



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:44 pm BST

PDB ID : 2QA2
Title : Crystal structure of CabE, an aromatic hydroxylase from angucycline biosynthesis, determined to 2.7 Å resolution
Authors : Koskiniemi, H.; Dobritsch, D.; Metsa-Ketela, M.; Kallio, P.; Niemi, J.; Schneider, G.
Deposited on : 2007-06-14
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

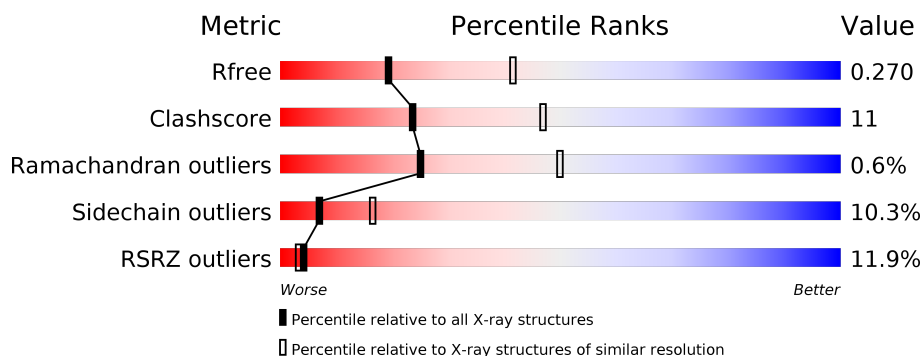
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	499	<div> <div>12%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>

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 Polyketide oxygenase CabE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	5	1	0
			3683	2289	684	694	16			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0

- Molecule 1: Polyketide oxygenase CabE



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	133.10Å 133.10Å 166.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.83 – 2.70 29.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.83-2.70) 99.4 (29.82-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.234 , 0.274 0.230 , 0.270	Depositor DCC
R_{free} test set	1220 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.3	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3760	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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 [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	A	0.52	0/3765	0.66	1/5115 (0.0%)

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	A	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	66	VAL	CA-CB-CG1	5.37	118.96	110.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	LEU	Peptide
1	A	447	PRO	Peptide
1	A	91	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	A	3683	0	3632	81	0
2	A	53	0	31	4	0
3	A	24	0	0	3	0
All	All	3760	0	3663	83	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 11.

