



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 5, 2026 – 01:36 AM UTC

PDB ID : 9U5W / pdb_00009u5w
Title : Crystal Structure of the Fluoroacetate Dehalogenase RPA1163 - Lys181Met/
Trp185Tyr/His280Ala with 2-fluoro-3-phenylpropanoic acid
Authors : Huang, H.S.; Zhang, Z.M.
Deposited on : 2025-03-22
Resolution : 2.08 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 Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

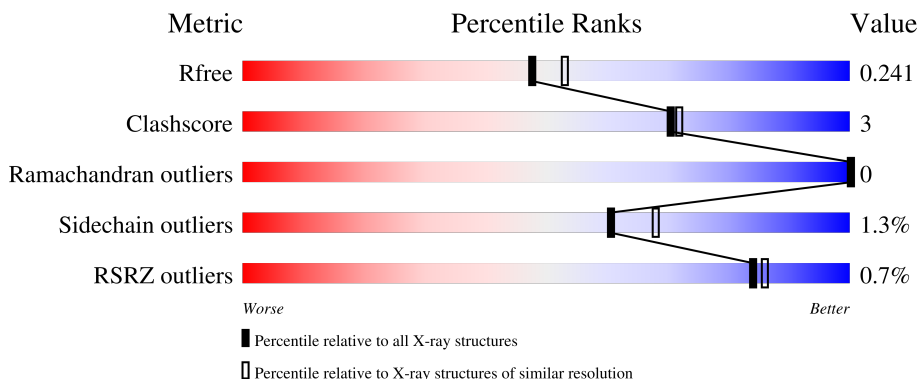
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	302	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	302	<div> <div></div> <div>92%</div> <div>5%</div> <div>..</div> </div>
1	C	302	<div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div>
1	D	302	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10352 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	298	Total	C	N	O	S	0	0	0
			2355	1516	408	421	10			
1	B	297	Total	C	N	O	S	0	0	0
			2341	1508	403	420	10			
1	C	299	Total	C	N	O	S	0	1	0
			2365	1524	408	423	10			
1	D	297	Total	C	N	O	S	0	0	0
			2346	1509	405	422	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	LYS	engineered mutation	UNP Q6NAM1
A	185	TYR	TRP	engineered mutation	UNP Q6NAM1
A	280	ALA	HIS	engineered mutation	UNP Q6NAM1
B	181	MET	LYS	engineered mutation	UNP Q6NAM1
B	185	TYR	TRP	engineered mutation	UNP Q6NAM1
B	280	ALA	HIS	engineered mutation	UNP Q6NAM1
C	181	MET	LYS	engineered mutation	UNP Q6NAM1
C	185	TYR	TRP	engineered mutation	UNP Q6NAM1
C	280	ALA	HIS	engineered mutation	UNP Q6NAM1
D	181	MET	LYS	engineered mutation	UNP Q6NAM1
D	185	TYR	TRP	engineered mutation	UNP Q6NAM1
D	280	ALA	HIS	engineered mutation	UNP Q6NAM1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	241	Total	O	0	0
			241	241		
2	B	237	Total	O	0	0
			237	237		

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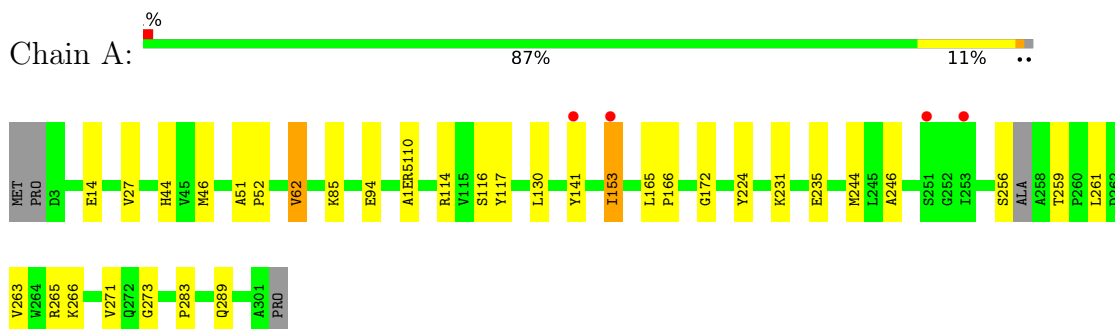
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	252	Total	O	0	0
			252	252		
2	D	215	Total	O	0	0
			215	215		

