



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2016 – 05:07 PM EDT

PDB ID : 1XGF
Title : Backbone Structure of COCOSIN, an 11S storage protein from *cocos nucifera*
Authors : Balasundaresan, D.; Ponnuswamy, M.N.
Deposited on : 2004-09-17
Resolution : 2.61 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

<http://wwpdb.org/validation/2016/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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

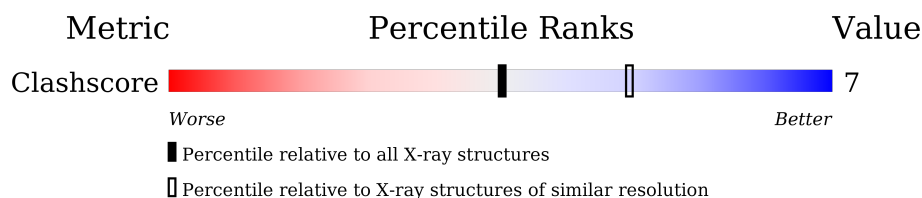
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	102246	3065 (2.64-2.60)

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. 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 $\leq 5\%$. 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	382	
1	B	382	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3056 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.

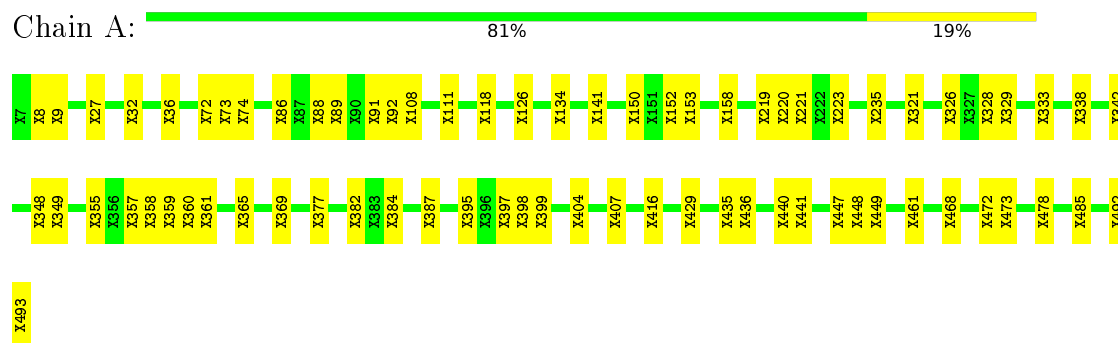
- Molecule 1 is a protein called cocosin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	0	0	0
			1528	764	382	382			
1	B	382	Total	C	N	O	0	0	0
			1528	764	382	382			

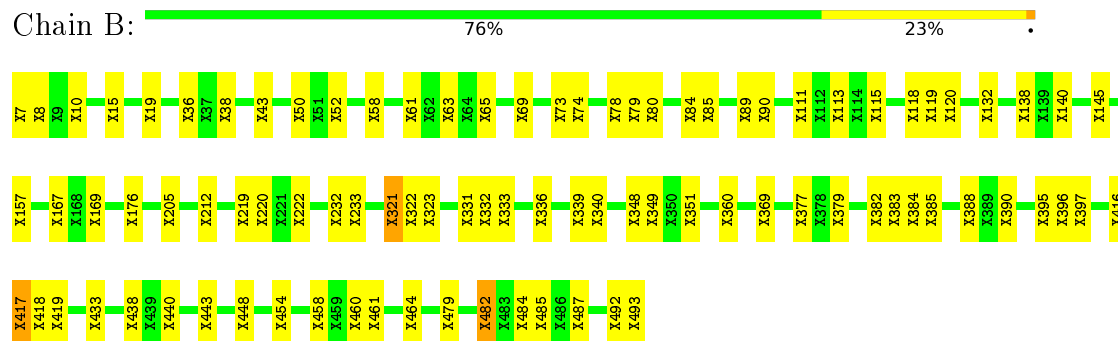
3 Residue-property plots

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: cocosin



- Molecule 1: cocosin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	93.66Å 93.66Å 216.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	2.80 – 2.61 29.60 – 2.61	Depositor EDS
% Data completeness (in resolution range)	(Not available) (2.80-2.61) 94.7 (29.60-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.61Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.240 , 0.294 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.08 , 159.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.099 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	3056	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

