



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 4FDC / pdb_00004fdc
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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

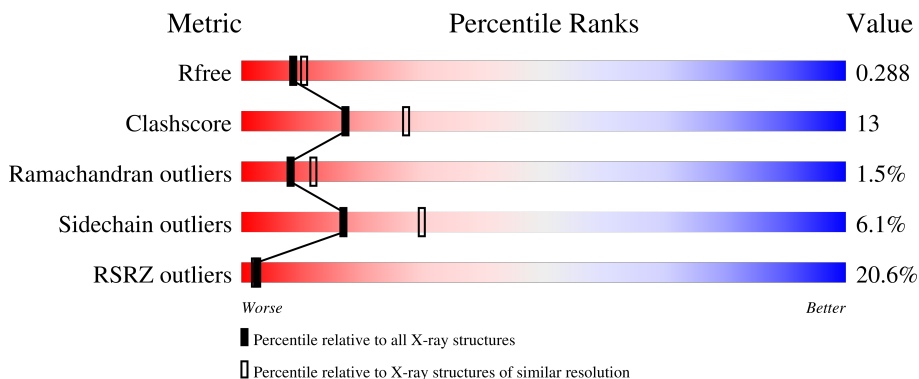
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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 $\leq 5\%$. 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	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3608 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.

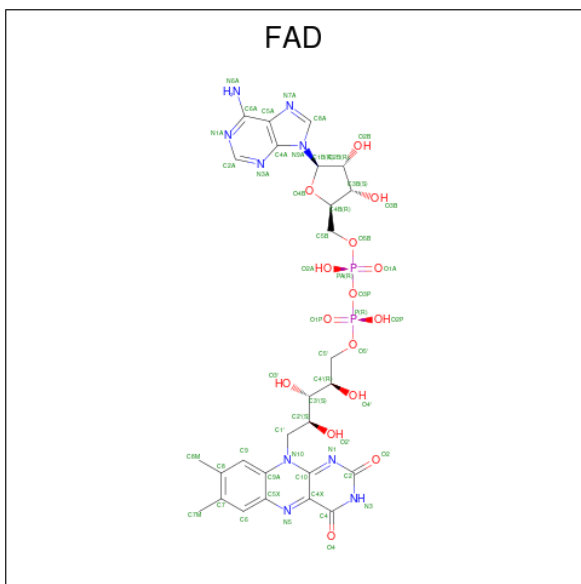
- Molecule 1 is a protein called Apoptosis-inducing factor 1, mitochondrial.

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

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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

