



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 07:00 AM EDT

PDB ID : 3KVS  
Title : The high resolution structure of C-Phycocyanin from *Galdieria Sulphuraria*  
Authors : Fromme, R.; Thangaraj, B.; Vanselow, C.; Fromme, P.  
Deposited on : 2009-11-30  
Resolution : 1.50 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 : 2.35  
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) : 2.35

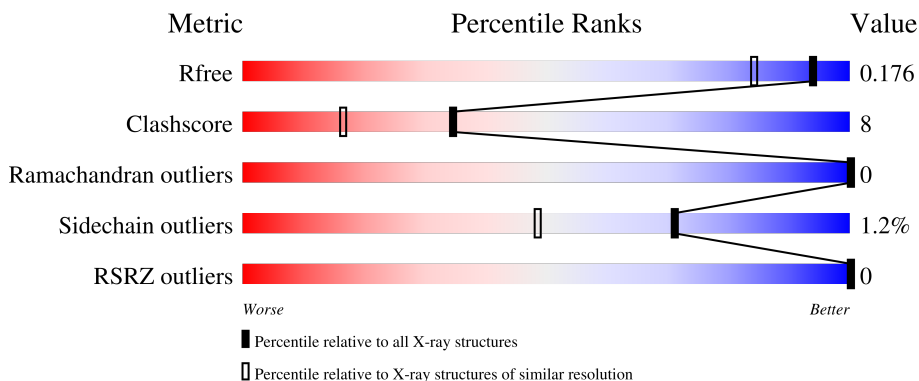
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

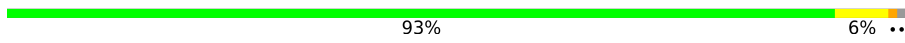

The reported resolution of this entry is 1.50 Å.

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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	162	 93% 6% ..
2	B	172	 90% 9% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3378 atoms, of which 137 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 C-phycoerythrin alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	161	1354	787	93	218	251	5	0	13	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLN	GLU	SEE REMARK 999	UNP P00306
A	136	VAL	ILE	SEE REMARK 999	UNP P00306
A	138	SER	ALA	SEE REMARK 999	UNP P00306

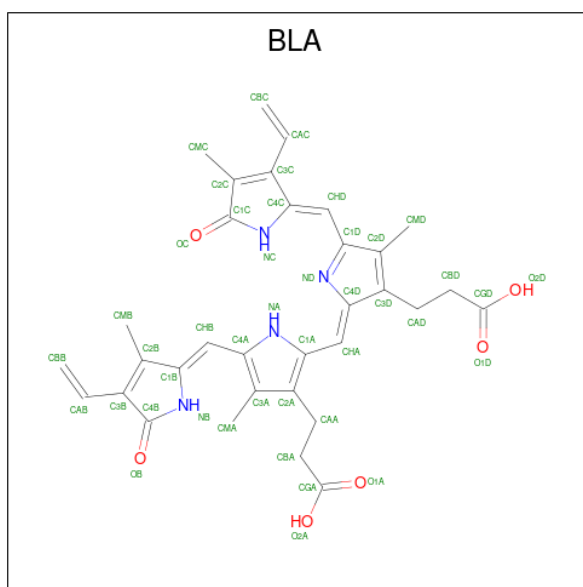
- Molecule 2 is a protein called C-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	170	1335	795	44	228	260	8	0	11	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	104	VAL	ILE	SEE REMARK 999	UNP P00311
B	131	VAL	ILE	SEE REMARK 999	UNP P00311

- Molecule 3 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: C<sub>33</sub>H<sub>34</sub>N<sub>4</sub>O<sub>6</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	0
			279	279		
4	B	281	Total	O	0	0
			281	281		

### 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: C-phycoerythrin alpha chain

Chain A:  93% 6% ..



- Molecule 2: C-phycoerythrin beta chain

Chain B:  90% 9% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.30Å 105.30Å 174.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.99 – 1.50 38.99 – 1.50	Depositor EDS
% Data completeness (in resolution range)	87.1 (38.99-1.50) 87.1 (38.99-1.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.62 (at 1.50Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.131 , 0.175 0.137 , 0.176	Depositor DCC
$R_{free}$ test set	2633 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.0	Xtrriage
Anisotropy	0.278	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.91% 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: BLA, MEN

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	0.62	2/1355 (0.1%)	0.56	1/1839 (0.1%)
2	B	0.38	0/1334	0.49	0/1805
All	All	0.52	2/2689 (0.1%)	0.52	1/3644 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	TYR	CE2-CZ	-6.74	1.29	1.38
1	A	116	GLU	CG-CD	6.00	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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	1261	93	1172	7	0
2	B	1291	44	1244	21	0
3	A	43	0	32	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	86	0	64	21	0
4	A	279	0	0	1	0
4	B	281	0	0	8	0
All	All	3241	137	2512	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 8.

