



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2021 – 02:10 PM EST

PDB ID : 6NDO
Title : Crystal structure of the dark-adapted full-length bacteriophytochrome Xc-cBphP mutant L193N from *Xanthomonas campestris*
Authors : Otero, L.H.; Sirigu, S.; Klinke, S.; Rinaldi, J.; Conforte, V.; Malamud, F.; Goldbaum, F.A.; Chavas, L.; Bonomi, H.R.
Deposited on : 2018-12-14
Resolution : 3.58 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 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 : 2.23.2
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) : 2.23.2

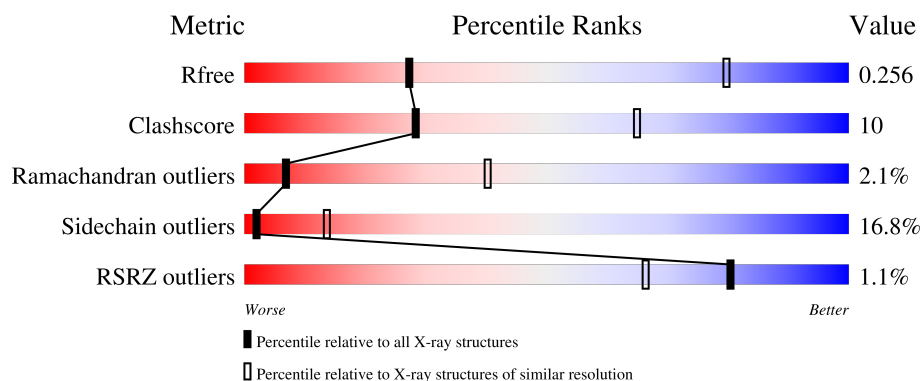
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.58 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	640	
1	B	640	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9462 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.

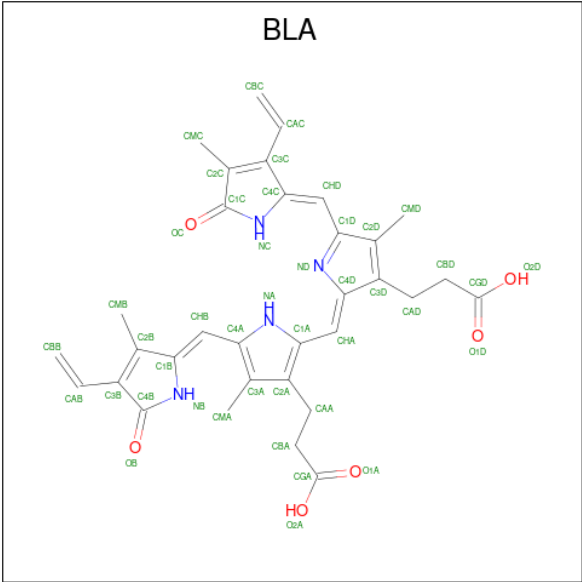
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	593	Total	C	N	O	S	0	0	0
			4644	2938	846	844	16			
1	B	604	Total	C	N	O	S	0	0	0
			4730	2992	861	861	16			

There are 16 discrepancies between the modelled and reference sequences:

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

- 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		

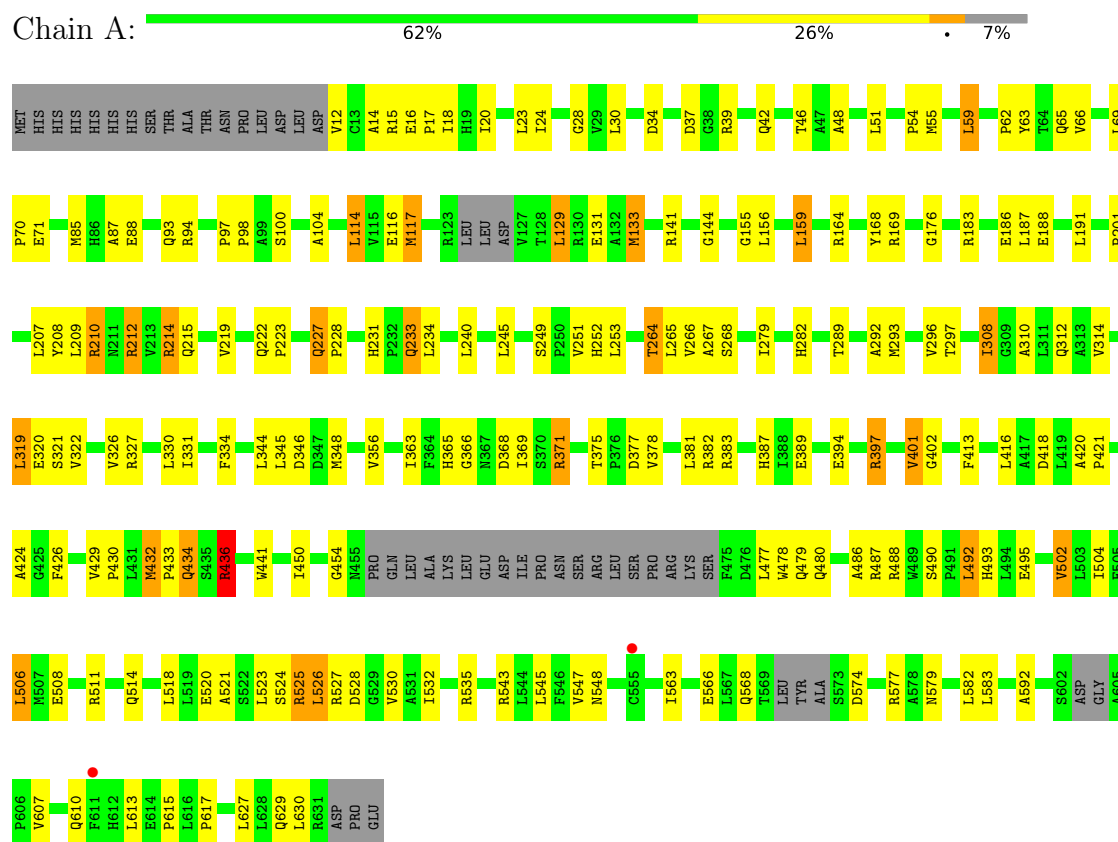
- Molecule 3 is water.

