wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 12:55 AM EDT

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 (i) 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 (i)) were used in the production of this report:

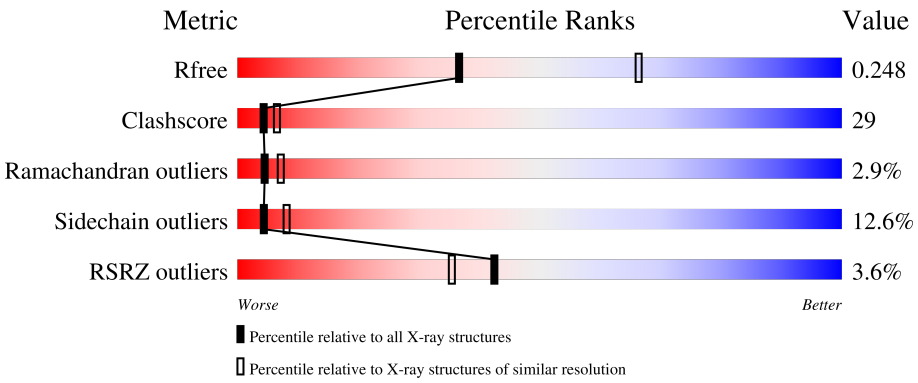
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

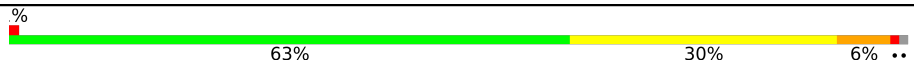
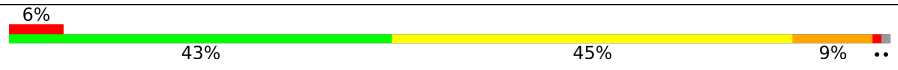
The reported resolution of this entry is 2.60 Å.

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 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 <=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	
1	B	584	

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)

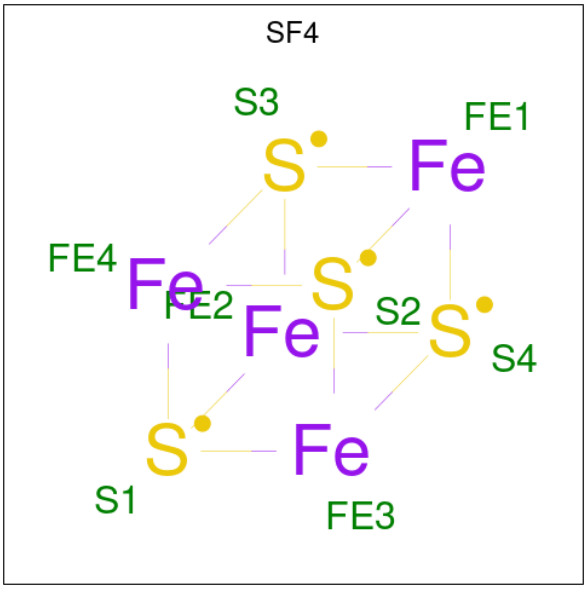
There are 5 unique types of molecules in this entry. The entry contains 9345 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

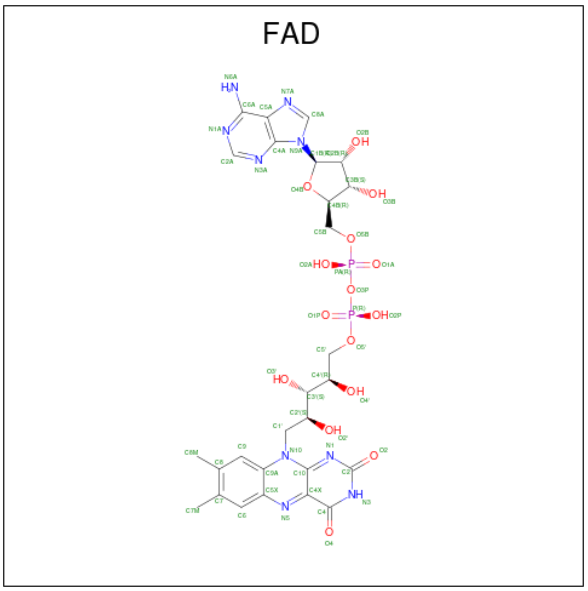
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	581	4553	2907	791	835	20	0	0	0
1	B	578	4531	2893	787	832	19	0	0	0

