



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 01:07 PM EDT

PDB ID : 4GPC  
Title : Structure of the biliverdin-HmuO, heme oxygenase from *Corynebacterium diphtheriae*  
Authors : Unno, M.; Ikeda-Saito, M.  
Deposited on : 2012-08-20  
Resolution : 1.85 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](mailto: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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

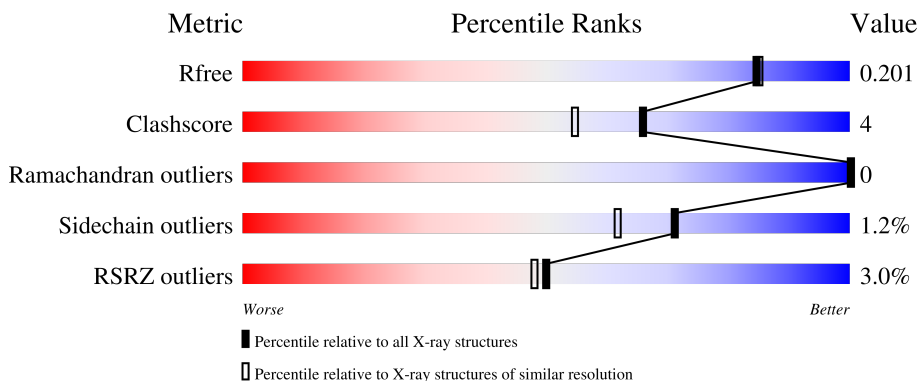
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	215	 5% 93% 5%
1	B	215	 % 91% 7%
1	C	215	 3% 91% 6%

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
3	SO4	A	902	-	X	-	-
3	SO4	A	903	-	X	-	-
3	SO4	B	602	-	X	-	-
3	SO4	B	603	-	X	-	-
3	SO4	B	604	-	X	-	-
3	SO4	C	903	-	X	X	-

## 2 Entry composition i

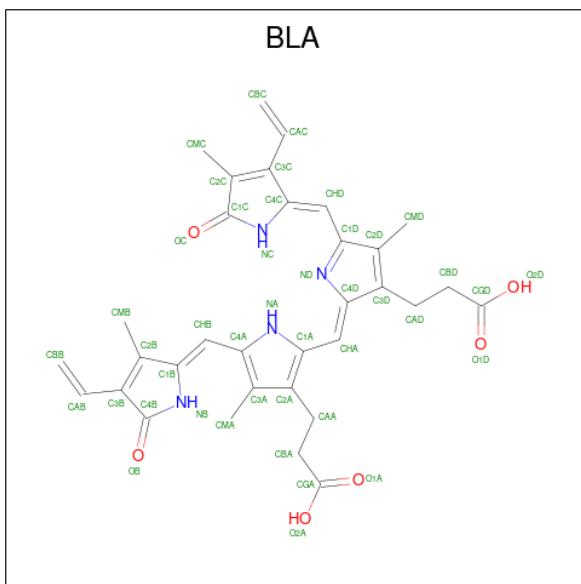
There are 5 unique types of molecules in this entry. The entry contains 5633 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Heme oxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	212	Total 1679	C 1059	N 298	O 319	S 3	0	1	0
1	B	211	Total 1694	C 1067	N 299	O 325	S 3	0	4	0
1	C	208	Total 1664	C 1048	N 294	O 319	S 3	0	2	0

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



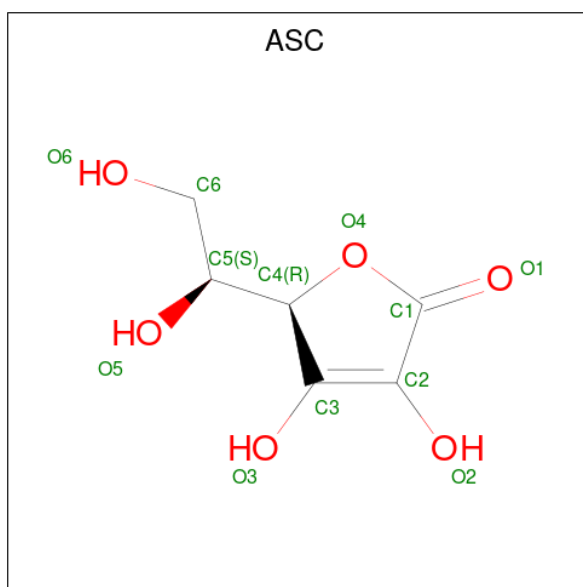
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0
2	C	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ASCORBIC ACID (three-letter code: ASC) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	105	Total O 105 105	0	0
5	B	168	Total O 168 168	0	0
5	C	152	Total O 152 152	0	0

### 3 Residue-property plots [i](#)

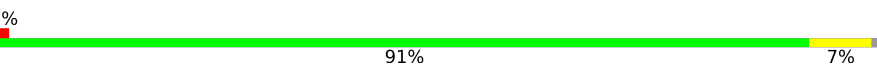
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Heme oxygenase

Chain A: 

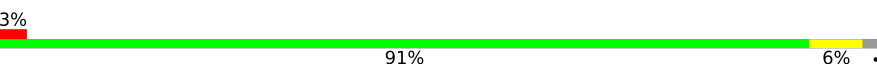


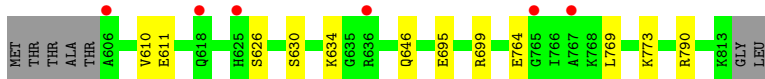
- Molecule 1: Heme oxygenase

Chain B: 



- Molecule 1: Heme oxygenase

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.11Å 63.09Å 107.56Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.23 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-1.85) 99.6 (30.23-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 1.85Å)	Xtrriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.168 , 0.203 0.165 , 0.201	Depositor DCC
$R_{free}$ test set	3067 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.1	Xtrriage
Anisotropy	0.380	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 51.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ASC, BLA, SO4

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	0.61	0/1715	0.64	0/2316
1	B	0.73	0/1743	0.71	0/2352
1	C	0.72	0/1706	0.68	0/2304
All	All	0.69	0/5164	0.68	0/6972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1679	0	1636	11	0
1	B	1694	0	1644	14	0
1	C	1664	0	1618	11	0
2	A	43	0	28	9	0
2	B	43	0	28	4	0
2	C	43	0	28	2	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	5	0	0	2	0
4	C	12	0	6	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	105	0	0	1	0
5	B	168	0	0	1	0
5	C	152	0	0	2	0
All	All	5633	0	4988	41	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 4.

