



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:24 AM UTC

PDB ID : 3FIM / pdb_00003fim
Title : Crystal structure of aryl-alcohol-oxidase from *Pleurotus eryngii*
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

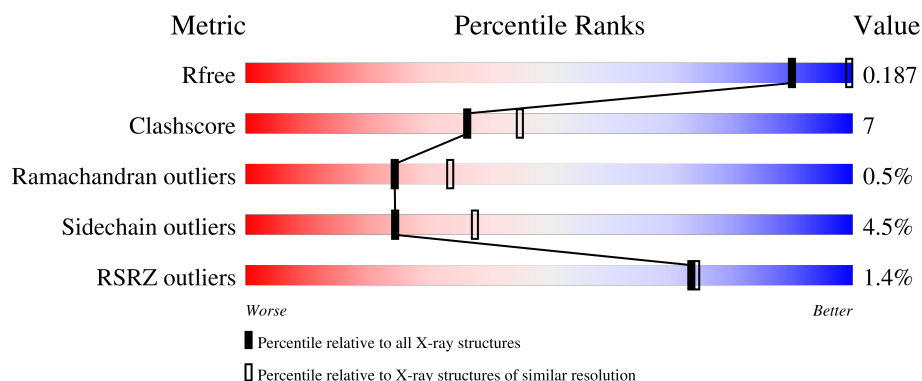
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

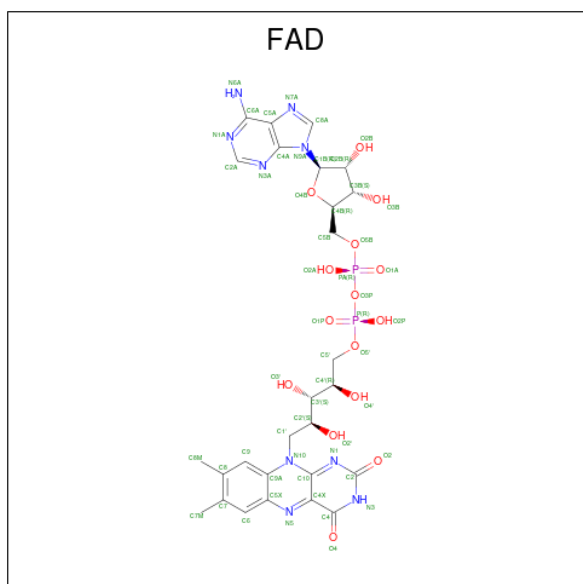
Mol	Chain	Length	Quality of chain
1	B	566	

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
1	B	565	Total	C	N	O	S	0	0	0
			4296	2707	739	839	11			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

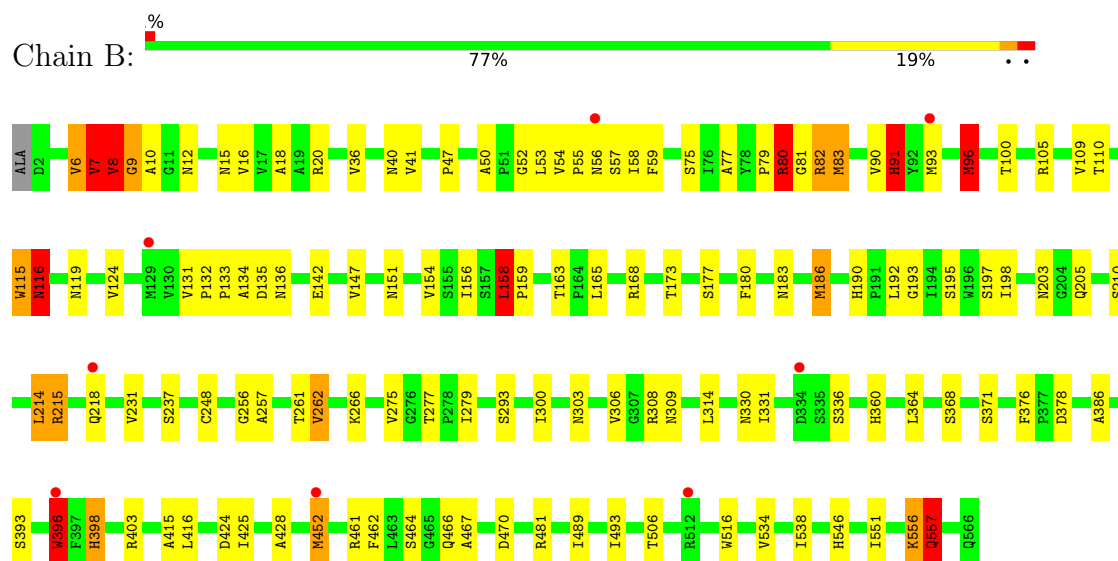
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	225	Total O 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



