Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:47 pm BST

PDB ID	:	5MIU
Title	:	G307E variant of Murine Apoptosis Inducing Factor (oxidized state)
Authors	:	Sorrentino, L.; Cossu, F.; Milani, M.; Aliverti, A.; Mastrangelo, E.
Deposited on	:	2016-11-29
Resolution	:	3.50 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:

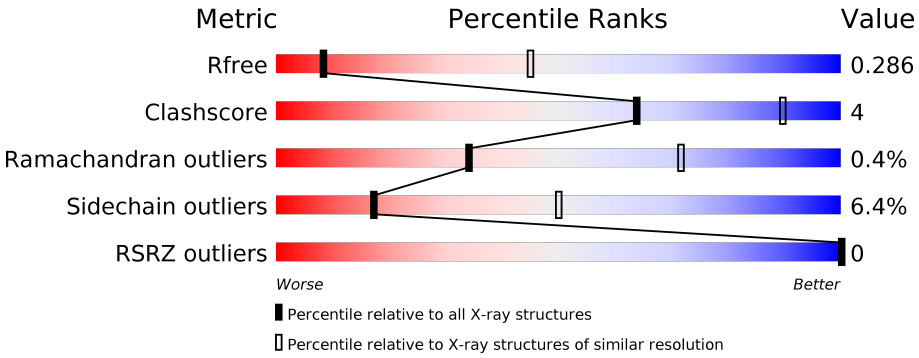
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	535	75% 9% • 15%
1	B	535	72% 10% • 16%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7086 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.

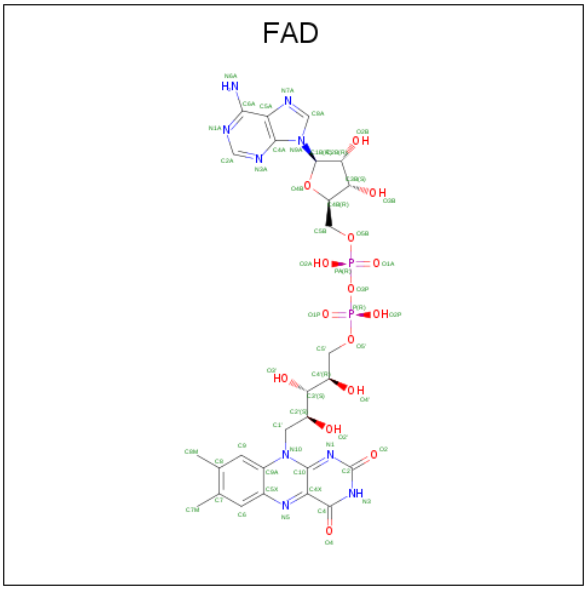
- Molecule 1 is a protein called Apoptosis-inducing factor 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3496	2217	624	644	11			
1	B	447	Total	C	N	O	S	0	0	0
			3459	2197	615	636	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	307	GLU	GLY	conflict	UNP Q9Z0X1
B	307	GLU	GLY	conflict	UNP Q9Z0X1

- 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
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is water.

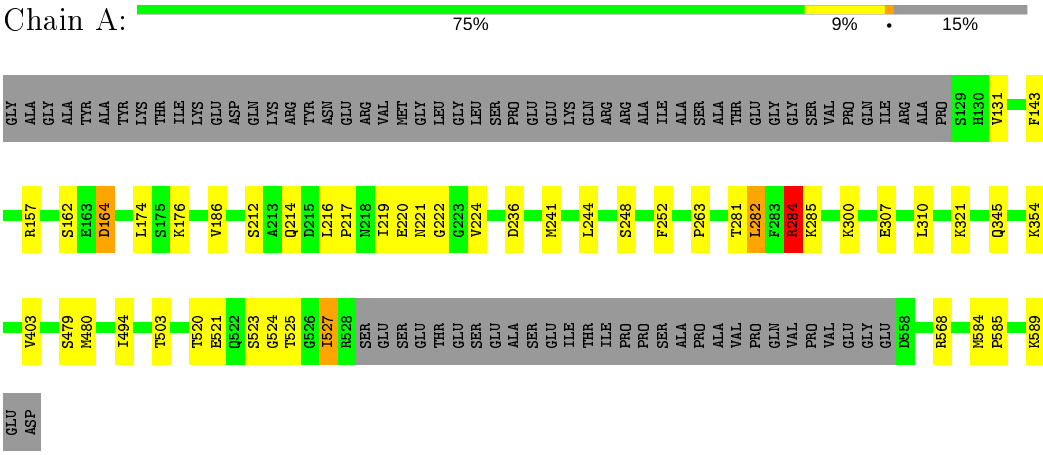
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	15	Total	O	0	0
			15	15		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

