



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 06:32 am BST

PDB ID : 4B1B
Title : Crystal structure of Plasmodium falciparum oxidised Thioredoxin Reductase at 2.9 angstrom
Authors : Boumis, G.; Giardina, G.; Dimastrogiovanni, D.; Angelucci, F.; Saccoccia, F.; Brunori, M.; Bellelli, A.; Miele, A.E.
Deposited on : 2012-07-09
Resolution : 2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	2.11
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)	:	2.11

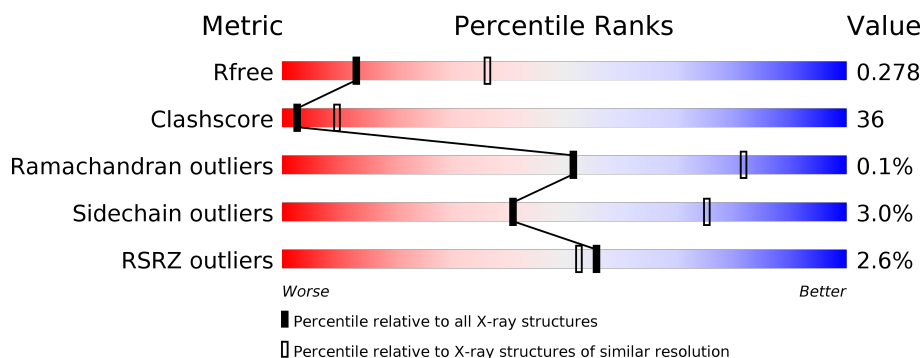
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	542	<div> <div>2%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	542	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>33%</div> <div>•</div> <div>19%</div> </div> </div>

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6887 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.

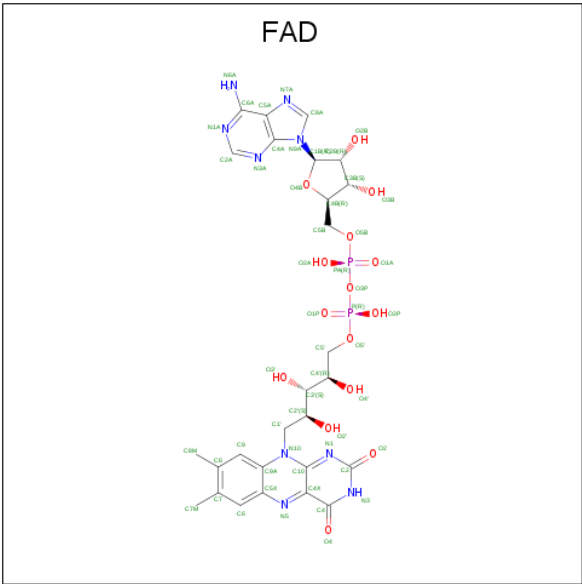
- Molecule 1 is a protein called THIOREDOXIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	1	0
			3389	2167	562	639	21			
1	B	437	Total	C	N	O	S	0	1	0
			3389	2167	562	639	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q25861
A	1	SER	-	expression tag	UNP Q25861
B	0	GLY	-	expression tag	UNP Q25861
B	1	SER	-	expression tag	UNP Q25861