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)
2:B:153:CYS:SG	3:B:555:BLA:HAC	1.59	1.43
1:A:75:ALA:HB1	1:A:81[B]:LYS:HD3	1.46	0.97
1:A:84:CYS:SG	3:A:484:BLA:HAC	2.11	0.89
3:B:584:BLA:HMD2	3:B:584:BLA:HC	1.42	0.84
3:A:484:BLA:HMD2	3:A:484:BLA:HC	1.47	0.80
2:B:30:MET:CE	4:B:328:HOH:O	2.33	0.77
2:B:153:CYS:CB	3:B:555:BLA:HAC	2.19	0.71
2:B:30:MET:SD	4:B:328:HOH:O	2.52	0.68
2:B:82:CYS:SG	3:B:584:BLA:CBC	2.85	0.65
1:A:137:LYS:HG3	1:A:154:ILE:HG21	1.80	0.63
2:B:78:ARG:NH2	4:B:425:HOH:O	2.32	0.63
2:B:88:ILE:HG21	3:B:584:BLA:HAB	1.81	0.62
2:B:153:CYS:SG	3:B:555:BLA:C4C	2.89	0.60
1:A:84:CYS:SG	3:A:484:BLA:CBC	2.91	0.58
2:B:65:GLN:HG2	4:B:542:HOH:O	2.02	0.58
3:B:584:BLA:HC	3:B:584:BLA:CMD	2.15	0.57
2:B:68:GLN:HG3	4:B:281:HOH:O	2.05	0.56
1:A:84:CYS:SG	3:A:484:BLA:C3C	2.94	0.56
2:B:82:CYS:SG	3:B:584:BLA:C3C	2.95	0.55
3:B:584:BLA:HMC1	3:B:584:BLA:HBC1	1.88	0.55
2:B:72:MEN:HE22	3:B:584:BLA:HBD2	1.89	0.54
3:B:555:BLA:HMD2	3:B:555:BLA:NC	2.21	0.54
3:B:555:BLA:HMD2	3:B:555:BLA:HC	1.74	0.51
2:B:153:CYS:SG	3:B:555:BLA:C3C	2.94	0.50
3:A:484:BLA:HMD2	3:A:484:BLA:NC	2.22	0.49
3:B:584:BLA:HHA	3:B:584:BLA:O1A	2.13	0.49
1:A:118:ILE:HD12	1:A:118:ILE:N	2.29	0.48
2:B:82:CYS:SG	3:B:584:BLA:HAC	2.48	0.47
3:B:555:BLA:HB	3:B:555:BLA:HMA1	1.79	0.47
2:B:62[A]:GLU:HG3	4:B:299:HOH:O	2.15	0.46

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLU:HG3	4:A:362:HOH:O	2.17	0.45
3:B:555:BLA:HMA1	3:B:555:BLA:NB	2.31	0.44
2:B:30:MET:HE2	4:B:328:HOH:O	2.06	0.43
2:B:36:LYS:HE2	3:B:555:BLA:HMD3	2.00	0.43
3:A:484:BLA:HC	3:A:484:BLA:CMD	2.26	0.43
2:B:95:TYR:O	2:B:98[A]:ILE:HG22	2.19	0.43
2:B:151:GLY:HA3	3:B:555:BLA:CMD	2.49	0.42
2:B:30:MET:HB3	4:B:328:HOH:O	2.20	0.42
2:B:158:ALA:O	2:B:162:THR:HG23	2.20	0.41
3:B:584:BLA:HMD2	3:B:584:BLA:NC	2.23	0.41
3:B:555:BLA:HB	3:B:555:BLA:CMA	2.33	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	173/162 (107%)	171 (99%)	2 (1%)	0	100	100
2	B	178/172 (104%)	175 (98%)	3 (2%)	0	100	100
All	All	351/334 (105%)	346 (99%)	5 (1%)	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	137/125 (110%)	135 (98%)	2 (2%)	65	39
2	B	139/132 (105%)	138 (99%)	1 (1%)	84	69
All	All	276/257 (107%)	273 (99%)	3 (1%)	71	53

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	50	ARG
2	B	91	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	MEN	B	72	2	7,8,9	1.27	1 (14%)	6,9,11	1.18	1 (16%)

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	MEN	B	72	2	-	2/7/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	72	MEN	CG-ND2	2.55	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	MEN	CB-CG-ND2	2.65	119.05	115.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	72	MEN	CA-CB-CG-ND2
2	B	72	MEN	CA-CB-CG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	72	MEN	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 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	$\# Z  > 2$
3	BLA	B	584	2	42,46,46	5.69	29 (69%)	53,67,67	3.36	24 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BLA	B	555	2	42,46,46	5.71	30 (71%)	53,67,67	3.51	24 (45%)
3	BLA	A	484	1	42,46,46	5.40	29 (69%)	53,67,67	3.36	28 (52%)

