Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:39 AM EDT

PDB ID	:	6MYJ
Title	:	Pleurotus ostreatus OstreolysinA plus sphingomyelin
Authors	:	Tomchick, D.R.; Radhakrishnan, A.; Endapally, S.
Deposited on	:	2018-11-01
Resolution	:	1.33 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) 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 1.33 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 5 unique types of molecules in this entry. The entry contains 9179 atoms, of which 4284 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 Ostreolysin A6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	135	Total	C	H	N	O	S	0	4	0
			2089	667	1029	178	214	1			
1	B	134	Total	C	H	N	O	S	0	6	0
			2110	671	1047	179	212	1			
1	C	135	Total	C	H	N	O	S	0	3	0
			2064	655	1015	180	213	1			
1	D	137	Total	C	H	N	O	S	0	5	0
			2139	680	1058	184	216	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P83467
A	62	SER	CYS	engineered mutation	UNP P83467
A	94	SER	CYS	engineered mutation	UNP P83467
B	0	GLY	-	expression tag	UNP P83467
B	62	SER	CYS	engineered mutation	UNP P83467
B	94	SER	CYS	engineered mutation	UNP P83467
C	0	GLY	-	expression tag	UNP P83467
C	62	SER	CYS	engineered mutation	UNP P83467
C	94	SER	CYS	engineered mutation	UNP P83467
D	0	GLY	-	expression tag	UNP P83467
D	62	SER	CYS	engineered mutation	UNP P83467
D	94	SER	CYS	engineered mutation	UNP P83467

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

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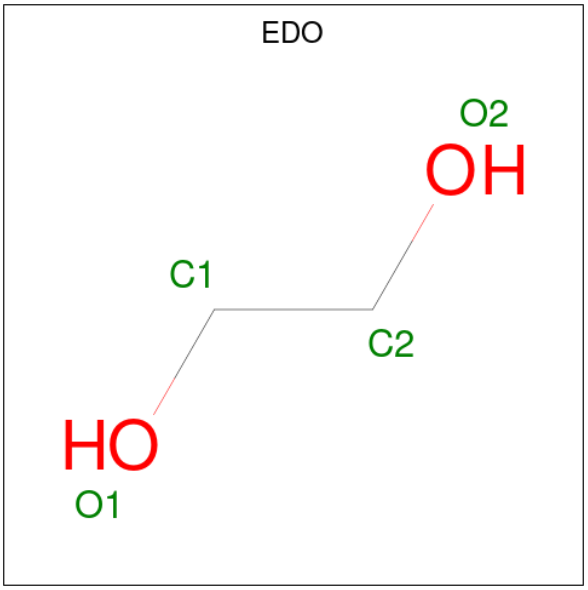
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	A	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0
3	B	1	Total C H O 10 2 6 2	0	0

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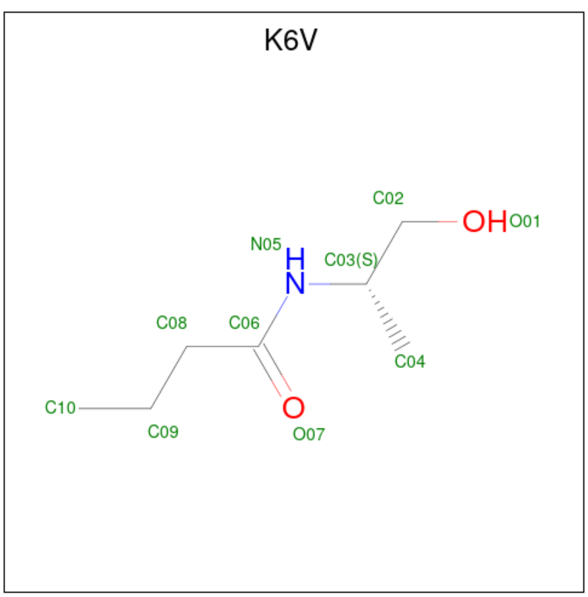
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	C	1	Total 10	C 2	H 6	O 2	0	0
3	D	1	Total 10	C 2	H 6	O 2	0	0
3	D	1	Total 10	C 2	H 6	O 2	0	0
3	D	1	Total 10	C 2	H 6	O 2	0	0
3	D	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 4 is N-[(2S)-1-hydroxypropan-2-yl]butanamide (three-letter code: K6V) (formula: $C_7H_{15}NO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	H	N	O	0	0
			25	7	15	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	132	Total	O	0	0
			132	132		
5	B	138	Total	O	0	0
			138	138		
5	C	136	Total	O	0	0
			136	136		
5	D	142	Total	O	0	0
			142	142		