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		

PRO	THR	ASP	ALA	GLU	SER	PHE	MET	ASN	LEU	PHE	VAL	THR	ILE	SER	SER	GLY	LEU	SER	TYR	ALA	GLY	GLY	CYS	GLY	GLY	LYS	CYS	GLY																									
LYS	HIS	ILE	ARG	ALA	GLN	LYS	ASP	GLU	TYR	ASP	VAL	ASP	VAL	SER	SER	GLY	LEU	SER	TYR	ALA	GLY	GLY	CYS	GLY	GLY	LYS	CYS	GLY																									
K371	E374	I375	R378	D383	S384	D385	E386	I387	K388	E389	Y390	Y391	Y392	I393	P394	T395	S396	I397	Y398	T399	P400	I401	E402	Y403	C406	G407	Y408	Y414	E415	L416	Y417	C418	K419	S420	N421	V422	E423	Y424	F425	L426	Q427	PHE	ASN	ASN	LEU	GLU	ILE	SER	ALA	VAL	HIS	ARG	GLN
D801	K302	T303	I306	Y307	D308	L311	I314	G318	E319	I320	L325	E326	S327	I328	N329	N330	N331	K334	S335	N336	N337	K338	I339	I340	A341	D342	H343	L344	S345	G346	T347	N348	I349	P350	S351	I352	P353	G356	D357	V358	A359	E360	N361	V362	P363	E364	I365	L366	P367	V368	A369	I370	
L189	G193	C194	I198	P199	D200	K206	T211	I215	K220	D221	V227	A230	C237	S238	G239	F240	L241	N242	S243	L244	V248	V252	R253	S254	I255	V256	L257	R258	Q262	V266	V277	I283	L284	P285	K286	K287	L288	D292	D293	K294	F299	S300											

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.19Å 109.24Å 182.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 2.90 46.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.91-2.90) 96.7 (46.91-2.90)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.265 , 0.288 0.259 , 0.278	Depositor DCC
R_{free} test set	1394 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	6887	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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: FAD

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	0.35	0/3455	0.36	0/4659
1	B	0.38	0/3455	0.41	2/4659 (0.0%)
All	All	0.36	0/6910	0.39	2/9318 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	479	GLY	C-N-CD	5.80	140.57	128.40
1	B	458	CYS	O-C-N	5.26	131.12	122.70

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	3389	0	3427	246	1
1	B	3389	0	3427	279	1
2	A	53	0	31	4	0
2	B	53	0	31	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	6887	0	6916	497	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 36.

The worst 5 of 497 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:B:489:MET:HE1	1:B:502:PHE:CZ	1.68	1.27
1:B:489:MET:CE	1:B:502:PHE:HZ	1.49	1.26
1:A:489:MET:CE	1:A:502:PHE:CZ	2.23	1.20
1:B:162:LYS:CE	1:B:172:TYR:HE1	1.56	1.17
1:B:492:ALA:HB1	1:B:497:VAL:HG21	1.22	1.16

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)
1:A:343:HIS:CG	1:B:38:HIS:CD2[3_544]	2.13	0.07

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	432/542 (80%)	399 (92%)	33 (8%)	0	100	100
1	B	432/542 (80%)	402 (93%)	29 (7%)	1 (0%)	47	78
All	All	864/1084 (80%)	801 (93%)	62 (7%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/457 (81%)	361 (97%)	10 (3%)	44	77
1	B	371/457 (81%)	359 (97%)	12 (3%)	39	73
All	All	742/914 (81%)	720 (97%)	22 (3%)	41	75

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	505	CYS
1	B	171	TYR
1	B	459	LEU
1	B	93	CYS
1	B	150	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	487	GLN
1	B	158	ASN
1	B	427	GLN
1	A	476	HIS
1	B	348	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	FAD	B	1506	-	51,58,58	1.34	6 (11%)	60,89,89	1.54	8 (13%)
2	FAD	A	1506	-	51,58,58	1.33	6 (11%)	60,89,89	1.53	7 (11%)

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	FAD	B	1506	-	-	8/30/50/50	0/6/6/6
2	FAD	A	1506	-	-	9/30/50/50	0/6/6/6

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1506	FAD	C10-N1	4.03	1.38	1.33
2	A	1506	FAD	C10-N1	3.98	1.38	1.33
2	B	1506	FAD	C2A-N3A	3.95	1.38	1.32
2	A	1506	FAD	C2A-N3A	3.94	1.38	1.32
2	B	1506	FAD	C4X-N5	3.63	1.38	1.33

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1506	FAD	C4-N3-C2	5.95	120.16	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1506	FAD	C4-N3-C2	5.93	120.15	115.14
2	A	1506	FAD	N3A-C2A-N1A	-5.52	120.06	128.68
2	B	1506	FAD	N3A-C2A-N1A	-5.42	120.20	128.68
2	B	1506	FAD	P-O3P-PA	-3.47	120.90	132.83

