W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 6, 2023 – 08:44 am GMT

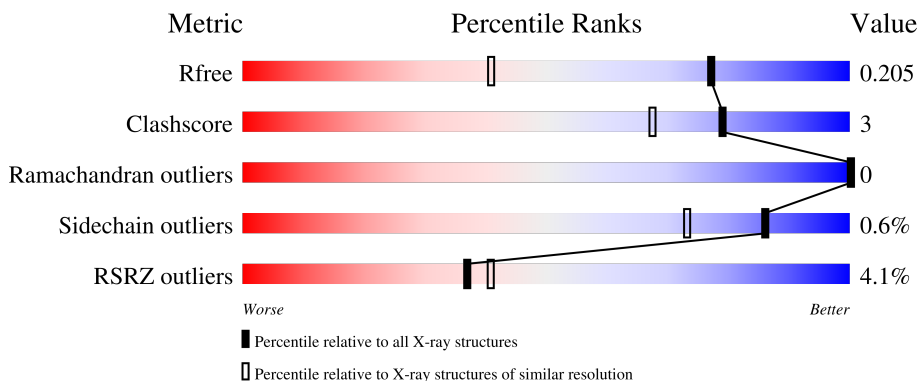|		
PDB ID	:	6QKT
Title	:	Crystal Structure of the Fluoroacetate Dehalogenase RPA1163 - Tyr219Phe - Fluoroacetate soaked 24hr - Glycolate bound
Authors	:	Mehrabi, P.; Kim, T.H.; Prosser, R.S.; Pai, E.F.
Deposited on	:	2019-01-30
Resolution	:	1.51 Å(reported)

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 1.51 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	Percentile Ranks	Value
Rfree		0.205
Clashscore		3
Ramachandran outliers		0
Sidechain outliers		0.6%
RSRZ outliers		4.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5349 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 Fluoroacetate dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	3	0
			2373	1527	415	422	9			
1	B	294	Total	C	N	O	S	0	2	0
			2342	1511	407	415	9			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A2R4GQN1
A	0	HIS	-	expression tag	UNP A0A2R4GQN1
A	2	PRO	SER	conflict	UNP A0A2R4GQN1
A	78	GLU	ASP	conflict	UNP A0A2R4GQN1
A	119	LEU	MET	conflict	UNP A0A2R4GQN1
A	197	ARG	GLN	conflict	UNP A0A2R4GQN1
A	199	VAL	ILE	conflict	UNP A0A2R4GQN1
A	219	PHE	TYR	conflict	UNP A0A2R4GQN1
A	232	ILE	ALA	conflict	UNP A0A2R4GQN1
A	295	VAL	MET	conflict	UNP A0A2R4GQN1
A	296	ARG	THR	conflict	UNP A0A2R4GQN1
A	303	GLY	-	expression tag	UNP A0A2R4GQN1
A	304	SER	-	expression tag	UNP A0A2R4GQN1
B	-1	GLY	-	expression tag	UNP A0A2R4GQN1
B	0	HIS	-	expression tag	UNP A0A2R4GQN1
B	2	PRO	SER	conflict	UNP A0A2R4GQN1
B	78	GLU	ASP	conflict	UNP A0A2R4GQN1
B	119	LEU	MET	conflict	UNP A0A2R4GQN1
B	197	ARG	GLN	conflict	UNP A0A2R4GQN1
B	199	VAL	ILE	conflict	UNP A0A2R4GQN1
B	219	PHE	TYR	conflict	UNP A0A2R4GQN1
B	232	ILE	ALA	conflict	UNP A0A2R4GQN1
B	295	VAL	MET	conflict	UNP A0A2R4GQN1
B	296	ARG	THR	conflict	UNP A0A2R4GQN1
B	303	GLY	-	expression tag	UNP A0A2R4GQN1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	304	SER	-	expression tag	UNP A0A2R4GQN1