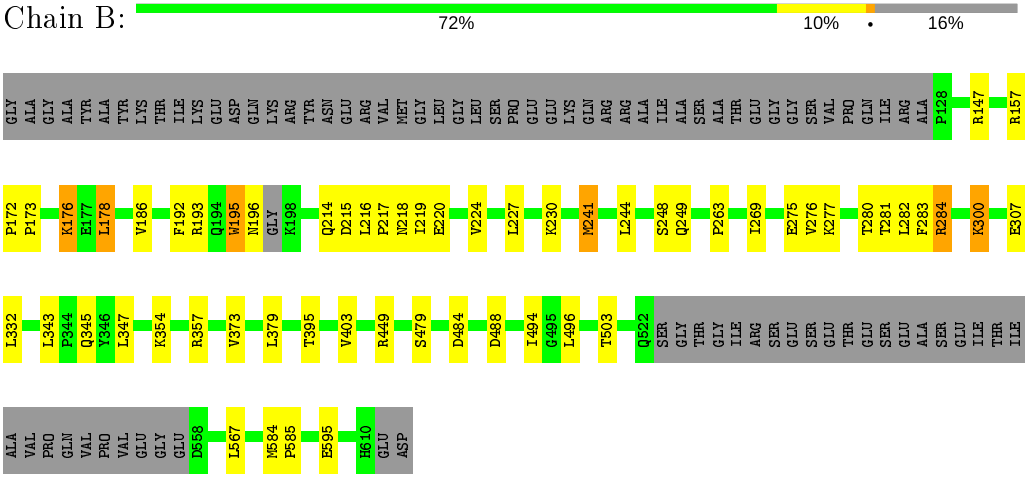
- Molecule 1: Apoptosis-inducing factor 1, mitochondrial

Chain A:



- Molecule 1: Apoptosis-inducing factor 1, mitochondrial

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.04Å 110.06Å 119.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 3.50 47.75 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.70-3.50) 99.4 (47.75-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.279 0.221 , 0.286	Depositor DCC
R_{free} test set	857 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7086	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	1/3565 (0.0%)	0.66	4/4816 (0.1%)
1	B	0.42	0/3528	0.62	1/4766 (0.0%)
All	All	0.44	1/7093 (0.0%)	0.64	5/9582 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	523	SER	CA-CB	11.01	1.69	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	523	SER	CB-CA-C	-13.81	83.87	110.10
1	B	196	ASN	N-CA-CB	7.55	124.19	110.60
1	A	523	SER	N-CA-C	-7.36	91.14	111.00
1	A	523	SER	N-CA-CB	-6.50	100.75	110.50
1	A	282	LEU	N-CA-C	-5.21	96.93	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	3496	0	3533	27	0
1	B	3459	0	3495	32	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
3	A	10	0	0	1	0
3	B	15	0	0	0	0
All	All	7086	0	7090	59	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 4.