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

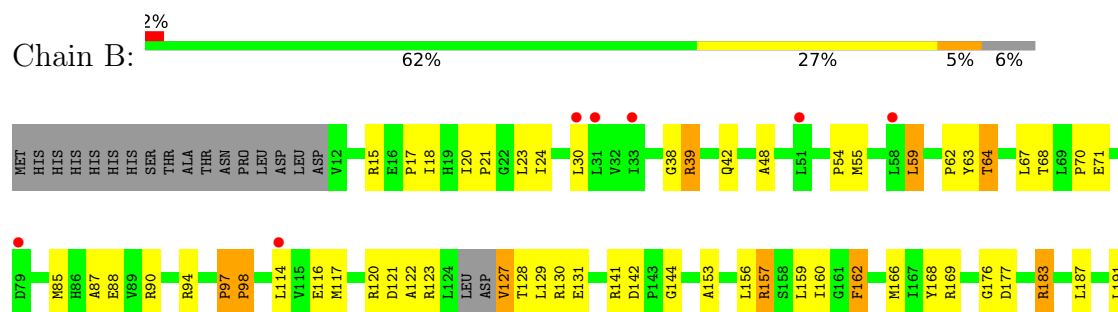
3 Residue-property plots [i](#)

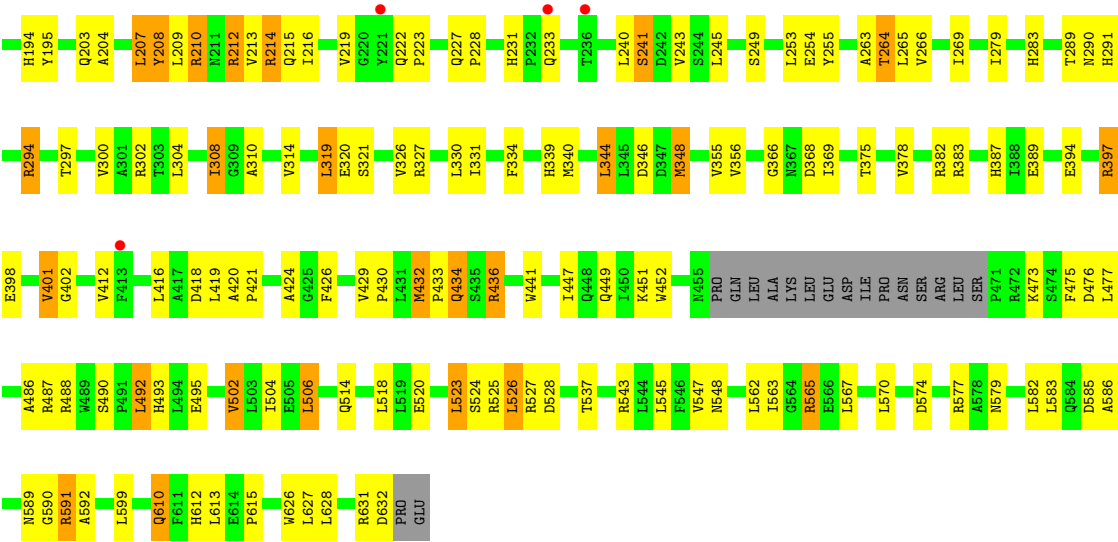
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	103.60Å 103.60Å 343.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.58 49.60 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.60-3.58) 99.4 (49.60-3.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.57Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.198 , 0.238 0.216 , 0.256	Depositor DCC
R_{free} test set	1141 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	142.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 125.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9462	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

5.1 Standard geometry

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	0.53	0/4748	0.73	0/6475
1	B	0.51	0/4838	0.72	0/6599
All	All	0.52	0/9586	0.72	0/13074

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

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	4644	0	4632	89	0
1	B	4730	0	4720	90	0
2	A	43	0	31	8	0
2	B	43	0	30	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	9462	0	9413	184	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 10.

