Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 03:12 am BST

PDB ID	:	2ALD
Title	:	HUMAN MUSCLE ALDOLASE
Authors	:	Dalby, A.R.; Littlechild, J.A.
Deposited on	:	1998-10-21
Resolution	:	2.10 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 following versions of software and data (see references ⓘ) were used in the production of this report:

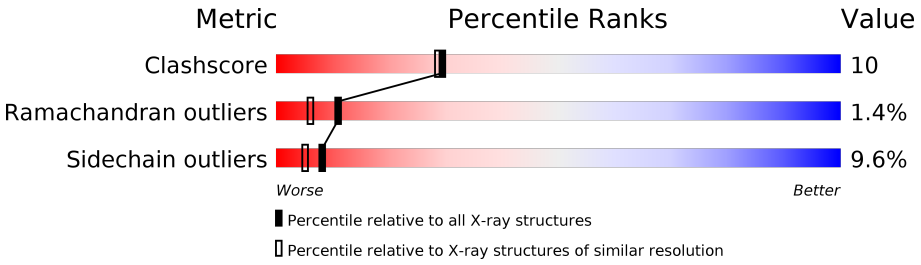
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 on 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	363	73% 19% 6% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2906 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2763	1741	486	525	11	45	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	143	143	143	0	0

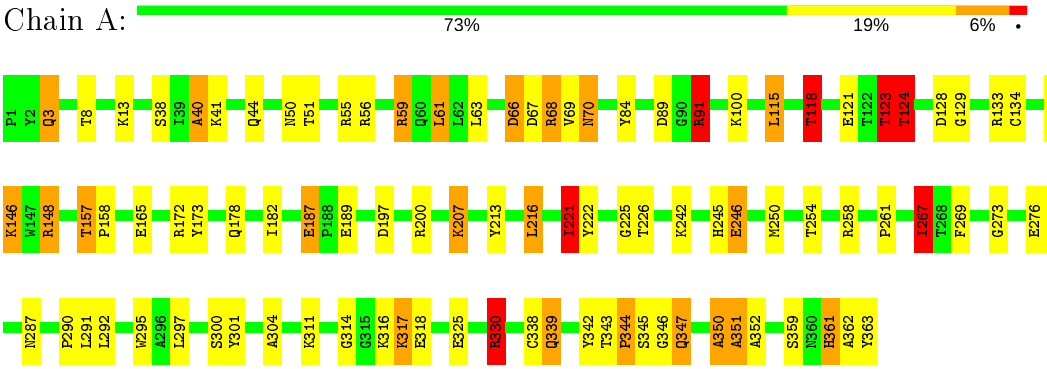
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: FRUCTOSE-BISPHOSPHATE ALDOLASE

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	96.50Å 96.50Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	78.7 (20.00-2.10)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.172 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2906	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.87	4/2816 (0.1%)	1.84	57/3815 (1.5%)

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	16

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	350	ALA	C-N	16.44	1.71	1.34
1	A	344	PRO	C-N	11.91	1.61	1.34
1	A	330	ARG	CD-NE	-5.65	1.36	1.46
1	A	246	GLU	CD-OE2	5.51	1.31	1.25