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	69
1	B	0	80
All	All	0	149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (149) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	UNK	Peptide
1	A	111	UNK	Mainchain
1	A	118	UNK	Mainchain
1	A	126	UNK	Mainchain
1	A	134	UNK	Mainchain
1	A	141	UNK	Mainchain,Peptide
1	A	150	UNK	Mainchain
1	A	152	UNK	Mainchain
1	A	153	UNK	Mainchain
1	A	158	UNK	Mainchain
1	A	219	UNK	Mainchain
1	A	220	UNK	Mainchain
1	A	221	UNK	Mainchain
1	A	223	UNK	Mainchain
1	A	235	UNK	Mainchain
1	A	27	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	32	UNK	Mainchain
1	A	321	UNK	Mainchain
1	A	326	UNK	Mainchain
1	A	333	UNK	Mainchain
1	A	338	UNK	Mainchain
1	A	342	UNK	Mainchain
1	A	348	UNK	Mainchain
1	A	349	UNK	Mainchain
1	A	355	UNK	Mainchain
1	A	357	UNK	Mainchain
1	A	358	UNK	Mainchain
1	A	36	UNK	Mainchain,Peptide
1	A	361	UNK	Mainchain
1	A	365	UNK	Mainchain
1	A	369	UNK	Mainchain
1	A	377	UNK	Mainchain
1	A	382	UNK	Mainchain
1	A	384	UNK	Mainchain
1	A	387	UNK	Mainchain
1	A	395	UNK	Mainchain
1	A	397	UNK	Mainchain
1	A	398	UNK	Mainchain
1	A	399	UNK	Mainchain
1	A	404	UNK	Mainchain
1	A	407	UNK	Mainchain
1	A	416	UNK	Mainchain,Peptide
1	A	429	UNK	Mainchain
1	A	435	UNK	Mainchain
1	A	436	UNK	Mainchain
1	A	440	UNK	Mainchain
1	A	441	UNK	Mainchain
1	A	447	UNK	Mainchain
1	A	448	UNK	Mainchain
1	A	449	UNK	Mainchain
1	A	461	UNK	Mainchain
1	A	468	UNK	Mainchain
1	A	472	UNK	Mainchain
1	A	473	UNK	Mainchain
1	A	478	UNK	Mainchain,Peptide
1	A	485	UNK	Mainchain
1	A	72	UNK	Mainchain
1	A	8	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	A	86	UNK	Mainchain
1	A	88	UNK	Mainchain
1	A	89	UNK	Mainchain
1	A	9	UNK	Mainchain
1	A	91	UNK	Mainchain
1	A	92	UNK	Mainchain,Peptide
1	B	10	UNK	Mainchain
1	B	111	UNK	Mainchain
1	B	113	UNK	Mainchain
1	B	115	UNK	Mainchain
1	B	118	UNK	Mainchain
1	B	120	UNK	Mainchain
1	B	138	UNK	Mainchain
1	B	140	UNK	Mainchain
1	B	145	UNK	Mainchain
1	B	15	UNK	Mainchain
1	B	157	UNK	Mainchain
1	B	167	UNK	Mainchain
1	B	169	UNK	Mainchain
1	B	176	UNK	Mainchain
1	B	19	UNK	Mainchain
1	B	205	UNK	Mainchain
1	B	212	UNK	Mainchain
1	B	219	UNK	Mainchain
1	B	220	UNK	Mainchain
1	B	222	UNK	Mainchain
1	B	232	UNK	Mainchain
1	B	233	UNK	Mainchain
1	B	321	UNK	Mainchain,Peptide
1	B	331	UNK	Mainchain
1	B	332	UNK	Mainchain
1	B	333	UNK	Mainchain
1	B	336	UNK	Mainchain
1	B	339	UNK	Mainchain
1	B	340	UNK	Mainchain
1	B	348	UNK	Mainchain,Peptide
1	B	349	UNK	Mainchain
1	B	351	UNK	Mainchain
1	B	36	UNK	Mainchain
1	B	360	UNK	Mainchain
1	B	369	UNK	Mainchain
1	B	377	UNK	Mainchain