All (184) 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:64:THR:HA	1:B:67:LEU:HB2	1.52	0.90
1:A:14:ALA:HB2	1:A:201:PRO:HB3	1.52	0.90
1:B:97:PRO:HB2	1:B:98:PRO:HD3	1.60	0.83
1:A:251:VAL:HG11	2:A:900:BLA:HBC1	1.60	0.83
2:A:900:BLA:NB	2:A:900:BLA:HMA1	1.94	0.81
1:A:12:VAL:HG13	1:A:15:ARG:NE	1.96	0.81
1:B:432:MET:HG2	1:B:433:PRO:HD2	1.63	0.80
1:A:432:MET:HG2	1:A:433:PRO:HD2	1.63	0.80
1:A:371:ARG:HH21	1:A:377:ASP:HA	1.46	0.80
1:A:524:SER:HA	1:A:548:ASN:HB2	1.69	0.74
1:A:16:GLU:HG3	1:A:17:PRO:HD2	1.68	0.73
2:B:900:BLA:NB	2:B:900:BLA:HMA1	2.03	0.72
1:B:121:ASP:HB3	1:B:290:ASN:HB3	1.72	0.71
1:B:265:LEU:HD21	1:B:297:THR:HG21	1.72	0.71
1:B:401:VAL:HG13	1:B:402:GLY:H	1.55	0.71
1:A:231:HIS:HD2	1:A:233:GLN:H	1.42	0.67
1:A:16:GLU:CG	1:A:17:PRO:HD2	2.25	0.66
1:B:231:HIS:HD2	1:B:233:GLN:H	1.42	0.66
1:A:401:VAL:HG13	1:A:402:GLY:H	1.62	0.65
1:A:156:LEU:HD11	1:A:297:THR:HG22	1.79	0.65
1:A:39:ARG:HA	1:A:62:PRO:HA	1.77	0.65
1:A:523:LEU:HA	1:A:526:LEU:HD12	1.80	0.63
1:A:436:ARG:HE	1:A:511:ARG:HG2	1.62	0.63
1:B:156:LEU:HD11	1:B:297:THR:HG22	1.80	0.62
2:B:900:BLA:CMA	2:B:900:BLA:HB	2.13	0.62
1:A:164:ARG:HG3	1:A:282:HIS:HB2	1.84	0.59
1:B:168:TYR:CZ	1:B:176:GLY:HA3	2.37	0.59
1:B:21:PRO:HD2	1:B:240:LEU:HD23	1.85	0.58
1:A:365:HIS:HE1	1:A:511:ARG:HD3	1.68	0.57
1:B:255:TYR:OH	2:B:900:BLA:HMB3	2.03	0.57
1:A:371:ARG:HG3	1:A:381:LEU:HD11	1.86	0.57
1:A:430:PRO:HD3	1:A:504:ILE:HG12	1.86	0.57
2:B:900:BLA:HBB1	2:B:900:BLA:OB	2.04	0.57
1:A:490:SER:HB3	1:A:493:HIS:ND1	2.19	0.57
1:B:327:ARG:O	1:B:331:ILE:HG12	2.05	0.56
1:B:490:SER:HB3	1:B:493:HIS:ND1	2.20	0.56
1:A:502:VAL:HG23	1:B:502:VAL:HA	1.87	0.56
1:A:327:ARG:O	1:A:331:ILE:HG12	2.06	0.56
1:A:523:LEU:O	1:A:526:LEU:HB2	2.06	0.56
1:B:610:GLN:HB2	1:B:632:ASP:HA	1.88	0.55
1:B:195:TYR:CD2	2:B:900:BLA:HMB1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:PRO:HG3	1:B:525:ARG:HH21	1.71	0.55
1:A:104:ALA:HB2	1:A:117:MET:HB3	1.89	0.55
1:A:155:GLY:O	1:A:159:LEU:HD12	2.07	0.55
1:B:524:SER:HA	1:B:548:ASN:HB2	1.89	0.54
1:B:17:PRO:HB2	1:B:20:ILE:HG13	1.90	0.53
1:B:208:TYR:CE2	2:B:900:BLA:HAA2	2.43	0.53
1:B:430:PRO:HD3	1:B:504:ILE:HG12	1.90	0.53
1:A:394:GLU:HG3	1:A:397:ARG:HH21	1.73	0.53
1:B:30:LEU:HD11	1:B:114:LEU:HD23	1.90	0.53
1:B:216:ILE:HB	1:B:264:THR:HB	1.90	0.53
1:B:502:VAL:O	1:B:506:LEU:HB2	2.08	0.53
1:A:227:GLN:HE21	1:A:227:GLN:HA	1.73	0.53
1:B:394:GLU:HG3	1:B:397:ARG:HH21	1.74	0.53
1:A:17:PRO:HB2	1:A:20:ILE:HG13	1.90	0.53
1:A:502:VAL:HA	1:B:502:VAL:HG23	1.91	0.53
1:A:502:VAL:O	1:A:506:LEU:HB2	2.08	0.53
1:A:265:LEU:HD21	1:A:297:THR:HG21	1.91	0.53
1:B:369:ILE:HD11	1:B:382:ARG:HG3	1.91	0.53
1:B:416:LEU:HB3	1:B:419:LEU:HD13	1.91	0.52
1:A:369:ILE:HD11	1:A:382:ARG:HG3	1.90	0.52
1:B:291:HIS:HA	1:B:294:ARG:HD3	1.91	0.52
1:A:521:ALA:O	1:A:525:ARG:HG3	2.09	0.52
2:A:900:BLA:NB	2:A:900:BLA:CMA	2.70	0.52
1:A:214:ARG:HH12	1:A:264:THR:CG2	2.23	0.52
1:A:436:ARG:HG2	1:A:508:GLU:OE2	2.10	0.52
1:B:195:TYR:CE2	2:B:900:BLA:HMB1	2.44	0.52
1:A:12:VAL:HG13	1:A:15:ARG:CZ	2.40	0.51
1:A:219:VAL:HG13	1:A:253:LEU:HD23	1.93	0.51
1:A:30:LEU:HD11	1:A:114:LEU:HD23	1.93	0.51
1:A:183:ARG:HH12	1:A:187:LEU:C	2.13	0.51
1:A:70:PRO:HD2	1:A:88:GLU:O	2.12	0.50
1:A:34:ASP:HB3	1:A:37:ASP:HB2	1.93	0.50
1:A:227:GLN:HB3	1:A:228:PRO:HD3	1.93	0.50
1:A:208:TYR:HB3	1:A:268:SER:OG	2.12	0.50
1:A:212:ARG:HD2	1:A:268:SER:HB2	1.93	0.50
1:A:418:ASP:C	1:A:420:ALA:H	2.15	0.50
1:A:365:HIS:CE1	1:A:511:ARG:HD3	2.46	0.49
1:A:51:LEU:HD22	1:A:66:VAL:HG22	1.94	0.49
1:B:219:VAL:HG13	1:B:253:LEU:HD23	1.93	0.49
1:B:70:PRO:HD2	1:B:88:GLU:O	2.13	0.49
1:B:120:ARG:C	1:B:122:ALA:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLN:HG2	1:B:204:ALA:N	2.26	0.49
2:B:900:BLA:NB	2:B:900:BLA:CMA	2.70	0.49
1:A:547:VAL:HG12	1:A:563:ILE:HG13	1.95	0.48
1:B:612:HIS:O	1:B:628:LEU:HA	2.13	0.48
1:B:208:TYR:CD1	1:B:208:TYR:N	2.82	0.48
1:A:292:ALA:O	1:A:296:VAL:HG23	2.14	0.48
1:B:547:VAL:HG12	1:B:563:ILE:HG13	1.94	0.48
1:B:562:LEU:O	1:B:565:ARG:HB2	2.13	0.48
1:B:227:GLN:HA	1:B:227:GLN:HE21	1.78	0.48
1:B:39:ARG:HA	1:B:62:PRO:HA	1.95	0.48
1:B:432:MET:C	1:B:434:GLN:H	2.17	0.48
1:A:319:LEU:HD23	1:A:492:LEU:HD12	1.96	0.48
1:B:213:VAL:C	1:B:214:ARG:HG3	2.34	0.47
1:B:418:ASP:C	1:B:420:ALA:H	2.17	0.47
1:A:23:LEU:HD22	1:A:223:PRO:HB2	1.96	0.47
1:A:432:MET:C	1:A:434:GLN:H	2.17	0.47
1:B:586:ALA:HA	1:B:591:ARG:HB2	1.95	0.47
1:B:592:ALA:HB2	1:B:615:PRO:HD3	1.96	0.47
