Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 01:09 PM EST

PDB ID	:	1OQ9
Title	:	The Crystal Structure of the Complex between Stearoyl Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean) and Acetate.
Authors	:	Moche, M.; Shanklin, J.; Ghoshal, A.K.; Lindqvist, Y.
Deposited on	:	2003-03-07
Resolution	:	2.40 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.

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

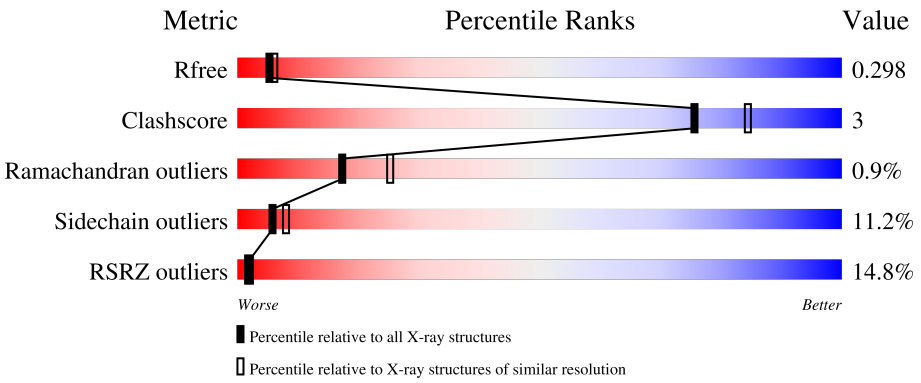
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

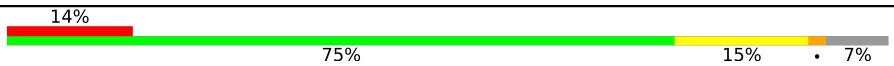
The reported resolution of this entry is 2.40 Å.

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	363	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2822 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.

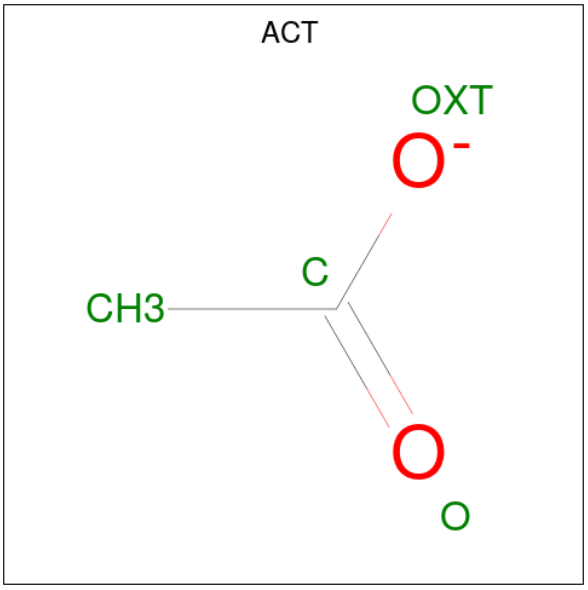
- Molecule 1 is a protein called Acyl-[acyl-carrier protein] desaturase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	338	2743	1745	472	512	14	0	0	0

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
2	A	2	2	2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0

- Molecule 4 is water.

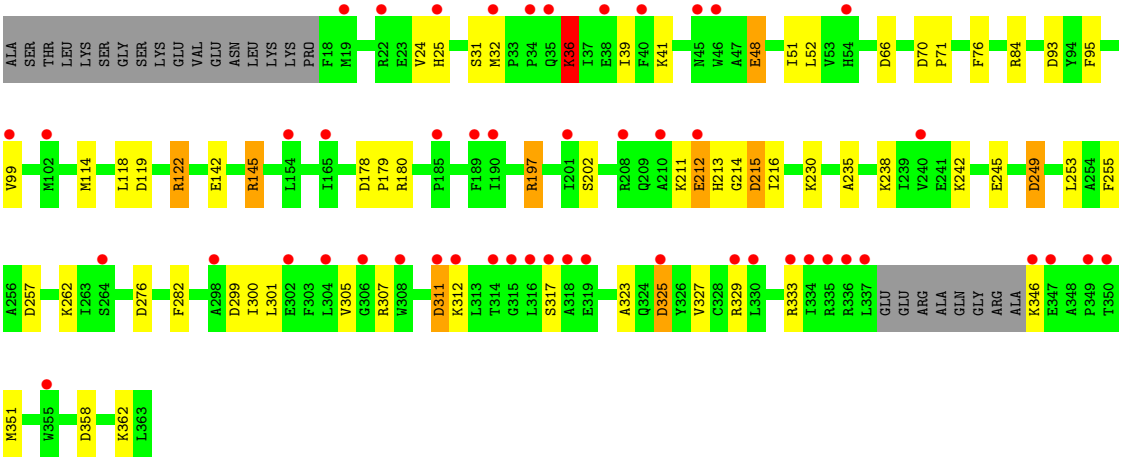
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	73	73	73	0	0

3 Residue-property plots (i)

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: Acyl-[acyl-carrier protein] desaturase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α, β, γ	94.11Å 94.11Å 81.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.40 24.60 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (25.00-2.40) 99.4 (24.60-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.216 , 0.264 0.257 , 0.298	Depositor DCC
R_{free} test set	820 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2822	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ACT, FE

