Worldwide PDB — Protein Data Bank

Full wwPDB X-ray Structure Validation Report (i)

May 16, 2020 – 11:20 am BST

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PDB ID	:	1UCW
Title	:	COMPLEX OF TRANSALDOLASE WITH THE REDUCED SCHIFF-BASE INTERMEDIATE
Authors	:	Jia, J.; Lindqvist, Y.; Schneider, G.
Deposited on	:	1996-11-14
Resolution	:	2.20 Å(reported)

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 2.20 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.
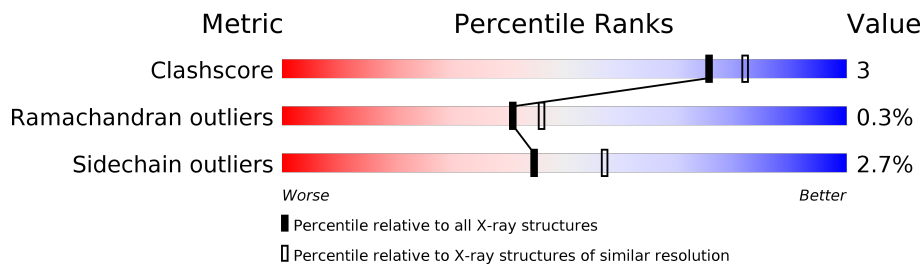
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Mol	Chain	Length	Quality of chain
1	A	317	90% 8% •
1	B	317	90% 9% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5463 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 TRANSALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total 2479	C 1568	N 420	O 484	S 7	0	1	0
1	B	316	Total 2479	C 1568	N 420	O 484	S 7	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LLY	LYS	MODIFIED RESIDUE	UNP P0A870
B	132	LLY	LYS	MODIFIED RESIDUE	UNP P0A870

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	249	Total 249	O 249	0	0
2	B	256	Total 256	O 256	0	0

3 Residue-property plots ⓘ

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.

- Molecule 1: TRANSALDOLASE

Chain A:

90%   8% ·

MET T2 L5 T13 R49 V56 A57 W58 Q62 L83 R92 E106 K132 N152 F159 S160 Q163 T190 D191 Q211 E215 S226 L234 R241 L249 A253 I259 D288 V292 R300 L309 L316 L317

- Molecule 1: TRANSALDOLASE

Chain B:

90%   9% ·

MET T2 L5 T13 R49 D54 A55 V56 A57 W58 Q62 L83 R92 E106 K132 N152 F159 S160 Q163 T190 D191 Q211 E215 S226 L234 R241 L249 A253 I259 D288 V292 R300 L309 L316

L317
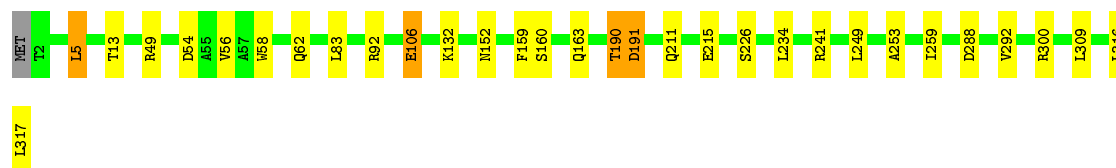
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.20Å 91.90Å 130.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 37.61 – 2.19	Depositor EDS
% Data completeness (in resolution range)	87.0 (10.00-2.20) 86.8 (37.61-2.19)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.84 (at 2.20Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.204 , 0.244 0.258 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 55.2	EDS
L-test for twinning[2]	$< |L| > = 0.53$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5463	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9134e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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)

Bond lengths and bond angles in the following residue types are not validated in this section: LLY

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	0.39	0/2506	0.70	3/3391 (0.1%)
1	B	0.39	0/2506	0.74	3/3391 (0.1%)
All	All	0.39	0/5012	0.72	6/6782 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	ARG	NE-CZ-NH2	-16.14	112.23	120.30
1	B	300	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	A	300	ARG	NE-CZ-NH2	-12.79	113.91	120.30
1	A	300	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	B	300	ARG	CD-NE-CZ	7.01	133.42	123.60
1	A	300	ARG	CD-NE-CZ	5.76	131.67	123.60

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	A	2479	0	2495	15	0
1	B	2479	0	2495	16	0
2	A	249	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	256	0	0	2	0
All	All	5463	0	4990	31	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 3.