All (59) 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:178:LEU:CD1	1:B:192:PHE:HB3	1.94	0.97
1:B:176:LYS:NZ	2:B:701:FAD:O4	2.10	0.84
1:B:157:ARG:NH2	1:B:219:ILE:O	2.18	0.75
1:A:157:ARG:NH1	1:A:217:PRO:O	2.26	0.69
1:A:281:THR:HG22	1:A:282:LEU:O	1.95	0.66
1:B:178:LEU:HD12	1:B:192:PHE:HB3	1.75	0.65
1:B:281:THR:HG22	1:B:282:LEU:O	1.98	0.63
1:B:178:LEU:HD11	1:B:192:PHE:HB3	1.80	0.60
1:B:195:TRP:HH2	1:B:484:ASP:OD2	1.84	0.60
1:A:281:THR:HG22	1:A:282:LEU:N	2.18	0.59
1:A:520:THR:HG22	1:A:524:GLY:HA2	1.85	0.59
1:B:281:THR:HG22	1:B:282:LEU:N	2.18	0.56
1:B:172:PRO:HB2	1:B:173:PRO:HD3	1.87	0.55
1:B:269:ILE:O	1:B:277:LYS:HE3	2.07	0.55
1:B:275:GLU:HG3	1:B:373:VAL:HG21	1.90	0.55
1:B:283:PHE:O	1:B:283:PHE:HD1	1.90	0.54
1:B:281:THR:CG2	1:B:282:LEU:N	2.74	0.50
1:A:310:LEU:HD11	2:A:701:FAD:HM73	1.92	0.50
1:A:263:PRO:HG3	1:A:284:ARG:HG3	1.92	0.50
1:A:520:THR:CG2	1:A:524:GLY:HA2	2.42	0.49
1:B:300:LYS:O	1:B:327:ILE:HG13	2.13	0.48
1:B:283:PHE:CD1	1:B:283:PHE:C	2.86	0.48
1:A:219:ILE:HG23	1:A:222:GLY:HA3	1.96	0.48
1:A:164:ASP:OD2	1:A:285:LYS:NZ	2.36	0.48
1:A:520:THR:O	1:A:524:GLY:CA	2.61	0.48
1:B:263:PRO:HG3	1:B:284:ARG:HD3	1.96	0.48
1:A:236:ASP:HB3	1:A:241:MET:HG3	1.96	0.47
1:A:527:ILE:O	1:A:527:ILE:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:LYS:NZ	3:A:802:HOH:O	2.42	0.47
1:A:281:THR:CG2	1:A:282:LEU:N	2.77	0.47
1:A:524:GLY:C	1:A:525:THR:HG23	2.36	0.46
1:A:310:LEU:CD1	2:A:701:FAD:HM73	2.45	0.46
1:B:277:LYS:HA	1:B:280:THR:OG1	2.16	0.45
1:B:172:PRO:HB2	1:B:173:PRO:CD	2.47	0.44
1:B:283:PHE:O	1:B:283:PHE:CD1	2.70	0.44
1:A:220:GLU:O	1:A:221:ASN:ND2	2.51	0.44
1:B:479:SER:O	1:B:494:ILE:HD12	2.18	0.44
1:A:143:PHE:CE2	1:A:147:ARG:HD2	2.53	0.44
1:B:584:MET:N	1:B:585:PRO:HD2	2.32	0.44
1:A:520:THR:O	1:A:524:GLY:HA2	2.18	0.43
1:A:216:LEU:N	1:A:217:PRO:HD2	2.34	0.43
1:A:584:MET:N	1:A:585:PRO:HD2	2.33	0.43
1:B:244:LEU:HD12	1:B:248:SER:HB2	2.01	0.42
1:A:174:LEU:HD12	1:A:284:ARG:O	2.20	0.42
1:A:174:LEU:CD1	1:A:284:ARG:O	2.68	0.42
1:A:479:SER:O	1:A:494:ILE:HD12	2.19	0.42
1:B:241:MET:SD	1:B:249:GLN:NE2	2.93	0.42
1:B:332:LEU:C	1:B:332:LEU:HD12	2.40	0.41
1:A:131:VAL:O	1:A:252:PHE:HA	2.20	0.41
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.76	0.41
1:B:488:ASP:N	1:B:488:ASP:OD1	2.54	0.41
1:A:153:ASP:C	1:A:153:ASP:OD1	2.59	0.41
1:B:178:LEU:HA	1:B:178:LEU:HD12	1.87	0.41
1:B:277:LYS:O	1:B:280:THR:OG1	2.34	0.41
1:B:343:LEU:HD22	1:B:347:LEU:HD23	2.02	0.41
1:B:216:LEU:N	1:B:217:PRO:HD2	2.35	0.41
1:B:227:LEU:HD22	1:B:230:LYS:HG3	2.03	0.41
1:B:449:ARG:HD2	1:B:496:LEU:CD2	2.51	0.41
1:A:244:LEU:HD12	1:A:248:SER:HB2	2.02	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	A	449/535 (84%)	416 (93%)	30 (7%)	3 (1%)	22 61
1	B	441/535 (82%)	410 (93%)	30 (7%)	1 (0%)	47 81
All	All	890/1070 (83%)	826 (93%)	60 (7%)	4 (0%)	34 72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	ARG
1	A	527	ILE
1	A	403	VAL
1	B	403	VAL