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
3	BLA	B	584	2	-	12/26/74/74	0/4/4/4
3	BLA	B	555	2	-	12/26/74/74	0/4/4/4
3	BLA	A	484	1	-	10/26/74/74	0/4/4/4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	584	BLA	CHA-C4D	20.99	1.52	1.35
3	B	555	BLA	CHA-C4D	20.83	1.52	1.35
3	A	484	BLA	CHA-C4D	19.40	1.51	1.35
3	B	584	BLA	CHB-C1B	9.11	1.53	1.34
3	B	584	BLA	OB-C4B	8.90	1.40	1.23
3	B	555	BLA	CHB-C1B	8.79	1.52	1.34
3	B	555	BLA	OB-C4B	8.77	1.40	1.23
3	B	555	BLA	C4C-NC	8.62	1.52	1.37
3	A	484	BLA	C4C-NC	8.43	1.51	1.37
3	A	484	BLA	OB-C4B	8.31	1.39	1.23
3	B	555	BLA	OC-C1C	8.29	1.39	1.23
3	A	484	BLA	CHB-C1B	8.26	1.51	1.34
3	B	584	BLA	C4C-NC	8.14	1.51	1.37
3	B	584	BLA	OC-C1C	8.01	1.38	1.23
3	A	484	BLA	OC-C1C	7.75	1.38	1.23
3	B	584	BLA	C3C-C2C	7.15	1.51	1.37
3	B	584	BLA	C3B-C2B	7.13	1.51	1.37
3	B	584	BLA	C1B-NB	7.10	1.49	1.37
3	B	555	BLA	C1D-ND	7.10	1.52	1.36
3	A	484	BLA	C3C-C2C	7.08	1.51	1.37
3	B	555	BLA	C1B-NB	7.08	1.49	1.37
3	B	555	BLA	C3C-C2C	7.03	1.51	1.37
3	B	555	BLA	C3B-C2B	6.84	1.51	1.37
3	A	484	BLA	C1B-NB	6.82	1.49	1.37
3	A	484	BLA	C3D-C2D	6.78	1.51	1.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	584	BLA	C1D-ND	6.68	1.51	1.36
3	B	584	BLA	C3D-C2D	6.64	1.50	1.36
3	A	484	BLA	C3B-C2B	6.55	1.50	1.37
3	A	484	BLA	C1D-ND	6.43	1.51	1.36
3	B	555	BLA	C3D-C2D	6.38	1.50	1.36
3	A	484	BLA	C1C-NC	6.28	1.51	1.38
3	B	555	BLA	CHD-C4C	6.12	1.52	1.38
3	B	555	BLA	C1C-NC	5.98	1.50	1.38
3	B	584	BLA	C1C-NC	5.85	1.50	1.38
3	B	584	BLA	CHD-C4C	5.83	1.51	1.38
3	B	555	BLA	C4D-ND	5.82	1.51	1.38
3	B	584	BLA	CHD-C1D	5.80	1.54	1.40
3	B	555	BLA	CHD-C1D	5.69	1.53	1.40
3	B	584	BLA	C4D-ND	5.69	1.50	1.38
3	B	555	BLA	O1D-CGD	5.57	1.40	1.22
3	B	584	BLA	O1A-CGA	5.55	1.40	1.22
3	A	484	BLA	CHD-C4C	5.54	1.51	1.38
3	B	584	BLA	O1D-CGD	5.52	1.40	1.22
3	B	555	BLA	O1A-CGA	5.42	1.40	1.22
3	A	484	BLA	CHD-C1D	5.41	1.53	1.40
3	A	484	BLA	O1D-CGD	5.34	1.39	1.22
3	A	484	BLA	C4D-ND	5.24	1.49	1.38
3	A	484	BLA	O1A-CGA	5.17	1.39	1.22
3	B	584	BLA	C4B-NB	4.86	1.48	1.38
3	A	484	BLA	C4B-NB	4.86	1.48	1.38
3	B	555	BLA	C4D-C3D	4.85	1.53	1.45
3	B	555	BLA	C4B-NB	4.82	1.48	1.38
3	B	555	BLA	C1D-C2D	4.78	1.56	1.45
3	A	484	BLA	C1D-C2D	4.71	1.56	1.45
3	B	584	BLA	C1D-C2D	4.48	1.55	1.45
3	B	584	BLA	C4D-C3D	4.48	1.52	1.45
3	B	584	BLA	C3C-C4C	4.46	1.53	1.45
3	A	484	BLA	C3C-C4C	4.41	1.52	1.45
3	B	555	BLA	C3C-C4C	4.25	1.52	1.45
3	B	584	BLA	C2A-C3A	4.20	1.50	1.37
3	A	484	BLA	C4D-C3D	4.16	1.52	1.45
3	B	555	BLA	C2A-C3A	4.09	1.49	1.37
3	B	555	BLA	C1B-C2B	3.85	1.52	1.45
3	A	484	BLA	C2A-C3A	3.77	1.48	1.37
3	B	584	BLA	C1B-C2B	3.71	1.51	1.45
3	B	584	BLA	O2D-CGD	-3.50	1.19	1.30
3	B	584	BLA	O2A-CGA	-3.47	1.19	1.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	555	BLA	O2D-CGD	-3.45	1.19	1.30
3	A	484	BLA	O2A-CGA	-3.38	1.19	1.30
3	B	555	BLA	O2A-CGA	-3.32	1.19	1.30
3	A	484	BLA	O2D-CGD	-3.27	1.19	1.30
3	B	555	BLA	C4A-CHB	3.16	1.53	1.41
3	B	555	BLA	CBC-CAC	3.11	1.45	1.30
3	A	484	BLA	C1B-C2B	3.09	1.50	1.45
3	B	584	BLA	C4A-CHB	2.95	1.52	1.41
3	B	584	BLA	C1A-CHA	2.81	1.52	1.41
3	B	555	BLA	C1A-CHA	2.74	1.51	1.41
3	A	484	BLA	C4A-CHB	2.62	1.51	1.41
3	A	484	BLA	C1A-CHA	2.51	1.50	1.41
3	A	484	BLA	CAC-C3C	2.46	1.54	1.47
3	B	555	BLA	CAB-C3B	2.41	1.54	1.47
3	B	584	BLA	CAB-C3B	2.40	1.54	1.47
3	B	584	BLA	C3B-C4B	2.31	1.54	1.47
3	A	484	BLA	CAB-C3B	2.25	1.53	1.47
3	B	584	BLA	CAC-C3C	2.22	1.53	1.47
3	B	555	BLA	C3B-C4B	2.20	1.54	1.47
3	B	555	BLA	C1C-C2C	2.09	1.53	1.47
3	A	484	BLA	C1C-C2C	2.01	1.53	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	484	BLA	C1A-CHA-C4D	-11.32	115.29	128.81
3	B	555	BLA	C1A-CHA-C4D	-11.22	115.40	128.81
3	B	584	BLA	C1A-CHA-C4D	-11.07	115.58	128.81
3	B	555	BLA	OB-C4B-C3B	-7.65	112.13	129.46
3	B	584	BLA	OB-C4B-C3B	-7.64	112.15	129.46
3	A	484	BLA	C4C-NC-C1C	-7.44	101.20	110.67
3	B	584	BLA	CHD-C4C-C3C	-6.97	109.94	127.91
3	A	484	BLA	CHD-C4C-C3C	-6.89	110.16	127.91
3	A	484	BLA	OB-C4B-C3B	-6.74	114.18	129.46
3	B	555	BLA	CAC-C3C-C4C	-6.39	105.02	123.54
3	B	555	BLA	CHD-C4C-NC	-6.34	112.44	126.06
3	B	555	BLA	C4C-CHD-C1D	-6.24	112.83	128.08
3	B	555	BLA	OC-C1C-NC	-6.17	110.74	125.08
3	B	555	BLA	CHD-C4C-C3C	-6.00	112.45	127.91
3	B	555	BLA	C4B-C3B-C2B	-5.98	100.25	107.92
3	B	584	BLA	OC-C1C-NC	-5.80	111.60	125.08
3	B	584	BLA	CHD-C4C-NC	-5.77	113.68	126.06

