



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:53 AM UTC

PDB ID : 8VGY / pdb_00008vgy
Title : Crystal structure of human apoptosis-inducing factor (AIF) bound to the fused N-terminal domain of CHCHD4
Authors : Brosey, C.A.; Tainer, J.A.
Deposited on : 2023-12-29
Resolution : 2.30 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)
Xtriage (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

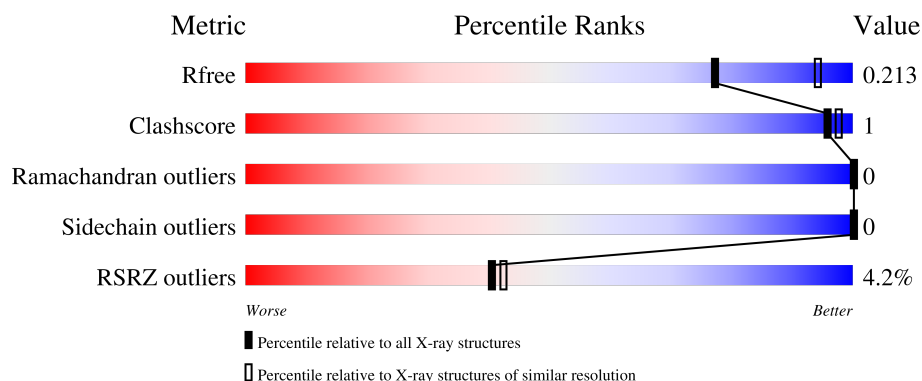
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	A	571	4% 81% 17%
1	C	571	3% 77% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14678 atoms, of which 7112 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,Mitochondrial intermembrane space import and assembly protein 40.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	473	Total	C	H	N	O	S	0	0	0
			7163	2275	3572	639	664	13			
1	C	456	Total	C	H	N	O	S	0	0	0
			6940	2208	3467	619	634	12			

There are 34 discrepancies between the modelled and reference sequences:

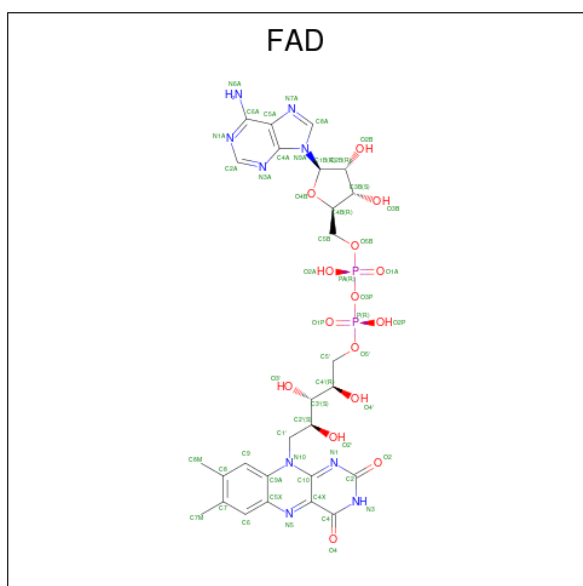
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	initiating methionine	UNP O95831
A	196	ALA	TRP	engineered mutation	UNP O95831
A	992	SER	-	linker	UNP O95831
A	993	GLY	-	linker	UNP O95831
A	994	SER	-	linker	UNP O95831
A	995	GLY	-	linker	UNP O95831
A	996	PRO	-	linker	UNP O95831
A	997	GLY	-	linker	UNP O95831
A	998	SER	-	linker	UNP O95831
A	999	GLY	-	linker	UNP O95831
A	1000	SER	-	linker	UNP O95831
A	1046	LEU	-	expression tag	UNP Q8N4Q1
A	1047	GLU	-	expression tag	UNP Q8N4Q1
A	1048	VAL	-	expression tag	UNP Q8N4Q1
A	1049	LEU	-	expression tag	UNP Q8N4Q1
A	1050	PHE	-	expression tag	UNP Q8N4Q1
A	1051	GLN	-	expression tag	UNP Q8N4Q1
C	103	MET	-	initiating methionine	UNP O95831
C	196	ALA	TRP	engineered mutation	UNP O95831
C	992	SER	-	linker	UNP O95831
C	993	GLY	-	linker	UNP O95831
C	994	SER	-	linker	UNP O95831
C	995	GLY	-	linker	UNP O95831
C	996	PRO	-	linker	UNP O95831