All (83) 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:A:200:MET:HG2	1:A:212:ILE:HB	1.58	0.86
1:A:43:GLY:HA3	3:A:513:HOH:O	1.77	0.85
1:A:83:VAL:HG11	1:A:363:SER:HB3	1.59	0.83
1:A:176:PHE:HB2	1:A:213:VAL:HG13	1.65	0.78
1:A:339:LEU:O	1:A:350:ARG:NH1	2.21	0.74
1:A:41:SER:HB3	1:A:97:SER:OG	1.88	0.73
1:A:15:LEU:HD22	1:A:104:GLU:HA	1.68	0.73
1:A:287:GLY:HA3	2:A:500:FAD:H1'2	1.75	0.68
1:A:337:GLY:O	1:A:341:LEU:HB3	1.94	0.67
1:A:447:PRO:O	1:A:449:GLN:N	2.30	0.65
1:A:458:VAL:HG13	1:A:469:ILE:HD12	1.82	0.62
1:A:266:ARG:HG3	1:A:271:LEU:HG	1.83	0.60
2:A:500:FAD:PA	2:A:500:FAD:H5'1	2.42	0.59
1:A:329:LEU:O	1:A:333:THR:HG22	2.02	0.58
1:A:1:SER:HA	1:A:144:THR:HG22	1.85	0.58
1:A:47:THR:HG23	1:A:289:ASN:CG	2.26	0.55
1:A:342:SER:HB2	1:A:346:MET:HB2	1.90	0.54
2:A:500:FAD:O1A	2:A:500:FAD:H5'1	2.07	0.54
1:A:422:ASP:O	1:A:425:VAL:HG22	2.09	0.53
1:A:17:LEU:HD13	1:A:298:LEU:HD23	1.88	0.53
1:A:186:THR:HB	1:A:188:ARG:HH21	1.74	0.53
1:A:226:PRO:HB3	1:A:252:VAL:O	2.09	0.52
1:A:56:GLN:NE2	1:A:464:GLY:HA3	2.24	0.52
1:A:194:VAL:O	1:A:195:PRO:C	2.48	0.52
1:A:204:LEU:HD12	1:A:208:VAL:HB	1.92	0.52
1:A:125:ASP:HA	1:A:130:VAL:HG22	1.92	0.51
1:A:96:GLN:OE1	2:A:500:FAD:O4'	2.27	0.51
1:A:152:ASP:N	1:A:152:ASP:OD1	2.40	0.50
1:A:168:GLY:HA3	1:A:259:ALA:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ARG:HH11	1:A:27:ASP:HA	1.77	0.49
1:A:173[A]:ARG:NH2	1:A:214:CYS:HB3	2.27	0.49
1:A:7:VAL:O	1:A:30:VAL:HA	2.12	0.49
1:A:165:ASP:O	1:A:262:VAL:HA	2.12	0.48
1:A:15:LEU:HD22	1:A:104:GLU:CA	2.39	0.48
1:A:154:GLY:O	1:A:159:ARG:NH2	2.47	0.48
1:A:390:ARG:HB3	3:A:511:HOH:O	2.13	0.47
1:A:173[B]:ARG:CZ	1:A:341:LEU:HD21	2.45	0.47
1:A:215:GLU:CD	1:A:238:ARG:HH12	2.18	0.46
1:A:323:HIS:HB3	1:A:324:PRO:HD3	1.97	0.46
1:A:194:VAL:O	1:A:196:LEU:N	2.47	0.46
1:A:74:PHE:HE1	1:A:369:MET:CE	2.28	0.45
1:A:40:GLU:HG3	1:A:251:TRP:CH2	2.52	0.45
1:A:267:ARG:O	1:A:268:GLY:C	2.55	0.45
1:A:280:HIS:HB3	1:A:330:LEU:CD2	2.47	0.45
1:A:290:VAL:HG21	1:A:329:LEU:HD13	1.98	0.45
1:A:77:ARG:N	1:A:77:ARG:HD2	2.31	0.45
1:A:343:GLY:C	1:A:345:GLU:H	2.17	0.45
1:A:477:LEU:HG	1:A:481:LEU:HD11	1.99	0.45
1:A:50:THR:HA	1:A:53:VAL:HG22	1.99	0.44
1:A:177:LEU:C	1:A:177:LEU:HD23	2.38	0.44
1:A:19:GLY:HA3	1:A:106:TRP:CZ3	2.53	0.44
1:A:347:GLN:HB3	1:A:348:PRO:HD3	2.00	0.44
1:A:206:ASP:O	1:A:208:VAL:HG23	2.17	0.43
1:A:194:VAL:CG2	1:A:239:LEU:HD23	2.48	0.43
1:A:298:LEU:HB2	1:A:318:TYR:CD1	2.53	0.43
1:A:74:PHE:CG	1:A:366:LEU:HD22	2.54	0.43
1:A:32:GLU:OE2	1:A:34:LEU:HB2	2.18	0.43
1:A:411:PRO:O	1:A:412:ALA:HB3	2.19	0.43
1:A:180:ILE:HD11	1:A:211:ILE:HD11	2.00	0.43
1:A:326:GLY:O	1:A:329:LEU:HB3	2.19	0.42
1:A:180:ILE:HG22	1:A:181:ARG:N	2.35	0.42
1:A:461:ARG:HB2	1:A:463:ASP:OD1	2.19	0.42
1:A:57:ARG:HB2	1:A:59:ILE:HD11	2.01	0.42
1:A:134:VAL:O	1:A:140:PRO:HA	2.20	0.42
1:A:16:MET:HG2	1:A:292:VAL:HG13	2.01	0.42
1:A:73:HIS:CD2	1:A:76:GLY:H	2.37	0.42
1:A:311:PRO:HB2	3:A:502:HOH:O	2.20	0.42
1:A:322:ARG:HD2	1:A:322:ARG:HA	1.79	0.41
1:A:173[B]:ARG:NE	1:A:341:LEU:HD21	2.35	0.41
1:A:74:PHE:CD1	1:A:366:LEU:HD22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG23	1:A:239:LEU:HD23	2.02	0.41
1:A:470:SER:HA	1:A:471:PRO:HA	1.83	0.41
1:A:434:ASP:HB3	1:A:489:ARG:NH1	2.35	0.41
1:A:22:ARG:NH1	1:A:27:ASP:HA	2.34	0.41
1:A:7:VAL:HB	1:A:30:VAL:HG22	2.03	0.41
1:A:75:GLY:CA	1:A:336:GLN:HG3	2.51	0.41
1:A:237:GLN:HG3	1:A:238:ARG:N	2.36	0.41
1:A:447:PRO:HA	1:A:448:PRO:HD3	1.99	0.41
1:A:74:PHE:CE1	1:A:369:MET:CE	3.04	0.40
1:A:482:ASP:HA	1:A:486:GLY:O	2.21	0.40
1:A:42:ARG:HG2	1:A:42:ARG:H	1.65	0.40
1:A:118:HIS:CE1	1:A:137:PRO:HD2	2.56	0.40
1:A:418:ASP:O	1:A:440:THR:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/499 (98%)	443 (91%)	42 (9%)	3 (1%)	25	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	GLY
1	A	299	GLY
1	A	195	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	381/389 (98%)	342 (90%)	39 (10%)	7 17

