



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:49 PM GMT

PDB ID : 2C7Z
Title : PLANT ENZYME CRYSTAL FORM II
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Deposited on : 2005-11-30
Resolution : 2.37 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

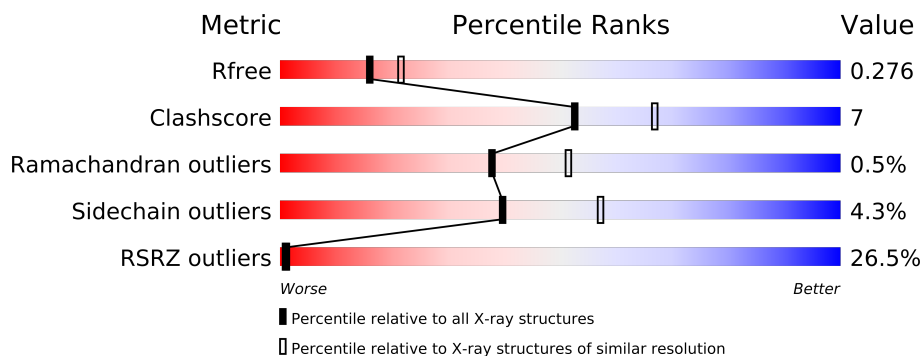
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.37 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}	66092	2963 (2.40-2.36)
Clashscore	79885	3668 (2.40-2.36)
Ramachandran outliers	78287	3600 (2.40-2.36)
Sidechain outliers	78261	3602 (2.40-2.36)
RSRZ outliers	66119	2966 (2.40-2.36)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	404	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3002 atoms, of which 0 are hydrogen and 0 are deuterium.

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 3-KETOACYL-COA THIOLASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	34	0	0
			2900	1816	514	551	19			

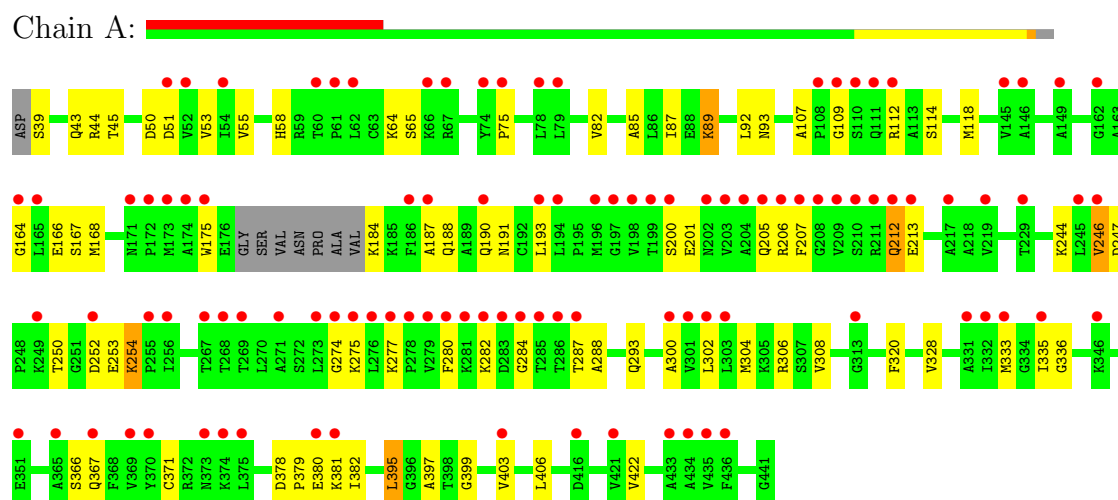
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	102	Total	O	0	0
			102	102		

