Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:32 PM EDT

PDB ID	:	3FIM
Title	:	Crystal structure of aryl-alcohol-oxidase from Pleurotus eryingii
Authors	:	Fernandez, I.S.
Deposited on	:	2008-12-12
Resolution	:	2.55 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 (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:

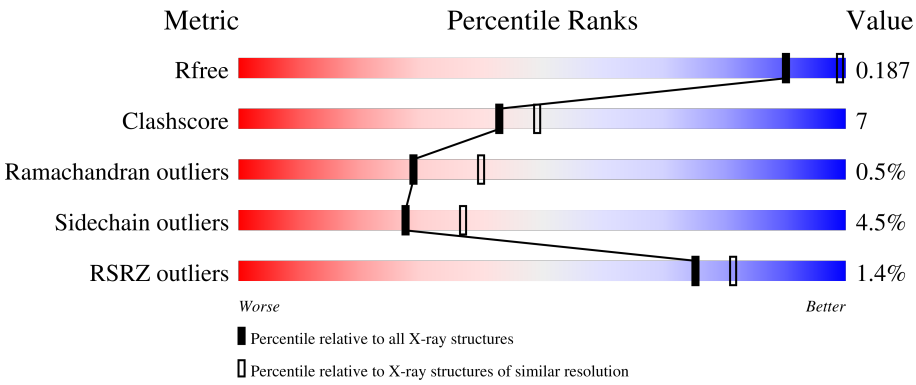
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

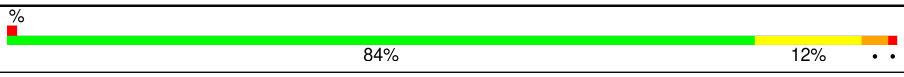
The reported resolution of this entry is 2.55 Å.

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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	B	566	

2 Entry composition (i)

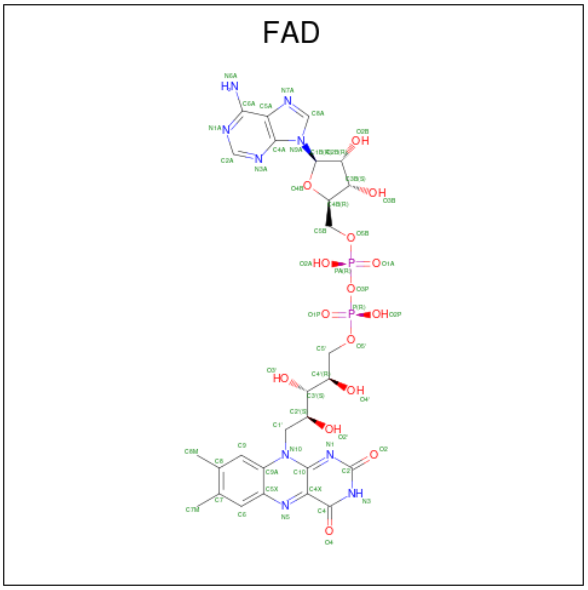
There are 3 unique types of molecules in this entry. The entry contains 4574 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aryl-alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	565	4296	2707	739	839	11	0	0	0

- 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	B	1	53	27	9	15	2	0	0

- Molecule 3 is water.

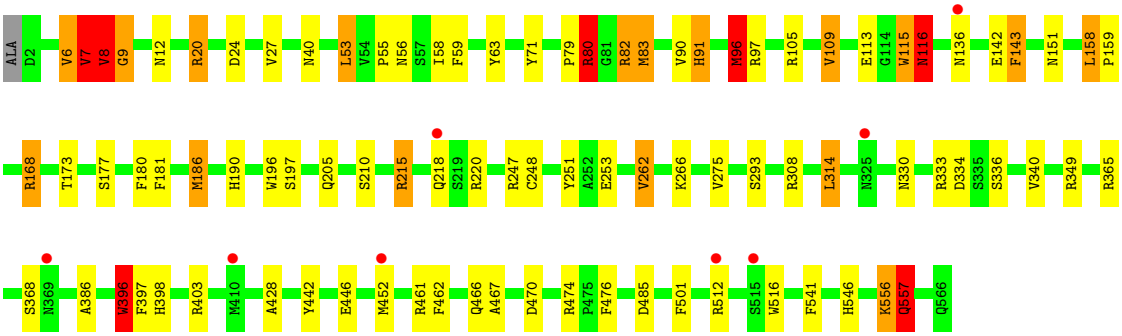
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	225	225	225	0	0

