



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:24 AM EDT

PDB ID : 1ZTU
Title : Structure of the chromophore binding domain of bacterial phytochrome
Authors : Wagner, J.R.; Brunzelle, J.S.; Forest, K.T.; Vierstra, R.D.
Deposited on : 2005-05-27
Resolution : 2.50 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : 2.23.2
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) : 2.23.2

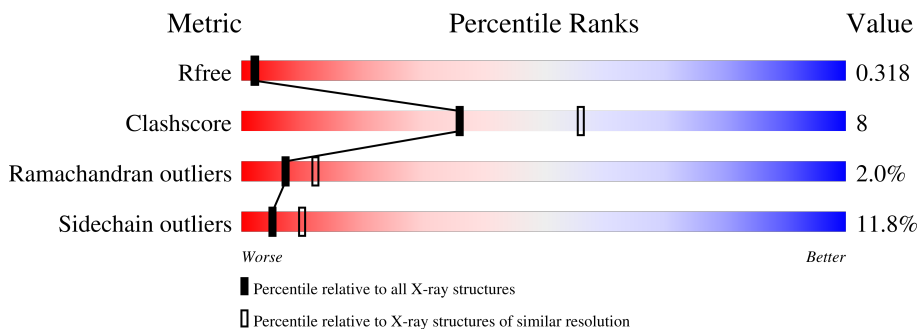
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	341	 70% 19% .. 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2485 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bacteriophytochrome.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	313	2408	1537	429	433	4	5	0	1	0

There are 27 discrepancies between the modelled and reference sequences:

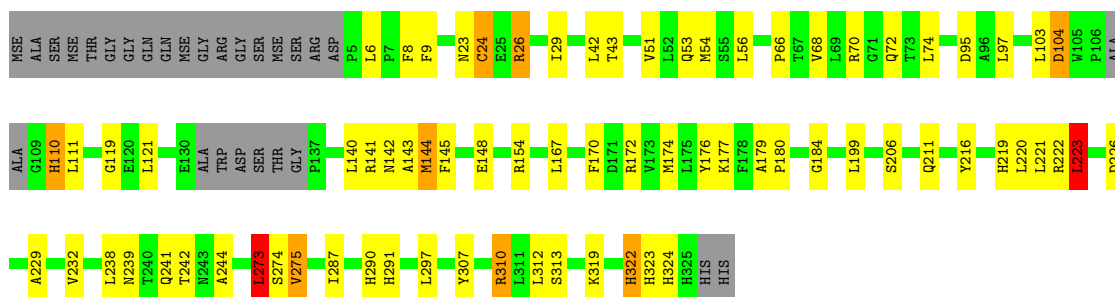
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MSE	-	cloning artifact	UNP Q9RZA4
A	-12	ALA	-	cloning artifact	UNP Q9RZA4
A	-11	SER	-	cloning artifact	UNP Q9RZA4
A	-10	MSE	-	cloning artifact	UNP Q9RZA4
A	-9	THR	-	cloning artifact	UNP Q9RZA4
A	-8	GLY	-	cloning artifact	UNP Q9RZA4
A	-7	GLY	-	cloning artifact	UNP Q9RZA4
A	-6	GLN	-	cloning artifact	UNP Q9RZA4
A	-5	GLN	-	cloning artifact	UNP Q9RZA4
A	-4	MSE	-	cloning artifact	UNP Q9RZA4
A	-3	GLY	-	cloning artifact	UNP Q9RZA4
A	-2	ARG	-	cloning artifact	UNP Q9RZA4
A	-1	GLY	-	cloning artifact	UNP Q9RZA4
A	0	SER	-	cloning artifact	UNP Q9RZA4
A	1	MSE	MET	modified residue	UNP Q9RZA4
A	144	MSE	MET	modified residue	UNP Q9RZA4
A	174	MSE	MET	modified residue	UNP Q9RZA4
A	240	THR	PRO	engineered mutation	UNP Q9RZA4
A	259	MSE	MET	modified residue	UNP Q9RZA4
A	261	MSE	MET	modified residue	UNP Q9RZA4
A	267	MSE	MET	modified residue	UNP Q9RZA4
A	322	HIS	-	expression tag	UNP Q9RZA4
A	323	HIS	-	expression tag	UNP Q9RZA4
A	324	HIS	-	expression tag	UNP Q9RZA4
A	325	HIS	-	expression tag	UNP Q9RZA4
A	326	HIS	-	expression tag	UNP Q9RZA4
A	327	HIS	-	expression tag	UNP Q9RZA4

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. 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.

