

wwPDB X-ray Structure Validation Summary Report (i)

Nov 30, 2021 – 11:09 am GMT

:	7B2O
:	Crystal structure of Chlamydomonas reinhardtii chloroplastic sedoheptulose-
	1,7-bisphosphatase
:	Le Moigne, T.; Lemaire, S.D.; Henri, J.
:	2020-11-27
:	3.09 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.09 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	Whole archive	Similar resolution
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	331	89%	5%	6%
1	В	331	85%	9%	7%
1	С	331	2% 84 %	9%	7%
1	D	331	2% 8 4%	10%	6%
1	Е	331	81%	13%	• 6%

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Mol	Chain	Length	Quality of chain		
			3%		
1	F	331	78%	15%	7%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14194 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		At	oms			ZeroOcc	AltConf	Trace
1	Δ	211	Total	С	Ν	0	S	0	0	0
1	А	311	2372	1509	393	449	21	0	0	0
1	р	200	Total	С	Ν	0	S	0	1	0
1	D	509	2363	1503	391	448	21	0	L	0
1	С	200	Total	С	Ν	0	S	0	0	0
1	U	509	2359	1501	390	447	21	0	0	0
1	а	210	Total	С	Ν	0	S	0	0	0
1	D	510	2362	1504	391	446	21	0	0	0
1	F	211	Total	С	Ν	0	S	0	0	0
	Ľ	311	2371	1509	392	449	21	0	0	0
1	Б	200	Total	С	Ν	0	S	0	1	0
	Г	509	2363	1504	392	446	21	0		

• Molecule 1 is a protein called FBPase domain-containing protein.

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	61	MET	-	initiating methionine	UNP A0A2K3DY10
А	62	HIS	-	expression tag	UNP A0A2K3DY10
А	63	HIS	-	expression tag	UNP A0A2K3DY10
А	64	HIS	-	expression tag	UNP A0A2K3DY10
А	65	HIS	-	expression tag	UNP A0A2K3DY10
А	66	HIS	-	expression tag	UNP A0A2K3DY10
А	67	HIS	-	expression tag	UNP A0A2K3DY10
А	68	HIS	-	expression tag	UNP A0A2K3DY10
А	69	MET	-	expression tag	UNP A0A2K3DY10
В	64	MET	-	initiating methionine	UNP A0A2K3DY10
В	65	HIS	-	expression tag	UNP A0A2K3DY10
В	66	HIS	-	expression tag	UNP A0A2K3DY10
В	67	HIS	-	expression tag	UNP A0A2K3DY10
В	68	HIS	-	expression tag	UNP A0A2K3DY10
В	69	HIS	-	expression tag	UNP A0A2K3DY10
В	70	HIS	-	expression tag	UNP A0A2K3DY10
В	71	HIS	-	expression tag	UNP A0A2K3DY10

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$1D_{2}O$

Chain	Residue	Modelled	Actual	Comment	Reference
В	72	MET	_	expression tag	UNP A0A2K3DY10
С	64	MET	_	initiating methionine	UNP A0A2K3DY10
С	65	HIS	-	expression tag	UNP A0A2K3DY10
С	66	HIS	-	expression tag	UNP A0A2K3DY10
С	67	HIS	-	expression tag	UNP A0A2K3DY10
С	68	HIS	-	expression tag	UNP A0A2K3DY10
С	69	HIS	-	expression tag	UNP A0A2K3DY10
С	70	HIS	-	expression tag	UNP A0A2K3DY10
С	71	HIS	-	expression tag	UNP A0A2K3DY10
С	72	MET	-	expression tag	UNP A0A2K3DY10
D	64	MET	-	initiating methionine	UNP A0A2K3DY10
D	65	HIS	-	expression tag	UNP A0A2K3DY10
D	66	HIS	-	expression tag	UNP A0A2K3DY10
D	67	HIS	-	expression tag	UNP A0A2K3DY10
D	68	HIS	-	expression tag	UNP A0A2K3DY10
D	69	HIS	-	expression tag	UNP A0A2K3DY10
D	70	HIS	-	expression tag	UNP A0A2K3DY10
D	71	HIS	-	expression tag	UNP A0A2K3DY10
D	72	MET	-	expression tag	UNP A0A2K3DY10
Е	64	MET	-	initiating methionine	UNP A0A2K3DY10
E	65	HIS	-	expression tag	UNP A0A2K3DY10
E	66	HIS	-	expression tag	UNP A0A2K3DY10
E	67	HIS	-	expression tag	UNP A0A2K3DY10
E	68	HIS	-	expression tag	UNP A0A2K3DY10
Е	69	HIS	-	expression tag	UNP A0A2K3DY10
E	70	HIS	-	expression tag	UNP A0A2K3DY10
E	71	HIS	-	expression tag	UNP A0A2K3DY10
E	72	MET	-	expression tag	UNP A0A2K3DY10
F	64	MET	-	initiating methionine	UNP A0A2K3DY10
F	65	HIS	-	expression tag	UNP A0A2K3DY10
F	66	HIS	-	expression tag	UNP A0A2K3DY10
F	67	HIS	-	expression tag	UNP A0A2K3DY10
F	68	HIS	-	expression tag	UNP A0A2K3DY10
F	69	HIS	-	expression tag	UNP A0A2K3DY10
F	70	HIS	-	expression tag	UNP A0A2K3DY10
F	71	HIS	-	expression tag	UNP A0A2K3DY10
F	72	MET	-	expression tag	UNP A0A2K3DY10

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• Molecule 2 is water.