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	38	THR
1	A	40	GLU
1	A	42	ARG
1	A	68	THR
1	A	70	THR
1	A	80	ASP
1	A	85	GLU
1	A	92	LYS
1	A	99	THR
1	A	119	THR
1	A	124	THR
1	A	144	THR
1	A	155	ARG
1	A	165	ASP
1	A	204	LEU
1	A	213	VAL
1	A	221	ARG
1	A	237	GLN
1	A	239	LEU
1	A	246	HIS
1	A	298	LEU
1	A	336	GLN
1	A	340	PHE
1	A	341	LEU
1	A	353	LEU
1	A	363	SER
1	A	390	ARG
1	A	395	GLU
1	A	398	ARG

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Mol	Chain	Res	Type
1	A	400	HIS
1	A	405	THR
1	A	410	HIS
1	A	440	THR
1	A	458	VAL
1	A	459	LEU
1	A	469	ILE
1	A	470	SER
1	A	478	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	73	HIS
1	A	96	GLN
1	A	246	HIS
1	A	334	GLN
1	A	336	GLN
1	A	394	GLN

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 carbohydrates 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	A	500	-	51,58,58	1.53	7 (13%)	60,89,89	1.58	8 (13%)

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	A	500	-	-	8/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C4X-N5	5.36	1.41	1.33
2	A	500	FAD	C10-N1	4.29	1.38	1.33
2	A	500	FAD	C2A-N3A	3.47	1.37	1.32
2	A	500	FAD	C1'-N10	3.33	1.51	1.48
2	A	500	FAD	C4-N3	3.13	1.38	1.33
2	A	500	FAD	C5X-N5	2.64	1.39	1.35
2	A	500	FAD	C2A-N1A	2.56	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-5.81	119.60	128.68
2	A	500	FAD	C4-N3-C2	4.96	119.33	115.14
2	A	500	FAD	C4X-N5-C5X	3.90	120.66	116.77
2	A	500	FAD	C5X-C9A-N10	2.98	119.88	117.72
2	A	500	FAD	C4-C4X-N5	2.65	121.63	118.60
2	A	500	FAD	P-O3P-PA	-2.65	123.73	132.83
2	A	500	FAD	C10-C4X-N5	-2.28	119.68	121.26
2	A	500	FAD	O3'-C3'-C4'	-2.01	103.96	108.81

There are no chirality outliers.

All (8) torsion outliers are listed below:

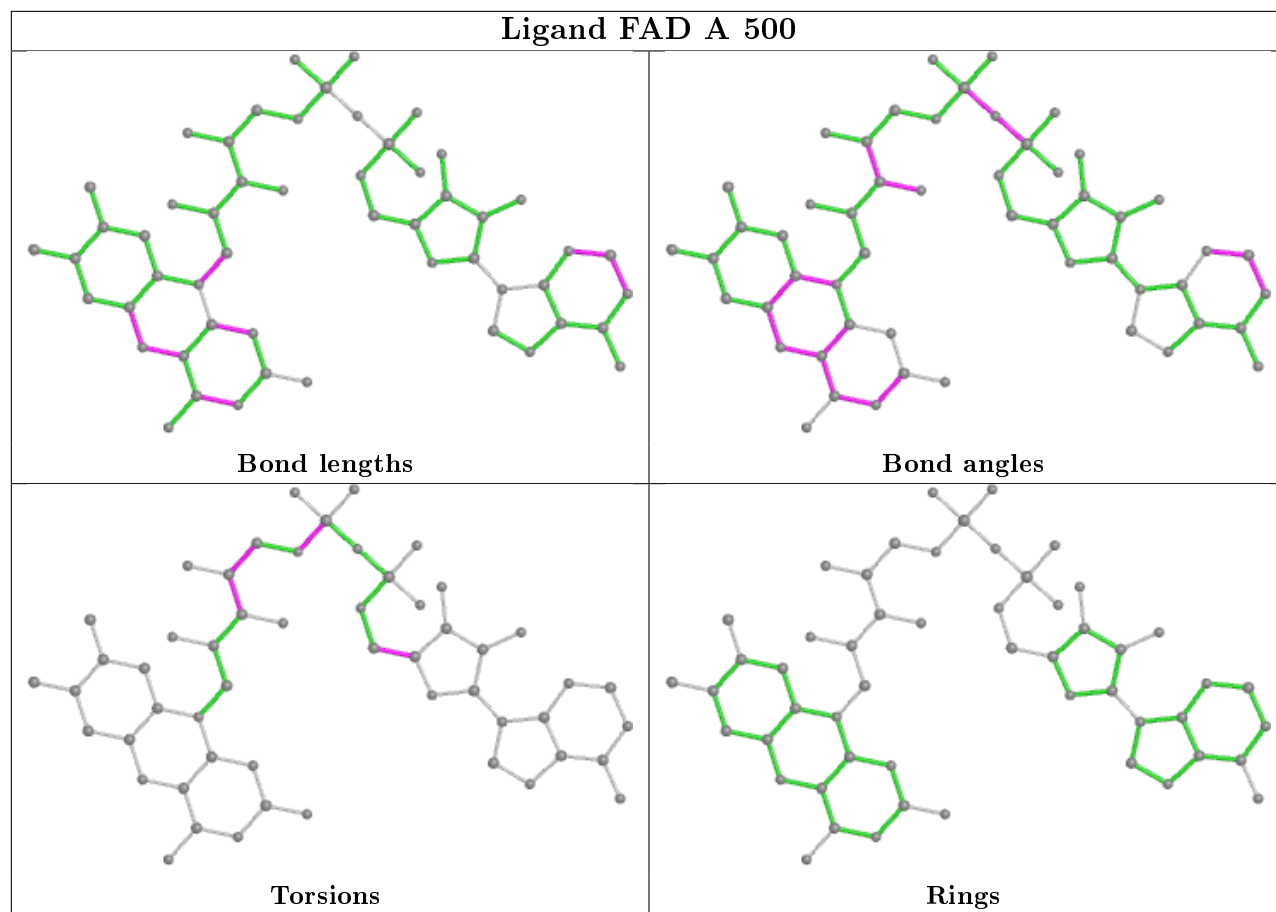
Mol	Chain	Res	Type	Atoms
2	A	500	FAD	C3'-C4'-C5'-O5'
2	A	500	FAD	O4'-C4'-C5'-O5'
2	A	500	FAD	C5'-O5'-P-O1P
2	A	500	FAD	C5'-O5'-P-O2P
2	A	500	FAD	C5'-O5'-P-O3P
2	A	500	FAD	O3'-C3'-C4'-O4'
2	A	500	FAD	C2'-C3'-C4'-O4'
2	A	500	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	489/499 (97%)	0.69	58 (11%) 4 3	41, 73, 90, 106	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	PRO	7.5
1	A	401	GLY	6.1
1	A	488	ALA	4.9
1	A	478	THR	4.8
1	A	167	PRO	4.6
1	A	447	PRO	4.2
1	A	474	ARG	4.2
1	A	149	VAL	3.9
1	A	383	ASP	3.8
1	A	137	PRO	3.7
1	A	17	LEU	3.7
1	A	402	LYS	3.6
1	A	205	GLY	3.4
1	A	36	GLN	3.3
1	A	7	VAL	3.2
1	A	197	GLY	3.2
1	A	381	GLY	3.1
1	A	400	HIS	3.1
1	A	206	ASP	3.0
1	A	446	ALA	3.0
1	A	223	ARG	3.0
1	A	14	GLY	2.9
1	A	151	CYS	2.9
1	A	146	ARG	2.9
1	A	449	GLN	2.8
1	A	219	PRO	2.8
1	A	296	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	307	SER	2.8
1	A	396	LEU	2.8
1	A	222	ARG	2.7
1	A	224	THR	2.7
1	A	39	GLY	2.6
1	A	67	GLU	2.6
1	A	467	ALA	2.5
1	A	248	GLU	2.5
1	A	84	LEU	2.5
1	A	34	LEU	2.5
1	A	380	ASP	2.5
1	A	13	ALA	2.4
1	A	150	GLY	2.4
1	A	303	ALA	2.4
1	A	244	ILE	2.4
1	A	91	VAL	2.4
1	A	273	ALA	2.3
1	A	173[A]	ARG	2.3
1	A	63	PHE	2.3
1	A	297	ASN	2.3
1	A	443	LEU	2.3
1	A	399	ALA	2.3
1	A	37	ARG	2.2
1	A	138	ASP	2.1
1	A	292	VAL	2.1
1	A	8	VAL	2.1
1	A	420	ALA	2.1
1	A	181	ARG	2.1
1	A	62	ALA	2.0
1	A	452	LEU	2.0
1	A	461	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