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	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.42Å 100.56Å 58.81Å 90.00° 106.29° 90.00°	Depositor
Resolution (Å)	44.56 – 1.33	Depositor
% Data completeness (in resolution range)	99.3 (44.56-1.33)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.81 (at 1.33Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.155 , 0.168	Depositor
Wilson B-factor (Å^2)	13.5	Xtriage
Anisotropy	0.036	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9179	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9215e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Of 25 ligands modelled in this entry, 4 are monoatomic - leaving 21 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	$\#\|Z\| > 2$
3	EDO	B	207	-	3,3,3	0.36	0	2,2,2	0.17	0
3	EDO	D	204	-	3,3,3	0.39	0	2,2,2	0.69	0
3	EDO	B	203	-	3,3,3	0.42	0	2,2,2	0.42	0
3	EDO	A	204	-	3,3,3	0.48	0	2,2,2	0.28	0
3	EDO	D	202	-	3,3,3	0.60	0	2,2,2	0.24	0
3	EDO	A	203	-	3,3,3	0.43	0	2,2,2	0.29	0
3	EDO	B	205	-	3,3,3	0.41	0	2,2,2	0.58	0
3	EDO	B	206	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	C	205	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	C	206	-	3,3,3	0.47	0	2,2,2	0.24	0
3	EDO	A	202	-	3,3,3	0.38	0	2,2,2	0.53	0
3	EDO	D	203	-	3,3,3	0.40	0	2,2,2	0.49	0
3	EDO	C	203	-	3,3,3	0.40	0	2,2,2	0.28	0
3	EDO	B	204	-	3,3,3	0.42	0	2,2,2	0.47	0
3	EDO	C	204	-	3,3,3	0.45	0	2,2,2	0.28	0
3	EDO	D	205	-	3,3,3	0.40	0	2,2,2	0.37	0
3	EDO	C	207	-	3,3,3	0.50	0	2,2,2	0.12	0
3	EDO	B	202	-	3,3,3	0.51	0	2,2,2	0.05	0
4	K6V	D	206	-	9,9,9	1.93	2 (22%)	10,10,10	1.42	3 (30%)
3	EDO	A	205	-	3,3,3	0.53	0	2,2,2	0.11	0
3	EDO	C	202	-	3,3,3	0.51	0	2,2,2	0.08	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
3	EDO	B	207	-	-	1/1/1/1	-
3	EDO	D	204	-	-	0/1/1/1	-
3	EDO	B	203	-	-	0/1/1/1	-
3	EDO	A	204	-	-	0/1/1/1	-
3	EDO	D	202	-	-	0/1/1/1	-
3	EDO	A	203	-	-	0/1/1/1	-
3	EDO	B	205	-	-	0/1/1/1	-
3	EDO	B	206	-	-	1/1/1/1	-
3	EDO	C	205	-	-	1/1/1/1	-
3	EDO	C	206	-	-	0/1/1/1	-
3	EDO	A	202	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	203	-	-	0/1/1/1	-
3	EDO	C	203	-	-	0/1/1/1	-
3	EDO	B	204	-	-	0/1/1/1	-
3	EDO	C	204	-	-	0/1/1/1	-
3	EDO	D	205	-	-	0/1/1/1	-
3	EDO	C	207	-	-	1/1/1/1	-
3	EDO	B	202	-	-	0/1/1/1	-
4	K6V	D	206	-	-	2/9/9/9	-
3	EDO	A	205	-	-	0/1/1/1	-
3	EDO	C	202	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	206	K6V	C06-N05	5.22	1.45	1.34
4	D	206	K6V	O07-C06	-2.14	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	206	K6V	C02-C03-N05	-2.52	105.86	109.62
4	D	206	K6V	C03-N05-C06	-2.47	118.40	123.33
4	D	206	K6V	C09-C08-C06	-2.10	107.51	112.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	206	K6V	O01-C02-C03-C04
4	D	206	K6V	O01-C02-C03-N05
3	B	207	EDO	O1-C1-C2-O2
3	B	206	EDO	O1-C1-C2-O2
3	C	205	EDO	O1-C1-C2-O2
3	C	207	EDO	O1-C1-C2-O2

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

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.