



wwPDB X-ray Structure Validation Summary Report ⓘ

May 31, 2020 – 02:23 am BST

PDB ID : 2GMJ
Title : Structure of Porcine Electron Transfer Flavoprotein-Ubiquinone Oxidoreductase
Authors : Zhang, J.; Frerman, F.E.; Kim, J.-J.P.
Deposited on : 2006-04-06
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

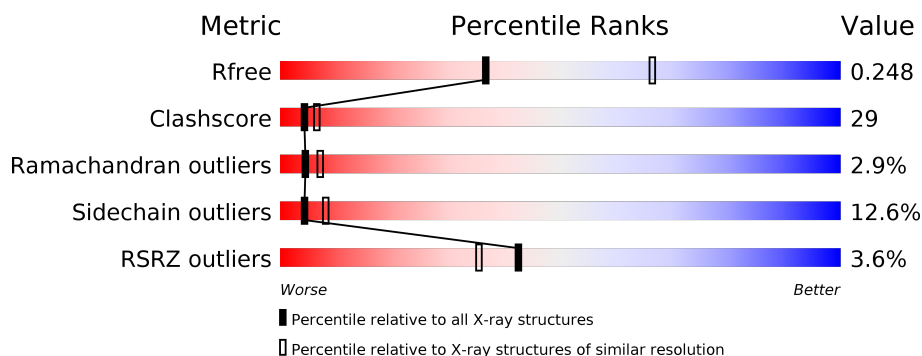
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	A	584	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 63% 30% 6% .. </div> </div>
1	B	584	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 6% 43% 45% 9% .. </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SF4	B	612	-	-	X	-

2 Entry composition [i](#)

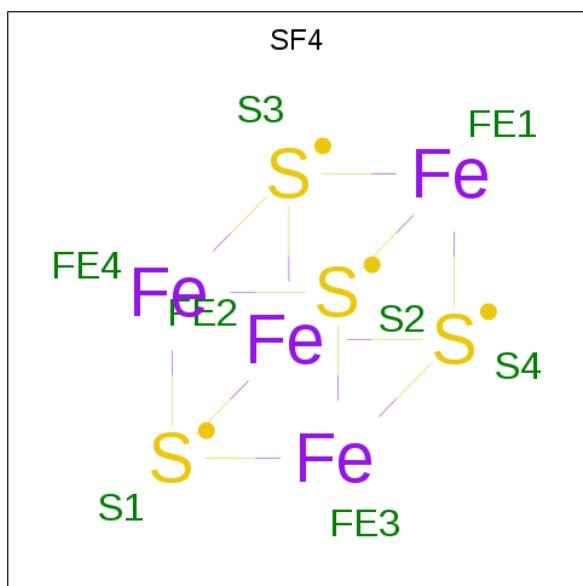
There are 5 unique types of molecules in this entry. The entry contains 9345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Electron transfer flavoprotein-ubiquinone oxidoreductase.

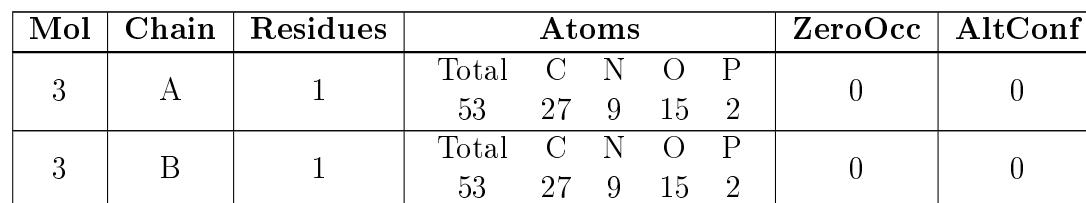
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4553	2907	791	835	20			
1	B	578	Total	C	N	O	S	0	0	0
			4531	2893	787	832	19			

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 4 1	0	0
4	A	1	Total C O 5 4 1	0	0



Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	4	1		
4	A	1	Total	C	O	0	0
			5	4	1		
4	B	1	Total	C	O	0	0
			5	4	1		
4	B	1	Total	C	O	0	0
			5	4	1		