All (31) 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:92:ARG:HH12	1:B:152:ASN:HD22	1.40	0.68
1:A:92:ARG:HH12	1:A:152:ASN:HD22	1.40	0.68
1:B:132:LLY:HE3	2:B:797:HOH:O	1.98	0.62
1:A:132:LLY:HE3	2:A:555:HOH:O	1.99	0.61
1:B:160:SER:H	1:B:163:GLN:HE21	1.49	0.59
1:A:160:SER:H	1:A:163:GLN:HE21	1.50	0.57
1:A:159:PHE:H	1:A:163:GLN:NE2	2.06	0.54
1:B:159:PHE:H	1:B:163:GLN:NE2	2.06	0.53
1:B:211:GLN:O	1:B:215:GLU:HB2	2.09	0.52
1:B:54:ASP:HB2	2:B:813:HOH:O	2.10	0.51
1:A:211:GLN:O	1:A:215:GLU:HB2	2.10	0.51
1:B:234:LEU:HD22	1:B:259:ILE:HG21	1.93	0.50
1:B:106:GLU:OE1	1:B:106:GLU:HA	2.12	0.49
1:A:234:LEU:HD22	1:A:259:ILE:HG21	1.94	0.49
1:A:106:GLU:OE1	1:A:106:GLU:HA	2.13	0.48
1:B:13:THR:HB	1:B:241:ARG:HG2	1.95	0.48
1:B:56:VAL:HG13	1:B:317:LEU:HD23	1.96	0.47
1:A:56:VAL:HG13	1:A:317:LEU:HD23	1.96	0.46
1:B:5:LEU:HD12	1:B:253:ALA:HB2	1.98	0.45
1:A:49:ARG:HH22	1:A:316:LEU:HD22	1.81	0.45
1:B:49:ARG:HH22	1:B:316:LEU:HD22	1.82	0.45
1:A:288:ASP:O	1:A:292:VAL:HG23	2.17	0.44
1:A:92:ARG:HH12	1:A:152:ASN:ND2	2.12	0.43
1:A:13:THR:HB	1:A:241:ARG:HG2	2.00	0.43
1:B:190:THR:CG2	1:B:191:ASP:N	2.81	0.43
1:B:58:TRP:O	1:B:62:GLN:HG2	2.19	0.43
1:B:288:ASP:O	1:B:292:VAL:HG23	2.19	0.42
1:A:190:THR:CG2	1:A:191:ASP:N	2.83	0.42
1:A:58:TRP:O	1:A:62:GLN:HG2	2.21	0.41
1:B:160:SER:H	1:B:163:GLN:NE2	2.15	0.41
1:A:5:LEU:HD12	1:A:253:ALA:HB2	2.02	0.40

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	314/317 (99%)	308 (98%)	5 (2%)	1 (0%)	41	46
1	B	314/317 (99%)	308 (98%)	5 (2%)	1 (0%)	41	46
All	All	628/634 (99%)	616 (98%)	10 (2%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	SER
1	B	226	SER

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	260/260 (100%)	253 (97%)	7 (3%)	44	57
1	B	260/260 (100%)	253 (97%)	7 (3%)	44	57
All	All	520/520 (100%)	506 (97%)	14 (3%)	44	57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU

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Mol	Chain	Res	Type
1	A	83	LEU
1	A	106	GLU
1	A	190	THR
1	A	191	ASP
1	A	249	LEU
1	A	309	LEU
1	B	5	LEU
1	B	83	LEU
1	B	106	GLU
1	B	190	THR
1	B	191	ASP
1	B	249	LEU
1	B	309	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	152	ASN
1	A	163	GLN
1	B	152	ASN
1	B	163	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	#$\|Z\|>2$
1	LLY	A	132	1	11,13,16	2.58	4 (36%)	3,14,20	1.05	0
1	LLY	B	132	1	11,13,16	2.53	2 (18%)	3,14,20	1.02	0

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
1	LLY	A	132	1	-	2/7/14/20	-
1	LLY	B	132	1	-	3/7/14/20	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	132	LLY	O1-C1	5.76	1.42	1.19
1	A	132	LLY	O1-C1	5.71	1.42	1.19
1	A	132	LLY	O3-C2	5.55	1.42	1.19
1	B	132	LLY	O3-C2	5.48	1.41	1.19
1	A	132	LLY	CH-C2	2.04	1.55	1.51
1	A	132	LLY	CH-C1	2.01	1.55	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	132	LLY	N-CA-CB-CG
1	A	132	LLY	C-CA-CB-CG
1	B	132	LLY	N-CA-CB-CG
1	B	132	LLY	C-CA-CB-CG
1	B	132	LLY	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	132	LLY	1	0
1	B	132	LLY	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.