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	484	BLA	OB-C4B-NB	-5.66	111.91	125.08
3	A	484	BLA	CHB-C1B-C2B	-5.41	116.29	126.97
3	B	555	BLA	CHB-C1B-C2B	-5.37	116.36	126.97
3	B	584	BLA	C1B-NB-C4B	-5.32	103.89	110.67
3	A	484	BLA	C4B-C3B-C2B	-5.19	101.27	107.92
3	B	555	BLA	OB-C4B-NB	-5.11	113.20	125.08
3	B	584	BLA	CAB-C3B-C2B	-5.10	111.80	128.60
3	A	484	BLA	C3B-C2B-C1B	-4.92	102.08	108.03
3	B	584	BLA	OB-C4B-NB	-4.89	113.72	125.08
3	B	555	BLA	CAB-C3B-C2B	-4.86	112.60	128.60
3	B	584	BLA	CHB-C1B-C2B	-4.86	117.38	126.97
3	A	484	BLA	CHD-C4C-NC	-4.71	115.95	126.06
3	A	484	BLA	OC-C1C-NC	-4.63	114.31	125.08
3	B	555	BLA	C1B-NB-C4B	-4.29	105.21	110.67
3	B	555	BLA	C4C-NC-C1C	-4.22	105.30	110.67
3	B	584	BLA	C4C-CHD-C1D	-4.12	118.01	128.08
3	B	584	BLA	C4C-NC-C1C	-4.08	105.47	110.67
3	B	584	BLA	CMC-C2C-C3C	-3.94	118.66	128.30
3	A	484	BLA	CHD-C1D-C2D	3.83	134.75	124.90
3	A	484	BLA	CHD-C1D-ND	-3.83	116.93	124.93
3	B	584	BLA	C4B-C3B-C2B	-3.82	103.02	107.92
3	A	484	BLA	C4C-CHD-C1D	-3.69	119.06	128.08
3	B	555	BLA	CMC-C2C-C3C	-3.55	119.60	128.30
3	B	555	BLA	OC-C1C-C2C	-3.42	112.96	128.48
3	A	484	BLA	C1B-NB-C4B	-3.39	106.36	110.67
3	B	555	BLA	CMD-C2D-C1D	3.28	130.11	125.06
3	B	584	BLA	OC-C1C-C2C	-3.27	113.62	128.48
3	A	484	BLA	C3B-C4B-NB	-3.24	102.53	106.19
3	B	584	BLA	CHD-C1D-C2D	3.24	133.23	124.90
3	B	584	BLA	CMC-C2C-C1C	-3.13	114.03	121.39
3	B	584	BLA	CMD-C2D-C1D	3.03	129.73	125.06
3	A	484	BLA	CAB-C3B-C2B	-3.01	118.69	128.60
3	B	555	BLA	CHB-C1B-NB	-2.97	120.41	130.40
3	B	555	BLA	C3B-C4B-NB	-2.91	102.90	106.19
3	A	484	BLA	OC-C1C-C2C	-2.74	116.02	128.48
3	B	584	BLA	CHD-C1D-ND	-2.67	119.35	124.93
3	B	584	BLA	CAD-CBD-CGD	-2.66	107.89	113.60
3	A	484	BLA	CMC-C2C-C3C	-2.62	121.88	128.30
3	A	484	BLA	CMD-C2D-C1D	2.62	129.10	125.06
3	B	555	BLA	CAC-C3C-C2C	-2.55	120.20	128.60
3	B	584	BLA	CHB-C1B-NB	-2.54	121.85	130.40
3	B	584	BLA	CAC-C3C-C2C	-2.54	120.23	128.60

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	584	BLA	CBD-CAD-C3D	-2.50	105.69	112.63
3	A	484	BLA	CBD-CAD-C3D	-2.47	105.76	112.63
3	B	584	BLA	CMB-C2B-C3B	-2.43	122.35	128.30
3	A	484	BLA	C4C-C3C-C2C	-2.39	99.40	107.09
3	B	555	BLA	CMB-C2B-C3B	-2.38	122.47	128.30
3	A	484	BLA	CHA-C4D-C3D	-2.36	119.86	125.32
3	A	484	BLA	CAD-C3D-C4D	-2.30	120.94	125.01
3	B	555	BLA	CMB-C2B-C1B	-2.28	121.32	124.17
3	A	484	BLA	O2A-CGA-CBA	2.24	121.21	114.03
3	A	484	BLA	CBB-CAB-C3B	-2.21	116.64	127.62
3	A	484	BLA	O2D-CGD-CBD	2.19	121.06	114.03
3	A	484	BLA	CMC-C2C-C1C	-2.18	116.26	121.39
3	B	555	BLA	CHA-C4D-C3D	-2.16	120.33	125.32
3	A	484	BLA	CHB-C1B-NB	-2.09	123.37	130.40
3	B	584	BLA	CMB-C2B-C1B	-2.09	121.55	124.17
3	B	555	BLA	CBA-CAA-C2A	-2.04	109.13	112.62
3	B	555	BLA	O2A-CGA-O1A	-2.02	118.27	123.30