All (41) 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:33:LEU:HD11	2:A:901:BLA:HMC1	1.43	1.00
1:C:695:GLU:HG3	3:C:903:SO4:O2	1.80	0.80
2:C:901:BLA:HMC1	2:C:901:BLA:HBC1	1.63	0.77
1:A:33:LEU:CD1	2:A:901:BLA:HMC1	2.23	0.67
1:A:33:LEU:HD11	2:A:901:BLA:CMC	2.24	0.67
1:B:454:ASP:HB3	1:B:456:GLU:OE1	1.98	0.62
1:B:322:LYS:HG2	1:B:505:HIS:CE1	2.35	0.61
1:B:509:ALA:O	1:B:513:LYS:HG3	2.00	0.61
1:C:699:ARG:NE	3:C:903:SO4:O4	2.33	0.61
1:A:208:PHE:CE2	2:A:901:BLA:HBB2	2.36	0.60
1:B:454:ASP:HB3	1:B:456:GLU:CD	2.24	0.58
1:A:208:PHE:HE2	2:A:901:BLA:HBB2	1.67	0.57
1:A:4:ALA:HB3	5:A:1090:HOH:O	2.04	0.57
1:B:333:LEU:HD11	2:B:601:BLA:HMC1	1.88	0.56
1:B:454:ASP:HB3	1:B:456:GLU:OE2	2.07	0.55
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.72	0.54
1:B:311:GLU:OE2	1:B:490:ARG:NH1	2.41	0.53
1:A:23:ALA:HB1	2:A:901:BLA:CBB	2.38	0.53
2:A:901:BLA:HMB1	2:A:901:BLA:HBB1	1.91	0.53
1:C:699:ARG:HG3	1:C:699:ARG:NH1	2.25	0.52
1:C:790:ARG:NH1	5:C:1125:HOH:O	2.37	0.50
1:B:443:ILE:HD11	2:B:601:BLA:HMC2	1.93	0.49
1:B:456:GLU:CD	1:B:456:GLU:H	2.16	0.48
1:C:610:VAL:HG23	5:C:1132:HOH:O	2.14	0.48
1:C:630:SER:O	1:C:634:LYS:HG3	2.13	0.48
2:A:901:BLA:CBB	2:A:901:BLA:HMB1	2.44	0.47
1:B:455:PRO:HD2	1:B:456:GLU:OE2	2.16	0.46
2:B:601:BLA:HBB1	2:B:601:BLA:OB	2.16	0.46
1:B:495:LYS:CE	5:B:828:HOH:O	2.64	0.46
1:C:769:LEU:HG	1:C:773:LYS:HE2	1.98	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:GLN:NE2	1:C:646:GLN:HA	2.32	0.44
1:A:18:GLN:CA	1:A:18:GLN:HE21	2.29	0.44
1:B:448:GLN:HG2	1:B:453:VAL:O	2.17	0.44
1:B:508:PHE:CE2	2:B:601:BLA:HBB2	2.52	0.44
2:C:901:BLA:HA	2:C:901:BLA:HB	1.66	0.43
1:A:131:VAL:HG21	1:A:200:ALA:HB3	2.02	0.42
1:C:646:GLN:HA	1:C:646:GLN:HE21	1.85	0.42
1:B:322:LYS:HE2	1:B:505:HIS:HE1	1.85	0.42
1:A:208:PHE:HE2	2:A:901:BLA:CBB	2.32	0.41
1:C:611:GLU:OE1	1:C:790:ARG:NH2	2.48	0.41
1:A:163:PHE:HB3	1:A:166:ILE:HD12	2.03	0.41

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	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
1	B	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
1	C	208/215 (97%)	204 (98%)	4 (2%)	0	100	100
All	All	632/645 (98%)	621 (98%)	11 (2%)	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	171/175 (98%)	168 (98%)	3 (2%)	59	45
1	B	175/175 (100%)	173 (99%)	2 (1%)	73	65
1	C	172/175 (98%)	170 (99%)	2 (1%)	71	62
All	All	518/525 (99%)	511 (99%)	7 (1%)	71	55

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	141	GLN
1	A	170	LYS
1	B	441[A]	GLN
1	B	441[B]	GLN
1	C	626	SER
1	C	764	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	78	ASN
1	A	148	GLN
1	A	182	ASN
1	B	378	ASN
1	B	505	HIS
1	C	625	HIS
1	C	646	GLN
1	C	678	ASN
1	C	762	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	C	901	-	42,46,46	3.99	23 (54%)	53,67,67	3.90	24 (45%)
3	SO4	C	903	-	4,4,4	0.39	0	6,6,6	3.38	4 (66%)
2	BLA	A	901	-	42,46,46	3.87	22 (52%)	53,67,67	3.95	26 (49%)
3	SO4	B	604	-	4,4,4	0.14	0	6,6,6	3.29	5 (83%)
3	SO4	B	602	-	4,4,4	0.29	0	6,6,6	3.51	5 (83%)
3	SO4	A	903	-	4,4,4	0.20	0	6,6,6	3.52	5 (83%)
3	SO4	A	902	-	4,4,4	0.17	0	6,6,6	3.01	5 (83%)
4	ASC	C	902	-	12,12,12	1.94	2 (16%)	17,17,17	1.97	6 (35%)
2	BLA	B	601	-	42,46,46	4.04	21 (50%)	53,67,67	4.13	28 (52%)
3	SO4	B	603	-	4,4,4	0.19	0	6,6,6	3.23	5 (83%)

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	901	-	-	3/26/74/74	0/4/4/4
2	BLA	B	601	-	-	9/26/74/74	0/4/4/4
4	ASC	C	902	-	-	0/6/22/22	0/1/1/1
2	BLA	A	901	-	-	10/26/74/74	0/4/4/4

