



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 29, 2025 – 08:22 AM EDT

PDB ID : 4FZW / pdb_00004fzw
Title : Crystal Structure of the PaaF-PaaG Hydratase-Isomerase Complex from E.coli
Authors : Grishin, A.M.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2012-07-08
Resolution : 2.55 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 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

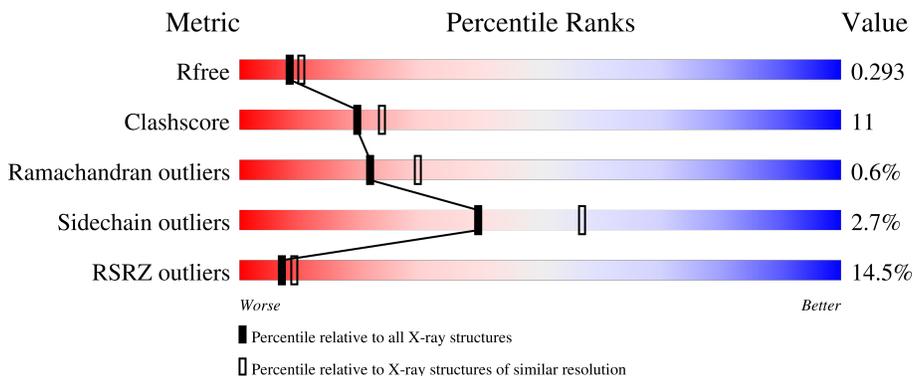
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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	258	 17% 72% 24% 9%
1	B	258	 13% 76% 22% 9%
2	C	274	 14% 71% 18% 9%
2	D	274	 11% 73% 16% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7617 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 2,3-dehydroadipyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	Total	C	N	O	S	0	0	0
			1885	1180	339	358	8			
1	B	256	Total	C	N	O	S	0	0	0
			1878	1177	336	356	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P76082
A	-1	ARG	-	expression tag	UNP P76082
A	0	SER	-	expression tag	UNP P76082
B	-2	MET	-	expression tag	UNP P76082
B	-1	ARG	-	expression tag	UNP P76082
B	0	SER	-	expression tag	UNP P76082

- Molecule 2 is a protein called 1,2-epoxyphenylacetyl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	249	Total	C	N	O	S	0	0	0
			1846	1159	329	347	11			
2	D	250	Total	C	N	O	S	0	1	0
			1869	1174	333	351	11			

There are 24 discrepancies between the modelled and reference sequences:

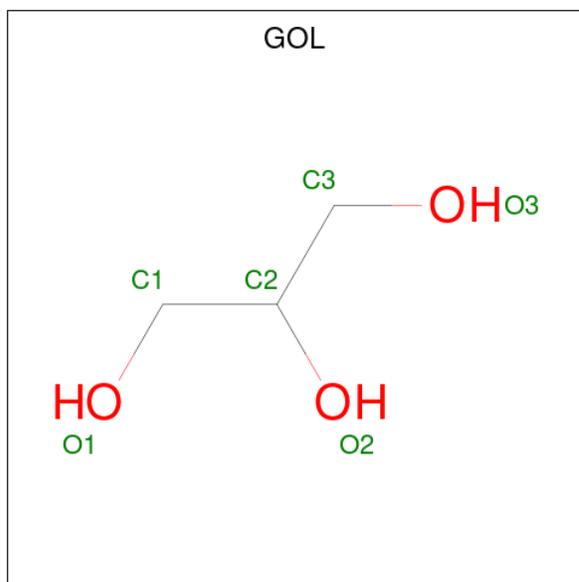
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP P77467
C	-10	GLY	-	expression tag	UNP P77467
C	-9	SER	-	expression tag	UNP P77467
C	-8	SER	-	expression tag	UNP P77467
C	-7	HIS	-	expression tag	UNP P77467
C	-6	HIS	-	expression tag	UNP P77467