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Chain	Residue	Modelled	Actual	Comment	Reference
C	997	GLY	-	linker	UNP O95831
C	998	SER	-	linker	UNP O95831
C	999	GLY	-	linker	UNP O95831
C	1000	SER	-	linker	UNP O95831
C	1046	LEU	-	expression tag	UNP Q8N4Q1
C	1047	GLU	-	expression tag	UNP Q8N4Q1
C	1048	VAL	-	expression tag	UNP Q8N4Q1
C	1049	LEU	-	expression tag	UNP Q8N4Q1
C	1050	PHE	-	expression tag	UNP Q8N4Q1
C	1051	GLN	-	expression tag	UNP Q8N4Q1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			83	27	30	9	15	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

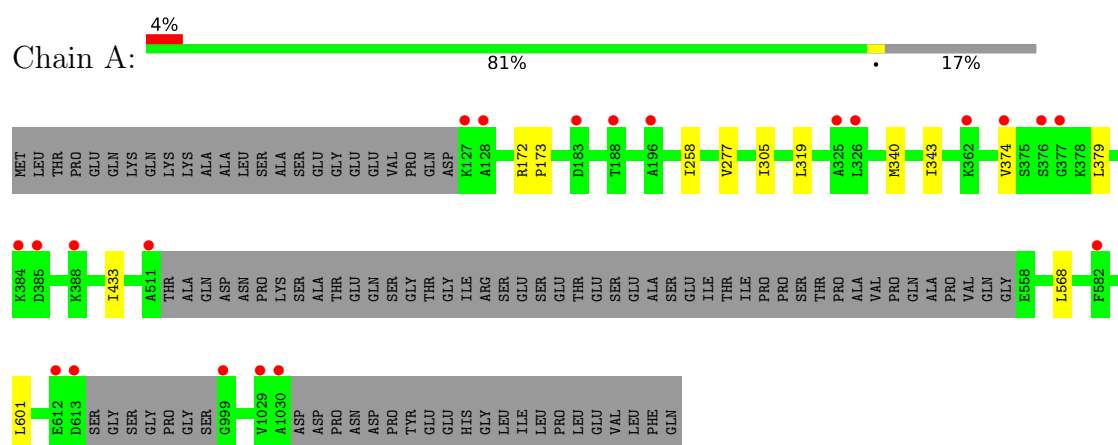
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	C	189	Total	O	0	0
			189	189		

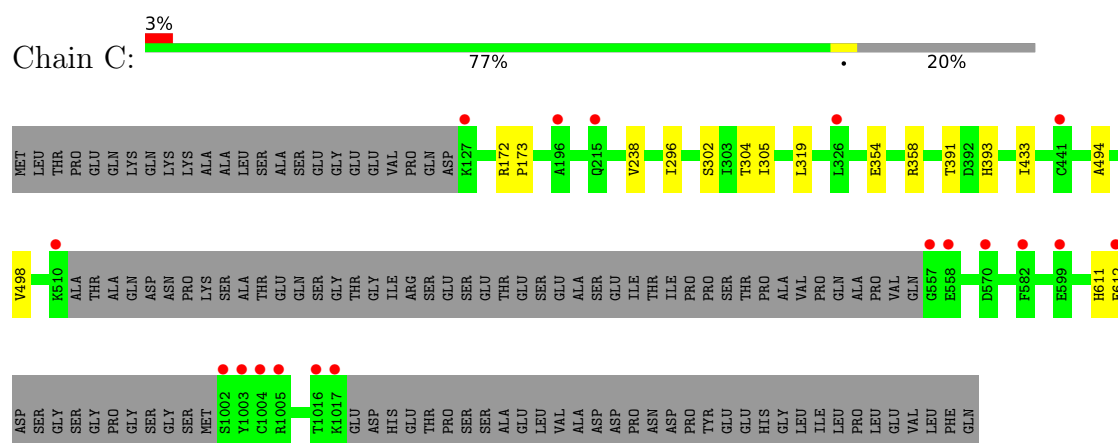
3 Residue-property plots [i](#)

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, Mitochondrial intermembrane space import and assembly protein 40



- Molecule 1: Apoptosis-inducing factor 1, mitochondrial, Mitochondrial intermembrane space import and assembly protein 40



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.61Å 109.20Å 174.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.59 – 2.30 92.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (92.59-2.30) 100.0 (92.59-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.181 , 0.212 0.182 , 0.213	Depositor DCC
R_{free} test set	2864 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14678	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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, EDO

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	0.13	0/3660	0.29	0/4952
1	C	0.11	0/3541	0.29	0/4789
All	All	0.12	0/7201	0.29	0/9741

There are no bond length outliers.