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	371/436 (85%)	351 (95%)	20 (5%)	22 55
1	B	368/436 (84%)	341 (93%)	27 (7%)	14 45
All	All	739/872 (85%)	692 (94%)	47 (6%)	17 50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	SER
1	A	164	ASP
1	A	176	LYS
1	A	186	VAL
1	A	212	SER
1	A	214	GLN
1	A	224	VAL
1	A	284	ARG
1	A	300	LYS

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Mol	Chain	Res	Type
1	A	307	GLU
1	A	321	LYS
1	A	345	GLN
1	A	354	LYS
1	A	379	LEU
1	A	395	THR
1	A	480	MET
1	A	503	THR
1	A	521	GLU
1	A	568	ARG
1	A	595	GLU
1	B	147	ARG
1	B	162	SER
1	B	164	ASP
1	B	176	LYS
1	B	178	LEU
1	B	186	VAL
1	B	193	ARG
1	B	195	TRP
1	B	214	GLN
1	B	215	ASP
1	B	218	ASN
1	B	220	GLU
1	B	224	VAL
1	B	241	MET
1	B	276	VAL
1	B	284	ARG
1	B	300	LYS
1	B	307	GLU
1	B	323	GLN
1	B	345	GLN
1	B	354	LYS
1	B	357	ARG
1	B	379	LEU
1	B	395	THR
1	B	503	THR
1	B	567	LEU
1	B	595	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	ASN
1	A	338	ASN
1	A	402	ASN
1	A	456	HIS
1	A	467	ASN
1	A	610	HIS
1	B	338	ASN
1	B	402	ASN
1	B	467	ASN
1	B	522	GLN
1	B	596	GLN
1	B	610	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

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	701	-	51,58,58	1.97	8 (15%)	60,89,89	1.92	10 (16%)
2	FAD	A	701	-	51,58,58	1.84	7 (13%)	60,89,89	1.95	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	701	-	-	5/30/50/50	0/6/6/6
2	FAD	A	701	-	-	4/30/50/50	0/6/6/6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C4X-C10	10.18	1.49	1.38
2	A	701	FAD	C4X-C10	9.68	1.48	1.38
2	B	701	FAD	C4-C4X	4.35	1.48	1.41
2	B	701	FAD	C9A-C5X	3.97	1.50	1.42
2	A	701	FAD	C9A-C5X	3.77	1.50	1.42
2	A	701	FAD	C4-C4X	3.77	1.47	1.41
2	B	701	FAD	C8-C7	3.07	1.48	1.40
2	A	701	FAD	C8-C7	2.96	1.48	1.40
2	A	701	FAD	C9A-N10	2.92	1.42	1.38
2	B	701	FAD	C9A-N10	2.84	1.42	1.38
2	B	701	FAD	C5A-C4A	2.48	1.47	1.40
2	A	701	FAD	C5A-C4A	2.35	1.47	1.40
2	B	701	FAD	C10-N1	2.34	1.36	1.33
2	A	701	FAD	C2A-N3A	2.10	1.35	1.32
2	B	701	FAD	C2A-N3A	2.08	1.35	1.32