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



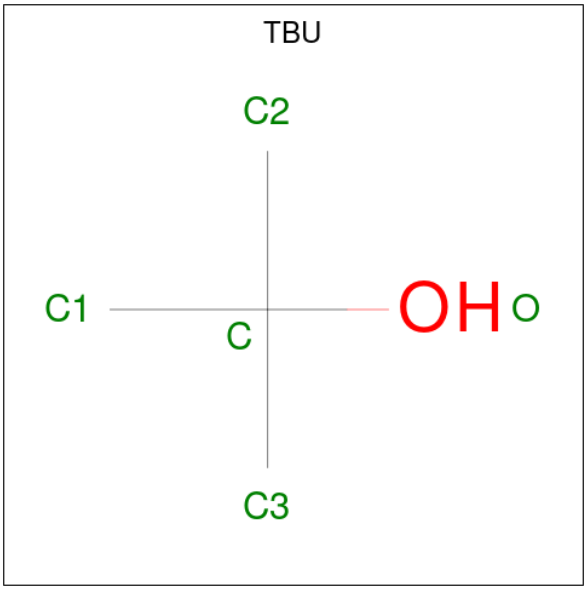
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	A	1	8	4	4	0	0
2	B	1	8	4	4	0	0

- Molecule 3 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		
3	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
3	B	1	53	27	9	15	2	0	0

- Molecule 4 is TERTIARY-BUTYL ALCOHOL (three-letter code: TBU) (formula: $C_4H_{10}O$).



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

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

- Molecule 5 is water.

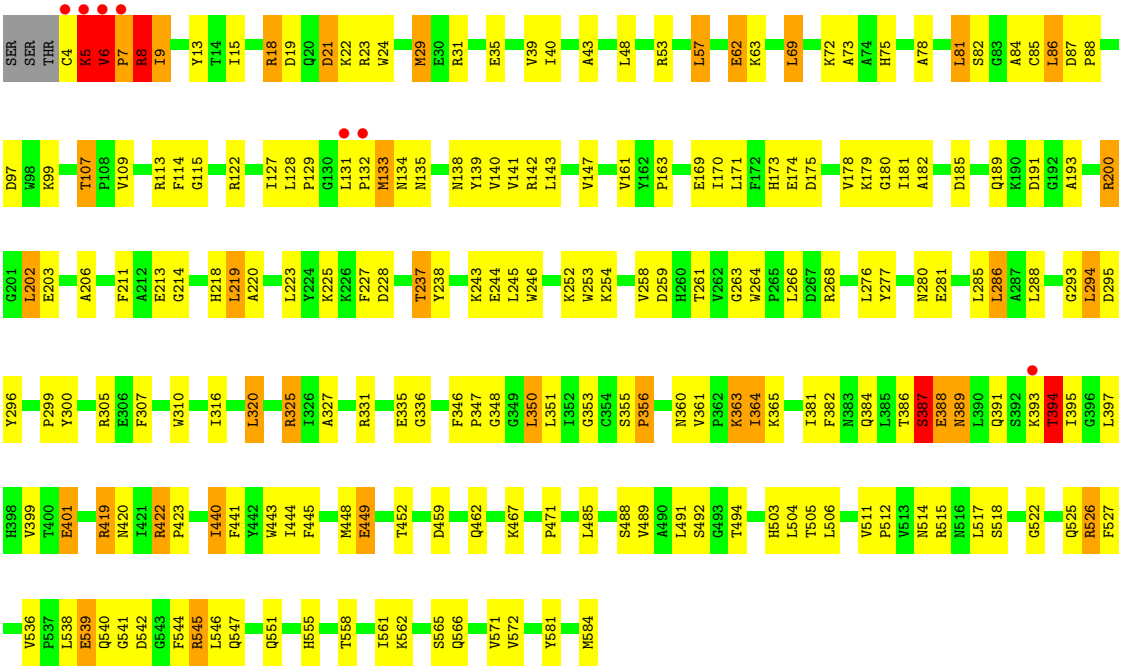
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	77	77	77	0	0
			Total	O		
5	B	32	32	32	0	0

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.