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	BLA	CHA-C4D	13.76	1.46	1.35
2	A	901	BLA	CHA-C4D	13.54	1.46	1.35
2	C	901	BLA	CHA-C4D	13.34	1.46	1.35
2	C	901	BLA	CBD-CGD	-10.01	1.27	1.50
2	B	601	BLA	CBD-CGD	-9.92	1.27	1.50
2	A	901	BLA	CBD-CGD	-8.38	1.31	1.50
2	B	601	BLA	CBD-CAD	-8.33	1.25	1.52
2	C	901	BLA	CBD-CAD	-8.24	1.25	1.52
2	A	901	BLA	CBD-CAD	-7.68	1.27	1.52
2	A	901	BLA	CBA-CGA	-6.79	1.34	1.50
2	C	901	BLA	CBA-CGA	-6.75	1.34	1.50
2	B	601	BLA	CBA-CGA	-6.54	1.35	1.50
4	C	902	ASC	O4-C1	6.08	1.45	1.36
2	B	601	BLA	CHB-C1B	6.02	1.46	1.34
2	C	901	BLA	CHB-C1B	5.62	1.46	1.34
2	A	901	BLA	CHB-C1B	5.49	1.45	1.34
2	A	901	BLA	C3B-C2B	5.36	1.48	1.37
2	B	601	BLA	C3B-C2B	5.35	1.48	1.37
2	C	901	BLA	C3C-C2C	5.28	1.48	1.37
2	B	601	BLA	C3C-C2C	4.81	1.47	1.37
2	A	901	BLA	C3C-C2C	4.70	1.46	1.37
2	C	901	BLA	C3B-C2B	4.70	1.46	1.37
2	C	901	BLA	CBB-CAB	4.68	1.53	1.30
2	B	601	BLA	CBB-CAB	4.67	1.53	1.30
2	A	901	BLA	CHD-C4C	4.49	1.48	1.38
2	A	901	BLA	CBB-CAB	4.47	1.52	1.30
2	B	601	BLA	C1D-C2D	-4.45	1.36	1.45
2	C	901	BLA	C1D-C2D	-4.43	1.36	1.45
2	C	901	BLA	CHD-C4C	4.40	1.48	1.38
2	A	901	BLA	C1D-C2D	-4.14	1.36	1.45
2	B	601	BLA	CHD-C4C	3.96	1.47	1.38
2	A	901	BLA	CBC-CAC	3.72	1.48	1.30
2	B	601	BLA	OB-C4B	3.71	1.30	1.23
2	B	601	BLA	CBC-CAC	3.64	1.48	1.30
2	C	901	BLA	OB-C4B	3.62	1.30	1.23
2	C	901	BLA	CHD-C1D	3.54	1.48	1.40
2	C	901	BLA	C3D-C2D	3.54	1.44	1.36
2	A	901	BLA	CHD-C1D	3.50	1.48	1.40
2	B	601	BLA	CHD-C1D	3.48	1.48	1.40
2	A	901	BLA	O1D-CGD	3.45	1.33	1.22
2	B	601	BLA	C1B-C2B	3.43	1.51	1.45
2	C	901	BLA	CBC-CAC	3.43	1.47	1.30
2	A	901	BLA	C1C-C2C	-3.38	1.38	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	BLA	C3D-C2D	3.35	1.43	1.36
2	B	601	BLA	C3D-C2D	3.32	1.43	1.36
2	A	901	BLA	C3C-C4C	-3.26	1.40	1.45
2	B	601	BLA	C3C-C4C	-3.24	1.40	1.45
2	C	901	BLA	C1B-C2B	3.18	1.50	1.45
2	A	901	BLA	OB-C4B	3.13	1.29	1.23
2	C	901	BLA	C3C-C4C	-3.12	1.40	1.45
2	B	601	BLA	C1C-C2C	-2.90	1.39	1.47
2	C	901	BLA	OC-C1C	2.88	1.29	1.23
2	A	901	BLA	OC-C1C	2.84	1.29	1.23
2	C	901	BLA	C1C-C2C	-2.78	1.40	1.47
2	B	601	BLA	OC-C1C	2.76	1.28	1.23
2	A	901	BLA	C1B-C2B	2.63	1.49	1.45
2	C	901	BLA	C4D-C3D	-2.48	1.41	1.45
4	C	902	ASC	C4-C3	2.47	1.53	1.50
2	A	901	BLA	O1A-CGA	2.46	1.30	1.22
2	B	601	BLA	O1A-CGA	2.32	1.29	1.22
2	B	601	BLA	O2A-CGA	-2.31	1.23	1.30
2	C	901	BLA	O1A-CGA	2.28	1.29	1.22
2	C	901	BLA	CAD-C3D	-2.23	1.45	1.51
2	B	601	BLA	CAA-C2A	-2.17	1.48	1.52
2	A	901	BLA	O2A-CGA	-2.15	1.23	1.30
2	C	901	BLA	CAA-CBA	-2.04	1.42	1.52
2	A	901	BLA	CAA-CBA	-2.02	1.42	1.52
2	C	901	BLA	C1A-CHA	2.01	1.48	1.41

