



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:25 PM UTC

PDB ID : 3UPM / pdb_00003upm
Title : Crystal Structure of PTE mutant H254Q/H257F/K185R/I274N
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Deposited on : 2011-11-18
Resolution : 1.95 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
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

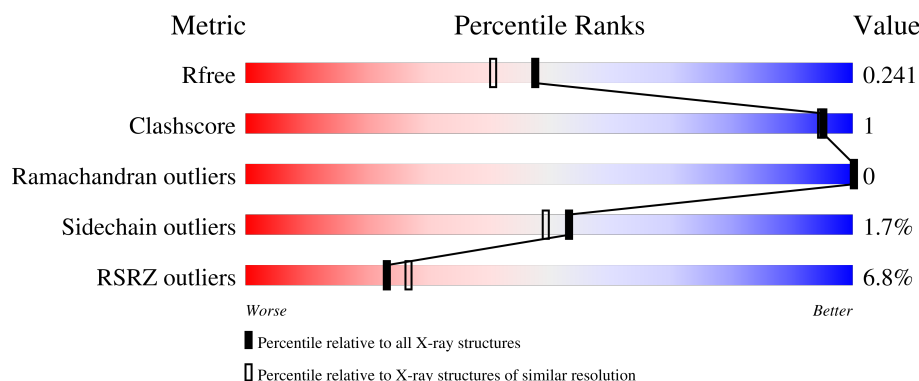
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	327	4% 92% 7%
1	B	327	9% 88% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5401 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2504	1582	444	471	7			
1	B	320	Total	C	N	O	S	0	0	0
			2454	1554	436	457	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	185	ARG	LYS	engineered mutation	UNP P0A434
A	254	GLN	HIS	engineered mutation	UNP P0A434
A	257	PHE	HIS	engineered mutation	UNP P0A434
A	274	ASN	ILE	engineered mutation	UNP P0A434
B	185	ARG	LYS	engineered mutation	UNP P0A434
B	254	GLN	HIS	engineered mutation	UNP P0A434
B	257	PHE	HIS	engineered mutation	UNP P0A434
B	274	ASN	ILE	engineered mutation	UNP P0A434

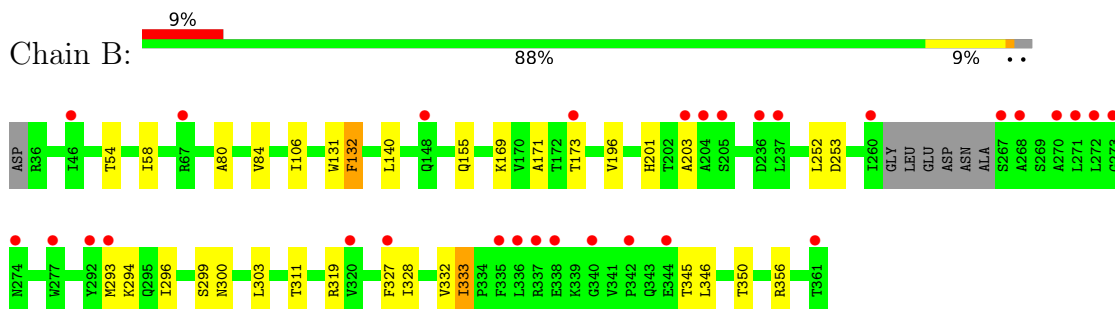
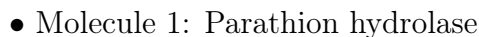
- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	2	Total	Co	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	266	Total	O	0	0
			266	266		
3	B	173	Total	O	0	0
			173	173		

- Molecule 1: Parathion hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 85.39Å 88.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 50.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-1.95) 99.3 (50.00-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.55 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.232 0.207 , 0.241	Depositor DCC
R_{free} test set	2407 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.583	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h 0.015 for -h,-l,-k 0.017 for k,h,-l 0.004 for l,h,k 0.004 for k,l,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5401	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.70	1/2538 (0.0%)	1.11	15/3445 (0.4%)
1	B	0.71	2/2487 (0.1%)	1.13	13/3374 (0.4%)
All	All	0.71	3/5025 (0.1%)	1.12	28/6819 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	ILE	CA-CB	9.72	1.59	1.54
1	A	333	ILE	CA-CB	8.19	1.59	1.53
1	B	333	ILE	CA-CB	5.33	1.57	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	THR	N-CA-C	8.86	123.90	113.18
1	A	253	ASP	N-CA-C	8.67	124.06	112.88
1	B	253	ASP	N-CA-C	8.65	124.89	113.30
1	A	54	THR	N-CA-C	8.31	123.23	113.18
1	A	106	ILE	N-CA-C	-7.73	103.91	112.80
1	B	106	ILE	N-CA-C	-7.57	105.17	112.29
1	B	58	ILE	N-CA-C	-7.46	103.67	111.58
1	A	132	PHE	N-CA-C	7.22	121.01	112.93
1	A	252	LEU	N-CA-C	-6.98	99.87	109.71
1	A	201	HIS	N-CA-C	-6.70	98.77	109.76
1	A	58	ILE	N-CA-C	-6.41	104.01	111.00
1	B	201	HIS	N-CA-C	-6.36	98.82	109.07
1	A	203	ALA	N-CA-C	-6.31	93.86	107.49
1	B	203	ALA	N-CA-C	-6.04	96.23	107.71
1	B	311	THR	N-CA-C	5.90	121.05	111.37
1	A	171	ALA	N-CA-C	5.80	117.93	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	ALA	N-CA-C	5.75	118.01	108.99
1	A	226	VAL	N-CA-C	5.64	116.86	108.46
1	A	311	THR	N-CA-C	5.59	122.70	110.80
1	B	332	VAL	N-CA-C	5.58	115.77	110.53
1	A	296	ILE	N-CA-C	5.57	116.33	108.36
1	B	252	LEU	N-CA-C	-5.50	101.96	109.71
1	A	139	ARG	N-CA-C	5.46	119.56	113.01
1	B	132	PHE	N-CA-C	5.30	119.37	113.01
1	B	155	GLN	N-CA-C	5.22	118.11	111.69
1	B	296	ILE	N-CA-C	5.13	115.69	108.36
1	A	200	THR	N-CA-C	5.04	117.81	109.85
1	A	65	PHE	N-CA-C	5.00	116.42	111.07

