



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:17 am BST

PDB ID : 4FDC
Title : Crystal structure of the E493V mutant of human apoptosis inducing factor (AIF)
Authors : Sevrioukova, I.F.
Deposited on : 2012-05-27
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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

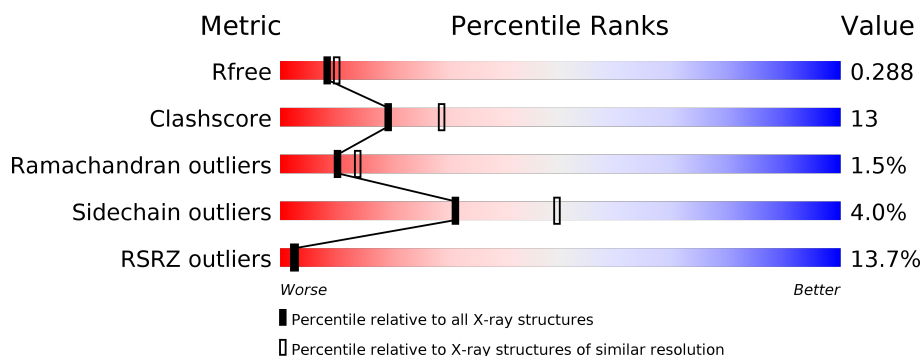
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	B	514	<div> <div>12%</div> <div>69%</div> <div>17%</div> <div>•</div> <div>10%</div> </div>

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.

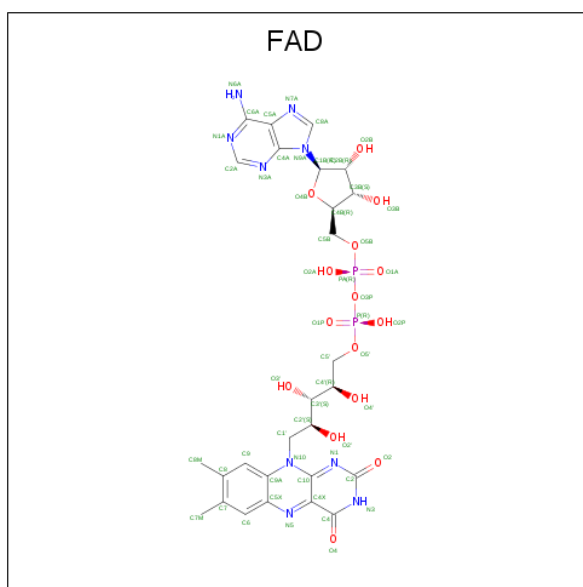
- Molecule 1 is a protein called Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	461	Total	C	N	O	S	0	0	0
			3555	2253	631	660	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	493	VAL	GLU	ENGINEERED MUTATION	UNP O95831
B	614	LEU	-	EXPRESSION TAG	UNP O95831
B	615	VAL	-	EXPRESSION TAG	UNP O95831
B	616	PRO	-	EXPRESSION TAG	UNP O95831

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 1: Apoptosis-inducing factor 1, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.40 Å 62.70 Å 101.92 Å 90.00° 118.57° 90.00°	Depositor
Resolution (Å)	39.50 – 2.40 29.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.50-2.40) 94.2 (29.84-2.40)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.39 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.253 , 0.297 0.256 , 0.288	Depositor DCC
R_{free} test set	1082 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3608	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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	B	0.50	3/3624 (0.1%)	0.57	0/4896

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	TRP	CD2-CE2	5.25	1.47	1.41
1	B	483	TRP	CD2-CE2	5.25	1.47	1.41
1	B	351	TRP	CD2-CE2	5.01	1.47	1.41

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	B	3555	0	3597	92	0
2	B	53	0	31	2	0
All	All	3608	0	3628	93	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 13.