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P77467
C	-4	HIS	-	expression tag	UNP P77467
C	-3	HIS	-	expression tag	UNP P77467
C	-2	HIS	-	expression tag	UNP P77467
C	-1	GLY	-	expression tag	UNP P77467
C	0	SER	-	expression tag	UNP P77467
D	-11	MET	-	initiating methionine	UNP P77467
D	-10	GLY	-	expression tag	UNP P77467
D	-9	SER	-	expression tag	UNP P77467
D	-8	SER	-	expression tag	UNP P77467
D	-7	HIS	-	expression tag	UNP P77467
D	-6	HIS	-	expression tag	UNP P77467
D	-5	HIS	-	expression tag	UNP P77467
D	-4	HIS	-	expression tag	UNP P77467
D	-3	HIS	-	expression tag	UNP P77467
D	-2	HIS	-	expression tag	UNP P77467
D	-1	GLY	-	expression tag	UNP P77467
D	0	SER	-	expression tag	UNP P77467

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

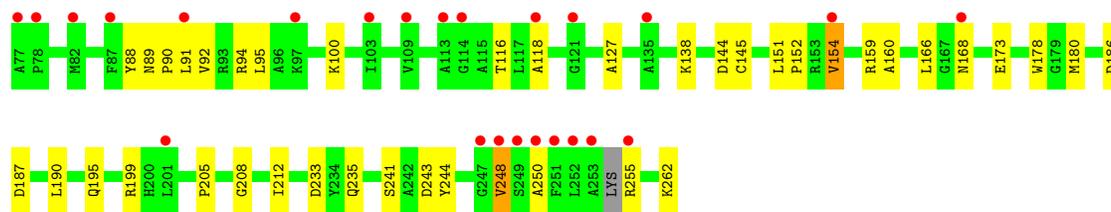
Continued on next page...

Continued from previous page...

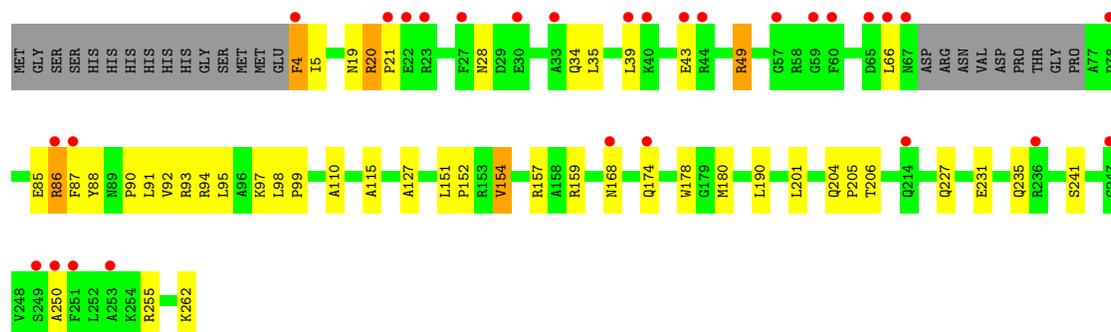
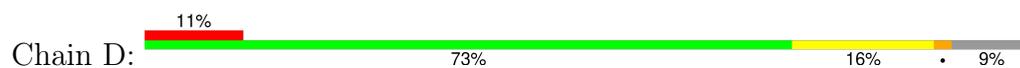
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	6	3	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total 29	O 29	0	0
4	B	36	Total 36	O 36	0	0
4	C	25	Total 25	O 25	0	0
4	D	31	Total 31	O 31	0	0



● Molecule 2: 1,2-epoxyphenylacetyl-CoA isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 131.98Å 153.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.79 – 2.55 46.79 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.79-2.55) 99.7 (46.79-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.54Å)	Xtrriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.280 , 0.321 0.285 , 0.293	Depositor DCC
R_{free} test set	2579 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtrriage
Anisotropy	0.719	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7617	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0751e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	0.59	0/1906	0.90	3/2583 (0.1%)
1	B	0.60	0/1899	0.90	3/2574 (0.1%)
2	C	0.59	0/1873	0.95	6/2536 (0.2%)
2	D	0.58	0/1901	0.91	3/2576 (0.1%)
All	All	0.59	0/7579	0.92	15/10269 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	20	ARG	CA-C-N	7.30	128.97	119.84
2	C	20	ARG	C-N-CA	7.30	128.97	119.84
2	D	20	ARG	CA-C-N	6.49	127.96	119.84
2	D	20	ARG	C-N-CA	6.49	127.96	119.84
1	A	102	TYR	N-CA-C	6.39	118.99	109.59

