



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2021 – 10:52 PM EDT

PDB ID : 1S9C
Title : Crystal structure analysis of the 2-enoyl-CoA hydratase 2 domain of human peroxisomal multifunctional enzyme type 2
Authors : Koski, M.K.; Haapalainen, A.M.; Hiltunen, J.K.; Glumoff, T.
Deposited on : 2004-02-04
Resolution : 3.00 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

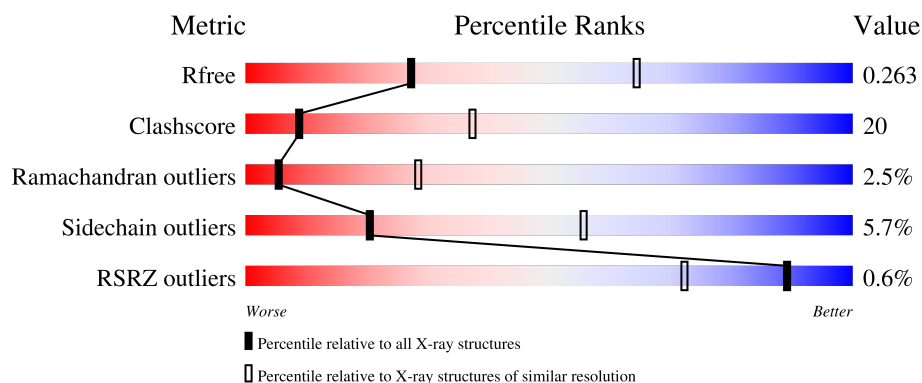
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	298	<div> <div>51%</div> <div>28%</div> <div>••</div> <div>17%</div> </div>
1	B	298	<div> <div>%</div> <div>54%</div> <div>25%</div> <div>•</div> <div>18%</div> </div>
1	C	298	<div> <div>62%</div> <div>25%</div> <div>•</div> <div>9%</div> </div>
1	D	298	<div> <div>59%</div> <div>26%</div> <div>•</div> <div>12%</div> </div>
1	E	298	<div> <div>%</div> <div>56%</div> <div>22%</div> <div>••</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	298	<div><div></div><div>57%31%<div></div>7%</div></div>
1	G	298	<div><div></div><div>60%29%6%5%</div></div>
1	H	298	<div><div>%<div></div></div><div>55%25%<div></div>16%</div></div>
1	I	298	<div><div></div><div>61%27%6%5%</div></div>
1	J	298	<div><div></div><div>52%29%<div></div>14%</div></div>
1	K	298	<div><div>%<div></div></div><div>52%28%5%14%</div></div>
1	L	298	<div><div>%<div></div></div><div>53%29%<div></div>14%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24524 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	9	0	0
			1945	1260	320	356	9			
1	B	245	Total	C	N	O	S	13	0	0
			1923	1246	318	352	7			
1	C	271	Total	C	N	O	S	34	0	0
			2101	1359	349	385	8			
1	D	261	Total	C	N	O	S	34	0	0
			2046	1325	339	373	9			
1	E	243	Total	C	N	O	S	37	0	0
			1909	1236	315	351	7			
1	F	276	Total	C	N	O	S	23	0	0
			2122	1368	355	390	9			
1	G	284	Total	C	N	O	S	32	0	0
			2179	1406	363	401	9			
1	H	250	Total	C	N	O	S	22	0	0
			1954	1262	326	359	7			
1	I	283	Total	C	N	O	S	45	0	0
			2175	1404	362	400	9			
1	J	255	Total	C	N	O	S	26	0	0
			2003	1295	332	367	9			
1	K	256	Total	C	N	O	S	42	0	0
			1995	1288	333	367	7			
1	L	256	Total	C	N	O	S	25	0	0
			1992	1284	333	366	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	SER	engineered mutation	UNP P51659
A	2	ALA	THR	engineered mutation	UNP P51659
A	242	VAL	ILE	engineered mutation	UNP P51659
A	298	LEU	THR	engineered mutation	UNP P51659
B	1	MET	SER	engineered mutation	UNP P51659