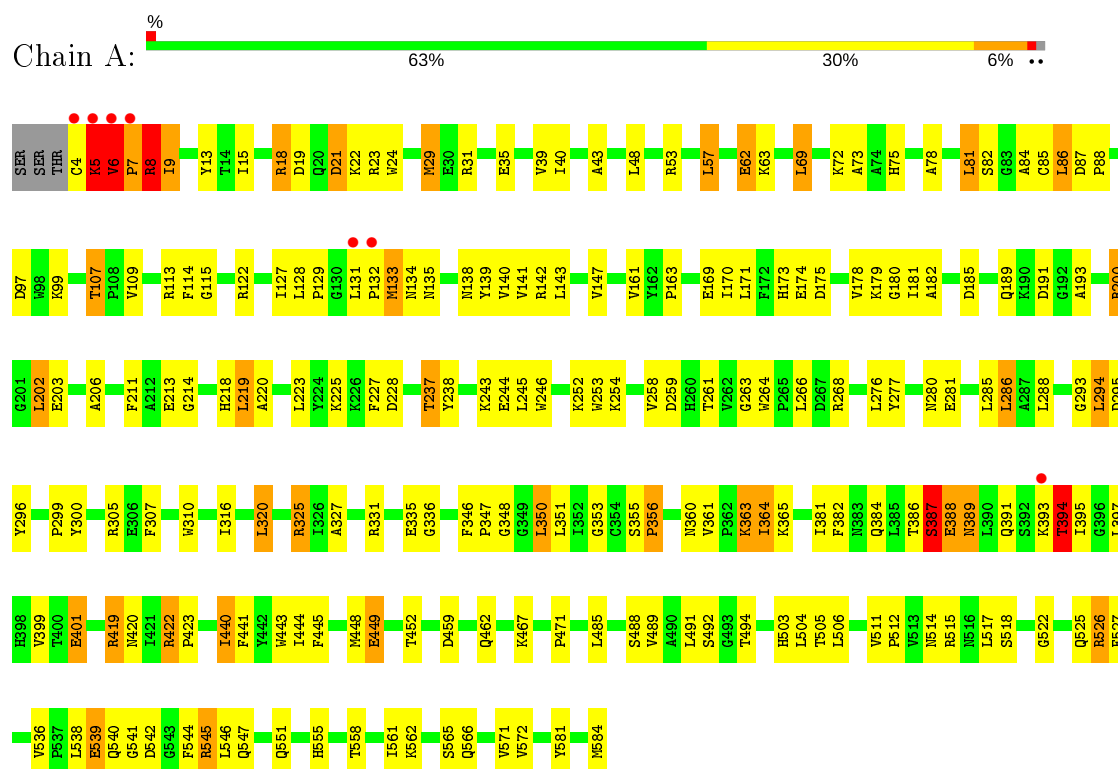
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	77	Total	O	0	0
			77	77		
5	B	32	Total	O	0	0
			32	32		

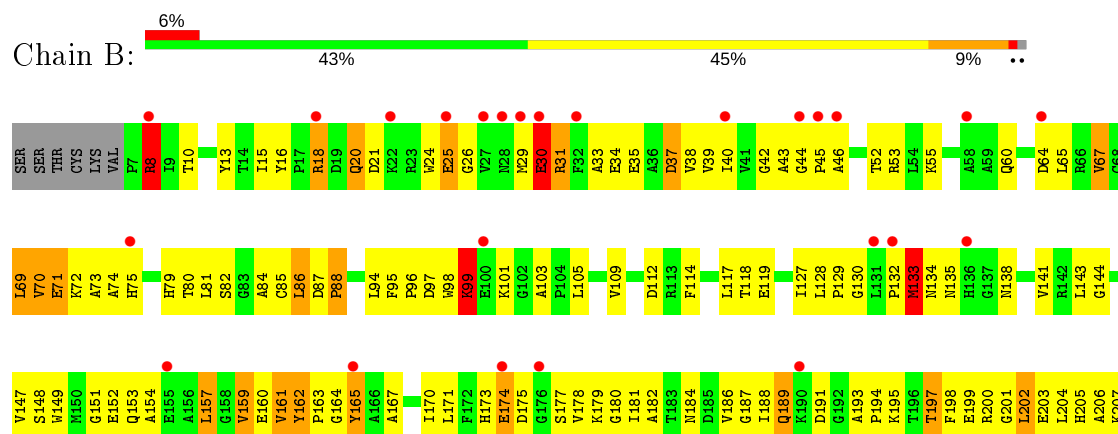
3 Residue-property plots

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: Electron transfer flavoprotein-ubiquinone oxidoreductase



- Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase



V208	L294	V361	G447	H526
T209	Q297	F362	M448	F527
I210	Q298	K363	E450	C528
F211	M298	I364	P450	P529
A212	P299	K365	M451	
E213	Y300	G366	T452	V532
	L301	T367	K456	V533
H216	S302	H368		E534
G217	P303	T369	K456	F535
H218	F304	H369	D459	V536
L219	R305	A370	S460	P537
	E306	M371	D461	L538
L223	F307	A378	Q462	E539
Y224	W310	E379	L463	Q540
F227	K311	S380	K467	G541
D228	H312	I381		D542
L229	H313	F382	P471	G543
R230		M383		F544
A231	I316	G384	P477	H545
M232	K317	L385		L546
C233	P318	T386	I481	Q551
E234	T319	M389	S482	
P235	L320	L390	F483	V554
Q236	E321	G391	D484	H555
		S392	L485	C556
I240	K324	K393	L486	K557
G241	R325	T394	S487	
L242	R326	I395	S488	I561
K243	A327	G396	V489	K562
E244		L397	A490	D563
L245	R331	H398	L491	
	A332		T494	N567
I248	L333	E401	N495	I568
D249	N334	Y402	H496	N569
E250	E335	E403		N570
K251	G336	L406	E497	V571
K252	S340	F407	H498	V572
	T341	M408		P573
R257	P342	W410	H503	E574
D259	K343	Y416	L504	
	I344	S417	T505	G577
W264	T345	V418	L506	G578
P265	P347	R419	V507	P579
L266	G348	M420	D508	
	G349	I421	D509	N584
F275	G349	R422	V510	
L276	L350	P423	P511	
Y277	L351		V512	
H278	I352	H426	V513	
L279	G353		N514	
	C354	I440	R515	
E283	S355	P441	N516	
P284	P356	Y442	L517	
L285	G357			
L286	F358		D521	
A287	M359	F445	G522	
	N360	R446	P523	
			E524	
			Q525	

4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	154.84Å 154.84Å 130.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.75 – 2.60 29.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.9 (28.75-2.60) 73.5 (29.57-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.255 0.222 , 0.248	Depositor DCC
R_{free} test set	3135 reflections (7.73%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9345	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: SF4, TBU, 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	0.48	0/4682	0.81	8/6356 (0.1%)
1	B	0.45	0/4660	0.81	5/6326 (0.1%)
All	All	0.46	0/9342	0.81	13/12682 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	541	GLY	N-CA-C	-8.53	91.78	113.10
1	B	544	PHE	N-CA-C	7.64	131.62	111.00
1	B	393	LYS	N-CA-C	-7.25	91.42	111.00
1	B	396	GLY	N-CA-C	-6.49	96.88	113.10
1	A	5	LYS	N-CA-C	6.40	128.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	162	TYR	Sidechain

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	4553	0	4450	169	0
1	B	4531	0	4424	361	0
2	A	8	0	0	0	0
2	B	8	0	0	3	0
3	A	53	0	30	2	0
3	B	53	0	30	4	0
4	A	20	0	40	5	0
4	B	10	0	20	0	0
5	A	77	0	0	2	0
5	B	32	0	0	1	0
All	All	9345	0	8994	530	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 29.

The worst 5 of 530 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:512:PRO:HB3	1:B:546:LEU:HD13	1.18	1.09
1:B:218:HIS:CE1	1:B:219:LEU:HG	1.88	1.08
1:B:393:LYS:CE	1:B:393:LYS:HA	1.83	1.06
1:B:351:LEU:HB3	1:B:356:PRO:HG3	1.38	1.05
1:B:299:PRO:HG3	1:B:463:LEU:HD22	1.41	1.02

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	579/584 (99%)	528 (91%)	38 (7%)	13 (2%)	6	12
1	B	576/584 (99%)	497 (86%)	58 (10%)	21 (4%)	3	4
All	All	1155/1168 (99%)	1025 (89%)	96 (8%)	34 (3%)	4	7

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	GLU
1	B	8	ARG
1	B	20	GLN
1	B	74	ALA
1	B	129	PRO