1:B:340:MET:HA	1:B:344:LEU:HD22	1.96	0.47
1:B:344:LEU:O	1:B:348:MET:HB2	2.14	0.47
1:A:454:GLY:HA2	1:A:478:TRP:HD1	1.79	0.47
1:A:424:ALA:HB3	1:A:486:ALA:HB2	1.95	0.47
1:A:97:PRO:N	1:A:98:PRO:HD3	2.30	0.47
1:A:308:ILE:O	1:A:312:GLN:HG3	2.15	0.47
1:B:266:VAL:HG11	2:B:900:BLA:HBA1	1.97	0.47
1:A:168:TYR:CE1	1:A:176:GLY:HA3	2.50	0.46
1:B:23:LEU:HD22	1:B:223:PRO:HB2	1.96	0.46
1:B:48:ALA:HB1	1:B:54:PRO:HA	1.97	0.46
1:B:59:LEU:HD21	1:B:228:PRO:HG3	1.98	0.46
1:B:590:GLY:HA2	1:B:626:TRP:HZ2	1.81	0.46
1:B:204:ALA:O	1:B:208:TYR:CD1	2.69	0.46
1:A:48:ALA:HB1	1:A:54:PRO:HA	1.97	0.46
1:A:530:VAL:HG22	1:A:629:GLN:HB3	1.97	0.46
1:B:97:PRO:HB2	1:B:98:PRO:CD	2.39	0.45
1:B:162:PHE:HA	1:B:283:HIS:ND1	2.30	0.45
1:B:209:LEU:O	1:B:212:ARG:HD2	2.16	0.45
1:A:168:TYR:CZ	1:A:176:GLY:HA3	2.51	0.45
1:A:579:ASN:HA	1:A:582:LEU:HD12	1.98	0.45
1:B:420:ALA:N	1:B:421:PRO:HD2	2.31	0.45
1:B:208:TYR:HE2	2:B:900:BLA:HAA2	1.80	0.45
1:A:592:ALA:HB2	1:A:615:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ALA:N	1:A:421:PRO:HD2	2.31	0.45
1:B:263:ALA:HB3	1:B:283:HIS:HB3	1.99	0.45
1:A:267:ALA:HB3	1:A:279:ILE:HB	1.98	0.45
1:A:12:VAL:HG12	1:A:12:VAL:O	2.16	0.45
1:B:447:ILE:H	1:B:447:ILE:HG13	1.52	0.45
1:A:14:ALA:CB	1:A:201:PRO:HB3	2.37	0.45
1:A:289:THR:HG22	1:A:293:MET:HB2	1.98	0.44
1:B:326:VAL:HG12	1:B:355:VAL:HG13	1.99	0.44
1:B:424:ALA:HB3	1:B:486:ALA:HB2	1.98	0.44
1:B:567:LEU:HD12	1:B:570:LEU:HD22	2.00	0.44
1:A:59:LEU:HD21	1:A:228:PRO:HG3	2.00	0.44
2:A:900:BLA:HMA1	2:A:900:BLA:C1B	2.45	0.44
1:A:320:GLU:HG2	1:A:492:LEU:HD11	1.98	0.44
1:B:249:SER:HB3	2:B:900:BLA:HBD2	2.00	0.44
1:A:12:VAL:HG13	1:A:15:ARG:CD	2.48	0.44
1:B:208:TYR:OH	2:B:900:BLA:HAA1	2.18	0.44
1:B:579:ASN:HA	1:B:582:LEU:HD12	1.98	0.44
1:A:249:SER:HB3	2:A:900:BLA:HBD2	2.00	0.44
1:A:133:MET:HE3	1:B:302:ARG:HH12	1.82	0.43
1:A:345:LEU:HD22	1:A:363:ILE:HD13	1.99	0.43
2:A:900:BLA:CMA	2:A:900:BLA:HB	2.31	0.43
1:B:71:GLU:HB2	1:B:87:ALA:HB1	1.99	0.43
1:B:369:ILE:HD12	1:B:378:VAL:HG13	2.01	0.43
1:A:369:ILE:HD12	1:A:378:VAL:HG13	2.01	0.43
1:A:310:ALA:O	1:A:314:VAL:HG23	2.19	0.43
1:B:207:LEU:HB3	1:B:214:ARG:HH21	1.84	0.42
1:B:240:LEU:HD12	1:B:243:VAL:HG21	2.01	0.42
1:B:319:LEU:HD23	1:B:492:LEU:HD12	1.99	0.42
1:A:71:GLU:HB2	1:A:87:ALA:HB1	2.00	0.42
1:B:153:ALA:O	1:B:157:ARG:HB2	2.20	0.42
1:B:310:ALA:O	1:B:314:VAL:HG23	2.20	0.42
1:A:532:ILE:HD13	1:A:532:ILE:HA	1.88	0.42
1:B:159:LEU:HB3	1:B:160:ILE:HD12	2.01	0.42
1:B:304:LEU:O	1:B:308:ILE:HG23	2.19	0.42
1:B:523:LEU:O	1:B:526:LEU:HB2	2.20	0.42
1:B:269:ILE:HD11	1:B:279:ILE:HG13	2.02	0.42
1:A:426:PHE:HA	1:A:441:TRP:O	2.19	0.42
1:B:42:GLN:HA	1:B:228:PRO:HG2	2.02	0.42
1:B:127:VAL:HA	1:B:130:ARG:HB2	2.01	0.42
1:B:207:LEU:HD21	1:B:241:SER:HA	2.02	0.42
1:B:227:GLN:HB2	1:B:228:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ALA:O	1:B:208:TYR:HD1	2.02	0.41
1:A:24:ILE:HD11	1:A:30:LEU:HD22	2.03	0.41
1:B:156:LEU:HD13	1:B:300:VAL:HG21	2.02	0.41
1:A:252:HIS:CE1	2:A:900:BLA:C1A	3.03	0.41
1:A:42:GLN:HA	1:A:228:PRO:HG2	2.03	0.41
1:B:320:GLU:HG2	1:B:492:LEU:HD11	2.02	0.41
2:A:900:BLA:HMA1	2:A:900:BLA:HB	1.80	0.41
1:B:426:PHE:HA	1:B:441:TRP:O	2.21	0.41
1:A:129:LEU:HG	1:A:296:VAL:HG22	2.02	0.41
1:A:231:HIS:HB3	1:A:234:LEU:HB2	2.03	0.41
1:B:24:ILE:HD11	1:B:30:LEU:HD22	2.02	0.41
1:A:308:ILE:C	1:A:308:ILE:HD12	2.40	0.41
1:A:450:ILE:HB	1:A:480:GLN:HB3	2.03	0.41
1:A:322:VAL:O	1:A:326:VAL:HG23	2.21	0.41
1:A:28:GLY:O	1:A:46:THR:HG21	2.20	0.40
1:B:120:ARG:O	1:B:122:ALA:N	2.48	0.40
1:A:94:ARG:HB3	1:A:97:PRO:HB3	2.03	0.40
1:B:183:ARG:HG3	1:B:187:LEU:HB2	2.02	0.40
1:A:413:PHE:CB	1:A:416:LEU:HD12	2.52	0.40
1:B:194:HIS:HD2	1:B:452:TRP:CZ3	2.40	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	583/640 (91%)	535 (92%)	37 (6%)	11 (2%)	8	42
1	B	598/640 (93%)	536 (90%)	48 (8%)	14 (2%)	6	38
All	All	1181/1280 (92%)	1071 (91%)	85 (7%)	25 (2%)	7	40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU
1	B	123	ARG
1	A	18	ILE
1	A	366	GLY
1	A	401	VAL
1	B	18	ILE
1	B	55	MET
1	B	97	PRO
1	B	144	GLY
1	B	162	PHE
1	B	366	GLY
1	B	401	VAL
1	B	475	PHE
1	A	55	MET
1	A	144	GLY
1	A	210	ARG
1	A	436	ARG
1	B	98	PRO
1	B	241	SER
1	B	436	ARG
1	A	100	SER
1	B	210	ARG
1	A	607	VAL
1	A	93	GLN
1	B	38	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	489/532 (92%)	413 (84%)	76 (16%)	2	18
1	B	498/532 (94%)	408 (82%)	90 (18%)	1	11
All	All	987/1064 (93%)	821 (83%)	166 (17%)	2	13

