE	2.45	0.47
2:B:900:BLA:NB	2:B:900:BLA:CMA	2.72	0.47
1:B:324:LEU:HD12	1:B:327:ARG:HH12	1.80	0.46
1:B:193:LEU:HG	1:B:453:ALA:HB2	1.97	0.46
1:B:167:ILE:HB	1:B:180:ALA:HB3	1.97	0.46
1:A:357:ASP:HB3	1:A:443:ARG:HH21	1.79	0.46
1:B:190:TYR:O	1:B:193:LEU:HB2	2.15	0.46
1:A:59:LEU:HD11	1:A:228:PRO:HD3	1.98	0.46
1:A:155:GLY:O	1:A:159:LEU:HD12	2.15	0.46
1:B:568:GLN:HA	1:B:571:TYR:CE2	2.50	0.45
1:B:418:ASP:C	1:B:420:ALA:H	2.20	0.45
1:A:45:THR:HA	1:A:55:MET:HE1	1.99	0.45
1:A:214:ARG:NH2	1:A:266:VAL:HG22	2.32	0.45
1:A:167:ILE:HB	1:A:180:ALA:HB3	1.99	0.45
1:A:609:ARG:HG2	1:A:630:LEU:HB3	1.98	0.45
1:B:340:MET:HA	1:B:344:LEU:HD22	1.98	0.45
1:B:543:ARG:HD2	1:B:564:GLY:O	2.16	0.45
1:A:356:VAL:HG13	1:A:489:TRP:CZ3	2.51	0.44
1:B:326:VAL:CG1	1:B:355:VAL:HG13	2.47	0.44
1:A:266:VAL:HA	1:A:279:ILE:O	2.18	0.44
1:A:369:ILE:HD11	1:A:382:ARG:HG3	2.00	0.44
1:A:376:PRO:HB2	1:A:380:ALA:HB3	1.98	0.44
1:A:627:LEU:HD13	1:B:522:SER:HB3	2.00	0.43
1:B:155:GLY:O	1:B:159:LEU:HD12	2.17	0.43
1:B:416:LEU:O	1:B:418:ASP:O	2.37	0.43
1:A:28:GLY:O	1:A:46:THR:HG21	2.19	0.43
1:A:430:PRO:HD3	1:A:504:ILE:HG12	2.01	0.43
1:B:214:ARG:HG3	2:B:900:BLA:O2A	2.19	0.43
1:B:255:TYR:CD2	2:B:900:BLA:OC	2.70	0.43
1:A:330:LEU:O	1:A:334:PHE:HB2	2.19	0.43
1:A:97:PRO:HD2	1:A:98:PRO:HD3	2.01	0.43
1:A:502:VAL:HG23	1:B:502:VAL:HA	2.00	0.43
1:A:518:LEU:HD22	1:B:532:ILE:HG21	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.53	0.42
1:B:201:PRO:HB2	1:B:203:GLN:OE1	2.18	0.42
1:A:529:GLY:O	1:A:629:GLN:HA	2.20	0.42
1:B:330:LEU:O	1:B:334:PHE:HB2	2.20	0.42
1:A:195:TYR:CD1	2:A:900:BLA:HMB1	2.54	0.42
1:B:94:ARG:NH1	1:B:95:ALA:H	2.17	0.42
1:B:266:VAL:HA	1:B:279:ILE:O	2.20	0.42
1:A:401:VAL:CG1	1:A:498:ARG:HH21	2.33	0.42
1:B:615:PRO:HB2	1:B:623:THR:HG21	2.01	0.41
1:A:255:TYR:CD2	2:A:900:BLA:OC	2.73	0.41
1:A:352:LEU:HD21	1:A:439:LEU:HD21	2.02	0.41
1:A:12:VAL:HA	1:A:15:ARG:HD2	2.02	0.41
1:B:94:ARG:CZ	1:B:95:ALA:H	2.33	0.41
1:A:532:ILE:HG21	1:B:518:LEU:HD22	2.03	0.41
1:A:420:ALA:O	1:A:424:ALA:HB2	2.19	0.41
1:B:369:ILE:HD11	1:B:382:ARG:HG3	2.02	0.41
1:A:550:ALA:O	1:A:554:VAL:HG23	2.21	0.41
1:B:64:THR:HA	1:B:67:LEU:HB3	2.03	0.41
1:A:418:ASP:C	1:A:420:ALA:H	2.24	0.41
1:B:67:LEU:HD11	1:B:69:LEU:HB2	2.03	0.41
1:A:97:PRO:CD	1:A:98:PRO:HD3	2.51	0.41
1:B:328:GLU:O	1:B:332:THR:HG23	2.21	0.41
1:B:436:ARG:CZ	1:B:511:ARG:HG2	2.51	0.41
1:B:28:GLY:O	1:B:46:THR:HG21	2.21	0.40
1:A:195:TYR:CZ	2:A:900:BLA:HAB	2.56	0.40
1:B:352:LEU:HD21	1:B:439:LEU:HD21	2.02	0.40
1:B:615:PRO:CB	1:B:623:THR:HG21	2.52	0.40
1:B:598:PRO:HA	1:B:608:TYR:HA	2.04	0.40
1:B:48:ALA:HB2	1:B:55:MET:HE2	2.03	0.40
1:B:282:HIS:HE1	2:B:900:BLA:OB	2.04	0.40