5.3.2 Protein sidechains ⓘ

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	482/486 (99%)	432 (90%)	50 (10%)	7	13
1	B	479/486 (99%)	408 (85%)	71 (15%)	3	5
All	All	961/972 (99%)	840 (87%)	121 (13%)	4	8

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	ARG
1	B	133	MET
1	B	505	THR
1	B	60	GLN
1	B	71	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	525	GLN
1	A	552	ASN
1	B	498	HIS
1	A	516	ASN
1	B	516	ASN

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 ⓘ

10 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	$\# Z > 2$
4	TBU	A	623	-	4,4,4	0.69	0	6,6,6	0.51	0
4	TBU	B	625	-	4,4,4	0.53	0	6,6,6	0.52	0
4	TBU	B	626	-	4,4,4	0.53	0	6,6,6	0.54	0
4	TBU	A	624	-	4,4,4	0.40	0	6,6,6	0.65	0
3	FAD	A	611	-	51,58,58	2.48	15 (29%)	60,89,89	3.00	18 (30%)
2	SF4	A	610	1	0,12,12	0.00	-	-	-	-
4	TBU	A	622	-	4,4,4	0.35	0	6,6,6	0.67	0
4	TBU	A	621	-	4,4,4	0.45	0	6,6,6	0.55	0
2	SF4	B	612	1	0,12,12	0.00	-	-	-	-
3	FAD	B	613	-	51,58,58	2.40	17 (33%)	60,89,89	3.17	19 (31%)

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	SF4	A	610	1	-	-	0/6/5/5
2	SF4	B	612	1	-	-	0/6/5/5
3	FAD	B	613	-	-	7/30/50/50	0/6/6/6
3	FAD	A	611	-	-	2/30/50/50	0/6/6/6

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	611	FAD	C1'-N10	-8.36	1.39	1.48
3	B	613	FAD	C9A-N10	7.70	1.48	1.38
3	A	611	FAD	C9A-N10	7.34	1.48	1.38
3	A	611	FAD	C4-N3	5.99	1.43	1.33
3	B	613	FAD	C4-N3	5.71	1.43	1.33

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	613	FAD	C4-N3-C2	14.95	127.77	115.14
3	A	611	FAD	C4-N3-C2	13.73	126.73	115.14
3	B	613	FAD	C10-C4X-N5	8.47	127.11	121.26
3	A	611	FAD	C10-C4X-N5	8.11	126.87	121.26
3	B	613	FAD	O3'-C3'-C2'	7.78	127.61	108.81