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	C4-N3-C2	8.56	122.37	115.14
2	B	701	FAD	C4-N3-C2	8.35	122.19	115.14
2	A	701	FAD	C1'-N10-C9A	5.41	122.55	118.29
2	B	701	FAD	C4-C4X-C10	-5.39	116.38	119.95
2	B	701	FAD	C1'-N10-C9A	5.00	122.23	118.29
2	A	701	FAD	N3A-C2A-N1A	-4.14	122.20	128.68
2	A	701	FAD	C4X-C4-N3	-3.94	118.04	123.43
2	B	701	FAD	N3A-C2A-N1A	-3.64	122.99	128.68
2	A	701	FAD	C4X-N5-C5X	3.63	120.40	116.77
2	A	701	FAD	C4-C4X-C10	-3.59	117.57	119.95
2	B	701	FAD	C9A-N10-C10	-3.40	117.45	121.91
2	A	701	FAD	C9A-N10-C10	-3.33	117.55	121.91
2	B	701	FAD	C4X-N5-C5X	3.25	120.02	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FAD	C4-C4X-N5	3.11	122.15	118.60
2	B	701	FAD	C4X-C4-N3	-2.90	119.46	123.43
2	B	701	FAD	C4A-C5A-N7A	-2.74	106.54	109.40
2	A	701	FAD	P-O3P-PA	-2.47	124.34	132.83
2	A	701	FAD	C4-C4X-N5	2.13	121.03	118.60
2	B	701	FAD	C1'-N10-C10	2.12	120.31	118.41
2	A	701	FAD	N6A-C6A-N1A	2.03	122.80	118.57
2	A	701	FAD	O2'-C2'-C1'	2.03	114.48	109.59

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	C3B-C4B-C5B-O5B
2	B	701	FAD	O3'-C3'-C4'-C5'
2	B	701	FAD	C2'-C3'-C4'-C5'
2	A	701	FAD	O3'-C3'-C4'-C5'
2	A	701	FAD	C2'-C3'-C4'-C5'
2	B	701	FAD	C2'-C3'-C4'-O4'

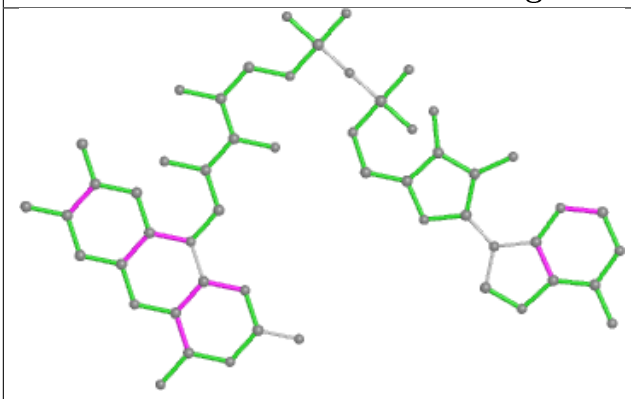
There are no ring outliers.

2 monomers are involved in 3 short contacts:

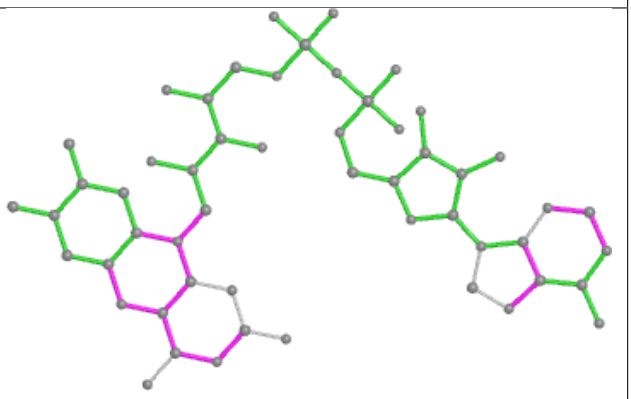
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	FAD	1	0
2	A	701	FAD	2	0

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 then 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.

