wwPDB X-ray Structure Validation Summary Report (i)

Dec 3, 2023 – 11:37 am GMT

PDB ID	:	2J6I
Title	:	Candida boidinii formate dehydrogenase (FDH) C-terminal mutant
Authors	:	Schirwitz, K.; Schmidt, A.; Lamzin, V.S.
Deposited on	:	2006-09-29
Resolution	:	1.55 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 (i)) were used in the production of this report:

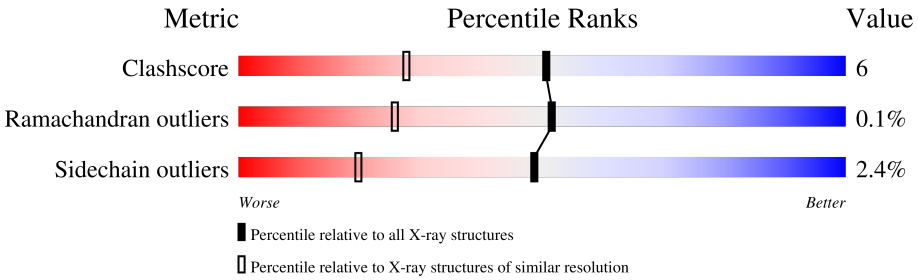
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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))
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13261 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.

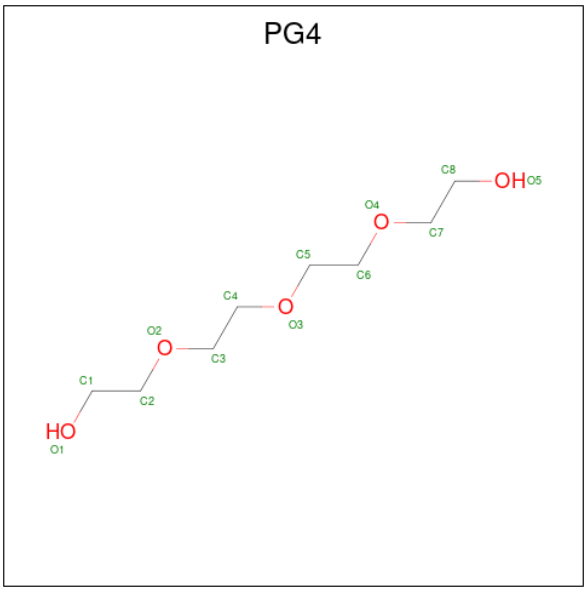
- Molecule 1 is a protein called FORMATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	2	0
			2759	1758	473	522	6			
1	B	353	Total	C	N	O	S	0	2	0
			2765	1763	473	523	6			
1	C	352	Total	C	N	O	S	0	2	0
			2755	1757	472	520	6			
1	D	352	Total	C	N	O	S	0	3	0
			2768	1765	473	524	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	VAL	LYS	engineered mutation	UNP O93968
B	328	VAL	LYS	engineered mutation	UNP O93968
C	328	VAL	LYS	engineered mutation	UNP O93968
D	328	VAL	LYS	engineered mutation	UNP O93968

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 8 5	0	0
2	C	1	Total C O 13 8 5	0	0
2	D	1	Total C O 13 8 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	578	Total O 578 578	0	0
3	B	534	Total O 534 534	0	0
3	C	560	Total O 560 560	0	0
3	D	503	Total O 503 503	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.36Å 68.14Å 109.15Å 78.07° 89.41° 81.27°	Depositor
Resolution (Å)	19.26 – 1.55	Depositor
% Data completeness (in resolution range)	96.1 (19.26-1.55)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.254	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13261	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4

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	0.51	0/2822	0.61	0/3832
1	B	0.53	0/2826	0.61	0/3838
1	C	0.53	0/2817	0.63	0/3823
1	D	0.55	3/2837 (0.1%)	0.60	0/3852
All	All	0.53	3/11302 (0.0%)	0.62	0/15345

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	TYR	CE2-CZ	-7.01	1.29	1.38
1	D	8	TYR	CD2-CE2	-6.96	1.28	1.39
1	D	8	TYR	CD1-CE1	-6.51	1.29	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2759	0	2762	23	0
1	B	2765	0	2762	45	0
1	C	2755	0	2763	32	0
1	D	2768	0	2769	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	13	0	18	0	0
2	C	13	0	18	1	0
2	D	13	0	18	0	0
3	A	578	0	0	6	0
3	B	534	0	0	11	0
3	C	560	0	0	8	0
3	D	503	0	0	8	0
All	All	13261	0	11110	126	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 6.

The worst 5 of 126 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:C:84:LYS:HG2	3:C:2048:HOH:O	1.67	0.92
1:C:344:GLN:H	1:C:344:GLN:HE21	1.15	0.90
1:B:10:ALA:HB3	1:B:14:ALA:HB2	1.53	0.90
1:D:216[C]:GLU:HG3	1:D:246:LYS:HD3	1.55	0.87
3:A:2072:HOH:O	1:C:12[B]:LYS:HE2	1.76	0.86

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 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	353/364 (97%)	342 (97%)	11 (3%)	0	100	100
1	B	353/364 (97%)	340 (96%)	13 (4%)	0	100	100
1	C	350/364 (96%)	341 (97%)	9 (3%)	0	100	100
1	D	352/364 (97%)	339 (96%)	12 (3%)	1 (0%)	41	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1408/1456 (97%)	1362 (97%)	45 (3%)	1 (0%)	51 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	200	PRO

4.3.2 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	290/296 (98%)	287 (99%)	3 (1%)	76 57
1	B	290/296 (98%)	284 (98%)	6 (2%)	53 24
1	C	290/296 (98%)	282 (97%)	8 (3%)	43 14
1	D	292/296 (99%)	280 (96%)	12 (4%)	30 5
All	All	1162/1184 (98%)	1133 (98%)	29 (2%)	49 18

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	249	LYS
1	D	213	GLU
1	D	12	LYS
1	D	119	ASN
1	C	349	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	350	ASN
1	D	232	HIS
1	D	350	ASN
1	D	311	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	214	ASN

4.3.3 RNA

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

3 ligands are 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	PG4	A	1354	-	12,12,12	0.44	0	11,11,11	0.34	0
2	PG4	C	1354	-	12,12,12	0.48	0	11,11,11	0.23	0
2	PG4	D	1354	-	12,12,12	0.47	0	11,11,11	0.28	0

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	PG4	A	1354	-	-	4/10/10/10	-
2	PG4	C	1354	-	-	5/10/10/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PG4	D	1354	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1354	PG4	O2-C3-C4-O3
2	C	1354	PG4	O4-C7-C8-O5
2	C	1354	PG4	O1-C1-C2-O2
2	C	1354	PG4	O3-C5-C6-O4
2	D	1354	PG4	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1354	PG4	1	0

4.7 Other polymers

There are no such residues in this entry.

4.8 Polymer linkage issues

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

5.3 Carbohydrates

EDS was not executed - this section is therefore empty.

5.4 Ligands

EDS was not executed - this section is therefore empty.

5.5 Other polymers

EDS was not executed - this section is therefore empty.