



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:32 AM UTC

PDB ID : 2QA2 / pdb\_00002qa2  
Title : Crystal structure of CabE, an aromatic hydroxylase from angucycline biosynthesis, determined to 2.7 Å resolution  
Authors : Koskiniemi, H.; Dobritzsch, 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](mailto: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>.

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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)  
Xtrriage (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

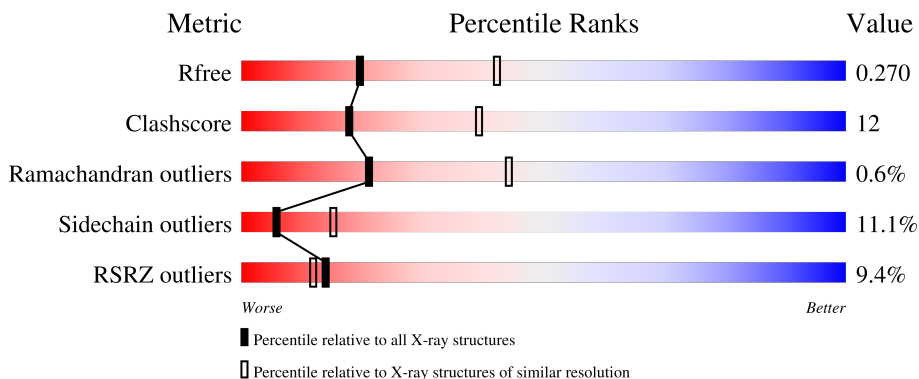
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3760 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 Polyketide oxygenase CabE.

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

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

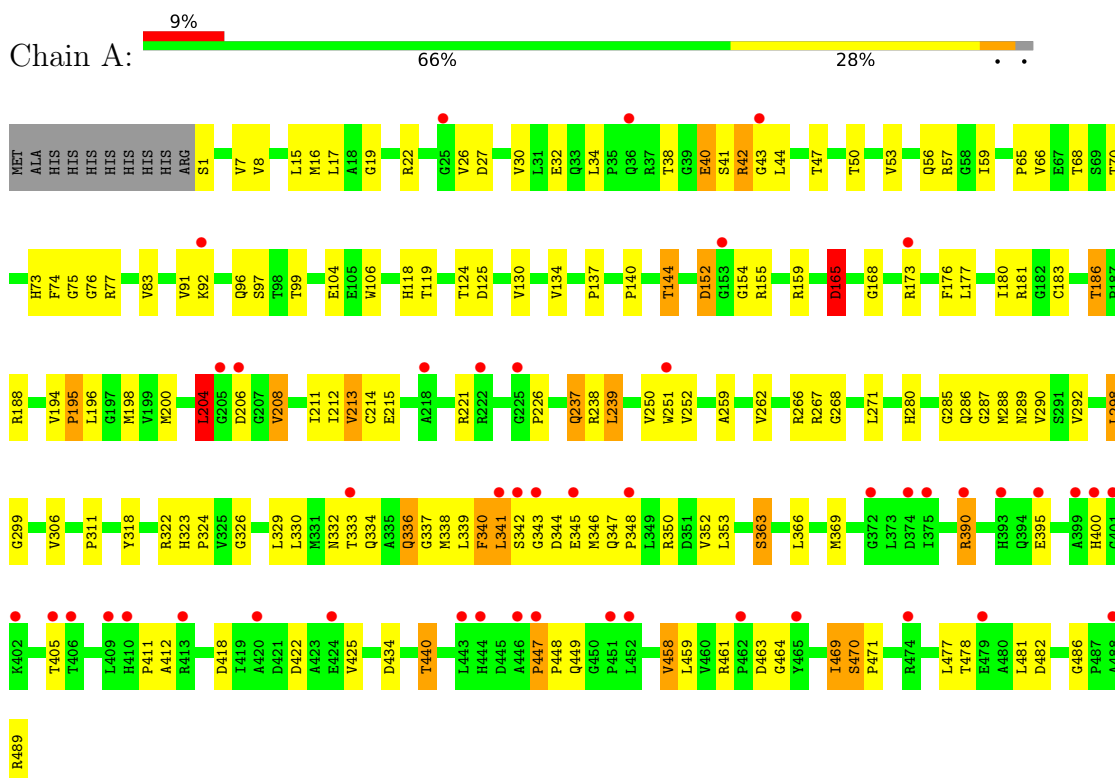
- Molecule 3 is water.