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: Aryl-alcohol oxidase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	180.23Å 180.23Å 160.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.04 – 2.55 20.04 – 2.57	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.04-2.55) 99.7 (20.04-2.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	18.86 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.206 0.183 , 0.187	Depositor DCC
R_{free} test set	2479 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4574	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 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	B	1.71	52/4405 (1.2%)	1.40	63/6026 (1.0%)

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	2	1

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	GLY	N-CA	22.92	1.80	1.46
1	B	116	ASN	N-CA	16.08	1.78	1.46
1	B	396	TRP	CG-CD1	13.40	1.55	1.36
1	B	396	TRP	CE3-CZ3	-12.07	1.18	1.38
1	B	396	TRP	CD2-CE2	10.16	1.53	1.41
1	B	56	ASN	N-CA	9.53	1.65	1.46
1	B	557	GLN	CB-CG	9.13	1.77	1.52
1	B	116	ASN	CB-CG	8.98	1.71	1.51
1	B	55	PRO	C-O	7.93	1.39	1.23
1	B	396	TRP	CZ3-CH2	7.37	1.51	1.40
1	B	556	LYS	CD-CE	-7.13	1.33	1.51
1	B	557	GLN	CD-NE2	7.10	1.50	1.32
1	B	196	TRP	CE3-CZ3	7.07	1.50	1.38
1	B	40	ASN	C-O	6.88	1.36	1.23
1	B	63	TYR	CG-CD1	6.87	1.48	1.39
1	B	40	ASN	CB-CG	6.78	1.66	1.51
1	B	557	GLN	CA-CB	6.65	1.68	1.53
1	B	396	TRP	CG-CD2	-6.63	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	TYR	CG-CD1	6.53	1.47	1.39
1	B	396	TRP	CE2-CZ2	-6.40	1.28	1.39
1	B	470	ASP	CB-CG	6.38	1.65	1.51
1	B	446	GLU	CG-CD	6.36	1.61	1.51
1	B	58	ILE	CB-CG2	6.32	1.72	1.52
1	B	516	TRP	CZ2-CH2	6.15	1.49	1.37
1	B	501	PHE	CE2-CZ	6.15	1.49	1.37
1	B	516	TRP	CD2-CE3	6.07	1.49	1.40
1	B	386	ALA	CA-CB	5.93	1.65	1.52
1	B	442	TYR	CG-CD1	5.72	1.46	1.39
1	B	8	VAL	C-O	5.68	1.34	1.23
1	B	330	ASN	CG-OD1	5.67	1.36	1.24
1	B	9	GLY	CA-C	5.67	1.60	1.51
1	B	476	PHE	CE2-CZ	5.63	1.48	1.37
1	B	541	PHE	CD1-CE1	5.59	1.50	1.39
1	B	397	PHE	CE2-CZ	5.51	1.47	1.37
1	B	403	ARG	CD-NE	-5.50	1.37	1.46
1	B	516	TRP	CE2-CZ2	5.50	1.49	1.39
1	B	181	PHE	CE2-CZ	5.48	1.47	1.37
1	B	6	VAL	CA-CB	5.46	1.66	1.54
1	B	428	ALA	CA-CB	5.44	1.63	1.52
1	B	275	VAL	CA-CB	5.42	1.66	1.54
1	B	205	GLN	CD-OE1	5.40	1.35	1.24
1	B	27	VAL	CB-CG2	5.39	1.64	1.52
1	B	83	MET	CB-CG	5.39	1.68	1.51
1	B	340	VAL	CB-CG2	5.39	1.64	1.52
1	B	516	TRP	CD2-CE2	5.28	1.47	1.41
1	B	253	GLU	CG-CD	5.28	1.59	1.51
1	B	113	GLU	CG-CD	5.25	1.59	1.51
1	B	151	ASN	CG-OD1	5.19	1.35	1.24
1	B	71	TYR	CD1-CE1	5.15	1.47	1.39
1	B	7	VAL	N-CA	-5.11	1.36	1.46
1	B	143	PHE	CD2-CE2	5.04	1.49	1.39
1	B	396	TRP	CB-CG	5.01	1.59	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	403	ARG	NE-CZ-NH2	-21.51	109.54	120.30
1	B	403	ARG	NE-CZ-NH1	20.94	130.77	120.30
1	B	80	ARG	NE-CZ-NH1	15.22	127.91	120.30
1	B	8	VAL	C-N-CA	-15.19	90.39	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	82	ARG	NE-CZ-NH2	-13.31	113.65	120.30
1	B	80	ARG	NE-CZ-NH2	-13.03	113.79	120.30