All (93) 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:417:ASP:OD2	1:B:449:ARG:NH2	1.63	1.30
1:B:407:ALA:O	1:B:413:GLU:CG	1.92	1.18
1:B:471:GLY:HA2	1:B:472:ALA:HB2	1.16	1.10
1:B:407:ALA:O	1:B:413:GLU:HG2	1.51	1.09
1:B:505:VAL:HG21	1:B:601:LEU:CD1	1.92	0.99
1:B:407:ALA:O	1:B:413:GLU:HG3	1.60	0.98
1:B:600:ASP:O	1:B:601:LEU:HB2	1.63	0.96
1:B:415:ASP:CG	1:B:416:SER:H	1.61	0.94
1:B:505:VAL:HG11	1:B:601:LEU:CD1	1.98	0.93
1:B:471:GLY:HA2	1:B:472:ALA:CB	1.95	0.93
1:B:412:LEU:HD21	1:B:430:ARG:HG2	1.51	0.91
1:B:505:VAL:HG21	1:B:601:LEU:HD11	1.52	0.91
1:B:505:VAL:HG11	1:B:601:LEU:HD13	1.57	0.86
1:B:415:ASP:CG	1:B:416:SER:N	2.30	0.83
1:B:131:HIS:HD2	1:B:252:THR:OG1	1.61	0.82
1:B:505:VAL:CG1	1:B:601:LEU:HD13	2.09	0.81
1:B:404:VAL:O	1:B:407:ALA:CB	2.30	0.80
1:B:505:VAL:CB	1:B:601:LEU:HD13	2.13	0.79
1:B:404:VAL:O	1:B:407:ALA:HB3	1.82	0.77
1:B:505:VAL:HG11	1:B:601:LEU:HD12	1.68	0.74
1:B:417:ASP:OD2	1:B:449:ARG:CZ	2.35	0.74
1:B:600:ASP:O	1:B:601:LEU:CB	2.36	0.73
1:B:471:GLY:CA	1:B:472:ALA:HB2	2.09	0.72
1:B:505:VAL:CG2	1:B:601:LEU:CD1	2.65	0.72
1:B:412:LEU:HD22	1:B:429:ALA:HB1	1.74	0.69
1:B:383:LEU:HD12	1:B:387:ARG:HB2	1.75	0.69
1:B:131:HIS:CD2	1:B:252:THR:OG1	2.45	0.68
1:B:505:VAL:CB	1:B:601:LEU:CD1	2.73	0.67
1:B:505:VAL:HB	1:B:601:LEU:HD13	1.78	0.64
1:B:505:VAL:CG1	1:B:601:LEU:CD1	2.69	0.61
1:B:412:LEU:CD2	1:B:430:ARG:HG2	2.29	0.60
1:B:533:GLU:HG2	1:B:585:MET:HB2	1.81	0.60
1:B:468:ASN:HA	1:B:472:ALA:HA	1.87	0.56
1:B:600:ASP:OD1	1:B:600:ASP:N	2.38	0.56
1:B:217:LEU:N	1:B:218:PRO:CD	2.68	0.56
1:B:285:ARG:NH1	2:B:1000:FAD:HM81	2.22	0.55
1:B:505:VAL:CG2	1:B:601:LEU:HD11	2.31	0.55
1:B:533:GLU:HG2	1:B:585:MET:CB	2.37	0.55
1:B:505:VAL:HG21	1:B:601:LEU:HD12	1.85	0.54
1:B:405:GLU:C	1:B:407:ALA:H	2.08	0.54
1:B:422:ARG:HH12	1:B:449:ARG:HH11	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASP:OD2	1:B:478:HIS:HE1	1.92	0.52
1:B:404:VAL:HA	1:B:421:PHE:CZ	2.44	0.52
1:B:178:GLU:HG2	1:B:195:GLN:HA	1.91	0.52
1:B:412:LEU:HD21	1:B:430:ARG:CG	2.33	0.51
1:B:443:TYR:CZ	1:B:448:GLY:HA2	2.44	0.51