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

### 3 Residue-property plots

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: Polyketide oxygenase CabE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.10Å 133.10Å 166.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.83 – 2.70 29.83 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.83-2.70) 99.3 (29.83-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.48 (at 2.68Å)	Xtrriage
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 (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtrriage
Anisotropy	0.283	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 86.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3760	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.66	0/3765	0.96	6/5115 (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	A	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ASP	N-CA-C	-6.71	105.08	113.20
1	A	250	VAL	N-CA-C	-5.42	106.90	111.56
1	A	165	ASP	CA-C-N	-5.09	117.19	122.89
1	A	165	ASP	C-N-CA	-5.09	117.19	122.89
1	A	65	PRO	CA-C-O	5.06	126.64	121.23
1	A	66	VAL	CA-CB-CG1	5.03	118.96	110.40

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

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	89	0
2	A	53	0	31	4	0
3	A	24	0	0	3	0
All	All	3760	0	3663	91	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 12.

All (91) 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:47:THR:HG23	1:A:289:ASN:CG	2.26	0.60
1:A:266:ARG:HG3	1:A:271:LEU:HG	1.83	0.60
2:A:500:FAD:H5'1	2:A:500:FAD:PA	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:334:GLN:HE21	1:A:338:MET:HE3	1.70	0.57
1:A:194:VAL:O	1:A:195:PRO:C	2.48	0.56
1:A:342:SER:HB2	1:A:346:MET:HB2	1.90	0.54
2:A:500:FAD:H5'1	2:A:500:FAD:O1A	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLN:NE2	1:A:464:GLY:HA3	2.24	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:215:GLU:CD	1:A:238:ARG:HH12	2.18	0.51
1:A:96:GLN:OE1	2:A:500:FAD:O4'	2.27	0.51
1:A:152:ASP:OD1	1:A:152:ASP:N	2.40	0.50
1:A:168:GLY:HA3	1:A:259:ALA:O	2.11	0.50
1:A:267:ARG:O	1:A:268:GLY:C	2.55	0.50
1:A:177:LEU:C	1:A:177:LEU:HD23	2.38	0.49
1:A:343:GLY:C	1:A:345:GLU:H	2.17	0.49
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:198:MET:HE3	1:A:340:PHE:O	2.14	0.48
1:A:96:GLN:HA	1:A:288:MET:HE1	1.97	0.47
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:323:HIS:HB3	1:A:324:PRO:HD3	1.97	0.46
1:A:332:ASN:CG	1:A:369:MET:HE3	2.40	0.46
1:A:194:VAL:O	1:A:196:LEU:N	2.47	0.46
1:A:40:GLU:HG3	1:A:251:TRP:CH2	2.52	0.45
1:A:74:PHE:HE1	1:A:369:MET:CE	2.28	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: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:19:GLY:HA3	1:A:106:TRP:CZ3	2.53	0.44
1:A:74:PHE:CE1	1:A:369:MET:HE1	2.52	0.44
1:A:347:GLN:HB3	1:A:348:PRO:HD3	2.00	0.44
1:A:194:VAL:CG2	1:A:239:LEU:HD23	2.48	0.43
1:A:206:ASP:O	1:A:208:VAL:HG23	2.17	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:286:GLN:O	1:A:287:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLY:O	1:A:329:LEU:HB3	2.19	0.42
1:A:57:ARG:HB2	1:A:59:ILE:HD11	2.01	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: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:173[B]:ARG:NE	1:A:341:LEU:HD21	2.35	0.41
1:A:322:ARG:HA	1:A:322:ARG:HD2	1.79	0.41
1:A:332:ASN:OD1	1:A:332:ASN:C	2.62	0.41
1:A:74:PHE:CD1	1:A:366:LEU:HD22	2.56	0.41
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:H	1:A:42:ARG:HG2	1.65	0.40
1:A:74:PHE:HE1	1:A:369:MET:HE1	1.87	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