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	A	3591	3572	3570	7	0
1	C	3473	3467	3467	9	0
2	A	53	31	31	0	0
2	C	53	30	31	0	0
3	A	8	12	12	0	0
4	A	199	0	0	0	0
4	C	189	0	0	0	0
All	All	7566	7112	7111	16	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 1.

All (16) 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:C:304:THR:OG1	1:C:391:THR:HG21	1.84	0.78
1:A:258:ILE:HG13	1:A:433:ILE:HD11	1.81	0.62
1:A:374:VAL:HG22	1:A:379:LEU:HD23	1.83	0.61
1:C:302:SER:OG	1:C:391:THR:HG22	2.02	0.60
1:C:238:VAL:HG22	1:C:433:ILE:CD1	2.41	0.51
1:A:568:LEU:HD21	1:A:601:LEU:HD11	1.95	0.48
1:C:172:ARG:N	1:C:173:PRO:CD	2.76	0.48
1:C:494:ALA:HB1	1:C:498:VAL:HG21	1.94	0.48
1:A:305:ILE:HD11	1:A:319:LEU:HD12	1.96	0.47
1:A:172:ARG:N	1:A:173:PRO:CD	2.78	0.46
1:C:354:GLU:O	1:C:358:ARG:HG2	2.17	0.45
1:C:305:ILE:HD11	1:C:319:LEU:HD12	1.99	0.44
1:A:277:VAL:HG23	1:A:374:VAL:HG23	2.02	0.42
1:A:340:MET:CE	1:A:343:ILE:HD11	2.49	0.41
1:C:296:ILE:HD13	1:C:393:HIS:CE1	2.56	0.41
1:C:611:HIS:O	1:C:612:GLU:C	2.64	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	467/571 (82%)	452 (97%)	15 (3%)	0	100	100
1	C	450/571 (79%)	436 (97%)	14 (3%)	0	100	100
All	All	917/1142 (80%)	888 (97%)	29 (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	372/471 (79%)	372 (100%)	0	100	100
1	C	359/471 (76%)	359 (100%)	0	100	100
All	All	731/942 (78%)	731 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	241	ASN
1	A	432	ASN
1	A	454	HIS
1	A	478	HIS
1	C	241	ASN
1	C	366	ASN
1	C	432	ASN
1	C	454	HIS
1	C	457	HIS
1	C	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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	$\# Z > 2$
3	EDO	A	1703	-	3,3,3	0.40	0	2,2,2	0.52	0
2	FAD	A	1701	-	58,58,58	1.45	4 (6%)	85,89,89	0.91	3 (3%)
3	EDO	A	1702	-	3,3,3	0.43	0	2,2,2	0.37	0
2	FAD	C	1701	-	58,58,58	1.48	5 (8%)	85,89,89	0.94	4 (4%)

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
3	EDO	A	1703	-	-	0/1/1/1	-
2	FAD	A	1701	-	-	4/34/50/50	0/6/6/6
3	EDO	A	1702	-	-	0/1/1/1	-
2	FAD	C	1701	-	-	3/34/50/50	0/6/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1701	FAD	C9-C9A	6.26	1.49	1.39
2	A	1701	FAD	C9-C9A	6.22	1.49	1.39
2	A	1701	FAD	C6-C5X	6.14	1.49	1.40
2	C	1701	FAD	C6-C5X	6.03	1.49	1.40
2	C	1701	FAD	O5'-C5'	3.25	1.56	1.44
2	A	1701	FAD	O5'-C5'	3.25	1.56	1.44
2	C	1701	FAD	PA-O2A	-2.39	1.44	1.55
2	A	1701	FAD	C1'-C2'	2.07	1.55	1.52
2	C	1701	FAD	C1'-C2'	2.06	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1701	FAD	C4-N3-C2	-2.83	120.62	125.64
2	A	1701	FAD	C4-N3-C2	-2.59	121.04	125.64
2	C	1701	FAD	C4'-C3'-C2'	-2.21	109.89	113.57
2	C	1701	FAD	C9-C9A-N10	2.14	124.73	121.85
2	A	1701	FAD	C5'-C4'-C3'	-2.11	108.24	112.22
2	A	1701	FAD	C4'-C3'-C2'	-2.08	110.11	113.57
2	C	1701	FAD	C5'-C4'-C3'	-2.06	108.33	112.22

There are no chirality outliers.