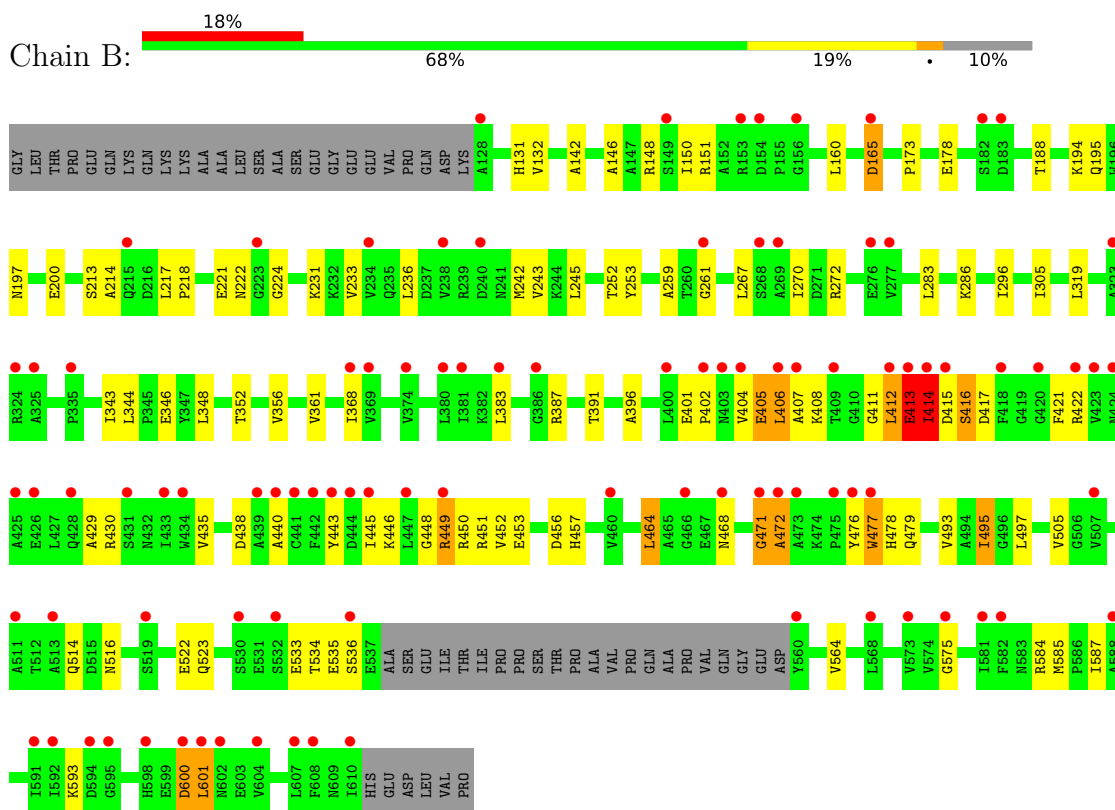


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0

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: Apoptosis-inducing factor 1, mitochondrial



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	102.40Å 62.70Å 101.92Å 90.00° 118.57° 90.00°	Depositor
Resolution (Å)	39.50 – 2.40 39.50 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.2 (39.50-2.40) 94.2 (39.50-2.40)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.253 , 0.297 0.256 , 0.288	Depositor DCC
R_{free} test set	1144 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtrriage
Anisotropy	0.151	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtrriage
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

Xtrriage'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	0.64	0/3624	0.84	8/4896 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	413	GLU	N-CA-C	5.70	122.94	110.80
1	B	412	LEU	N-CA-C	-5.65	106.55	113.50
1	B	173	PRO	N-CA-C	5.62	117.56	110.70
1	B	414	ILE	N-CA-C	5.61	121.02	109.34
1	B	173	PRO	CA-C-N	-5.46	113.27	119.28
1	B	173	PRO	C-N-CA	-5.46	113.27	119.28
1	B	214	ALA	N-CA-C	-5.15	106.83	113.01
1	B	450	ARG	N-CA-C	5.12	116.84	108.55

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	90	0
2	B	53	0	31	1	0
All	All	3608	0	3628	91	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 (91) 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:415:ASP:CG	1:B:416:SER:H	1.61	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: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:415:ASP:CG	1:B:416:SER:N	2.30	0.87
1:B:505:VAL:HG11	1:B:601:LEU:HD13	1.57	0.86
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:505:VAL:CG2	1:B:601:LEU:CD1	2.65	0.72
1:B:471:GLY:CA	1:B:472:ALA:HB2	2.09	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:405:GLU:C	1:B:407:ALA:H	2.08	0.60
1:B:468:ASN:HA	1:B:472:ALA:HA	1.87	0.56
1:B:600:ASP:N	1:B:600:ASP:OD1	2.38	0.56
1:B:217:LEU:N	1:B:218:PRO:CD	2.68	0.56
1:B:505:VAL:CG2	1:B:601:LEU:HD11	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:422:ARG:HH12	1:B:449:ARG:HH11	1.57	0.53
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:413:GLU:C	1:B:414:ILE:HG23	2.42	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:405:GLU:C	1:B:407:ALA:N	2.71	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:477:TRP:CE3	2.56	0.41
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: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%)	8 12

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%)	355 (94%)	23 (6%)	17 30

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	148	ARG
1	B	165	ASP
1	B	188	THR
1	B	213	SER
1	B	272	ARG
1	B	296	ILE
1	B	343	ILE
1	B	346	GLU
1	B	368	ILE
1	B	391	THR
1	B	401	GLU
1	B	405	GLU
1	B	408	LYS
1	B	414	ILE
1	B	445	ILE
1	B	449	ARG
1	B	453	GLU
1	B	464	LEU
1	B	477	TRP
1	B	495	ILE
1	B	516	ASN
1	B	564	VAL
1	B	600	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	131	HIS
1	B	219	HIS

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Mol	Chain	Res	Type
1	B	235	GLN
1	B	366	ASN
1	B	478	HIS
1	B	479	GLN
1	B	523	GLN
1	B	580	ASN
1	B	583	ASN

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 oligosaccharides 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	-	58,58,58	1.77	10 (17%)	85,89,89	1.57	17 (20%)