1	B	55	PRO	C-N-CA	-11.95	91.82	121.70
1	B	6	VAL	C-N-CA	11.24	149.81	121.70
1	B	83	MET	CG-SD-CE	-9.94	84.29	100.20
1	B	557	GLN	CA-CB-CG	9.89	135.16	113.40
1	B	116	ASN	N-CA-CB	9.87	128.37	110.60
1	B	8	VAL	O-C-N	-9.19	107.57	123.20
1	B	82	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	B	24	ASP	CB-CG-OD1	8.83	126.24	118.30
1	B	6	VAL	O-C-N	-8.62	108.90	122.70
1	B	403	ARG	CD-NE-CZ	8.45	135.43	123.60
1	B	557	GLN	N-CA-CB	8.35	125.63	110.60
1	B	115	TRP	C-N-CA	-8.26	101.06	121.70
1	B	6	VAL	CA-C-N	7.88	134.53	117.20
1	B	461	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	452	MET	CG-SD-CE	7.74	112.59	100.20
1	B	333	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	B	158	LEU	CA-CB-CG	-7.53	97.99	115.30
1	B	24	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	B	168	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	349	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	248	CYS	CA-CB-SG	-7.28	100.90	114.00
1	B	105	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	B	158	LEU	CB-CG-CD2	6.91	122.74	111.00
1	B	557	GLN	CB-CG-CD	6.82	129.34	111.60
1	B	314	LEU	CA-CB-CG	6.82	130.98	115.30
1	B	485	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	82	ARG	CG-CD-NE	-6.74	97.66	111.80
1	B	186	MET	CG-SD-CE	-6.61	89.63	100.20
1	B	8	VAL	CA-C-N	6.52	129.24	116.20
1	B	396	TRP	CH2-CZ2-CE2	-6.47	110.93	117.40
1	B	53	LEU	CA-CB-CG	6.44	130.10	115.30
1	B	55	PRO	O-C-N	-6.37	112.51	122.70
1	B	115	TRP	O-C-N	-6.32	112.60	122.70
1	B	247	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	365	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	151	ASN	CB-CA-C	-6.04	98.32	110.40
1	B	333	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	262	VAL	CB-CA-C	-6.00	99.99	111.40
1	B	82	ARG	CD-NE-CZ	5.92	131.89	123.60
1	B	20	ARG	NE-CZ-NH1	-5.88	117.36	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	396	TRP	CD1-NE1-CE2	-5.87	103.72	109.00
1	B	461	ARG	CG-CD-NE	-5.86	99.50	111.80
1	B	403	ARG	CG-CD-NE	-5.84	99.53	111.80
1	B	96	MET	CG-SD-CE	-5.75	91.00	100.20
1	B	557	GLN	CB-CA-C	5.72	121.83	110.40
1	B	215	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	220	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	556	LYS	CB-CG-CD	-5.59	97.07	111.60
1	B	334	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	109	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	B	365	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	403	ARG	CA-CB-CG	5.31	125.08	113.40
1	B	40	ASN	CB-CA-C	5.30	120.99	110.40
1	B	308	ARG	CG-CD-NE	-5.18	100.93	111.80
1	B	8	VAL	CG1-CB-CG2	5.16	119.15	110.90
1	B	512	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	97	ARG	NE-CZ-NH2	-5.07	117.77	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	7	VAL	CA
1	B	8	VAL	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	6	VAL	Peptide

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	B	4296	0	4138	53	0
2	B	53	0	31	7	0
3	B	225	0	0	6	0
All	All	4574	0	4169	58	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 7.