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BLA	CAD-CBD-CGD	21.21	159.24	113.60
2	A	901	BLA	CAD-CBD-CGD	19.29	155.12	113.60
2	C	901	BLA	CAD-CBD-CGD	17.36	150.97	113.60
2	C	901	BLA	C3B-C4B-NB	9.56	117.00	106.19
2	A	901	BLA	C3B-C4B-NB	9.12	116.50	106.19
2	B	601	BLA	C3B-C4B-NB	8.42	115.71	106.19
2	C	901	BLA	CBD-CAD-C3D	7.04	132.19	112.63
2	C	901	BLA	C1B-NB-C4B	-6.84	101.96	110.67
2	A	901	BLA	C1B-NB-C4B	-6.56	102.31	110.67
2	C	901	BLA	C4C-NC-C1C	-6.45	102.45	110.67
2	A	901	BLA	C4C-NC-C1C	-6.26	102.69	110.67
2	B	601	BLA	C4C-NC-C1C	-6.20	102.77	110.67
2	A	901	BLA	C2B-C1B-NB	6.13	115.97	106.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	901	BLA	C2B-C1B-NB	5.99	115.75	106.99
3	C	903	SO4	O4-S-O3	-5.74	84.56	109.06
3	A	903	SO4	O4-S-O3	-5.72	84.64	109.06
3	B	602	SO4	O4-S-O3	-5.67	84.87	109.06
2	B	601	BLA	C1B-NB-C4B	-5.48	103.69	110.67
2	B	601	BLA	C2B-C1B-NB	5.29	114.73	106.99
3	B	604	SO4	O4-S-O3	-5.14	87.13	109.06
2	A	901	BLA	C3B-C2B-C1B	-4.95	102.05	108.03
2	C	901	BLA	C1A-CHA-C4D	-4.88	122.97	128.81
2	B	601	BLA	CBD-CAD-C3D	4.85	126.11	112.63
2	C	901	BLA	C3C-C4C-NC	4.84	114.36	106.80
2	B	601	BLA	CMB-C2B-C1B	4.82	130.19	124.17
3	B	603	SO4	O3-S-O1	-4.79	84.29	109.31
2	B	601	BLA	C3C-C4C-NC	4.78	114.27	106.80
2	B	601	BLA	C1A-CHA-C4D	-4.67	123.23	128.81
2	B	601	BLA	C3B-C2B-C1B	-4.61	102.46	108.03
2	C	901	BLA	C3B-C2B-C1B	-4.54	102.54	108.03
2	A	901	BLA	CBD-CAD-C3D	4.45	124.99	112.63
2	A	901	BLA	C3C-C4C-NC	4.36	113.61	106.80
2	C	901	BLA	CMB-C2B-C1B	4.32	129.56	124.17
2	A	901	BLA	CAD-C3D-C4D	4.15	132.35	125.01
3	B	604	SO4	O4-S-O2	-4.10	87.89	109.31
2	C	901	BLA	C4B-C3B-C2B	-4.04	102.74	107.92
2	A	901	BLA	CMB-C2B-C1B	3.90	129.04	124.17
3	B	602	SO4	O4-S-O2	-3.90	88.95	109.31
2	B	601	BLA	C2C-C1C-NC	3.90	116.87	106.45
2	C	901	BLA	CAA-CBA-CGA	3.89	124.67	113.76
3	B	603	SO4	O4-S-O1	-3.87	89.10	109.31
3	C	903	SO4	O3-S-O2	3.85	129.40	109.31
3	A	903	SO4	O4-S-O1	-3.83	89.34	109.31
3	A	902	SO4	O3-S-O1	-3.82	89.36	109.31
3	A	903	SO4	O4-S-O2	-3.78	89.56	109.31
2	C	901	BLA	C2C-C1C-NC	3.78	116.56	106.45
3	B	602	SO4	O4-S-O1	-3.77	89.64	109.31
2	B	601	BLA	CHD-C4C-NC	-3.76	117.98	126.06
2	A	901	BLA	C2C-C1C-NC	3.72	116.41	106.45
2	A	901	BLA	C4B-C3B-C2B	-3.70	103.18	107.92
3	A	902	SO4	O4-S-O1	-3.65	90.24	109.31
2	A	901	BLA	CHA-C4D-ND	-3.62	123.80	128.83
2	B	601	BLA	C4B-C3B-C2B	-3.52	103.40	107.92
4	C	902	ASC	C4-O4-C1	-3.51	105.29	109.25
3	A	902	SO4	O2-S-O1	-3.47	83.79	109.43