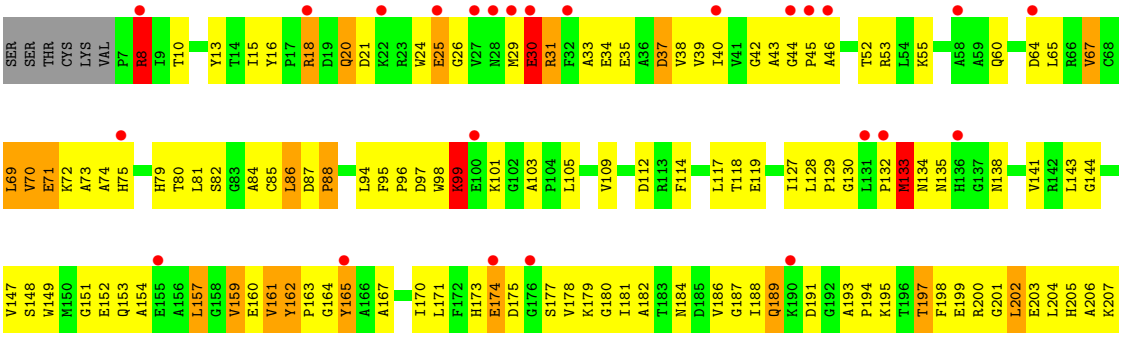
• Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase

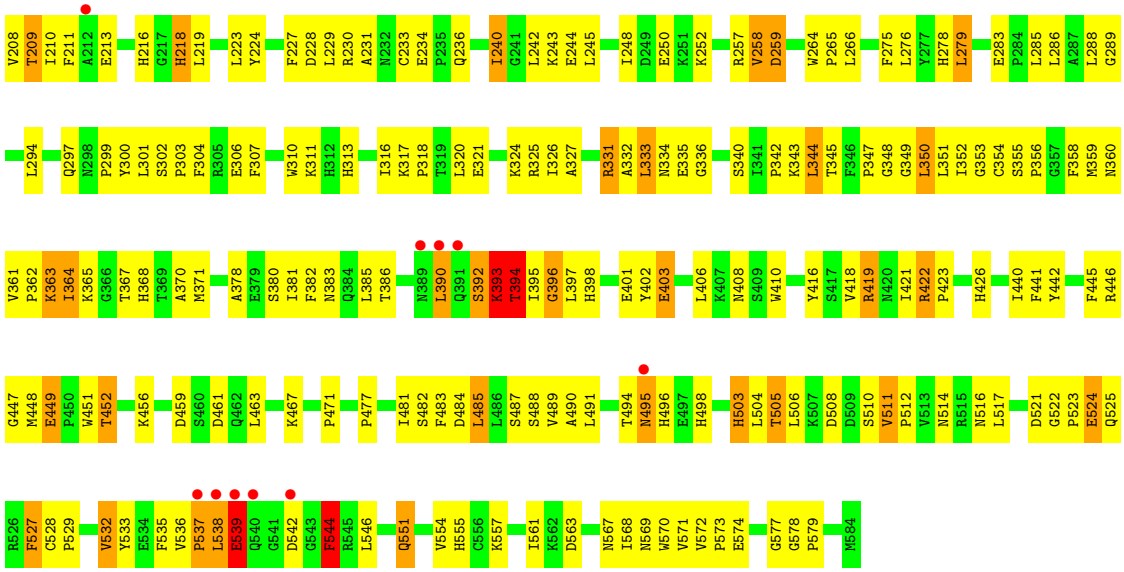
Chain A:



• Molecule 1: Electron transfer flavoprotein-ubiquinone oxidoreductase

Chain B:




V208 T209 I210 F211 A212 E213 H216 G217 H218 L219 L223 Y224 F227 D228 L229 R230 A231 N232 C233 E234 P235 Q236 I240 G241 L242 K243 E244 L245 I248 D249 E250 K251 K252 R257 V258 D259 W264 P265 L266 F275 L276 Y277 H278 L279 E283 P284 L285 L286 A287 L288 G289
L294 Q297 N298 P299 Y300 L301 S302 P303 F304 R305 E306 F307 W310 K311 H312 H313 I316 K317 P318 T319 L320 E321 K324 R325 I326 A327 R331 A332 L333 N334 E335 G336 S340 I341 P342 K343 L344 T345 F346 P347 G348 G349 L350 L351 I352 G353 C354 S355 P356 G357 F358 M359 N360
V361 P362 K363 I364 K365 G366 T367 H368 T369 A370 M371 A378 E379 S380 I381 F382 N383 Q384 L385 T386 N389 L390 Q391 S392 K393 T394 I395 G396 L397 H398 E401 Y402 E403 L406 K407 N408 S409 W410 Y416 S417 V418 R419 N420 I421 R422 P423 H426 I440 F441 Y442 F445 R446
G447 M448 E449 P450 W451 T452 K456 D459 S460 D461 Q462 L463 K467 P471 P477 I481 S482 F483 D484 L485 L486 S487 S488 V489 A490 L491 T494 N495 H496 E497 H498 H503 L504 T505 L506 K507 D508 D509 S510 V511 P512 V513 N514 R515 N516 L517 D521 G522 P523 E524 Q525
R526 F527 C528 P529 V532 Y533 E534 F535 V536 P537 L538 E539 Q540 G541 D542 G543 F544 R545 L546 Q551 V554 H555 C556 K557 I561 K562 D563 N567 I568 N569 W570 V571 V572 P573 E574 G577 G578 P579 M584

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	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.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: TBU, FAD, SF4

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(^{o})	Ideal(^{o})
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 (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	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:HA	1:B:393:LYS:CE	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 (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	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 (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	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	64	ASP
1	B	503	HIS
1	B	159	VAL
1	B	495	ASN
1	B	544	PHE

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

Mol	Chain	Res	Type
1	B	334	ASN
1	B	498	HIS
1	B	555	HIS
1	B	516	ASN
1	B	495	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	622	-	4,4,4	0.35	0	6,6,6	0.67	0
4	TBU	A	624	-	4,4,4	0.40	0	6,6,6	0.65	0
3	FAD	A	611	-	53,58,58	2.05	14 (26%)	68,89,89	1.74	13 (19%)
4	TBU	B	625	-	4,4,4	0.53	0	6,6,6	0.52	0
3	FAD	B	613	-	53,58,58	2.00	16 (30%)	68,89,89	1.83	14 (20%)
2	SF4	B	612	1	0,12,12	-	-	-		
4	TBU	A	623	-	4,4,4	0.69	0	6,6,6	0.51	0
4	TBU	A	621	-	4,4,4	0.45	0	6,6,6	0.55	0
4	TBU	B	626	-	4,4,4	0.53	0	6,6,6	0.54	0
2	SF4	A	610	1	0,12,12	-	-	-		

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

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	613	FAD	C10-N10	5.73	1.49	1.37
3	A	611	FAD	C1'-C2'	-5.64	1.44	1.52
3	B	613	FAD	C6-C5X	4.70	1.47	1.40
3	A	611	FAD	C10-N10	4.60	1.47	1.37
3	A	611	FAD	C4X-N5	4.53	1.39	1.30

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	613	FAD	O3'-C3'-C2'	7.78	127.61	108.81
3	A	611	FAD	O3'-C3'-C2'	6.18	123.74	108.81
3	B	613	FAD	O4B-C1B-C2B	-5.54	98.83	106.93
3	A	611	FAD	O4B-C1B-C2B	-4.92	99.74	106.93
3	B	613	FAD	P-O5'-C5'	4.45	147.77	121.68

