



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:52 PM UTC

PDB ID : 3NOT / pdb_00003not
Title : Light-induced intermediate structure L2 of P. aeruginosa bacteriophytochrome
Authors : Yang, X.; Ren, Z.; Moffat, K.
Deposited on : 2010-06-25
Resolution : 2.70 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

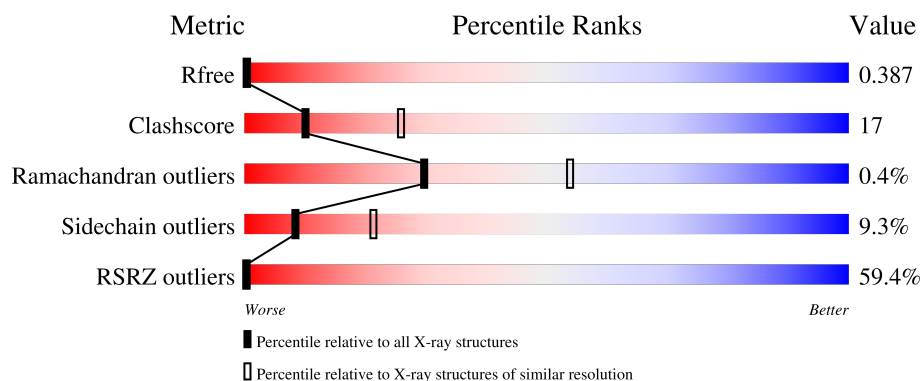
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	C	505	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BLA	C	900	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3860 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.

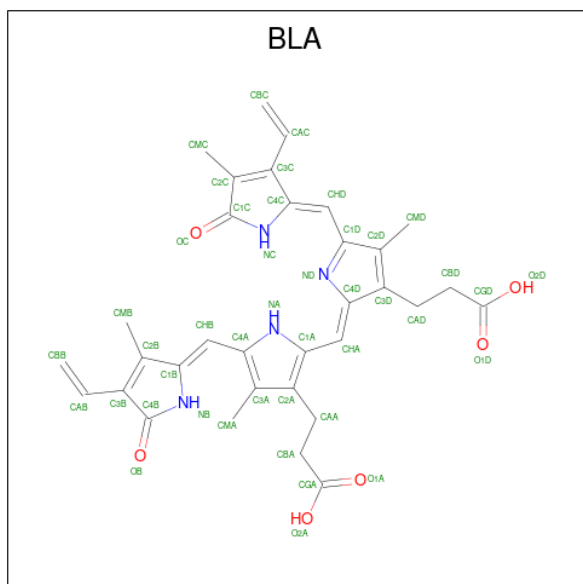
- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	483	3817	2401	689	708	19	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	500	HIS	-	expression tag	UNP Q9HWR3
C	501	HIS	-	expression tag	UNP Q9HWR3
C	502	HIS	-	expression tag	UNP Q9HWR3
C	503	HIS	-	expression tag	UNP Q9HWR3
C	504	HIS	-	expression tag	UNP Q9HWR3
C	505	HIS	-	expression tag	UNP Q9HWR3

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: BLA) (formula: $C_{33}H_{34}N_4O_6$).



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

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.38Å 162.98Å 436.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.70) 99.2 (50.00-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.51Å)	Xtriage
Refinement program	DynamiX	Depositor
R, R_{free}	(Not available) , (Not available) 0.384 , 0.387	Depositor DCC
R_{free} test set	8759 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.61	EDS
Total number of atoms	3860	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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	C	0.40	3/3902 (0.1%)	0.83	7/5296 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	TYR	C-N	-10.53	1.18	1.33
1	C	189	ARG	C-N	-5.97	1.26	1.33
1	C	276	CYS	C-N	-5.08	1.26	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GLN	N-CA-C	-10.57	100.45	113.97
1	C	163	TYR	O-C-N	-10.12	111.35	123.29
1	C	448	GLY	CA-C-N	5.76	125.61	119.28
1	C	448	GLY	C-N-CA	5.76	125.61	119.28
1	C	193	SER	CA-C-N	-5.22	112.94	122.38
1	C	193	SER	C-N-CA	-5.22	112.94	122.38
1	C	103	LYS	CB-CA-C	-5.20	110.15	117.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	194	ASP	Mainchain
1	C	62	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3817	0	3752	127	0
2	C	43	0	31	25	0
All	All	3860	0	3783	132	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 17.

