

wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2023 – 05:05 PM EDT

:	4Q5O
:	Crystal structure of EctD from S. alaskensis with 2-oxoglutarate and 5-
	hydroxyectoine
:	Hoeppner, A.; Widderich, N.; Bremer, E.; Smits, S.H.
	2014-04-17
:	2.64 Å(reported)
	: : :

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

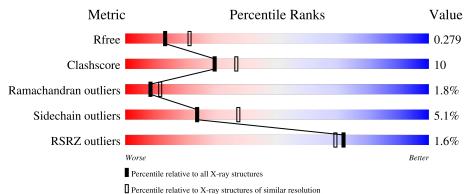
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.64 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472(2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	А	314	% 69%	18%	• 10%		
1	В	314	^{2%} 68%	19%	•• 10%		

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AKG	А	402	-	Х	-	-
4	6CS	В	403	-	-	Х	-



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4469 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 Ectoine hydroxylase.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	282	Total	С	Ν	Ο	S	0	0	0
	I A		2198	1389	397	403	9	0		
1	В	282	Total	С	Ν	Ο	S	0	0	0
1	D	262	2198	1389	397	403	9			

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	HIS	-	expression tag	UNP Q1GNW5
А	-6	HIS	-	expression tag	UNP Q1GNW5
А	-5	HIS	-	expression tag	UNP Q1GNW5
A	-4	HIS	-	expression tag	UNP Q1GNW5
А	-3	HIS	-	expression tag	UNP Q1GNW5
A	-2	HIS	-	expression tag	UNP Q1GNW5
А	-1	SER	-	expression tag	UNP Q1GNW5
A	0	GLU	-	expression tag	UNP Q1GNW5
В	-7	HIS	-	expression tag	UNP Q1GNW5
В	-6	HIS	-	expression tag	UNP Q1GNW5
В	-5	HIS	-	expression tag	UNP Q1GNW5
В	-4	HIS	-	expression tag	UNP Q1GNW5
В	-3	HIS	-	expression tag	UNP Q1GNW5
В	-2	HIS	-	expression tag	UNP Q1GNW5
В	-1	SER	-	expression tag	UNP Q1GNW5
В	0	GLU	-	expression tag	UNP Q1GNW5

There are 16 discrepancies between the modelled and reference sequences:

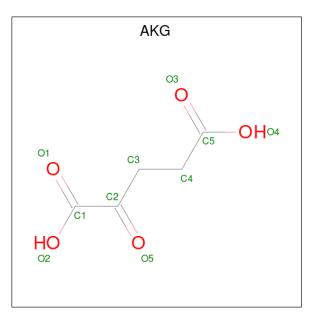
• Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Fe 1 1	0	0
2	В	1	Total Fe 1 1	0	0



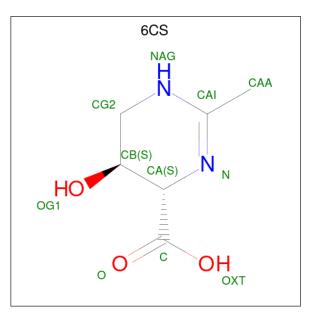


• Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 10 5 5	0	0
3	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 10 5 5 \end{array}$	0	0

• Molecule 4 is (4S,5S)-5-HYDROXY-2-METHYL-1,4,5,6-TETRAHYDROPYRIMIDINE-4-CARBOXYLIC ACID (three-letter code: 6CS) (formula: $C_6H_{10}N_2O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total C N O 11 6 2 3	0	0
4	В	1	Total C N O 11 6 2 3	0	0

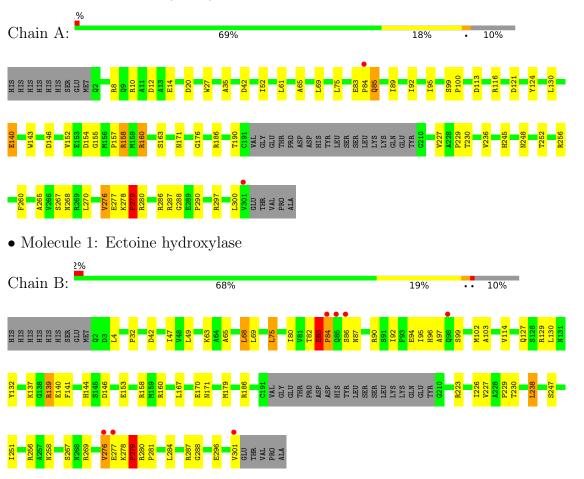
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	14	Total O 14 14	0	0
5	В	15	Total O 15 15	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: Ectoine hydroxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	81.00Å 87.08Å 94.88Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 - 2.64	Depositor
Resolution (A)	40.94 – 2.64	EDS
% Data completeness	99.8 (30.00-2.64)	Depositor
(in resolution range)	$99.8 \ (40.94 - 2.64)$	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.81 (at 2.65 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.206 , 0.279	Depositor
IV, IVfree	0.206 , 0.279	DCC
R_{free} test set	1035 reflections $(5.11%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	57.6	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.35, 48.8	EDS
L-test for twinning ²	$< L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4469	wwPDB-VP
Average B, all atoms $(Å^2)$	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: AKG, $6\mathrm{CS},\,\mathrm{FE}$

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.43	0/2255	0.62	1/3070~(0.0%)	
1	В	0.44	0/2255	0.62	1/3070~(0.0%)	
All	All	0.44	0/4510	0.62	2/6140~(0.0%)	

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	279	PRO	N-CA-CB	6.26	110.81	103.30
1	В	279	PRO	N-CA-CB	5.92	110.41	103.30

There are no chirality outliers.