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	484	BLA	NA-C4A-CHB-C1B
3	A	484	BLA	C3A-C4A-CHB-C1B
3	A	484	BLA	NB-C1B-CHB-C4A
3	A	484	BLA	C4B-C3B-CAB-CBB
3	A	484	BLA	C2D-C1D-CHD-C4C
3	B	555	BLA	C3A-C4A-CHB-C1B
3	B	555	BLA	NB-C1B-CHB-C4A
3	B	555	BLA	C4C-C3C-CAC-CBC
3	B	584	BLA	NA-C1A-CHA-C4D
3	B	584	BLA	C2A-C1A-CHA-C4D
3	B	584	BLA	NA-C4A-CHB-C1B
3	B	584	BLA	C3A-C4A-CHB-C1B
3	B	584	BLA	NC-C4C-CHD-C1D
3	A	484	BLA	NC-C4C-CHD-C1D
3	B	555	BLA	NC-C4C-CHD-C1D
3	B	584	BLA	C2D-C1D-CHD-C4C
3	A	484	BLA	ND-C1D-CHD-C4C
3	B	555	BLA	ND-C1D-CHD-C4C
3	B	584	BLA	ND-C1D-CHD-C4C
3	B	555	BLA	C2D-C1D-CHD-C4C

*Continued on next page...*



*Continued from previous page...*

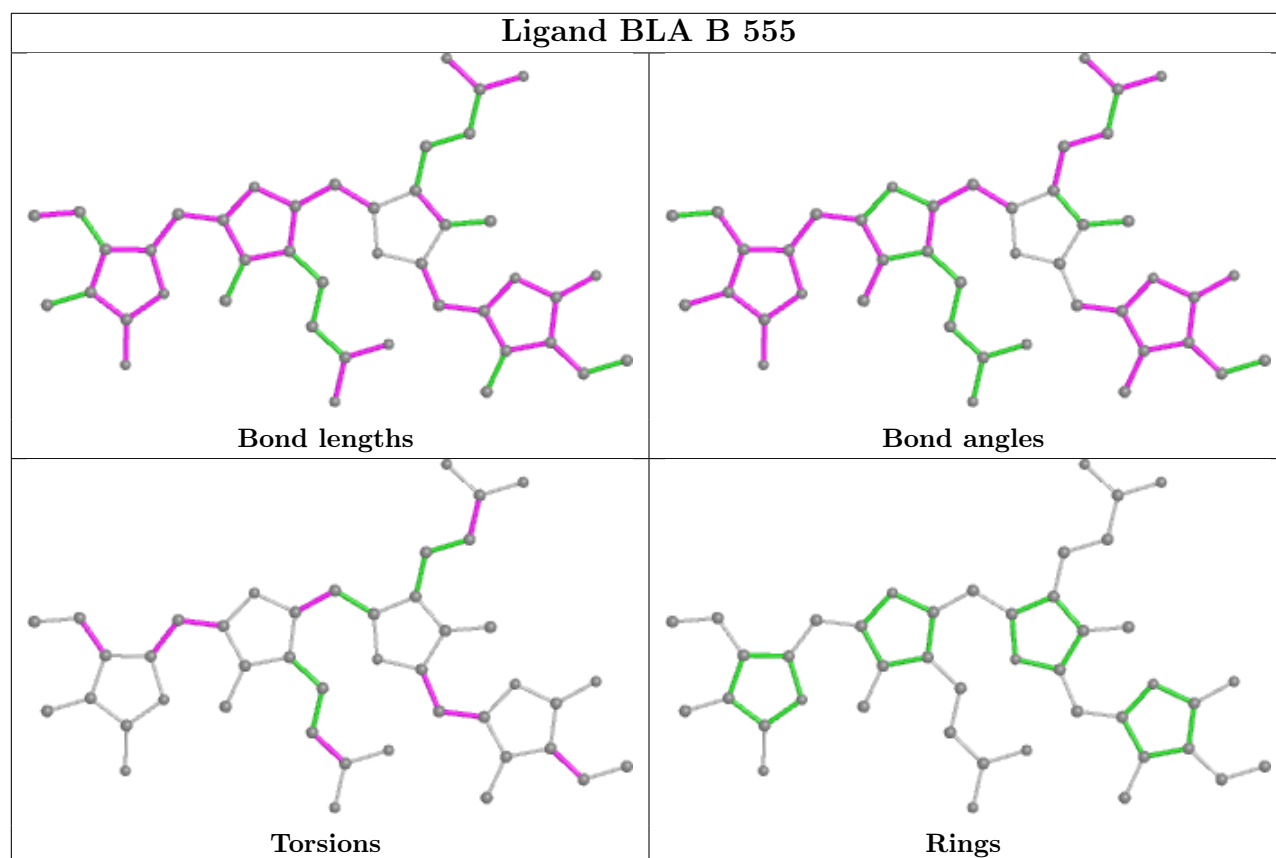
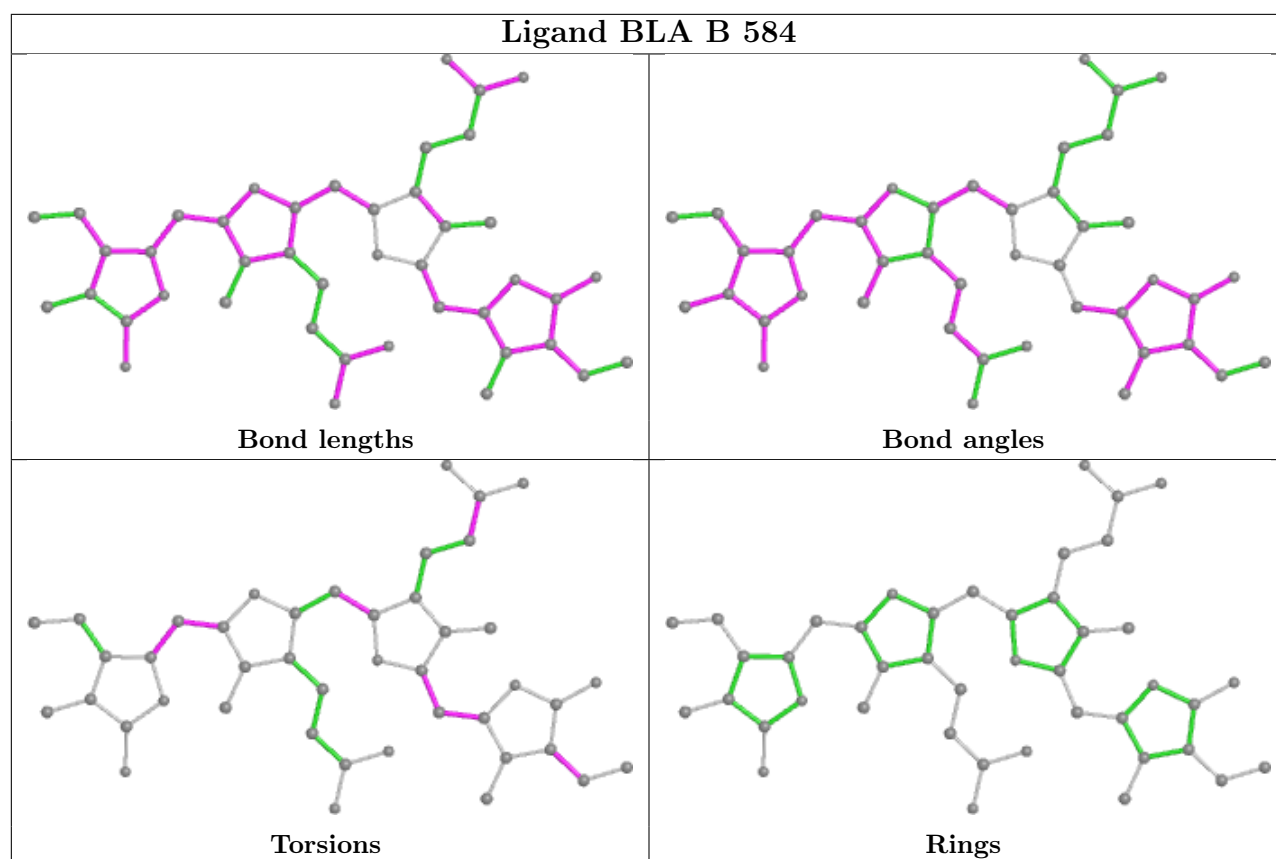
Mol	Chain	Res	Type	Atoms
3	B	584	BLA	C4B-C3B-CAB-CBB
3	A	484	BLA	C2C-C3C-CAC-CBC
3	B	555	BLA	C2B-C3B-CAB-CBB
3	B	584	BLA	C2B-C3B-CAB-CBB
3	B	555	BLA	ND-C4D-CHA-C1A
3	B	584	BLA	NB-C1B-CHB-C4A
3	B	555	BLA	C4B-C3B-CAB-CBB
3	B	555	BLA	CAA-CBA-CGA-O2A
3	B	555	BLA	CAA-CBA-CGA-O1A
3	A	484	BLA	CAA-CBA-CGA-O1A
3	A	484	BLA	CAA-CBA-CGA-O2A
3	B	584	BLA	CAA-CBA-CGA-O2A
3	B	584	BLA	CAA-CBA-CGA-O1A
3	B	555	BLA	CAD-CBD-CGD-O1D

