



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:03 AM UTC

PDB ID : 3NOU / pdb_00003nou
Title : Light-induced intermediate structure L3 of P. aeruginosa bacteriophytochrome
Authors : Yang, X.; Ren, Z.; Moffat, K.
Deposited on : 2010-06-25
Resolution : 3.00 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

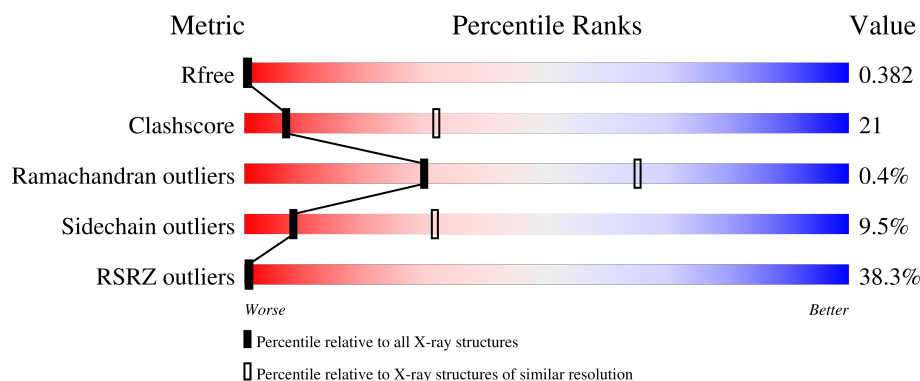
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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.

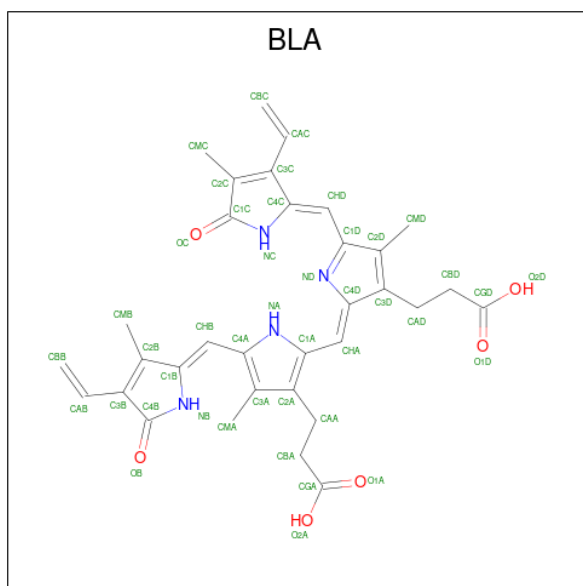
- Molecule 1 is a protein called Bacteriophytochrome.

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

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	498	LEU	ALA	conflict	UNP Q9HWR3
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 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-3.00) 99.1 (50.00-3.00)	Depositor EDS
R_{merge}	0.11	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) 0.379 , 0.382	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 , 24.8	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	0.54	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	0.51	1/3902 (0.0%)	0.84	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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	188	GLN	C-N	-22.29	1.01	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	188	GLN	O-C-N	-13.16	105.51	123.01
1	C	63	GLN	N-CA-C	-10.57	100.45	113.97
1	C	188	GLN	CA-C-N	7.39	133.66	122.65
1	C	188	GLN	C-N-CA	7.39	133.66	122.65
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	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	188	GLN	Mainchain
1	C	62	GLU	Peptide

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	C	3817	0	3751	160	0
2	C	43	0	30	34	0
All	All	3860	0	3781	162	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 21.