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	ALA	THR	engineered mutation	UNP P51659
B	242	VAL	ILE	engineered mutation	UNP P51659
B	298	LEU	THR	engineered mutation	UNP P51659
C	1	MET	SER	engineered mutation	UNP P51659
C	2	ALA	THR	engineered mutation	UNP P51659
C	242	VAL	ILE	engineered mutation	UNP P51659
C	298	LEU	THR	engineered mutation	UNP P51659
D	1	MET	SER	engineered mutation	UNP P51659
D	2	ALA	THR	engineered mutation	UNP P51659
D	242	VAL	ILE	engineered mutation	UNP P51659
D	298	LEU	THR	engineered mutation	UNP P51659
E	1	MET	SER	engineered mutation	UNP P51659
E	2	ALA	THR	engineered mutation	UNP P51659
E	242	VAL	ILE	engineered mutation	UNP P51659
E	298	LEU	THR	engineered mutation	UNP P51659
F	1	MET	SER	engineered mutation	UNP P51659
F	2	ALA	THR	engineered mutation	UNP P51659
F	242	VAL	ILE	engineered mutation	UNP P51659
F	298	LEU	THR	engineered mutation	UNP P51659
G	1	MET	SER	engineered mutation	UNP P51659
G	2	ALA	THR	engineered mutation	UNP P51659
G	242	VAL	ILE	engineered mutation	UNP P51659
G	298	LEU	THR	engineered mutation	UNP P51659
H	1	MET	SER	engineered mutation	UNP P51659
H	2	ALA	THR	engineered mutation	UNP P51659
H	242	VAL	ILE	engineered mutation	UNP P51659
H	298	LEU	THR	engineered mutation	UNP P51659
I	1	MET	SER	engineered mutation	UNP P51659
I	2	ALA	THR	engineered mutation	UNP P51659
I	242	VAL	ILE	engineered mutation	UNP P51659
I	298	LEU	THR	engineered mutation	UNP P51659
J	1	MET	SER	engineered mutation	UNP P51659
J	2	ALA	THR	engineered mutation	UNP P51659
J	242	VAL	ILE	engineered mutation	UNP P51659
J	298	LEU	THR	engineered mutation	UNP P51659
K	1	MET	SER	engineered mutation	UNP P51659
K	2	ALA	THR	engineered mutation	UNP P51659
K	242	VAL	ILE	engineered mutation	UNP P51659
K	298	LEU	THR	engineered mutation	UNP P51659
L	1	MET	SER	engineered mutation	UNP P51659
L	2	ALA	THR	engineered mutation	UNP P51659
L	242	VAL	ILE	engineered mutation	UNP P51659

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Chain	Residue	Modelled	Actual	Comment	Reference
L	298	LEU	THR	engineered mutation	UNP P51659