1:B:443:TYR:CE2	1:B:448:GLY:HA2	2.46	0.51
1:B:132:VAL:O	1:B:253:TYR:HA	2.10	0.51
1:B:404:VAL:O	1:B:407:ALA:N	2.40	0.51
1:B:283:LEU:HD23	1:B:396:ALA:HB3	1.93	0.51
1:B:261:GLY:HA2	1:B:438:ASP:HB2	1.94	0.50
1:B:464:LEU:HD22	1:B:476:TYR:HB2	1.93	0.50
1:B:267:LEU:H	1:B:270:ILE:HD12	1.78	0.49
1:B:493:VAL:HG12	1:B:585:MET:CE	2.42	0.49
1:B:452:VAL:CG2	1:B:457:HIS:CG	2.97	0.48
1:B:142:ALA:HB3	1:B:259:ALA:HB1	1.96	0.48
1:B:242:MET:HG2	1:B:243:VAL:N	2.29	0.48
1:B:194:LYS:HG2	1:B:200:GLU:HG2	1.96	0.47
1:B:217:LEU:HB3	1:B:218:PRO:HD3	1.96	0.47
1:B:233:VAL:O	1:B:406:LEU:HD21	2.13	0.47
1:B:305:ILE:HD11	1:B:319:LEU:HD12	1.97	0.46
1:B:497:LEU:O	1:B:575:GLY:HA3	2.16	0.45
1:B:146:ALA:O	1:B:150:ILE:HG13	2.15	0.45
1:B:446:LYS:HE3	1:B:593:LYS:O	2.16	0.45
1:B:534:THR:HG22	1:B:535:GLU:N	2.31	0.45
1:B:411:GLY:HA2	1:B:413:GLU:OE1	2.17	0.44
1:B:132:VAL:HG21	1:B:160:LEU:HB3	2.00	0.44
1:B:435:VAL:HG12	1:B:440:ALA:HB2	1.98	0.44
1:B:534:THR:HG22	1:B:536:SER:H	1.83	0.44
1:B:197:ASN:HB2	1:B:522:GLU:HG3	1.99	0.43
1:B:402:PRO:HG3	1:B:451:ARG:HD2	2.00	0.43
1:B:404:VAL:HB	1:B:407:ALA:CB	2.48	0.43
1:B:221:GLU:O	1:B:222:ASN:HB2	2.18	0.43
1:B:405:GLU:C	1:B:407:ALA:N	2.71	0.43
1:B:151:ARG:CZ	1:B:224:GLY:HA2	2.49	0.43
1:B:479:GLN:HB3	1:B:495:ILE:HD11	2.00	0.43
1:B:404:VAL:HB	1:B:407:ALA:HB2	2.02	0.42
1:B:356:VAL:HG12	1:B:361:VAL:HB	2.01	0.42
1:B:584:ARG:HD2	1:B:587:ILE:HD12	2.02	0.42
1:B:452:VAL:HG21	1:B:457:HIS:CG	2.55	0.41
1:B:412:LEU:HD22	1:B:429:ALA:CB	2.45	0.41
1:B:477:TRP:CE3	1:B:477:TRP:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:LEU:N	1:B:218:PRO:HD3	2.36	0.41
1:B:344:LEU:HD22	1:B:348:LEU:HD23	2.02	0.41
1:B:231:LYS:HB3	1:B:245:LEU:HD13	2.02	0.41
1:B:514:GLN:HB2	1:B:523:GLN:NE2	2.35	0.41
1:B:165:ASP:OD1	1:B:286:LYS:HD2	2.21	0.41
1:B:236:LEU:HD12	1:B:243:VAL:HG12	2.02	0.40
1:B:352:THR:O	1:B:356:VAL:HG23	2.22	0.40
2:B:1000:FAD:H9	2:B:1000:FAD:H1'1	1.72	0.40
1:B:413:GLU:C	1:B:414:ILE:HG23	2.42	0.40
1:B:414:ILE:CG1	1:B:415:ASP:N	2.85	0.40
1:B:601:LEU:HD23	1:B:601:LEU:HA	1.92	0.40