All (132) 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:C:247:HIS:CE1	2:C:900:BLA:CAA	2.18	1.25
1:C:247:HIS:CE1	2:C:900:BLA:HAA2	1.84	1.13
1:C:247:HIS:CE1	2:C:900:BLA:HAA1	1.97	1.00
1:C:247:HIS:HE1	2:C:900:BLA:CAA	1.81	0.91
1:C:163:TYR:OH	1:C:275:SER:HB3	1.78	0.82
1:C:203:TYR:OH	2:C:900:BLA:HBA1	1.80	0.82
1:C:45:ILE:HD12	1:C:46:GLN:H	1.44	0.82
1:C:188:GLN:NE2	2:C:900:BLA:HAB	1.96	0.80
1:C:84:ASN:HD22	1:C:85:SER:H	1.29	0.79
1:C:247:HIS:CE1	2:C:900:BLA:C2A	2.66	0.78
1:C:163:TYR:CE1	1:C:275:SER:HB2	2.18	0.78
1:C:247:HIS:NE2	2:C:900:BLA:HAA2	2.00	0.77
1:C:475:SER:HB2	1:C:478:ASP:H	1.50	0.76
2:C:900:BLA:HMC1	2:C:900:BLA:HBC1	1.71	0.73
1:C:171:GLY:HA3	1:C:190:TYR:CZ	2.25	0.72
1:C:247:HIS:HE1	2:C:900:BLA:HAA1	1.46	0.72
1:C:45:ILE:HD12	1:C:46:GLN:N	2.06	0.71
1:C:62:GLU:OE2	1:C:62:GLU:HA	1.90	0.70
1:C:247:HIS:HE1	2:C:900:BLA:C2A	2.06	0.67
1:C:358:MET:HE1	1:C:378:LEU:HD22	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.76	0.67
1:C:163:TYR:OH	1:C:275:SER:CB	2.43	0.66
1:C:185:TYR:HB3	1:C:188:GLN:HG3	1.78	0.65
1:C:209:ARG:HG2	1:C:209:ARG:HH11	1.61	0.65
1:C:328:ARG:HH12	1:C:344:ASP:HB2	1.60	0.65
1:C:247:HIS:NE2	2:C:900:BLA:CAA	2.56	0.65
1:C:257:ARG:HD3	1:C:281:PRO:HD3	1.77	0.65
1:C:250:TYR:OH	2:C:900:BLA:HMB3	1.97	0.65
1:C:161:MET:HE3	1:C:163:TYR:OH	1.97	0.64
1:C:84:ASN:ND2	1:C:85:SER:H	1.96	0.63
1:C:188:GLN:HE21	2:C:900:BLA:HAB	1.61	0.63
1:C:417:HIS:HD2	1:C:420:GLU:H	1.48	0.61
1:C:163:TYR:CD1	1:C:273:LEU:CD1	2.84	0.60
1:C:148:THR:HG23	1:C:160:VAL:HG22	1.82	0.60
1:C:129:ARG:HE	1:C:154:MET:HG2	1.65	0.60
2:C:900:BLA:HBC1	2:C:900:BLA:CMC	2.31	0.60
1:C:209:ARG:NH1	2:C:900:BLA:O1D	2.35	0.60
1:C:347:ALA:HB2	1:C:366:ILE:HD11	1.83	0.59
1:C:220:ARG:HG3	1:C:220:ARG:HH11	1.67	0.59
1:C:210:LEU:HD12	1:C:289:ARG:HD3	1.86	0.58
1:C:366:ILE:O	1:C:367:ARG:HB2	2.03	0.58
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.69	0.57
1:C:163:TYR:CZ	1:C:275:SER:CB	2.88	0.57
2:C:900:BLA:HBD2	2:C:900:BLA:CMD	2.35	0.57
1:C:229:THR:HG23	1:C:231:GLU:H	1.69	0.56
1:C:315:LEU:O	1:C:319:THR:HG23	2.04	0.56
1:C:347:ALA:CB	1:C:366:ILE:HD11	2.35	0.56
1:C:165:PHE:CD1	1:C:272:GLY:HA2	2.41	0.56
1:C:134:VAL:HG12	1:C:302:ILE:HG12	1.88	0.55
1:C:163:TYR:CD1	1:C:273:LEU:HD12	2.42	0.55
1:C:209:ARG:HH12	2:C:900:BLA:CGD	2.18	0.55
1:C:94:LEU:H	1:C:94:LEU:HD22	1.72	0.54
1:C:467:VAL:O	1:C:470:HIS:HB2	2.06	0.54
1:C:84:ASN:HD22	1:C:85:SER:N	2.00	0.54
1:C:188:GLN:HE21	2:C:900:BLA:CAB	2.20	0.54
1:C:163:TYR:CD1	1:C:273:LEU:HD11	2.42	0.54
1:C:319:THR:HG22	1:C:322:ARG:HH21	1.71	0.54
1:C:250:TYR:OH	2:C:900:BLA:CMB	2.55	0.54
1:C:163:TYR:CE1	1:C:273:LEU:HD11	2.43	0.53
1:C:391:HIS:HA	1:C:411:VAL:O	2.08	0.53
2:C:900:BLA:HBB1	2:C:900:BLA:OB	2.07	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:GLU:O	1:C:317:VAL:HG13	2.10	0.52
1:C:24:GLN:HE22	1:C:211:ILE:HA	1.75	0.52
1:C:163:TYR:CZ	1:C:275:SER:HB2	2.44	0.52
1:C:220:ARG:HG3	1:C:220:ARG:NH1	2.24	0.52
1:C:171:GLY:HA3	1:C:190:TYR:CE2	2.46	0.51
1:C:257:ARG:HH11	1:C:281:PRO:HG3	1.76	0.51