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	598/640 (93%)	542 (91%)	45 (8%)	11 (2%)	8	33
1	B	602/640 (94%)	550 (91%)	43 (7%)	9 (2%)	10	38
All	All	1200/1280 (94%)	1092 (91%)	88 (7%)	20 (2%)	9	34

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	435	SER
1	A	455	ASN
1	A	526	LEU
1	A	537	THR
1	B	455	ASN
1	A	366	GLY
1	B	18	ILE
1	B	366	GLY
1	B	529	GLY
1	A	572	ALA
1	B	435	SER
1	B	94	ARG
1	A	436	ARG
1	A	227	GLN
1	A	418	ASP
1	A	607	VAL
1	A	401	VAL
1	B	401	VAL
1	B	227	GLN
1	B	604	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/532 (94%)	427 (85%)	74 (15%)	3	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	502/532 (94%)	425 (85%)	77 (15%)	2	11
All	All	1003/1064 (94%)	852 (85%)	151 (15%)	3	12

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	13	CYS
1	A	24	ILE
1	A	37	ASP
1	A	59	LEU
1	A	63	TYR
1	A	66	VAL
1	A	67	LEU
1	A	69	LEU
1	A	82	GLN
1	A	94	ARG
1	A	116	GLU
1	A	117	MET
1	A	118	GLU
1	A	123	ARG
1	A	129	LEU
1	A	133	MET
1	A	135	LEU
1	A	136	LEU
1	A	141	ARG
1	A	157	ARG
1	A	158	SER
1	A	159	LEU
1	A	188	GLU
1	A	193	LEU
1	A	207	LEU
1	A	210	ARG
1	A	212	ARG
1	A	214	ARG
1	A	222	GLN
1	A	226	ILE
1	A	230	VAL
1	A	234	LEU
1	A	238	VAL
1	A	244	SER
1	A	254	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	264	THR
1	A	268	SER
1	A	300	VAL
1	A	307	ARG
1	A	319	LEU
1	A	323	LEU
1	A	335	ASN
1	A	343	GLU
1	A	344	LEU
1	A	346	ASP
1	A	348	MET
1	A	355	VAL
1	A	371	ARG
1	A	375	THR
1	A	383	ARG
1	A	385	ARG
1	A	387	HIS
1	A	391	GLU
1	A	429	VAL
1	A	432	MET
1	A	437	SER
1	A	449	GLN
1	A	450	ILE
1	A	472	ARG
1	A	474	SER
1	A	476	ASP
1	A	492	LEU
1	A	518	LEU
1	A	525	ARG
1	A	527	ARG
1	A	535	ARG
1	A	543	ARG
1	A	545	LEU
1	A	566	GLU
1	A	570	LEU
1	A	571	TYR
1	A	585	ASP
1	A	614	GLU
1	B	13	CYS
1	B	18	ILE
1	B	37	ASP
1	B	50	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	59	LEU
1	B	67	LEU
1	B	69	LEU
1	B	82	GLN
1	B	85	MET
1	B	94	ARG
1	B	96	THR
1	B	116	GLU
1	B	117	MET
1	B	118	GLU
1	B	123	ARG
1	B	124	LEU
1	B	128	THR
1	B	129	LEU
1	B	135	LEU
1	B	139	VAL
1	B	142	ASP
1	B	157	ARG
1	B	158	SER
1	B	159	LEU
1	B	160	ILE
1	B	169	ARG
1	B	210	ARG
1	B	214	ARG
1	B	222	GLN
1	B	229	THR
1	B	230	VAL
1	B	234	LEU
1	B	238	VAL
1	B	244	SER
1	B	254	GLU
1	B	264	THR
1	B	268	SER
1	B	291	HIS
1	B	300	VAL
1	B	319	LEU
1	B	323	LEU
1	B	335	ASN
1	B	338	GLU
1	B	343	GLU
1	B	344	LEU
1	B	348	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	VAL
1	B	375	THR
1	B	383	ARG
1	B	385	ARG
1	B	387	HIS
1	B	391	GLU
1	B	397	ARG
1	B	429	VAL
1	B	432	MET
1	B	437	SER
1	B	449	GLN
1	B	456	PRO
1	B	472	ARG
1	B	476	ASP
1	B	488	ARG
1	B	492	LEU
1	B	496	SER
1	B	514	GLN
1	B	518	LEU
1	B	527	ARG
1	B	528	ASP
1	B	539	ASN
1	B	545	LEU