4 Data and refinement statistics

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) 99.4 (20.04-2.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.05%)	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)	0.35 , 28.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

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: 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	2.07	97/4405 (2.2%)	1.63	67/6026 (1.1%)

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	2	1

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	GLY	N-CA	30.16	1.80	1.45
1	B	116	ASN	N-CA	25.06	1.78	1.46
1	B	56	ASN	N-CA	13.38	1.65	1.46
1	B	40	ASN	C-O	11.08	1.36	1.23
1	B	557	GLN	CA-CB	9.80	1.68	1.53
1	B	6	VAL	CA-CB	9.54	1.66	1.54
1	B	8	VAL	C-O	8.47	1.34	1.24
1	B	557	GLN	CD-NE2	8.26	1.50	1.33
1	B	557	GLN	CB-CG	8.25	1.77	1.52
1	B	279	ILE	CA-CB	8.22	1.65	1.54
1	B	275	VAL	CA-CB	8.18	1.66	1.54
1	B	55	PRO	C-O	7.93	1.39	1.23
1	B	116	ASN	CB-CG	7.86	1.71	1.52
1	B	8	VAL	CA-C	-7.82	1.42	1.52
1	B	198	ILE	CA-C	7.46	1.61	1.52
1	B	396	TRP	CG-CD1	7.43	1.55	1.36
1	B	386	ALA	CA-CB	7.41	1.65	1.53
1	B	396	TRP	CD2-CE2	7.17	1.53	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	LEU	C-O	6.93	1.32	1.23
1	B	396	TRP	CE3-CZ3	-6.91	1.18	1.38
1	B	557	GLN	N-CA	6.82	1.54	1.46
1	B	116	ASN	CA-C	-6.81	1.43	1.52
1	B	330	ASN	CG-OD1	6.78	1.36	1.23
1	B	277	THR	CA-C	6.70	1.60	1.52
1	B	163	THR	CA-CB	6.68	1.62	1.53
1	B	303	ASN	C-O	6.68	1.31	1.24
1	B	428	ALA	CA-CB	6.61	1.63	1.53
1	B	257	ALA	CA-C	6.55	1.61	1.53
1	B	403	ARG	CD-NE	-6.54	1.37	1.46
1	B	205	GLN	CD-OE1	6.47	1.35	1.23
1	B	147	VAL	CA-CB	6.41	1.63	1.54
1	B	156	ILE	C-O	6.37	1.30	1.24
1	B	133	PRO	C-O	6.36	1.31	1.23
1	B	556	LYS	CD-CE	-6.34	1.33	1.52
1	B	115	TRP	N-CA	6.32	1.53	1.45
1	B	396	TRP	CG-CD2	-6.32	1.32	1.43
1	B	151	ASN	CG-OD1	6.21	1.35	1.23
1	B	193	GLY	C-O	6.21	1.31	1.23
1	B	516	TRP	CZ2-CH2	6.20	1.49	1.37
1	B	538	ILE	CA-CB	6.14	1.61	1.54