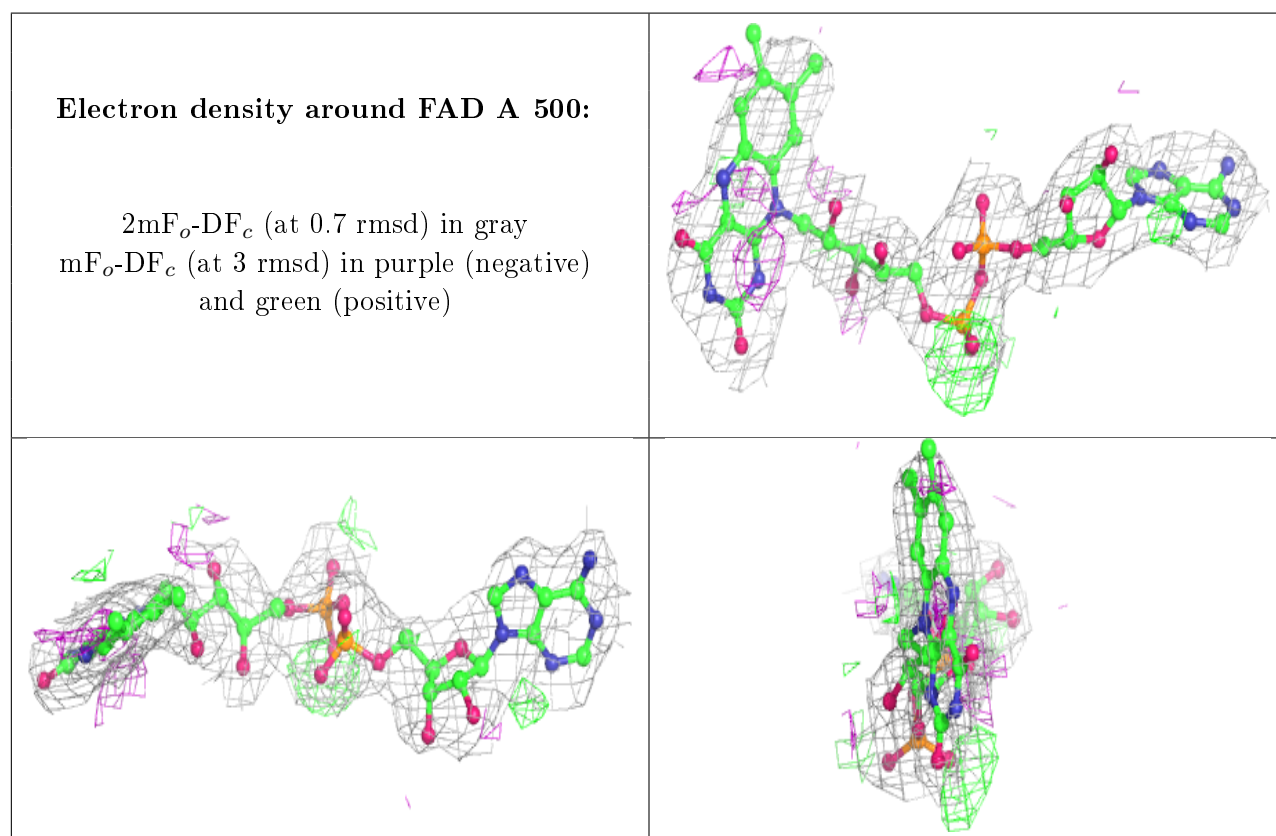
There are no carbohydrates in this entry.

6.4 Ligands [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
2	FAD	A	500	53/53	0.92	0.18	69,76,83,84	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.