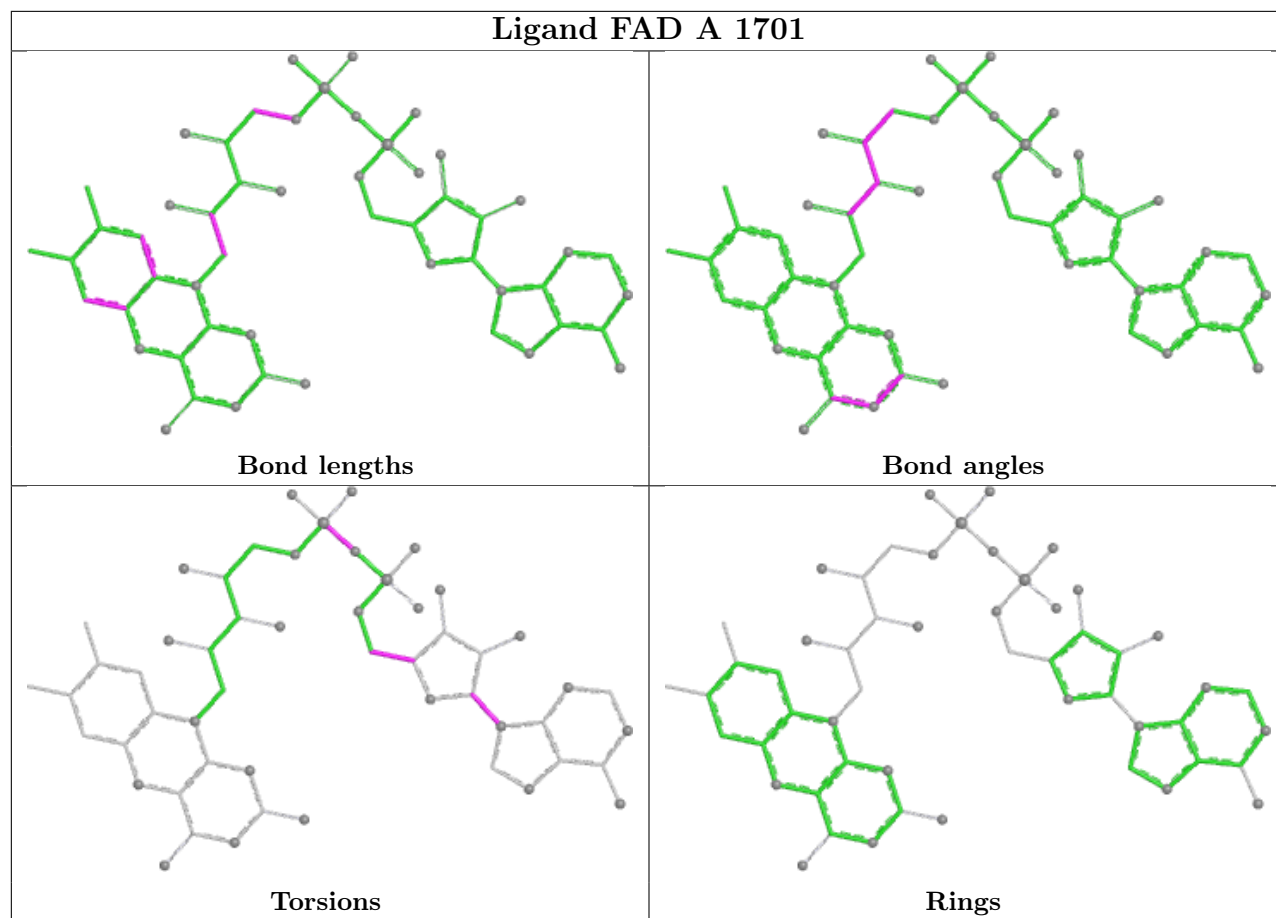
All (7) torsion outliers are listed below:

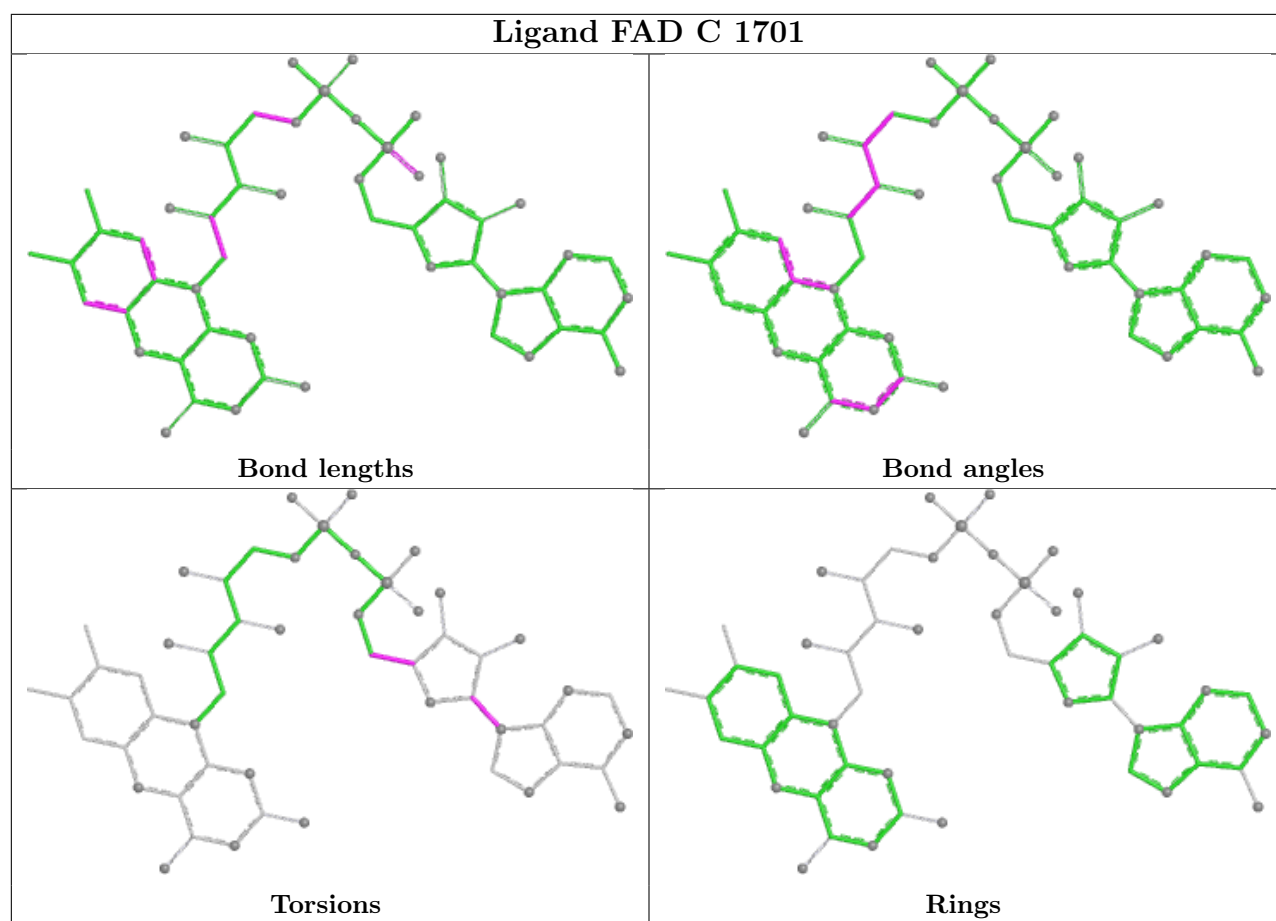
Mol	Chain	Res	Type	Atoms
2	C	1701	FAD	C3B-C4B-C5B-O5B
2	C	1701	FAD	O4B-C4B-C5B-O5B
2	A	1701	FAD	C3B-C4B-C5B-O5B
2	A	1701	FAD	C2B-C1B-N9A-C8A
2	C	1701	FAD	C2B-C1B-N9A-C8A
2	A	1701	FAD	O4B-C4B-C5B-O5B
2	A	1701	FAD	PA-O3P-P-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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	A	473/571 (82%)	0.14	21 (4%) 39 41	32, 51, 91, 116	0
1	C	456/571 (79%)	0.19	18 (3%) 43 45	34, 58, 95, 120	0
All	All	929/1142 (81%)	0.17	39 (4%) 40 42	32, 55, 93, 120	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	ASP	7.8
1	C	612	GLU	7.0
1	A	1030	ALA	6.5
1	A	999	GLY	6.0
1	C	1003	TYR	5.0
1	C	557	GLY	4.9
1	A	127	LYS	4.8
1	C	326	LEU	4.7
1	C	127	LYS	4.5
1	A	326	LEU	4.5
1	C	510	LYS	4.3
1	C	1017	LYS	4.3
1	C	441	CYS	4.3
1	A	612	GLU	4.1
1	C	1002	SER	4.0
1	C	215	GLN	3.5
1	A	196	ALA	3.4
1	A	183	ASP	3.3
1	C	599	GLU	3.2
1	C	1016	THR	3.2
1	C	1004	CYS	3.1
1	C	558	GLU	2.9
1	A	388	LYS	2.8
1	A	511	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	188	THR	2.7
1	C	570	ASP	2.7
1	A	1029	VAL	2.6
1	A	384	LYS	2.5
1	C	1005	ARG	2.4
1	A	377	GLY	2.4
1	C	196	ALA	2.4
1	A	385	ASP	2.3
1	A	582	PHE	2.3
1	A	325	ALA	2.3
1	A	128	ALA	2.2
1	A	374	VAL	2.1
1	C	582	PHE	2.1
1	A	376	SER	2.0
1	A	362	LYS	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](#)