1:C:163:TYR:CZ	1:C:275:SER:HB3	2.45	0.51
1:C:42:SER:O	1:C:45:ILE:HG13	2.10	0.51
1:C:260:MET:HE1	1:C:292:PHE:CD2	2.46	0.50
1:C:201:ARG:O	1:C:205:GLN:HG2	2.12	0.50
1:C:339:LEU:HD12	1:C:357:VAL:HG11	1.95	0.49
1:C:341:HIS:O	1:C:345:GLY:HA3	2.13	0.49
2:C:900:BLA:HBD2	2:C:900:BLA:HMD1	1.94	0.48
1:C:284:ILE:HG22	1:C:289:ARG:HG2	1.94	0.48
1:C:7:VAL:HG23	1:C:7:VAL:O	2.12	0.48
1:C:440:LYS:O	1:C:441:PRO:C	2.57	0.48
1:C:44:ASN:CG	1:C:219:MET:HG2	2.40	0.47
1:C:60:THR:H	1:C:63:GLN:HE21	1.60	0.47
1:C:286:TYR:N	1:C:287:PRO:HD2	2.30	0.47
1:C:417:HIS:CD2	1:C:420:GLU:H	2.30	0.47
1:C:288:VAL:O	1:C:291:SER:HB2	2.15	0.47
1:C:247:HIS:NE2	2:C:900:BLA:HAA1	2.28	0.46
1:C:444:LEU:HD12	1:C:444:LEU:N	2.29	0.46
1:C:94:LEU:N	1:C:94:LEU:HD13	2.31	0.46
1:C:475:SER:HB2	1:C:478:ASP:CG	2.41	0.46
1:C:124:THR:O	1:C:128:GLN:HG3	2.16	0.46
1:C:152:ARG:HB2	1:C:160:VAL:CG1	2.45	0.45
1:C:131:ILE:HG22	1:C:295:PHE:HD1	1.81	0.45
1:C:155:THR:OG1	1:C:157:TYR:HD1	2.00	0.45
1:C:8:THR:H	1:C:11:ASN:HD22	1.65	0.45
1:C:260:MET:HE1	1:C:292:PHE:HD2	1.80	0.45
1:C:194:ASP:OD2	1:C:453:ARG:NH2	2.42	0.45
1:C:30:VAL:HG12	1:C:32:LEU:CD1	2.48	0.44
1:C:51:PHE:CE2	1:C:63:GLN:O	2.71	0.44
1:C:257:ARG:NH1	1:C:281:PRO:HG3	2.32	0.44
1:C:354:GLY:HA3	1:C:370:PHE:CE1	2.51	0.44
1:C:159:ARG:NH1	1:C:183:GLU:O	2.51	0.44
1:C:139:ASP:HB3	1:C:142:SER:OG	2.18	0.44
1:C:284:ILE:HG22	1:C:289:ARG:CG	2.47	0.44
1:C:33:ARG:HB3	1:C:39:LEU:HD11	1.99	0.43
1:C:152:ARG:HB2	1:C:160:VAL:HG13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ILE:HB	1:C:272:GLY:O	2.19	0.43
1:C:17:ILE:CD1	2:C:900:BLA:HMD1	2.48	0.43
1:C:32:LEU:HD23	1:C:72:LEU:HD21	2.01	0.42
1:C:356:LEU:HB3	1:C:425:PHE:HB2	2.00	0.42
1:C:188:GLN:NE2	2:C:900:BLA:CAB	2.74	0.42
1:C:140:THR:HG21	1:C:307:GLU:OE2	2.18	0.42
1:C:147:VAL:HG21	1:C:274:PHE:CZ	2.55	0.42
1:C:358:MET:HG2	1:C:358:MET:O	2.19	0.42
1:C:134:VAL:HG12	1:C:134:VAL:O	2.19	0.42
1:C:147:VAL:O	1:C:151:LEU:HG	2.20	0.42
1:C:60:THR:O	1:C:63:GLN:HG2	2.20	0.42
1:C:186:LEU:HD23	1:C:186:LEU:HA	1.89	0.41
1:C:283:LEU:C	1:C:284:ILE:HD12	2.45	0.41
1:C:305:ARG:HA	1:C:305:ARG:HD2	1.99	0.41
1:C:163:TYR:CE1	1:C:273:LEU:CD1	3.03	0.41
1:C:163:TYR:CE1	1:C:275:SER:CB	2.98	0.41
1:C:209:ARG:HH11	1:C:209:ARG:CG	2.31	0.41
1:C:485:LEU:O	1:C:488:ASP:HB2	2.20	0.41
1:C:19:VAL:O	1:C:19:VAL:HG23	2.19	0.41
1:C:364:LEU:HD23	1:C:364:LEU:HA	1.87	0.41
1:C:464:GLU:O	1:C:468:ARG:HG2	2.21	0.41
1:C:356:LEU:HD13	1:C:357:VAL:N	2.35	0.41
1:C:64:VAL:O	1:C:68:VAL:HG21	2.20	0.41
1:C:261:SER:HA	1:C:274:PHE:O	2.21	0.41
1:C:284:ILE:CG2	1:C:289:ARG:HG2	2.51	0.41
1:C:45:ILE:HG13	1:C:45:ILE:H	1.66	0.41
1:C:5:THR:HA	1:C:6:PRO:HD3	1.99	0.40
1:C:62:GLU:N	1:C:65:GLY:H	2.19	0.40
1:C:18:HIS:C	1:C:20:PRO:HD3	2.46	0.40
1:C:67:GLU:CD	1:C:67:GLU:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	C	479/505 (95%)	456 (95%)	21 (4%)	2 (0%)	30	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	PRO
1	C	66	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	410/431 (95%)	372 (91%)	38 (9%)	8	21

