



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM 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.; Metsä-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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

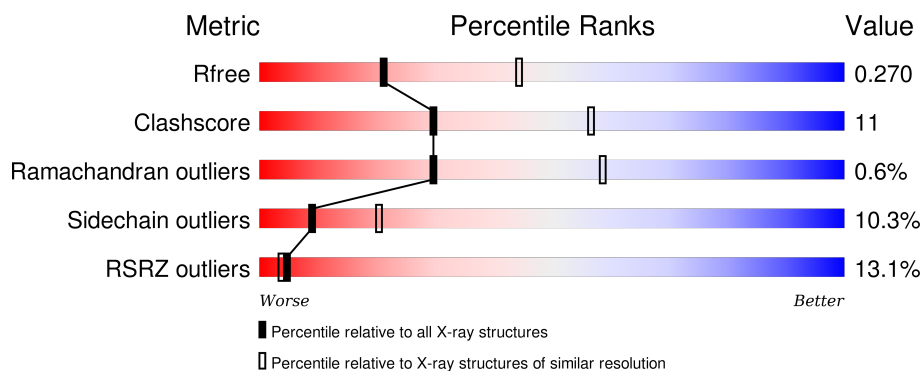
# 1 Overall quality at a glance

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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>13%</div> <div>68%</div> <div>27%</div> <div>• •</div> </div>

## 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
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:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 3 is water.

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

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 29.82 – 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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 83.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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
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	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: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

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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: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 [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%)	30	59

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%)	9 21

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	-	48,58,58	1.38	6 (12%)	54,89,89	2.17	8 (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	-	-	0/30/50/50	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	FAD	C2A-N1A	2.51	1.38	1.33
2	A	500	FAD	C5X-N5	2.75	1.39	1.35
2	A	500	FAD	C4-N3	2.90	1.38	1.33
2	A	500	FAD	C1'-N10	3.07	1.51	1.48
2	A	500	FAD	C2A-N3A	3.11	1.37	1.32
2	A	500	FAD	C4X-N5	4.88	1.41	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	-12.14	119.60	128.89
2	A	500	FAD	P-O3P-PA	-3.20	123.73	132.73
2	A	500	FAD	C9A-C5X-N5	-2.06	119.31	122.36
2	A	500	FAD	C1B-N9A-C4A	-2.03	123.88	126.94
2	A	500	FAD	C4-C4X-N5	2.40	121.63	118.72
2	A	500	FAD	C5X-C9A-N10	2.97	119.88	117.62
2	A	500	FAD	C4X-N5-C5X	3.39	120.66	116.76
2	A	500	FAD	C4-N3-C2	4.73	119.33	115.25

There are no chirality outliers.

There are no torsion outliers.

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

## 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, 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%)	0.74	64 (13%) 5 4	41, 73, 90, 106	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	448	PRO	7.7
1	A	401	GLY	6.2
1	A	488	ALA	5.1
1	A	478	THR	4.8
1	A	167	PRO	4.6
1	A	447	PRO	4.3
1	A	474	ARG	4.3
1	A	149	VAL	4.0
1	A	383	ASP	3.9
1	A	137	PRO	3.9
1	A	402	LYS	3.7
1	A	17	LEU	3.7
1	A	205	GLY	3.4
1	A	36	GLN	3.3
1	A	7	VAL	3.3
1	A	400	HIS	3.2
1	A	197	GLY	3.2
1	A	206	ASP	3.1
1	A	446	ALA	3.1
1	A	381	GLY	3.1
1	A	146	ARG	3.0
1	A	14	GLY	3.0
1	A	151	CYS	3.0
1	A	223	ARG	3.0
1	A	449	GLN	3.0
1	A	219	PRO	2.9
1	A	307	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	396	LEU	2.9
1	A	222	ARG	2.8
1	A	296	VAL	2.8
1	A	39	GLY	2.7
1	A	224	THR	2.6
1	A	248	GLU	2.6
1	A	67	GLU	2.6
1	A	84	LEU	2.6
1	A	13	ALA	2.5
1	A	467	ALA	2.5
1	A	380	ASP	2.5
1	A	150	GLY	2.5
1	A	34	LEU	2.5
1	A	244	ILE	2.4
1	A	273	ALA	2.4
1	A	303	ALA	2.4
1	A	173[A]	ARG	2.4
1	A	91	VAL	2.4
1	A	297	ASN	2.4
1	A	443	LEU	2.3
1	A	63	PHE	2.3
1	A	138	ASP	2.3
1	A	399	ALA	2.3
1	A	37	ARG	2.2
1	A	62	ALA	2.2
1	A	8	VAL	2.2
1	A	452	LEU	2.1
1	A	292	VAL	2.1
1	A	181	ARG	2.1
1	A	461	ARG	2.1
1	A	89	TYR	2.1
1	A	445	ASP	2.1
1	A	243	ASP	2.1
1	A	420	ALA	2.0
1	A	88	HIS	2.0
1	A	204	LEU	2.0
1	A	327	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 [i](#)

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. 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	500	53/53	0.92	0.18	-0.70	69,76,83,84	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.