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 errors 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: 3-KETOACYL-COA THIOLASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.39Å 95.82Å 56.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.54 – 2.37 18.54 – 2.37	Depositor EDS
% Data completeness (in resolution range)	87.4 (18.54-2.37) 87.4 (18.54-2.37)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.276 0.198 , 0.276	Depositor DCC
R_{free} test set	725 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 14473 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3002	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.72	6/2944 (0.2%)	0.72	8/3983 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	LYS	CB-CG	-21.54	0.94	1.52
1	A	206	ARG	CB-CG	-13.16	1.17	1.52
1	A	275	LYS	CB-CG	9.24	1.77	1.52
1	A	205	GLN	CG-CD	-9.20	1.29	1.51
1	A	282	LYS	CG-CD	-5.56	1.33	1.52
1	A	246	VAL	CB-CG1	5.12	1.63	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	254	LYS	CA-CB-CG	13.26	142.56	113.40
1	A	254	LYS	CB-CG-CD	10.19	138.10	111.60
1	A	282	LYS	CB-CG-CD	8.22	132.98	111.60
1	A	252	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	280	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	A	280	PHE	CB-CG-CD2	5.49	124.64	120.80
1	A	205	GLN	CB-CG-CD	5.22	125.17	111.60
1	A	205	GLN	CG-CD-OE1	-5.15	111.29	121.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2900	0	2939	41	0
2	A	102	0	0	6	0
All	All	3002	0	2939	41	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (41) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:85:ALA:O	1:A:89:LYS:HD3	1.79	0.82
1:A:114:SER:HB2	1:A:175:TRP:HB3	1.65	0.79
1:A:184:LYS:N	2:A:2039:HOH:O	2.21	0.73
1:A:107:ALA:HB3	1:A:112:ARG:HG2	1.72	0.71
1:A:212:GLN:HG2	1:A:213:GLU:H	1.60	0.66
1:A:274:GLY:HA3	2:A:2059:HOH:O	1.95	0.64
1:A:371:CYS:SG	2:A:2074:HOH:O	2.55	0.64
1:A:50:ASP:O	1:A:306:ARG:NH1	2.31	0.64
1:A:187:ALA:O	1:A:191:ASN:HB2	1.98	0.64
1:A:65:SER:HB3	1:A:168:MET:HG3	1.80	0.62
1:A:82:VAL:HG12	1:A:300:ALA:HB3	1.81	0.61
1:A:212:GLN:CG	1:A:213:GLU:N	2.64	0.60
1:A:246:VAL:HG22	1:A:253:GLU:HG2	1.84	0.60
1:A:166:GLU:HG3	1:A:395:LEU:HB2	1.84	0.59
1:A:64:LYS:HE2	1:A:293:GLN:HB2	1.84	0.58
1:A:207:PHE:O	2:A:2042:HOH:O	2.17	0.58
1:A:212:GLN:CG	1:A:213:GLU:H	2.20	0.54
1:A:75:PRO:HG3	1:A:167:SER:HB3	1.89	0.54
1:A:200:SER:HB3	1:A:366:SER:OG	2.09	0.53
1:A:190:GLN:HB2	2:A:2040:HOH:O	2.09	0.52
1:A:378:ASP:HB3	1:A:381:LYS:HD2	1.91	0.52
1:A:335:ILE:HA	2:A:2074:HOH:O	2.10	0.51
1:A:399:GLY:O	1:A:403:VAL:HG23	2.11	0.51
1:A:65:SER:HB3	1:A:168:MET:CG	2.42	0.49
1:A:200:SER:OG	1:A:367:GLN:HB2	2.12	0.49
1:A:43:GLN:NE2	1:A:45:THR:OG1	2.46	0.49
1:A:406:LEU:HD22	1:A:422:VAL:HG23	1.95	0.49
1:A:287:THR:HG22	1:A:288:ALA:N	2.29	0.47
1:A:164:GLY:HA3	1:A:397:ALA:HA	1.98	0.46
1:A:379:PRO:HA	1:A:382:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:53:VAL:HG22	1:A:304:MET:O	2.17	0.44
1:A:118:MET:HG2	1:A:175:TRP:HB2	2.00	0.44
1:A:190:GLN:HA	1:A:193:LEU:HB2	2.00	0.43
1:A:58:HIS:NE2	1:A:89:LYS:HE3	2.33	0.43
1:A:201:GLU:OE2	1:A:284:GLY:HA3	2.19	0.42
1:A:328:VAL:HG11	1:A:336:GLY:HA2	2.01	0.42
1:A:107:ALA:CB	1:A:112:ARG:HG2	2.47	0.42
1:A:378:ASP:OD2	1:A:380:GLU:HB3	2.19	0.42
1:A:247:ASP:OD2	1:A:250:THR:HG23	2.20	0.41
1:A:55:VAL:HG23	1:A:302:LEU:HD23	2.02	0.40
1:A:87:ILE:HG23	1:A:92:LEU:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	392/404 (97%)	368 (94%)	22 (6%)	2 (0%)	38 51