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	BLA	CBC-CAC-C3C	-3.43	110.55	127.62
4	C	902	ASC	O3-C3-C2	-3.42	123.29	132.29
2	B	601	BLA	CMC-C2C-C1C	3.40	129.39	121.39
2	B	601	BLA	CAD-C3D-C4D	3.35	130.93	125.01
2	A	901	BLA	CAD-C3D-C2D	-3.35	121.65	127.88
2	A	901	BLA	OB-C4B-C3B	-3.25	122.10	129.46
2	B	601	BLA	CHA-C4D-ND	-3.20	124.38	128.83
2	C	901	BLA	OB-C4B-C3B	-3.17	122.27	129.46
3	B	604	SO4	O4-S-O1	-3.15	92.84	109.31
3	B	603	SO4	O2-S-O1	-3.08	86.70	109.43
3	C	903	SO4	O4-S-O1	-3.05	93.39	109.31
2	A	901	BLA	CBC-CAC-C3C	-3.01	112.64	127.62
3	C	903	SO4	O4-S-O2	-3.00	93.67	109.31
2	A	901	BLA	CBB-CAB-C3B	-2.98	112.78	127.62
2	C	901	BLA	C1D-C2D-C3D	-2.95	103.12	106.51
2	B	601	BLA	OB-C4B-C3B	-2.95	122.78	129.46
2	B	601	BLA	CBA-CAA-C2A	2.94	117.64	112.62
4	C	902	ASC	O3-C3-C4	2.90	125.65	118.08
4	C	902	ASC	O1-C1-C2	-2.88	124.86	129.37
2	C	901	BLA	CBB-CAB-C3B	-2.87	113.34	127.62
2	A	901	BLA	CHB-C1B-C2B	-2.85	121.34	126.97
3	B	603	SO4	O4-S-O3	2.77	120.90	109.06
2	B	601	BLA	OC-C1C-NC	-2.77	118.63	125.08
2	C	901	BLA	CHB-C1B-NB	-2.71	121.30	130.40
3	B	602	SO4	O3-S-O2	2.70	123.39	109.31
2	B	601	BLA	CBB-CAB-C3B	-2.69	114.23	127.62
2	C	901	BLA	CHA-C4D-ND	-2.68	125.11	128.83
2	B	601	BLA	CAD-C3D-C2D	-2.65	122.94	127.88
2	B	601	BLA	CHB-C1B-NB	-2.64	121.54	130.40
3	A	903	SO4	O3-S-O1	2.62	122.98	109.31
2	C	901	BLA	CMA-C3A-C2A	2.60	129.84	124.94
2	C	901	BLA	CAD-C3D-C2D	-2.52	123.19	127.88
2	A	901	BLA	CMC-C2C-C1C	2.49	127.25	121.39
4	C	902	ASC	O4-C1-O1	2.43	124.12	121.25
3	A	902	SO4	O4-S-O3	2.38	119.22	109.06
2	C	901	BLA	CAD-C3D-C4D	2.37	129.21	125.01
2	C	901	BLA	CMC-C2C-C1C	2.35	126.93	121.39
3	B	604	SO4	O3-S-O2	2.35	121.58	109.31
3	A	902	SO4	O3-S-O2	2.33	121.46	109.31
3	B	603	SO4	O3-S-O2	2.32	121.43	109.31
3	A	903	SO4	O3-S-O2	2.32	121.41	109.31
2	B	601	BLA	C1D-C2D-C3D	-2.30	103.87	106.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	BLA	CHB-C1B-NB	-2.30	122.69	130.40
2	B	601	BLA	C2D-C1D-ND	2.24	115.32	110.53
3	B	604	SO4	O3-S-O1	2.24	120.98	109.31
2	A	901	BLA	CBA-CAA-C2A	2.21	116.38	112.62
2	C	901	BLA	CBC-CAC-C3C	-2.18	116.79	127.62
2	B	601	BLA	CMA-C3A-C2A	2.17	129.04	124.94
2	A	901	BLA	C1A-CHA-C4D	-2.15	126.24	128.81
2	B	601	BLA	CAA-C2A-C3A	2.15	133.41	127.25
2	A	901	BLA	CMA-C3A-C2A	2.08	128.87	124.94
4	C	902	ASC	C6-C5-C4	2.08	115.44	111.86
2	A	901	BLA	CMD-C2D-C1D	2.08	128.26	125.06
2	C	901	BLA	CHB-C1B-C2B	-2.04	122.93	126.97
2	B	601	BLA	CHD-C1D-ND	-2.04	120.67	124.93
2	A	901	BLA	C2D-C1D-ND	2.03	114.87	110.53
2	A	901	BLA	C1D-C2D-C3D	-2.03	104.18	106.51
3	B	602	SO4	O3-S-O1	2.03	119.89	109.31

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	BLA	NA-C4A-CHB-C1B
2	A	901	BLA	C3A-C4A-CHB-C1B
2	A	901	BLA	C2C-C3C-CAC-CBC
2	A	901	BLA	C4C-C3C-CAC-CBC
2	A	901	BLA	C2D-C3D-CAD-CBD
2	A	901	BLA	C4D-C3D-CAD-CBD
2	B	601	BLA	NA-C4A-CHB-C1B
2	B	601	BLA	C3A-C4A-CHB-C1B
2	B	601	BLA	C2C-C3C-CAC-CBC
2	B	601	BLA	C4C-C3C-CAC-CBC
2	B	601	BLA	ND-C1D-CHD-C4C
2	B	601	BLA	C2D-C1D-CHD-C4C
2	C	901	BLA	CAD-CBD-CGD-O2D
2	C	901	BLA	CAD-CBD-CGD-O1D
2	B	601	BLA	CAA-CBA-CGA-O2A
2	B	601	BLA	CAA-CBA-CGA-O1A
2	A	901	BLA	CAA-CBA-CGA-O2A
2	A	901	BLA	CAD-CBD-CGD-O1D
2	C	901	BLA	ND-C4D-CHA-C1A
2	A	901	BLA	CAA-CBA-CGA-O1A
2	A	901	BLA	CAD-CBD-CGD-O2D

