



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 5XTY / pdb\_00005xty  
Title : Crystal Structure of 11S allergen from Cocos nucifera L.  
Authors : Vajravijayan, S.; Nandhagopal, N.; Gunasekaran, K.  
Deposited on : 2017-06-21  
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

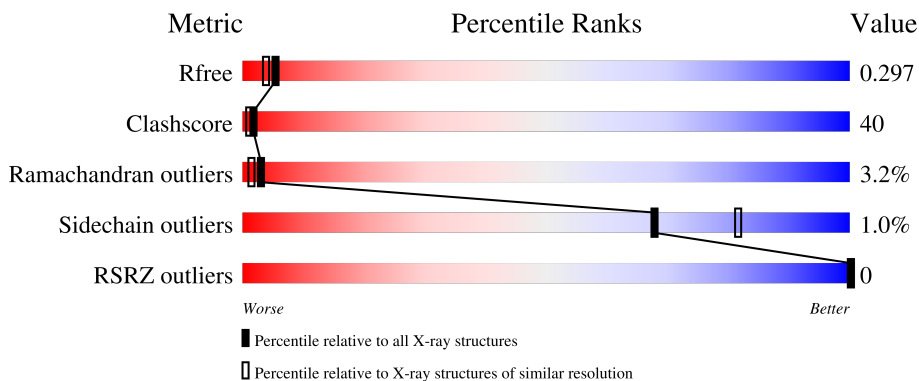
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

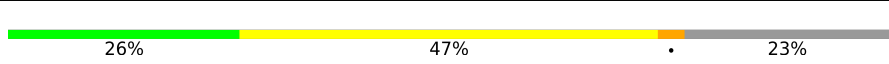
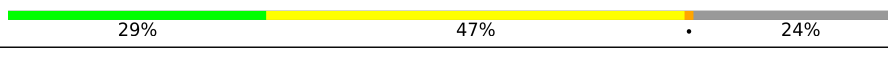
The reported resolution of this entry is 2.20 Å.

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))
$R_{free}$	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	466	 26% 47% 23%
1	B	466	 29% 47% 24%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5768 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 11S globulin isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	359	2812	1745	522	526	19	0	0	0
1	B	356	2800	1740	524	519	17	0	0	0

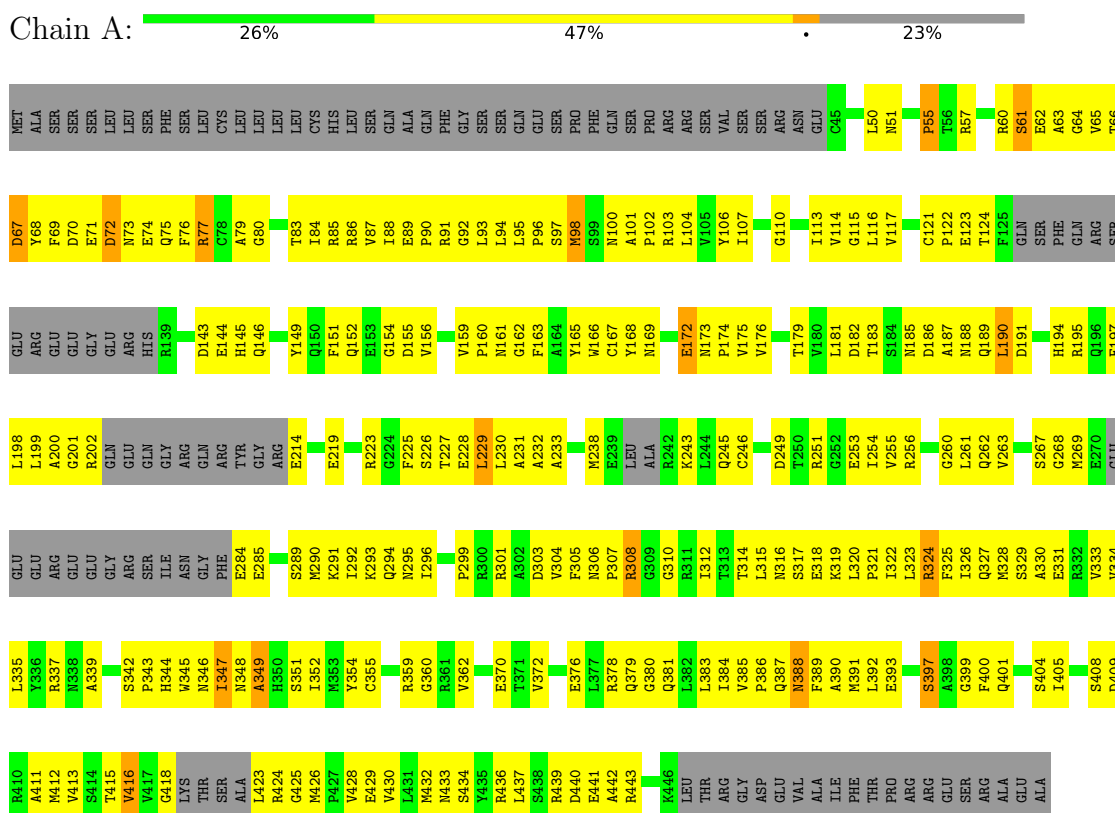
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	70	Total	O	0	0
			70	70		
2	B	86	Total	O	0	0
			86	86		