- Molecule 1: Bacteriophytochrome

Chain A:  70% 19% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.88Å 133.67Å 49.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.84 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.50) 97.0 (19.84-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.76 (at 2.50Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.266 0.288 , 0.318	Depositor DCC
R_{free} test set	752 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtrriage
Anisotropy	0.115	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2485	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.51	0/2472	0.73	4/3372 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	LEU	CA-CB-CG	7.19	131.84	115.30
1	A	273	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	221	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	24	CYS	N-CA-C	5.39	125.56	111.00

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	2408	0	2403	39	3
2	A	43	0	31	4	0
3	A	34	0	0	4	0
All	All	2485	0	2434	39	3

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 (39) 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:172:ARG:HD2	1:A:174:MSE:HE2	1.56	0.87
1:A:42:LEU:HD22	1:A:54:MET:HG3	1.61	0.80
1:A:8[B]:PHE:HE1	1:A:211:GLN:HB2	1.52	0.74
1:A:242:THR:HG23	1:A:244:ALA:H	1.54	0.72
1:A:275:VAL:HG13	1:A:287:ILE:HB	1.79	0.65
1:A:170:PHE:HD1	1:A:291:HIS:HB2	1.63	0.63
1:A:9:PHE:HE1	1:A:23:ASN:HB2	1.67	0.59
1:A:287:ILE:HD11	1:A:312:LEU:HD23	1.84	0.58
1:A:176:TYR:CZ	1:A:184:GLY:HA3	2.38	0.58
1:A:51:VAL:HG23	1:A:70:ARG:HA	1.85	0.58
1:A:145:PHE:HA	1:A:148:GLU:HB2	1.85	0.58
1:A:179:ALA:HB1	1:A:180:PRO:HD2	1.87	0.57
1:A:170:PHE:CD1	1:A:291:HIS:HB2	2.43	0.54
1:A:104:ASP:HB3	1:A:110:HIS:H	1.72	0.53
1:A:174:MSE:HE1	1:A:290:HIS:CE1	2.43	0.53
1:A:9:PHE:CE1	1:A:23:ASN:HB2	2.44	0.52
1:A:216:TYR:HA	3:A:361:HOH:O	2.11	0.50
1:A:274:SER:OG	2:A:328:BLA:HBA1	2.10	0.50
1:A:290:HIS:CE1	2:A:328:BLA:OB	2.65	0.50
1:A:322:HIS:CG	1:A:322:HIS:O	2.66	0.49
1:A:142:ASN:C	1:A:144:MSE:H	2.16	0.49
1:A:23:ASN:O	1:A:26:ARG:HG2	2.13	0.48
1:A:322:HIS:C	1:A:324:HIS:H	2.17	0.48
1:A:287:ILE:HD11	1:A:312:LEU:CD2	2.44	0.48
1:A:239:ASN:HB3	1:A:242:THR:HG22	1.96	0.47
1:A:42:LEU:CD2	1:A:54:MET:HG3	2.37	0.47
1:A:140:LEU:HD21	1:A:307:TYR:CE1	2.50	0.47
1:A:43:THR:OG1	1:A:53:GLN:HB2	2.16	0.46
1:A:310:ARG:HG3	3:A:360:HOH:O	2.16	0.45
1:A:219:HIS:C	3:A:361:HOH:O	2.54	0.45
1:A:274:SER:OG	2:A:328:BLA:CBA	2.65	0.44
1:A:9:PHE:CE1	1:A:26:ARG:HG3	2.53	0.44
1:A:239:ASN:OD1	1:A:241:GLN:HB2	2.18	0.44
1:A:223:LEU:HB3	1:A:273:LEU:HD22	2.00	0.43
1:A:29:ILE:HG21	2:A:328:BLA:HMD1	2.00	0.43
1:A:322:HIS:C	1:A:324:HIS:N	2.73	0.42
1:A:68:VAL:O	1:A:68:VAL:HG13	2.20	0.41
1:A:226:ASP:HB3	1:A:229:ALA:HB2	2.03	0.41
1:A:216:TYR:C	3:A:361:HOH:O	2.60	0.40

