



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2016 – 12:27 PM EST

PDB ID : 5FMH
Title : Crystal structure of the E405K mutant of human apoptosis inducing factor
Authors : Sevrioukova, I.
Deposited on : 2015-11-04
Resolution : 1.80 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

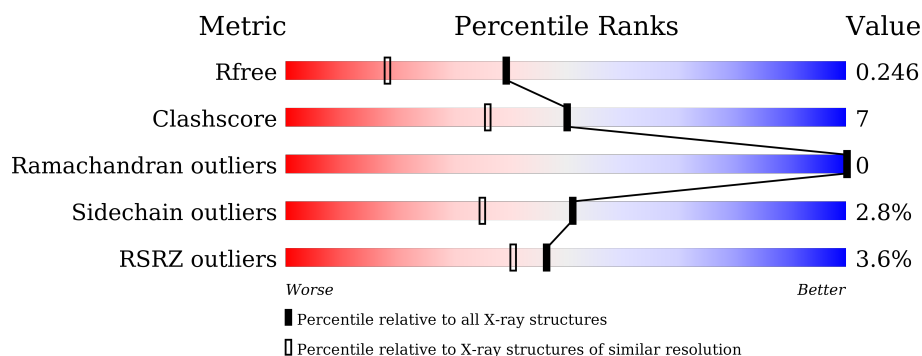
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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. 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	510	<div> <div>3%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4090 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.

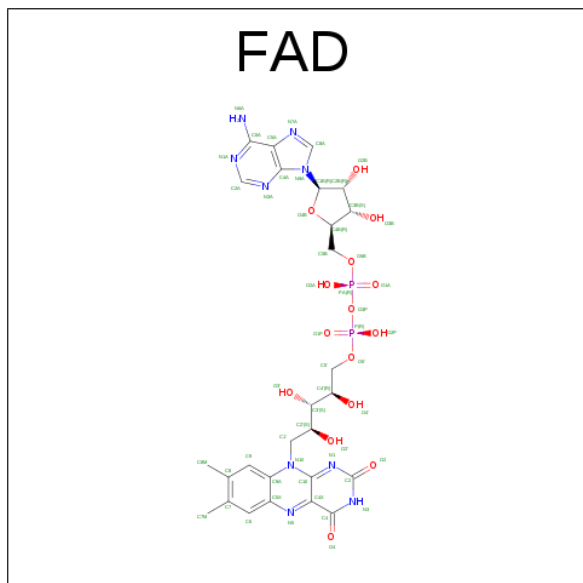
- Molecule 1 is a protein called APOPTOSIS-INDUCING FACTOR 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	3703	2350	657	685	11	0	11	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	405	LYS	GLU	ENGINEERED MUTATION	UNP O95831

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

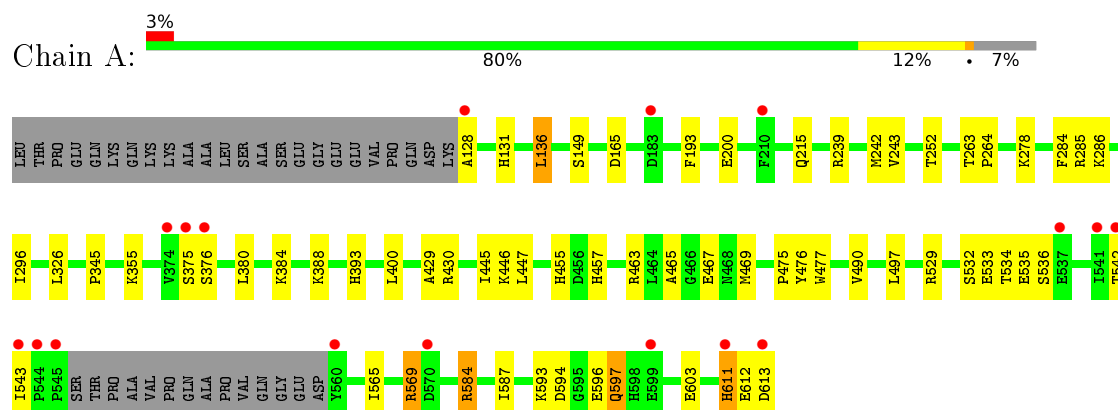


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	334	Total 334	O 334	0	0

- 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	109.30Å 49.23Å 81.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.48 – 1.80 45.39 – 1.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (81.48-1.80) 93.2 (45.39-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.191 , 0.243 0.199 , 0.246	Depositor DCC
R_{free} test set	1901 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4090	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.21% 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

5.1 Standard geometry

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	0.53	0/3802	0.73	1/5136 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	136	LEU	CB-CG-CD1	5.67	120.64	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3703	0	3778	53	1
2	A	53	0	31	0	0
3	A	334	0	0	7	2
All	All	4090	0	3809	53	2

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 7.