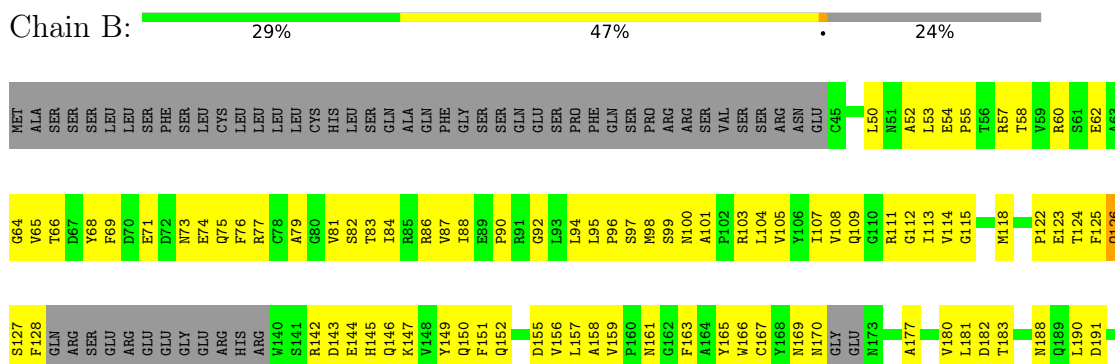
### 3 Residue-property plots

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: 11S globulin isoform 1



- Molecule 1: 11S globulin isoform 1



ARG	ALA
GLU	ALA
SER	ALA
ARG	ALA
ALA	ALA
GLU	ALA
ALA	ALA
A398	ARG
G399	GLU
F400	SER
Q401	ARG
L402	ALA
V403	GLU
S404	ALA
I405	ALA
K406	ALA
T407	ALA
S408	ALA
D409	ALA
R410	ALA
A411	ALA
M412	ALA
T415	ALA
VAL	ALA
VAL	ALA
GLY	ALA
LYS	ALA
THR	ALA
S421	ALA
A422	ALA
L423	ALA
R424	ALA
G425	ALA
M426	ALA
P427	ALA
V430	ALA
L431	ALA
M432	ALA
N433	ALA
S434	ALA
Y435	ALA
R436	ALA
L437	ALA
S438	ALA
R439	ALA
D440	ALA
E441	ALA
R444	ALA
V445	ALA
K446	ALA
L447	ALA
T448	ALA
ARG	ALA
GLY	ALA
ASP	ALA
GLU	ALA
VAL	ALA
VAL	ALA
ALA	ALA
ILE	ALA
PHE	ALA
THR	ALA
PRO	ALA
ARG	ALA
M328	ALA
S329	ALA
A330	ALA
E331	ALA
V334	ALA
I335	ALA
Y336	ALA
R337	ALA
N338	ALA
A339	ALA
K340	ALA
V341	ALA
S342	ALA
F343	ALA
H344	ALA
W345	ALA
N346	ALA
I347	ALA
N348	ALA
S351	ALA
I352	ALA
M353	ALA
Y354	ALA
C355	ALA
T356	ALA
R359	ALA
G360	ALA
R361	ALA
V362	ALA
E363	ALA
V364	ALA
A365	ALA
D366	ALA
D367	ALA
F373	ALA
D374	ALA
G375	ALA
E376	ALA
L377	ALA
R378	ALA
Q379	ALA
L382	ALA
L383	ALA
I384	ALA
V385	ALA
P386	ALA
Q387	ALA
N388	ALA
F389	ALA
A390	ALA
M391	ALA
L392	ALA
E393	ALA
R394	ALA
A395	ALA
L264	ALA
P265	ALA
R266	ALA
S267	ALA
GLY	ALA
MET	ALA
GLU	ALA
GLU	ALA
GLU	ALA
GLU	ALA
GLY	ALA
ARG	ALA
GLN	ALA
GLY	ALA
TYR	ALA
GLY	ALA
ARG	ALA
ILE	ALA
GLU	ALA
GLY	ALA
SER	ALA
ASN	ALA
G282	ALA
F283	ALA
E284	ALA
E285	ALA
T286	ALA
Y287	ALA
C288	ALA
S289	ALA
M290	ALA
K291	ALA
I292	ALA
K293	ALA
Q294	ALA
N295	ALA
D298	ALA
R301	ALA
A302	ALA
D303	ALA
N306	ALA
P307	ALA
R308	ALA
G309	ALA
I312	ALA
T313	ALA
T314	ALA
L315	ALA
E318	ALA
K319	ALA
L320	ALA
P321	ALA
I322	ALA
L323	ALA
R324	ALA
F325	ALA
I326	ALA
Q327	ALA
R195	ALA
Q196	ALA
F197	ALA
L198	ALA
G201	ALA
R202	ALA
GLN	ALA
GLU	ALA
GLN	ALA
GLY	ALA
ARG	ALA
GLN	ALA
ARG	ALA
GLU	ALA
SER	ALA
GLY	ALA
ILE	ALA
LYS	ALA
E219	ALA
N220	ALA
I221	ALA
L222	ALA
R223	ALA
T227	ALA
E228	ALA
L229	ALA
L230	ALA
A231	ALA
A232	ALA
A233	ALA
F234	ALA
G235	ALA
V236	ALA
N237	ALA
M238	ALA
E239	ALA
L240	ALA
A241	ALA
R242	ALA
Q245	ALA
C246	ALA
R247	ALA
D248	ALA
D249	ALA
T250	ALA
R251	ALA
G252	ALA
E253	ALA
I254	ALA
V255	ALA
R256	ALA
A257	ALA
G260	ALA