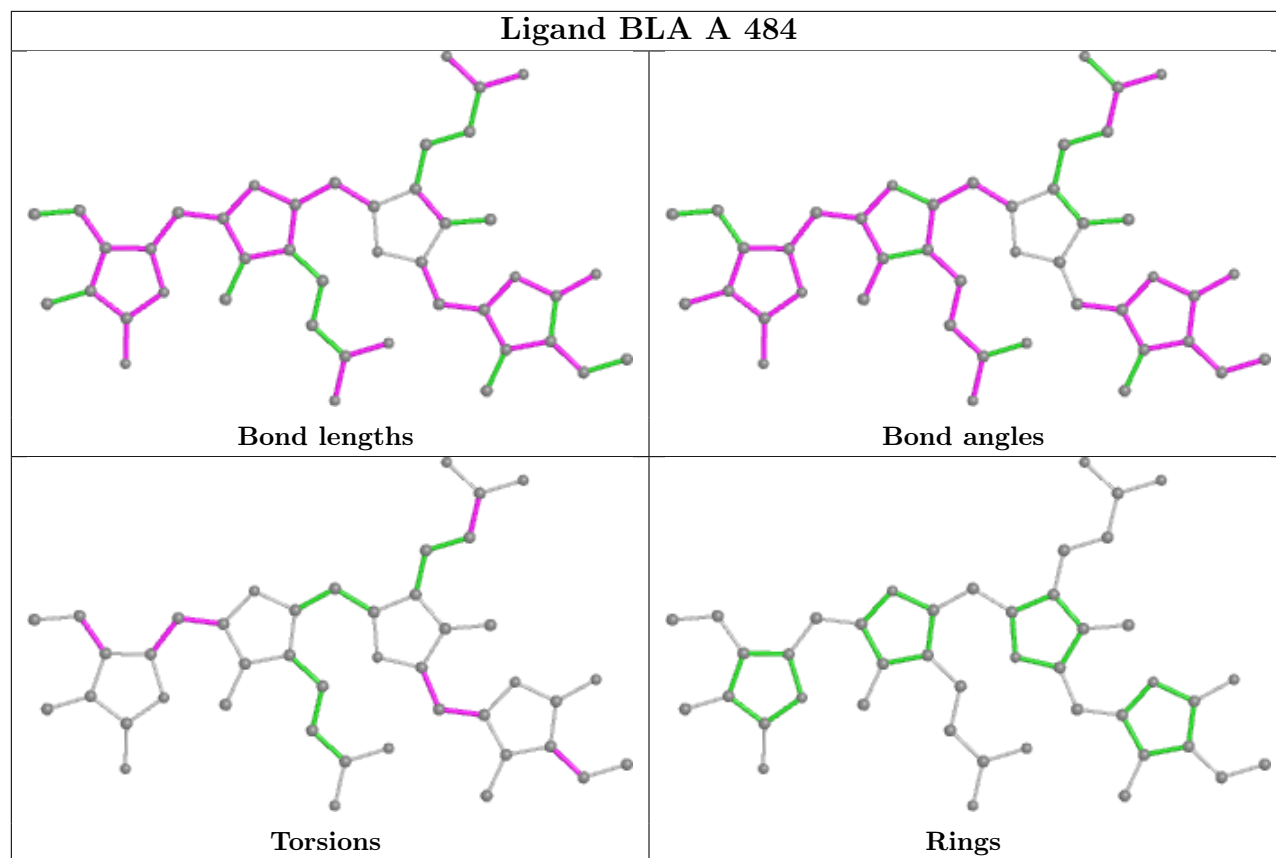
There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	584	BLA	10	0
3	B	555	BLA	11	0
3	A	484	BLA	6	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	161/162 (99%)	-0.66	0 100 100	6, 11, 19, 27	0
2	B	169/172 (98%)	-0.58	0 100 100	7, 13, 23, 31	0
All	All	330/334 (98%)	-0.62	0 100 100	6, 12, 21, 31	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
2	MEN	B	72	9/10	0.98	0.04	10,11,15,15	0