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	B	457/514 (89%)	417 (91%)	33 (7%)	7 (2%)	10 14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	413	GLU
1	B	414	ILE
1	B	472	ALA
1	B	416	SER
1	B	471	GLY
1	B	601	LEU
1	B	406	LEU

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	B	378/422 (90%)	363 (96%)	15 (4%)	31 49

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	165	ASP
1	B	188	THR
1	B	272	ARG
1	B	285	ARG
1	B	405	GLU
1	B	414	ILE
1	B	445	ILE
1	B	449	ARG
1	B	464	LEU
1	B	477	TRP
1	B	495	ILE
1	B	516	ASN
1	B	564	VAL
1	B	593	LYS
1	B	600	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	HIS
1	B	366	ASN
1	B	478	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 carbohydrates 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	FAD	B	1000	-	51,58,58	1.57	7 (13%)	60,89,89	1.77	11 (18%)

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	1000	-	-	5/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	FAD	C9-C9A	-5.87	1.29	1.40
2	B	1000	FAD	C4-C4X	4.55	1.49	1.41
2	B	1000	FAD	C9-C8	-3.43	1.28	1.37
2	B	1000	FAD	C8-C7	3.06	1.48	1.40
2	B	1000	FAD	C9A-N10	3.04	1.42	1.38
2	B	1000	FAD	C10-N1	2.31	1.36	1.33
2	B	1000	FAD	C4X-N5	2.14	1.36	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	FAD	C4-N3-C2	6.49	120.63	115.14
2	B	1000	FAD	N3A-C2A-N1A	-4.24	122.05	128.68
2	B	1000	FAD	C5X-C9A-N10	3.59	120.32	117.72
2	B	1000	FAD	C1'-N10-C10	3.59	121.62	118.41
2	B	1000	FAD	C4-C4X-C10	-3.34	117.74	119.95
2	B	1000	FAD	C4X-C4-N3	-3.19	119.06	123.43
2	B	1000	FAD	C4X-N5-C5X	2.93	119.70	116.77
2	B	1000	FAD	C9A-N10-C10	-2.45	118.69	121.91
2	B	1000	FAD	C7-C6-C5X	-2.41	117.81	121.22
2	B	1000	FAD	P-O3P-PA	-2.26	125.06	132.83
2	B	1000	FAD	C1B-N9A-C4A	-2.26	122.67	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