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

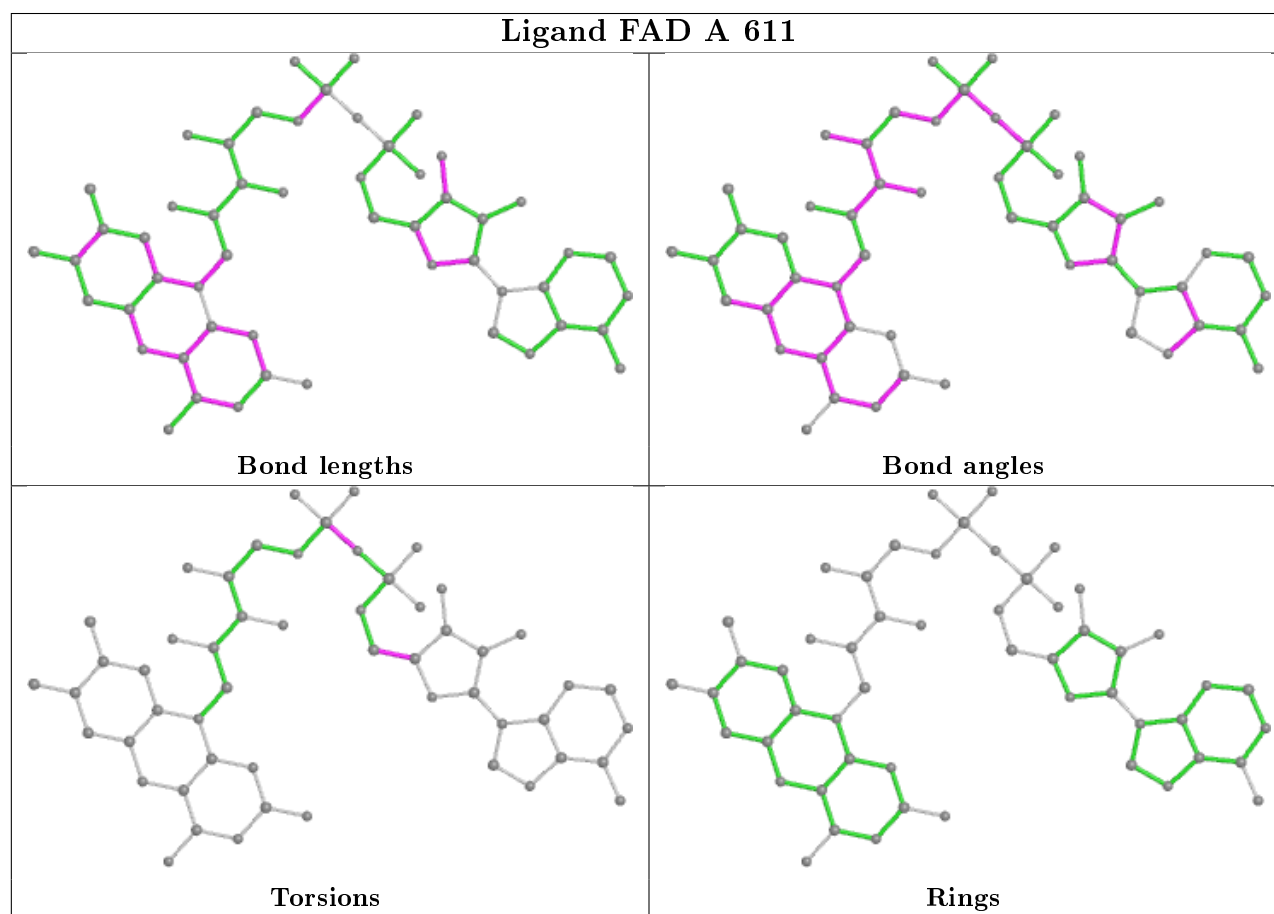
Mol	Chain	Res	Type	Atoms
3	A	611	FAD	PA-O3P-P-O5'
3	B	613	FAD	O2'-C2'-C3'-O3'
3	B	613	FAD	C2'-C3'-C4'-O4'
3	B	613	FAD	PA-O3P-P-O5'
3	B	613	FAD	C2'-C3'-C4'-C5'

