



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:51 pm GMT

PDB ID : 3OML
Title : Structure of full-length peroxisomal multifunctional enzyme type 2 from *Drosophila melanogaster*
Authors : Haataja, T.J.K.; Koski, M.K.; Glumoff, T.; Hiltunen, J.K.
Deposited on : 2010-08-27
Resolution : 2.15 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

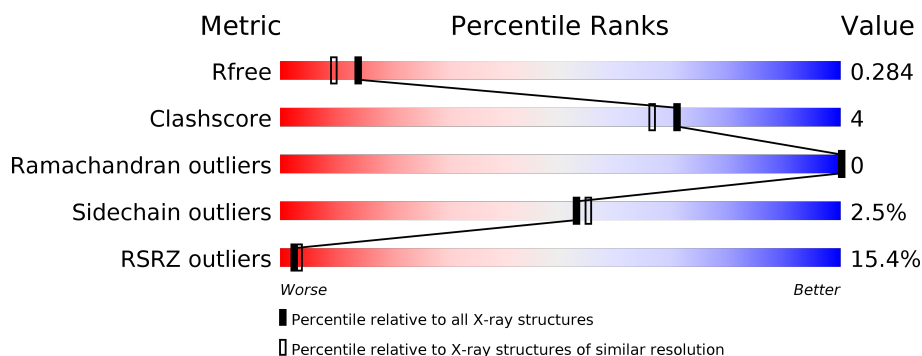
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	613	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4176 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 Peroxisomal Multifunctional Enzyme Type 2, CG3415.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	130	0	0
			4038	2567	687	770	14			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	EXPRESSION TAG	UNP Q9VXJ0
A	-5	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	-4	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	-3	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	-2	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	-1	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	0	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	599	LEU	-	EXPRESSION TAG	UNP Q9VXJ0
A	600	GLU	-	EXPRESSION TAG	UNP Q9VXJ0
A	601	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	602	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	603	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	604	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	605	HIS	-	EXPRESSION TAG	UNP Q9VXJ0
A	606	HIS	-	EXPRESSION TAG	UNP Q9VXJ0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total	O	0	0
			138	138		

- Molecule 1: Peroxisomal Multifunctional Enzyme Type 2, CG3415



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.48Å 114.48Å 89.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.10 – 2.15 28.10 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.10-2.15) 99.7 (28.10-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.234 , 0.285 0.235 , 0.284	Depositor DCC
R_{free} test set	1636 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	42.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4176	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	15/4104 (0.4%)	0.85	21/5563 (0.4%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	VAL	CB-CG2	-15.57	1.20	1.52
1	A	61	VAL	CB-CG2	-12.50	1.26	1.52
1	A	73	VAL	CB-CG2	-11.29	1.29	1.52
1	A	9	ARG	CA-CB	-9.95	1.32	1.53
1	A	87	GLU	CA-CB	9.84	1.75	1.53
1	A	135	GLN	CD-OE1	9.60	1.45	1.24
1	A	65	ILE	CB-CG1	-9.10	1.28	1.54
1	A	87	GLU	C-O	8.95	1.40	1.23
1	A	138	PHE	CB-CG	-7.75	1.38	1.51
1	A	60	ILE	CB-CG1	-7.50	1.33	1.54
1	A	372	LYS	CG-CD	-7.19	1.28	1.52
1	A	60	ILE	CB-CG2	7.08	1.74	1.52
1	A	34	GLU	CA-CB	-6.96	1.38	1.53
1	A	65	ILE	CB-CG2	6.80	1.74	1.52
1	A	128	LYS	CG-CD	5.09	1.69	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	PHE	CB-CG-CD1	-16.01	109.59	120.80
1	A	138	PHE	CB-CG-CD2	15.40	131.58	120.80
1	A	73	VAL	CG1-CB-CG2	14.56	134.20	110.90
1	A	62	VAL	CA-CB-CG2	11.09	127.53	110.90
1	A	67	LYS	CB-CA-C	-10.99	88.43	110.40
1	A	34	GLU	N-CA-CB	10.15	128.87	110.60
1	A	34	GLU	CA-CB-CG	8.33	131.73	113.40
1	A	63	ASP	CB-CA-C	-8.33	93.75	110.40
1	A	113	LYS	CB-CG-CD	8.20	132.93	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LYS	CB-CG-CD	8.01	132.42	111.60
1	A	67	LYS	CA-CB-CG	7.80	130.56	113.40
1	A	372	LYS	CB-CG-CD	7.44	130.95	111.60
1	A	205	GLU	N-CA-CB	-6.88	98.22	110.60
1	A	73	VAL	CA-CB-CG1	-6.66	100.91	110.90
1	A	459	ASP	N-CA-CB	-6.32	99.22	110.60
1	A	84	LYS	CA-CB-CG	6.06	126.73	113.40
1	A	63	ASP	N-CA-CB	6.02	121.43	110.60
1	A	9	ARG	CB-CA-C	5.96	122.31	110.40
1	A	474	GLN	CA-CB-CG	5.45	125.39	113.40
1	A	71	GLU	N-CA-CB	5.34	120.22	110.60
1	A	459	ASP	CB-CG-OD2	5.21	122.99	118.30