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	-	-	6/34/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	FAD	C9-C8	-7.88	1.28	1.39
2	B	1000	FAD	C9-C9A	-6.59	1.29	1.39
2	B	1000	FAD	C8-C7	3.15	1.48	1.40
2	B	1000	FAD	C5A-C6A	2.85	1.48	1.41
2	B	1000	FAD	C4X-N5	2.61	1.36	1.30
2	B	1000	FAD	C4A-N9A	-2.36	1.32	1.37
2	B	1000	FAD	C5A-N7A	-2.21	1.35	1.39
2	B	1000	FAD	C4-N3	-2.18	1.34	1.38
2	B	1000	FAD	C5X-N5	-2.16	1.35	1.39
2	B	1000	FAD	C2-N3	-2.14	1.34	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	FAD	C5A-C4A-N3A	-4.36	120.71	126.72
2	B	1000	FAD	N3A-C2A-N1A	-4.32	122.05	128.58
2	B	1000	FAD	C2A-N3A-C4A	3.54	120.47	111.83
2	B	1000	FAD	N9A-C8A-N7A	-3.35	109.18	113.94
2	B	1000	FAD	C4-N3-C2	-2.82	120.63	125.64
2	B	1000	FAD	C4A-C5A-N7A	-2.78	107.41	110.58
2	B	1000	FAD	C9A-C5X-N5	-2.70	119.59	122.45
2	B	1000	FAD	N3A-C4A-N9A	2.62	131.62	127.17
2	B	1000	FAD	C5X-C9A-N10	2.60	120.32	117.97
2	B	1000	FAD	C4A-N9A-C8A	2.57	108.44	105.74
2	B	1000	FAD	O4-C4-C4X	-2.48	119.97	126.53
2	B	1000	FAD	C5A-N7A-C8A	2.45	107.30	103.45
2	B	1000	FAD	C4X-C10-N1	-2.45	118.59	124.59
2	B	1000	FAD	C9A-C9-C8	2.43	124.10	119.22
2	B	1000	FAD	C10-N1-C2	2.36	121.96	116.85
2	B	1000	FAD	C4X-C4-N3	2.28	119.06	113.25
2	B	1000	FAD	C4X-C10-N10	2.10	119.49	116.48