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	63	TYR
1	A	65	GLN
1	A	69	LEU
1	A	85	MET
1	A	114	LEU
1	A	116	GLU
1	A	117	MET
1	A	129	LEU
1	A	131	GLU
1	A	133	MET
1	A	141	ARG
1	A	159	LEU
1	A	169	ARG
1	A	188	GLU
1	A	191	LEU
1	A	207	LEU
1	A	209	LEU
1	A	210	ARG
1	A	212	ARG
1	A	214	ARG
1	A	215	GLN
1	A	222	GLN
1	A	227	GLN
1	A	233	GLN
1	A	240	LEU
1	A	245	LEU
1	A	264	THR
1	A	266	VAL
1	A	308	ILE
1	A	319	LEU
1	A	321	SER
1	A	330	LEU
1	A	334	PHE
1	A	344	LEU
1	A	346	ASP
1	A	348	MET
1	A	356	VAL
1	A	368	ASP
1	A	371	ARG
1	A	375	THR
1	A	383	ARG
1	A	387	HIS

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Mol	Chain	Res	Type
1	A	389	GLU
1	A	397	ARG
1	A	429	VAL
1	A	432	MET
1	A	434	GLN
1	A	436	ARG
1	A	477	LEU
1	A	479	GLN
1	A	487	ARG
1	A	488	ARG
1	A	492	LEU
1	A	495	GLU
1	A	502	VAL
1	A	506	LEU
1	A	514	GLN
1	A	518	LEU
1	A	520	GLU
1	A	525	ARG
1	A	526	LEU
1	A	527	ARG
1	A	528	ASP
1	A	535	ARG
1	A	543	ARG
1	A	545	LEU
1	A	566	GLU
1	A	568	GLN
1	A	574	ASP
1	A	577	ARG
1	A	583	LEU
1	A	610	GLN
1	A	613	LEU
1	A	627	LEU
1	A	630	LEU
1	B	15	ARG
1	B	39	ARG
1	B	59	LEU
1	B	63	TYR
1	B	64	THR
1	B	68	THR
1	B	85	MET
1	B	90	ARG
1	B	94	ARG

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Mol	Chain	Res	Type
1	B	116	GLU
1	B	117	MET
1	B	127	VAL
1	B	128	THR
1	B	129	LEU
1	B	131	GLU
1	B	141	ARG
1	B	142	ASP
1	B	157	ARG
1	B	166	MET
1	B	169	ARG
1	B	177	ASP
1	B	183	ARG
1	B	191	LEU
1	B	207	LEU
1	B	208	TYR
1	B	210	ARG
1	B	212	ARG
1	B	214	ARG
1	B	215	GLN
1	B	222	GLN
1	B	245	LEU
1	B	254	GLU
1	B	264	THR
1	B	289	THR
1	B	294	ARG
1	B	308	ILE
1	B	319	LEU
1	B	321	SER
1	B	330	LEU
1	B	334	PHE
1	B	339	HIS
1	B	344	LEU
1	B	346	ASP
1	B	348	MET
1	B	356	VAL
1	B	368	ASP
1	B	375	THR
1	B	383	ARG
1	B	387	HIS
1	B	389	GLU
1	B	397	ARG

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Mol	Chain	Res	Type
1	B	398	GLU
1	B	412	VAL
1	B	429	VAL
1	B	432	MET
1	B	434	GLN
1	B	436	ARG
1	B	449	GLN
1	B	451	LYS
1	B	473	LYS
1	B	476	ASP
1	B	477	LEU
1	B	487	ARG
1	B	488	ARG
1	B	492	LEU
1	B	495	GLU
1	B	502	VAL
1	B	506	LEU
1	B	514	GLN
1	B	518	LEU
1	B	520	GLU
1	B	523	LEU
1	B	526	LEU
1	B	527	ARG
1	B	528	ASP
1	B	537	THR
1	B	543	ARG
1	B	545	LEU
1	B	565	ARG
1	B	574	ASP
1	B	577	ARG
1	B	583	LEU
1	B	585	ASP
1	B	589	ASN
1	B	591	ARG
1	B	599	LEU
1	B	610	GLN
1	B	613	LEU
1	B	627	LEU
1	B	631	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	215	GLN
1	A	231	HIS
1	A	252	HIS
1	A	365	HIS
1	B	227	GLN
1	B	231	HIS
1	B	233	GLN
1	B	392	HIS
1	B	449	GLN
1	B	610	GLN
1	B	629	GLN

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 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	B	900	1	36,46,46	2.17	10 (27%)	47,67,67	2.06	10 (21%)
2	BLA	A	900	1	36,46,46	2.37	5 (13%)	47,67,67	1.13	3 (6%)