1	B	132	PRO	CA-C	6.11	1.55	1.51
1	B	12	ASN	CG-ND2	-6.08	1.20	1.33
1	B	16	VAL	CA-CB	6.08	1.61	1.54
1	B	163	THR	C-N	6.05	1.40	1.34
1	B	58	ILE	CB-CG2	6.03	1.72	1.52
1	B	261	THR	CA-CB	5.99	1.62	1.53
1	B	18	ALA	CA-CB	5.88	1.62	1.53
1	B	415	ALA	N-CA	5.87	1.53	1.46
1	B	40	ASN	CB-CG	5.84	1.66	1.52
1	B	82	ARG	CD-NE	-5.83	1.38	1.46
1	B	83	MET	SD-CE	-5.83	1.65	1.79
1	B	364	LEU	N-CA	5.82	1.53	1.45
1	B	415	ALA	CA-C	5.82	1.59	1.52
1	B	309	ASN	CG-OD1	5.82	1.34	1.23
1	B	516	TRP	CD2-CE3	5.75	1.49	1.40
1	B	256	GLY	C-O	-5.75	1.16	1.24
1	B	80	ARG	CD-NE	-5.74	1.38	1.46
1	B	371	SER	CA-C	5.71	1.60	1.52
1	B	10	ALA	N-CA	5.69	1.54	1.46
1	B	214	LEU	C-O	-5.69	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	ASN	CA-CB	5.68	1.63	1.53
1	B	425	ILE	CA-CB	5.67	1.61	1.54
1	B	551	ILE	CA-CB	5.66	1.61	1.54
1	B	134	ALA	CA-CB	5.63	1.62	1.53
1	B	81	GLY	C-O	5.61	1.29	1.23
1	B	424	ASP	C-O	5.61	1.30	1.23
1	B	54	VAL	CA-C	5.60	1.58	1.52
1	B	40	ASN	CA-C	5.55	1.60	1.53
1	B	237	SER	C-O	-5.55	1.16	1.24
1	B	398	HIS	ND1-CE1	5.51	1.38	1.32
1	B	376	PHE	CA-C	5.49	1.58	1.52
1	B	124	VAL	CA-CB	5.48	1.61	1.54
1	B	50	ALA	C-O	5.47	1.29	1.24
1	B	183	ASN	CA-C	5.45	1.58	1.52
1	B	154	VAL	N-CA	5.44	1.52	1.46
1	B	493	ILE	CA-CB	5.39	1.61	1.54
1	B	131	VAL	C-O	5.39	1.31	1.24
1	B	83	MET	CB-CG	5.38	1.68	1.52
1	B	131	VAL	C-N	5.38	1.38	1.33
1	B	393	SER	CA-C	5.35	1.59	1.52
1	B	135	ASP	N-CA	5.35	1.53	1.46
1	B	7	VAL	N-CA	-5.33	1.36	1.46
1	B	36	VAL	CA-CB	5.31	1.61	1.54
1	B	119	ASN	CG-OD1	5.26	1.33	1.23
1	B	470	ASP	CB-CG	5.24	1.65	1.52
1	B	506	THR	CA-C	5.24	1.59	1.52
1	B	115	TRP	C-N	-5.24	1.26	1.33
1	B	534	VAL	CA-CB	5.24	1.59	1.53
1	B	396	TRP	CE2-CZ2	-5.23	1.28	1.39
1	B	203	ASN	CA-C	5.21	1.59	1.53
1	B	96	MET	SD-CE	-5.16	1.66	1.79
1	B	306	VAL	C-O	5.13	1.30	1.24
1	B	464	SER	C-O	-5.11	1.17	1.24
1	B	77	ALA	CA-CB	5.05	1.61	1.53
1	B	231	VAL	CA-CB	5.05	1.60	1.53
1	B	110	THR	N-CA	5.01	1.52	1.46
1	B	50	ALA	N-CA	-5.01	1.41	1.46