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

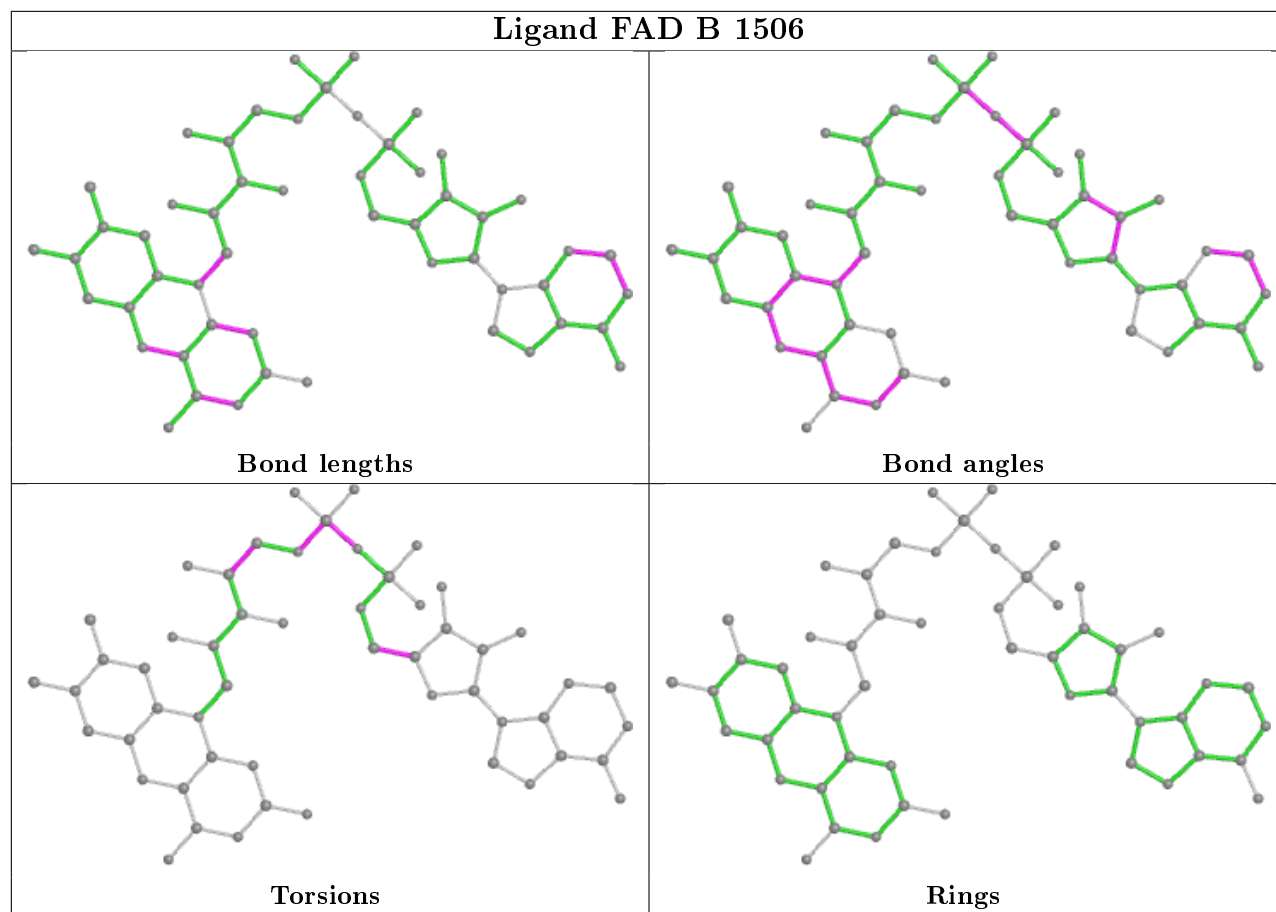
Mol	Chain	Res	Type	Atoms
2	B	1506	FAD	C3'-C4'-C5'-O5'
2	B	1506	FAD	O4'-C4'-C5'-O5'
2	B	1506	FAD	C5'-O5'-P-O2P
2	B	1506	FAD	PA-O3P-P-O5'
2	A	1506	FAD	O4B-C4B-C5B-O5B