1	B	565	ARG
1	B	568	GLN
1	B	585	ASP
1	B	601	VAL
1	B	603	ASP
1	B	610	GLN
1	B	614	GLU
1	B	634	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	291	HIS
1	B	584	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 monosaccharides 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	42,46,46	1.81	10 (23%)	53,67,67	2.01	15 (28%)
2	BLA	B	900	1	42,46,46	1.82	7 (16%)	53,67,67	2.12	15 (28%)

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	-	3/26/74/74	0/4/4/4
2	BLA	B	900	1	-	3/26/74/74	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	CHB-C1B	6.32	1.47	1.34
2	A	900	BLA	C3D-C2D	5.46	1.48	1.36
2	B	900	BLA	CHA-C4D	4.99	1.39	1.35
2	A	900	BLA	C3B-C2B	4.94	1.47	1.37
2	A	900	BLA	CHA-C4D	4.93	1.39	1.35
2	B	900	BLA	C3B-C2B	4.89	1.47	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	BLA	C2A-C3A	3.44	1.47	1.37
2	A	900	BLA	C2A-C3A	3.19	1.47	1.37
2	A	900	BLA	C3C-C4C	2.49	1.49	1.45
2	B	900	BLA	C3C-C4C	2.45	1.49	1.45
2	A	900	BLA	OB-C4B	2.38	1.28	1.23
2	B	900	BLA	OB-C4B	2.37	1.28	1.23
2	A	900	BLA	C1B-C2B	2.28	1.49	1.45
2	A	900	BLA	C4D-C3D	2.17	1.49	1.45
2	A	900	BLA	C1A-CHA	2.16	1.49	1.41
2	A	900	BLA	C4B-NB	-2.13	1.33	1.38
2	B	900	BLA	C4B-NB	-2.03	1.33	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3B-C4B-NB	7.08	114.19	106.19
2	A	900	BLA	C3B-C4B-NB	6.22	113.22	106.19
2	B	900	BLA	C2B-C1B-NB	5.82	115.51	106.99
2	B	900	BLA	C3B-C2B-C1B	-5.69	101.16	108.03
2	A	900	BLA	C3B-C2B-C1B	-5.43	101.47	108.03
2	B	900	BLA	C1B-NB-C4B	-4.65	104.74	110.67
2	A	900	BLA	C2B-C1B-NB	4.49	113.56	106.99
2	A	900	BLA	CMB-C2B-C1B	4.05	129.22	124.17
2	A	900	BLA	CBA-CAA-C2A	-3.60	106.48	112.62
2	A	900	BLA	C1B-NB-C4B	-3.20	106.60	110.67
2	B	900	BLA	C1A-CHA-C4D	3.11	132.53	128.81
2	B	900	BLA	CHB-C1B-NB	-2.98	120.39	130.40
2	A	900	BLA	OB-C4B-C3B	-2.98	122.71	129.46
2	B	900	BLA	OB-C4B-C3B	-2.91	122.86	129.46
2	A	900	BLA	CHB-C1B-NB	-2.86	120.79	130.40
2	B	900	BLA	CMB-C2B-C1B	2.80	127.66	124.17
2	B	900	BLA	C4B-C3B-C2B	-2.75	104.39	107.92
2	B	900	BLA	CBA-CAA-C2A	-2.74	107.94	112.62
2	A	900	BLA	C4D-C3D-C2D	-2.60	103.90	106.78
2	A	900	BLA	CBB-CAB-C3B	-2.47	115.32	127.62
2	B	900	BLA	CAA-CBA-CGA	-2.36	107.14	113.76
2	A	900	BLA	C4C-CHD-C1D	2.35	133.82	128.08
2	B	900	BLA	C4C-CHD-C1D	2.30	133.71	128.08
2	B	900	BLA	CMA-C3A-C2A	2.30	129.28	124.94
2	B	900	BLA	CHA-C4D-ND	-2.25	125.71	128.83
2	B	900	BLA	CBB-CAB-C3B	-2.23	116.53	127.62
2	A	900	BLA	CHA-C4D-ND	-2.17	125.82	128.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	BLA	C4B-C3B-C2B	-2.17	105.14	107.92
2	A	900	BLA	CMA-C3A-C2A	2.15	128.99	124.94
2	A	900	BLA	C1D-C2D-C3D	-2.14	104.05	106.51

There are no chirality outliers.