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'

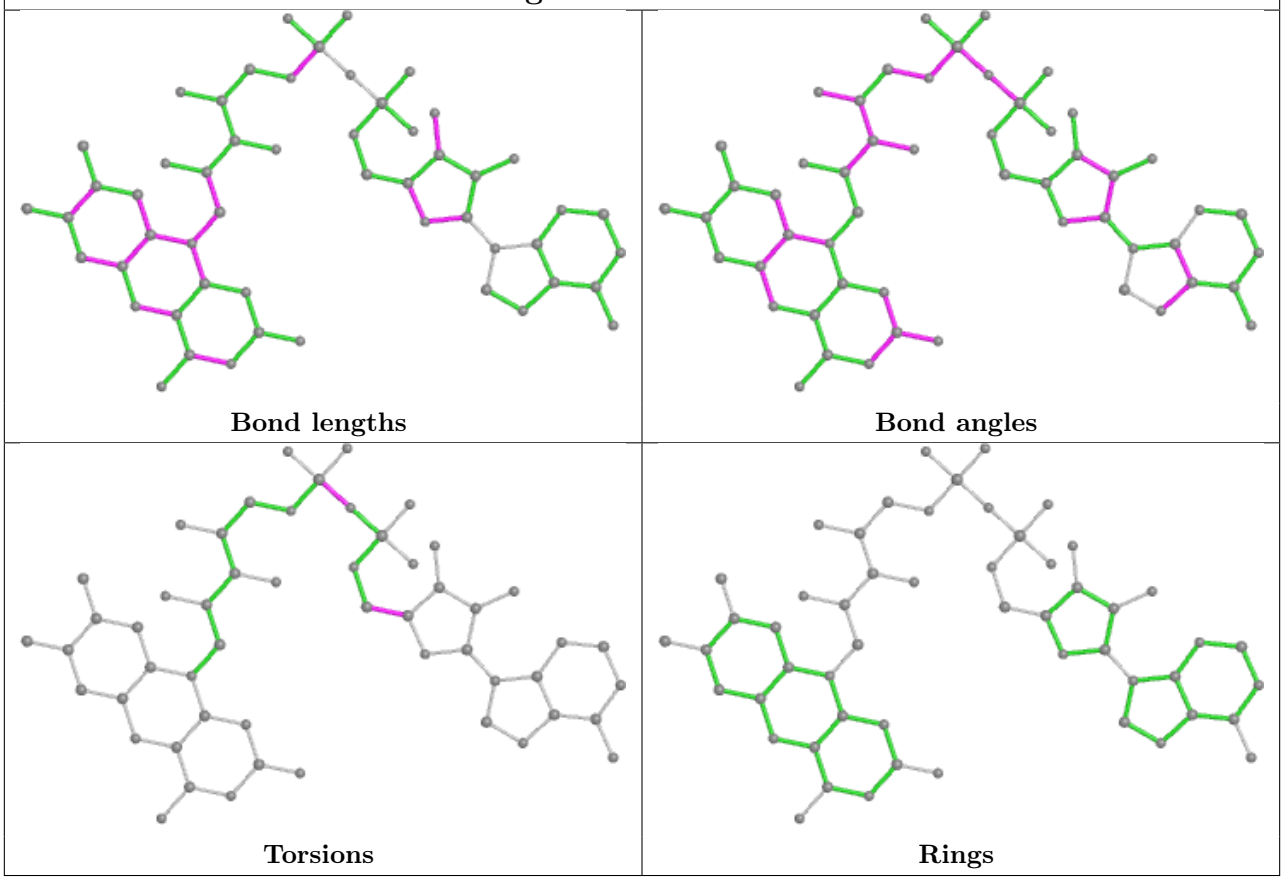
There are no ring outliers.