*Continued on next page...*

*Continued from previous page...*

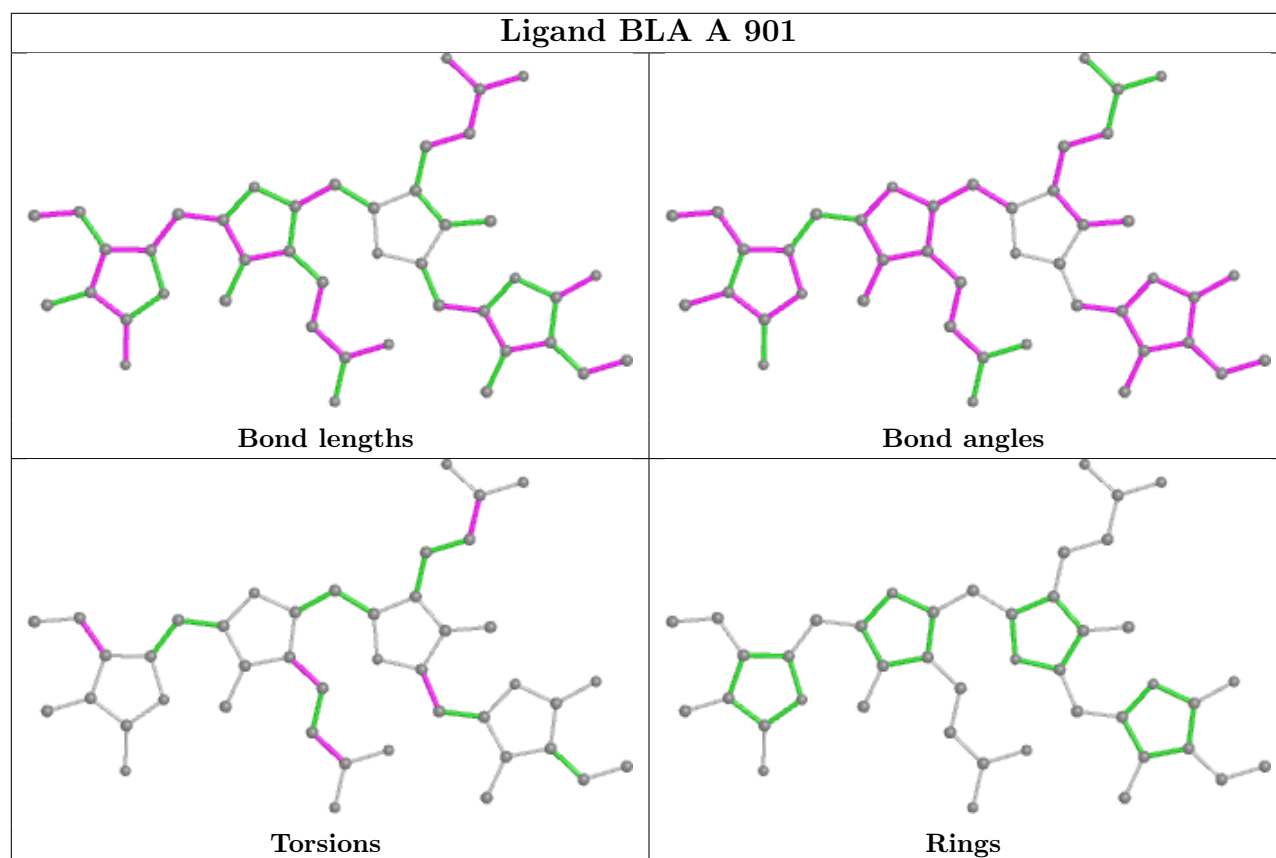
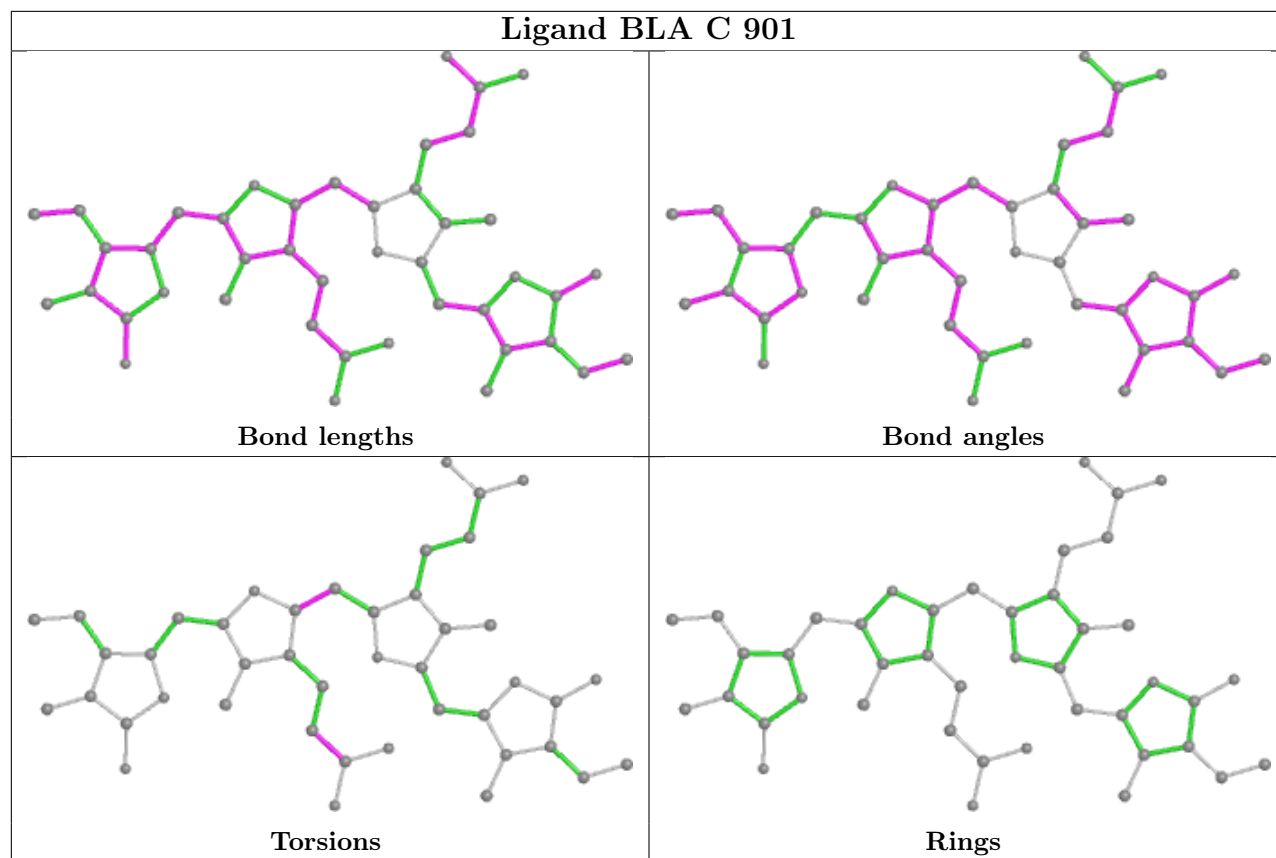
Mol	Chain	Res	Type	Atoms
2	B	601	BLA	CAD-CBD-CGD-O2D