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	FAD	C3B-C4B-C5B-O5B

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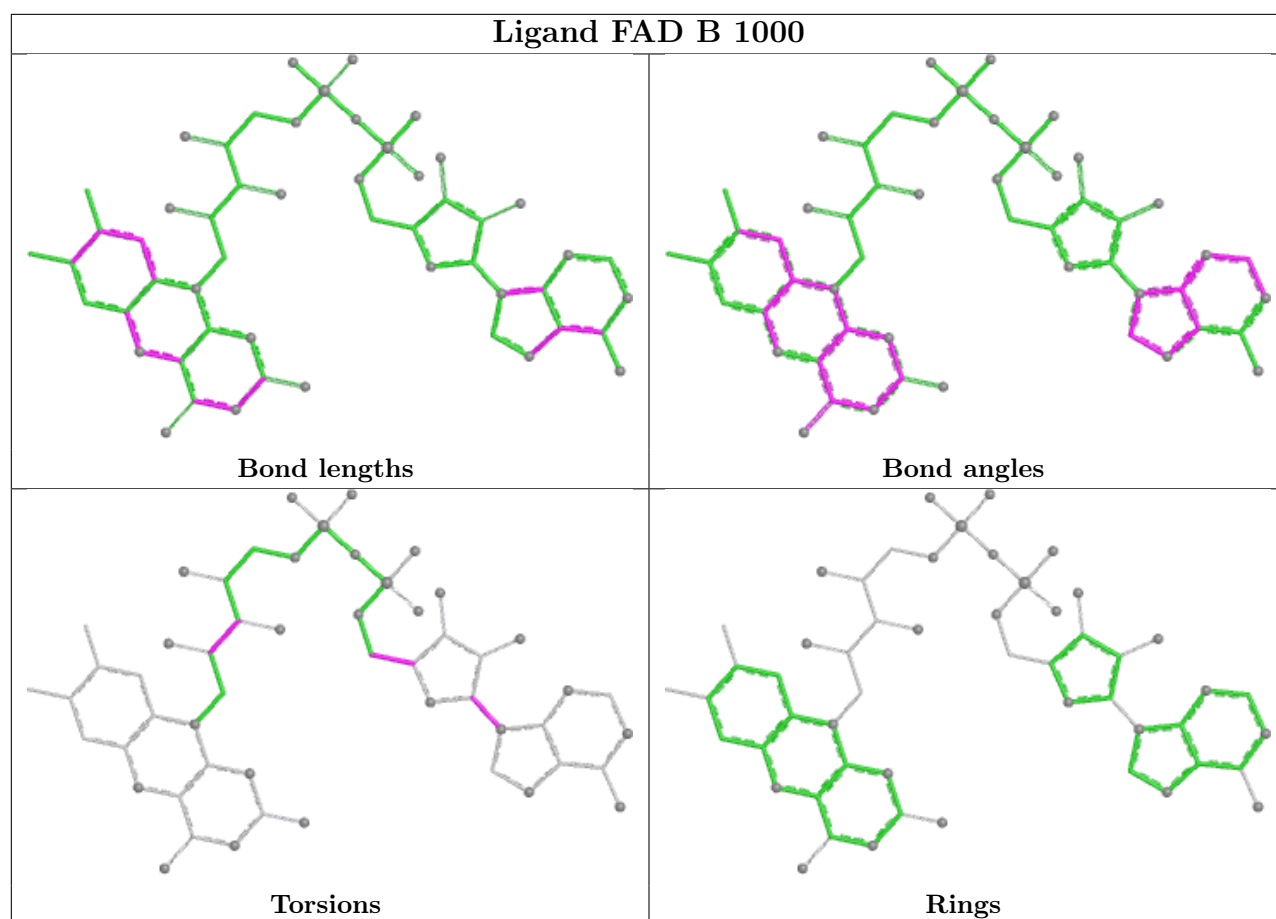
Mol	Chain	Res	Type	Atoms
2	B	1000	FAD	O4B-C4B-C5B-O5B
2	B	1000	FAD	O2'-C2'-C3'-C4'
2	B	1000	FAD	C1'-C2'-C3'-O3'
2	B	1000	FAD	O2'-C2'-C3'-O3'
2	B	1000	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	FAD	1	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%)	1.32	95 (20%) 2 2	62, 123, 208, 313	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	443	TYR	6.8
1	B	473	ALA	6.7
1	B	472	ALA	6.4
1	B	440	ALA	5.2
1	B	414	ILE	4.0
1	B	442	PHE	3.9
1	B	601	LEU	3.9
1	B	536	SER	3.9
1	B	471	GLY	3.8
1	B	610	ILE	3.8
1	B	475	PRO	3.7
1	B	445	ILE	3.7
1	B	530	SER	3.6
1	B	215	GLN	3.6
1	B	238	VAL	3.5
1	B	268	SER	3.5
1	B	415	ASP	3.5
1	B	422	ARG	3.5
1	B	165	ASP	3.4
1	B	404	VAL	3.3
1	B	277	VAL	3.3
1	B	441	CYS	3.2
1	B	507	VAL	3.2
1	B	407	ALA	3.2
1	B	568	LEU	3.1
1	B	128	ALA	3.1
1	B	269	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	412	LEU	3.1
1	B	413	GLU	3.0
1	B	324	ARG	3.0
1	B	400	LEU	3.0
1	B	234	VAL	2.9
1	B	604	VAL	2.9
1	B	418	PHE	2.9
1	B	477	TRP	2.9
1	B	149	SER	2.9
1	B	425	ALA	2.9
1	B	468	ASN	2.8
1	B	581	ILE	2.7
1	B	403	ASN	2.7
1	B	573	VAL	2.7
1	B	434	TRP	2.7
1	B	420	GLY	2.7
1	B	374	VAL	2.7
1	B	449	ARG	2.7
1	B	466	GLY	2.6
1	B	608	PHE	2.6
1	B	183	ASP	2.6
1	B	423	VAL	2.6
1	B	426	GLU	2.6
1	B	261	GLY	2.6
1	B	276	GLU	2.5
1	B	433	ILE	2.5
1	B	240	ASP	2.5
1	B	476	TYR	2.5
1	B	409	THR	2.4
1	B	156	GLY	2.4
1	B	592	ILE	2.4
1	B	153	ARG	2.4
1	B	380	LEU	2.4
1	B	383	LEU	2.4
1	B	511	ALA	2.3
1	B	532	SER	2.3
1	B	591	ILE	2.3
1	B	602	ASN	2.3
1	B	431	SER	2.3
1	B	607	LEU	2.3
1	B	560	TYR	2.3
1	B	588	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	582	PHE	2.3
1	B	182	SER	2.2
1	B	323	ALA	2.2
1	B	325	ALA	2.2
1	B	575	GLY	2.2
1	B	444	ASP	2.2
1	B	223	GLY	2.2
1	B	154	ASP	2.2
1	B	460	VAL	2.2
1	B	594	ASP	2.2
1	B	335	PRO	2.2
1	B	386	GLY	2.1
1	B	447	LEU	2.1
1	B	368	ILE	2.1
1	B	381	ILE	2.1
1	B	424	ASN	2.1
1	B	595	GLY	2.1
1	B	519	SER	2.1
1	B	428	GLN	2.0
1	B	369	VAL	2.0
1	B	600	ASP	2.0
1	B	406	LEU	2.0
1	B	439	ALA	2.0
1	B	513	ALA	2.0
1	B	402	PRO	2.0
1	B	598	HIS	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 [\(i\)](#)