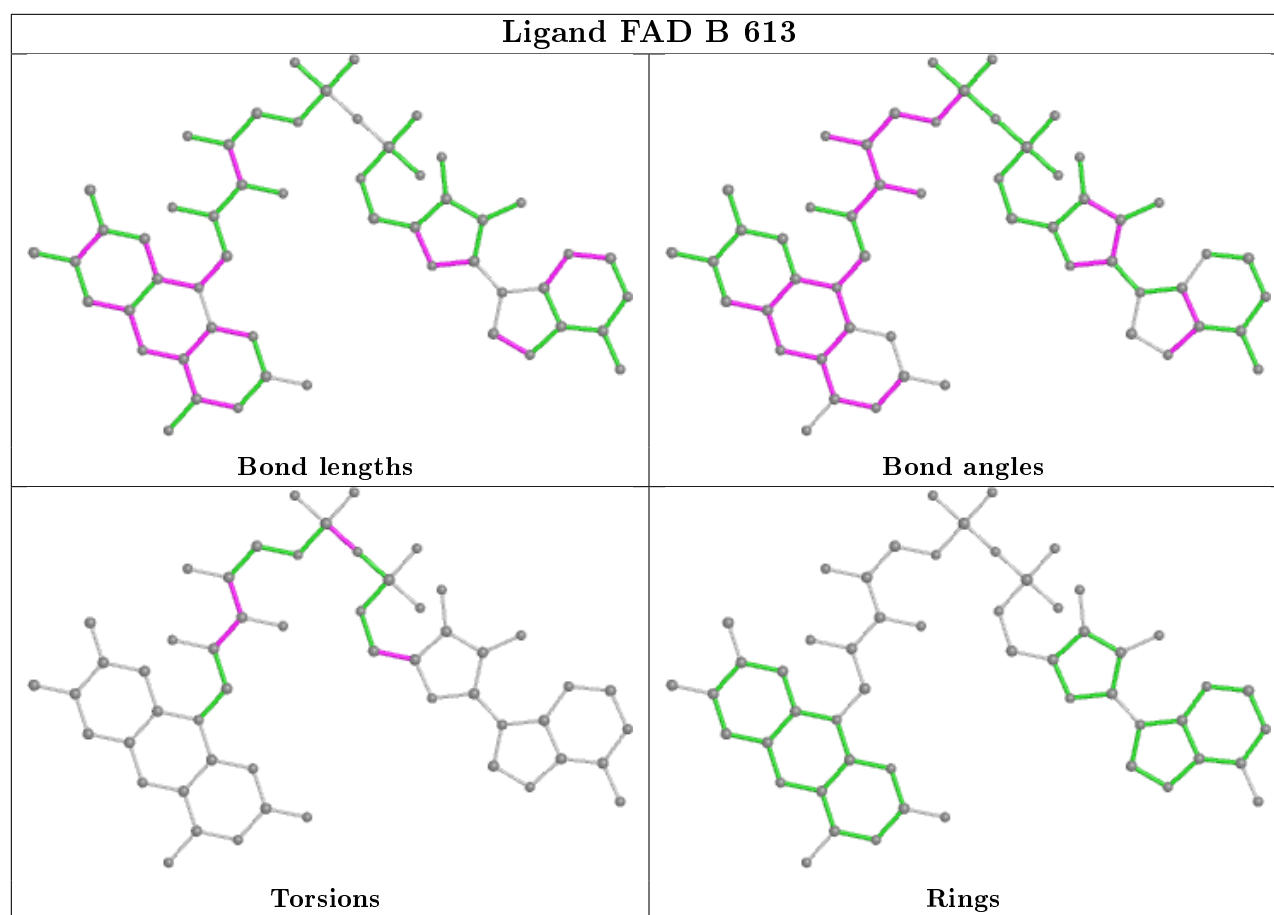
There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	623	TBU	2	0
3	A	611	FAD	2	0
4	A	621	TBU	3	0
2	B	612	SF4	3	0
3	B	613	FAD	4	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 [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	581/584 (99%)	-0.53	7 (1%) 79 76	7, 23, 56, 89	0
1	B	578/584 (98%)	0.19	35 (6%) 21 16	29, 63, 85, 95	0
All	All	1159/1168 (99%)	-0.17	42 (3%) 42 35	7, 45, 83, 95	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	PRO	9.6
1	B	542	ASP	4.9
1	A	4	CYS	4.6
1	B	32	PHE	4.4
1	A	6	VAL	4.1

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](#)

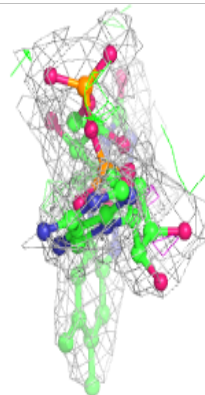
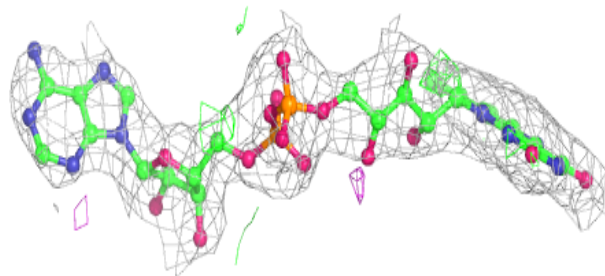
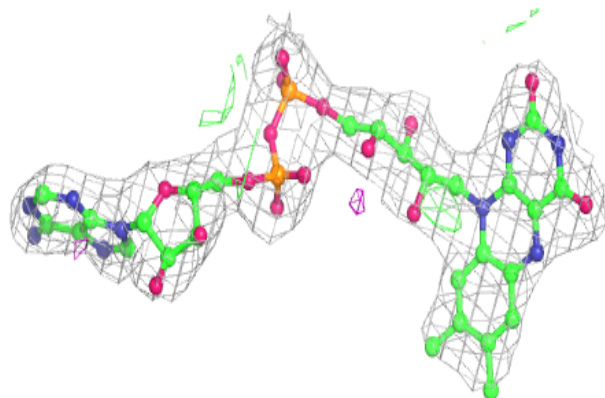
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

