WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 06:47 pm GMT

PDB ID	:	2C7Z
Title	:	Plant enzyme crystal form II
Authors	:	Sundaramoorthy, R.; Micossi, E.; Alphey, M.S.; Leonard, G.A.; Hunter, W.N.
Deposited on	:	2005-11-30
Resolution	:	2.37 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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	Percentile Ranks	Value
Rfree		0.278
Clashscore		7
Ramachandran outliers		0.5%
Sidechain outliers		4.3%
RSRZ outliers		19.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
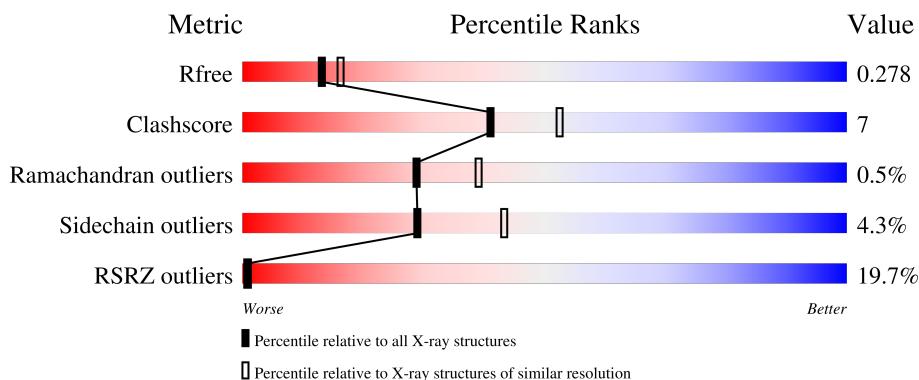
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 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	404	19% 78% 19% ··
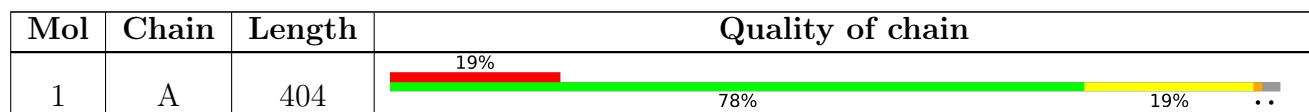
2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 3002 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 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, 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: 3-KETOACYL-COA THIOLASE 2
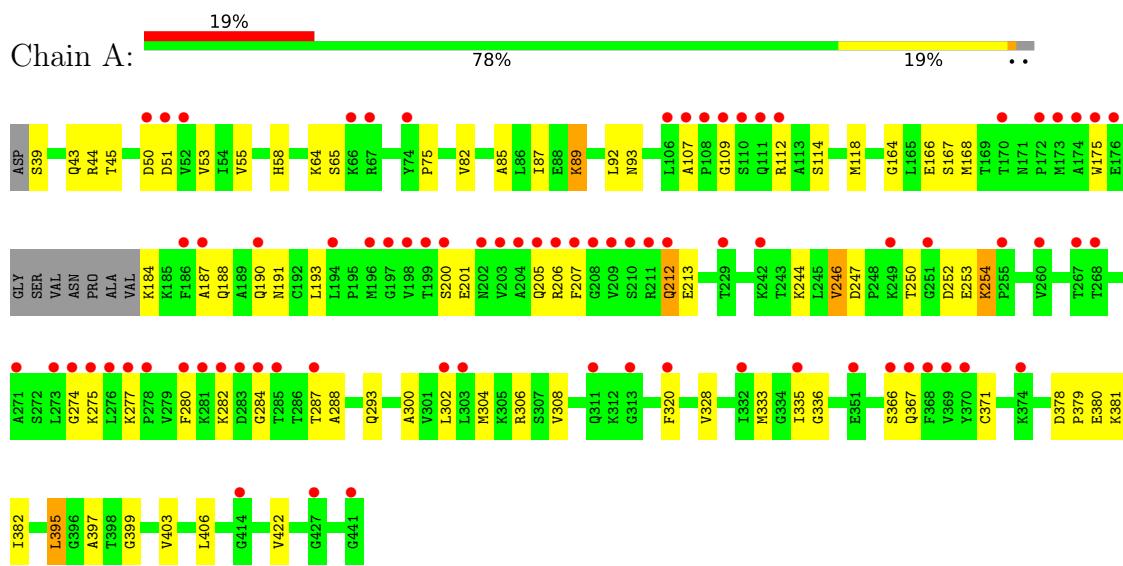
4 Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [1]	1.21 (at 2.38Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.276 0.197 , 0.278	Depositor DCC
R_{free} test set	725 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 66.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