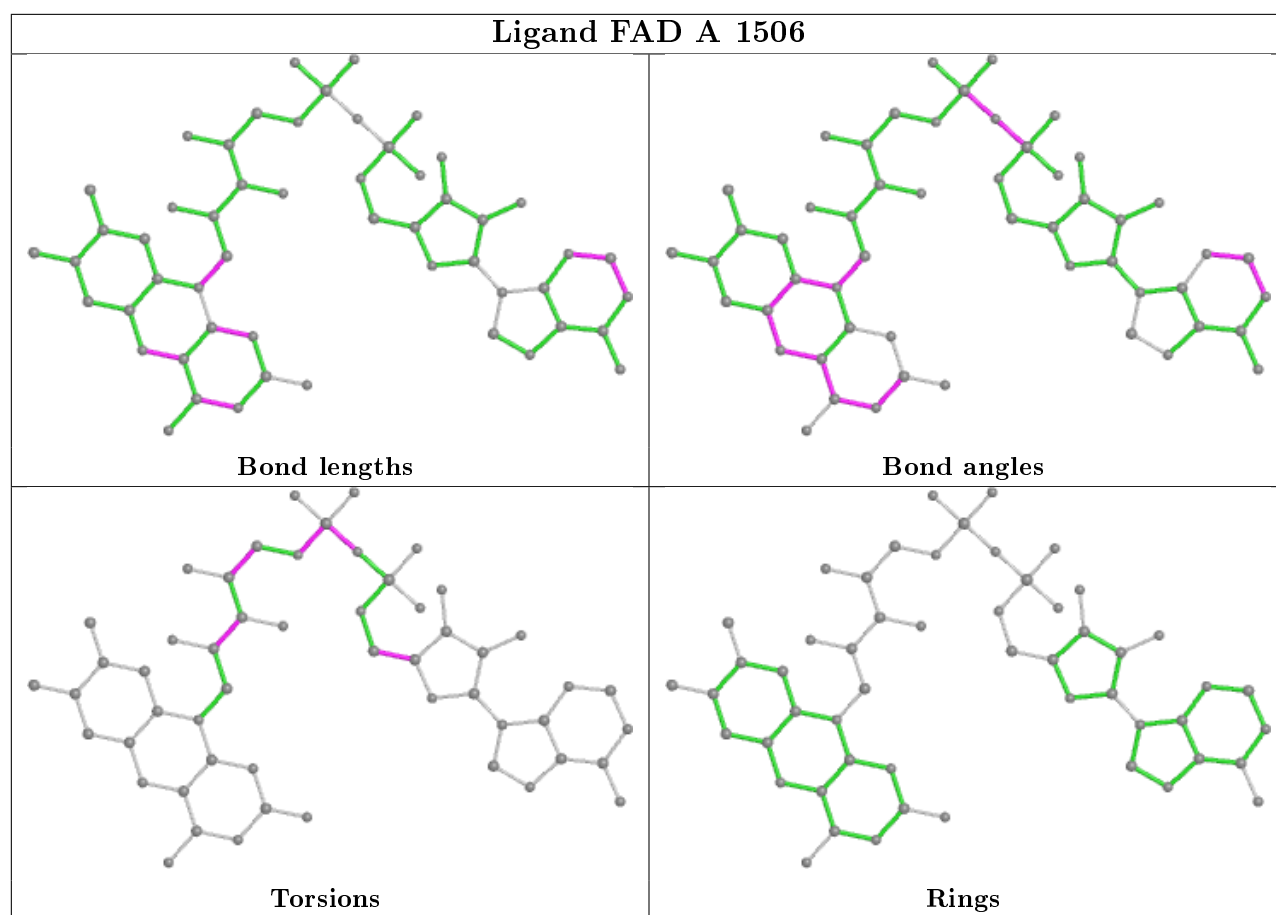
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1506	FAD	2	0
2	A	1506	FAD	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/542 (80%)	0.12	10 (2%) 60 58	17, 27, 66, 77	2 (0%)
1	B	437/542 (80%)	0.21	13 (2%) 50 45	17, 34, 64, 86	6 (1%)
All	All	874/1084 (80%)	0.17	23 (2%) 56 52	17, 30, 65, 86	8 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	177	LEU	4.7
1	A	426	LEU	4.2
1	B	172	TYR	4.1
1	A	459	LEU	3.7
1	A	467	ASN	3.6