All (58) 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:557:GLN:CB	1:B:557:GLN:CG	1.77	1.62
2:B:0:FAD:C1'	2:B:0:FAD:N10	1.68	1.52
1:B:116:ASN:CA	1:B:116:ASN:N	1.78	1.46
1:B:9:GLY:N	1:B:9:GLY:CA	1.80	1.45
1:B:8:VAL:O	1:B:9:GLY:CA	1.75	1.32
1:B:8:VAL:O	1:B:9:GLY:HA2	1.26	1.26
1:B:8:VAL:C	1:B:9:GLY:CA	2.20	1.08
1:B:20:ARG:HE	1:B:556:LYS:CE	1.74	1.00
2:B:0:FAD:C1'	2:B:0:FAD:C10	2.40	1.00
1:B:115:TRP:O	1:B:116:ASN:CA	2.17	0.92
1:B:115:TRP:C	1:B:116:ASN:CA	2.37	0.92
1:B:20:ARG:HE	1:B:556:LYS:HE3	1.37	0.89
2:B:0:FAD:C1'	2:B:0:FAD:N1	2.35	0.88
2:B:0:FAD:N1	2:B:0:FAD:H1'2	1.89	0.87
1:B:115:TRP:O	1:B:116:ASN:HB3	1.74	0.86
1:B:115:TRP:O	1:B:116:ASN:CB	2.26	0.83
1:B:83:MET:HE3	1:B:90:VAL:HG13	1.62	0.82
1:B:20:ARG:HE	1:B:556:LYS:HE2	1.46	0.78
1:B:79:PRO:O	1:B:80:ARG:HD2	1.83	0.78
1:B:186:MET:CE	3:B:758:HOH:O	2.32	0.76
1:B:96:MET:HE3	1:B:546:HIS:HB2	1.66	0.76
1:B:190:HIS:ND1	3:B:709:HOH:O	2.28	0.66
1:B:20:ARG:NE	1:B:556:LYS:HE3	2.09	0.65
1:B:83:MET:CE	1:B:90:VAL:CG1	2.75	0.65
1:B:20:ARG:NE	1:B:556:LYS:CE	2.53	0.64
1:B:83:MET:HE3	1:B:90:VAL:CG1	2.28	0.63
1:B:20:ARG:NE	1:B:556:LYS:HE2	2.13	0.63
2:B:0:FAD:N10	2:B:0:FAD:C2'	2.59	0.62
1:B:20:ARG:HH21	1:B:556:LYS:CE	2.15	0.58
1:B:186:MET:HE2	3:B:758:HOH:O	1.99	0.58
1:B:215:ARG:O	1:B:218:GLN:HG2	2.08	0.53
1:B:20:ARG:HH21	1:B:556:LYS:HE2	1.73	0.53
1:B:59:PHE:HB3	1:B:83:MET:CE	2.43	0.49
1:B:96:MET:HE3	1:B:546:HIS:CB	2.40	0.48
1:B:20:ARG:NH2	1:B:556:LYS:HE2	2.30	0.47
1:B:59:PHE:HB3	1:B:83:MET:HE1	1.97	0.47
1:B:96:MET:CE	3:B:582:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:GLN:CG	1:B:557:GLN:HB3	2.20	0.46
1:B:91:HIS:HB2	2:B:0:FAD:C4X	2.45	0.46
1:B:396:TRP:CH2	1:B:398:HIS:HB3	2.51	0.45
1:B:142:GLU:HB3	1:B:158:LEU:HD22	1.99	0.44
1:B:173:THR:O	1:B:177:SER:HB3	2.17	0.44
1:B:83:MET:HE1	1:B:90:VAL:CG1	2.47	0.43
1:B:116:ASN:N	1:B:116:ASN:HA	2.09	0.43
1:B:186:MET:HE3	3:B:758:HOH:O	2.09	0.43
1:B:159:PRO:HD3	1:B:197:SER:O	2.18	0.43
1:B:546:HIS:HB3	2:B:0:FAD:C2	2.49	0.43
1:B:20:ARG:NH2	1:B:556:LYS:CE	2.81	0.43
1:B:168:ARG:HD3	1:B:467:ALA:O	2.19	0.42
1:B:116:ASN:N	1:B:116:ASN:C	2.63	0.42
1:B:96:MET:CE	1:B:96:MET:N	2.82	0.42
1:B:293:SER:HB3	3:B:720:HOH:O	2.20	0.41
1:B:556:LYS:HA	1:B:556:LYS:HD3	1.72	0.41
1:B:180:PHE:CZ	1:B:462:PHE:HB2	2.56	0.41
1:B:266:LYS:HE3	1:B:266:LYS:HB3	1.85	0.41
1:B:557:GLN:CG	1:B:557:GLN:HB2	2.20	0.40
1:B:20:ARG:CZ	1:B:556:LYS:HE2	2.50	0.40
1:B:96:MET:HE3	1:B:546:HIS:N	2.36	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	B	563/566 (100%)	539 (96%)	21 (4%)	3 (0%)	29 40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	8	VAL
1	B	116	ASN

