



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 3FCX / pdb_00003fcx
Title : Crystal structure of human esterase D
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Deposited on : 2008-11-24
Resolution : 1.50 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 ⓘ 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
Xtriage (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

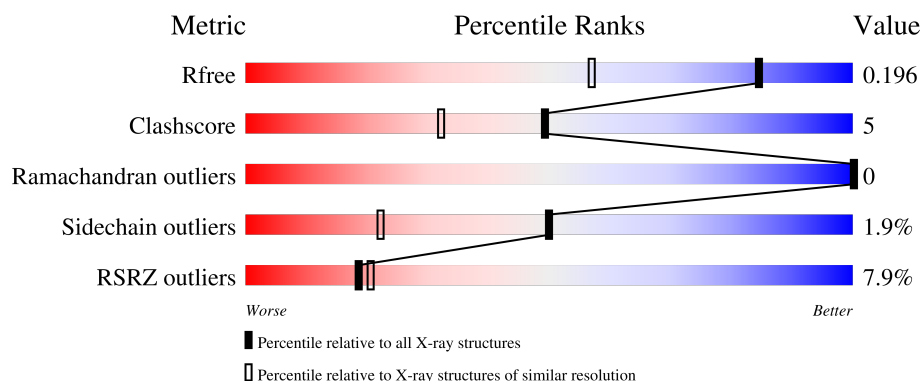
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	282	10% 83% 11% • 5%
1	B	282	6% 93% • • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4900 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 S-formylglutathione hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	1	0
			2119	1369	352	384	14			
1	B	275	Total	C	N	O	S	0	0	0
			2174	1399	359	403	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	ASP	GLY	engineered mutation	UNP P10768
B	257	ASP	GLY	engineered mutation	UNP P10768

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	2	Total	Ca	0	0
			2	2		

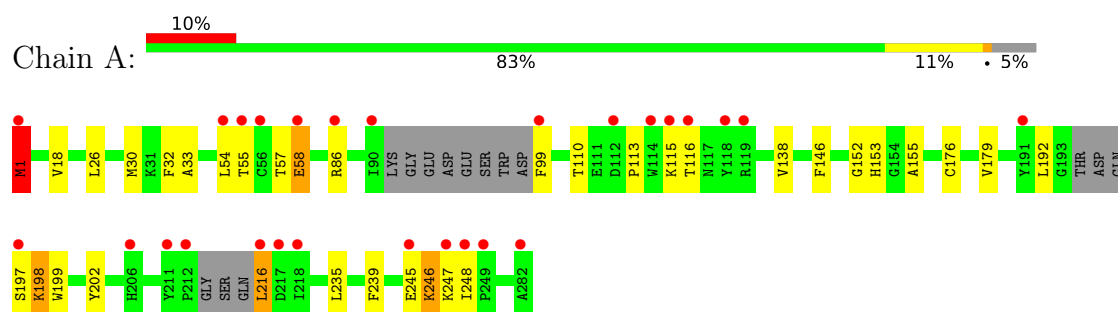
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	329	Total	O	0	0
			329	329		

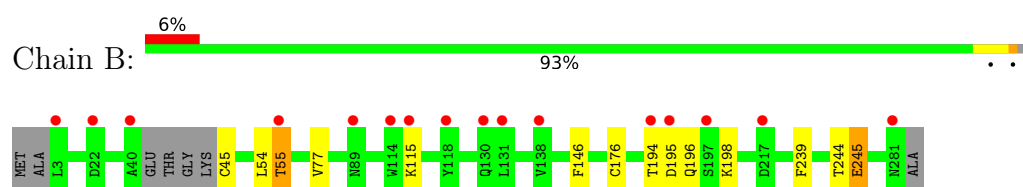
3 Residue-property plots [i](#)

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: S-formylglutathione hydrolase



- Molecule 1: S-formylglutathione hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.54Å 70.72Å 65.01Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	40.16 – 1.50 40.16 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.16-1.50) 98.2 (40.16-1.50)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	0.33	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.176 , 0.196 0.179 , 0.196	Depositor DCC
R_{free} test set	3500 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4900	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.54% 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