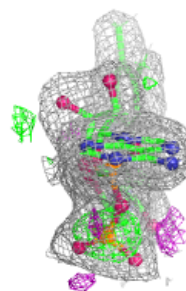
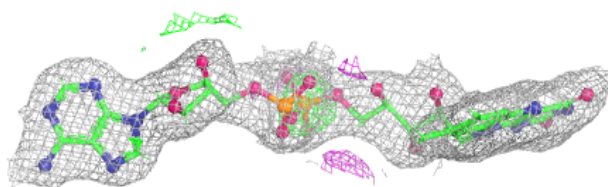
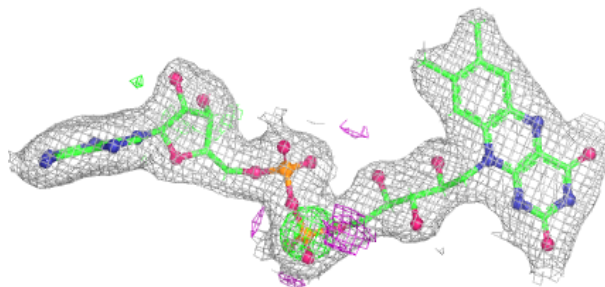
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	1703	4/4	0.90	0.16	44,52,59,68	0
3	EDO	A	1702	4/4	0.93	0.14	39,48,57,57	0
2	FAD	A	1701	53/53	0.96	0.07	34,42,53,78	0
2	FAD	C	1701	53/53	0.97	0.06	33,40,52,65	0

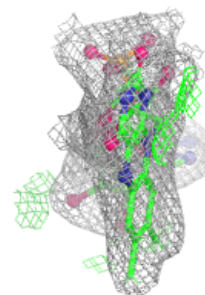
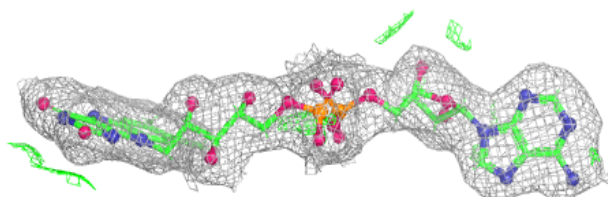
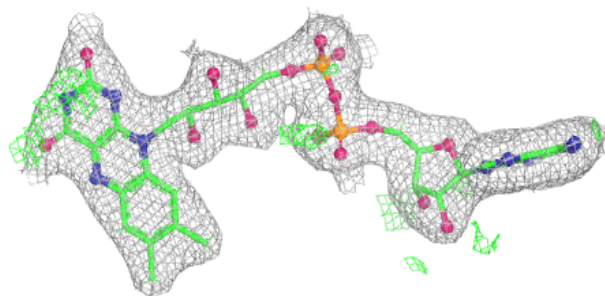
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD A 1701:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD C 1701:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.