Full wwPDB X-ray Structure Validation Report (i)

Apr 4, 2022 – 08:35 PM EDT

PDB ID	:	5TNP
Title	:	Crystal structure of the E153Q mutant of the CFTR inhibitory factor Cif containing the adducted Styrene oxide hydrolysis intermediate
Authors	:	Hvorecny, K.L.; Madden, D.R.
Deposited on	:	2016-10-14
Resolution	:	1.85 Å(reported)

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

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.27

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 1.85 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10371 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.
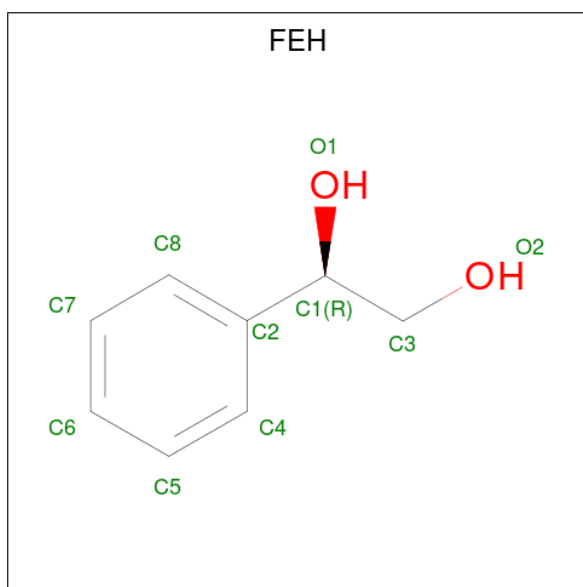
- Molecule 1 is a protein called CFTR inhibitory factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	11	0
			2409	1550	410	438	11			
1	B	293	Total	C	N	O	S	0	2	0
			2347	1511	402	423	11			
1	C	293	Total	C	N	O	S	0	11	0
			2407	1549	410	437	11			
1	D	293	Total	C	N	O	S	0	3	0
			2358	1516	405	426	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLN	GLU	engineered mutation	UNP A0A0M3KL26
B	153	GLN	GLU	engineered mutation	UNP A0A0M3KL26
C	153	GLN	GLU	engineered mutation	UNP A0A0M3KL26
D	153	GLN	GLU	engineered mutation	UNP A0A0M3KL26

- Molecule 2 is (1R)-1-phenylethane-1,2-diol (three-letter code: FEH) (formula: $C_8H_{10}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 9	C 8	O 1	0	1
2	A	1	Total 9	C 8	O 1	0	1
2	B	1	Total 9	C 8	O 1	0	1
2	B	1	Total 9	C 8	O 1	0	1
2	C	1	Total 9	C 8	O 1	0	1
2	C	1	Total 9	C 8	O 1	0	1
2	D	1	Total 9	C 8	O 1	0	1
2	D	1	Total 9	C 8	O 1	0	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	199	Total 199	O 199	0	0
3	B	184	Total 184	O 184	0	0
3	C	200	Total 200	O 200	0	0
3	D	195	Total 195	O 195	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.01Å 84.01Å 89.46Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	19.82 – 1.85	Depositor
% Data completeness (in resolution range)	99.7 (19.82-1.85)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.52 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.167 , 0.207	Depositor
Wilson B-factor (Å²)	21.4	Xtriage
Anisotropy	0.375	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10371	wwPDB-VP
Average B, all atoms (Å²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA ⓘ

MolProbity failed to run properly - this section is therefore empty.

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 ⓘ

8 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	FEH	D	402[B]	1	9,9,10	0.80	0	11,11,12	0.47	0
2	FEH	C	401[A]	1	9,9,10	0.32	0	11,11,12	0.58	0
2	FEH	B	402[B]	1	9,9,10	0.86	0	11,11,12	0.65	0
2	FEH	A	401[A]	1	9,9,10	0.34	0	11,11,12	0.59	0
2	FEH	C	402[B]	1	9,9,10	0.85	0	11,11,12	0.61	0
2	FEH	B	401[A]	1	9,9,10	0.33	0	11,11,12	0.62	0
2	FEH	D	401[A]	1	9,9,10	0.31	0	11,11,12	0.67	0
2	FEH	A	402[B]	1	9,9,10	0.83	0	11,11,12	0.50	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	FEH	D	402[B]	1	-	4/4/4/6	0/1/1/1
2	FEH	C	401[A]	1	-	0/4/4/6	0/1/1/1
2	FEH	B	402[B]	1	-	3/4/4/6	0/1/1/1
2	FEH	A	401[A]	1	-	1/4/4/6	0/1/1/1
2	FEH	C	402[B]	1	-	1/4/4/6	0/1/1/1
2	FEH	B	401[A]	1	-	1/4/4/6	0/1/1/1
2	FEH	D	401[A]	1	-	4/4/4/6	0/1/1/1
2	FEH	A	402[B]	1	-	4/4/4/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401[A]	FEH	C3-C1-C2-C8
2	B	402[B]	FEH	C3-C1-C2-C8
2	C	402[B]	FEH	C3-C1-C2-C8
2	A	402[B]	FEH	C3-C1-C2-C4
2	D	401[A]	FEH	C3-C1-C2-C8
2	D	402[B]	FEH	C3-C1-C2-C4

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Mol	Chain	Res	Type	Atoms
2	A	402[B]	FEH	C3-C1-C2-C8
2	B	402[B]	FEH	C3-C1-C2-C4
2	A	401[A]	FEH	C3-C1-C2-C8
2	D	401[A]	FEH	C3-C1-C2-C4
2	D	402[B]	FEH	C3-C1-C2-C8
2	A	402[B]	FEH	O1-C1-C2-C8
2	B	402[B]	FEH	O1-C1-C2-C4
2	A	402[B]	FEH	O1-C1-C2-C4
2	D	401[A]	FEH	O1-C1-C2-C4
2	D	401[A]	FEH	O1-C1-C2-C8
2	D	402[B]	FEH	O1-C1-C2-C4
2	D	402[B]	FEH	O1-C1-C2-C8

There are no ring outliers.

No monomer is involved in short contacts.

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 failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3   Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

5.4   Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

5.5   Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.