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.06Å 92.06Å 212.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.83 – 2.20 29.83 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.83-2.20) 99.7 (29.83-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	22.14 (at 2.20Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.199 , 0.299 0.200 , 0.297	Depositor DCC
$R_{free}$ test set	1708 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.9	Xtrriage
Anisotropy	0.310	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 125.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	0.398 for h,-h-k,-l	Xtrriage
Reported twinning fraction	0.530 for k,h,-l	Depositor
Outliers	0 of 33978 reflections	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.50	0/2853	0.64	0/3845
1	B	0.50	0/2843	0.63	0/3833
All	All	0.50	0/5696	0.64	0/7678

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ALA	Peptide

### 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	2812	0	2772	239	3
1	B	2800	0	2765	222	3
2	A	70	0	0	36	1

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	86	0	0	25	1
All	All	5768	0	5537	447	6

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 40.

The worst 5 of 447 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:100:ASN:O	1:B:161:ASN:ND2	1.98	0.96
1:B:88:ILE:O	1:B:169:ASN:ND2	1.96	0.96
1:A:323:LEU:O	1:A:409:ASP:OD2	1.83	0.95
1:B:238:MET:SD	1:B:238:MET:N	2.37	0.93
1:A:318:GLU:HB3	1:B:290:MET:HB3	1.52	0.91

The worst 5 of 6 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:B:504:HOH:O	2:B:562:HOH:O[3_545]	2.00	0.20
1:B:144:GLU:O	1:B:446:LYS:NZ[2_445]	2.12	0.08
1:A:426:MET:O	2:A:507:HOH:O[2_445]	2.13	0.07
1:A:243:LYS:NZ	1:A:441:GLU:OE2[3_545]	2.18	0.02
1:B:195:ARG:NH2	1:B:367:ASP:OD1[2_445]	2.18	0.02

## 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	347/466 (74%)	283 (82%)	46 (13%)	18 (5%)	<b>1</b> <b>0</b>
1	B	344/466 (74%)	298 (87%)	42 (12%)	4 (1%)	<b>10</b> <b>8</b>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	691/932 (74%)	581 (84%)	88 (13%)	22 (3%)	<b>3</b> <b>1</b>

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	SER
1	B	266	PRO
1	A	61	SER
1	A	347	ILE
1	A	388	ASN

### 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	299/399 (75%)	296 (99%)	3 (1%)	68 81
1	B	299/399 (75%)	296 (99%)	3 (1%)	68 81
All	All	598/798 (75%)	592 (99%)	6 (1%)	68 81

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	126	GLN
1	B	170	ASN
1	B	253	GLU
1	A	98	MET
1	A	67	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	295	ASN
1	A	350	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	388	ASN

### 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 oligosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/466 (77%)	-0.89	0 <a href="#">100</a> <a href="#">100</a>	36, 52, 76, 149	0
1	B	356/466 (76%)	-0.94	0 <a href="#">100</a> <a href="#">100</a>	35, 48, 67, 88	0
All	All	715/932 (76%)	-0.91	0 <a href="#">100</a> <a href="#">100</a>	35, 50, 73, 149	0

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 oligosaccharides 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.