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	B	470/470 (100%)	449 (96%)	21 (4%)	27 37

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	B	8	VAL
1	B	12	ASN
1	B	53	LEU
1	B	80	ARG
1	B	82	ARG
1	B	91	HIS
1	B	96	MET
1	B	109	VAL
1	B	116	ASN
1	B	136	ASN
1	B	143	PHE
1	B	210	SER
1	B	262	VAL
1	B	314	LEU
1	B	336	SER
1	B	368	SER
1	B	396	TRP
1	B	466	GLN
1	B	474	ARG
1	B	557	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	B	0	-	54,58,58	2.47	17 (31%)	71,89,89	3.34	30 (42%)

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	0	-	-	6/30/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	FAD	C1'-N10	8.69	1.68	1.47
2	B	0	FAD	O4B-C1B	5.69	1.48	1.40
2	B	0	FAD	O4-C4	5.16	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	0	FAD	C7M-C7	4.70	1.59	1.51
2	B	0	FAD	C6-C5X	4.48	1.46	1.40
2	B	0	FAD	C2-N1	4.45	1.46	1.36
2	B	0	FAD	C4X-N5	4.08	1.39	1.30
2	B	0	FAD	C9A-N10	3.61	1.47	1.41
2	B	0	FAD	C10-N1	3.49	1.40	1.33
2	B	0	FAD	P-O3P	3.39	1.63	1.59
2	B	0	FAD	C2'-C3'	2.60	1.58	1.53
2	B	0	FAD	C8-C7	-2.40	1.35	1.40
2	B	0	FAD	O2B-C2B	2.39	1.48	1.43
2	B	0	FAD	C5'-C4'	-2.35	1.48	1.51
2	B	0	FAD	C9A-C5X	2.31	1.44	1.41
2	B	0	FAD	PA-O3P	2.18	1.61	1.59
2	B	0	FAD	O2'-C2'	2.02	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	FAD	O4-C4-N3	-11.54	98.42	120.11
2	B	0	FAD	C1'-N10-C9A	10.80	141.62	120.63
2	B	0	FAD	C4-C4X-N5	9.15	130.85	118.21
2	B	0	FAD	C4X-C4-N3	7.25	131.70	113.25
2	B	0	FAD	C7M-C7-C6	-6.09	108.83	119.57
2	B	0	FAD	O4B-C1B-N9A	-5.48	101.48	108.75
2	B	0	FAD	N3A-C2A-N1A	-5.26	121.53	128.67
2	B	0	FAD	C4-N3-C2	-5.01	116.75	125.64
2	B	0	FAD	O3P-PA-O1A	-4.85	96.10	110.70
2	B	0	FAD	O2P-P-O3P	4.71	120.00	107.27
2	B	0	FAD	C4-C4X-C10	-4.63	109.00	116.93
2	B	0	FAD	C4X-C10-N10	4.46	122.86	116.48
2	B	0	FAD	C5X-C6-C7	-3.84	113.71	120.83
2	B	0	FAD	C7M-C7-C8	3.56	128.03	120.76
2	B	0	FAD	C8M-C8-C9	-3.34	113.70	119.57
2	B	0	FAD	O4B-C4B-C5B	-3.32	98.69	109.33
2	B	0	FAD	C9-C8-C7	3.28	124.50	119.69
2	B	0	FAD	C10-N1-C2	3.28	123.95	116.85
2	B	0	FAD	C4B-O4B-C1B	-3.14	107.05	109.92
2	B	0	FAD	C9A-N10-C10	-3.10	116.02	120.75
2	B	0	FAD	C6-C5X-N5	-2.75	113.88	118.44
2	B	0	FAD	O3P-P-O1P	-2.70	102.57	110.70
2	B	0	FAD	O5'-P-O1P	-2.70	98.25	108.94
2	B	0	FAD	C4'-C3'-C2'	-2.64	109.17	113.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	0	FAD	C6-C7-C8	2.34	123.12	119.69
2	B	0	FAD	C6-C5X-C9A	2.33	122.25	119.05
2	B	0	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	B	0	FAD	O5B-C5B-C4B	-2.24	101.35	108.99
2	B	0	FAD	O4'-C4'-C5'	-2.11	105.33	109.99
2	B	0	FAD	O2P-P-O1P	2.08	122.12	112.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