All (6) torsion outliers are listed below:

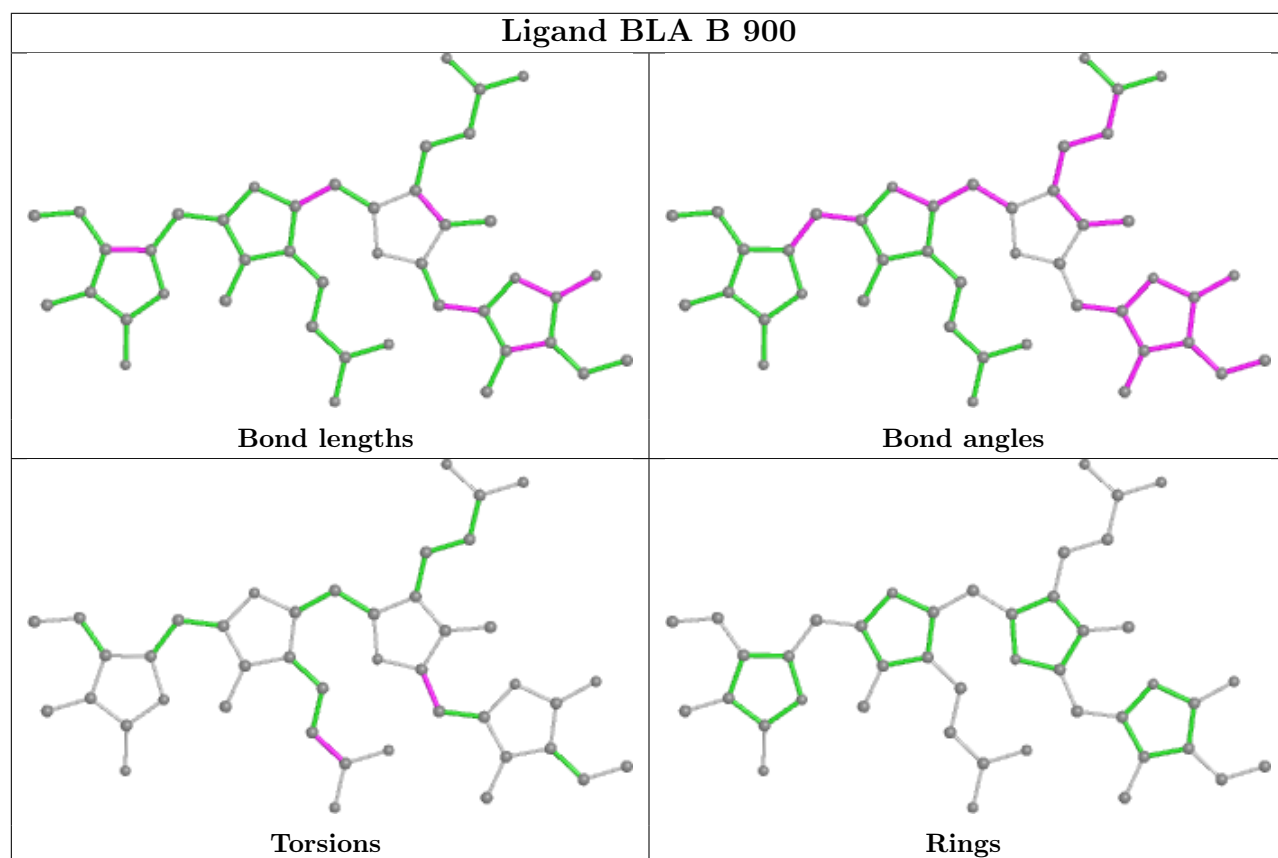
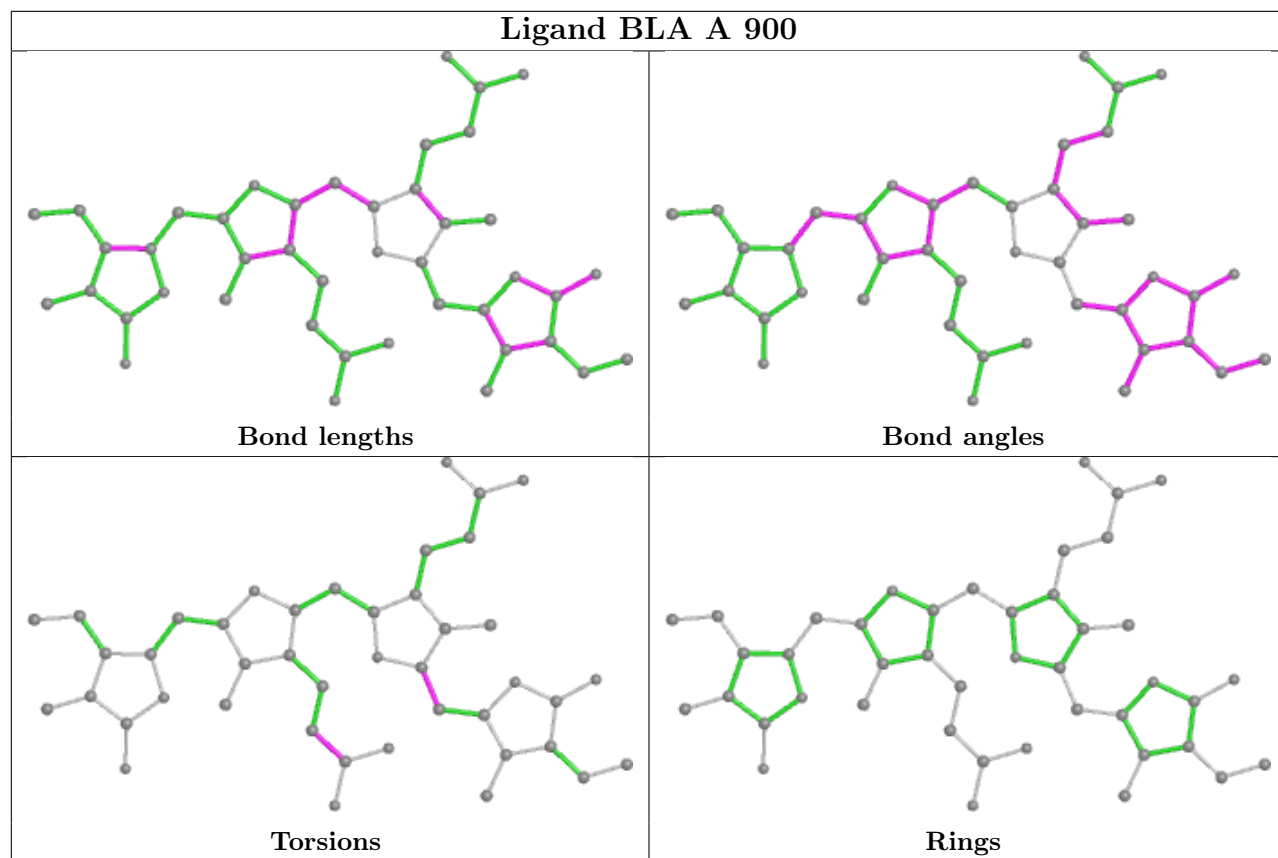
Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	CAD-CBD-CGD-O2D
2	A	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O1D
2	B	900	BLA	CAD-CBD-CGD-O2D

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	BLA	11	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

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, 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	606/640 (94%)	0.49	27 (4%) 33 21	79, 116, 167, 184	0
1	B	608/640 (95%)	0.59	49 (8%) 12 6	77, 115, 172, 203	0