All (53) 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:285:ARG:HD2	3:A:2131:HOH:O	1.43	1.18
1:A:445[B]:ILE:HD11	1:A:477:TRP:CE3	2.12	0.85
1:A:284:PHE:O	1:A:285:ARG:HG2	1.83	0.79
1:A:611:HIS:CD2	1:A:611:HIS:H	2.03	0.76
1:A:611:HIS:HB3	1:A:613:ASP:OD2	1.85	0.75
1:A:296:ILE:HD11	3:A:2075:HOH:O	1.92	0.68
1:A:534:THR:HG22	1:A:536:SER:H	1.57	0.68
1:A:597:GLN:HE21	1:A:597:GLN:N	1.94	0.66
1:A:534:THR:HG21	3:A:2315:HOH:O	1.95	0.65
1:A:445[B]:ILE:HD11	1:A:477:TRP:HE3	1.60	0.65
1:A:612:GLU:HB2	1:A:613:ASP:HA	1.79	0.65
1:A:533:GLU:O	1:A:534:THR:HB	2.00	0.62
1:A:128:ALA:N	3:A:2001:HOH:O	2.33	0.61
1:A:611:HIS:HB2	1:A:613:ASP:HB2	1.84	0.60
1:A:131:HIS:HD2	1:A:252:THR:OG1	1.85	0.59
1:A:284:PHE:C	1:A:285:ARG:HG2	2.22	0.59
1:A:534:THR:HG22	1:A:535:GLU:N	2.18	0.59
1:A:296:ILE:HD13	1:A:393:HIS:CE1	2.37	0.58
1:A:429:ALA:O	1:A:430:ARG:NH1	2.37	0.58
1:A:611:HIS:CB	1:A:613:ASP:HB2	2.37	0.54
1:A:457:HIS:HD2	1:A:476:TYR:OH	1.91	0.54
1:A:165:ASP:OD1	1:A:286:LYS:NZ	2.36	0.53
1:A:131:HIS:CD2	1:A:252:THR:OG1	2.62	0.53
1:A:447:LEU:HD21	1:A:497:LEU:HB2	1.90	0.52
1:A:355:LYS:HE2	1:A:490:VAL:HG21	1.92	0.51
1:A:285:ARG:CZ	1:A:400:LEU:HD21	2.40	0.51
1:A:529[B]:ARG:HD3	1:A:532:SER:OG	2.11	0.51
1:A:611:HIS:C	1:A:613:ASP:HB2	2.32	0.50
1:A:584:ARG:HG3	1:A:587:ILE:HD12	1.94	0.50
1:A:446:LYS:CE	1:A:593:LYS:O	2.60	0.49
1:A:569:ARG:HB2	1:A:569:ARG:HH11	1.77	0.49
1:A:465:ALA:O	1:A:469:MET:HG3	2.15	0.47
1:A:612:GLU:N	1:A:613:ASP:HB2	2.30	0.46
1:A:463:ARG:O	1:A:467:GLU:HG3	2.16	0.45
1:A:534:THR:CG2	1:A:535:GLU:N	2.79	0.45
1:A:543:ILE:HG21	1:A:603:GLU:HB3	1.99	0.44
1:A:455:HIS:HD2	3:A:2017:HOH:O	1.99	0.44
1:A:380:LEU:HD11	1:A:388:LYS:HE2	1.99	0.44
1:A:242:MET:HG2	1:A:243:VAL:N	2.32	0.43
1:A:475:PRO:HG2	1:A:477:TRP:CE2	2.54	0.43
1:A:445[B]:ILE:HD12	1:A:445[B]:ILE:HA	1.62	0.43
1:A:375:SER:O	1:A:376:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLU:O	1:A:534:THR:CB	2.65	0.42
1:A:149[B]:SER:HB3	1:A:463:ARG:HG3	2.01	0.42
1:A:263:THR:HG23	1:A:264:PRO:HD2	2.02	0.42
1:A:597:GLN:HE21	1:A:597:GLN:CA	2.33	0.41
1:A:529[A]:ARG:NH1	3:A:2295:HOH:O	2.53	0.41
1:A:193:PHE:O	1:A:200:GLU:HA	2.21	0.41
1:A:345:PRO:CD	1:A:565:ILE:HD13	2.51	0.41
1:A:529[B]:ARG:HA	1:A:529[B]:ARG:HD3	1.52	0.41
1:A:430:ARG:NH1	3:A:2229:HOH:O	2.54	0.41
1:A:594:ASP:HB3	1:A:596:GLU:HG2	2.02	0.41
1:A:612:GLU:CB	1:A:613:ASP:HA	2.48	0.40