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	HIS
1	C	29	LEU
1	C	32	LEU
1	C	45	ILE
1	C	62	GLU
1	C	76	LEU
1	C	94	LEU
1	C	98	ILE
1	C	114	THR
1	C	117	THR
1	C	143	LEU
1	C	160	VAL
1	C	164	ARG
1	C	166	ARG
1	C	186	LEU
1	C	188	GLN
1	C	194	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	210	LEU
1	C	221	VAL
1	C	232	SER
1	C	252	THR
1	C	259	SER
1	C	260	MET
1	C	297	GLN
1	C	304	GLU
1	C	305	ARG
1	C	306	LEU
1	C	317	VAL
1	C	325	LEU
1	C	356	LEU
1	C	364	LEU
1	C	366	ILE
1	C	373	GLN
1	C	378	LEU
1	C	393	ASP
1	C	412	LEU
1	C	483	GLU
1	C	485	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	11	ASN
1	C	24	GLN
1	C	61	GLN
1	C	63	GLN
1	C	84	ASN
1	C	93	HIS
1	C	100	HIS
1	C	126	ASN
1	C	137	HIS
1	C	188	GLN
1	C	198	GLN
1	C	247	HIS
1	C	278	HIS
1	C	293	GLN
1	C	394	ASN
1	C	417	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	C	900	1	46,46,46	2.71	16 (34%)	66,67,67	1.76	15 (22%)