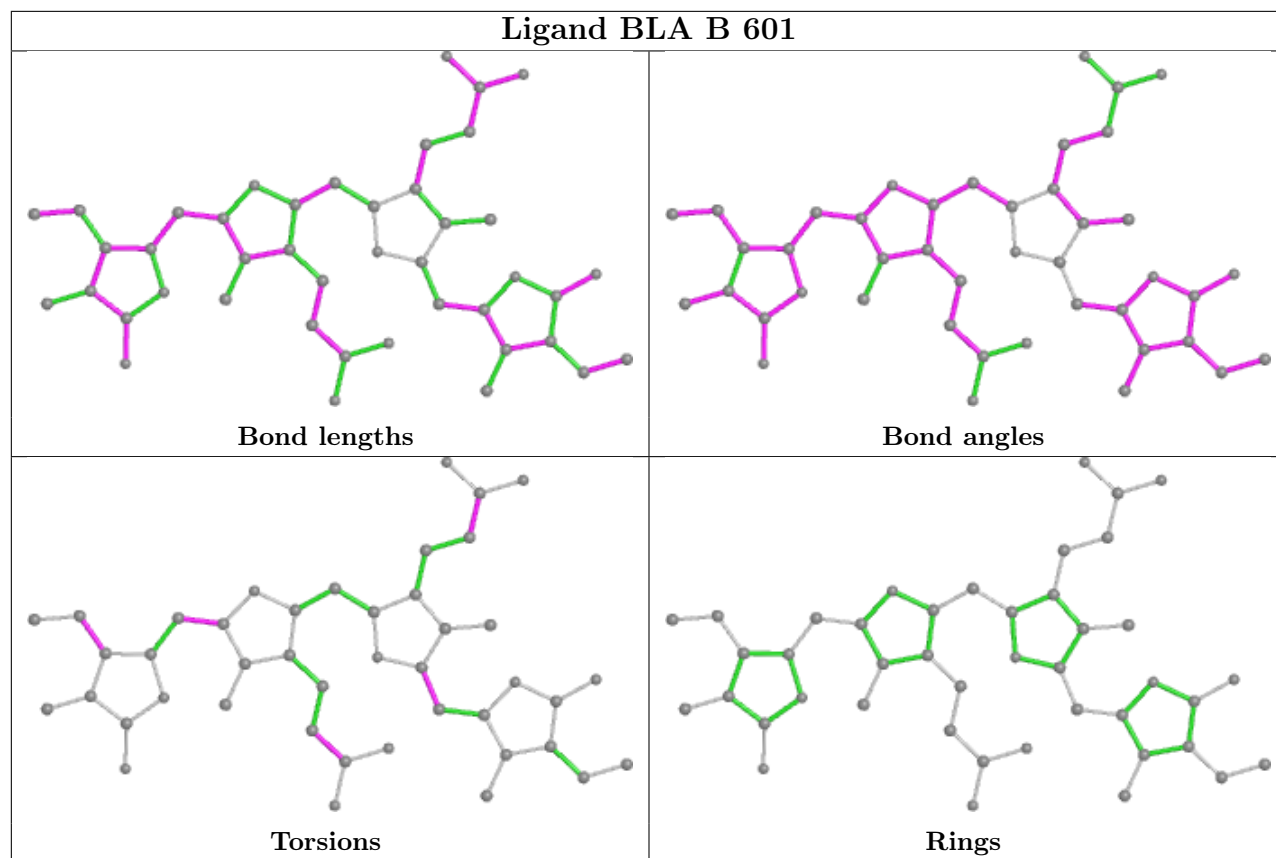
There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	BLA	2	0
3	C	903	SO4	2	0
2	A	901	BLA	9	0
2	B	601	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	212/215 (98%)	0.05	10 (4%) 31 30	17, 28, 43, 54	0
1	B	211/215 (98%)	-0.16	3 (1%) 75 76	12, 21, 36, 50	0
1	C	208/215 (96%)	-0.16	6 (2%) 51 50	13, 22, 35, 41	0
All	All	631/645 (97%)	-0.09	19 (3%) 50 48	12, 24, 39, 54	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	9.8
1	A	215	LEU	7.5
1	A	4	ALA	6.8
1	A	6	ALA	5.7
1	C	606	ALA	3.8
1	A	5	THR	3.4
1	A	92	GLY	2.9
1	A	18	GLN	2.8
1	A	167	ALA	2.8
1	A	94	SER	2.8
1	C	636	ARG	2.8
1	C	618	GLN	2.7
1	B	306	ALA	2.7
1	B	325	HIS	2.4
1	C	767	ALA	2.2
1	A	213	LYS	2.2
1	C	765	GLY	2.2
1	C	625	HIS	2.1
1	B	464[A]	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

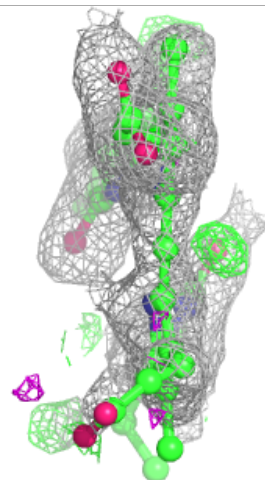
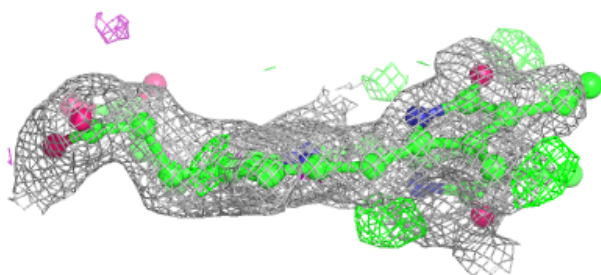
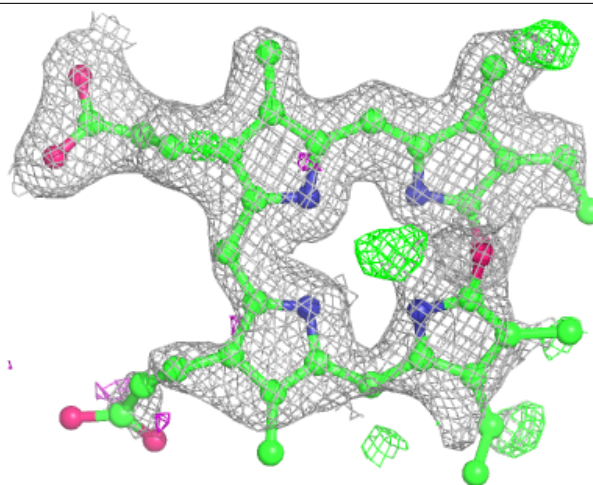
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	B	601	43/43	0.83	0.17	25,40,73,94	0
4	ASC	C	902	12/12	0.90	0.12	29,32,37,42	0
2	BLA	A	901	43/43	0.91	0.13	27,44,70,74	0
3	SO4	C	903	5/5	0.93	0.22	20,21,39,40	0
3	SO4	B	602	5/5	0.94	0.30	49,51,52,53	0
3	SO4	B	603	5/5	0.94	0.14	70,70,70,70	0
2	BLA	C	901	43/43	0.94	0.11	19,26,35,43	0
3	SO4	A	902	5/5	0.94	0.20	46,48,51,51	0
3	SO4	A	903	5/5	0.97	0.26	54,55,55,56	0
3	SO4	B	604	5/5	0.97	0.17	55,55,55,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around BLA B 601:**