All (3) 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)
1:A:307:TYR:CD2	1:A:307:TYR:CE2[2_665]	1.86	0.34
1:A:307:TYR:CE2	1:A:307:TYR:CZ[2_665]	2.00	0.20
1:A:307:TYR:CD2	1:A:307:TYR:CZ[2_665]	2.14	0.06

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	308/341 (90%)	288 (94%)	14 (4%)	6 (2%)	8 13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	CYS
1	A	110	HIS
1	A	66	PRO
1	A	143	ALA
1	A	119	GLY
1	A	323	HIS

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	255/264 (97%)	225 (88%)	30 (12%)	5 10

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	26	ARG
1	A	56	LEU
1	A	72	GLN
1	A	74	LEU
1	A	95	ASP
1	A	97	LEU
1	A	103	LEU
1	A	104	ASP
1	A	111	LEU
1	A	121	LEU
1	A	141	ARG
1	A	144	MSE
1	A	154	ARG
1	A	167	LEU
1	A	177	LYS
1	A	199	LEU
1	A	206	SER
1	A	220	LEU
1	A	222	ARG
1	A	223	LEU
1	A	232	VAL
1	A	238	LEU
1	A	273	LEU
1	A	275	VAL
1	A	297	LEU
1	A	310	ARG
1	A	313	SER
1	A	319	LYS
1	A	322	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	290	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](#)

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	328	1	36,46,46	3.81	13 (36%)	47,67,67	2.61	23 (48%)

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	A	328	1	-	7/22/74/74	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	328	BLA	CHA-C4D	16.38	1.48	1.35
2	A	328	BLA	CHB-C1B	7.92	1.50	1.34
2	A	328	BLA	C3D-C2D	5.30	1.48	1.36
2	A	328	BLA	C3C-C2C	4.90	1.47	1.37
2	A	328	BLA	C3B-C2B	4.77	1.46	1.37
2	A	328	BLA	CBC-CAC	4.42	1.52	1.30
2	A	328	BLA	CHD-C4C	4.36	1.48	1.38
2	A	328	BLA	C2A-C3A	3.92	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	328	BLA	CHD-C1D	3.60	1.48	1.40
2	A	328	BLA	C1B-C2B	3.04	1.50	1.45
2	A	328	BLA	OC-C1C	2.53	1.28	1.23
2	A	328	BLA	C4A-CHB	2.48	1.50	1.41
2	A	328	BLA	OB-C4B	2.25	1.27	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	328	BLA	C3B-C4B-NB	7.26	114.39	106.19
2	A	328	BLA	C1A-CHA-C4D	5.15	134.97	128.81
2	A	328	BLA	C4C-NC-C1C	-5.13	104.14	110.67
2	A	328	BLA	C3C-C4C-NC	4.54	113.89	106.80
2	A	328	BLA	C4B-C3B-C2B	-4.22	102.51	107.92
2	A	328	BLA	CMC-C2C-C1C	3.90	130.55	121.39
2	A	328	BLA	C2C-C1C-NC	3.67	116.25	106.45
2	A	328	BLA	CAA-CBA-CGA	3.36	118.31	112.67
2	A	328	BLA	CMB-C2B-C1B	3.30	128.29	124.17
2	A	328	BLA	C4D-C3D-C2D	-3.22	103.22	106.78
2	A	328	BLA	OB-C4B-C3B	-3.03	122.58	129.46
2	A	328	BLA	C3D-C4D-ND	2.92	114.30	110.05
2	A	328	BLA	CAA-C2A-C3A	2.78	135.22	127.25
2	A	328	BLA	CHB-C1B-C2B	-2.72	121.61	126.97
2	A	328	BLA	C1D-C2D-C3D	-2.70	103.41	106.51
2	A	328	BLA	C1B-NB-C4B	-2.60	107.35	110.67
2	A	328	BLA	CHA-C4D-ND	-2.57	125.26	128.83
2	A	328	BLA	CAC-C3C-C4C	2.44	130.61	123.54
2	A	328	BLA	CBC-CAC-C3C	-2.40	115.68	127.62
2	A	328	BLA	C2B-C1B-NB	2.30	110.35	106.99
2	A	328	BLA	C3B-C2B-C1B	-2.18	105.39	108.03
2	A	328	BLA	CHA-C4D-C3D	-2.11	120.44	125.32
2	A	328	BLA	CHD-C4C-NC	-2.03	121.70	126.06