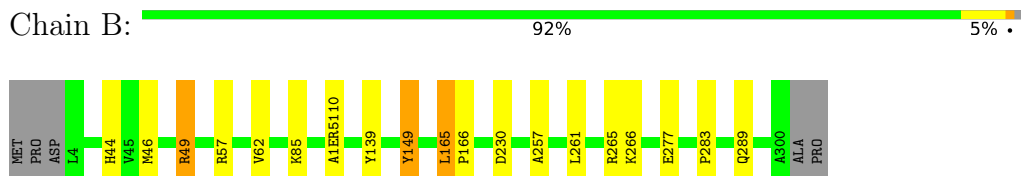
3 Residue-property plots [i](#)

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.

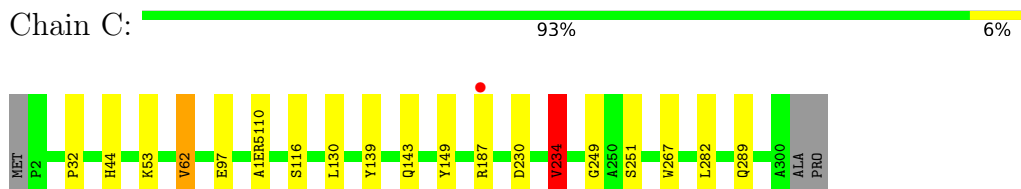
- Molecule 1: Fluoroacetate dehalogenase



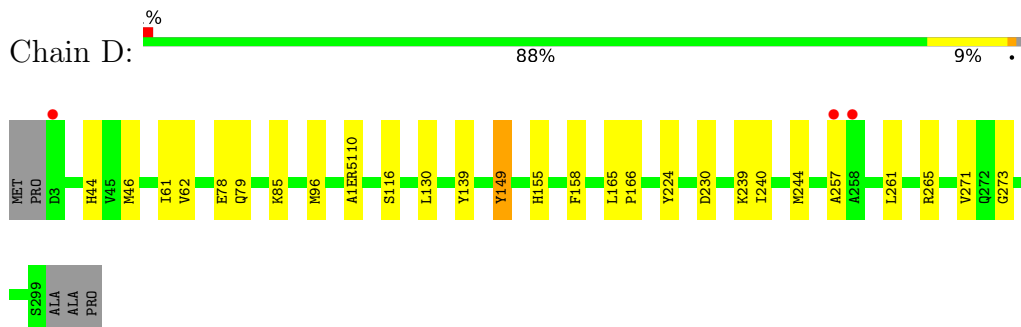
- Molecule 1: Fluoroacetate dehalogenase



- Molecule 1: Fluoroacetate dehalogenase



- Molecule 1: Fluoroacetate dehalogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.59Å 86.39Å 85.79Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	27.13 – 2.08 27.13 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.6 (27.13-2.08) 98.6 (27.13-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.9_1692+SVN	Depositor
R, R_{free}	0.190 , 0.239 0.192 , 0.241	Depositor DCC
R_{free} test set	1983 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	17.3	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.003 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10352	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% 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: A1ER5

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	0.79	1/2408 (0.0%)	0.94	0/3275
1	B	0.81	0/2395	0.92	0/3261
1	C	0.79	0/2420	0.93	3/3293 (0.1%)
1	D	0.81	1/2400 (0.0%)	0.93	0/3268
All	All	0.80	2/9623 (0.0%)	0.93	3/13097 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	224	TYR	CA-C	6.04	1.55	1.52
1	A	224	TYR	CA-C	6.04	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	VAL	CB-CA-C	-5.91	104.07	112.22
1	C	32	PRO	CA-C-N	5.83	126.02	119.90
1	C	32	PRO	C-N-CA	5.83	126.02	119.90

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	2355	0	2260	21	0
1	B	2341	0	2239	11	0
1	C	2365	0	2270	11	1
1	D	2346	0	2238	19	1
2	A	241	0	0	4	0
2	B	237	0	0	4	0
2	C	252	0	0	4	0
2	D	215	0	0	1	0
All	All	10352	0	9007	62	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 3.