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	488/499 (98%)	443 (91%)	42 (9%)	3 (1%)	21 44

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 [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	381/389 (98%)	339 (89%)	42 (11%)	6 15

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	26	VAL
1	A	38	THR
1	A	40	GLU
1	A	42	ARG
1	A	44	LEU
1	A	68	THR
1	A	70	THR
1	A	92	LYS
1	A	99	THR
1	A	119	THR
1	A	124	THR
1	A	144	THR
1	A	152	ASP
1	A	155	ARG
1	A	165	ASP
1	A	183	CYS
1	A	186	THR

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Mol	Chain	Res	Type
1	A	204	LEU
1	A	208	VAL
1	A	213	VAL
1	A	221	ARG
1	A	237	GLN
1	A	239	LEU
1	A	298	LEU
1	A	306	VAL
1	A	336	GLN
1	A	340	PHE
1	A	341	LEU
1	A	352	VAL
1	A	353	LEU
1	A	363	SER
1	A	390	ARG
1	A	395	GLU
1	A	400	HIS
1	A	405	THR
1	A	440	THR
1	A	458	VAL
1	A	459	LEU
1	A	469	ILE
1	A	470	SER
1	A	478	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	73	HIS
1	A	96	GLN
1	A	129	HIS
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 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	A	500	-	58,58,58	1.23	7 (12%)	85,89,89	1.59	17 (20%)

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	-	-	8/34/50/50	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	4.74	1.41	1.30
2	A	500	FAD	C10-N1	2.75	1.38	1.33
2	A	500	FAD	C2A-N1A	2.67	1.38	1.33
2	A	500	FAD	C8A-N7A	2.25	1.36	1.31
2	A	500	FAD	C2A-N3A	2.11	1.37	1.33
2	A	500	FAD	P-O3P	2.08	1.61	1.59
2	A	500	FAD	PA-O3P	2.05	1.61	1.59

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-5.93	119.60	128.58
2	A	500	FAD	C4-N3-C2	-3.55	119.33	125.64
2	A	500	FAD	C5A-C4A-N3A	-3.52	121.88	126.72
2	A	500	FAD	N9A-C8A-N7A	-3.48	109.00	113.94
2	A	500	FAD	C4X-C4-N3	3.25	121.52	113.25
2	A	500	FAD	C2A-N3A-C4A	3.20	119.64	111.83
2	A	500	FAD	C9A-C5X-N5	-2.96	119.31	122.45
2	A	500	FAD	O4-C4-C4X	-2.80	119.15	126.53
2	A	500	FAD	C5A-N7A-C8A	2.56	107.47	103.45
2	A	500	FAD	C10-C4X-N5	-2.51	119.68	124.81
2	A	500	FAD	C4-C4X-N5	2.48	121.63	118.21
2	A	500	FAD	C10-N1-C2	2.45	122.15	116.85
2	A	500	FAD	N3A-C4A-N9A	2.41	131.26	127.17
2	A	500	FAD	C4X-C10-N1	-2.32	118.90	124.59
2	A	500	FAD	C4X-C10-N10	2.30	119.78	116.48
2	A	500	FAD	O3'-C3'-C4'	-2.19	103.96	108.93
2	A	500	FAD	C5X-C9A-N10	2.11	119.88	117.97

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	O3'-C3'-C4'-C5'

