



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:28 AM UTC

PDB ID : 1BVD / pdb_00001bvd
Title : STRUCTURE OF A BILIVERDIN APOMYOGLOBIN COMPLEX (FORM B) AT 98 K
Authors : Wagner, U.G.; Mueller, N.; Schmitzberger, W.; Falk, H.; Kratky, C.
Deposited on : 1994-12-16
Resolution : 1.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

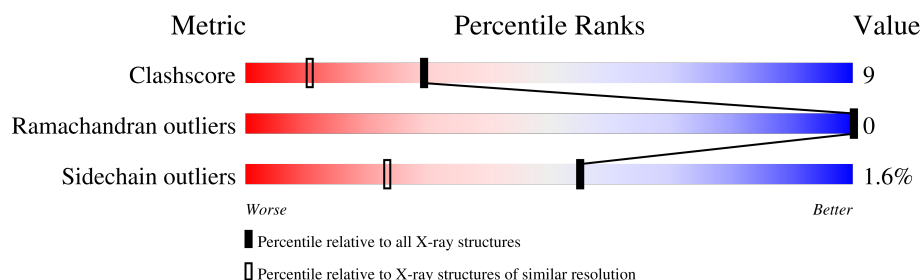
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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))
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	 65% 29% 5%

2 Entry composition [i](#)

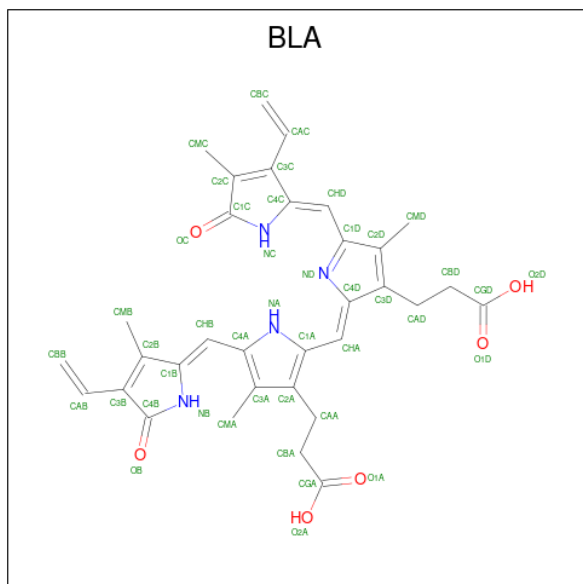
There are 3 unique types of molecules in this entry. The entry contains 1528 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 APOMYOGLOBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	3	0
			1226	789	216	219	2			

- Molecule 2 is BILIVERDINE IX ALPHA (CCD ID: 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		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	259	Total	O	0	0
			259	259		

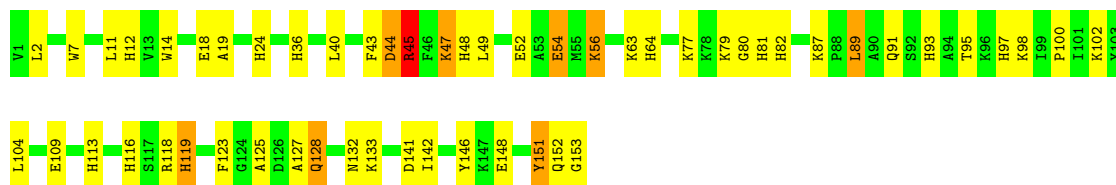
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: APOMYOGLOBIN

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	39.80Å 50.60Å 74.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.40	Depositor
% Data completeness (in resolution range)	90.5 (8.00-1.40)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.212 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1528	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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	1.66	15/1266 (1.2%)	1.95	46/1701 (2.7%)