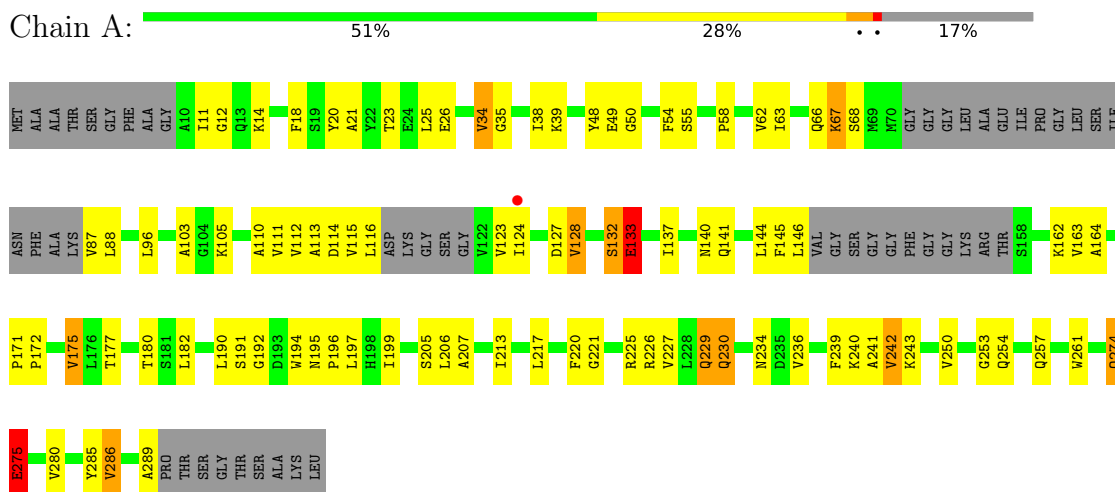
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	16	Total O 16 16	0	0
2	B	7	Total O 7 7	0	0
2	C	21	Total O 21 21	0	0
2	D	12	Total O 12 12	0	0
2	E	16	Total O 16 16	0	0
2	F	29	Total O 29 29	0	0
2	G	11	Total O 11 11	0	0
2	H	15	Total O 15 15	0	0
2	I	26	Total O 26 26	0	0
2	J	12	Total O 12 12	0	0
2	K	9	Total O 9 9	0	0
2	L	6	Total O 6 6	0	0

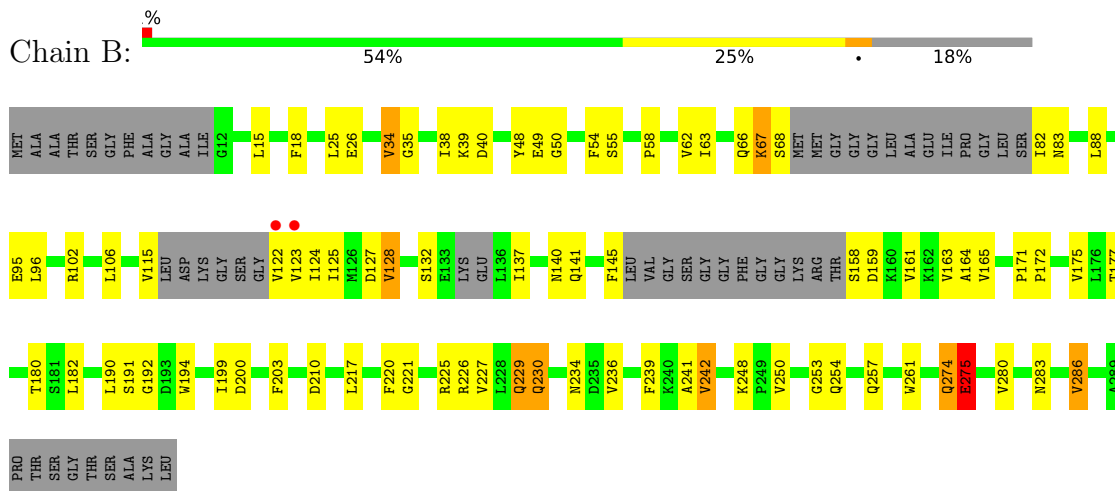
3 Residue-property plots

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: Peroxisomal multifunctional enzyme type 2