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	-	5/22/74/74	0/4/4/4
2	BLA	A	900	1	-	5/22/74/74	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	BLA	CHA-C4D	11.62	1.44	1.35
2	A	900	BLA	CHB-C1B	6.05	1.47	1.34
2	B	900	BLA	CHA-C4D	-5.27	1.30	1.35
2	B	900	BLA	C3B-C2B	5.22	1.47	1.37
2	B	900	BLA	CHB-C1B	4.88	1.44	1.34
2	B	900	BLA	C4D-C3D	3.91	1.51	1.45
2	B	900	BLA	CAA-C2A	-3.74	1.46	1.52
2	B	900	BLA	OC-C1C	3.37	1.30	1.23
2	B	900	BLA	C1C-NC	-2.95	1.31	1.38
2	A	900	BLA	OB-C4B	2.88	1.29	1.23
2	A	900	BLA	C2A-C3A	2.73	1.45	1.37
2	B	900	BLA	OB-C4B	2.68	1.28	1.23
2	B	900	BLA	C1B-C2B	2.38	1.49	1.45
2	A	900	BLA	CBD-CAD	2.36	1.64	1.52
2	B	900	BLA	C3D-C2D	2.03	1.41	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	BLA	C3B-C4B-NB	6.51	113.54	106.19
2	B	900	BLA	C3B-C2B-C1B	-5.53	101.34	108.03
2	A	900	BLA	C1A-CHA-C4D	-5.02	122.81	128.81
2	B	900	BLA	C2B-C1B-NB	5.00	114.31	106.99
2	B	900	BLA	CMB-C2B-C1B	4.23	129.46	124.17
2	B	900	BLA	CHB-C1B-NB	-4.17	116.40	130.40
2	B	900	BLA	C1B-NB-C4B	-3.62	106.06	110.67
2	B	900	BLA	CAA-CBA-CGA	3.01	117.71	112.67
2	B	900	BLA	OB-C4B-C3B	-2.87	122.95	129.46
2	A	900	BLA	CMA-C3A-C2A	-2.86	119.55	124.94
2	B	900	BLA	C4B-C3B-C2B	-2.49	104.73	107.92
2	B	900	BLA	C3D-C4D-ND	-2.18	106.89	110.05
2	A	900	BLA	CHB-C1B-NB	-2.08	123.42	130.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	BLA	NA-C4A-CHB-C1B
2	A	900	BLA	C3A-C4A-CHB-C1B
2	B	900	BLA	C1A-C2A-CAA-CBA
2	B	900	BLA	C3A-C2A-CAA-CBA
2	B	900	BLA	NA-C4A-CHB-C1B
2	B	900	BLA	C2C-C3C-CAC-CBC
2	B	900	BLA	C4C-C3C-CAC-CBC
2	A	900	BLA	C2C-C3C-CAC-CBC
2	A	900	BLA	C4C-C3C-CAC-CBC
2	A	900	BLA	NB-C1B-CHB-C4A

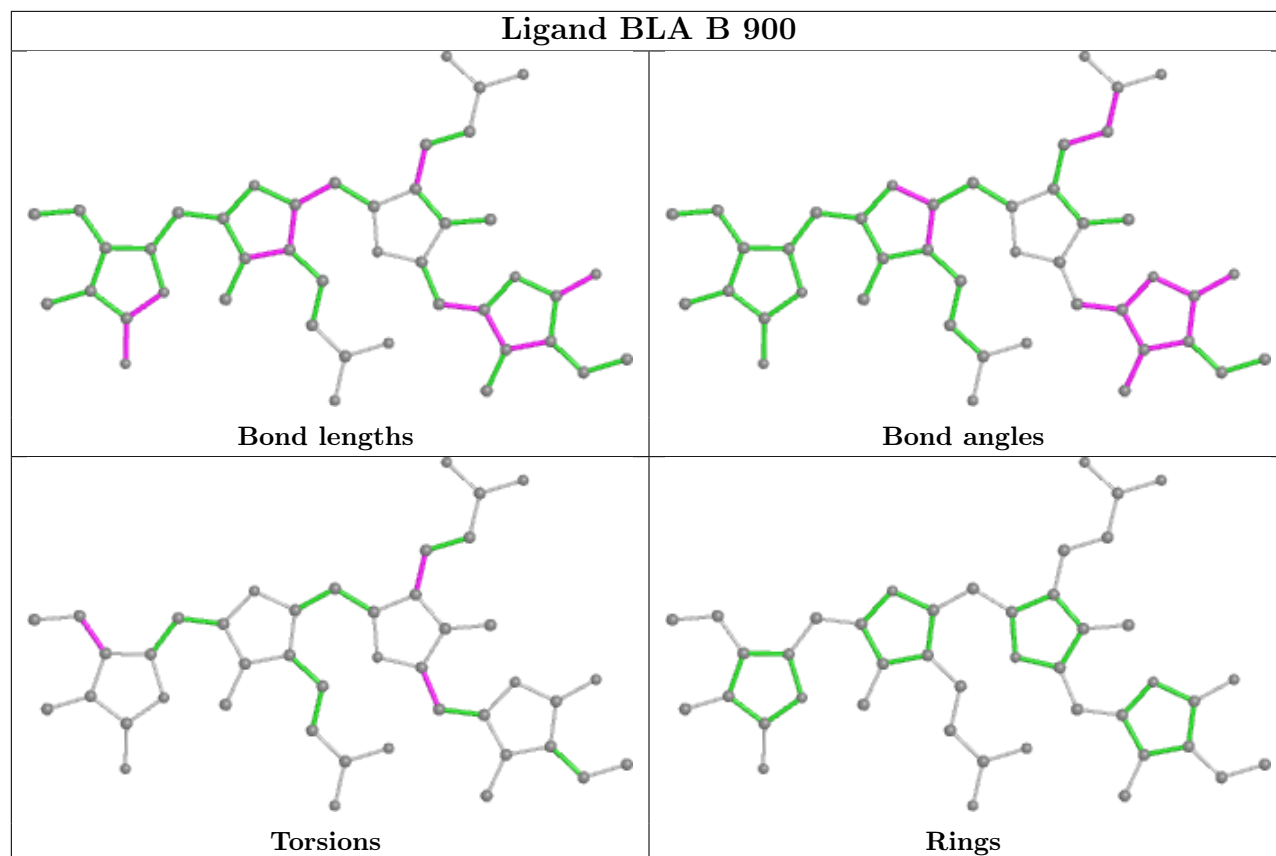
There are no ring outliers.