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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 ⓘ

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 Too-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 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	2900	0	2939	41	0
2	A	102	0	0	6	0
All	All	3002	0	2939	41	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 7.

All (41) 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: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:50:ASP:O	1:A:306:ARG:NH1	2.31	0.64
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: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:43:GLN:NE2	1:A:45:THR:OG1	2.46	0.49
1:A:200:SER:OG	1:A:367:GLN:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:HA	1:A:382:ILE:HD12	1.99	0.45
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%)	29 39

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%)	29	43

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

Sometimes 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 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 monosaccharides 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%)	1.01	78 (19%)	1	1	35, 44, 63, 67	8 (2%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	ALA	9.1
1	A	273	LEU	8.1
1	A	110	SER	7.2
1	A	278	PRO	6.6
1	A	173	MET	6.5
1	A	67	ARG	6.0
1	A	281	LYS	5.9
1	A	172	PRO	5.7
1	A	209	VAL	5.5
1	A	208	GLY	5.3
1	A	274	GLY	5.2
1	A	204	ALA	4.9
1	A	197	GLY	4.9
1	A	108	PRO	4.8
1	A	207	PHE	4.8
1	A	284	GLY	4.6
1	A	186	PHE	4.2
1	A	199	THR	4.1
1	A	194	LEU	4.0
1	A	200	SER	3.9
1	A	313	GLY	3.8
1	A	111	GLN	3.8
1	A	190	GLN	3.7
1	A	276	LEU	3.6
1	A	268	THR	3.6
1	A	212	GLN	3.4
1	A	170	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	112	ARG	3.4
1	A	206	ARG	3.3
1	A	255	PRO	3.3
1	A	283	ASP	3.3
1	A	277	LYS	3.2
1	A	198	VAL	3.2
1	A	109	GLY	3.2
1	A	203	VAL	3.1
1	A	260	VAL	3.0
1	A	196	MET	3.0
1	A	175	TRP	3.0
1	A	367	GLN	3.0
1	A	202	ASN	2.9
1	A	332	ILE	2.9
1	A	370	TYR	2.8
1	A	414	GLY	2.8
1	A	275	LYS	2.7
1	A	267	THR	2.7
1	A	74	TYR	2.6
1	A	280	PHE	2.6
1	A	302	LEU	2.6
1	A	51	ASP	2.6
1	A	366	SER	2.6
1	A	271	ALA	2.5
1	A	441	GLY	2.5
1	A	52	VAL	2.5
1	A	369	VAL	2.4
1	A	106	LEU	2.4
1	A	107	ALA	2.4
1	A	176	GLU	2.4
1	A	368	PHE	2.4
1	A	229	THR	2.3
1	A	311	GLN	2.3
1	A	251	GLY	2.3
1	A	427	GLY	2.3
1	A	66	LYS	2.2
1	A	374	LYS	2.2
1	A	287	THR	2.2
1	A	282	LYS	2.2
1	A	187	ALA	2.2
1	A	210	SER	2.2
1	A	351	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	GLN	2.2
1	A	320	PHE	2.1
1	A	211	ARG	2.1
1	A	242	LYS	2.1
1	A	285	THR	2.1
1	A	303	LEU	2.1
1	A	249	LYS	2.0
1	A	50	ASP	2.0
1	A	335	ILE	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 monosaccharides 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.