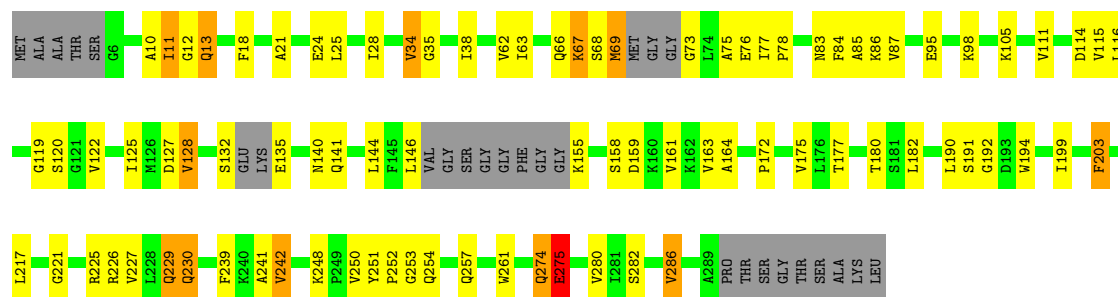


• Molecule 1: Peroxisomal multifunctional enzyme type 2



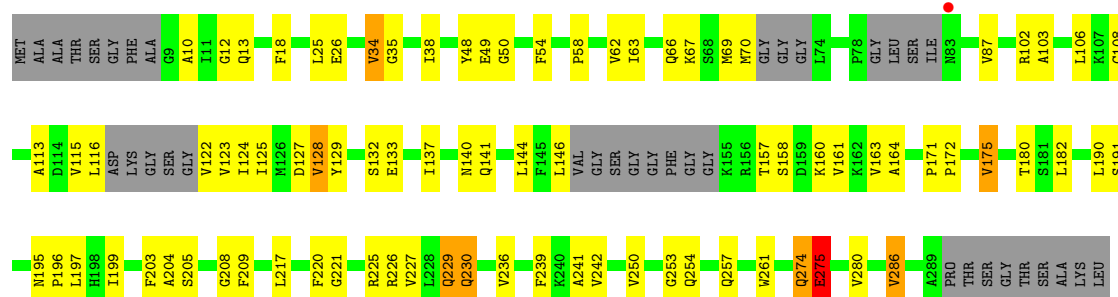
• Molecule 1: Peroxisomal multifunctional enzyme type 2





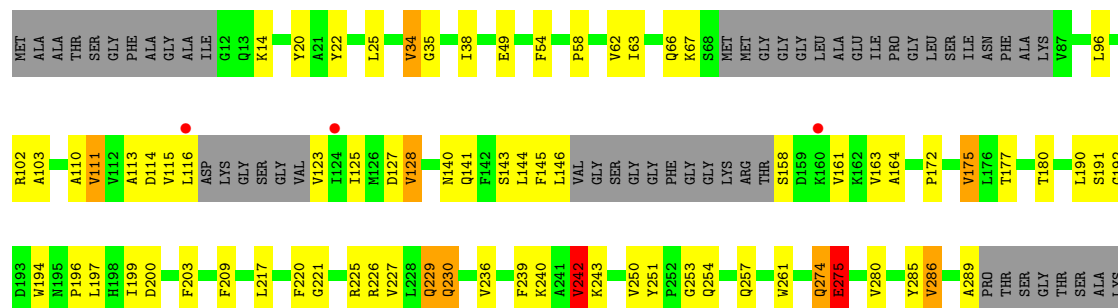
- Molecule 1: Peroxisomal multifunctional enzyme type 2

Chain D: 59% 26% 12%



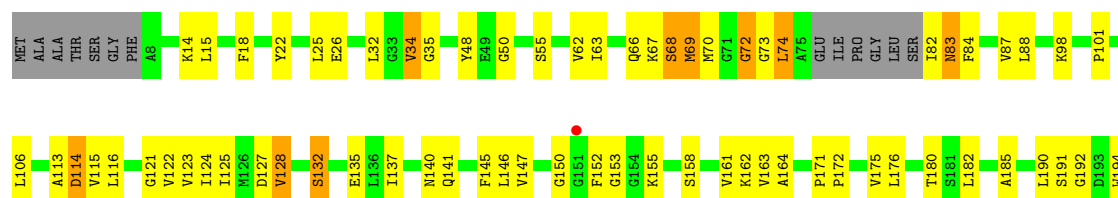
- Molecule 1: Peroxisomal multifunctional enzyme type 2