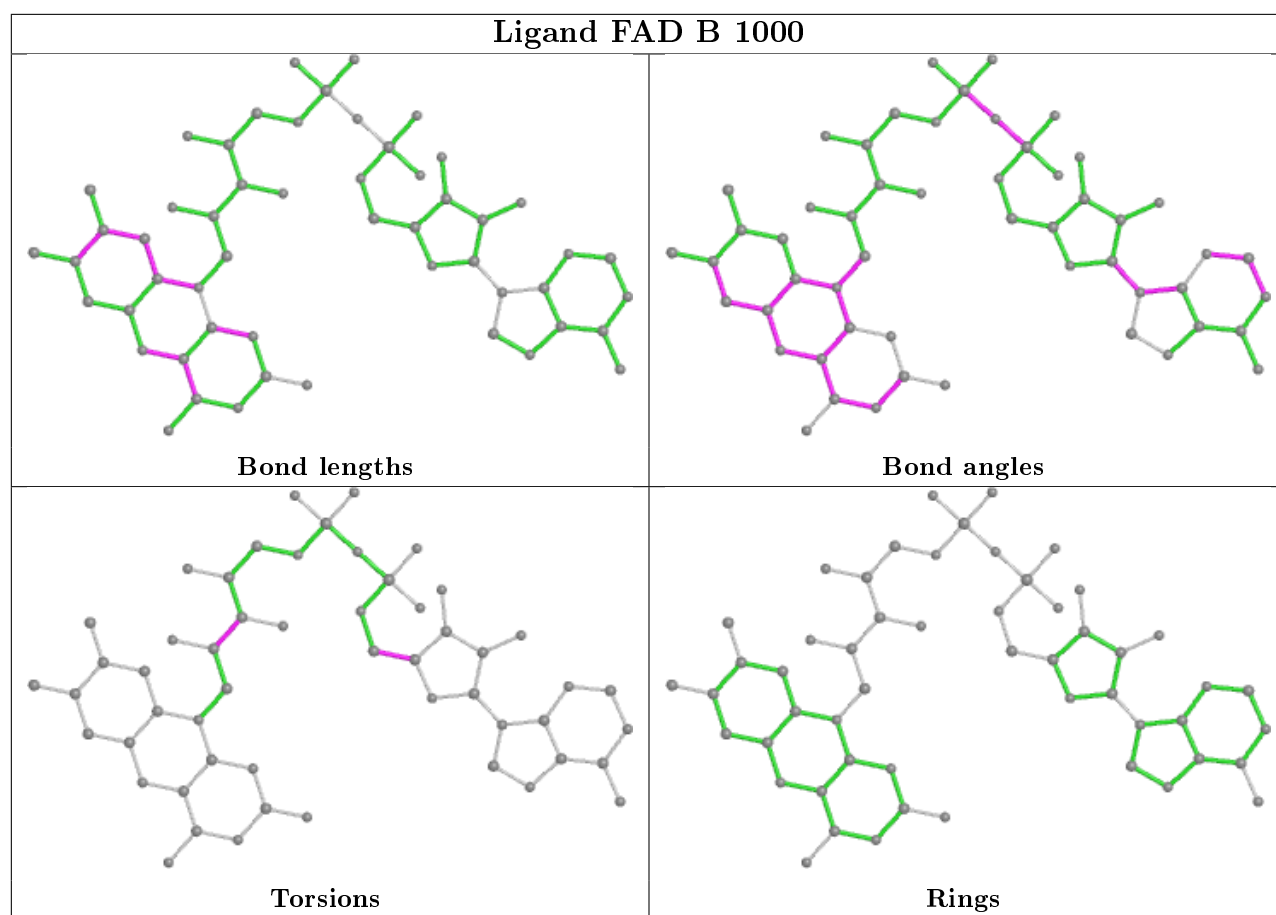
Mol	Chain	Res	Type	Atoms
2	B	1000	FAD	O4B-C4B-C5B-O5B
2	B	1000	FAD	C3B-C4B-C5B-O5B
2	B	1000	FAD	C1'-C2'-C3'-O3'
2	B	1000	FAD	O2'-C2'-C3'-C4'
2	B	1000	FAD	O2'-C2'-C3'-O3'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	FAD	2	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, 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	B	461/514 (89%)	0.92	63 (13%) 3 2	62, 123, 208, 313	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	415	ASP	6.4
1	B	239	ARG	6.2
1	B	510	LYS	6.0
1	B	598	HIS	5.6
1	B	503	PRO	5.2
1	B	407	ALA	5.0
1	B	607	LEU	4.5
1	B	414	ILE	4.5
1	B	610	ILE	4.3
1	B	152	ALA	4.2
1	B	374	VAL	4.1
1	B	511	ALA	4.1
1	B	183	ASP	3.9
1	B	569	ARG	3.6
1	B	536	SER	3.5
1	B	153	ARG	3.5
1	B	512	THR	3.4
1	B	513	ALA	3.4
1	B	571	LYS	3.3
1	B	443	TYR	3.1
1	B	472	ALA	3.1
1	B	535	GLU	3.0
1	B	537	GLU	3.0
1	B	603	GLU	3.0
1	B	471	GLY	3.0
1	B	271	ASP	2.9
1	B	315	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	356	VAL	2.8
1	B	601	LEU	2.8
1	B	197	ASN	2.8
1	B	275	ALA	2.8
1	B	368	ILE	2.7
1	B	583	ASN	2.7
1	B	435	VAL	2.6
1	B	605	ALA	2.6
1	B	272	ARG	2.6
1	B	514	GLN	2.5
1	B	507	VAL	2.5
1	B	574	VAL	2.5
1	B	312	GLY	2.5
1	B	440	ALA	2.5
1	B	560	TYR	2.5
1	B	573	VAL	2.4
1	B	421	PHE	2.4
1	B	482	PHE	2.4
1	B	597	GLN	2.3
1	B	256	CYS	2.3
1	B	418	PHE	2.3
1	B	582	PHE	2.3
1	B	608	PHE	2.3
1	B	502	LEU	2.2
1	B	493	VAL	2.2
1	B	604	VAL	2.2
1	B	276	GLU	2.1
1	B	155	PRO	2.1
1	B	599	GLU	2.1
1	B	156	GLY	2.1
1	B	561	GLY	2.1
1	B	492	TYR	2.1
1	B	442	PHE	2.1
1	B	411	GLY	2.1
1	B	602	ASN	2.0
1	B	565	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