All (162) 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:163:TYR:OH	1:C:275:SER:CB	1.77	1.30
1:C:163:TYR:OH	1:C:275:SER:HB3	1.21	1.30
1:C:247:HIS:CE1	2:C:900:BLA:HAA2	1.76	1.18
1:C:161:MET:CE	1:C:277:HIS:HE1	1.70	1.03
1:C:247:HIS:CE1	2:C:900:BLA:CAA	2.41	1.03
1:C:161:MET:CE	1:C:277:HIS:CE1	2.43	1.00
1:C:163:TYR:CZ	1:C:275:SER:HB2	1.99	0.97
1:C:163:TYR:CZ	1:C:275:SER:CB	2.51	0.93
1:C:171:GLY:HA3	1:C:190:TYR:CZ	2.03	0.93
1:C:203:TYR:OH	2:C:900:BLA:HBA1	1.67	0.93
1:C:203:TYR:OH	2:C:900:BLA:CBA	2.19	0.90
1:C:163:TYR:HH	1:C:275:SER:CB	1.82	0.88
1:C:171:GLY:HA3	1:C:190:TYR:CE2	2.08	0.88
1:C:247:HIS:NE2	2:C:900:BLA:HAA2	1.92	0.83
1:C:45:ILE:HD12	1:C:46:GLN:H	1.44	0.82
1:C:84:ASN:HD22	1:C:85:SER:H	1.29	0.79
1:C:173:VAL:CG2	2:C:900:BLA:CBB	2.59	0.79
1:C:161:MET:HE3	1:C:277:HIS:HE1	1.47	0.79
1:C:161:MET:HE2	1:C:277:HIS:CE1	2.18	0.79
1:C:475:SER:HB2	1:C:478:ASP:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:HIS:HE1	2:C:900:BLA:CAA	2.01	0.73
1:C:173:VAL:CG2	2:C:900:BLA:HBB1	2.20	0.71
1:C:45:ILE:HD12	1:C:46:GLN:N	2.06	0.71
1:C:163:TYR:CZ	1:C:275:SER:HB3	2.19	0.71
1:C:163:TYR:CD2	1:C:163:TYR:N	2.55	0.71
1:C:62:GLU:OE2	1:C:62:GLU:HA	1.90	0.70
1:C:247:HIS:CE1	2:C:900:BLA:C2A	2.75	0.69
1:C:172:GLU:HB2	1:C:189:ARG:HD2	1.74	0.68
1:C:163:TYR:N	1:C:163:TYR:HD2	1.89	0.67
1:C:358:MET:HE1	1:C:378:LEU:HD22	1.76	0.67
1:C:414:ILE:HD12	1:C:486:ARG:HB2	1.76	0.67
1:C:188:GLN:HB3	2:C:900:BLA:HBB2	1.75	0.66
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:257:ARG:HD3	1:C:281:PRO:HD3	1.77	0.65
1:C:196:PRO:HD3	2:C:900:BLA:CHD	2.27	0.64
1:C:163:TYR:HB3	1:C:190:TYR:OH	1.98	0.64
1:C:84:ASN:ND2	1:C:85:SER:H	1.96	0.63
1:C:199:ALA:HB1	2:C:900:BLA:CAD	2.29	0.62
1:C:203:TYR:OH	2:C:900:BLA:HBA2	1.99	0.62
1:C:173:VAL:HG23	2:C:900:BLA:CBB	2.30	0.62
1:C:173:VAL:HG21	2:C:900:BLA:CBB	2.29	0.61
1:C:162:ALA:C	1:C:163:TYR:HD2	2.08	0.61
1:C:247:HIS:HE1	2:C:900:BLA:C2A	2.14	0.61
1:C:417:HIS:HD2	1:C:420:GLU:H	1.48	0.61
1:C:453:ARG:NH2	2:C:900:BLA:HMC2	2.16	0.60
1:C:148:THR:HG23	1:C:160:VAL:HG22	1.82	0.60
1:C:161:MET:HB2	1:C:163:TYR:HE2	1.66	0.60
1:C:172:GLU:HB2	1:C:189:ARG:CD	2.32	0.60
1:C:129:ARG:HE	1:C:154:MET:HG2	1.65	0.60
1:C:347:ALA:HB2	1:C:366:ILE:HD11	1.83	0.59
1:C:250:TYR:OH	2:C:900:BLA:CMB	2.50	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:161:MET:HE3	1:C:277:HIS:CE1	2.29	0.58
1:C:173:VAL:HG21	2:C:900:BLA:HBB2	1.86	0.58
1:C:165:PHE:HD1	1:C:272:GLY:HA2	1.69	0.57
1:C:161:MET:HE2	1:C:277:HIS:ND1	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:453:ARG:NH2	2:C:900:BLA:CMC	2.69	0.55