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](#)

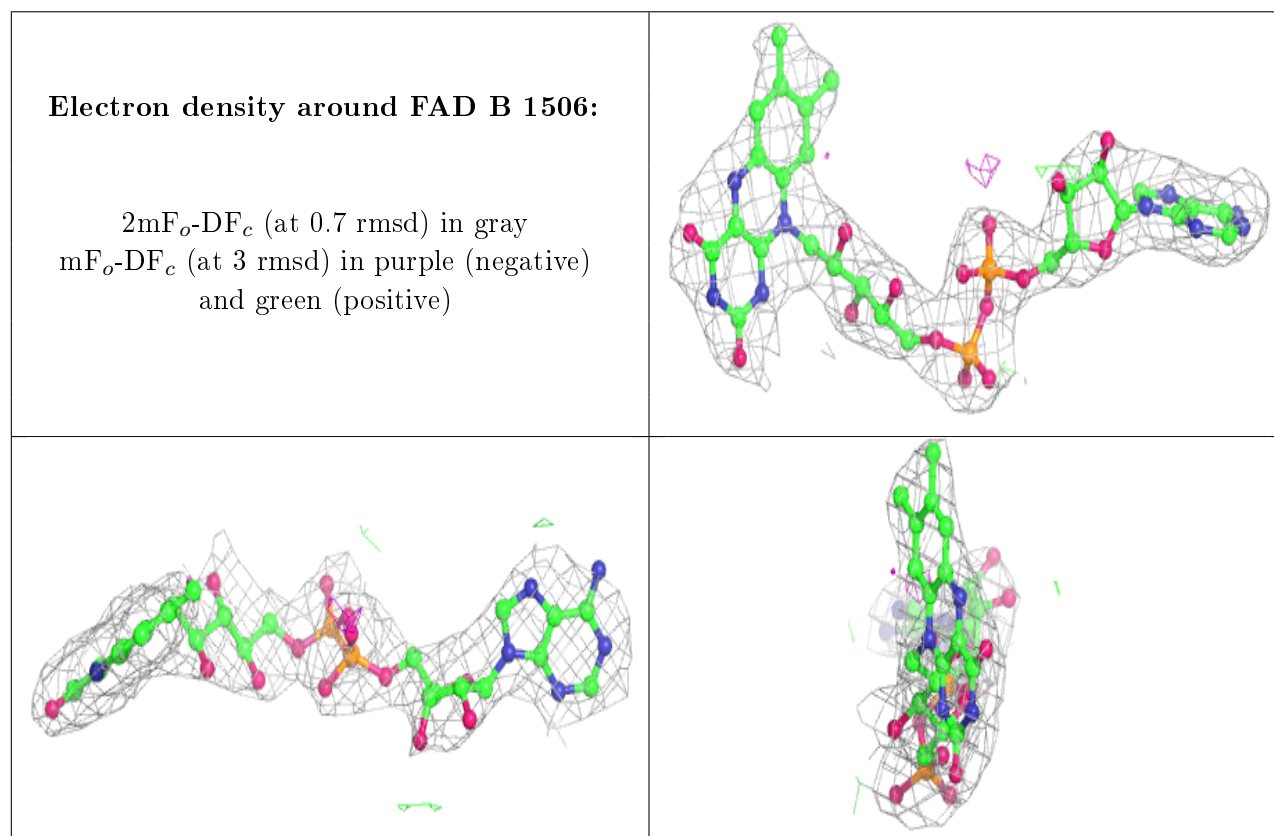
There are no carbohydrates in this entry.