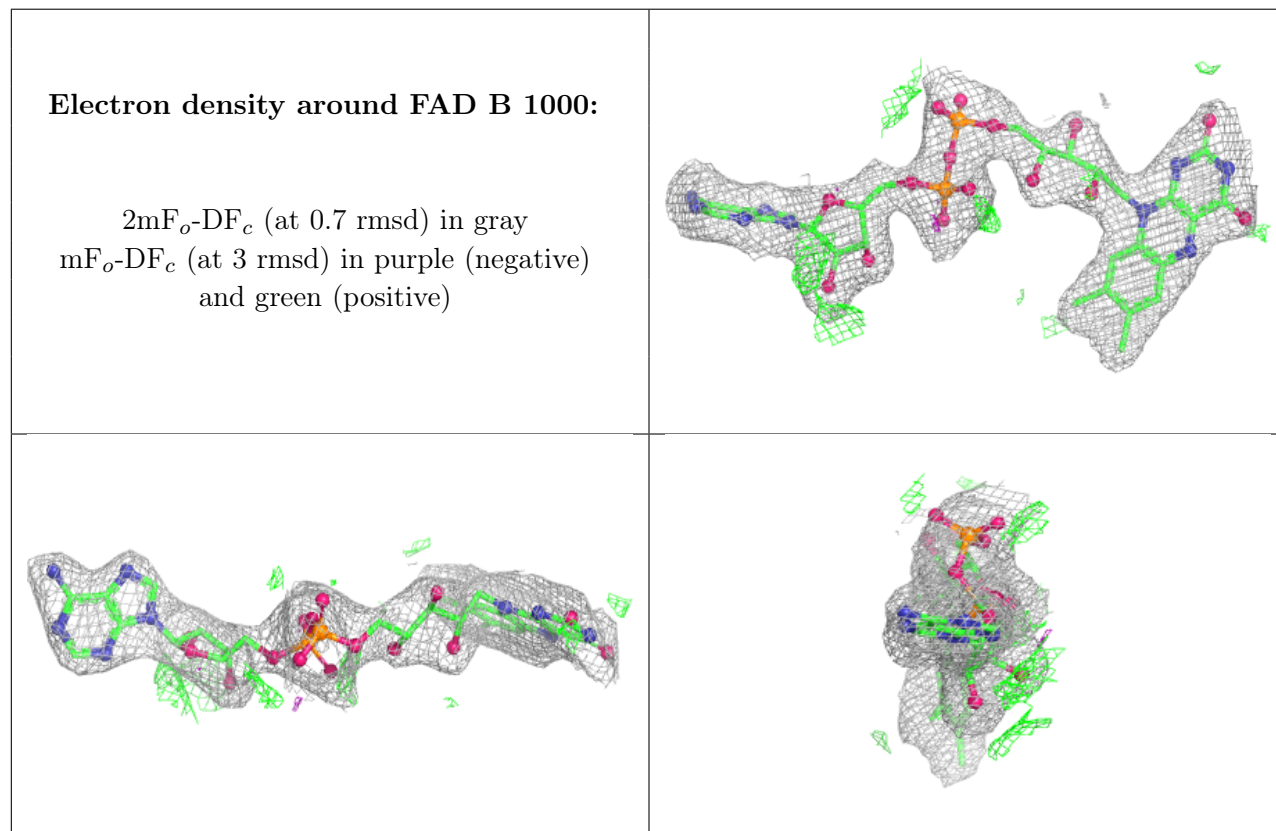
There are no oligosaccharides in this entry.

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	0.94	0.11	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.