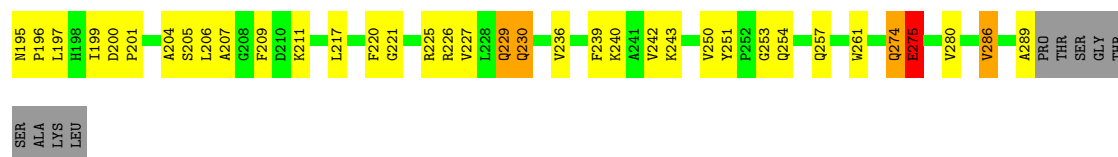
Chain E: % 56% 22% 18%



- Molecule 1: Peroxisomal multifunctional enzyme type 2

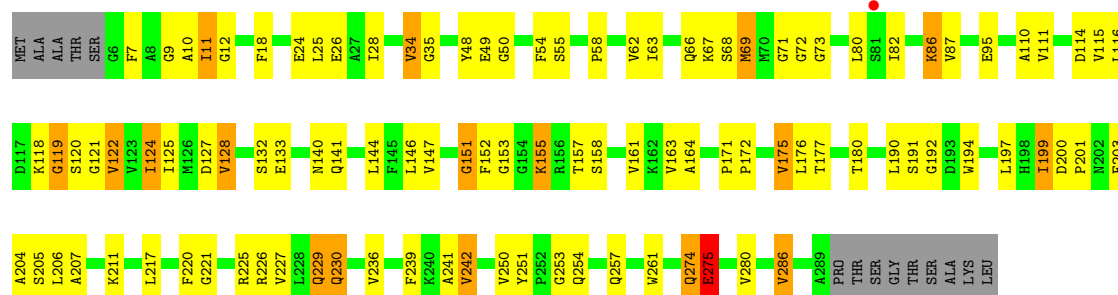
Chain F: 57% 31% 7%





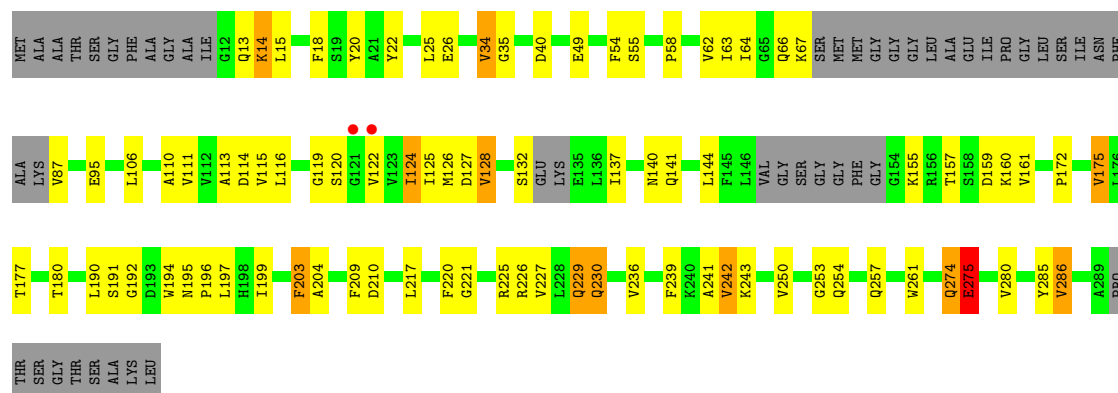
- Molecule 1: Peroxisomal multifunctional enzyme type 2

Chain G: 60% 29% 6% 5%



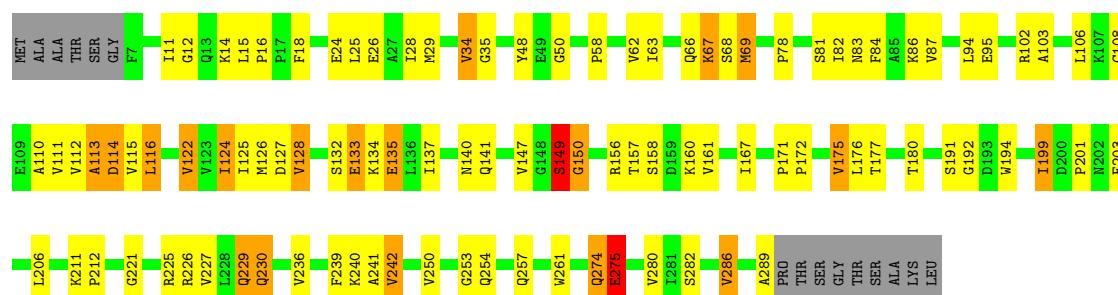
- Molecule 1: Peroxisomal multifunctional enzyme type 2