1:C:173:VAL:CG2	2:C:900:BLA:HBB2	2.34	0.55
1:C:169:ASP:O	1:C:192:ALA:HA	2.06	0.55
1:C:199:ALA:HB1	2:C:900:BLA:HAD2	1.89	0.55
2:C:900:BLA:HBB1	2:C:900:BLA:OB	2.07	0.54
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:319:THR:HG22	1:C:322:ARG:HH21	1.71	0.54
1:C:196:PRO:CD	2:C:900:BLA:CHD	2.86	0.53
1:C:391:HIS:HA	1:C:411:VAL:O	2.08	0.53
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:220:ARG:HG3	1:C:220:ARG:NH1	2.24	0.52
1:C:199:ALA:HB2	2:C:900:BLA:HMD2	1.92	0.51
1:C:171:GLY:N	1:C:190:TYR:O	2.42	0.51
1:C:257:ARG:HH11	1:C:281:PRO:HG3	1.76	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:161:MET:HE1	1:C:277:HIS:CE1	2.42	0.49
1:C:185:TYR:O	1:C:188:GLN:HB2	2.13	0.49
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
1:C:196:PRO:HD2	2:C:900:BLA:C2D	2.43	0.48
1:C:188:GLN:CB	2:C:900:BLA:HBB2	2.42	0.48
1:C:168:ASP:O	1:C:192:ALA:HB2	2.14	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:161:MET:CB	1:C:163:TYR:HE2	2.25	0.48
1:C:163:TYR:CE1	1:C:275:SER:HB2	2.47	0.48
1:C:440:LYS:O	1:C:441:PRO:C	2.57	0.48
1:C:161:MET:HE1	1:C:277:HIS:HE1	1.68	0.47
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:165:PHE:CE2	1:C:190:TYR:HE2	2.32	0.47
1:C:196:PRO:HD2	2:C:900:BLA:C1D	2.45	0.47
1:C:286:TYR:N	1:C:287:PRO:HD2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:193:SER:C	1:C:195:ILE:H	2.24	0.45
1:C:199:ALA:HB2	2:C:900:BLA:CMD	2.47	0.45
1:C:30:VAL:HG12	1:C:32:LEU:CD1	2.48	0.44
1:C:161:MET:HB2	1:C:163:TYR:CE2	2.51	0.44
1:C:172:GLU:CG	1:C:189:ARG:HD3	2.47	0.44
1:C:51:PHE:CE2	1:C:63:GLN:O	2.71	0.44
1:C:250:TYR:OH	2:C:900:BLA:HMB2	2.17	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:161:MET:HE2	1:C:277:HIS:HD1	1.81	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:250:TYR:OH	2:C:900:BLA:HMB1	2.17	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
1:C:188:GLN:NE2	1:C:189:ARG:O	2.52	0.43
2:C:900:BLA:HBA2	2:C:900:BLA:HHA	2.00	0.43
1:C:264:ILE:HB	1:C:272:GLY:O	2.19	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: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:171:GLY:O	1:C:189:ARG:HA	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:TYR:CE1	1:C:273:LEU:HD11	2.55	0.41
1:C:305:ARG:HA	1:C:305:ARG:HD2	1.99	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:193:SER:C	1:C:195:ILE:N	2.78	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:199:ALA:CB	2:C:900:BLA:CAD	2.97	0.40
1:C:5:THR:HA	1:C:6:PRO:HD3	1.99	0.40
1:C:199:ALA:CB	2:C:900:BLA:HAD1	2.51	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 65