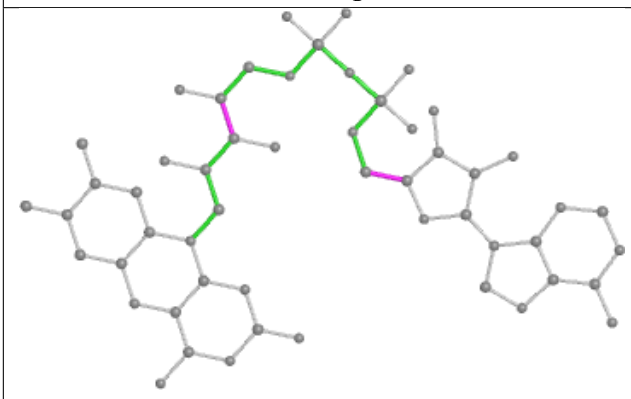
Ligand FAD B 701



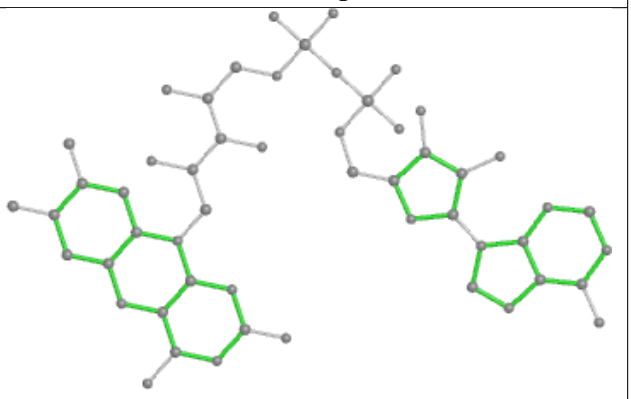
Bond lengths



Bond angles

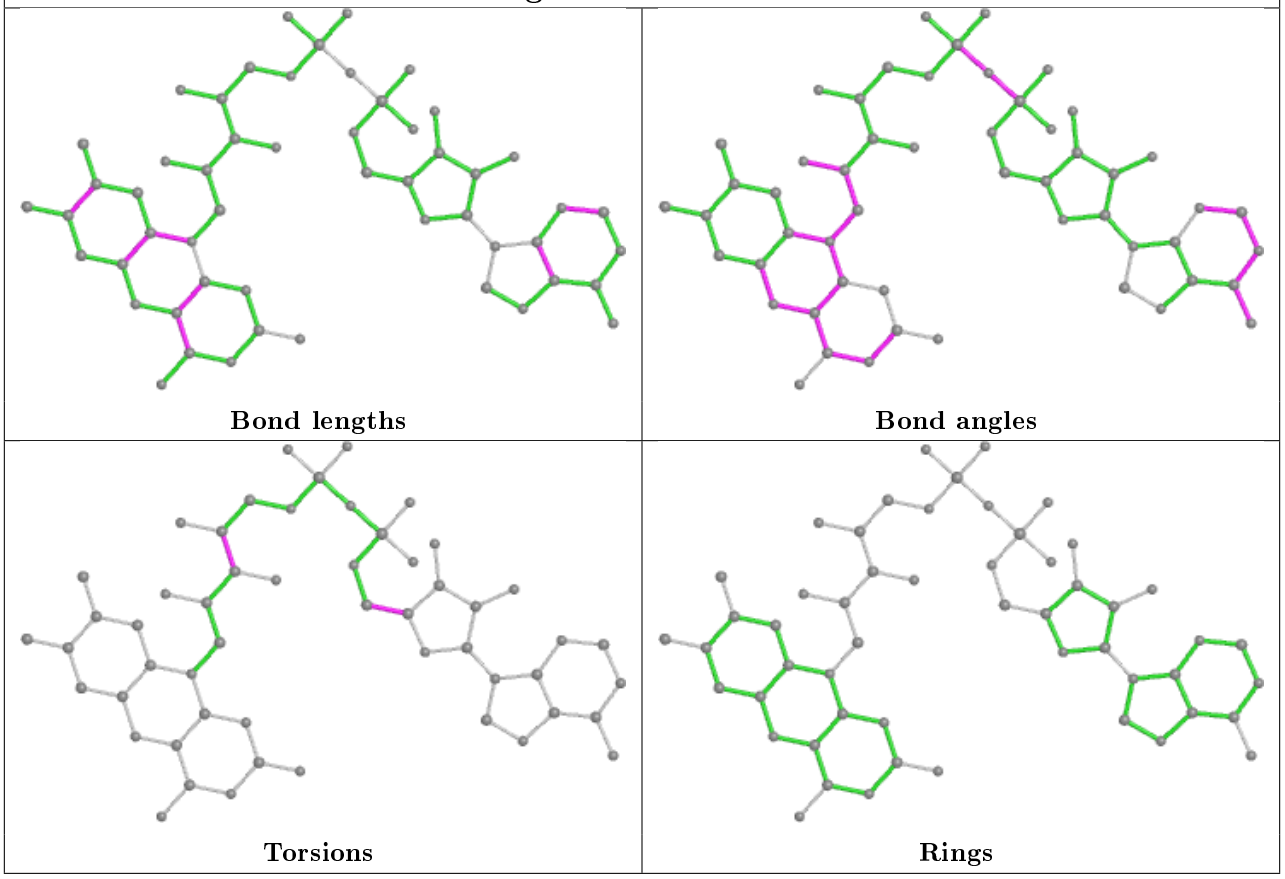


Torsions



Rings

Ligand FAD A 701



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

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, 95^{th} 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	453/535 (84%)	-0.47	0	100	100	30, 68, 100, 118	0
1	B	447/535 (83%)	-0.47	0	100	100	48, 73, 101, 130	1 (0%)