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	4038	0	4072	32	2
2	A	138	0	0	3	0
All	All	4176	0	4072	32	2

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 4.

All (32) 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:130:SER:HB3	1:A:151:MET:CE	2.13	0.78
1:A:27:GLU:HG2	1:A:219:LYS:HA	1.71	0.72
1:A:130:SER:HB3	1:A:151:MET:HE3	1.71	0.70
1:A:296:SER:O	2:A:648:HOH:O	2.11	0.68
1:A:314:ILE:HG22	1:A:366:LEU:HD11	1.76	0.67
1:A:282:ASP:O	2:A:646:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASN:HA	1:A:75:ASP:HB3	1.82	0.62
1:A:18:THR:HA	1:A:42:ASN:HB3	1.83	0.61
1:A:392:GLU:HB2	1:A:445:THR:HB	1.84	0.59
1:A:111:LEU:O	1:A:114:THR:HG22	2.04	0.58
1:A:130:SER:HB3	1:A:151:MET:HE1	1.84	0.58
1:A:342:MET:HG2	2:A:721:HOH:O	2.08	0.54
1:A:433:ASP:OD1	1:A:437:ARG:HB3	2.09	0.53
1:A:503:ASP:OD2	1:A:506:MET:HG2	2.08	0.52
1:A:429:SER:HB2	1:A:442:ASN:HB3	1.92	0.52
1:A:346:TYR:CZ	1:A:348:ASN:HB2	2.46	0.49
1:A:289:LEU:HD22	1:A:294:GLU:HB3	1.94	0.48
1:A:422:GLY:HA2	1:A:450:GLY:HA2	1.95	0.48
1:A:107:ARG:HH22	1:A:117:GLN:NE2	2.11	0.48
1:A:41:VAL:HG23	1:A:41:VAL:O	2.16	0.44
1:A:316:ASP:HB2	1:A:366:LEU:HD13	1.99	0.44
1:A:359:PHE:HB3	1:A:440:VAL:HG21	1.98	0.44
1:A:530:VAL:HG22	1:A:563:LEU:HD23	2.00	0.44
1:A:193:ASN:OD1	1:A:238:SER:HB2	2.17	0.43
1:A:592:LYS:HE3	1:A:592:LYS:HB2	1.76	0.43
1:A:562:ASP:HB2	1:A:573:ARG:HG2	2.01	0.42
1:A:395:LEU:HD11	1:A:440:VAL:HG11	2.02	0.41
1:A:158:ILE:HD13	1:A:250:LEU:HD13	2.02	0.41
1:A:62:VAL:O	1:A:66:ARG:HG3	2.19	0.41
1:A:151:MET:HG3	1:A:178:ALA:HB2	2.03	0.41
1:A:151:MET:CE	1:A:177:LEU:HD22	2.51	0.40
1:A:105:ILE:HG13	1:A:125:VAL:HG21	2.04	0.40