5 monomers are involved in 14 short contacts:

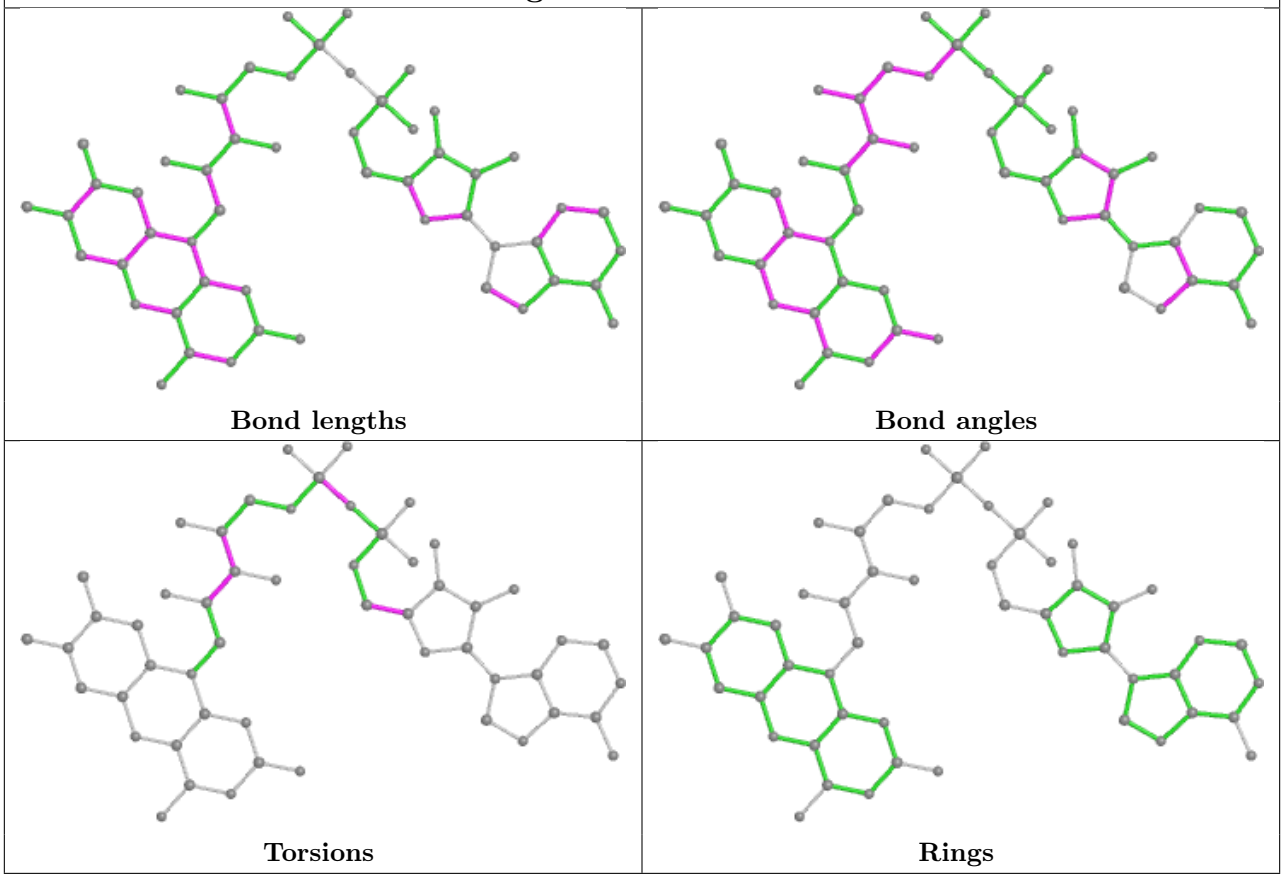
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	611	FAD	2	0
3	B	613	FAD	4	0
2	B	612	SF4	3	0
4	A	623	TBU	2	0
4	A	621	TBU	3	0

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 A 611



Ligand FAD B 613



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 monosaccharides in this entry.