### 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.

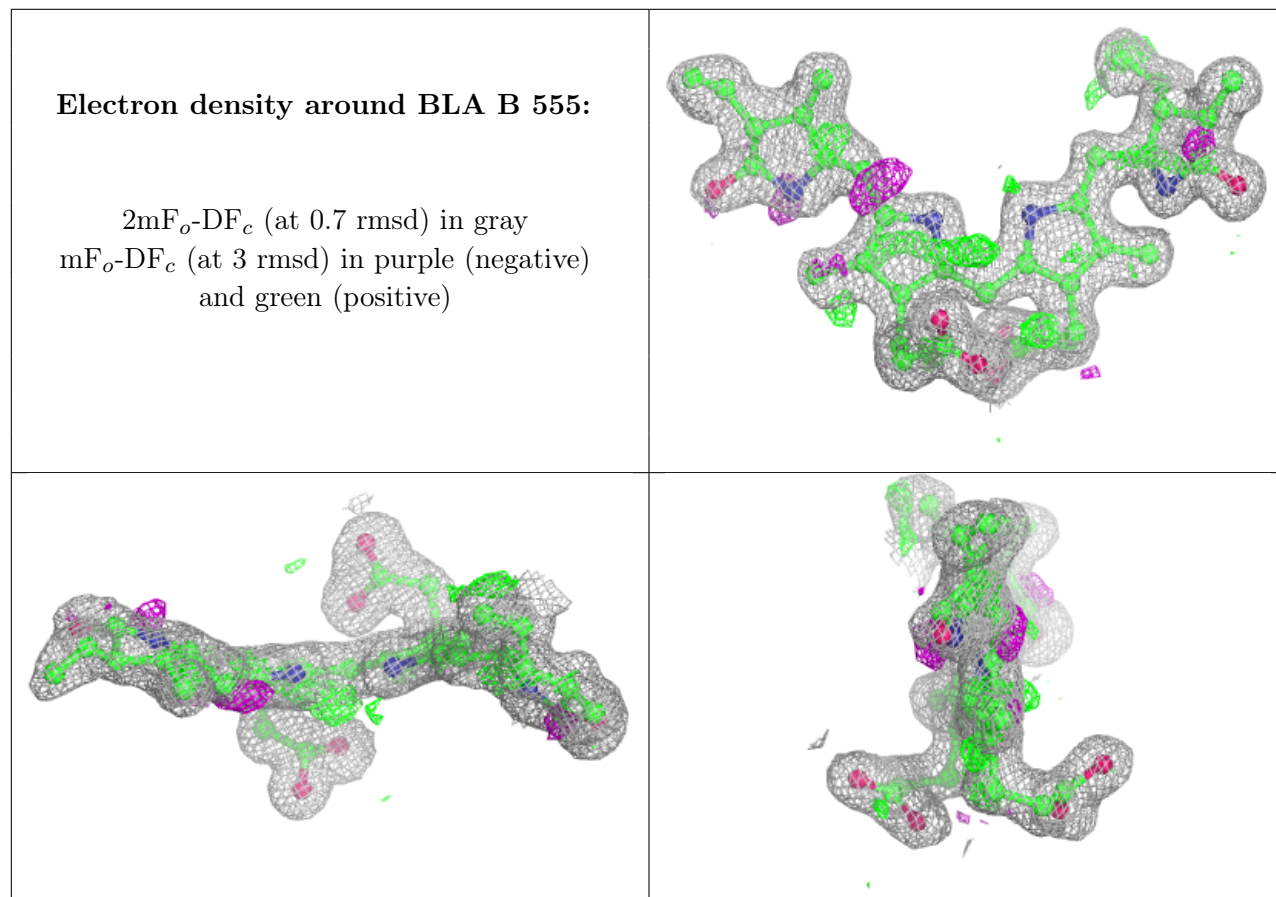
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	BLA	B	555	43/43	0.92	0.09	12,16,23,26	0

*Continued on next page...*

Continued from previous page...