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%)	371 (90%)	39 (10%)	8 31

All (39) 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	163	TYR
1	C	164	ARG
1	C	166	ARG
1	C	186	LEU
1	C	188	GLN
1	C	194	ASP
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

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Mol	Chain	Res	Type
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 (15) 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	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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	-	12/26/74/74	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	7.90	1.58	1.40
2	C	900	BLA	CHB-C1B	6.56	1.53	1.37
2	C	900	BLA	CHD-C4C	6.00	1.52	1.37
2	C	900	BLA	CHD-C1D	5.26	1.52	1.40
2	C	900	BLA	CBC-CAC	4.67	1.52	1.30
2	C	900	BLA	C4D-C3D	-4.30	1.39	1.45
2	C	900	BLA	C1C-C2C	-4.03	1.38	1.48
2	C	900	BLA	C1D-C2D	-3.67	1.37	1.45
2	C	900	BLA	C3C-C4C	-3.46	1.39	1.45
2	C	900	BLA	C1B-C2B	-3.14	1.39	1.45
2	C	900	BLA	CAB-C3B	-3.01	1.39	1.47
2	C	900	BLA	CAC-C3C	2.53	1.54	1.47
2	C	900	BLA	C4A-NA	-2.42	1.33	1.37
2	C	900	BLA	C1A-NA	-2.31	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	-6.21	112.80	128.06
2	C	900	BLA	C1A-CHA-C4D	-4.56	118.26	128.22
2	C	900	BLA	CHA-C4D-ND	4.17	133.36	124.60
2	C	900	BLA	CHA-C1A-C2A	-3.18	120.38	127.22
2	C	900	BLA	CHA-C4D-C3D	-2.95	118.58	125.40
2	C	900	BLA	C3B-C4B-NB	2.81	109.66	106.13
2	C	900	BLA	CBC-CAC-C3C	-2.66	114.22	127.53
2	C	900	BLA	C4A-CHB-C1B	-2.40	123.91	130.82
2	C	900	BLA	CHD-C1D-ND	2.30	129.92	124.95
2	C	900	BLA	C3C-C4C-NC	2.25	110.31	106.64
2	C	900	BLA	C4C-NC-C1C	-2.20	107.96	110.66
2	C	900	BLA	CHA-C1A-NA	2.20	130.26	125.29
2	C	900	BLA	C1A-C2A-C3A	-2.15	105.12	107.62
2	C	900	BLA	O1D-CGD-CBD	-2.14	116.30	123.09
2	C	900	BLA	C1D-C2D-C3D	2.01	108.75	106.48

There are no chirality outliers.

All (12) 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	NA-C4A-CHB-C1B
2	C	900	BLA	C3A-C4A-CHB-C1B
2	C	900	BLA	C2A-CAA-CBA-CGA
2	C	900	BLA	NB-C1B-CHB-C4A
2	C	900	BLA	NC-C4C-CHD-C1D
2	C	900	BLA	C2B-C1B-CHB-C4A
2	C	900	BLA	C1A-C2A-CAA-CBA
2	C	900	BLA	CAD-CBD-CGD-O2D
2	C	900	BLA	CAD-CBD-CGD-O1D
2	C	900	BLA	C3C-C4C-CHD-C1D