All	All	1214/1280 (94%)	0.54	76 (6%) 20 11	77, 116, 170, 203	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	471	PRO	6.2
1	B	79	ASP	5.4
1	B	413	PHE	4.6
1	B	471	PRO	4.4
1	B	58	LEU	4.2
1	B	51	LEU	4.2
1	B	128	THR	3.9
1	B	113	TRP	3.8
1	A	472	ARG	3.8
1	B	41	VAL	3.8
1	B	412	VAL	3.8
1	B	55	MET	3.7
1	B	77	VAL	3.6
1	B	78	ASP	3.6
1	B	36	ALA	3.5
1	B	233	GLN	3.5
1	B	609	ARG	3.3
1	B	236	THR	3.2
1	A	570	LEU	3.1
1	B	34	ASP	3.1
1	A	51	LEU	3.0
1	A	579	ASN	3.0
1	B	32	VAL	3.0
1	B	334	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	2.9
1	B	222	GLN	2.9
1	A	567	LEU	2.8
1	B	602	SER	2.8
1	B	539	ASN	2.7
1	B	59	LEU	2.7
1	A	535	ARG	2.7
1	B	234	LEU	2.7
1	A	590	GLY	2.7
1	B	570	LEU	2.6
1	B	60	GLY	2.6
1	A	602	SER	2.6
1	B	38	GLY	2.5
1	B	634	GLU	2.5
1	B	603	ASP	2.5
1	A	475	PHE	2.4
1	A	58	LEU	2.4
1	B	391	GLU	2.4
1	A	340	MET	2.4
1	A	626	TRP	2.4
1	A	334	PHE	2.3
1	B	426	PHE	2.3
1	A	122	ALA	2.3
1	B	633	PRO	2.3
1	B	67	LEU	2.3
1	A	559	VAL	2.3
1	A	523	LEU	2.3
1	B	115	VAL	2.3
1	B	63	TYR	2.3
1	B	33	ILE	2.2
1	B	594	TYR	2.2
1	B	583	LEU	2.2
1	A	539	ASN	2.2
1	B	235	GLY	2.2
1	A	416	LEU	2.2
1	B	472	ARG	2.2
1	B	40	ILE	2.2
1	B	396	LEU	2.2
1	B	80	GLN	2.2
1	B	606	PRO	2.2
1	A	41	VAL	2.2
1	A	594	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	123	ARG	2.1
1	B	35	PRO	2.1
1	B	89	VAL	2.1