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Mol	Chain	Res	Type	Group
1	B	379	UNK	Mainchain
1	B	38	UNK	Mainchain
1	B	382	UNK	Mainchain
1	B	383	UNK	Mainchain
1	B	384	UNK	Mainchain
1	B	385	UNK	Mainchain
1	B	388	UNK	Mainchain
1	B	390	UNK	Mainchain
1	B	395	UNK	Mainchain
1	B	396	UNK	Mainchain
1	B	397	UNK	Mainchain
1	B	417	UNK	Mainchain
1	B	43	UNK	Mainchain
1	B	433	UNK	Mainchain
1	B	438	UNK	Mainchain
1	B	440	UNK	Mainchain
1	B	443	UNK	Mainchain
1	B	448	UNK	Mainchain
1	B	454	UNK	Mainchain
1	B	458	UNK	Mainchain
1	B	460	UNK	Mainchain
1	B	461	UNK	Mainchain
1	B	464	UNK	Mainchain
1	B	482	UNK	Mainchain
1	B	484	UNK	Mainchain
1	B	485	UNK	Mainchain,Peptide
1	B	487	UNK	Mainchain
1	B	50	UNK	Mainchain
1	B	52	UNK	Mainchain
1	B	58	UNK	Mainchain
1	B	61	UNK	Mainchain
1	B	63	UNK	Mainchain
1	B	65	UNK	Mainchain
1	B	69	UNK	Mainchain
1	B	7	UNK	Mainchain
1	B	73	UNK	Mainchain
1	B	8	UNK	Mainchain
1	B	84	UNK	Mainchain
1	B	85	UNK	Peptide
1	B	89	UNK	Mainchain
1	B	90	UNK	Mainchain

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	1528	0	54	9	0
1	B	1528	0	47	13	0
All	All	3056	0	101	22	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 (22) 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:492:UNK:C	1:A:493:UNK:H	1.27	1.48
1:A:492:UNK:C	1:A:493:UNK:N	1.93	1.30
1:B:416:UNK:C	1:B:417:UNK:N	1.96	1.27
1:B:416:UNK:C	1:B:417:UNK:H2	1.57	1.11
1:A:492:UNK:CA	1:A:493:UNK:H	1.72	1.02
1:B:416:UNK:CA	1:B:417:UNK:H2	1.83	0.90
1:A:492:UNK:C	1:A:493:UNK:C	2.57	0.82
1:A:492:UNK:CA	1:A:493:UNK:N	2.39	0.79
1:B:416:UNK:CA	1:B:417:UNK:N	2.43	0.76
1:A:492:UNK:C	1:A:493:UNK:CA	2.73	0.65
1:A:328:UNK:O	1:A:329:UNK:C	2.49	0.60
1:B:416:UNK:C	1:B:417:UNK:H	2.11	0.59
1:B:479:UNK:O	1:B:482:UNK:O	2.26	0.53
1:B:492:UNK:O	1:B:493:UNK:C	2.60	0.49
1:B:79:UNK:O	1:B:132:UNK:N	2.50	0.45
1:B:418:UNK:O	1:B:419:UNK:C	2.65	0.43
1:A:359:UNK:O	1:A:360:UNK:C	2.66	0.43
1:B:321:UNK:O	1:B:322:UNK:C	2.67	0.43
1:B:78:UNK:O	1:B:80:UNK:N	2.53	0.41
1:B:74:UNK:O	1:B:119:UNK:N	2.53	0.41
1:B:322:UNK:O	1:B:323:UNK:C	2.67	0.40
1:A:73:UNK:O	1:A:74:UNK:C	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 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](#)

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(\AA^2)	Q<0.9
1	A	0/382	-	-	-	-
1	B	0/382	-	-	-	-
All	All	0/764	-	-	-	-

There are no RSRZ outliers to report.

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 carbohydrates 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.