- Molecule 2 is GLYCOLIC ACID (three-letter code: GOA) (formula: $C_2H_4O_3$).
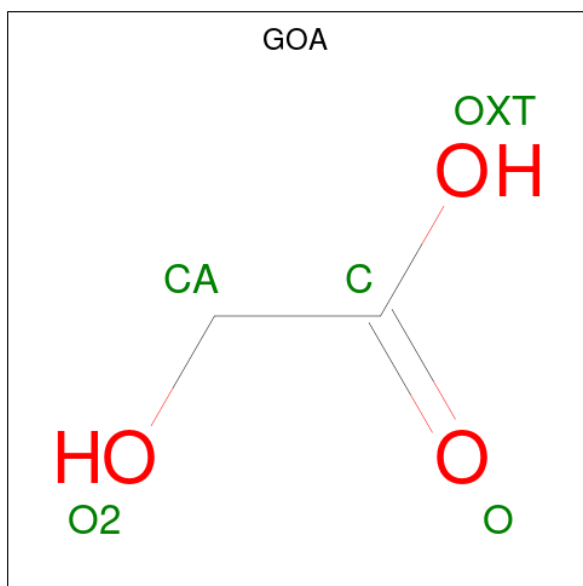
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	C 2	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	358	Total 358	O 358	0	0
3	B	271	Total 271	O 271	0	0

SEQUENCE-PLOTS INFOmissingINFO

3   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	41.85Å 79.51Å 84.83Å 90.00° 102.84° 90.00°	Depositor
Resolution (Å)	28.66 – 1.51 28.66 – 1.51	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.66-1.51) 98.2 (28.66-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 1.51Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.176 , 0.205 0.176 , 0.205	Depositor DCC
R_{free} test set	4143 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	11.4	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5349	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

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	0.57	2/2450 (0.1%)	0.72	1/3336 (0.0%)
1	B	0.53	0/2418	0.69	2/3291 (0.1%)
All	All	0.55	2/4868 (0.0%)	0.71	3/6627 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	MET	CB-CG	6.25	1.71	1.51
1	A	164	PRO	N-CD	-5.25	1.40	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	B	220	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	226	ASP	CB-CG-OD2	-5.21	113.61	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2373	0	2290	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2342	0	2254	14	0
2	A	5	0	0	0	0
3	A	358	0	0	2	0
3	B	271	0	0	4	0
All	All	5349	0	4544	26	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.

The worst 5 of 26 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:289:GLN:NE2	3:A:501:HOH:O	2.22	0.73
1:A:149[B]:TYR:CE2	1:A:257:ALA:HB3	2.29	0.66
1:B:141[B]:TYR:OH	1:B:253:ILE:O	2.13	0.66
1:A:4:LEU:N	3:A:502:HOH:O	2.31	0.64
1:B:4:LEU:N	3:B:401:HOH:O	2.31	0.63

There are no symmetry-related clashes.

4.3 Torsion angles ⓘ

4.3.1 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	298/306 (97%)	289 (97%)	9 (3%)	0	100	100
1	B	292/306 (95%)	285 (98%)	7 (2%)	0	100	100
All	All	590/612 (96%)	574 (97%)	16 (3%)	0	100	100

There are no Ramachandran outliers to report.

4.3.2 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	239/242 (99%)	236 (99%)	3 (1%)	69	43
1	B	235/242 (97%)	234 (100%)	1 (0%)	91	82
All	All	474/484 (98%)	470 (99%)	4 (1%)	86	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	TRP
1	A	149[A]	TYR
1	A	149[B]	TYR
1	B	15	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

4.6 Ligand geometry ⓘ

1 ligand is 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	$\#|Z| > 2$
2	GOA	A	401	-	4,4,4	1.14	0	4,4,4	1.17	0

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
2	GOA	A	401	-	-	0/2/2/2	-

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.

4.7 Other polymers ⓘ

There are no such residues in this entry.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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5 Fit of model and data ⓘ

5.1 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	297/306 (97%)	0.12	8 (2%)	54	59	5, 11, 23, 41	0
1	B	294/306 (96%)	0.37	16 (5%)	25	28	8, 15, 30, 46	0
All	All	591/612 (96%)	0.24	24 (4%)	37	41	5, 13, 27, 46	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ALA	8.7
1	B	253	ILE	8.1
1	B	300	ALA	7.4
1	B	4	LEU	6.3
1	A	300	ALA	6.1

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	GOA	A	401	5/5	0.94	0.10	9,10,12,12	0

5.5　Other polymers ⓘ

There are no such residues in this entry.