Chain H: 55% 25% 16%

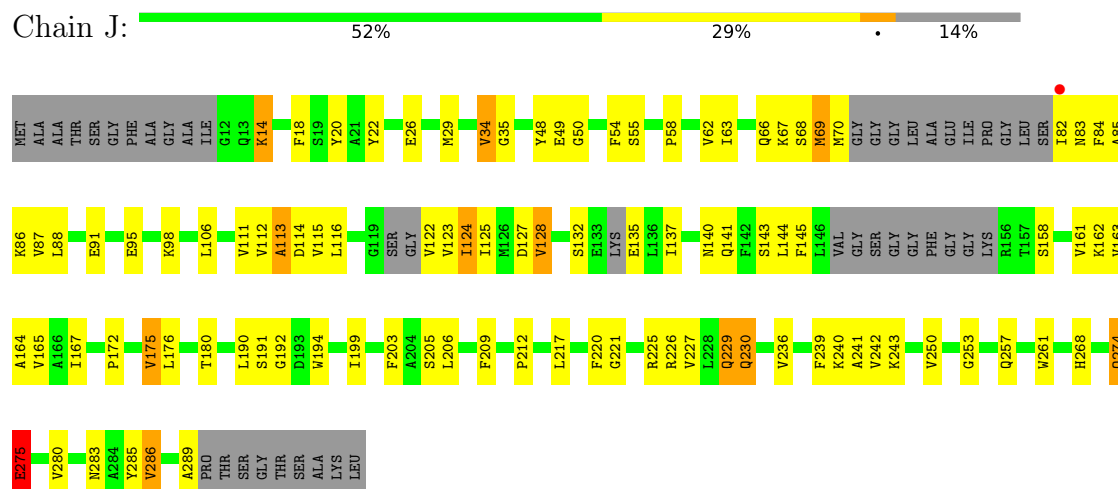


- Molecule 1: Peroxisomal multifunctional enzyme type 2

Chain I: 61% 27% 6% 5%



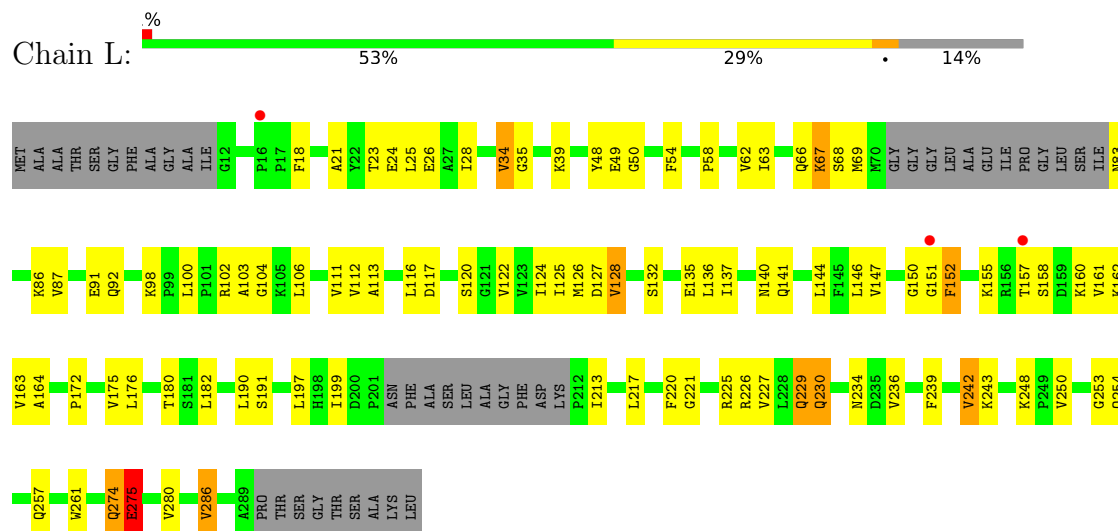
- Molecule 1: Peroxisomal multifunctional enzyme type 2