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	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	TYR	C-N	-15.85	1.11	1.33
1	A	89	LEU	C-N	12.29	1.50	1.33
1	A	45	ARG	NE-CZ	8.44	1.42	1.33
1	A	91	GLN	C-N	6.93	1.44	1.33
1	A	12	HIS	CD2-NE2	-6.71	1.30	1.37
1	A	116	HIS	CD2-NE2	-6.39	1.30	1.37
1	A	98	LYS	C-N	5.96	1.38	1.33
1	A	45	ARG	CZ-NH1	5.88	1.41	1.32
1	A	44	ASP	CA-CB	-5.72	1.44	1.53
1	A	36	HIS	CG-ND1	-5.46	1.32	1.38
1	A	48	HIS	CD2-NE2	-5.39	1.31	1.37
1	A	93	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	152	GLN	CB-CG	5.29	1.68	1.52
1	A	93	HIS	CG-ND1	-5.26	1.32	1.38
1	A	82	HIS	CG-CD2	5.01	1.41	1.35

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	LEU	O-C-N	8.06	130.74	122.03
1	A	152	GLN	CB-CA-C	7.90	124.06	110.79
1	A	113	HIS	CA-CB-CG	-7.19	106.61	113.80
1	A	128	GLN	CG-CD-NE2	-7.07	105.79	116.40
1	A	151	TYR	CA-C-N	-6.60	109.68	120.71
1	A	151	TYR	C-N-CA	-6.60	109.68	120.71
1	A	80	GLY	CA-C-O	-6.39	112.63	119.27
1	A	77	LYS	CA-CB-CG	-6.32	101.45	114.10
1	A	148	GLU	CB-CA-C	-6.29	98.26	110.46
1	A	95	THR	N-CA-C	6.23	121.01	113.41
1	A	113	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	A	56	LYS	CA-CB-CG	-6.08	101.95	114.10
1	A	44	ASP	N-CA-C	6.02	118.63	111.71
1	A	132[A]	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	132[B]	ASN	OD1-CG-ND2	-5.99	116.61	122.60
1	A	148	GLU	N-CA-CB	5.97	119.57	110.14
1	A	14	TRP	CG-CD1-NE1	-5.94	102.48	110.20
1	A	36	HIS	CA-C-N	5.91	126.32	119.47
1	A	36	HIS	C-N-CA	5.91	126.32	119.47
1	A	152	GLN	N-CA-CB	-5.89	101.42	110.13
1	A	45	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	A	113	HIS	CG-CD2-NE2	-5.76	101.44	107.20
1	A	128	GLN	CA-CB-CG	-5.74	102.62	114.10
1	A	146	TYR	N-CA-C	-5.74	104.93	111.07
1	A	64	HIS	CA-CB-CG	-5.67	108.13	113.80
1	A	152	GLN	O-C-N	-5.64	115.34	122.17
1	A	100	PRO	O-C-N	-5.60	115.88	122.99
1	A	7	TRP	CG-CD1-NE1	-5.54	103.00	110.20
1	A	54	GLU	O-C-N	5.46	128.37	122.15
1	A	116	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	113	HIS	CE1-NE2-CD2	5.41	114.41	109.00
1	A	118	ARG	CB-CG-CD	-5.35	99.00	111.30
1	A	87	LYS	O-C-N	-5.32	115.50	120.55
1	A	63	LYS	CG-CD-CE	-5.32	99.06	111.30
1	A	36	HIS	CA-CB-CG	-5.30	108.50	113.80
1	A	119	HIS	CB-CG-CD2	-5.29	124.33	131.20
1	A	19	ALA	N-CA-C	-5.28	105.70	111.82
1	A	128	GLN	CG-CD-OE1	5.26	131.33	120.80
1	A	141	ASP	O-C-N	-5.26	116.15	122.15
1	A	109	GLU	CA-C-O	-5.19	114.92	120.42
1	A	79	LYS	CA-C-O	5.18	127.85	121.84
1	A	93	HIS	CA-CB-CG	-5.17	108.62	113.80
1	A	81	HIS	CA-CB-CG	-5.17	108.63	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	HIS	CB-CG-ND1	5.11	130.36	122.70
1	A	152	GLN	CG-CD-NE2	5.04	123.96	116.40
1	A	81	HIS	CB-CG-CD2	-5.02	124.67	131.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ARG	Sidechain

