



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2YYK / pdb_00002yyk
Title : Crystal structure of the mutant of HpaB (T198I, A276G, and R466H)
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Deposited on : 2007-04-30
Resolution : 1.60 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

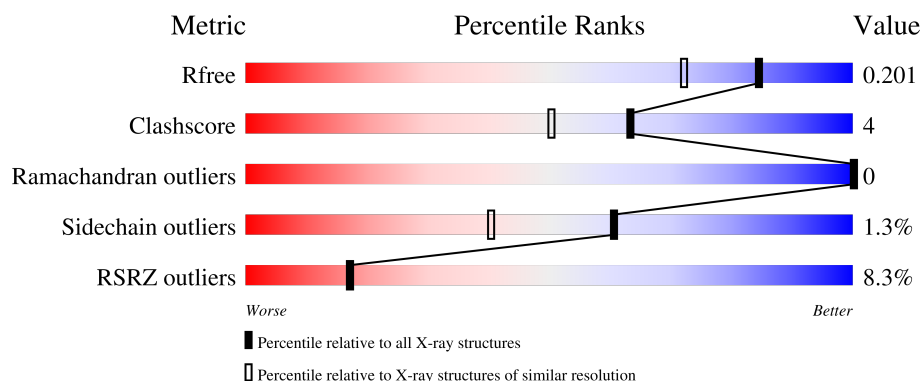
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	481	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	601	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4178 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 4-hydroxyphenylacetate-3-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3759	2416	644	684	15			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ILE	THR	engineered mutation	UNP Q5SJP8
A	276	GLY	ALA	engineered mutation	UNP Q5SJP8
A	466	HIS	ARG	engineered mutation	UNP Q5SJP8

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

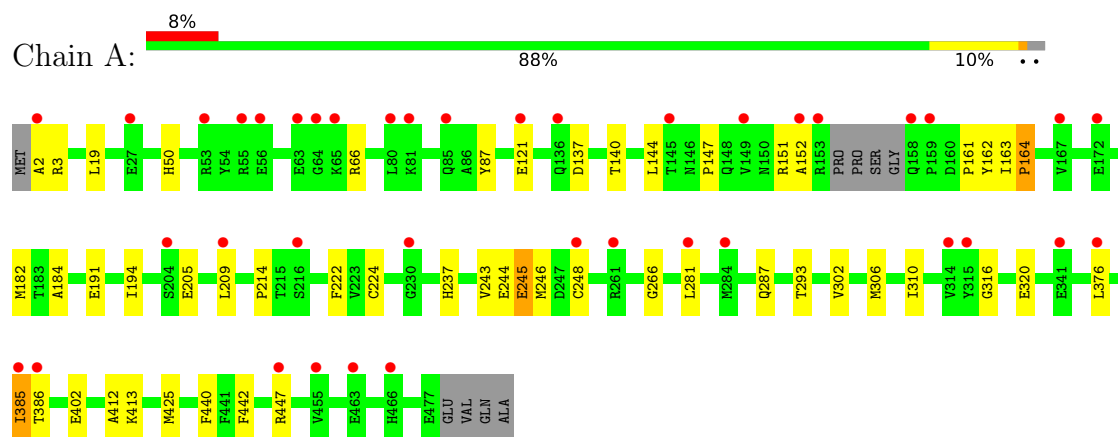
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	400	Total 400	O 400	0	0

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: 4-hydroxyphenylacetate-3-hydroxylase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.82Å 99.61Å 131.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.53 – 1.60 41.53 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (41.53-1.60) 98.4 (41.53-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.90 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.203 0.192 , 0.201	Depositor DCC
R_{free} test set	3939 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: GOL, NA, ACY

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	0.33	0/3851	0.85	9/5220 (0.2%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	ALA	N-CA-C	-6.77	105.05	113.38
1	A	440	PHE	N-CA-C	5.89	122.93	114.39
1	A	164	PRO	N-CA-C	-5.70	102.91	111.57
1	A	385	ILE	N-CA-C	5.68	118.45	112.83
1	A	293	THR	N-CA-C	-5.36	105.51	111.36
1	A	245	GLU	N-CA-C	5.21	117.87	111.82
1	A	214	PRO	N-CA-C	-5.13	103.22	111.38
1	A	224	CYS	N-CA-C	5.12	117.73	110.50
1	A	412	ALA	N-CA-C	5.05	117.18	111.02

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	3759	0	3717	30	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	9	0	0
4	A	6	0	4	0	0
5	A	400	0	0	2	0
All	All	4178	0	3730	30	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 4.