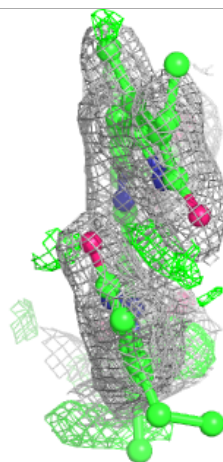
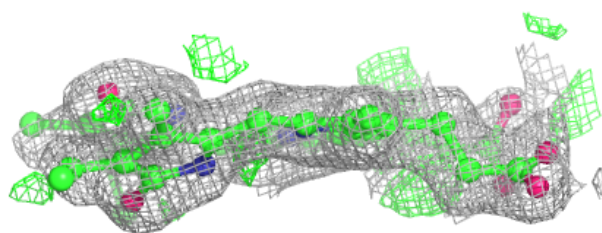
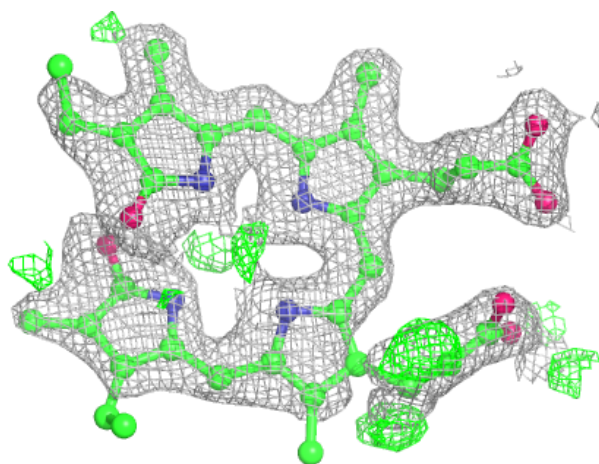
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

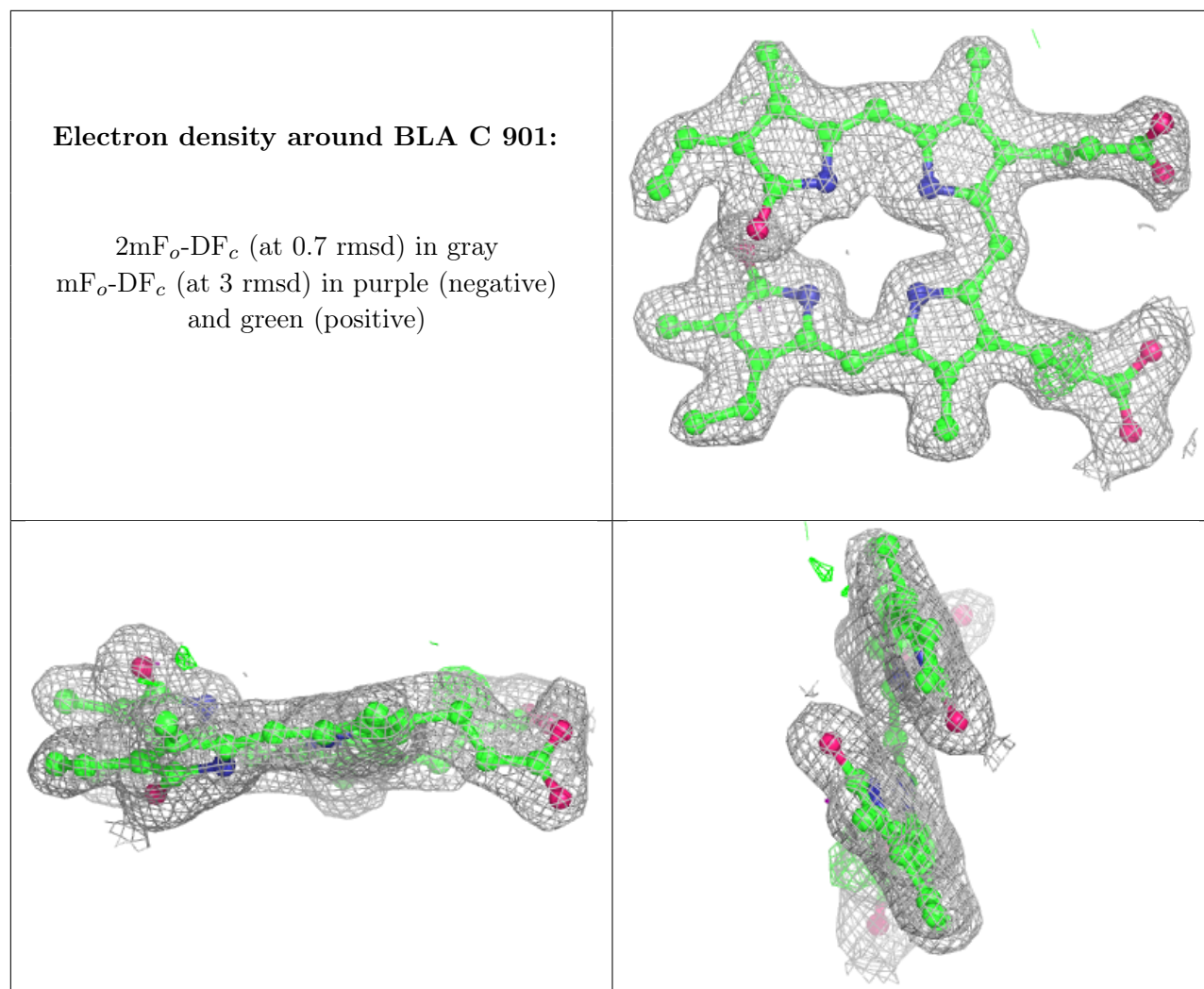




**Electron density around BLA A 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.