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	1226	0	1242	21	0
2	A	43	0	34	4	0
3	A	259	0	0	7	1
All	All	1528	0	1276	22	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (22) 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:45:ARG:NH1	3:A:404:HOH:O	1.89	1.05
1:A:11:LEU:HD22	3:A:372:HOH:O	1.59	1.03
1:A:45:ARG:NH1	2:A:154:BLA:O2D	2.24	0.71
1:A:24:HIS:NE2	1:A:119:HIS:HE1	1.88	0.71
1:A:18:GLU:OE1	3:A:338:HOH:O	2.12	0.67
1:A:104:LEU:HD11	1:A:142:ILE:HG21	1.78	0.65
1:A:119:HIS:HD2	3:A:161:HOH:O	1.87	0.57
1:A:89:LEU:HD11	2:A:154:BLA:CHB	2.41	0.51
1:A:125:ALA:HA	3:A:412:HOH:O	2.11	0.51
1:A:49:LEU:HD22	1:A:54:GLU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG2	1:A:56:LYS:HD2	1.94	0.48
1:A:44:ASP:HA	1:A:47:LYS:HE3	1.95	0.47
1:A:104:LEU:CD1	1:A:142:ILE:HG21	2.45	0.46
1:A:102:LYS:HD2	3:A:297:HOH:O	2.15	0.46
1:A:40:LEU:HG	1:A:47:LYS:HA	1.99	0.44
1:A:128:GLN:NE2	3:A:389:HOH:O	2.50	0.43
2:A:154:BLA:HB	2:A:154:BLA:HA	1.67	0.43
1:A:43:PHE:O	1:A:47:LYS:HB3	2.19	0.43
1:A:89:LEU:HD21	2:A:154:BLA:HMB2	2.02	0.42
1:A:123:PHE:HA	1:A:127:ALA:HB3	2.03	0.41
1:A:151:TYR:CE2	1:A:153:GLY:HA2	2.54	0.41
1:A:2:LEU:HG	1:A:133:LYS:HE2	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:284:HOH:O	3:A:373:HOH:O[1_655]	1.75	0.45

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	154/153 (101%)	149 (97%)	5 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	127/125 (102%)	125 (98%)	2 (2%)	55 23

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	47	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	26	GLN
1	A	91	GLN
1	A	119	HIS
1	A	128	GLN
1	A	152	GLN

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	A	154	-	46,46,46	1.49	9 (19%)	66,67,67	1.79	17 (25%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	A	154	-	-	3/26/74/74	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	BLA	C3C-C4C	3.91	1.53	1.45
2	A	154	BLA	CBC-CAC	2.96	1.44	1.30
2	A	154	BLA	CAB-C3B	-2.85	1.39	1.47
2	A	154	BLA	C1B-C2B	2.84	1.50	1.45
2	A	154	BLA	CHA-C4D	2.46	1.43	1.38
2	A	154	BLA	CAC-C3C	-2.42	1.40	1.47
2	A	154	BLA	O2A-CGA	2.39	1.38	1.30
2	A	154	BLA	C1A-C2A	2.38	1.48	1.42
2	A	154	BLA	C4A-C3A	2.01	1.46	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	BLA	C3B-C4B-NB	6.13	113.84	106.13
2	A	154	BLA	C1B-NB-C4B	-5.05	104.46	110.66
2	A	154	BLA	C4C-NC-C1C	-4.25	105.45	110.66
2	A	154	BLA	CAC-C3C-C4C	3.16	132.93	123.66
2	A	154	BLA	C2B-C1B-NB	2.98	111.31	106.97
2	A	154	BLA	O2D-CGD-O1D	-2.93	115.78	123.33
2	A	154	BLA	O2D-CGD-CBD	2.74	122.65	114.00
2	A	154	BLA	C2C-C1C-NC	2.61	112.39	106.55
2	A	154	BLA	CAC-C3C-C2C	-2.59	120.02	128.43
2	A	154	BLA	C1A-C2A-C3A	-2.47	104.74	107.62
2	A	154	BLA	C2A-C1A-NA	2.43	110.62	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	BLA	C4B-C3B-C2B	-2.38	104.87	107.92
2	A	154	BLA	CHB-C1B-NB	-2.36	121.03	126.06
2	A	154	BLA	C3B-C2B-C1B	-2.21	105.46	107.92
2	A	154	BLA	OB-C4B-C3B	-2.14	124.54	129.71
2	A	154	BLA	CHD-C4C-NC	-2.11	121.55	126.06
2	A	154	BLA	CMB-C2B-C1B	2.04	126.64	124.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