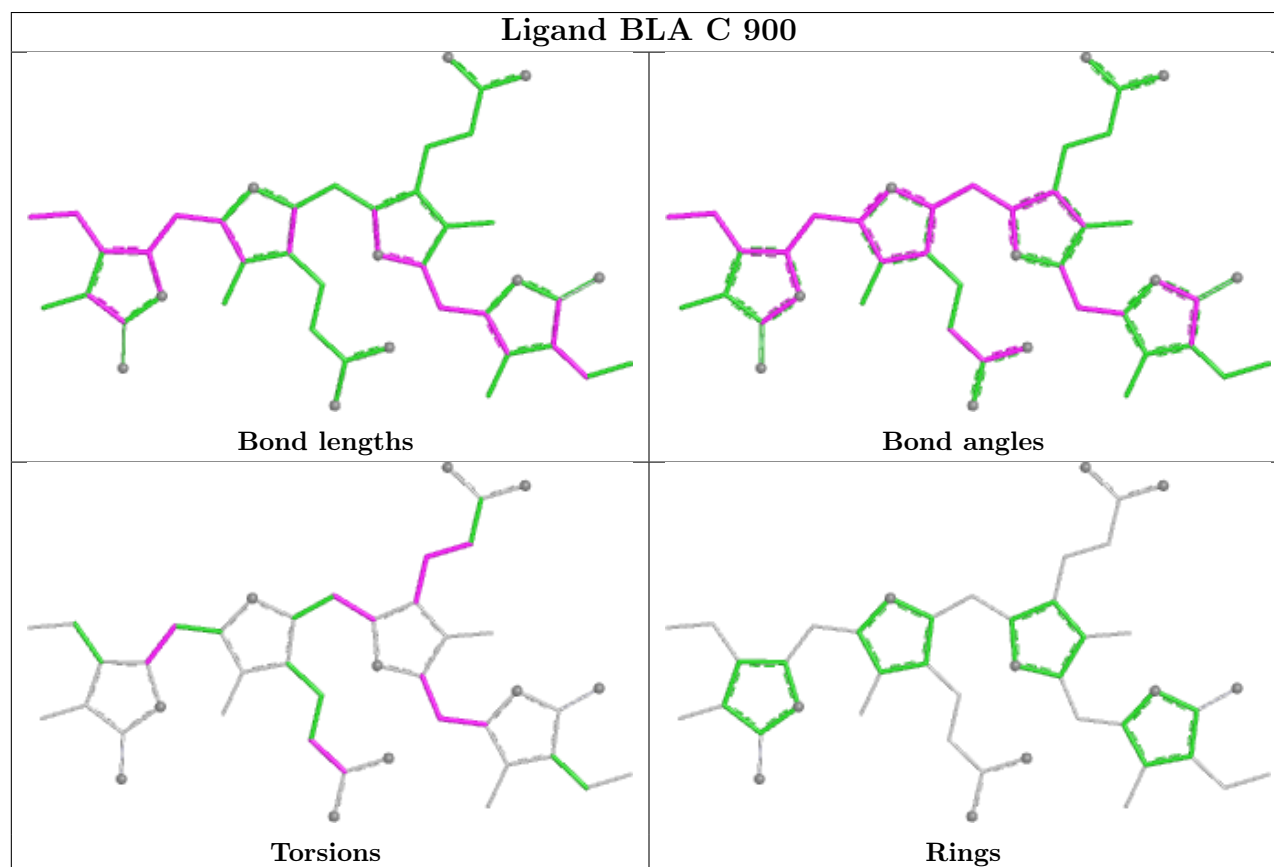
There are no ring outliers.

1 monomer is involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	BLA	34	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	188:GLN	C	189:ARG	N	1.01