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	C	900	1	-	13/26/74/74	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	CHB-C4A	7.92	1.58	1.40
2	C	900	BLA	CHB-C1B	6.54	1.53	1.37
2	C	900	BLA	CHD-C4C	5.98	1.52	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	BLA	CHD-C1D	5.28	1.52	1.40
2	C	900	BLA	CBC-CAC	4.66	1.52	1.30
2	C	900	BLA	C4D-C3D	-4.28	1.39	1.45
2	C	900	BLA	C1C-C2C	-4.01	1.38	1.48
2	C	900	BLA	C1D-C2D	-3.66	1.37	1.45
2	C	900	BLA	C3C-C4C	-3.45	1.39	1.45
2	C	900	BLA	C1B-C2B	-3.14	1.39	1.45
2	C	900	BLA	CAB-C3B	-2.99	1.39	1.47
2	C	900	BLA	CAC-C3C	2.54	1.54	1.47
2	C	900	BLA	C4A-NA	-2.41	1.33	1.37
2	C	900	BLA	C1A-NA	-2.32	1.33	1.37
2	C	900	BLA	C4C-NC	-2.18	1.34	1.37
2	C	900	BLA	C3B-C4B	-2.15	1.38	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	BLA	C4C-CHD-C1D	-6.22	112.78	128.06
2	C	900	BLA	C1A-CHA-C4D	-4.56	118.27	128.22
2	C	900	BLA	CHA-C4D-ND	4.17	133.35	124.60
2	C	900	BLA	CHA-C1A-C2A	-3.18	120.38	127.22
2	C	900	BLA	CHA-C4D-C3D	-2.94	118.60	125.40
2	C	900	BLA	C3B-C4B-NB	2.79	109.64	106.13
2	C	900	BLA	CBC-CAC-C3C	-2.67	114.19	127.53
2	C	900	BLA	C4A-CHB-C1B	-2.39	123.95	130.82
2	C	900	BLA	CHD-C1D-ND	2.30	129.92	124.95
2	C	900	BLA	C3C-C4C-NC	2.21	110.25	106.64
2	C	900	BLA	CHA-C1A-NA	2.19	130.24	125.29
2	C	900	BLA	C4C-NC-C1C	-2.17	107.99	110.66
2	C	900	BLA	C1A-C2A-C3A	-2.17	105.10	107.62
2	C	900	BLA	O1D-CGD-CBD	-2.13	116.33	123.09
2	C	900	BLA	C1D-C2D-C3D	2.01	108.76	106.48