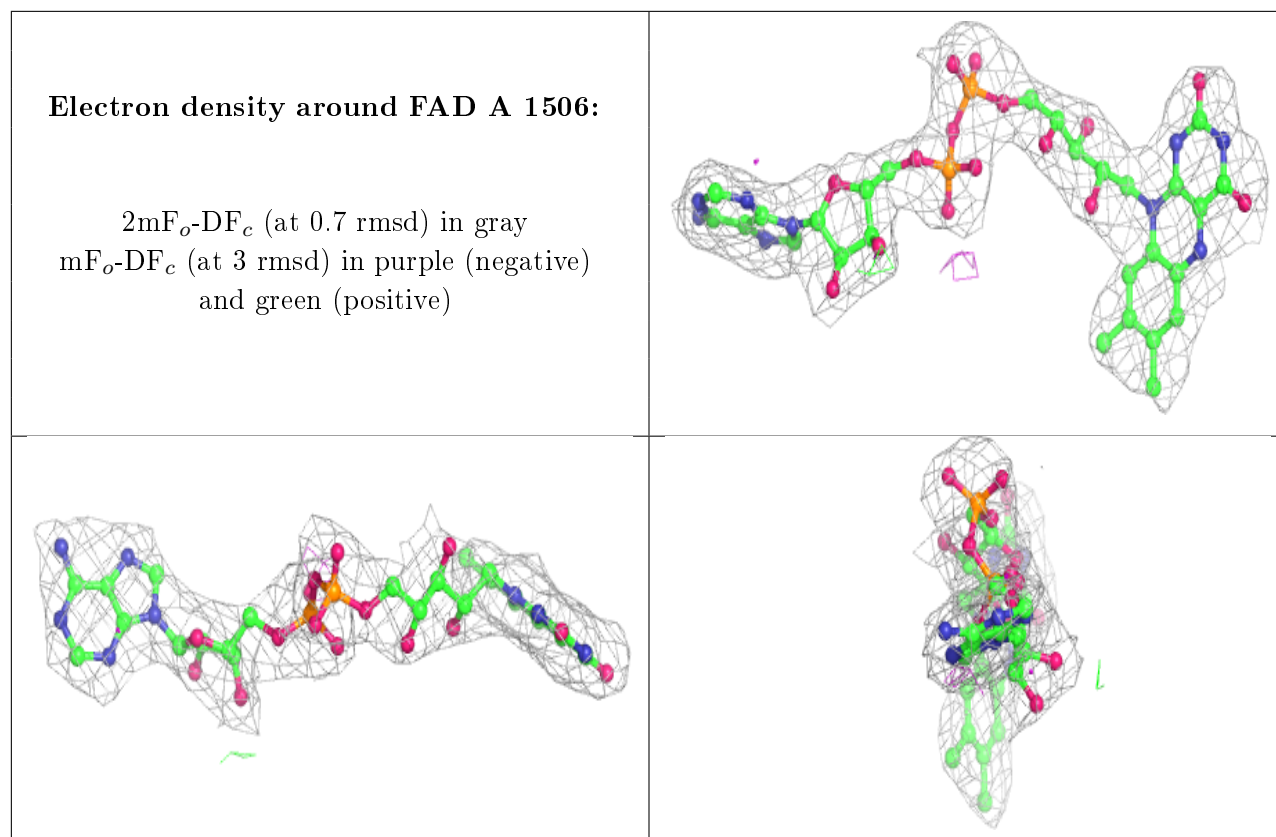
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FAD	B	1506	53/53	0.95	0.18	26,30,37,39	0
2	FAD	A	1506	53/53	0.96	0.17	18,19,20,20	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.