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	VAL	CA-C-N	-21.46	90.39	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	VAL	C-N-CA	-21.46	90.39	121.30
1	B	55	PRO	CA-C-N	-20.59	91.82	123.12
1	B	55	PRO	C-N-CA	-20.59	91.82	123.12
1	B	6	VAL	CA-C-N	15.62	149.81	121.70
1	B	6	VAL	C-N-CA	15.62	149.81	121.70
1	B	6	VAL	O-C-N	-13.49	108.90	123.20
1	B	8	VAL	O-C-N	-12.00	107.57	122.57
1	B	403	ARG	NE-CZ-NH2	-10.73	109.54	119.20
1	B	115	TRP	CA-C-N	-10.72	101.06	121.54
1	B	115	TRP	C-N-CA	-10.72	101.06	121.54
1	B	116	ASN	N-CA-CB	10.58	128.37	110.49
1	B	557	GLN	N-CA-CB	10.55	125.63	110.12
1	B	557	GLN	CA-CB-CG	10.53	135.16	114.10
1	B	557	GLN	CB-CG-CD	9.85	129.34	112.60
1	B	403	ARG	NE-CZ-NH1	9.27	130.77	121.50
1	B	403	ARG	CD-NE-CZ	7.88	135.43	124.40
1	B	83	MET	CG-SD-CE	-7.55	84.29	100.90
1	B	116	ASN	CA-CB-CG	7.41	120.01	112.60
1	B	115	TRP	O-C-N	-7.21	112.60	121.83
1	B	331	ILE	N-CA-C	-7.21	103.27	110.62
1	B	262	VAL	CB-CA-C	-6.69	99.99	110.69
1	B	557	GLN	CB-CA-C	6.65	121.83	110.79
1	B	151	ASN	CB-CA-C	-6.65	98.32	109.75
1	B	398	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	B	52	GLY	N-CA-C	6.55	121.67	114.40
1	B	82	ARG	CG-CD-NE	-6.52	97.66	112.00
1	B	556	LYS	CA-C-O	-6.42	114.26	121.00
1	B	80	ARG	NE-CZ-NH1	6.41	127.91	121.50
1	B	360	HIS	CB-CG-CD2	-6.35	122.94	131.20
1	B	8	VAL	N-CA-CB	6.33	121.68	111.23
1	B	57	SER	N-CA-C	6.23	117.69	108.60
1	B	556	LYS	CB-CG-CD	-6.19	97.07	111.30
1	B	82	ARG	NE-CZ-NH2	-6.17	113.65	119.20
1	B	132	PRO	N-CA-C	6.11	116.34	110.47
1	B	300	ILE	N-CA-C	-6.09	106.57	111.81
1	B	91	HIS	N-CA-C	6.05	117.70	110.19
1	B	80	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	B	398	HIS	CB-CG-ND1	5.92	131.57	122.70
1	B	248	CYS	CA-CB-SG	-5.87	100.90	114.40
1	B	481	ARG	N-CA-C	5.83	117.72	111.36
1	B	115	TRP	N-CA-C	-5.76	100.94	109.86
1	B	56	ASN	N-CA-C	5.75	118.09	107.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ASN	CB-CA-C	5.69	120.99	112.06
1	B	461	ARG	CG-CD-NE	-5.68	99.50	112.00
1	B	403	ARG	CG-CD-NE	-5.67	99.53	112.00
1	B	403	ARG	CB-CA-C	5.59	118.06	109.50
1	B	41	VAL	N-CA-C	-5.52	98.74	106.53
1	B	215	ARG	N-CA-C	5.52	120.26	112.75
1	B	403	ARG	CA-CB-CG	5.49	125.08	114.10
1	B	378	ASP	CA-C-N	-5.39	114.47	120.45
1	B	378	ASP	C-N-CA	-5.39	114.47	120.45
1	B	9	GLY	N-CA-C	5.35	121.34	112.89
1	B	82	ARG	CD-NE-CZ	5.35	131.89	124.40
1	B	75	SER	CB-CA-C	-5.33	100.74	109.53
1	B	452	MET	CG-SD-CE	5.31	112.59	100.90
1	B	158	LEU	CA-CB-CG	-5.23	97.99	116.30
1	B	556	LYS	N-CA-C	5.23	116.67	110.97
1	B	360	HIS	CB-CG-ND1	5.22	130.53	122.70
1	B	105	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	B	489	ILE	N-CA-C	5.12	115.34	110.42
1	B	186	MET	CG-SD-CE	-5.12	89.63	100.90
1	B	8	VAL	CB-CA-C	5.11	119.67	111.29
1	B	58	ILE	CB-CG1-CD1	-5.10	103.10	113.80
1	B	393	SER	N-CA-C	5.06	117.22	109.07
1	B	396	TRP	CH2-CZ2-CE2	-5.05	110.93	117.50
1	B	308	ARG	CG-CD-NE	-5.03	100.93	112.00