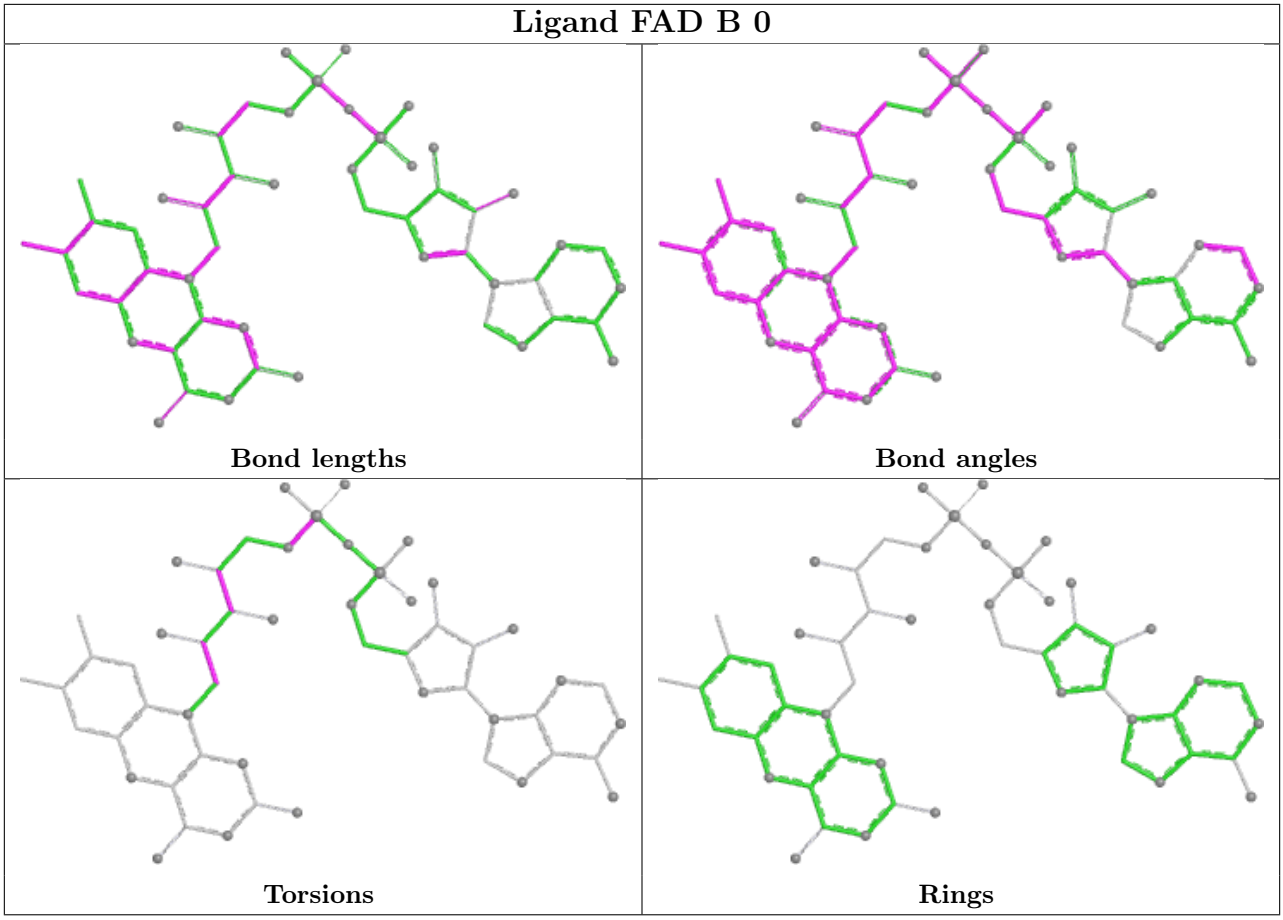
Mol	Chain	Res	Type	Atoms
2	B	0	FAD	N10-C1'-C2'-O2'
2	B	0	FAD	N10-C1'-C2'-C3'
2	B	0	FAD	C5'-O5'-P-O1P
2	B	0	FAD	O3'-C3'-C4'-C5'
2	B	0	FAD	O3'-C3'-C4'-O4'
2	B	0	FAD	C5'-O5'-P-O3P