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	2504	0	2514	4	0
1	B	2454	0	2474	8	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	266	0	0	0	0
3	B	173	0	0	1	0
All	All	5401	0	4988	12	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 1.

All (12) 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:B:131:TRP:CG	1:B:132:PHE:H	2.21	0.59
1:B:333:ILE:HG23	1:B:346:LEU:HD13	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:MET:HG3	1:B:345:THR:HG23	1.95	0.49
1:B:80:ALA:O	1:B:84:VAL:HG23	2.15	0.46
1:A:131:TRP:CG	1:A:132:PHE:H	2.35	0.44
1:B:319:ARG:NH2	3:B:1436:HOH:O	2.49	0.44
1:B:333:ILE:HD11	1:B:350:THR:HG21	2.01	0.42
1:A:106:ILE:O	1:A:106:ILE:HG22	2.20	0.41
1:A:46:ILE:HG21	1:A:359:SER:OG	2.21	0.41
1:B:300:ASN:OD1	1:B:327:PHE:HB3	2.22	0.40
1:B:294:LYS:O	1:B:356:ARG:NH1	2.53	0.40
1:A:194:THR:OG1	1:A:196:VAL:HG22	2.22	0.40

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	324/327 (99%)	314 (97%)	10 (3%)	0	100	100
1	B	315/327 (96%)	306 (97%)	9 (3%)	0	100	100
All	All	639/654 (98%)	620 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	262/262 (100%)	258 (98%)	4 (2%)	57	54
1	B	257/262 (98%)	252 (98%)	5 (2%)	50	45
All	All	519/524 (99%)	510 (98%)	9 (2%)	53	49

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

Mol	Chain	Res	Type
1	A	178	PRO
1	A	262	LEU
1	A	299	SER
1	A	303	LEU
1	B	140	LEU
1	B	173	THR
1	B	196	VAL
1	B	299	SER
1	B	303	LEU

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	38	ASN
1	B	38	ASN
1	B	155	GLN
1	B	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	KCX	B	169	1,2	10,11,12	0.93	1 (10%)	6,12,14	1.91	1 (16%)
1	KCX	A	169	1,2	10,11,12	0.92	1 (10%)	6,12,14	1.97	1 (16%)

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	KCX	B	169	1,2	-	0/9/10/12	-
1	KCX	A	169	1,2	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	KCX	OQ1-CX	2.12	1.25	1.21
1	B	169	KCX	OQ1-CX	2.10	1.25	1.21

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	KCX	OQ1-CX-NZ	-4.69	117.79	124.92
1	B	169	KCX	OQ1-CX-NZ	-4.49	118.11	124.92

There are no chirality outliers.

There are no torsion outliers.

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](#)

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

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

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	326/327 (99%)	0.31	14 (4%) 40 46	23, 32, 51, 69	0
1	B	319/327 (97%)	0.67	30 (9%) 14 16	24, 37, 66, 84	0
All	All	645/654 (98%)	0.49	44 (6%) 23 27	23, 34, 60, 84	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	270	ALA	4.7
1	B	271	LEU	4.6
1	B	204	ALA	4.3
1	B	205	SER	3.7
1	B	237	LEU	3.5
1	A	293	MET	3.5
1	B	268	ALA	3.4
1	B	338	GLU	3.2
1	B	340	GLY	3.2
1	A	340	GLY	3.1
1	B	267	SER	3.0
1	B	203	ALA	3.0
1	B	274	ASN	2.9
1	B	173	THR	2.8
1	B	361	THR	2.8
1	B	273	GLY	2.8
1	B	335	PHE	2.6
1	A	344	GLU	2.6
1	A	173	THR	2.6
1	A	361	THR	2.6
1	A	338	GLU	2.5
1	A	46	ILE	2.4
1	B	293	MET	2.4
1	B	67	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	337	ARG	2.3
1	B	336	LEU	2.3
1	B	277	TRP	2.2
1	A	132	PHE	2.2
1	B	292	TYR	2.2
1	B	46	ILE	2.2
1	B	148	GLN	2.2
1	B	344	GLU	2.2
1	A	360	PRO	2.2
1	A	89	ARG	2.2
1	B	320	VAL	2.1
1	B	327	PHE	2.1
1	B	260	ILE	2.1
1	A	262	LEU	2.1
1	B	272	LEU	2.1
1	B	236	ASP	2.1
1	A	342	PRO	2.1
1	A	311	THR	2.0
1	A	334	PRO	2.0
1	B	342	PRO	2.0

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	KCX	B	169	12/13	0.87	0.11	27,30,41,43	0
1	KCX	A	169	12/13	0.93	0.08	21,25,30,31	0

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
2	CO	A	801	1/1	0.99	0.04	29,29,29,29	0
2	CO	B	803	1/1	0.99	0.10	39,39,39,39	0
2	CO	B	804	1/1	0.99	0.15	47,47,47,47	0
2	CO	A	802	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.