All	All	900/1070 (84%)	-0.47	0	100	100	30, 71, 101, 130	1 (0%)

There are no RSRZ outliers to report.

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

There are no carbohydrates in this entry.

6.4 Ligands

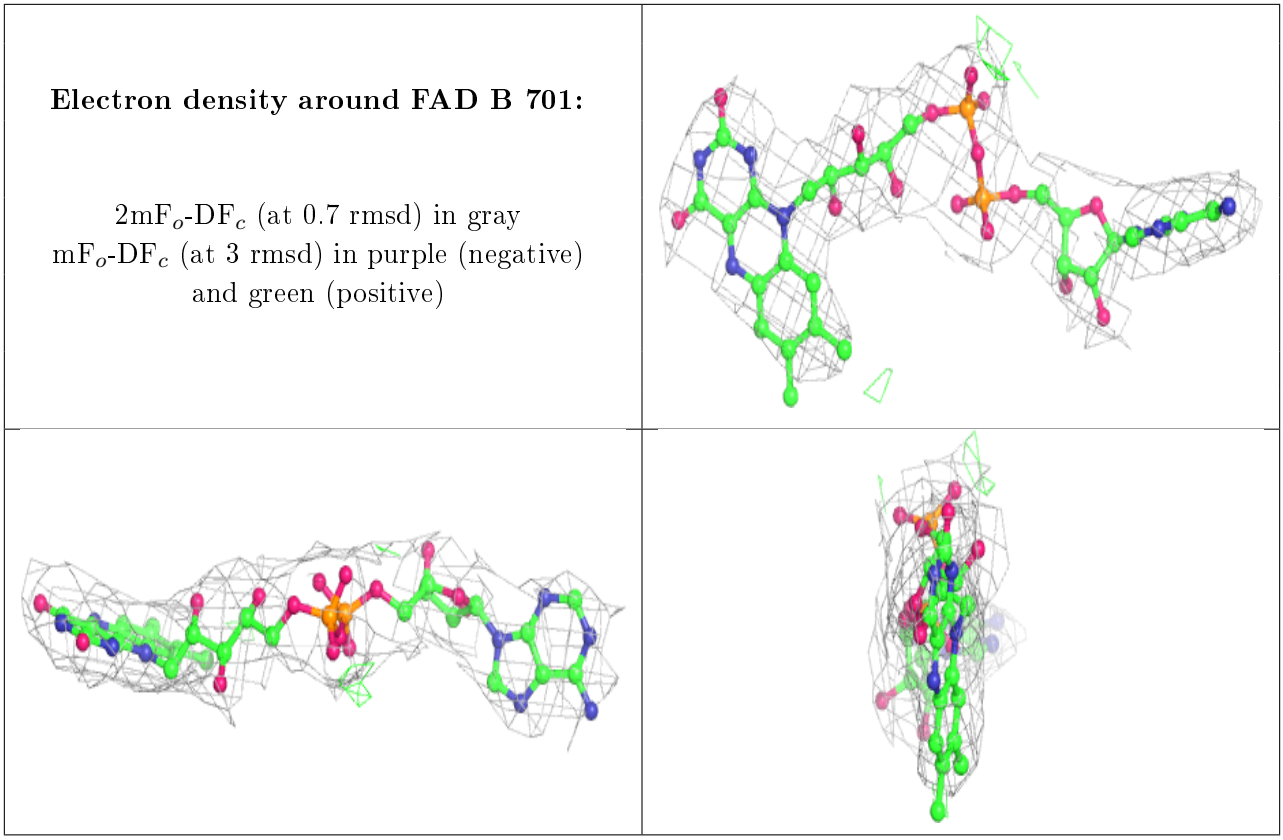
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	701	53/53	0.95	0.17	52,61,65,68	0
2	FAD	A	701	53/53	0.96	0.17	42,50,56,58	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.