6.4 Ligands (i)

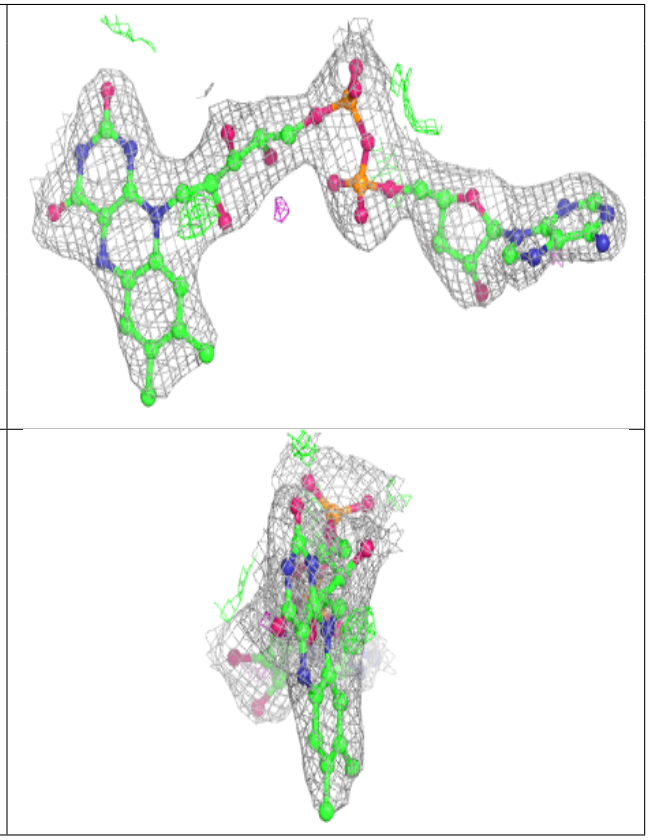
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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	622	5/5	0.91	0.22	26,27,28,28	0
4	TBU	A	623	5/5	0.91	0.32	29,33,34,38	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
4	TBU	A	621	5/5	0.96	0.20	25,25,27,28	0
3	FAD	A	611	53/53	0.96	0.16	7,13,20,21	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.

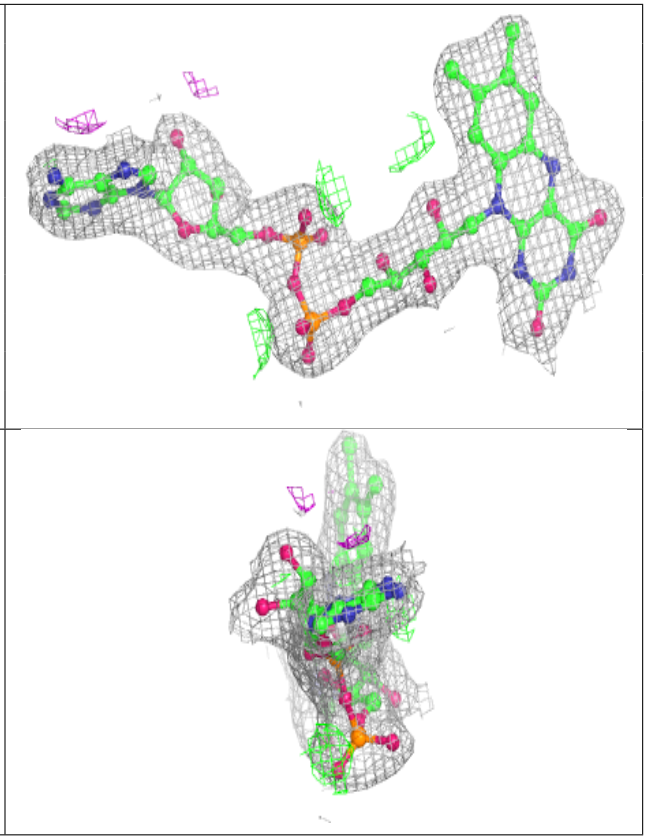
Electron density around FAD B 613:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around FAD A 611:

$2mF_o$-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.