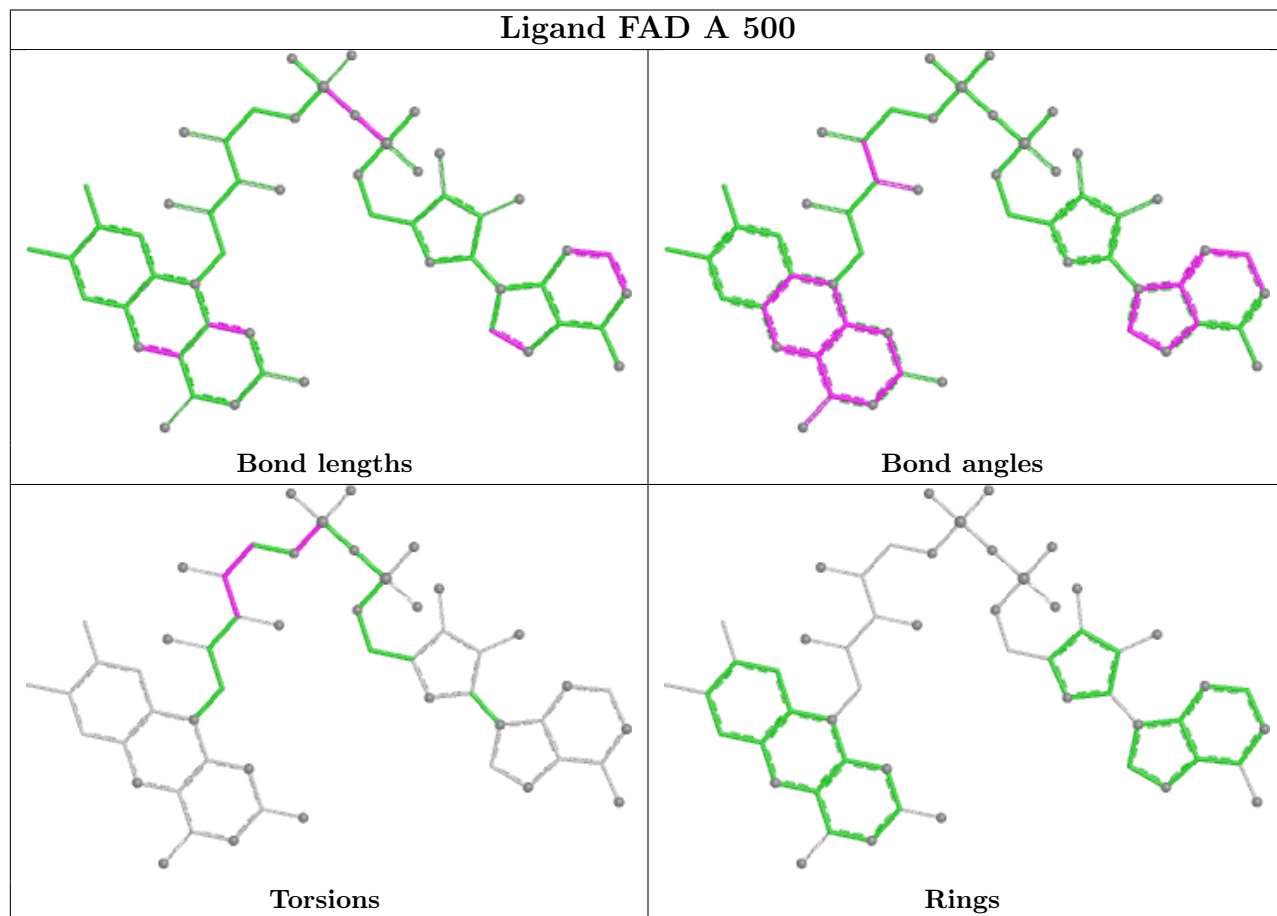
There are no ring outliers.

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	489/499 (97%)	0.87	46 (9%) <b>14</b> <b>12</b>	37, 73, 90, 106	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	GLY	4.5
1	A	25	GLY	4.3
1	A	173[A]	ARG	4.2
1	A	375	ILE	3.7
1	A	465	TYR	3.4
1	A	374	ASP	3.4
1	A	390	ARG	3.3
1	A	443	LEU	3.3
1	A	206	ASP	3.3
1	A	343	GLY	3.2
1	A	222	ARG	3.1
1	A	447	PRO	2.9
1	A	462	PRO	2.8
1	A	409	LEU	2.8
1	A	348	PRO	2.7
1	A	474	ARG	2.7
1	A	406	THR	2.6
1	A	452	LEU	2.6
1	A	43	GLY	2.6
1	A	218	ALA	2.6
1	A	393	HIS	2.5
1	A	420	ALA	2.5
1	A	153	GLY	2.5
1	A	251	TRP	2.5
1	A	402	LYS	2.4
1	A	36	GLN	2.4
1	A	400	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	444	HIS	2.4
1	A	488	ALA	2.4
1	A	345	GLU	2.3
1	A	446	ALA	2.3
1	A	92	LYS	2.3
1	A	333	THR	2.2
1	A	405	THR	2.2
1	A	479	GLU	2.2
1	A	342	SER	2.2
1	A	410	HIS	2.2
1	A	399	ALA	2.1
1	A	424	GLU	2.1
1	A	451	PRO	2.1
1	A	372	GLY	2.1
1	A	413	ARG	2.1
1	A	341	LEU	2.1
1	A	225	GLY	2.1
1	A	395	GLU	2.0
1	A	401	GLY	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.