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	BLA	NA-C1A-CHA-C4D
2	C	900	BLA	C2A-C1A-CHA-C4D
2	C	900	BLA	C2D-C3D-CAD-CBD
2	C	900	BLA	NA-C4A-CHB-C1B
2	C	900	BLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

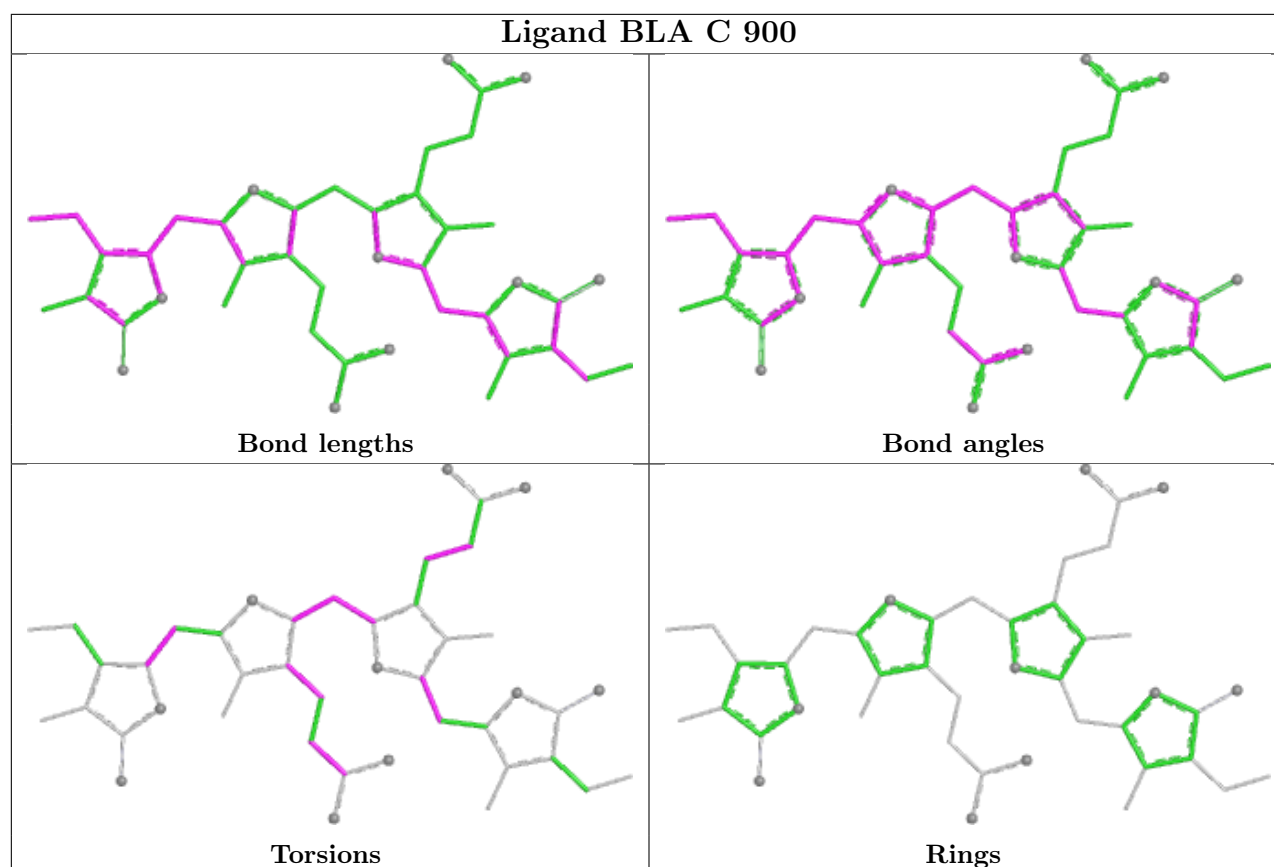
Mol	Chain	Res	Type	Atoms
2	C	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	C4D-C3D-CAD-CBD
2	C	900	BLA	ND-C4D-CHA-C1A
2	C	900	BLA	C3D-C4D-CHA-C1A
2	C	900	BLA	NC-C4C-CHD-C1D
2	C	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	CAD-CBD-CGD-O1D
2	C	900	BLA	C3C-C4C-CHD-C1D

There are no ring outliers.