- Molecule 1: Peroxisomal multifunctional enzyme type 2



- Molecule 1: Peroxisomal multifunctional enzyme type 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.30Å 105.43Å 206.94Å 90.00° 103.37° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-3.00) 93.7 (29.96-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 3.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.265 0.228 , 0.263	Depositor DCC
R_{free} test set	3870 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24524	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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	0.50	0/1989	0.66	1/2694 (0.0%)
1	B	0.43	0/1967	0.63	0/2664
1	C	0.50	0/2148	0.66	0/2907
1	D	0.49	0/2091	0.66	0/2829
1	E	0.50	1/1953 (0.1%)	0.65	0/2646
1	F	0.53	0/2170	0.75	2/2935 (0.1%)
1	G	0.46	0/2230	0.71	2/3018 (0.1%)
1	H	0.47	0/1998	0.65	0/2705
1	I	0.50	0/2226	0.71	0/3013
1	J	0.48	0/2047	0.66	0/2769
1	K	0.43	0/2039	0.64	0/2760
1	L	0.43	0/2037	0.63	0/2754
All	All	0.48	1/24895 (0.0%)	0.67	5/33694 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	VAL	CB-CG1	-5.18	1.42	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	74	LEU	N-CA-C	-8.64	87.66	111.00
1	G	151	GLY	N-CA-C	6.78	130.04	113.10
1	F	72	GLY	N-CA-C	-6.73	96.27	113.10
1	A	133	GLU	N-CA-C	-5.12	97.16	111.00
1	G	133	GLU	N-CA-C	-5.00	97.49	111.00

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	1945	0	1951	95	0
1	B	1923	0	1919	74	0
1	C	2101	0	2110	78	0
1	D	2046	0	2059	83	0
1	E	1909	0	1908	70	0
1	F	2122	0	2129	86	0
1	G	2179	0	2185	90	0
1	H	1954	0	1957	73	1
1	I	2175	0	2182	84	0
1	J	2003	0	2005	94	0
1	K	1995	0	2005	96	0
1	L	1992	0	1999	86	1
2	A	16	0	0	3	0
2	B	7	0	0	1	0
2	C	21	0	0	2	0
2	D	12	0	0	1	0
2	E	16	0	0	0	0
2	F	29	0	0	2	0
2	G	11	0	0	1	0
2	H	15	0	0	0	0
2	I	26	0	0	3	0
2	J	12	0	0	1	0
2	K	9	0	0	0	0
2	L	6	0	0	1	0
All	All	24524	0	24409	976	1

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 20.

The worst 5 of 976 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:I:86:LYS:HB3	1:I:147:VAL:HG22	1.41	0.99
1:K:196:PRO:HB2	1:K:203:PHE:HD2	1.28	0.98
1:L:69:MET:HE2	1:L:144:LEU:HD11	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:VAL:HG11	1:H:286:VAL:HG11	1.46	0.96
1:D:227:VAL:HG11	1:D:286:VAL:HG11	1.47	0.96

All (1) 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:H:159:ASP:OD2	1:L:136:LEU:O[2_745]	2.16	0.04