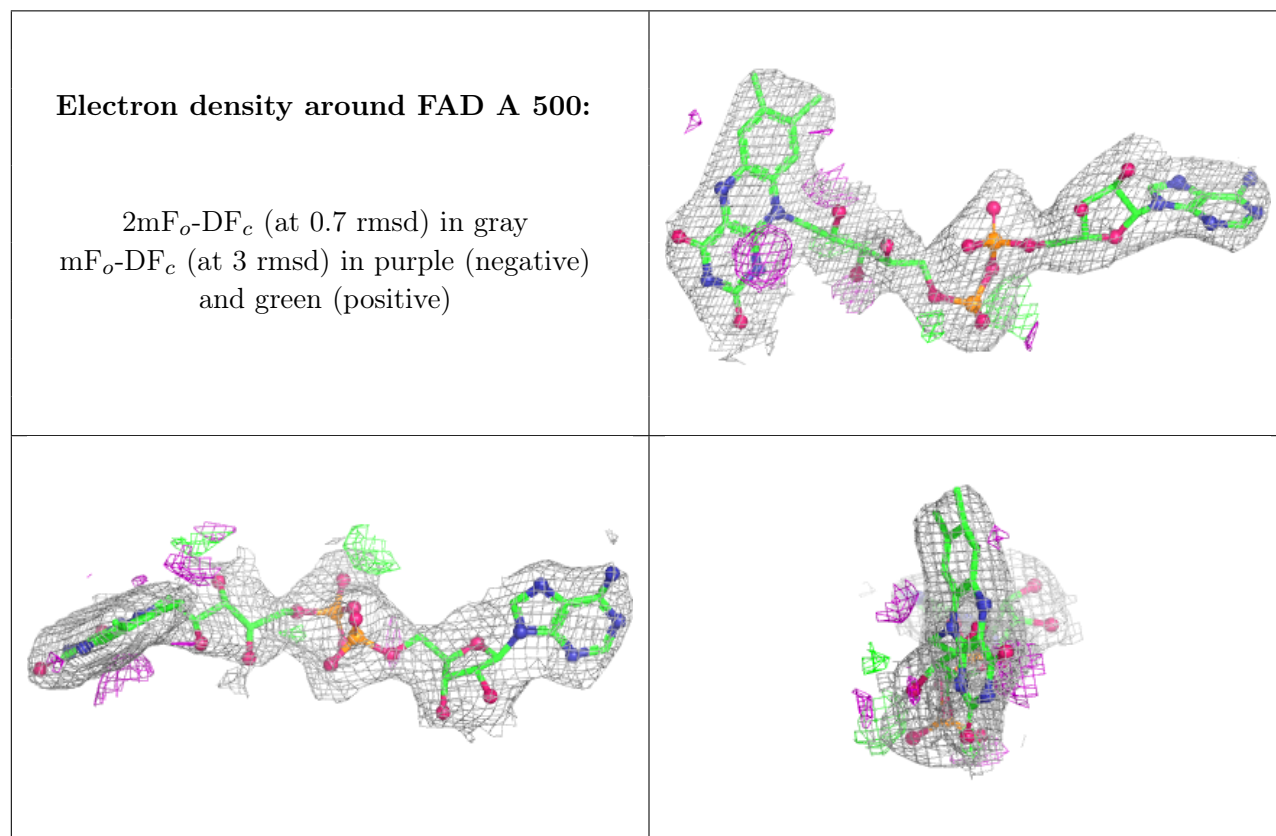
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	FAD	A	500	53/53	0.95	0.11	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.