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 ⓘ

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	4139	56	0
2	B	53	0	31	7	0
3	B	225	0	0	5	0
All	All	4574	0	4170	61	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 (61) 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	1.13
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:C	1:B:116:ASN:CA	2.37	0.96
1:B:115:TRP:O	1:B:116:ASN:CA	2.17	0.92
1:B:20:ARG:HE	1:B:556:LYS:HE3	1.37	0.89
1:B:96:MET:N	1:B:96:MET:HE2	1.88	0.88
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:186:MET:HE2	1:B:195:SER:OG	1.78	0.84
1:B:115:TRP:O	1:B:116:ASN:CB	2.26	0.83
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:96:MET:HE1	1:B:546:HIS:HB2	1.66	0.76
1:B:186:MET:CE	3:B:758:HOH:O	2.32	0.76
1:B:186:MET:HE3	3:B:758:HOH:O	1.85	0.76
1:B:96:MET:HE2	1:B:96:MET:H	1.55	0.71
1:B:83:MET:HE3	1:B:90:VAL:HG13	1.72	0.69
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:MET:HE1	1:B:90:VAL:CG1	2.34	0.57
1:B:83:MET:CE	1:B:90:VAL:HG13	2.36	0.56
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:83:MET:HE1	1:B:90:VAL:HG12	1.94	0.48
1:B:20:ARG:NH2	1:B:556:LYS:HE2	2.30	0.47
1:B:116:ASN:N	1:B:116:ASN:C	2.63	0.47
1:B:96:MET:CE	3:B:582:HOH:O	2.63	0.47
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:59:PHE:HB3	1:B:83:MET:HE2	1.97	0.45
1:B:396:TRP:CH2	1:B:398:HIS:HB3	2.51	0.45
1:B:47:PRO:HA	1:B:93:MET:HE1	1.99	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:116:ASN:N	1:B:116:ASN:HA	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:15:ASN:CG	1:B:214:LEU:HG	2.45	0.41
1:B:416:LEU:HD13	1:B:452:MET:HE3	2.01	0.41
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

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	B	563/566 (100%)	539 (96%)	21 (4%)	3 (0%)	24	34

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 ⓘ

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%)	24	38

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	53	LEU
1	B	80	ARG
1	B	82	ARG
1	B	91	HIS
1	B	96	MET
1	B	100	THR
1	B	109	VAL
1	B	116	ASN
1	B	136	ASN
1	B	158	LEU
1	B	165	LEU
1	B	210	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	557	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	ASN
1	B	414	ASN
1	B	441	GLN
1	B	459	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 oligosaccharides 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	-	58,58,58	2.33	18 (31%)	85,89,89	3.24	38 (44%)

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	-	-	6/34/50/50	0/6/6/6

All (18) 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	O4-C4	5.16	1.33	1.23
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	O4B-C1B	2.75	1.48	1.42
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	C5A-N7A	-2.19	1.35	1.39
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 (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	C5A-C4A-N3A	-5.46	119.19	126.72
2	B	0	FAD	C4-N3-C2	-5.01	116.75	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	0	FAD	N9A-C8A-N7A	-4.87	107.03	113.94
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	N3A-C2A-N1A	-4.66	121.53	128.58
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	N3A-C4A-N9A	4.28	134.45	127.17
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	C5A-N7A-C8A	3.48	108.93	103.45
2	B	0	FAD	C4A-N9A-C8A	3.46	109.38	105.74
2	B	0	FAD	O4B-C1B-N9A	-3.44	101.48	108.09
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	C2A-N3A-C4A	3.18	119.59	111.83
2	B	0	FAD	C9A-N10-C10	-3.10	116.02	120.75
2	B	0	FAD	C2B-C1B-N9A	2.98	120.70	113.30
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
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	C2A-N1A-C6A	2.27	122.45	118.73
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
2	B	0	FAD	C4A-C5A-N7A	-2.06	108.23	110.58

There are no chirality outliers.