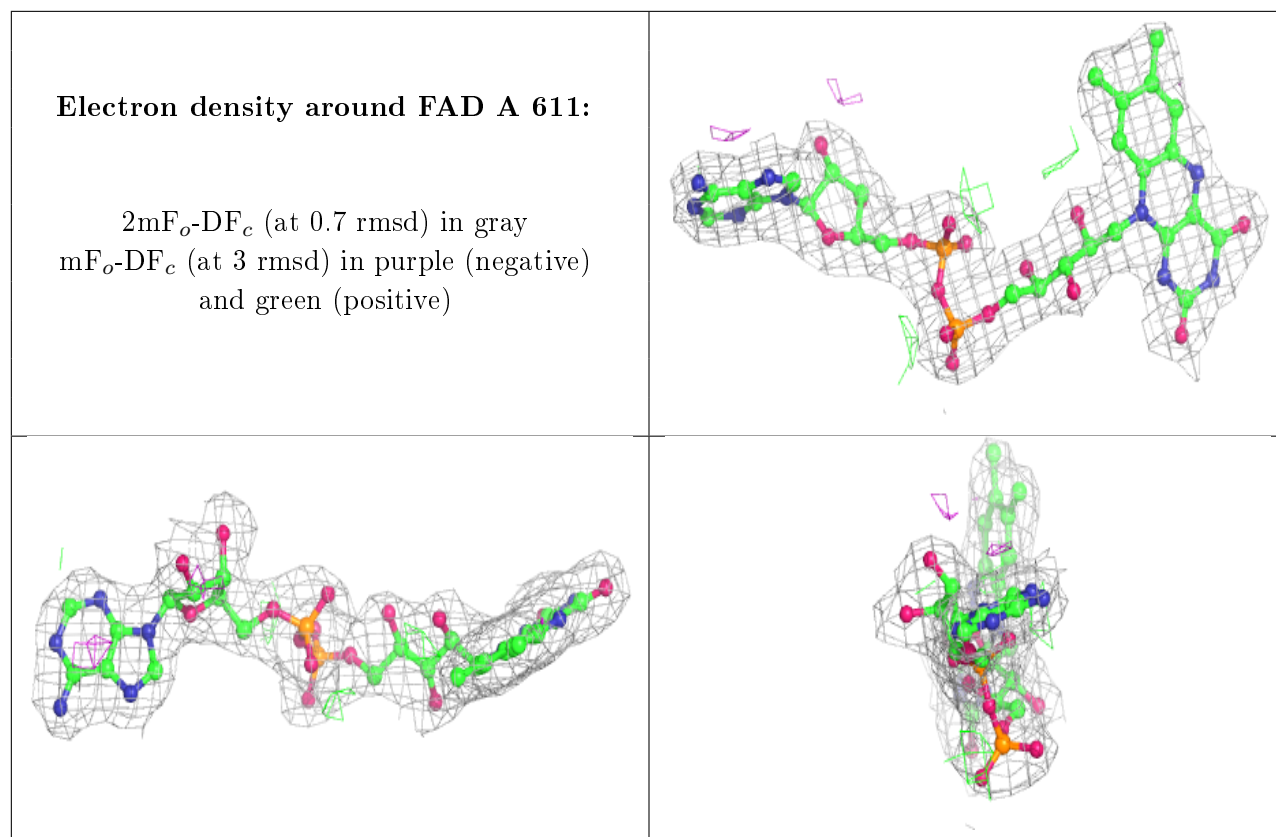
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TBU	B	626	5/5	0.84	0.34	57,57,59,59	0
2	SF4	A	610	8/8	0.89	0.11	6,8,9,10	0
4	TBU	A	624	5/5	0.90	0.18	51,51,51,52	0
4	TBU	A	623	5/5	0.91	0.32	29,33,34,38	0
4	TBU	A	622	5/5	0.91	0.22	26,27,28,28	0
3	FAD	B	613	53/53	0.92	0.24	42,58,74,74	0
2	SF4	B	612	8/8	0.94	0.10	51,53,54,54	0
4	TBU	B	625	5/5	0.95	0.23	56,56,57,57	0
3	FAD	A	611	53/53	0.96	0.16	7,13,20,21	0
4	TBU	A	621	5/5	0.96	0.20	25,25,27,28	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 613:

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.