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	GLY
1	A	395	LEU

5.3.2 Protein sidechains ⓘ

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	300/307 (98%)	287 (96%)	13 (4%)	40 57

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	44	ARG
1	A	51	ASP
1	A	89	LYS
1	A	93	ASN
1	A	188	GLN
1	A	212	GLN
1	A	244	LYS
1	A	254	LYS
1	A	277	LYS
1	A	308	VAL
1	A	320	PHE
1	A	333	MET

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	43	GLN
1	A	93	ASN
1	A	212	GLN
1	A	214	GLN
1	A	361	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	396/404 (98%)	1.45	105 (26%) 1 1	35, 44, 63, 67	8 (2%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	PRO	7.1
1	A	208	GLY	6.5
1	A	276	LEU	6.4
1	A	207	PHE	5.8
1	A	281	LYS	5.6
1	A	273	LEU	5.6
1	A	172	PRO	5.6
1	A	279	VAL	5.5
1	A	108	PRO	5.4
1	A	110	SER	5.4
1	A	284	GLY	5.1
1	A	277	LYS	5.0
1	A	280	PHE	4.9
1	A	186	PHE	4.8
1	A	274	GLY	4.8
1	A	204	ALA	4.8
1	A	173	MET	4.6
1	A	369	VAL	4.3
1	A	331	ALA	3.9
1	A	212	GLN	3.9
1	A	206	ARG	3.8
1	A	174	ALA	3.8
1	A	67	ARG	3.8
1	A	210	SER	3.8
1	A	198	VAL	3.8
1	A	283	ASP	3.8
1	A	74	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	66	LYS	3.7
1	A	200	SER	3.7
1	A	370	TYR	3.7
1	A	209	VAL	3.7
1	A	269	THR	3.6
1	A	267	THR	3.5
1	A	112	ARG	3.5
1	A	365	ALA	3.3
1	A	203	VAL	3.3
1	A	335	ILE	3.2
1	A	202	ASN	3.2
1	A	434	ALA	3.1
1	A	79	LEU	3.1
1	A	229	THR	3.0
1	A	109	GLY	3.0
1	A	367	GLN	3.0
1	A	171	ASN	3.0
1	A	271	ALA	2.9
1	A	111	GLN	2.9
1	A	60	THR	2.9
1	A	245	LEU	2.9
1	A	303	LEU	2.8
1	A	268	THR	2.8
1	A	416	ASP	2.8
1	A	275	LYS	2.8
1	A	374	LYS	2.8
1	A	213	GLU	2.8
1	A	287	THR	2.8
1	A	255	PRO	2.8
1	A	285	THR	2.8
1	A	51	ASP	2.8
1	A	286	THR	2.7
1	A	332	ILE	2.7
1	A	282	LYS	2.7
1	A	301	VAL	2.6
1	A	175	TRP	2.6
1	A	351	GLU	2.6
1	A	164	GLY	2.6
1	A	302	LEU	2.6
1	A	196	MET	2.5
1	A	199	THR	2.4
1	A	75	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	381	LYS	2.4
1	A	149	ALA	2.4
1	A	54	ILE	2.4
1	A	165	LEU	2.3
1	A	194	LEU	2.3
1	A	52	VAL	2.3
1	A	256	ILE	2.3
1	A	373	ASN	2.3
1	A	78	LEU	2.3
1	A	219	VAL	2.3
1	A	313	GLY	2.3
1	A	146	ALA	2.3
1	A	187	ALA	2.3
1	A	145	VAL	2.2
1	A	403	VAL	2.2
1	A	197	GLY	2.2
1	A	211	ARG	2.2
1	A	162	GLY	2.2
1	A	193	LEU	2.2
1	A	252	ASP	2.2
1	A	433	ALA	2.2
1	A	217	ALA	2.2
1	A	62	LEU	2.2
1	A	61	PRO	2.2
1	A	436	PHE	2.1
1	A	249	LYS	2.1
1	A	246	VAL	2.1
1	A	380	GLU	2.1
1	A	333	MET	2.0
1	A	421	VAL	2.0
1	A	190	GLN	2.0
1	A	300	ALA	2.0
1	A	346	LYS	2.0
1	A	375	LEU	2.0
1	A	435	VAL	2.0
1	A	205	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.