wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 11:01 PM EDT

PDB ID	:	6UFE
Title	:	The structure of a potassium selective ion channel at atomic resolution
Authors	:	Langan, P.S.; Vandavasi, V.G.; Sullivan, B.; Afonine, P.V.; Weiss, K.L.
Deposited on	:	2019-09-24
Resolution	:	1.20 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	:	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)	:	2.35.1

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 1.20 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 (i)

There are 4 unique types of molecules in this entry. The entry contains 3500 atoms, of which 1792 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.

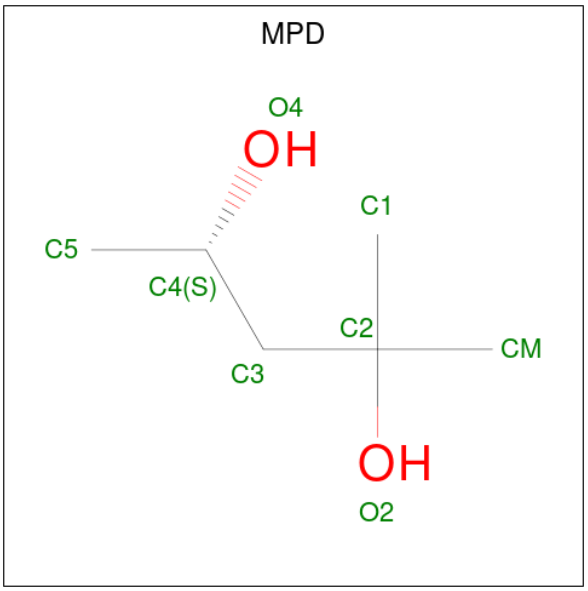
- Molecule 1 is a protein called Transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	A	90	1551	517	799	103	132	0	9	0
1	B	92	1616	533	839	111	133	0	11	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	TYR	ASP	engineered mutation	UNP A0A164U772
A	68	ASP	ASN	engineered mutation	UNP A0A164U772
A	111	LEU	-	expression tag	UNP A0A164U772
A	112	VAL	-	expression tag	UNP A0A164U772
A	113	PRO	-	expression tag	UNP A0A164U772
A	114	ARG	-	expression tag	UNP A0A164U772
B	66	TYR	ASP	engineered mutation	UNP A0A164U772
B	68	ASP	ASN	engineered mutation	UNP A0A164U772
B	111	LEU	-	expression tag	UNP A0A164U772
B	112	VAL	-	expression tag	UNP A0A164U772
B	113	PRO	-	expression tag	UNP A0A164U772
B	114	ARG	-	expression tag	UNP A0A164U772

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O 22 6 14 2	0	0
2	A	1	Total C H O 22 6 14 2	0	0
2	A	1	Total C H O 44 12 28 4	0	1
2	A	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0
2	B	1	Total C H O 22 6 14 2	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total K 4 4	0	0
3	B	4	Total K 4 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	39	39	39	0	0
			Total	O		
4	B	44	44	44	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	I 4	Depositor
Cell constants a, b, c, α, β, γ	67.86Å 67.86Å 89.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.46 – 1.20	Depositor
% Data completeness (in resolution range)	97.4 (21.46-1.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.48 (at 1.20Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.133 , 0.148	Depositor
Wilson B-factor (Å^2)	15.0	Xtriage
Anisotropy	0.020	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.047 for -h,k,-l	Xtriage
Total number of atoms	3500	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

4.4 Non-standard residues in protein, DNA, RNA chains (i)

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

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MPD	A	702	-	7,7,7	0.28	0	9,10,10	0.34	0
2	MPD	B	210	-	7,7,7	0.30	0	9,10,10	0.29	0
2	MPD	B	201	-	7,7,7	0.26	0	9,10,10	0.18	0
2	MPD	B	207	-	7,7,7	0.30	0	9,10,10	0.32	0
2	MPD	A	704	-	7,7,7	0.30	0	9,10,10	0.23	0
2	MPD	B	202	-	7,7,7	0.30	0	9,10,10	0.34	0
2	MPD	B	209	-	7,7,7	0.28	0	9,10,10	0.26	0
2	MPD	A	701	-	7,7,7	0.25	0	9,10,10	0.41	0
2	MPD	B	208	-	7,7,7	0.31	0	9,10,10	0.31	0
2	MPD	A	703[A]	-	7,7,7	0.30	0	9,10,10	0.39	0
2	MPD	A	703[B]	-	7,7,7	0.29	0	9,10,10	0.21	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	MPD	A	702	-	-	1/5/5/5	-
2	MPD	B	210	-	-	1/5/5/5	-
2	MPD	B	201	-	-	0/5/5/5	-
2	MPD	B	207	-	-	0/5/5/5	-
2	MPD	A	704	-	-	1/5/5/5	-
2	MPD	B	202	-	-	1/5/5/5	-
2	MPD	B	209	-	-	1/5/5/5	-
2	MPD	A	701	-	-	0/5/5/5	-
2	MPD	B	208	-	-	2/5/5/5	-
2	MPD	A	703[A]	-	-	1/5/5/5	-
2	MPD	A	703[B]	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	202	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	208	MPD	C2-C3-C4-C5
2	A	702	MPD	C2-C3-C4-C5
2	A	703[A]	MPD	C2-C3-C4-C5
2	A	704	MPD	C2-C3-C4-C5

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data (i)

5.1 Protein, DNA and RNA chains (i)

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

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

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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