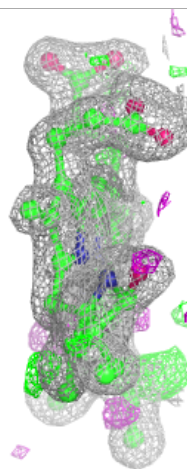
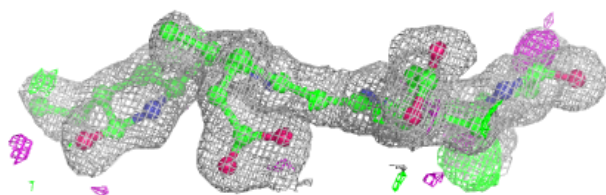
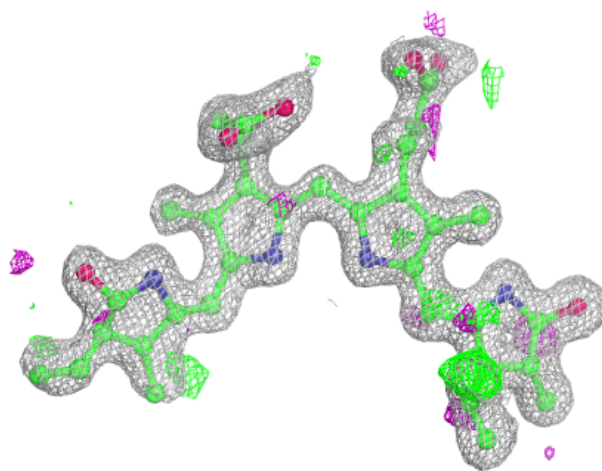
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BLA	B	584	43/43	0.92	0.12	8,18,28,31	0
3	BLA	A	484	43/43	0.96	0.08	6,9,12,13	0

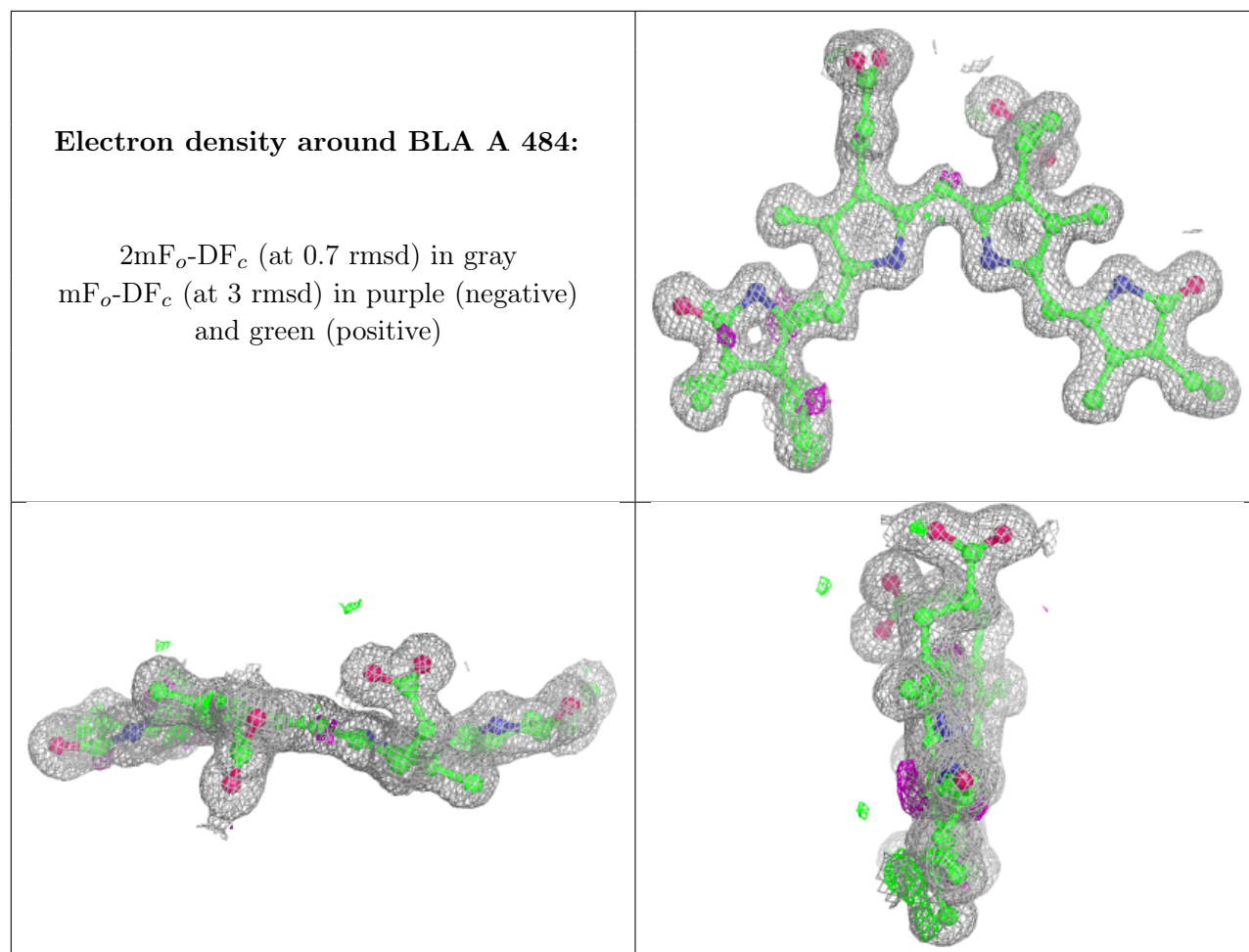
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



**Electron density around BLA B 584:**

$2mF_o-DF_c$  (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.