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	328	BLA	C1A-C2A-CAA-CBA
2	A	328	BLA	C3A-C2A-CAA-CBA
2	A	328	BLA	NA-C4A-CHB-C1B
2	A	328	BLA	C3A-C4A-CHB-C1B
2	A	328	BLA	C4C-C3C-CAC-CBC

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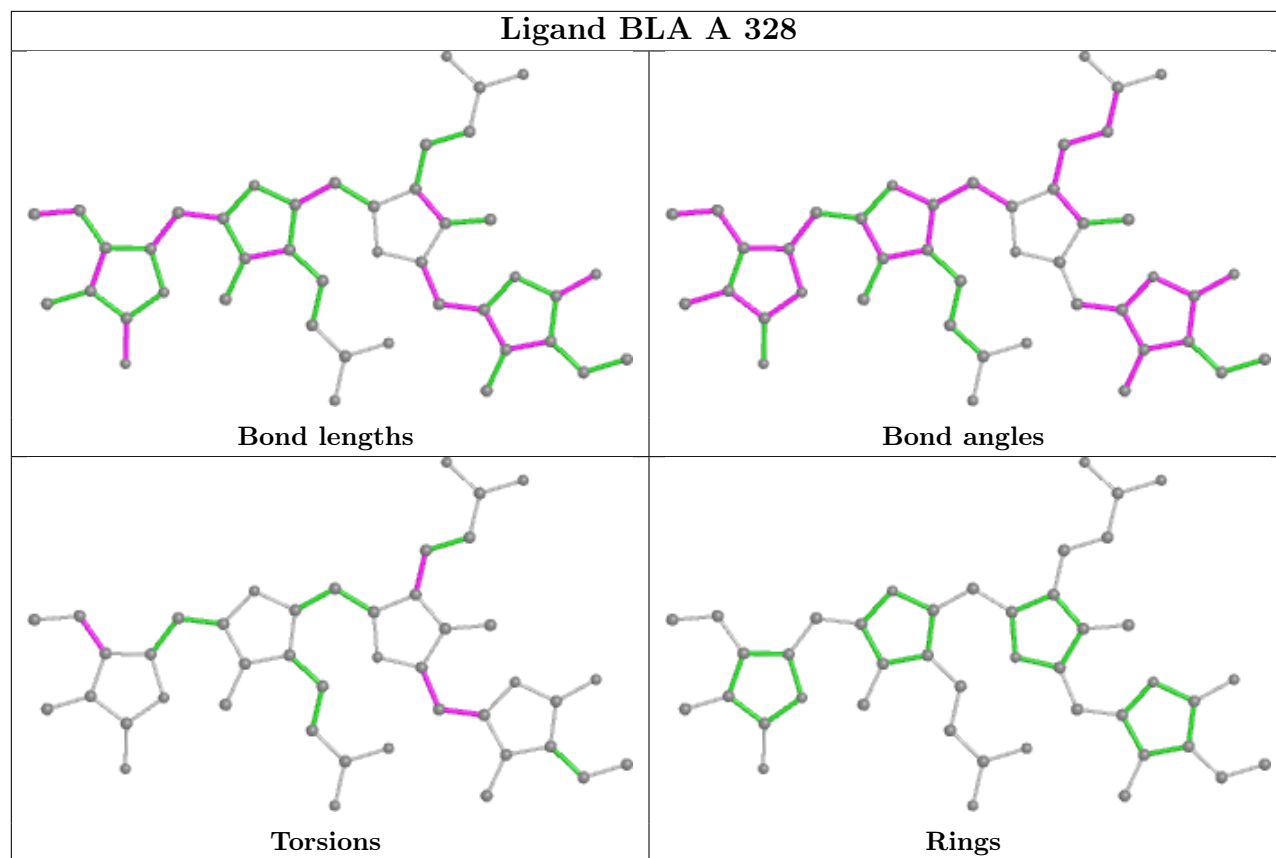
Mol	Chain	Res	Type	Atoms
2	A	328	BLA	C2C-C3C-CAC-CBC
2	A	328	BLA	NB-C1B-CHB-C4A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	328	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

