W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 08:59 PM EST

PDB ID	:	2IE3
Title	:	Structure of the Protein Phosphatase 2A Core Enzyme Bound to Tumor-inducing Toxins
Authors	:	Xing, Y.; Xu, Y.; Chen, Y.; Jeffrey, P.D.; Chao, Y.; Shi, Y.
Deposited on	:	2006-09-17
Resolution	:	2.80 Å(reported)

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

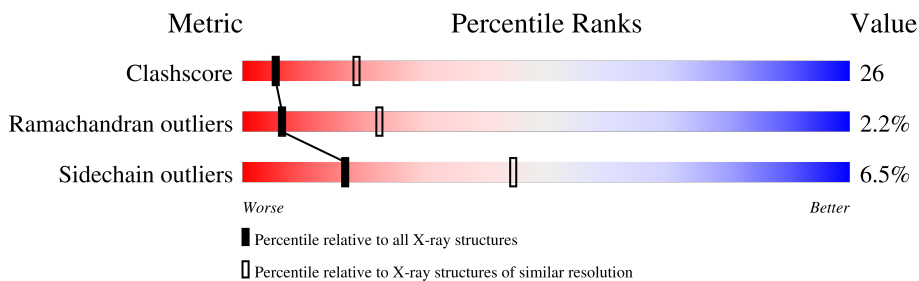|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		2.2%
Sidechain outliers		6.5%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	589	51% · 41% · 6% ··
2	C	309	56% · 34% · · 7%
3	I	7	29% · 43% · 29%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 6922 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 Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4527	2877	763	860	27			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	5	LEU	VAL	conflict	UNP P67775

- Molecule 3 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

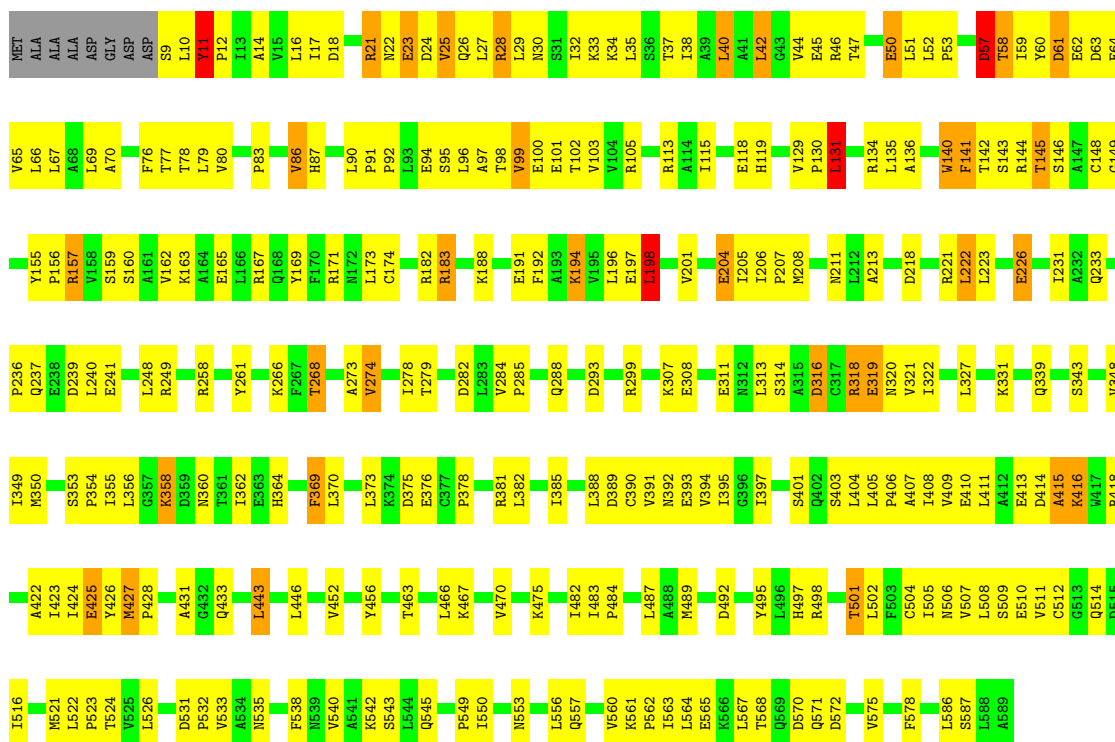| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Mn	0	0
			2	2		

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. 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. 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.
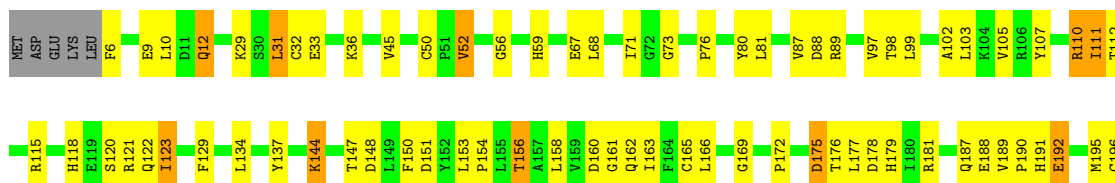
Note EDS was not executed.