1 monomer is involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	BLA	25	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	163:TYR	C	164:ARG	N	1.18

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	C	483/505 (95%)	2.55	287 (59%) 0 0	38, 60, 105, 147	0

All (287) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	ASP	9.5
1	C	496	HIS	8.8
1	C	197	ALA	8.1
1	C	418	ARG	8.1
1	C	78	GLY	7.8
1	C	363	THR	7.8
1	C	4	ILE	7.8
1	C	128	GLN	7.8
1	C	365	SER	7.5
1	C	407	ASP	7.0
1	C	443	LYS	6.8
1	C	334	ASP	6.5
1	C	119	SER	6.4
1	C	388	ASP	6.1
1	C	360	GLY	6.1
1	C	333	ASP	6.0
1	C	442	GLU	5.9
1	C	90	ILE	5.9
1	C	52	VAL	5.9
1	C	253	ASN	5.8
1	C	362	ARG	5.8
1	C	468	ARG	5.8
1	C	350	ILE	5.8
1	C	406	GLY	5.7
1	C	79	ASN	5.6
1	C	74	GLU	5.5
1	C	439	GLY	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	58	TYR	5.5
1	C	31	THR	5.3
1	C	308	GLN	5.3
1	C	494	LEU	5.3
1	C	73	GLU	5.2
1	C	224	ALA	5.1
1	C	229	THR	5.0
1	C	367	ARG	4.9
1	C	370	PHE	4.9
1	C	311	ILE	4.8
1	C	103	LYS	4.8
1	C	239	VAL	4.8
1	C	95	PHE	4.7
1	C	80	GLY	4.6
1	C	63	GLN	4.6
1	C	34	ALA	4.6
1	C	101	SER	4.5
1	C	342	PRO	4.5
1	C	269	LYS	4.5
1	C	444	LEU	4.5
1	C	99	GLY	4.5
1	C	297	GLN	4.5
1	C	379	GLN	4.5
1	C	117	THR	4.4
1	C	249	GLU	4.4
1	C	419	GLN	4.3
1	C	116	ASP	4.3
1	C	361	GLY	4.3
1	C	37	MET	4.3
1	C	472	THR	4.2
1	C	5	THR	4.2
1	C	107	TYR	4.2
1	C	231	GLU	4.2
1	C	394	ASN	4.2
1	C	115	ALA	4.1
1	C	408	CYS	4.1
1	C	62	GLU	4.1
1	C	343	ASP	4.1
1	C	233	PHE	4.1
1	C	208	ILE	4.1
1	C	32	LEU	4.0
1	C	81	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	327	ARG	4.0
1	C	372	ARG	4.0
1	C	474	TRP	4.0
1	C	70	ARG	3.9
1	C	415	ARG	3.9
1	C	432	VAL	3.9
1	C	104	GLU	3.9
1	C	380	ARG	3.9
1	C	387	ARG	3.9
1	C	120	ILE	3.8
1	C	10	ALA	3.8
1	C	452	PRO	3.8
1	C	54	SER	3.8
1	C	183	GLU	3.8
1	C	21	GLY	3.7
1	C	476	GLU	3.7
1	C	409	CYS	3.7
1	C	98	ILE	3.7
1	C	129	ARG	3.7
1	C	57	SER	3.7
1	C	383	ARG	3.6
1	C	118	LEU	3.6
1	C	232	SER	3.6
1	C	465	GLU	3.6
1	C	235	LEU	3.6
1	C	112	ILE	3.6
1	C	440	LYS	3.6
1	C	181	ASP	3.5
1	C	135	GLN	3.5
1	C	77	THR	3.5
1	C	94	LEU	3.4
1	C	366	ILE	3.4
1	C	446	THR	3.4
1	C	236	SER	3.4
1	C	13	GLU	3.4
1	C	267	GLY	3.4
1	C	93	HIS	3.4
1	C	263	SER	3.4
1	C	59	LEU	3.4
1	C	127	ALA	3.4
1	C	137	HIS	3.4
1	C	369	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	180	GLU	3.3
1	C	40	ALA	3.3
1	C	332	ALA	3.3
1	C	138	ASN	3.3
1	C	160	VAL	3.3
1	C	6	PRO	3.3
1	C	441	PRO	3.3
1	C	355	ALA	3.3
1	C	125	LEU	3.3
1	C	392	THR	3.3
1	C	330	ARG	3.2
1	C	491	GLU	3.2
1	C	382	GLN	3.2
1	C	11	ASN	3.2
1	C	344	ASP	3.2
1	C	270	LEU	3.2
1	C	202	LEU	3.2
1	C	445	LEU	3.2
1	C	60	THR	3.2
1	C	204	ILE	3.2
1	C	96	ASP	3.1
1	C	328	ARG	3.1
1	C	216	TYR	3.1
1	C	69	LEU	3.1
1	C	336	PHE	3.1
1	C	136	LEU	3.1
1	C	139	ASP	3.1
1	C	200	ARG	3.1
1	C	67	GLU	3.1
1	C	228	GLU	3.1
1	C	320	GLU	3.1
1	C	331	ASP	3.1
1	C	187	GLY	3.1
1	C	252	THR	3.1
1	C	105	VAL	3.1
1	C	393	ASP	3.0
1	C	113	ARG	3.0
1	C	201	ARG	3.0
1	C	189	ARG	3.0
1	C	486	ARG	3.0
1	C	431	GLU	2.9
1	C	33	ARG	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	87	GLU	2.9
1	C	259	SER	2.9
1	C	471	SER	2.9
1	C	89	ARG	2.9
1	C	196	PRO	2.9
1	C	122	SER	2.9
1	C	280	SER	2.9
1	C	389	ILE	2.9
1	C	282	LYS	2.9
1	C	198	GLN	2.8
1	C	48	LEU	2.8
1	C	364	LEU	2.8
1	C	140	THR	2.8
1	C	217	THR	2.8
1	C	64	VAL	2.8
1	C	420	GLU	2.8
1	C	178	ARG	2.8
1	C	451	GLY	2.8
1	C	35	ASP	2.8
1	C	30	VAL	2.8
1	C	434	ARG	2.8
1	C	326	ALA	2.8
1	C	237	TYR	2.8
1	C	244	SER	2.7
1	C	134	VAL	2.7
1	C	227	PRO	2.7
1	C	205	GLN	2.7
1	C	493	CYS	2.7
1	C	15	GLU	2.7
1	C	221	VAL	2.7
1	C	188	GLN	2.7
1	C	39	LEU	2.7
1	C	283	LEU	2.7
1	C	345	GLY	2.7
1	C	457	ARG	2.7
1	C	425	PHE	2.7
1	C	9	LEU	2.7
1	C	354	GLY	2.7
1	C	177	SER	2.7
1	C	206	ASN	2.7
1	C	449	PRO	2.7
1	C	49	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	309	GLY	2.6
1	C	28	ALA	2.6
1	C	53	ALA	2.6
1	C	384	ASP	2.6
1	C	323	LEU	2.6
1	C	114	THR	2.6
1	C	295	PHE	2.6
1	C	414	ILE	2.6
1	C	91	GLY	2.6
1	C	238	SER	2.6
1	C	109	GLU	2.6
1	C	371	GLU	2.6
1	C	483	GLU	2.6
1	C	395	TRP	2.5
1	C	164	ARG	2.5
1	C	61	GLN	2.5
1	C	121	THR	2.5
1	C	454	LEU	2.5
1	C	484	LYS	2.5
1	C	429	HIS	2.5
1	C	492	LEU	2.5
1	C	266	VAL	2.5
1	C	373	GLN	2.5
1	C	325	LEU	2.4
1	C	26	HIS	2.4
1	C	437	TRP	2.4
1	C	163	TYR	2.4
1	C	82	TRP	2.4
1	C	25	PRO	2.4
1	C	467	VAL	2.4
1	C	88	THR	2.4
1	C	438	GLY	2.4
1	C	133	GLN	2.4
1	C	268	GLY	2.4
1	C	293	GLN	2.4
1	C	487	LEU	2.3
1	C	346	ILE	2.3
1	C	463	TRP	2.3
1	C	305	ARG	2.3
1	C	102	TYR	2.3
1	C	391	HIS	2.3
1	C	495	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	353	ASP	2.3
1	C	426	TRP	2.3
1	C	38	VAL	2.3
1	C	338	ALA	2.3
1	C	481	ILE	2.3
1	C	341	HIS	2.3
1	C	286	TYR	2.3
1	C	176	GLU	2.3
1	C	14	ASP	2.3
1	C	287	PRO	2.3
1	C	130	ILE	2.3
1	C	329	ALA	2.3
1	C	65	GLY	2.3
1	C	51	PHE	2.3
1	C	12	CYS	2.2
1	C	185	TYR	2.2
1	C	473	PRO	2.2
1	C	123	PHE	2.2
1	C	47	ALA	2.2
1	C	347	ALA	2.2
1	C	423	TRP	2.2
1	C	416	PHE	2.2
1	C	8	THR	2.2
1	C	477	THR	2.2
1	C	335	LEU	2.2
1	C	422	GLY	2.2
1	C	435	ILE	2.2
1	C	175	ALA	2.2
1	C	376	ASN	2.2
1	C	273	LEU	2.2
1	C	277	HIS	2.2
1	C	110	PHE	2.2
1	C	337	GLY	2.1
1	C	106	PHE	2.1
1	C	462	ALA	2.1
1	C	260	MET	2.1
1	C	190	TYR	2.1
1	C	86	VAL	2.1
1	C	215	ALA	2.1
1	C	92	GLU	2.1
1	C	250	TYR	2.1
1	C	213	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	427	PHE	2.1
1	C	304	GLU	2.1
1	C	7	VAL	2.1
1	C	478	ASP	2.0
1	C	359	LEU	2.0
1	C	448	GLY	2.0
1	C	45	ILE	2.0
1	C	256	VAL	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](#)