2 monomers are involved in 20 short contacts:

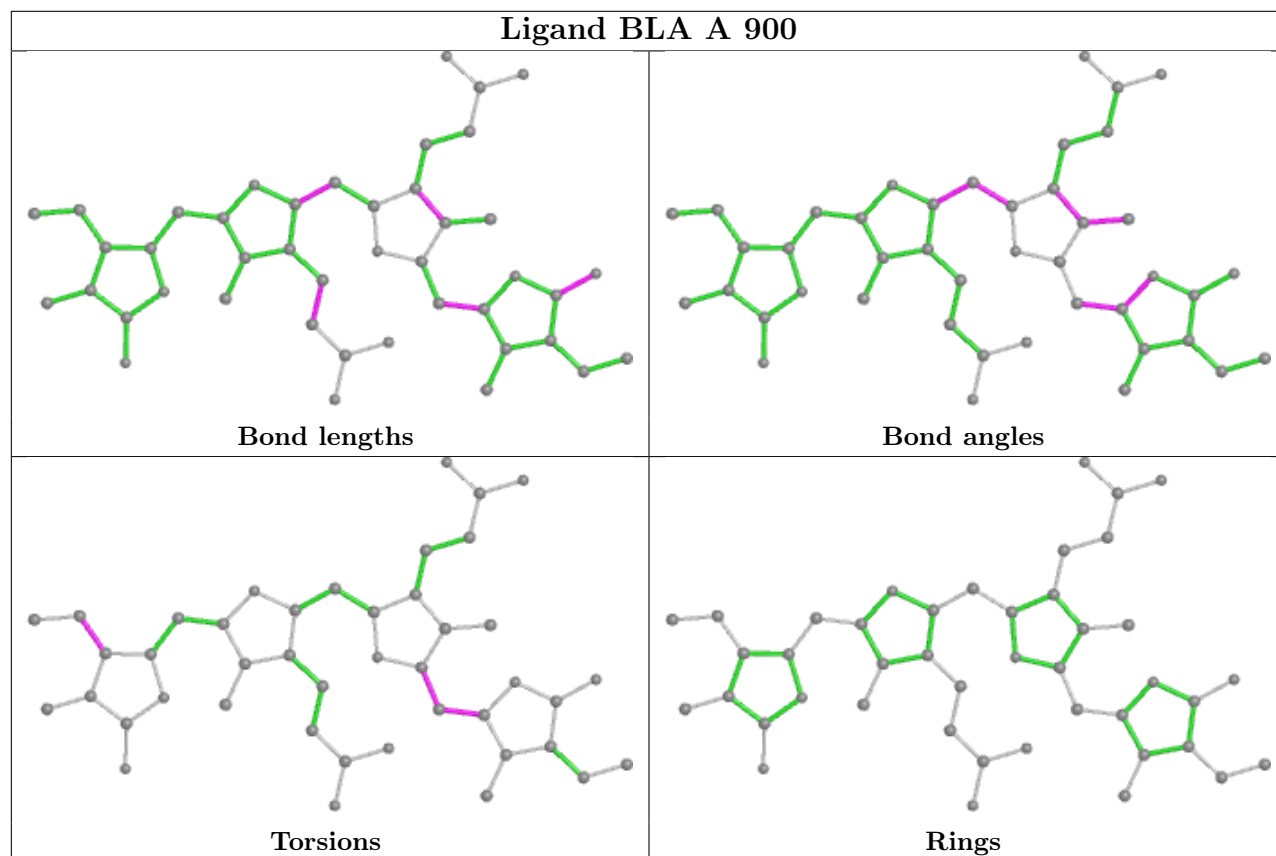
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	BLA	12	0
2	A	900	BLA	8	0

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 900



Ligand BLA A 900



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	593/640 (92%)	-0.09	2 (0%) 94 88	98, 149, 209, 238	0
1	B	604/640 (94%)	0.01	11 (1%) 68 51	99, 154, 231, 265	0
All	All	1197/1280 (93%)	-0.04	13 (1%) 80 66	98, 152, 223, 265	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	ASP	3.0
1	B	413	PHE	2.6
1	B	31	LEU	2.6
1	A	555	CYS	2.5
1	B	233	GLN	2.4
1	B	236	THR	2.4
1	B	221	TYR	2.3
1	B	30	LEU	2.2
1	B	51	LEU	2.2
1	B	58	LEU	2.1
1	B	114	LEU	2.1
1	B	33	ILE	2.1
1	A	611	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