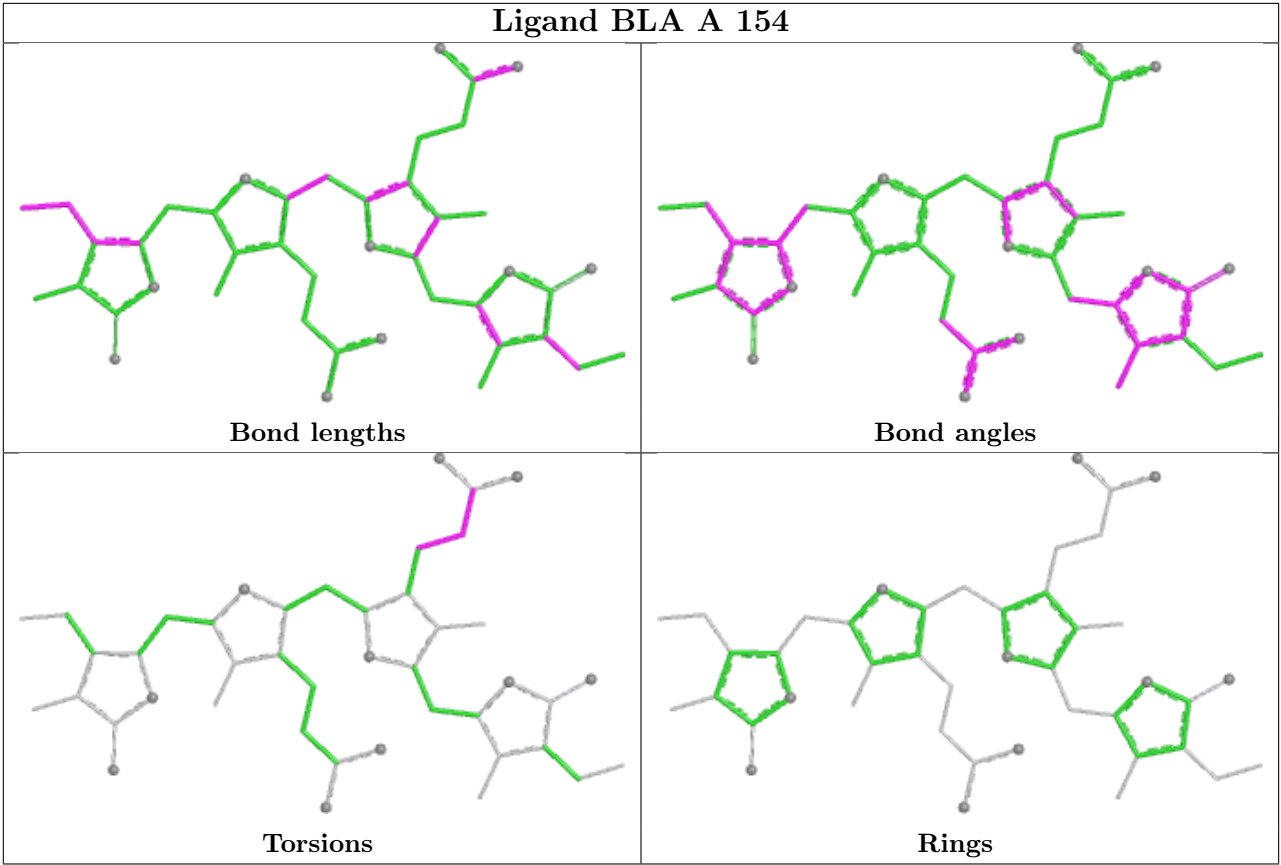
Mol	Chain	Res	Type	Atoms
2	A	154	BLA	CAA-CBA-CGA-O1A
2	A	154	BLA	CAA-CBA-CGA-O2A
2	A	154	BLA	C2A-CAA-CBA-CGA

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	BLA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	151:TYR	C	152:GLN	N	1.11

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.