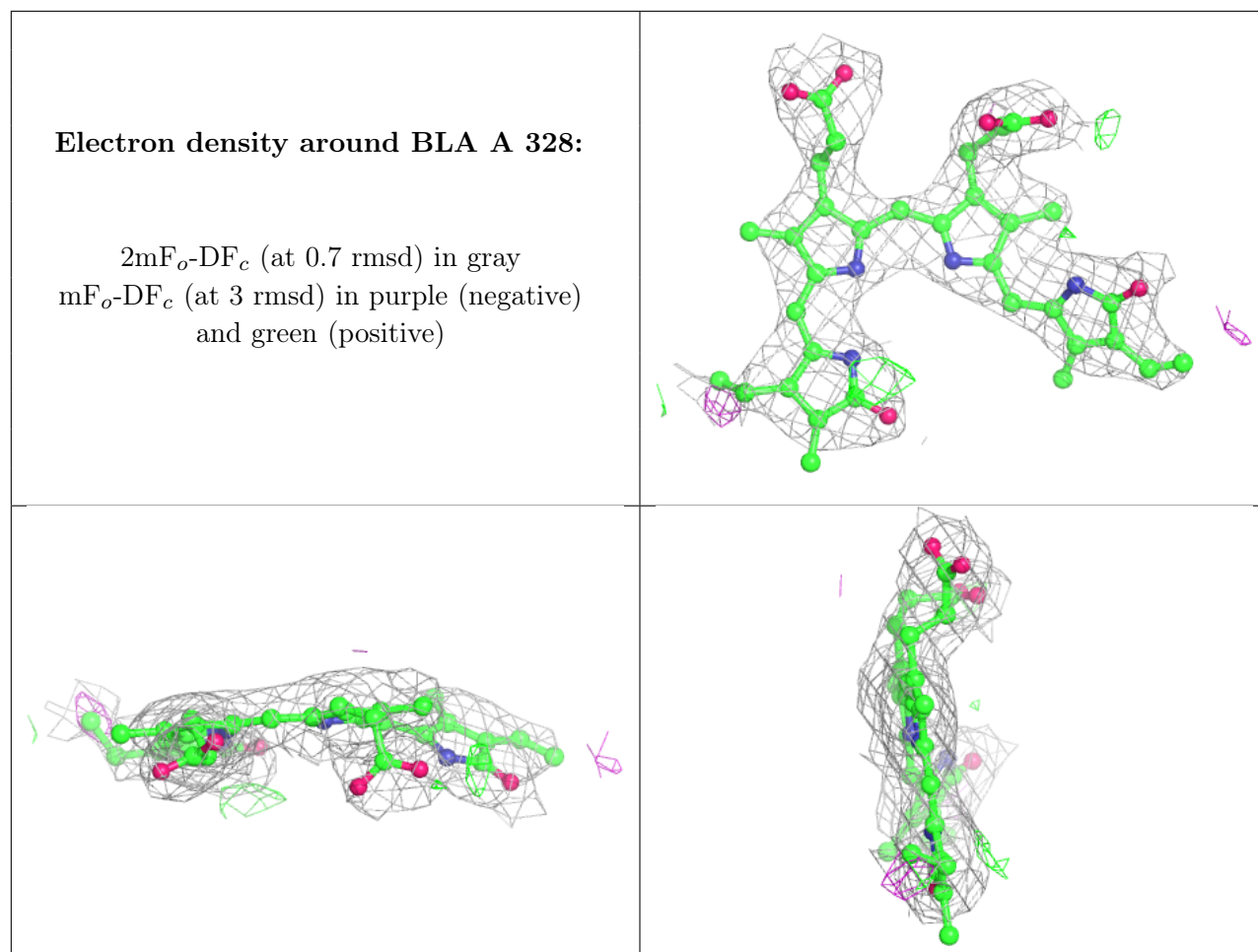
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.