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

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	0.61	3/2182 (0.1%)	0.83	7/2954 (0.2%)
1	B	0.56	4/2238 (0.2%)	0.72	2/3035 (0.1%)
All	All	0.59	7/4420 (0.2%)	0.77	9/5989 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	58	GLU	C-N	-10.49	1.20	1.33
1	B	194	THR	C-O	-8.84	1.12	1.24
1	A	57	THR	C-N	-8.03	1.22	1.34
1	A	138	VAL	C-O	-6.66	1.17	1.24
1	B	245	GLU	C-N	-6.08	1.24	1.33
1	B	196	GLN	C-O	-5.87	1.16	1.24
1	B	196	GLN	CG-CD	-5.06	1.39	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	GLU	CA-C-N	9.59	133.13	120.28
1	A	58	GLU	C-N-CA	9.59	133.13	120.28
1	A	58	GLU	O-C-N	-7.68	112.82	122.27
1	A	57	THR	O-C-N	7.51	130.47	122.20
1	A	57	THR	CA-C-N	-7.42	109.03	120.31
1	A	57	THR	C-N-CA	-7.42	109.03	120.31
1	A	1	MET	CA-CB-CG	6.08	126.26	114.10
1	B	196	GLN	N-CA-C	5.88	119.92	112.87
1	B	244	THR	O-C-N	5.66	128.12	122.12

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	2119	0	2071	41	1
1	B	2174	0	2096	6	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	274	0	0	15	1
4	B	329	0	0	2	0
All	All	4900	0	4167	46	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 5.

All (46) 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:1:MET:HE2	4:A:414:HOH:O	1.58	1.02
1:A:216:LEU:HD23	1:A:216:LEU:N	1.78	0.99
1:A:198:LYS:NZ	4:A:540:HOH:O	1.93	0.99
1:A:198:LYS:NZ	1:A:198:LYS:HB2	1.80	0.97
1:A:198:LYS:HB2	1:A:198:LYS:HZ3	1.27	0.97
1:A:197:SER:OG	4:A:527:HOH:O	1.80	0.94
1:A:216:LEU:HD11	4:B:519:HOH:O	1.73	0.87
1:A:18:VAL:CG1	1:A:58:GLU:OE2	2.23	0.85
1:A:18:VAL:HG13	1:A:58:GLU:OE2	1.79	0.81
1:A:86:ARG:NH2	4:A:383:HOH:O	2.12	0.81
1:A:26:LEU:HD12	1:A:30:MET:HG3	1.67	0.76
1:A:54:LEU:HG	4:A:302:HOH:O	1.86	0.74
1:A:235:LEU:HD21	4:A:565:HOH:O	1.88	0.73
1:A:246:LYS:O	1:A:246:LYS:HG3	1.91	0.71
1:A:18:VAL:HG11	1:A:58:GLU:OE2	1.92	0.69
1:B:54:LEU:O	1:B:55:THR:HG22	1.92	0.69
1:A:54:LEU:O	1:A:55:THR:OG1	2.11	0.68
1:A:245:GLU:OE2	4:A:426:HOH:O	2.14	0.66
1:A:192:LEU:O	1:A:198:LYS:HE2	1.96	0.65
1:A:245:GLU:HG3	4:A:372:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PHE:C	1:A:58:GLU:OE1	2.44	0.59
1:B:245:GLU:HG2	4:B:468:HOH:O	2.04	0.58
1:A:246:LYS:HG2	1:A:248:ILE:HG12	1.85	0.58
1:A:86:ARG:CD	4:A:597:HOH:O	2.52	0.57
1:A:86:ARG:HD3	4:A:597:HOH:O	2.07	0.54
1:A:152:GLY:HA2	4:A:463:HOH:O	2.07	0.54
1:A:18:VAL:HG13	1:A:58:GLU:CD	2.33	0.52
1:A:58:GLU:HG2	4:A:314:HOH:O	2.11	0.51
1:A:155:ALA:HB3	4:A:463:HOH:O	2.12	0.50
1:A:99:PHE:N	4:A:525:HOH:O	2.45	0.49
1:B:176:CYS:HB3	1:B:239:PHE:HB2	1.94	0.49
1:A:33:ALA:N	1:A:58:GLU:OE1	2.46	0.48
1:B:195:ASP:HB3	1:B:198:LYS:HD2	1.95	0.48
1:A:198:LYS:HB2	1:A:198:LYS:HZ2	1.72	0.48
1:A:1:MET:HE3	1:A:1:MET:HB2	1.56	0.47
1:A:216:LEU:HB3	4:A:400:HOH:O	2.14	0.47
1:A:246:LYS:HG2	1:A:248:ILE:CG1	2.45	0.46
1:A:153:HIS:HE1	1:A:202:TYR:O	1.99	0.45
1:A:176:CYS:HB3	1:A:239:PHE:HB2	1.98	0.44
1:A:198:LYS:NZ	1:A:198:LYS:CB	2.55	0.43
1:A:179:VAL:HG12	1:A:199:TRP:HB3	2.00	0.43
1:A:192:LEU:O	1:A:198:LYS:CE	2.65	0.43
1:A:216:LEU:N	1:A:216:LEU:CD2	2.56	0.42
1:A:110:THR:HG22	1:B:115:LYS:HE3	2.02	0.42
1:B:45:CYS:HB2	1:B:77:VAL:HG23	2.01	0.42
1:A:113:PRO:O	1:A:116:THR:HG22	2.21	0.41