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	ARG	CD-NE-CZ	33.00	169.81	123.60
1	A	133	ARG	NE-CZ-NH1	19.88	130.24	120.30
1	A	133	ARG	NE-CZ-NH2	-19.71	110.45	120.30
1	A	68	ARG	NE-CZ-NH2	-15.36	112.62	120.30
1	A	56	ARG	NE-CZ-NH1	14.26	127.43	120.30
1	A	55	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	68	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	A	172	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	A	330	ARG	NE-CZ-NH1	-8.75	115.92	120.30
1	A	91	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	343	THR	CA-C-O	-8.71	101.81	120.10
1	A	55	ARG	NE-CZ-NH2	-8.64	115.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	THR	N-CA-CB	-8.51	94.14	110.30
1	A	133	ARG	CD-NE-CZ	8.49	135.48	123.60
1	A	61	LEU	CA-CB-CG	8.05	133.81	115.30
1	A	352	ALA	CA-C-O	7.97	136.85	120.10
1	A	67	ASP	CB-CG-OD2	-7.85	111.23	118.30
1	A	344	PRO	O-C-N	-7.80	110.22	122.70
1	A	56	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	128	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	343	THR	O-C-N	7.59	135.53	121.10
1	A	187	GLU	OE1-CD-OE2	-7.25	114.61	123.30
1	A	143	ASP	CB-CG-OD1	6.88	124.50	118.30
1	A	246	GLU	CB-CG-CD	6.80	132.55	114.20
1	A	213	TYR	CA-CB-CG	-6.67	100.73	113.40
1	A	123	THR	N-CA-CB	6.65	122.94	110.30
1	A	157	THR	CA-C-O	-6.63	106.17	120.10
1	A	124	THR	N-CA-CB	6.47	122.59	110.30
1	A	84	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	A	140	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	267	ILE	CA-CB-CG2	6.24	123.39	110.90
1	A	344	PRO	N-CA-CB	6.24	110.79	103.30
1	A	123	THR	CB-CA-C	-6.20	94.86	111.60
1	A	197	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	40	ALA	CB-CA-C	-6.04	101.04	110.10
1	A	350	ALA	O-C-N	-6.00	113.09	122.70
1	A	301	TYR	CB-CG-CD1	5.91	124.55	121.00
1	A	361	HIS	CA-CB-CG	5.90	123.63	113.60
1	A	344	PRO	N-CD-CG	5.89	112.03	103.20
1	A	148	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	A	123	THR	OG1-CB-CG2	5.81	123.36	110.00
1	A	221	ILE	CB-CG1-CD1	-5.77	97.74	113.90
1	A	189	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	311	LYS	CA-CB-CG	5.72	125.97	113.40
1	A	66	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	59	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	352	ALA	CB-CA-C	5.50	118.35	110.10
1	A	124	THR	CA-CB-OG1	5.41	120.36	109.00
1	A	158	PRO	N-CA-CB	5.41	109.79	103.30
1	A	146	LYS	CB-CG-CD	-5.40	97.57	111.60
1	A	339	GLN	O-C-N	-5.38	114.05	123.20
1	A	352	ALA	O-C-N	-5.37	114.11	122.70
1	A	221	ILE	CA-CB-CG2	5.25	121.39	110.90
1	A	301	TYR	CB-CG-CD2	-5.23	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	258	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	67	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	330	ARG	CG-CD-NE	5.05	122.41	111.80

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	GLY	Mainchain
1	A	157	THR	Mainchain
1	A	225	GLY	Mainchain
1	A	254	THR	Mainchain
1	A	261	PRO	Mainchain
1	A	273	GLY	Mainchain
1	A	287	ASN	Mainchain
1	A	290	PRO	Mainchain
1	A	3	GLN	Mainchain
1	A	300	SER	Mainchain
1	A	314	GLY	Mainchain
1	A	338	CYS	Mainchain
1	A	339	GLN	Mainchain
1	A	344	PRO	Mainchain
1	A	51	THR	Mainchain
1	A	8	THR	Mainchain

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	2763	0	2781	52	0
2	A	143	0	0	2	1
All	All	2906	0	2781	52	1

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 10.