All (2) 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)
1:A:143:LYS:NZ	1:A:348:ASN:CA[8_555]	1.62	0.58
1:A:143:LYS:NZ	1:A:348:ASN:CB[8_555]	2.01	0.19

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	520/613 (85%)	501 (96%)	19 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	432/496 (87%)	421 (98%)	11 (2%)	53	55

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	110	SER
1	A	120	ASN
1	A	134	THR
1	A	188	ASN
1	A	235	ASP
1	A	251	HIS
1	A	312	ASP
1	A	444	SER
1	A	449	VAL
1	A	563	LEU

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	77	ASN
1	A	117	GLN
1	A	120	ASN

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	533	GLN

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

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	532/613 (86%)	0.70	82 (15%) 2 3	25, 62, 130, 154	32 (6%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	GLY	5.4
1	A	146	TYR	5.2
1	A	69	GLY	5.2
1	A	8	LEU	5.2
1	A	115	SER	5.0
1	A	68	ALA	4.8
1	A	311	GLY	4.6
1	A	472	ASN	4.5
1	A	194	VAL	4.2
1	A	371	ASP	4.0
1	A	12	GLY	4.0
1	A	449	VAL	4.0
1	A	423	ALA	3.9
1	A	119	TRP	3.8
1	A	175	ILE	3.7
1	A	388	ILE	3.7
1	A	450	GLY	3.7
1	A	520	LEU	3.6
1	A	435	SER	3.6
1	A	11	ASP	3.5
1	A	151	MET	3.5
1	A	523	LEU	3.4
1	A	545	VAL	3.4
1	A	357	THR	3.3
1	A	79	VAL	3.3
1	A	187	ARG	3.3
1	A	395	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	360	VAL	3.3
1	A	64	GLU	3.3
1	A	14	VAL	3.3
1	A	420	GLY	3.3
1	A	150	ILE	3.3
1	A	173	GLY	3.2
1	A	36	GLY	3.2
1	A	312	ASP	3.2
1	A	15	ALA	3.2
1	A	290	GLY	3.1
1	A	174	LEU	3.1
1	A	145	ASN	3.0
1	A	522	THR	3.0
1	A	422	GLY	2.9
1	A	196	VAL	2.9
1	A	474	GLN	2.8
1	A	172	MET	2.8
1	A	527	VAL	2.8
1	A	195	ILE	2.8
1	A	114	THR	2.8
1	A	418	ASP	2.8
1	A	206	GLY	2.7
1	A	143	LYS	2.7
1	A	332	ILE	2.7
1	A	121	LEU	2.6
1	A	188	ASN	2.6
1	A	419	LYS	2.6
1	A	169	ALA	2.5
1	A	475	PRO	2.5
1	A	105	ILE	2.5
1	A	158	ILE	2.5
1	A	225	VAL	2.5
1	A	521	CYS	2.5
1	A	462	ALA	2.5
1	A	149	ILE	2.4
1	A	35	ARG	2.4
1	A	564	TRP	2.4
1	A	141	MET	2.4
1	A	39	VAL	2.4
1	A	152	THR	2.3
1	A	106	LEU	2.3
1	A	317	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	147	GLY	2.3
1	A	389	LEU	2.3
1	A	107	ARG	2.3
1	A	100	VAL	2.2
1	A	41	VAL	2.2
1	A	369	SER	2.1
1	A	308	GLU	2.1
1	A	80	ILE	2.1
1	A	228	LEU	2.1
1	A	198	THR	2.0
1	A	524	GLY	2.0
1	A	176	GLY	2.0
1	A	526	SER	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 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.