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%)	1.90	185 (38%) 1 1	38, 60, 105, 147	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	ASP	7.7
1	C	496	HIS	7.5
1	C	365	SER	7.4
1	C	4	ILE	6.5
1	C	128	GLN	6.5
1	C	363	THR	6.2
1	C	334	ASP	5.8
1	C	418	ARG	5.8
1	C	197	ALA	5.6
1	C	407	ASP	5.6
1	C	78	GLY	5.5
1	C	333	ASP	5.4
1	C	119	SER	5.3
1	C	443	LYS	5.3
1	C	74	GLU	5.2
1	C	308	GLN	5.1
1	C	442	GLU	5.0
1	C	253	ASN	5.0
1	C	90	ILE	4.9
1	C	388	ASP	4.9
1	C	350	ILE	4.7
1	C	360	GLY	4.7
1	C	406	GLY	4.7
1	C	468	ARG	4.6
1	C	31	THR	4.5
1	C	362	ARG	4.5
1	C	63	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	58	TYR	4.4
1	C	249	GLU	4.3
1	C	99	GLY	4.3
1	C	439	GLY	4.3
1	C	52	VAL	4.3
1	C	116	ASP	4.2
1	C	73	GLU	4.2
1	C	101	SER	4.2
1	C	297	GLN	4.1
1	C	79	ASN	4.0
1	C	231	GLU	4.0
1	C	367	ARG	4.0
1	C	379	GLN	3.9
1	C	81	PRO	3.7
1	C	311	ILE	3.6
1	C	370	PHE	3.6
1	C	343	ASP	3.6
1	C	37	MET	3.5
1	C	95	PHE	3.5
1	C	444	LEU	3.5
1	C	183	GLU	3.5
1	C	494	LEU	3.5
1	C	229	THR	3.4
1	C	419	GLN	3.4
1	C	476	GLU	3.3
1	C	103	LYS	3.3
1	C	394	ASN	3.3
1	C	224	ALA	3.3
1	C	181	ASP	3.3
1	C	13	GLU	3.2
1	C	115	ALA	3.2
1	C	342	PRO	3.2
1	C	117	THR	3.2
1	C	233	PHE	3.1
1	C	104	GLU	3.1
1	C	369	ASP	3.1
1	C	465	GLU	3.1
1	C	380	ARG	3.1
1	C	107	TYR	3.1
1	C	491	GLU	3.1
1	C	32	LEU	3.0
1	C	34	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	472	THR	3.0
1	C	409	CYS	3.0
1	C	269	LYS	3.0
1	C	432	VAL	3.0
1	C	452	PRO	3.0
1	C	372	ARG	3.0
1	C	62	GLU	2.9
1	C	239	VAL	2.9
1	C	232	SER	2.9
1	C	280	SER	2.9
1	C	135	GLN	2.9
1	C	304	GLU	2.9
1	C	96	ASP	2.9
1	C	67	GLU	2.9
1	C	21	GLY	2.9
1	C	198	GLN	2.9
1	C	331	ASP	2.9
1	C	80	GLY	2.9
1	C	5	THR	2.8
1	C	93	HIS	2.8
1	C	57	SER	2.8
1	C	177	SER	2.8
1	C	236	SER	2.8
1	C	474	TRP	2.8
1	C	327	ARG	2.8
1	C	408	CYS	2.8
1	C	217	THR	2.8
1	C	252	THR	2.8
1	C	187	GLY	2.8
1	C	361	GLY	2.8
1	C	259	SER	2.7
1	C	70	ARG	2.7
1	C	139	ASP	2.7
1	C	137	HIS	2.7
1	C	267	GLY	2.7
1	C	54	SER	2.7
1	C	244	SER	2.7
1	C	344	ASP	2.6
1	C	15	GLU	2.6
1	C	235	LEU	2.6
1	C	129	ARG	2.6
1	C	109	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	392	THR	2.6
1	C	180	GLU	2.6
1	C	320	GLU	2.6
1	C	387	ARG	2.6
1	C	383	ARG	2.6
1	C	434	ARG	2.6
1	C	140	THR	2.6
1	C	201	ARG	2.5
1	C	127	ALA	2.5
1	C	112	ILE	2.5
1	C	382	GLN	2.5
1	C	441	PRO	2.5
1	C	138	ASN	2.5
1	C	393	ASP	2.5
1	C	415	ARG	2.5
1	C	486	ARG	2.5
1	C	295	PHE	2.4
1	C	11	ASN	2.4
1	C	446	THR	2.4
1	C	277	HIS	2.4
1	C	336	PHE	2.4
1	C	14	ASP	2.4
1	C	384	ASP	2.4
1	C	122	SER	2.4
1	C	204	ILE	2.4
1	C	206	ASN	2.4
1	C	9	LEU	2.4
1	C	431	GLU	2.4
1	C	94	LEU	2.3
1	C	228	GLU	2.3
1	C	440	LYS	2.3
1	C	98	ILE	2.3
1	C	33	ARG	2.3
1	C	449	PRO	2.3
1	C	125	LEU	2.3
1	C	205	GLN	2.3
1	C	87	GLU	2.3
1	C	118	LEU	2.3
1	C	120	ILE	2.3
1	C	345	GLY	2.3
1	C	60	THR	2.3
1	C	77	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	35	ASP	2.2
1	C	323	LEU	2.2
1	C	105	VAL	2.2
1	C	10	ALA	2.2
1	C	196	PRO	2.2
1	C	282	LYS	2.2
1	C	328	ARG	2.2
1	C	341	HIS	2.2
1	C	263	SER	2.2
1	C	208	ILE	2.2
1	C	283	LEU	2.2
1	C	483	GLU	2.2
1	C	191	PRO	2.2
1	C	26	HIS	2.2
1	C	355	ALA	2.1
1	C	69	LEU	2.1
1	C	133	GLN	2.1
1	C	471	SER	2.1
1	C	347	ALA	2.1
1	C	330	ARG	2.1
1	C	425	PHE	2.1
1	C	376	ASN	2.1
1	C	478	ASP	2.1
1	C	216	TYR	2.1
1	C	53	ALA	2.1
1	C	326	ALA	2.1
1	C	163	TYR	2.0
1	C	293	GLN	2.0
1	C	309	GLY	2.0
1	C	364	LEU	2.0
1	C	457	ARG	2.0
1	C	270	LEU	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](#)