All (52) 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:178:GLN:HE22	1:A:222:TYR:H	1.18	0.90
1:A:118:THR:HG23	1:A:121:GLU:H	1.37	0.87
1:A:66:ASP:OD1	1:A:68:ARG:HD3	1.76	0.85
1:A:89:ASP:OD1	1:A:91:ARG:HG2	1.82	0.78
1:A:118:THR:CG2	1:A:121:GLU:H	1.99	0.75
1:A:267:ILE:HG12	1:A:297:LEU:HD23	1.69	0.74
1:A:276:GLU:OE1	1:A:351:ALA:HB1	1.88	0.73
1:A:123:THR:HG21	1:A:165:GLU:OE2	1.88	0.72
1:A:330:ARG:HH11	1:A:351:ALA:HB3	1.55	0.71
1:A:123:THR:HG23	1:A:165:GLU:HG3	1.76	0.68
1:A:124:THR:HG21	1:A:148:ARG:O	1.94	0.67
1:A:70:ASN:HD21	1:A:100:LYS:NZ	1.93	0.66
1:A:250:MET:HE3	1:A:291:LEU:HD11	1.79	0.64
1:A:317:LYS:HE3	1:A:317:LYS:H	1.64	0.63
1:A:361:HIS:CG	1:A:362:ALA:H	2.17	0.62
1:A:330:ARG:HE	1:A:351:ALA:HB3	1.67	0.59
1:A:221:ILE:HD11	1:A:226:THR:HG21	1.85	0.57
1:A:330:ARG:NH1	1:A:351:ALA:HB3	2.20	0.56
1:A:40:ALA:HB2	1:A:50:ASN:ND2	2.22	0.55
1:A:134:CYS:HB3	1:A:182:ILE:HD12	1.89	0.54
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.92	0.53
1:A:216:LEU:HG	1:A:221:ILE:HG12	1.92	0.52
1:A:267:ILE:HG12	1:A:297:LEU:CD2	2.40	0.52
1:A:250:MET:CE	1:A:291:LEU:HD11	2.39	0.51
1:A:40:ALA:HB2	1:A:50:ASN:HD22	1.75	0.51
1:A:178:GLN:HE22	1:A:222:TYR:N	1.99	0.50
1:A:68:ARG:NH1	1:A:325:GLU:OE2	2.42	0.50
1:A:267:ILE:HD11	1:A:269:PHE:CE1	2.46	0.50
1:A:317:LYS:HG2	1:A:318:GLU:OE2	2.12	0.50
1:A:330:ARG:NE	1:A:351:ALA:HB3	2.26	0.49
1:A:267:ILE:HG13	1:A:267:ILE:O	2.10	0.49
1:A:267:ILE:HD11	1:A:269:PHE:CZ	2.49	0.47
1:A:70:ASN:HD21	1:A:100:LYS:HZ2	1.61	0.47
1:A:115:LEU:O	1:A:118:THR:HB	2.15	0.47
1:A:207:LYS:HD2	1:A:207:LYS:HA	1.55	0.46
1:A:123:THR:HG22	1:A:124:THR:H	1.80	0.45
1:A:123:THR:CG2	1:A:165:GLU:HG3	2.43	0.44
1:A:245:HIS:CD2	1:A:282:ASN:OD1	2.71	0.44
1:A:148:ARG:HD3	2:A:456:HOH:O	2.18	0.44
1:A:200:ARG:HH11	1:A:200:ARG:HG3	1.83	0.44
1:A:178:GLN:NE2	1:A:222:TYR:H	1.99	0.43
1:A:276:GLU:HG2	1:A:304:ALA:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LYS:HE3	1:A:316:LYS:HB3	1.75	0.43
1:A:70:ASN:HD21	1:A:100:LYS:HZ1	1.62	0.43
1:A:148:ARG:HH11	1:A:148:ARG:HD3	1.65	0.43
1:A:146:LYS:HE2	1:A:187:GLU:OE1	2.19	0.42
1:A:317:LYS:H	1:A:317:LYS:CE	2.31	0.42
1:A:277:GLU:OE2	1:A:342:TYR:OH	2.30	0.42
1:A:146:LYS:HE3	2:A:394:HOH:O	2.19	0.42
1:A:89:ASP:OD1	1:A:91:ARG:CG	2.60	0.41
1:A:361:HIS:CG	1:A:362:ALA:N	2.85	0.41
1:A:59:ARG:O	1:A:63:LEU:HG	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:499:HOH:O	2:A:499:HOH:O[9_555]	1.04	1.16

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	360/363 (99%)	337 (94%)	18 (5%)	5 (1%)	11 6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	350	ALA
1	A	351	ALA
1	A	347	GLN
1	A	345	SER
1	A	346	GLY

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%)	263 (90%)	28 (10%)	8 5

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LYS
1	A	38	SER
1	A	41	LYS
1	A	44	GLN
1	A	61	LEU
1	A	69	VAL
1	A	70	ASN
1	A	91	ARG
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	124	THR
1	A	173	TYR
1	A	207	LYS
1	A	216	LEU
1	A	221	ILE
1	A	242	LYS
1	A	246	GLU
1	A	267	ILE
1	A	278	GLU
1	A	292	LEU
1	A	295	TRP
1	A	317	LYS
1	A	330	ARG
1	A	347	GLN
1	A	359	SER
1	A	363	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	70	ASN
1	A	80	HIS
1	A	119	ASN
1	A	178	GLN
1	A	245	HIS
1	A	306	GLN
1	A	324	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	362:ALA	C	363:TYR	N	2.13
1	A	350:ALA	C	351:ALA	N	1.71
1	A	344:PRO	C	345:SER	N	1.61

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.