All (6) torsion outliers are listed below:

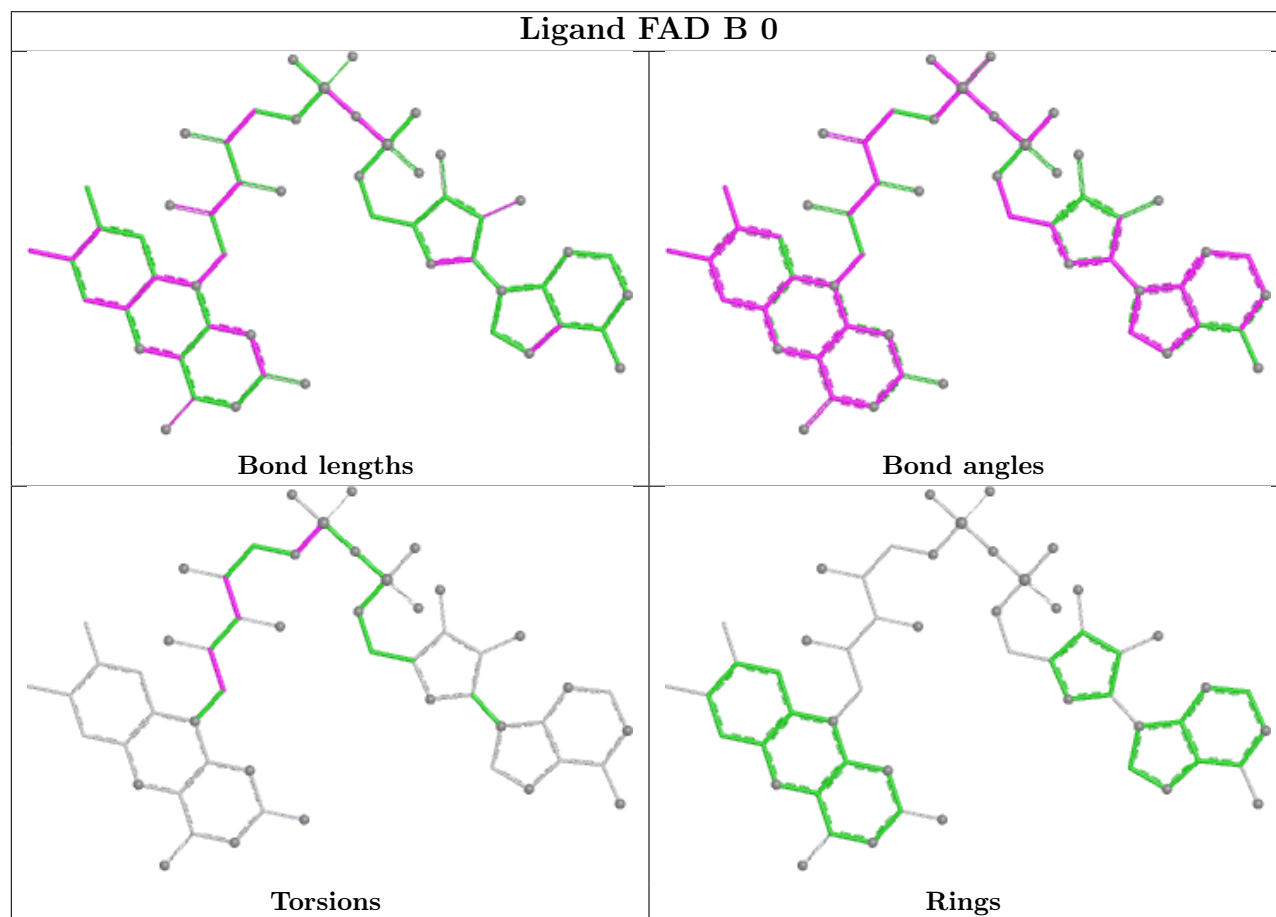
Mol	Chain	Res	Type	Atoms
2	B	0	FAD	N10-C1'-C2'-O2'
2	B	0	FAD	N10-C1'-C2'-C3'
2	B	0	FAD	C5'-O5'-P-O1P
2	B	0	FAD	O3'-C3'-C4'-C5'
2	B	0	FAD	O3'-C3'-C4'-O4'
2	B	0	FAD	C5'-O5'-P-O3P