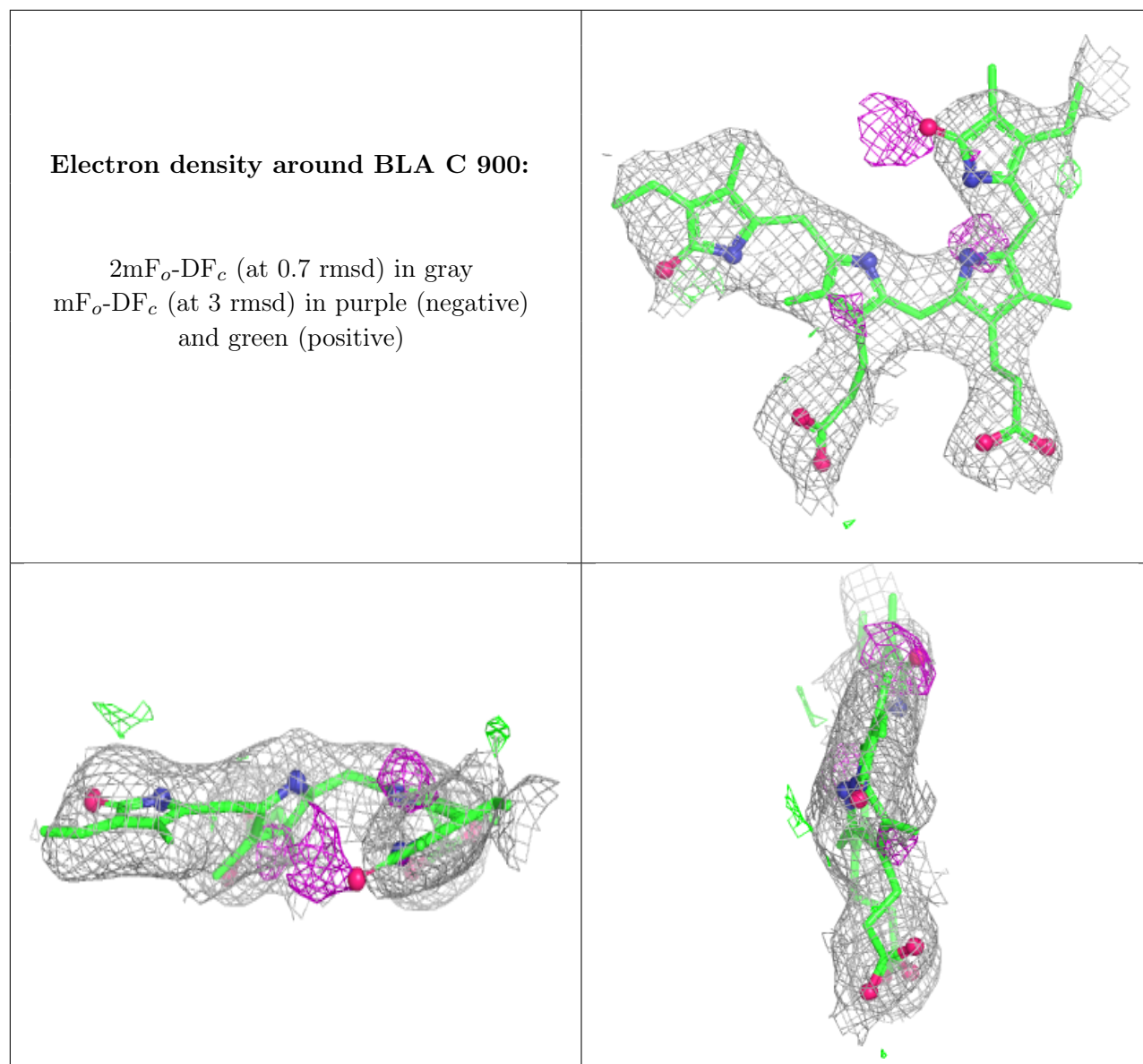
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	BLA	C	900	43/43	0.81	0.28	41,57,91,100	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.