Mol	Chain	Residues	Aton	ns	ZeroOcc	AltConf
2	А	1	Total 1	0 1	0	0
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	3	Total O 3 3	0	0



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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

• Molecule 1: FBPase domain-containing protein









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	178.22Å 183.65Å 75.20Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	47.47 - 3.09	Depositor
Resolution (A)	48.72 - 3.09	EDS
% Data completeness	99.4 (47.47-3.09)	Depositor
(in resolution range)	99.4 (48.72-3.09)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.69 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D	0.193 , 0.238	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.194 , 0.239	DCC
R_{free} test set	1989 reflections (4.36%)	wwPDB-VP
Wilson B-factor $(Å^2)$	64.7	Xtriage
Anisotropy	0.826	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14194	wwPDB-VP
Average B, all atoms $(Å^2)$	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond angles	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.33	0/2421	0.53	0/3275
1	В	0.33	0/2412	0.52	0/3264
1	С	0.30	0/2408	0.50	0/3259
1	D	0.31	0/2411	0.51	0/3263
1	Ε	0.29	0/2420	0.49	0/3275
1	F	0.30	0/2412	0.51	0/3263
All	All	0.31	0/14484	0.51	0/19599

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	2372	0	2353	14	0
1	В	2363	0	2339	19	0
1	С	2359	0	2337	18	0
1	D	2362	0	2345	28	0
1	Ε	2371	0	2351	30	0
1	F	2363	0	2346	29	0
2	А	1	0	0	0	0
2	В	3	0	0	0	0
All	All	14194	0	14071	124	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 4.

The worst 5 of 124 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:E:329:VAL:HG13	1:E:366:ILE:HD12	1.53	0.89
1:E:325:ILE:HA	1:E:329:VAL:HB	1.56	0.85
1:F:325:ILE:HA	1:F:329:VAL:HG22	1.64	0.80
1:D:366:ILE:HD12	1:D:366:ILE:O	1.83	0.77
1:F:325:ILE:HD12	1:F:326:LEU:N	1.98	0.77

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	Perce	\mathbf{ntiles}
1	А	309/331~(93%)	299~(97%)	10 (3%)	0	100	100
1	В	308/331~(93%)	292 (95%)	16 (5%)	0	100	100
1	С	307/331~(93%)	288 (94%)	19 (6%)	0	100	100
1	D	308/331~(93%)	292 (95%)	16 (5%)	0	100	100
1	Ε	309/331~(93%)	283~(92%)	23 (7%)	3(1%)	15	49
1	F	308/331~(93%)	288 (94%)	19 (6%)	1 (0%)	41	73
All	All	1849/1986~(93%)	1742 (94%)	103 (6%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Е	325	ILE
1	Е	167	ASP
1	Е	236	CYS

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Mol	Chain	Res	Type
1	F	255	HIS

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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percei	ntiles
1	А	254/270~(94%)	253~(100%)	1 (0%)	91	96
1	В	253/270~(94%)	249~(98%)	4 (2%)	62	84
1	С	253/270~(94%)	252 (100%)	1 (0%)	91	96
1	D	253/270~(94%)	251~(99%)	2(1%)	81	92
1	Ε	254/270~(94%)	251~(99%)	3~(1%)	71	88
1	F	253/270~(94%)	248~(98%)	5(2%)	55	80
All	All	1520/1620~(94%)	1504 (99%)	16 (1%)	76	89

5 of 16 residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	F	346	ASP
1	F	291	ARG
1	Е	133	GLN
1	F	268	ARG
1	D	266	ASN

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such side chains are listed below:

Mol	Chain	Res	Type
1	D	266	ASN

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)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RS	SRZ:	>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	А	311/331~(93%)	-0.23	1 (0%)	94	88	33, 52, 76, 97	0
1	В	309/331~(93%)	-0.16	1 (0%)	94	88	36, 52, 79, 106	0
1	С	309/331~(93%)	-0.03	7 (2%)	60	39	44, 63, 88, 102	0
1	D	310/331~(93%)	-0.02	6 (1%)	66	46	44, 65, 92, 109	0
1	Ε	311/331~(93%)	0.09	2 (0%)	89	78	47, 72, 106, 120	0
1	F	309/331~(93%)	0.18	9 (2%)	51	28	55, 84, 114, 123	1 (0%)
All	All	1859/1986~(93%)	-0.03	26(1%)	75	56	33, 64, 102, 123	1 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	318	THR	4.3
1	Е	131	ASP	3.4
1	С	132	GLU	3.3
1	D	131	ASP	3.1
1	С	131	ASP	2.9

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