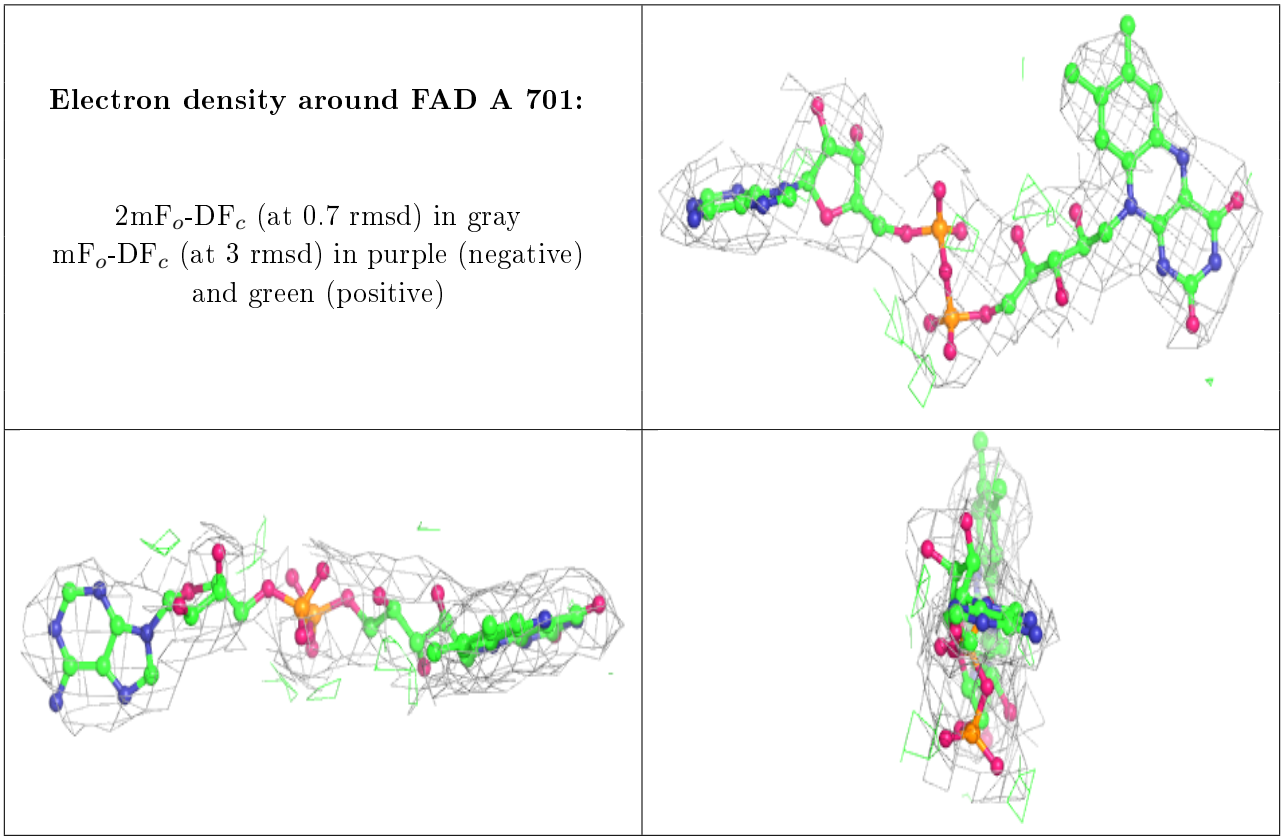
Electron density around FAD B 701:

$2mF_o$-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 A 701:

$2mF_o$-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.