The worst 5 of 62 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:141:TYR:HE1	1:A:153:ILE:HD12	1.53	0.72
1:B:277:GLU:OE2	2:B:401:HOH:O	2.11	0.68
1:C:97:GLU:OE1	2:C:401:HOH:O	2.15	0.63
1:D:130:LEU:HD23	1:D:244:MET:HE2	1.80	0.62
1:B:49:ARG:NH1	2:B:408:HOH:O	2.34	0.61

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:C:187:ARG:NH1	1:D:288:ASP:OD1[2_546]	2.13	0.07

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	293/302 (97%)	284 (97%)	9 (3%)	0	100	100
1	B	294/302 (97%)	284 (97%)	10 (3%)	0	100	100
1	C	297/302 (98%)	286 (96%)	11 (4%)	0	100	100
1	D	294/302 (97%)	286 (97%)	8 (3%)	0	100	100
All	All	1178/1208 (98%)	1140 (97%)	38 (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	234/238 (98%)	231 (99%)	3 (1%)	61	68
1	B	232/238 (98%)	228 (98%)	4 (2%)	53	60
1	C	235/238 (99%)	232 (99%)	3 (1%)	61	68
1	D	233/238 (98%)	231 (99%)	2 (1%)	70	77
All	All	934/952 (98%)	922 (99%)	12 (1%)	61	68

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	62	VAL
1	C	149	TYR
1	D	296	ARG
1	C	234	VAL
1	B	49	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	161	GLN
1	C	161	GLN

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Mol	Chain	Res	Type
1	D	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	A1ER5	B	110	1	18,19,20	1.63	2 (11%)	19,24,26	2.72	5 (26%)
1	A1ER5	D	110	1	18,19,20	1.80	3 (16%)	19,24,26	2.30	4 (21%)
1	A1ER5	C	110	1	18,19,20	1.07	1 (5%)	19,24,26	2.19	6 (31%)
1	A1ER5	A	110	1	18,19,20	1.29	3 (16%)	19,24,26	1.77	4 (21%)

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
1	A1ER5	B	110	1	-	7/17/18/20	0/1/1/1
1	A1ER5	D	110	1	-	5/17/18/20	0/1/1/1
1	A1ER5	C	110	1	-	7/17/18/20	0/1/1/1
1	A1ER5	A	110	1	-	5/17/18/20	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	110	A1ER5	OD2-CAH	-5.95	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	A1ER5	OD2-CAH	-5.57	1.35	1.45
1	C	110	A1ER5	OD2-CG	-3.14	1.25	1.34
1	A	110	A1ER5	OD2-CG	-3.04	1.25	1.34
1	A	110	A1ER5	OD2-CAH	-2.88	1.40	1.45

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	A1ER5	OD2-CAH-CAG	8.67	125.08	107.37
1	D	110	A1ER5	OD2-CAH-CAG	7.20	122.07	107.37
1	C	110	A1ER5	CAH-OD2-CG	5.20	124.02	116.25
1	D	110	A1ER5	OD2-CG-CB	4.92	120.25	111.43
1	B	110	A1ER5	CAH-OD2-CG	4.87	123.54	116.25

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	110	A1ER5	O-C-CA-CB
1	B	110	A1ER5	CAA-CAG-CAH-CAI
1	B	110	A1ER5	O-C-CA-CB
1	C	110	A1ER5	O-C-CA-CB
1	D	110	A1ER5	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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	297/302 (98%)	-0.16	4 (1%) 75 77	12, 15, 25, 37	0
1	B	296/302 (98%)	-0.35	0 100 100	11, 13, 20, 33	0
1	C	298/302 (98%)	-0.30	1 (0%) 90 91	7, 15, 23, 33	1 (0%)
1	D	296/302 (98%)	-0.22	3 (1%) 79 82	11, 15, 26, 41	0
All	All	1187/1208 (98%)	-0.26	8 (0%) 84 86	7, 15, 23, 41	1 (0%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	187	ARG	3.3
1	A	153	ILE	3.3
1	D	257	ALA	3.0
1	A	251	SER	2.9
1	D	258	ALA	2.8

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	A1ER5	B	110	19/20	0.94	0.07	11,11,12,13	0
1	A1ER5	D	110	19/20	0.94	0.06	11,11,13,13	0
1	A1ER5	C	110	19/20	0.95	0.06	11,11,11,11	0
1	A1ER5	A	110	19/20	0.96	0.06	12,12,15,16	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.