



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 05:39 PM GMT

PDB ID : 2QA2
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

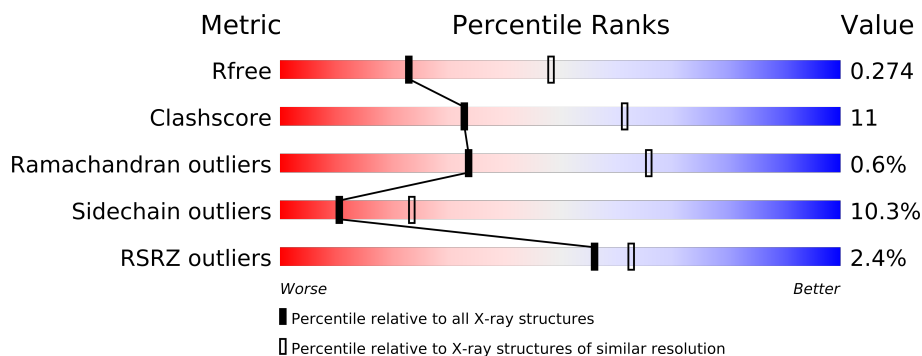
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	499	

2 Entry composition i

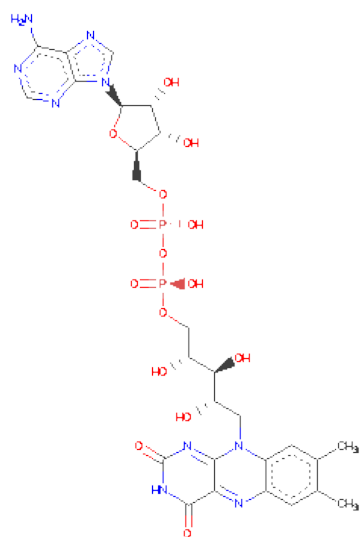
There are 3 unique types of molecules in this entry. The entry contains 3760 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (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	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

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 0.231 , 0.274	Depositor DCC
R_{free} test set	1217 reflections (4.99%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 24412 reflections	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.

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	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
2:A:500:FAD:O1A	2:A:500:FAD:H5'1	2.07	0.54
1:A:342:SER:HB2	1:A:346:MET:HB2	1.90	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	Distance(Å)	Clash(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:298:LEU:HB2	1:A:318:TYR:CD1	2.53	0.43
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: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:73:HIS:CD2	1:A:76:GLY:H	2.37	0.42
1:A:16:MET:HG2	1:A:292:VAL:HG13	2.01	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:HD2	1:A:322:ARG:HA	1.79	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:447:PRO:HA	1:A:448:PRO:HD3	1.99	0.41
1:A:237:GLN:HG3	1:A:238:ARG:N	2.36	0.41
1:A:75:GLY:CA	1:A:336:GLN:HG3	2.51	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

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%)	33	66

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%)	11	24

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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.11	5 (8%)	85,89,89	1.93	12 (14%)

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	-	-	0/34/50/50	0/1/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C1'-N10	3.07	1.51	1.48
2	A	500	FAD	C5X-N5	2.87	1.39	1.35
2	A	500	FAD	C2A-N3A	2.79	1.37	1.32
2	A	500	FAD	C2A-N1A	2.42	1.38	1.33
2	A	500	FAD	C4X-N5	2.31	1.41	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	FAD	N3A-C2A-N1A	-10.90	119.60	128.71
2	A	500	FAD	C2-N1-C10	7.12	122.15	114.98
2	A	500	FAD	C4X-C10-N1	-3.83	118.90	122.73
2	A	500	FAD	C4X-N5-C5X	3.54	120.66	116.69
2	A	500	FAD	N3A-C4A-N9A	3.23	131.26	125.43
2	A	500	FAD	C5X-C9A-N10	3.12	119.88	116.80
2	A	500	FAD	C4-N3-C2	-2.95	119.33	125.39
2	A	500	FAD	O4B-C1B-N9A	-2.94	105.71	108.44
2	A	500	FAD	P-O3P-PA	-2.71	123.73	131.68
2	A	500	FAD	C2'-C1'-N10	-2.10	109.66	112.45
2	A	500	FAD	C4X-C4-N3	2.09	121.52	115.39
2	A	500	FAD	N1-C10-N10	2.03	121.31	115.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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%)	-0.07	11 (2%) 59 65	41, 73, 90, 106	1 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	PRO	4.2
1	A	36	GLN	3.1
1	A	149	VAL	3.1
1	A	400	HIS	2.8
1	A	205	GLY	2.5
1	A	402	LYS	2.3
1	A	224	THR	2.2
1	A	399	ALA	2.2
1	A	381	GLY	2.1
1	A	474	ARG	2.1
1	A	151	CYS	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	A	500	53/53	0.25	1.60	69,76,83,84	0

6.5 Other polymers ⓘ

There are no such residues in this entry.