• Molecule 1: Protein Phosphatase 2, regulatory subunit A (PR 65), alpha isoform

• Molecule 2: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

D197 L198 L199 D202 P203 D204 D205 R206 G207 G208 W209 G217 Y218 T219 I224 S225 T235 L236 V237 S238 R239 C251 H252 V256 I259 P263 N264 Y265 C266 Y267 R268 C269 I275 M276 E277 L278 D279 D280 T281 L282 K283 L287 Q288 F289 D290 P291 A292 P293 ARG ARG

GLY GLU PRO HIS VAL THR ARG ARG THR PRO ASP TYR PHE LEU

• Molecule 3: microcystin LR

Chain I:

29%　　　　43%　　　　29%

A1 L2 D3 R4 1ZN5 E6 DAM7
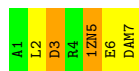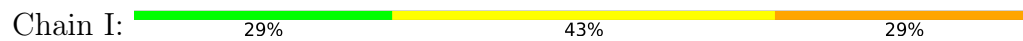
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	93.07Å 195.09Å 201.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	92.9 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.221 , 0.264	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6922	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACB, DAM, DAL, MN, FGA, 1ZN

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	0.45	0/4601	0.71	4/6246 (0.1%)
2	C	0.51	0/2379	0.76	2/3227 (0.1%)
3	I	0.52	0/17	0.82	0/19
All	All	0.47	0/6997	0.73	6/9492 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	11	TYR	N-CA-C	6.67	129.00	111.00
1	A	11	TYR	C-N-CD	6.33	141.69	128.40
2	C	206	ARG	N-CA-C	-6.28	94.06	111.00
1	A	131	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	11	TYR	C-N-CA	-5.44	99.15	122.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	5	1ZN	Mainchain,Peptide

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	A	4527	0	4633	259	0
2	C	2322	0	2223	107	0
3	I	71	0	61	3	0
4	C	2	0	0	0	0
All	All	6922	0	6917	361	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 26.

The worst 5 of 361 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:99:VAL:HG12	1:A:100:GLU:H	1.05	1.11
1:A:526:LEU:HD22	1:A:563:ILE:HG13	1.51	0.91
2:C:115:ARG:HH12	2:C:151:ASP:HA	1.33	0.90
1:A:99:VAL:HG12	1:A:100:GLU:N	1.83	0.90
2:C:115:ARG:HH21	2:C:189:VAL:HG23	1.37	0.90

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	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	579/589 (98%)	499 (86%)	62 (11%)	18 (3%)	4	14
2	C	286/309 (93%)	255 (89%)	30 (10%)	1 (0%)	41	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	1/7 (14%)	1 (100%)	0	0	100	100
All	All	866/905 (96%)	755 (87%)	92 (11%)	19 (2%)	6	22

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	ASP
1	A	63	ASP
1	A	319	GLU
1	A	21	ARG
1	A	23	GLU

5.3.2 Protein sidechains ⓘ

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	508/512 (99%)	473 (93%)	35 (7%)	15	41
2	C	254/274 (93%)	239 (94%)	15 (6%)	19	49
3	I	2/2 (100%)	2 (100%)	0	100	100
All	All	764/788 (97%)	714 (94%)	50 (6%)	17	44

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LYS
2	C	12	GLN
2	C	239	ARG
1	A	425	GLU
1	A	495	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	122	GLN
2	C	252	HIS
2	C	191	HIS
1	A	392	ASN
2	C	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
3	1ZN	I	5	3	23,23,24	1.65	4 (17%)	24,29,31	1.39	3 (12%)
3	ACB	I	3	3	7,8,9	2.53	3 (42%)	8,10,12	0.78	0
3	FGA	I	6	3	7,8,9	2.26	2 (28%)	7,9,11	1.86	2 (28%)
3	DAM	I	7	2,3	4,5,6	2.39	1 (25%)	3,5,7	3.94	3 (100%)

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	1ZN	I	5	3	-	5/22/25/27	0/1/1/1
3	ACB	I	3	3	-	1/9/10/12	-
3	FGA	I	6	3	-	2/7/8/9	-
3	DAM	I	7	2,3	-	0/0/4/6	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	6	FGA	O-C	4.76	1.36	1.22
3	I	3	ACB	CA-N	4.46	1.60	1.47
3	I	7	DAM	C-CA	4.26	1.52	1.45
3	I	3	ACB	CB-CA	3.88	1.58	1.55
3	I	5	1ZN	C3-C2	3.65	1.57	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	7	DAM	CM-N-CA	-4.76	116.21	123.45
3	I	5	1ZN	CA-C18-C	-4.58	105.05	110.72
3	I	7	DAM	O-C-CA	-4.35	119.64	125.22
3	I	6	FGA	OXT-C-CA	3.46	125.16	113.38
3	I	6	FGA	O-C-CA	-3.35	110.33	122.14

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	5	1ZN	C12-C13-C15-C16
3	I	5	1ZN	C14-C13-C15-C16
3	I	6	FGA	O-C-CA-N
3	I	3	ACB	CA-CB-CG-OD1
3	I	5	1ZN	C10-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	3	ACB	1	0

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.