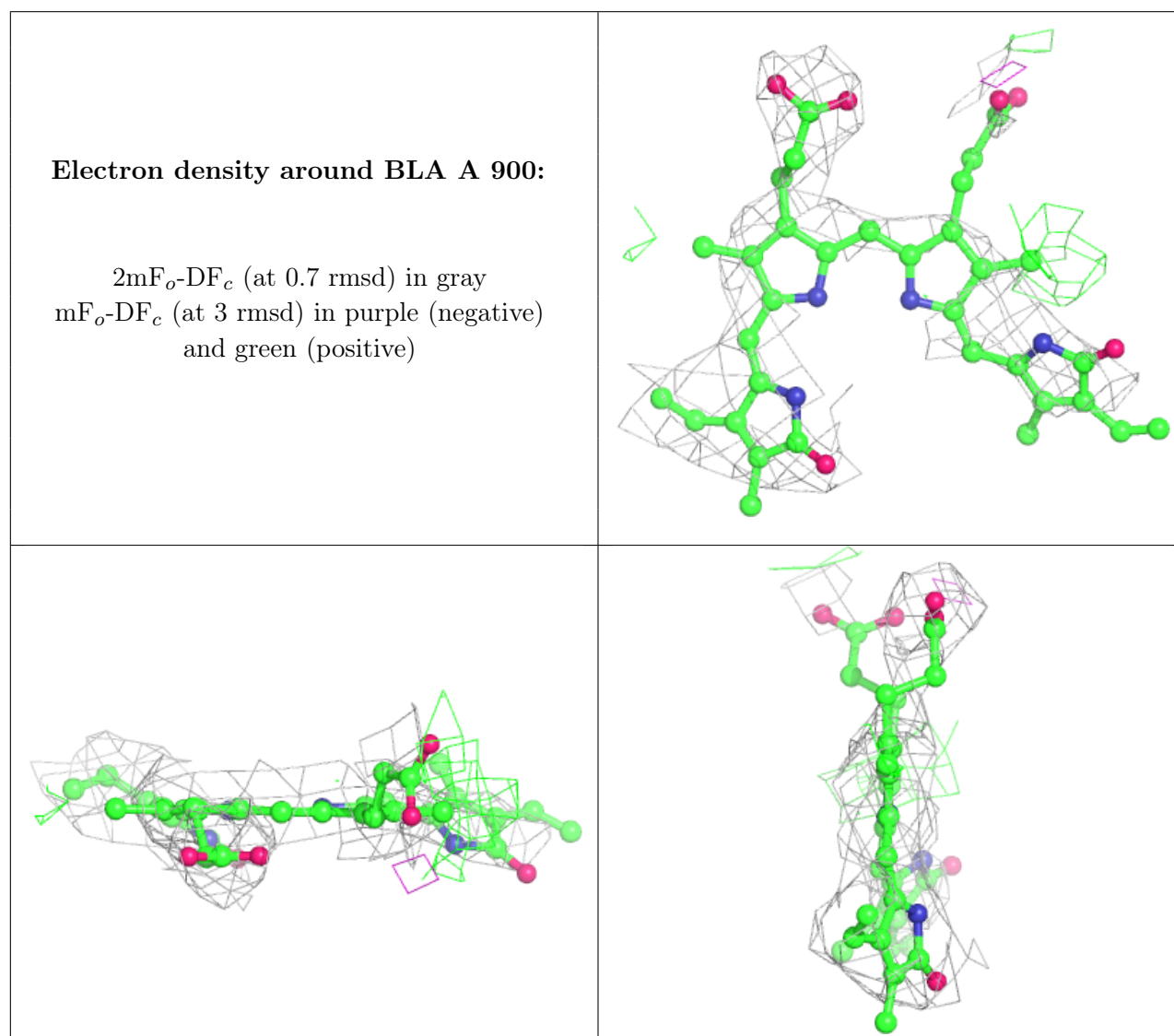
There are no monosaccharides in this entry.

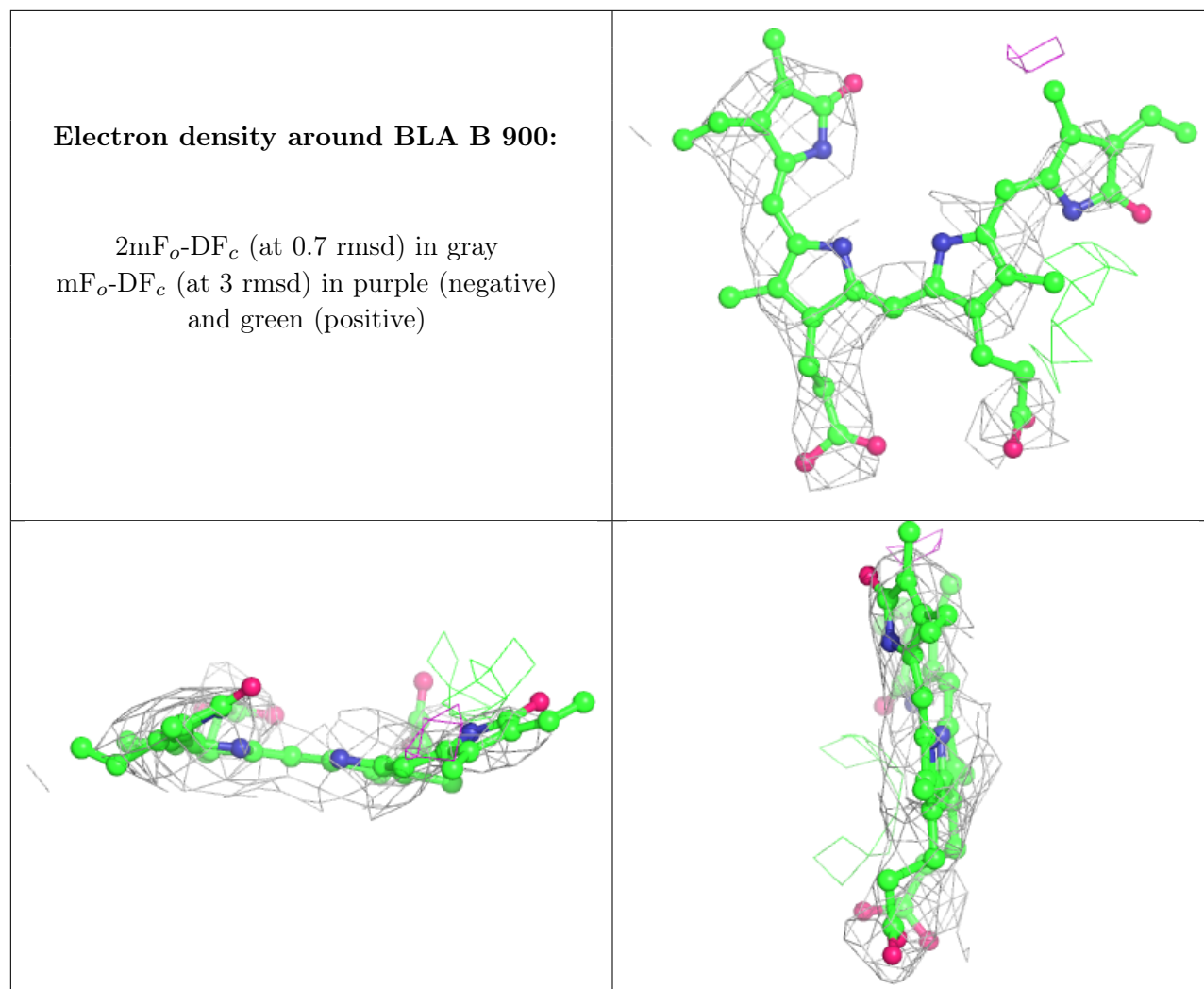
6.4 Ligands ⓘ

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	0.89	0.50	129,134,135,136	43
2	BLA	B	900	43/43	0.89	0.53	126,130,131,132	43

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.