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	1885	0	1925	55	0
1	B	1878	0	1911	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1846	0	1821	40	0
2	D	1869	0	1853	38	0
3	A	6	0	8	0	0
3	B	12	0	15	1	0
4	A	29	0	0	1	0
4	B	36	0	0	0	0
4	C	25	0	0	2	0
4	D	31	0	0	0	0
All	All	7617	0	7533	171	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 11.

The worst 5 of 171 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:77:LEU:HD21	1:B:230:LEU:HD11	1.39	1.04
2:D:154:VAL:HG13	2:D:180:MET:HA	1.43	0.99
2:C:4:PHE:HD1	2:C:34:GLN:HE22	1.15	0.92
2:D:4:PHE:HD1	2:D:34:GLN:HE22	1.17	0.89
2:C:39:LEU:HB2	2:C:94:ARG:HH11	1.41	0.86

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	252/258 (98%)	236 (94%)	13 (5%)	3 (1%)	11	14
1	B	254/258 (98%)	243 (96%)	9 (4%)	2 (1%)	16	23
2	C	243/274 (89%)	224 (92%)	19 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	247/274 (90%)	235 (95%)	11 (4%)	1 (0%)	30	40
All	All	996/1064 (94%)	938 (94%)	52 (5%)	6 (1%)	22	29

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	70	GLU
1	B	195	ALA
1	A	134	ILE
2	D	205	PRO

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	192/200 (96%)	185 (96%)	7 (4%)	30	44
1	B	189/200 (94%)	183 (97%)	6 (3%)	34	49
2	C	184/216 (85%)	182 (99%)	2 (1%)	70	82
2	D	188/216 (87%)	183 (97%)	5 (3%)	40	57
All	All	753/832 (90%)	733 (97%)	20 (3%)	40	57

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	154	VAL
2	D	49	ARG
2	D	154	VAL
2	D	86	ARG
1	A	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	142	GLN
1	B	211	GLN
2	D	174	GLN
1	B	246	GLN
2	C	195	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	GOL	B	302	-	5,5,5	0.60	0	5,5,5	1.71	2 (40%)
3	GOL	A	301	-	5,5,5	0.46	0	5,5,5	1.15	0
3	GOL	B	301	-	5,5,5	0.40	0	5,5,5	2.05	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	302	-	-	2/4/4/4	-
3	GOL	A	301	-	-	4/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GOL	C3-C2-C1	3.35	124.07	111.80
3	B	302	GOL	C3-C2-C1	2.48	120.89	111.80
3	B	301	GOL	O2-C2-C1	2.47	119.41	109.18
3	B	302	GOL	O2-C2-C3	2.18	118.19	109.18

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	301	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
3	A	301	GOL	C1-C2-C3-O3
3	A	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GOL	1	0

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	254/258 (98%)	0.94	45 (17%) 4 6	31, 42, 86, 95	0
1	B	256/258 (99%)	0.79	34 (13%) 8 11	33, 41, 82, 94	0
2	C	249/274 (90%)	0.95	38 (15%) 6 8	33, 45, 76, 113	0
2	D	250/274 (91%)	0.93	29 (11%) 11 13	34, 48, 76, 115	1 (0%)
All	All	1009/1064 (94%)	0.90	146 (14%) 7 9	31, 44, 80, 115	1 (0%)

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASN	8.2
1	A	233	ALA	6.4
2	C	33	ALA	6.0
1	A	242	SER	5.8
1	A	241	ILE	5.5

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	B	301	6/6	0.63	0.23	61,77,84,89	0
3	GOL	A	301	6/6	0.65	0.26	49,63,67,70	0
3	GOL	B	302	6/6	0.76	0.19	44,54,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.