wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 04:44 AM EDT

PDB ID	:	1ZAH
Title	:	Fructose-1,6-bisphosphate aldolase from rabbit muscle
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Deposited on	:	2005-04-06
Resolution	:	1.80 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:

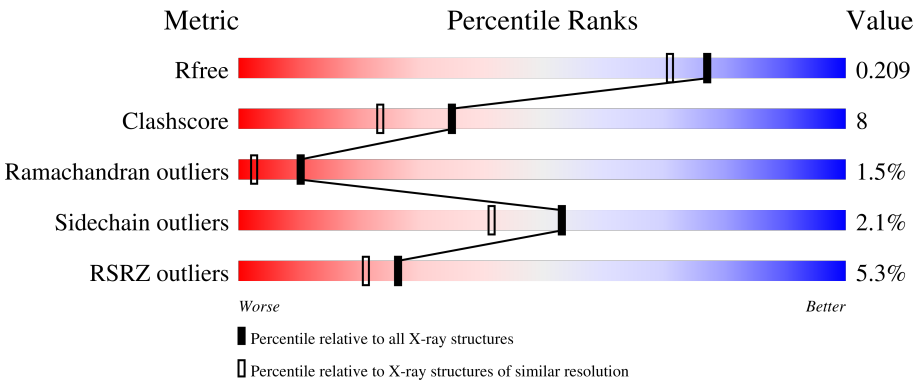
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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% 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	A	363	4% 85% 14%
1	B	363	5% 80% 19% •
1	C	363	4% 83% 16% •
1	D	363	7% 80% 19% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13459 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 Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2758	1733	489	525	11	0	0	0
1	B	363	2758	1733	489	525	11	0	0	0
1	C	363	2758	1733	489	525	11	0	0	0
1	D	363	2758	1733	489	525	11	0	0	0

- Molecule 2 is water.

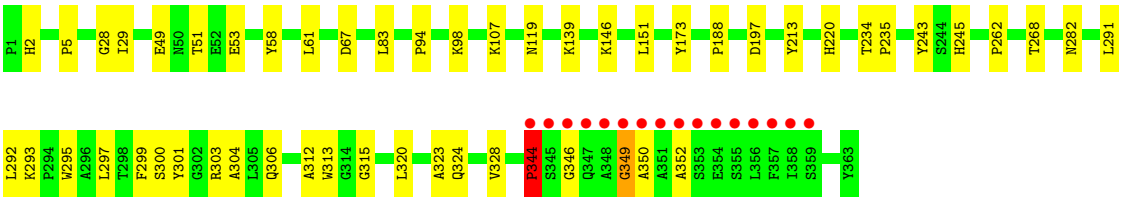
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	604	604	604	0	0
2	B	604	604	604	0	0
2	C	601	601	601	0	0
2	D	618	618	618	0	0

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: Fructose-bisphosphate aldolase A

Chain A:

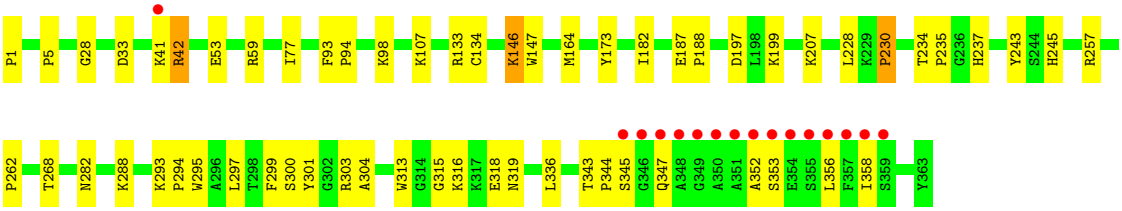


• Molecule 1: Fructose-bisphosphate aldolase A

Chain B:

• Molecule 1: Fructose-bisphosphate aldolase A

Chain C:



• Molecule 1: Fructose-bisphosphate aldolase A

Chain D:

7%
80%
19%

P1 P5 P25 G28 I29 D33 T36 A40 K41 R42 L43 Q44 S45 I46 G47 N50 Y58 R59 Q60 L61 L62 L63 V69 N70 P71 I77 E81 T82 L83 Y84 Q85 P92 F93 P94 R133 K146 E155 M164 Y173 I185 P188
P192 D193 D197 R200 K207 Y213 L228 K229 P230 T234 P235 Q241 K242 Y243 R257 P261 P262 V267 T268 E276 E277 N284 K293 P294 W295 A296 L297 T298 F299 S300 Y301 G302 R303 A304 A307 K316 N319 V328 Y342 T343 P344
S345 G346 Q347 A348 G349 A350 A351 A352 S353 E354 S355 L356 F357 I358 S359 N360 H361 A362 Y363

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.10Å 102.92Å 84.66Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 43.85 – 1.79	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-1.80) 94.5 (43.85-1.79)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.167 , 0.205 0.170 , 0.209	Depositor DCC
R_{free} test set	6370 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 64.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	13459	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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.

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	A	0.30	0/2812	0.60	0/3810
1	B	0.30	0/2812	0.58	0/3810
1	C	0.30	0/2812	0.58	0/3810
1	D	0.28	0/2812	0.57	0/3810
All	All	0.29	0/11248	0.58	0/15240

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
1	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	213	TYR	Sidechain
1	B	213	TYR	Sidechain
1	D	213	TYR	Sidechain

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	2758	0	2776	36	0
1	B	2758	0	2776	55	0
1	C	2758	0	2776	43	0
1	D	2758	0	2776	55	0
2	A	604	0	0	8	0
2	B	604	0	0	11	0
2	C	601	0	0	10	0
2	D	618	0	0	14	0
All	All	13459	0	11104	181	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 8.

The worst 5 of 181 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:D:146:LYS:HE2	2:D:367:HOH:O	1.84	0.78
1:D:284:ASN:ND2	1:D:342:TYR:H	1.85	0.74
1:A:146:LYS:HE2	2:A:368:HOH:O	1.88	0.71
1:B:358:ILE:HG22	1:B:359:SER:H	1.56	0.71
1:C:199:LYS:HG3	2:C:527:HOH:O	1.92	0.69

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	361/363 (99%)	335 (93%)	19 (5%)	7 (2%)	8 1
1	B	361/363 (99%)	338 (94%)	18 (5%)	5 (1%)	11 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	361/363 (99%)	342 (95%)	15 (4%)	4 (1%)	14 4
1	D	361/363 (99%)	341 (94%)	14 (4%)	6 (2%)	9 2
All	All	1444/1452 (99%)	1356 (94%)	66 (5%)	22 (2%)	10 2

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	346	GLY
1	A	346	GLY
1	A	349	GLY
1	D	349	GLY
1	A	5	PRO

5.3.2 Protein sidechains (i)

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	291/291 (100%)	286 (98%)	5 (2%)	60 51
1	B	291/291 (100%)	286 (98%)	5 (2%)	60 51
1	C	291/291 (100%)	283 (97%)	8 (3%)	44 31
1	D	291/291 (100%)	284 (98%)	7 (2%)	49 36
All	All	1164/1164 (100%)	1139 (98%)	25 (2%)	53 42

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	173	TYR
1	C	344	PRO
1	D	343	THR
1	C	295	TRP
1	D	59	ARG

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	C	241	GLN
1	C	347	GLN
1	C	319	ASN
1	D	50	ASN
1	A	319	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, 95th 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>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	363/363 (100%)	0.13	16 (4%)	34	28	10, 19, 44, 101	15 (4%)
1	B	363/363 (100%)	0.46	18 (4%)	28	23	10, 19, 50, 105	15 (4%)
1	C	363/363 (100%)	0.45	16 (4%)	34	28	10, 19, 47, 104	15 (4%)
1	D	363/363 (100%)	0.22	27 (7%)	14	11	11, 23, 70, 104	3 (0%)
All	All	1452/1452 (100%)	0.32	77 (5%)	26	21	10, 20, 60, 105	48 (3%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	349	GLY	35.7
1	B	348	ALA	35.6
1	B	349	GLY	33.3
1	C	352	ALA	32.6
1	C	351	ALA	30.9

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.