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	0.46	0/2810	0.75	12/3806 (0.3%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	CB-CG-OD2	7.35	124.91	118.30
1	A	358	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	215	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	70	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	178	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	257	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	311	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	276	ASP	CB-CG-OD2	5.30	123.08	118.30
1	A	325	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	119	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	66	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	299	ASP	CB-CG-OD2	5.10	122.89	118.30

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	2743	0	2688	17	0
2	A	2	0	0	0	0
3	A	4	0	3	0	0
4	A	73	0	0	1	0
All	All	2822	0	2691	17	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 (17) 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:25:HIS:CE1	1:A:180:ARG:HD3	2.22	0.75
1:A:145:ARG:HH11	1:A:145:ARG:HG3	1.55	0.71
1:A:249:ASP:O	1:A:253:LEU:HD12	1.96	0.65
1:A:36:LYS:O	1:A:39:ILE:HG22	2.03	0.59
1:A:145:ARG:HG3	1:A:145:ARG:NH1	2.20	0.56
1:A:114:MET:HG3	1:A:179:PRO:HG3	1.89	0.55
1:A:323:ALA:O	1:A:327:VAL:HG23	2.07	0.54
1:A:197:ARG:HG2	1:A:300:ILE:HG12	1.94	0.50
1:A:95:PHE:O	1:A:99:VAL:HG23	2.14	0.47
1:A:118:LEU:O	1:A:122:ARG:HB3	2.15	0.47
1:A:71:PRO:HA	1:A:76:PHE:CD1	2.50	0.46
1:A:212:GLU:C	1:A:214:GLY:H	2.20	0.45
1:A:142:GLU:O	1:A:145:ARG:HG3	2.17	0.44
1:A:51:ILE:HG23	1:A:235:ALA:HB1	1.99	0.44
1:A:212:GLU:C	1:A:214:GLY:N	2.73	0.41
1:A:84:ARG:NH1	4:A:460:HOH:O	2.54	0.40
1:A:48:GLU:HG2	1:A:52:LEU:HD12	2.04	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	334/363 (92%)	318 (95%)	13 (4%)	3 (1%)	17 25

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	213	HIS
1	A	262	LYS

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	295/315 (94%)	262 (89%)	33 (11%)	6 8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	31	SER
1	A	32	MET
1	A	36	LYS
1	A	41	LYS
1	A	48	GLU
1	A	122	ARG
1	A	145	ARG
1	A	197	ARG
1	A	202	SER
1	A	211	LYS
1	A	212	GLU
1	A	215	ASP
1	A	216	ILE
1	A	230	LYS
1	A	238	LYS
1	A	242	LYS
1	A	245	GLU

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Mol	Chain	Res	Type
1	A	249	ASP
1	A	255	PHE
1	A	282	PHE
1	A	301	LEU
1	A	305	VAL
1	A	307	ARG
1	A	311	ASP
1	A	312	LYS
1	A	317	SER
1	A	325	ASP
1	A	329	ARG
1	A	333	ARG
1	A	346	LYS
1	A	351	MET
1	A	362	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
3	ACT	A	366	2	3,3,3	0.85	0	3,3,3	1.86	2 (66%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	366	ACT	OXT-C-O	-2.35	113.38	122.05
3	A	366	ACT	OXT-C-CH3	2.20	124.25	115.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	338/363 (93%)	0.90	50 (14%) 2 2	34, 44, 57, 63	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	337	LEU	6.4
1	A	336	ARG	5.9
1	A	35	GLN	5.7
1	A	315	GLY	5.7
1	A	329	ARG	4.8
1	A	346	LYS	4.5
1	A	314	THR	4.1
1	A	45	ASN	3.8
1	A	54	HIS	3.8
1	A	317	SER	3.6
1	A	347	GLU	3.6
1	A	350	THR	3.6
1	A	318	ALA	3.5
1	A	190	ILE	3.4
1	A	34	PRO	3.4
1	A	334	ILE	3.3
1	A	330	LEU	3.2
1	A	325	ASP	3.2
1	A	306	GLY	3.2
1	A	40	PHE	3.0
1	A	319	GLU	2.9
1	A	335	ARG	2.9
1	A	201	ILE	2.8
1	A	99	VAL	2.8
1	A	264	SER	2.8
1	A	312	LYS	2.6
1	A	349	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	MET	2.6
1	A	311	ASP	2.6
1	A	165	ILE	2.5
1	A	333	ARG	2.5
1	A	240	VAL	2.5
1	A	355	TRP	2.4
1	A	185	PRO	2.4
1	A	189	PHE	2.3
1	A	210	ALA	2.3
1	A	102	MET	2.3
1	A	298	ALA	2.2
1	A	212	GLU	2.2
1	A	304	LEU	2.2
1	A	316	LEU	2.2
1	A	19	MET	2.2
1	A	25	HIS	2.1
1	A	46	TRP	2.1
1	A	308	TRP	2.1
1	A	154	LEU	2.1
1	A	22	ARG	2.1
1	A	208	ARG	2.1
1	A	38	GLU	2.0
1	A	302	GLU	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	A	366	4/4	0.86	0.23	34,34,34,35	0
2	FE	A	364	1/1	0.95	0.05	60,60,60,60	0
2	FE	A	365	1/1	0.98	0.04	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.