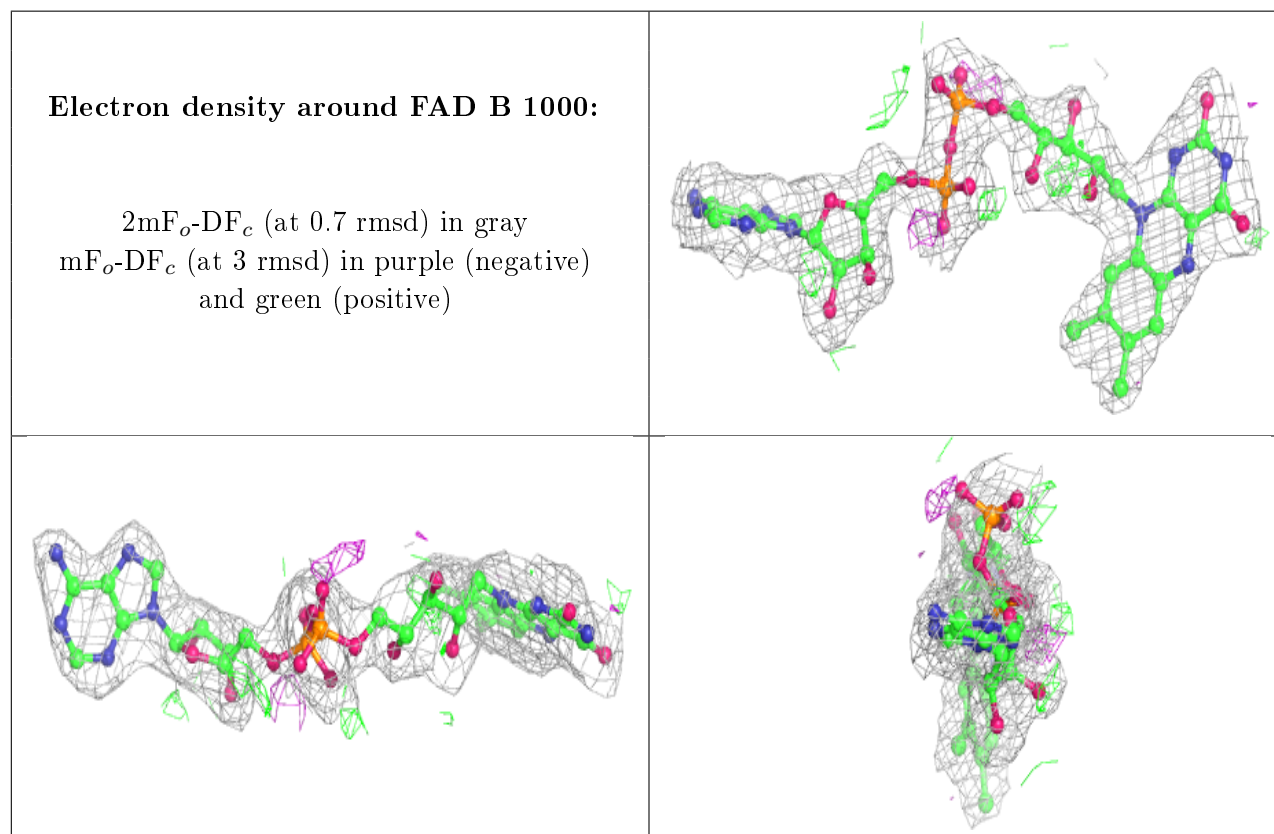
There are no carbohydrates in this entry.

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	1000	53/53	0.92	0.19	71,84,92,93	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.