1	A	240	LEU	2.0
1	A	470	SER	2.0
1	B	227	GLN	2.0
1	A	633	PRO	2.0
1	B	75	PHE	2.0
1	A	13	CYS	2.0
1	A	14	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

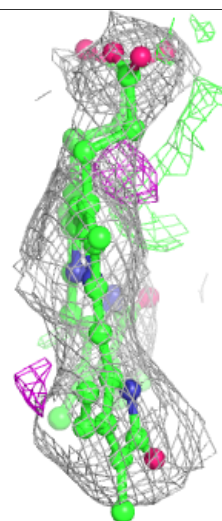
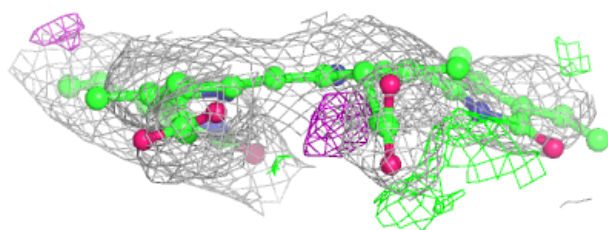
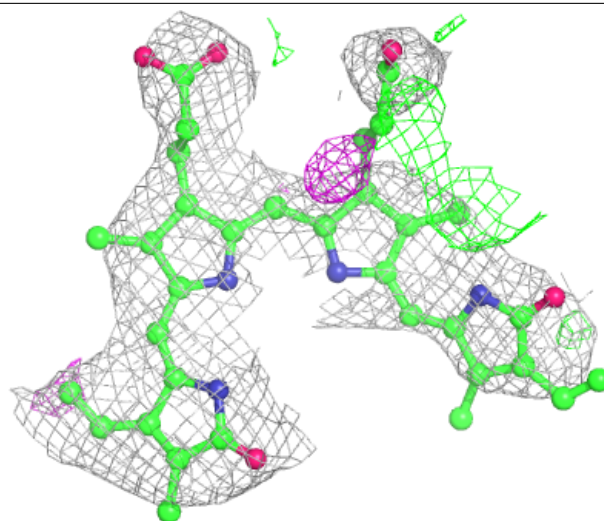
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

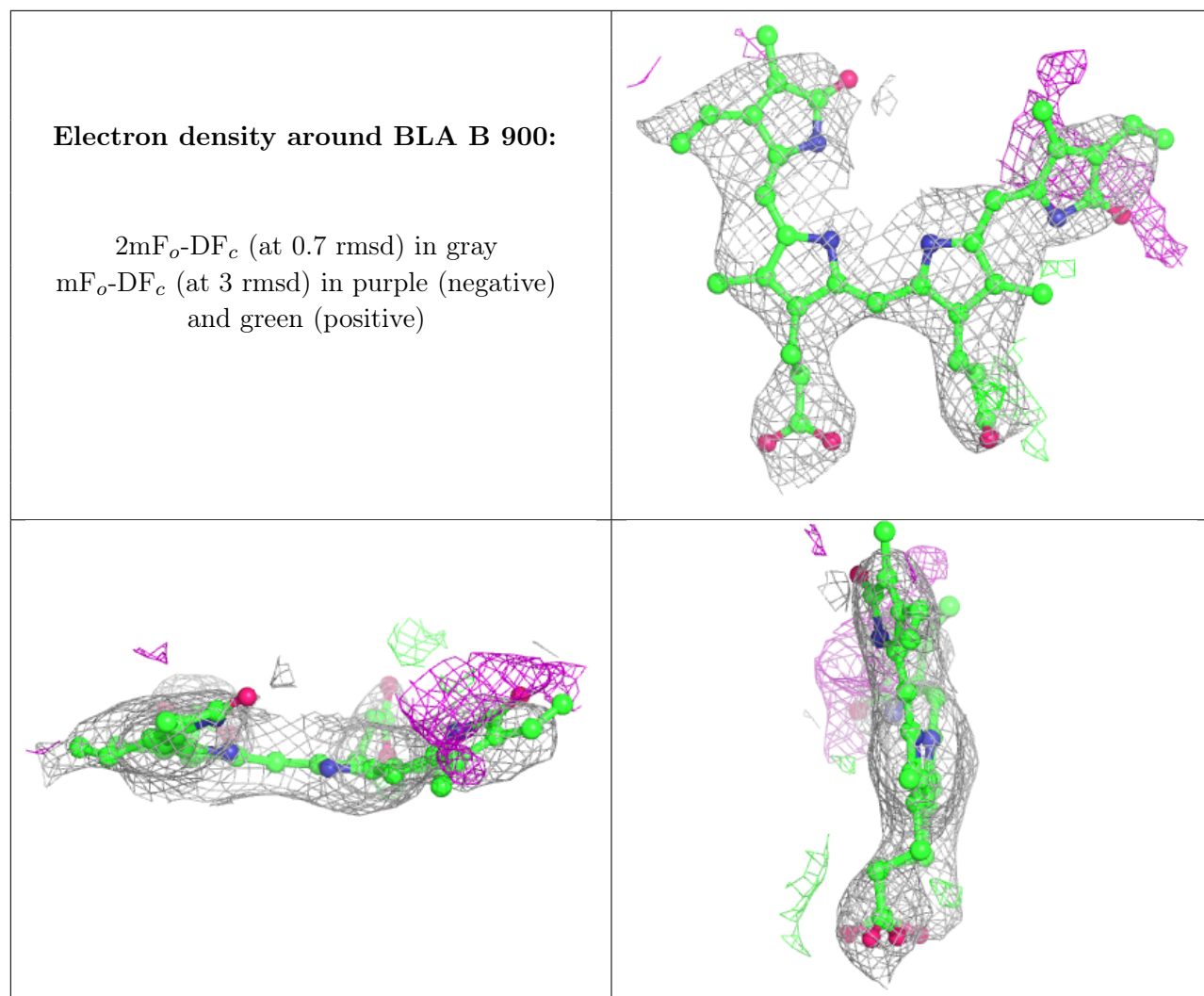
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BLA	A	900	43/43	0.88	0.34	122,129,145,159	0
2	BLA	B	900	43/43	0.88	0.37	116,123,137,151	0

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 A 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.