All (2) 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)
3:A:2124:HOH:O	3:A:2244:HOH:O[2_556]	1.37	0.83
1:A:613:ASP:C	3:A:2226:HOH:O[1_565]	2.01	0.19

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	479/510 (94%)	464 (97%)	15 (3%)	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	399/419 (95%)	388 (97%)	11 (3%)	51 35

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	LEU
1	A	215	GLN
1	A	239	ARG
1	A	278	LYS
1	A	326	LEU
1	A	384	LYS
1	A	542	THR
1	A	569	ARG
1	A	584	ARG
1	A	597	GLN
1	A	611	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	366	ASN
1	A	455	HIS
1	A	457	HIS
1	A	479	GLN
1	A	597	GLN
1	A	611	HIS

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 [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	A	1000	-	52,58,58	1.32	8 (15%)	52,89,89	2.52	14 (26%)

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	A	1000	-	-	0/30/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C2-N1	-2.55	1.32	1.38
2	A	1000	FAD	C9A-N10	2.01	1.41	1.38
2	A	1000	FAD	C2A-N3A	2.19	1.36	1.32
2	A	1000	FAD	C5A-C4A	2.40	1.45	1.40
2	A	1000	FAD	C8-C7	2.56	1.47	1.41
2	A	1000	FAD	C9A-C5X	3.47	1.49	1.42
2	A	1000	FAD	C4-C4X	3.58	1.48	1.41
2	A	1000	FAD	C4X-C10	3.59	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	C4-C4X-C10	-7.40	115.21	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	N3A-C2A-N1A	-6.65	123.65	128.87
2	A	1000	FAD	N3-C2-N1	-3.84	121.22	127.69
2	A	1000	FAD	C4X-C4-N3	-3.73	118.65	123.52
2	A	1000	FAD	C4X-C10-N10	-2.80	118.49	120.52
2	A	1000	FAD	C1B-N9A-C4A	-2.49	124.02	126.81
2	A	1000	FAD	C9A-C5X-N5	-2.13	118.71	122.18
2	A	1000	FAD	C6-C5X-N5	2.12	121.56	118.92
2	A	1000	FAD	C1'-N10-C9A	2.61	121.86	118.83
2	A	1000	FAD	C5X-C9A-N10	2.90	119.75	117.58
2	A	1000	FAD	N6A-C6A-N1A	3.27	124.00	118.52
2	A	1000	FAD	C4-C4X-N5	3.57	123.04	118.70
2	A	1000	FAD	C4X-N5-C5X	4.25	121.73	116.72
2	A	1000	FAD	C4-N3-C2	9.18	122.82	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	472/510 (92%)	0.00	17 (3%) 46 40	12, 25, 46, 89	1 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	544	PRO	4.7
1	A	545	PRO	4.3
1	A	560	TYR	4.1
1	A	543	ILE	4.0
1	A	613	ASP	3.8
1	A	599	GLU	3.4
1	A	570	ASP	3.2
1	A	541	ILE	3.1
1	A	611	HIS	2.8
1	A	537	GLU	2.7
1	A	183	ASP	2.7
1	A	375	SER	2.5
1	A	376	SER	2.5
1	A	374	VAL	2.4
1	A	210	PHE	2.3
1	A	542	THR	2.1
1	A	128	ALA	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	A	1000	53/53	0.96	0.09	-0.31	14,17,20,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.