

wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 02:55 PM EST

PDB ID	:	1P32
Title	:	CRYSTAL STRUCTURE OF HUMAN P32, A DOUGHNUT-SHAPED
		ACIDIC MITOCHONDRIAL MATRIX PROTEIN
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Deposited on		
Resolution	:	2.25 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 (1)) were used in the production of this report:

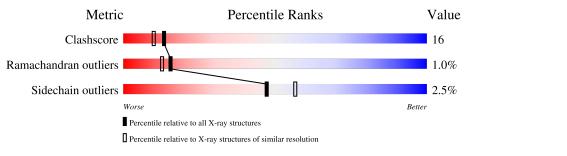
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.25 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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	А	209	65%	21%	• 13%				
1	В	209	56%	26%	18%				
1	С	209	59%	24%	• 16%				



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4663 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.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A 182	Total	С	Ν	0	\mathbf{S}	0	0	0	
	A	. 182	1464	924	235	301	4	0	0	0
1	р	171	Total	С	Ν	0	S	0	0	0
	1 В	1/1	1381	873	224	280	4	0		
1	С	C 176	Total	С	Ν	0	S	0	0	0
			1420	899	229	288	4	0	0	0

• Molecule 1 is a protein called MITOCHONDRIAL MATRIX PROTEIN, SF2P32.

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	74	MET	LEU	engineered mutation	UNP Q07021
В	74	MET	LEU	engineered mutation	UNP Q07021
С	74	MET	LEU	engineered mutation	UNP Q07021

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	143	Total O 143 143	0	0
2	В	123	Total O 123 123	0	0
2	С	132	Total O 132 132	0	0

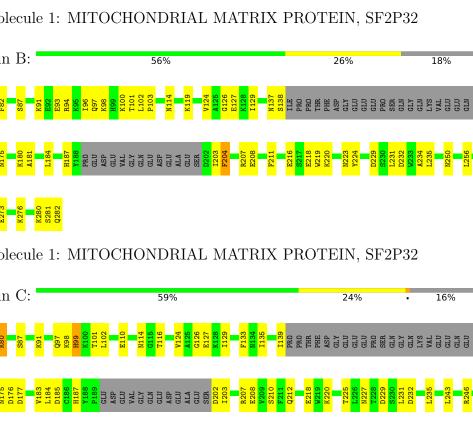


Residue-property plots (i) 3

• Molecule 1: MITOCHONDRIAL MATRIX PROTEIN, SF2P32

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.

- Chain A: 65% 21% 13% PHE ASP 3LV 3LU 3LU 3LU 3LU SER GLY GLN GLN CYS CYS CLV GLU GLU GLU GLU IAL VAL • Molecule 1: MITOCHONDRIAL MATRIX PROTEIN, SF2P32 Chain B: 56% 26% 18% SER CLASSER CL • Molecule 1: MITOCHONDRIAL MATRIX PROTEIN, SF2P32 Chain C: 59% 24% 16%
- Note EDS was not executed.



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	58.62Å 56.48Å 93.83Å	Depositor
a, b, c, α , β , γ	90.00° 95.99° 90.00°	Depositor
Resolution (Å)	30.00 - 2.25	Depositor
% Data completeness	91.7 (30.00-2.25)	Depositor
(in resolution range)	51.1 (50.00 2.25)	Depositor
R_{merge}	0.04	Depositor
R _{sym}	0.11	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.173 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4663	wwPDB-VP
Average B, all atoms $(Å^2)$	34.0	wwPDB-VP



5 Model quality (i)

5.1 Standard geometry (i)

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	А	0.33	0/1490	0.57	0/2011	
1	В	0.34	0/1405	0.54	0/1893	
1	С	0.33	0/1445	0.55	0/1949	
All	All	0.33	0/4340	0.55	0/5853	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	А	1464	0	1404	46	0
1	В	1381	0	1329	60	0
1	С	1420	0	1371	42	0
2	А	143	0	0	5	0
2	В	123	0	0	12	0
2	С	132	0	0	6	0
All	All	4663	0	4104	135	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 16.

The worst 5 of 135 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:B:231:LEU:HD11	1:B:235:LEU:HD23	1.36	1.03
1:A:174:LYS:HD2	1:B:282:GLN:CG	2.00	0.91
1:A:176:ASP:H	1:B:282:GLN:NE2	1.71	0.89
1:A:174:LYS:HD2	1:B:282:GLN:HG3	1.55	0.86
1:C:129:ILE:HD13	1:C:246:ARG:HB3	1.61	0.83

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		Allowed	Outliers	Perce	ntiles
1	А	176/209~(84%)	162 (92%)	12~(7%)	2(1%)	14	10
1	В	165/209~(79%)	159 (96%)	6 (4%)	0	100	100
1	С	170/209~(81%)	162 (95%)	5(3%)	3~(2%)	8	4
All	All	511/627~(82%)	483 (94%)	23~(4%)	5 (1%)	15	13

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	98	LYS
1	С	99	HIS
1	А	102	LEU
1	С	177	ASP
1	А	96	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	165/189~(87%)	161~(98%)	4 (2%)	49 58
1	В	155/189~(82%)	152 (98%)	3~(2%)	57 66
1	С	160/189~(85%)	155~(97%)	5(3%)	40 49
All	All	480/567~(85%)	468 (98%)	12 (2%)	47 56

analysed, and the total number of residues.

5 of 12 residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	80	LYS
1	С	114	ASN
1	С	274	ASP
1	С	176	ASP
1	А	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	В	282	GLN
1	С	114	ASN
1	С	97	GLN
1	С	167	ASN
1	А	265	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