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	0	FAD	7	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.



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	B	565/566 (99%)	-0.41	8 (1%) 75 81	29, 35, 45, 60	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	GLN	3.4
1	B	369	ASN	2.4
1	B	515	SER	2.3
1	B	452	MET	2.3
1	B	325	ASN	2.3
1	B	136	ASN	2.1
1	B	512	ARG	2.1
1	B	410	MET	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 monosaccharides in this entry.

6.4 Ligands (i)

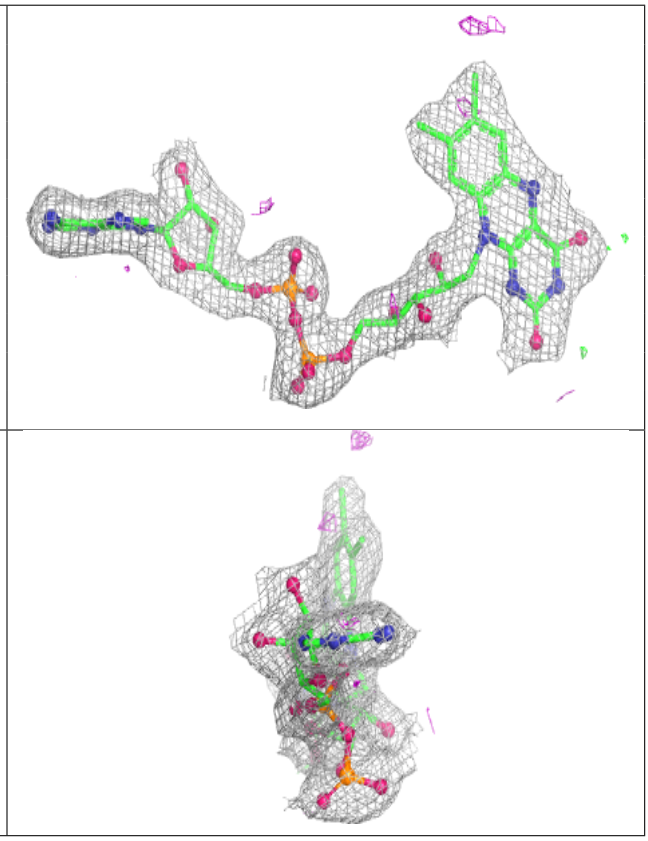
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	B	0	53/53	0.98	0.09	29,33,39,40	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 0:

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.