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:A:99:PHE:CD1	4:A:462:HOH:O[2_546]	2.13	0.07

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	261/282 (93%)	253 (97%)	8 (3%)	0	100	100
1	B	271/282 (96%)	262 (97%)	9 (3%)	0	100	100
All	All	532/564 (94%)	515 (97%)	17 (3%)	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	228/239 (95%)	221 (97%)	7 (3%)	35	9
1	B	235/239 (98%)	233 (99%)	2 (1%)	70	49
All	All	463/478 (97%)	454 (98%)	9 (2%)	50	22

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	115	LYS
1	A	146	PHE
1	A	198	LYS
1	A	216	LEU
1	A	246	LYS
1	A	247	LYS
1	B	55	THR
1	B	146	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN

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Mol	Chain	Res	Type
1	A	27	ASN
1	A	117	ASN
1	A	153	HIS
1	B	5	GLN
1	B	16	GLN
1	B	130	GLN
1	B	275	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	58:GLU	C	59:GLN	N	1.20

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	268/282 (95%)	0.53	27 (10%) 12 13	9, 14, 29, 37	1 (0%)
1	B	275/282 (97%)	0.28	16 (5%) 29 31	8, 13, 24, 35	0
All	All	543/564 (96%)	0.40	43 (7%) 18 20	8, 14, 27, 37	1 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	58	GLU	5.6
1	A	114	TRP	5.5
1	A	55	THR	4.9
1	A	212	PRO	4.8
1	B	114	TRP	4.4
1	A	197	SER	4.2
1	A	282	ALA	4.0
1	A	116	THR	3.8
1	A	249	PRO	3.7
1	A	118	TYR	3.7
1	A	99	PHE	3.6
1	A	216	LEU	3.5
1	A	115	LYS	3.3
1	A	245	GLU	3.3
1	A	90	ILE	3.2
1	A	56	CYS	3.2
1	B	281	ASN	3.1
1	B	3	LEU	3.1
1	B	89	ASN	3.0
1	B	138	VAL	3.0
1	A	86	ARG	3.0
1	B	217	ASP	3.0
1	A	1	MET	2.8
1	B	194	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	197	SER	2.7
1	A	54	LEU	2.7
1	A	248	ILE	2.5
1	A	211	TYR	2.5
1	B	118	TYR	2.4
1	B	40	ALA	2.4
1	A	112	ASP	2.4
1	A	217	ASP	2.3
1	B	55	THR	2.3
1	B	195	ASP	2.2
1	B	115	LYS	2.2
1	B	22	ASP	2.2
1	A	206	HIS	2.2
1	A	191	TYR	2.1
1	B	131	LEU	2.1
1	A	247	LYS	2.1
1	A	218	ILE	2.1
1	A	119[A]	ARG	2.1
1	B	130	GLN	2.1

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](#)

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($\text{\AA}^2$)	Q<0.9
3	CA	B	284	1/1	0.96	0.25	28,28,28,28	0
3	CA	B	283	1/1	0.98	0.18	35,35,35,35	0
2	MG	A	283	1/1	0.99	0.03	18,18,18,18	0
3	CA	A	284	1/1	0.99	0.07	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.