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	240/298 (80%)	216 (90%)	19 (8%)	5 (2%)	7	33
1	B	235/298 (79%)	209 (89%)	22 (9%)	4 (2%)	9	39
1	C	263/298 (88%)	229 (87%)	27 (10%)	7 (3%)	5	26
1	D	251/298 (84%)	227 (90%)	21 (8%)	3 (1%)	13	48
1	E	235/298 (79%)	211 (90%)	21 (9%)	3 (1%)	12	45
1	F	272/298 (91%)	238 (88%)	25 (9%)	9 (3%)	4	21
1	G	282/298 (95%)	246 (87%)	28 (10%)	8 (3%)	5	25
1	H	242/298 (81%)	212 (88%)	23 (10%)	7 (3%)	4	24
1	I	281/298 (94%)	238 (85%)	32 (11%)	11 (4%)	3	17
1	J	245/298 (82%)	220 (90%)	19 (8%)	6 (2%)	6	29
1	K	248/298 (83%)	211 (85%)	29 (12%)	8 (3%)	4	22
1	L	250/298 (84%)	215 (86%)	29 (12%)	6 (2%)	6	29
All	All	3044/3576 (85%)	2672 (88%)	295 (10%)	77 (2%)	5	28

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	GLU
1	B	275	GLU
1	C	275	GLU
1	D	275	GLU
1	E	275	GLU

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	211/241 (88%)	200 (95%)	11 (5%)	23	59
1	B	208/241 (86%)	197 (95%)	11 (5%)	22	58
1	C	225/241 (93%)	210 (93%)	15 (7%)	16	49
1	D	221/241 (92%)	213 (96%)	8 (4%)	35	70
1	E	207/241 (86%)	198 (96%)	9 (4%)	29	66
1	F	225/241 (93%)	211 (94%)	14 (6%)	18	52
1	G	231/241 (96%)	217 (94%)	14 (6%)	18	53
1	H	211/241 (88%)	199 (94%)	12 (6%)	20	56
1	I	231/241 (96%)	214 (93%)	17 (7%)	13	44
1	J	217/241 (90%)	206 (95%)	11 (5%)	24	60
1	K	216/241 (90%)	200 (93%)	16 (7%)	13	44
1	L	215/241 (89%)	204 (95%)	11 (5%)	24	60
All	All	2618/2892 (90%)	2469 (94%)	149 (6%)	20	56

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	203	PHE
1	L	229	GLN
1	J	274	GLN
1	K	202	ASN
1	E	229	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	234	ASN
1	L	230	GLN
1	H	257	GLN
1	L	83	ASN
1	K	202	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 monosaccharides 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(Å ²)	Q<0.9
1	A	248/298 (83%)	-0.50	1 (0%) 92 79	21, 41, 70, 80	2 (0%)
1	B	245/298 (82%)	-0.24	2 (0%) 86 65	31, 60, 80, 94	3 (1%)
1	C	271/298 (90%)	-0.61	0 100 100	17, 32, 76, 104	7 (2%)
1	D	261/298 (87%)	-0.56	1 (0%) 92 79	19, 39, 70, 104	8 (3%)
1	E	243/298 (81%)	-0.46	3 (1%) 79 54	21, 39, 75, 86	8 (3%)
1	F	276/298 (92%)	-0.58	1 (0%) 92 79	14, 31, 78, 92	4 (1%)
1	G	284/298 (95%)	-0.42	1 (0%) 92 79	25, 46, 88, 110	8 (2%)
1	H	250/298 (83%)	-0.35	2 (0%) 86 65	28, 48, 80, 87	5 (2%)
1	I	283/298 (94%)	-0.48	0 100 100	22, 40, 86, 97	10 (3%)
1	J	255/298 (85%)	-0.54	1 (0%) 92 79	26, 44, 68, 78	6 (2%)
1	K	256/298 (85%)	-0.21	4 (1%) 72 44	36, 55, 88, 95	10 (3%)
1	L	256/298 (85%)	-0.19	3 (1%) 79 54	40, 66, 87, 104	5 (1%)
All	All	3128/3576 (87%)	-0.43	19 (0%) 89 72	14, 45, 82, 110	76 (2%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	VAL	3.9
1	K	117	ASP	3.7
1	E	124	ILE	3.0
1	L	151	GLY	2.9
1	K	122	VAL	2.7

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.