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 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

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 [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%)	-0.11	8 (1%) 73 74	29, 35, 45, 60	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	512	ARG	2.8
1	B	56	ASN	2.5
1	B	334	ASP	2.4
1	B	129	MET	2.3
1	B	452	MET	2.3
1	B	396	TRP	2.3
1	B	218	GLN	2.2
1	B	93	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](#)

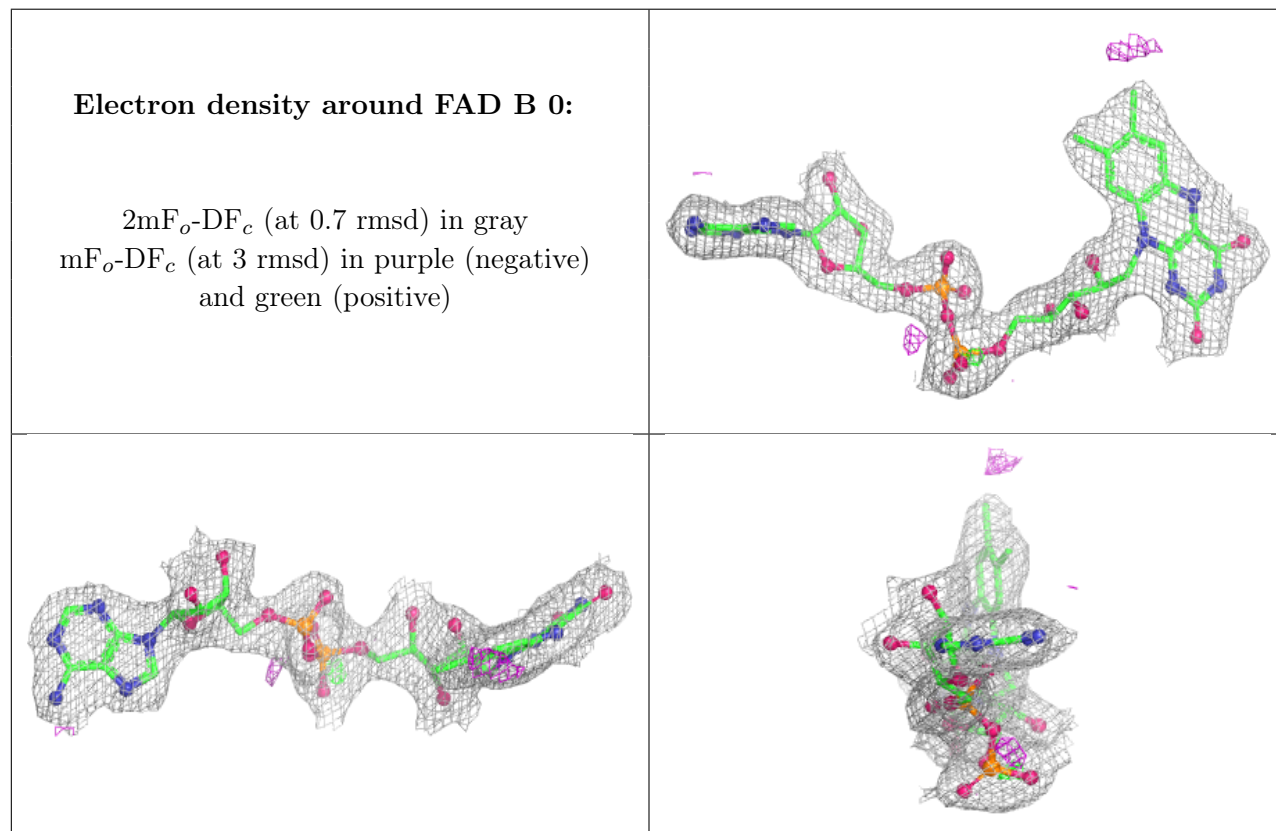
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	0	53/53	0.98	0.07	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.