There are no planarity outliers.

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	А	2198	0	2123	42	0
1	В	2198	0	2123	44	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
3	А	10	0	4	0	0
3	В	10	0	4	2	0
4	А	11	0	8	2	0

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Mol	Chain	Non-H	H(model)	$H(model) \mid H(added) \mid$		Symm-Clashes				
4	В	11	0	9	8	0				
5	А	14	0	0	0	0				
5	В	15	0	0	0	0				
All	All	4469	0	4271	83	0				

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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 10.

The worst 5 of 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:146:ASP:OD1	4:A:403:6CS:OG1	1.75	1.05
1:B:146:ASP:OD1	4:B:403:6CS:OG1	1.89	0.90
1:B:127:GLN:HE22	4:B:403:6CS:HAA1	1.45	0.80
1:A:227:VAL:HG12	1:A:229:PRO:HD3	1.67	0.75
1:B:127:GLN:NE2	1:B:284:LEU:O	2.23	0.71

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	Chain Analysed Favoured Allowed		Outliers	Perce	entiles	
1	А	278/314~(88%)	261 (94%)	12~(4%)	5(2%)	8	11
1	В	278/314~(88%)	253~(91%)	20~(7%)	5(2%)	8	11
All	All	556/628~(88%)	514 (92%)	32~(6%)	10 (2%)	8	11

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	85	GLN

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Mol	Chain	Res	Type
1	А	277	GLU
1	А	279	PRO
1	В	83	GLU
1	В	84	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Analysed Rotameric Outliers		Percentiles		
1	А	227/262~(87%)	222~(98%)	5(2%)	52 70		
1	В	227/262~(87%)	209~(92%)	18 (8%)	12 18		
All	All	454/524 (87%)	431 (95%)	23~(5%)	24 37		

5 of 23 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	В	170	GLU
1	В	256	ARG
1	В	238	LEU
1	В	267	SER
1	В	68	LEU

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:

Mol	Chain	Res	Type
1	В	171	ASN
1	В	258	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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		Res Link Bond lengths				Bond angles		
	Mol Type Chain Re	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2	
3	AKG	А	402	2	9,9,9	0.96	0	11,11,11	2.13	<mark>6 (54%)</mark>
3	AKG	В	402	2	9,9,9	0.95	0	11,11,11	2.03	2 (18%)
4	6CS	А	403	2	9,11,11	2.35	3 (33%)	9,15,15	4.55	<mark>6 (66%)</mark>
4	6CS	В	403	-	9,11,11	3.08	4 (44%)	$9,\!15,\!15$	2.94	2 (22%)

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
3	AKG	А	402	2	-	7/9/9/9	-
3	AKG	В	402	2	-	6/9/9/9	-
4	6CS	А	403	2	-	0/4/17/17	0/1/1/1
4	6CS	В	403	-	_	0/4/17/17	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	В	403	6CS	CG2-NAG	-6.62	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	403	6CS	CG2-NAG	-4.93	1.41	1.46
4	В	403	6CS	CA-N	-4.34	1.42	1.46
4	А	403	6CS	CA-N	-3.42	1.42	1.46
4	В	403	6CS	CA-C	-3.18	1.49	1.52

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The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	403	6CS	CB-CG2-NAG	11.05	121.28	109.83
4	В	403	6CS	CB-CG2-NAG	8.09	118.22	109.83
4	А	403	6CS	CB-CA-C	5.52	120.36	111.72
3	В	402	AKG	C3-C4-C5	-4.50	103.93	113.60
4	А	403	6CS	CG2-NAG-CAI	-3.07	115.12	123.00

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	402	AKG	O1-C1-C2-O5
3	А	402	AKG	O1-C1-C2-C3
3	А	402	AKG	O2-C1-C2-C3
3	А	402	AKG	C1-C2-C3-C4
3	В	402	AKG	O2-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	В	402	AKG	2	0
4	А	403	6CS	2	0
4	В	403	6CS	8	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 (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^{th} 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	$\langle RSRZ \rangle$	#RSRZ>2		OW	$/AB(A^2)$	Q<0.9
1	А	282/314~(89%)	-0.05	2(0%)	87 86	32, 4	19, 75, 100	0
1	В	282/314~(89%)	0.13	7 (2%)	57 53	36, 5	55, 81, 103	0
All	All	564/628~(89%)	0.04	9 (1%)	72 69	32, 5	52, 80, 103	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	277	GLU	4.5
1	В	84	PRO	4.2
1	В	276	VAL	3.8
1	В	301	VAL	3.7
1	В	85	GLN	3.1

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 monosaccharides 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^{th} 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 ²)	Q<0.9
4	6CS	А	403	11/11	0.72	0.30	69,77,80,82	0
3	AKG	А	402	10/10	0.80	0.27	66,78,86,90	0
4	6CS	В	403	11/11	0.81	0.37	66,70,76,77	0
2	\mathbf{FE}	А	401	1/1	0.92	0.16	61,61,61,61	0
3	AKG	В	402	10/10	0.92	0.19	54,59,71,72	0
2	FE	В	401	1/1	0.95	0.14	52,52,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.