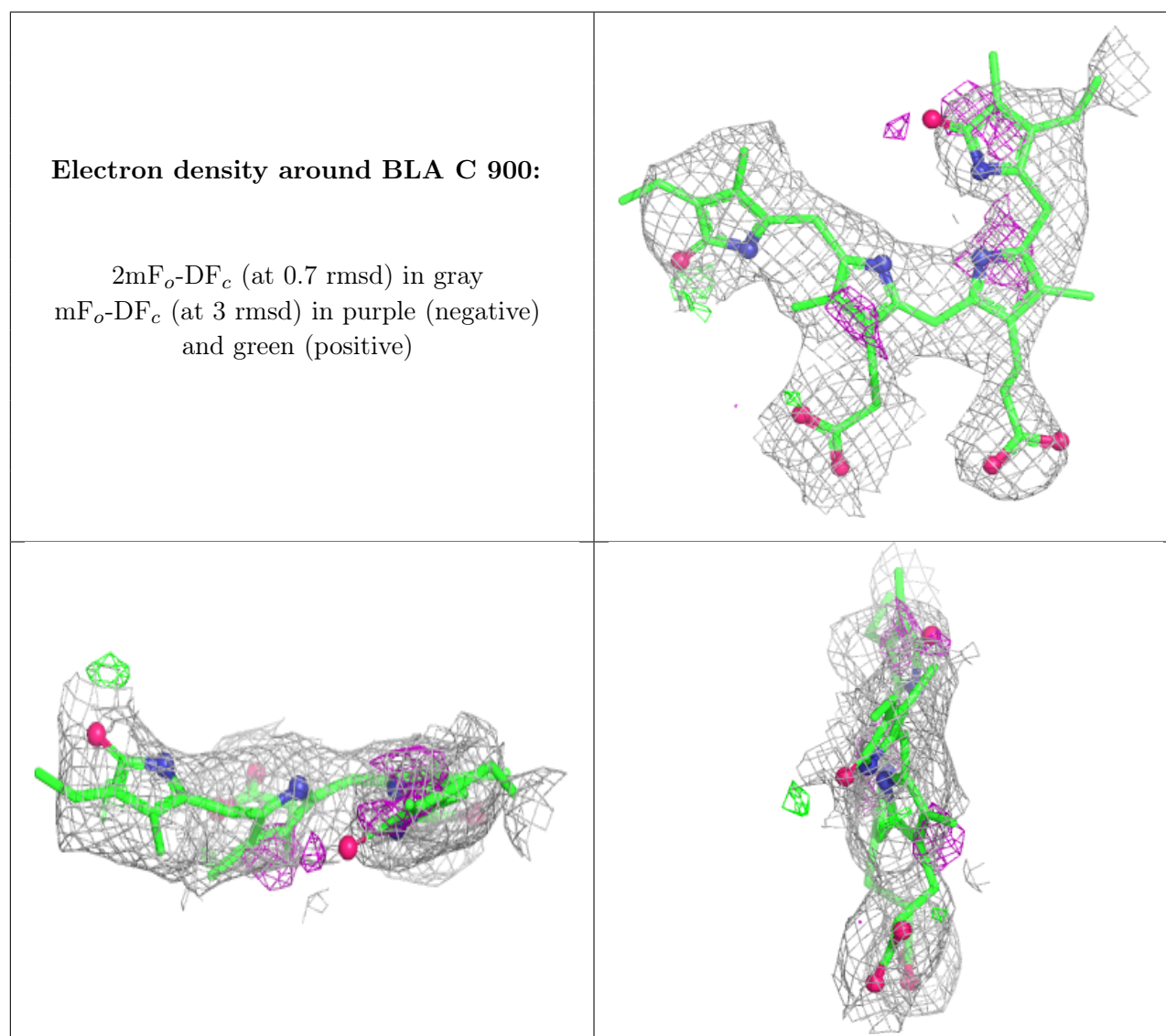
There are no oligosaccharides in this entry.

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	0.76	0.32	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 [i](#)

There are no such residues in this entry.