All (30) 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:147:PRO:HG3	1:A:182:MET:HE3	1.48	0.96
1:A:3:ARG:HB2	1:A:137:ASP:HB3	1.66	0.77
1:A:121:GLU:H	1:A:121:GLU:CD	1.97	0.72
1:A:151:ARG:HD2	5:A:1914:HOH:O	1.91	0.71
1:A:2:ALA:HB2	1:A:66:ARG:O	1.90	0.70
1:A:316:GLY:O	1:A:320:GLU:HG3	2.01	0.60
1:A:447:ARG:O	1:A:447:ARG:HD2	2.03	0.58
1:A:184:ALA:HB3	1:A:248:CYS:SG	2.48	0.54
1:A:281:LEU:HD13	1:A:281:LEU:C	2.33	0.54
1:A:3:ARG:O	1:A:50:HIS:HE1	1.91	0.53
1:A:147:PRO:HG3	1:A:182:MET:CE	2.32	0.53
1:A:163:ILE:HB	1:A:164:PRO:CD	2.40	0.51
1:A:163:ILE:HB	1:A:164:PRO:HD3	1.92	0.50
1:A:140:THR:HG22	1:A:191:GLU:HB2	1.95	0.49
1:A:161:PRO:HG2	1:A:162:TYR:CE1	2.47	0.48
1:A:182:MET:HA	1:A:182:MET:HE2	1.95	0.48
1:A:194:ILE:N	1:A:194:ILE:HD12	2.28	0.48
1:A:385:ILE:HG23	1:A:386:THR:HG23	1.95	0.48
1:A:447:ARG:HD2	1:A:447:ARG:C	2.39	0.47
1:A:3:ARG:HD2	1:A:137:ASP:O	2.15	0.47
1:A:19:LEU:HD23	1:A:222:PHE:HB2	1.98	0.46
1:A:205:GLU:O	1:A:266:GLY:HA2	2.16	0.46
1:A:237:HIS:HD2	5:A:1519:HOH:O	1.98	0.46
1:A:87:TYR:CD2	1:A:287:GLN:HA	2.50	0.46
1:A:245:GLU:O	1:A:246:MET:HB3	2.18	0.43
1:A:302:VAL:HG21	1:A:425:MET:SD	2.59	0.43
1:A:402:GLU:OE2	1:A:413:LYS:HE3	2.20	0.42
1:A:163:ILE:H	1:A:164:PRO:HD2	1.84	0.42
1:A:306:MET:O	1:A:310:ILE:HG12	2.21	0.40
1:A:144:LEU:HD23	1:A:144:LEU:H	1.86	0.40

There are no symmetry-related clashes.

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	468/481 (97%)	456 (97%)	12 (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	385/394 (98%)	380 (99%)	5 (1%)	61	40

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	209	LEU
1	A	243	VAL
1	A	244	GLU
1	A	376	LEU
1	A	442	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	49	GLN
1	A	50	HIS
1	A	85	GLN
1	A	94	ASN
1	A	125	ASN
1	A	136	GLN
1	A	170	GLN
1	A	201	GLN
1	A	237	HIS
1	A	317	HIS
1	A	378	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](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	ACY	A	500	-	3,3,3	5.22	1 (33%)	3,3,3	1.40	0
3	ACY	A	501	-	3,3,3	5.11	1 (33%)	3,3,3	1.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	A	502	-	3,3,3	5.35	1 (33%)	3,3,3	1.38	0
4	GOL	A	601	-	5,5,5	4.78	5 (100%)	5,5,5	3.83	3 (60%)

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
4	GOL	A	601	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ACY	O-C	9.09	1.61	1.22
3	A	500	ACY	O-C	8.81	1.60	1.22
3	A	501	ACY	O-C	8.62	1.59	1.22
4	A	601	GOL	C3-C2	-8.00	1.21	1.51
4	A	601	GOL	O1-C1	4.53	1.61	1.42
4	A	601	GOL	O3-C3	3.42	1.56	1.42
4	A	601	GOL	C1-C2	-3.09	1.40	1.51
4	A	601	GOL	O2-C2	-2.93	1.34	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	GOL	O2-C2-C3	6.94	137.91	109.18
4	A	601	GOL	O3-C3-C2	3.54	126.31	110.38
4	A	601	GOL	O1-C1-C2	3.41	125.75	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	GOL	C1-C2-C3-O3
4	A	601	GOL	O1-C1-C2-O2

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 [i](#)

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	472/481 (98%)	0.35	39 (8%) 17 17	3, 15, 27, 64	24 (5%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	VAL	12.6
1	A	248	CYS	9.9
1	A	80	LEU	9.2
1	A	81	LYS	9.1
1	A	27	GLU	8.3
1	A	204	SER	8.1
1	A	56	GLU	7.1
1	A	261	ARG	7.0
1	A	284	MET	5.7
1	A	455	VAL	5.3
1	A	153	ARG	4.8
1	A	55	ARG	4.7
1	A	167	VAL	4.5
1	A	152	ALA	4.3
1	A	158	GLN	4.3
1	A	385	ILE	4.1
1	A	281	LEU	4.0
1	A	121	GLU	3.8
1	A	159	PRO	3.8
1	A	376	LEU	3.7
1	A	145	THR	3.7
1	A	447	ARG	3.6
1	A	85	GLN	3.5
1	A	136	GLN	3.4
1	A	314	VAL	3.4
1	A	2	ALA	3.2
1	A	466	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	172	GLU	3.1
1	A	315	TYR	2.9
1	A	386	THR	2.9
1	A	463	GLU	2.9
1	A	64	GLY	2.6
1	A	230	GLY	2.5
1	A	216	SER	2.5
1	A	209	LEU	2.4
1	A	341	GLU	2.4
1	A	63	GLU	2.4
1	A	53	ARG	2.2
1	A	65	LYS	2.0

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	ACY	A	502	4/4	0.75	0.17	40,40,40,41	0
4	GOL	A	601	6/6	0.79	0.23	31,46,46,48	0
3	ACY	A	500	4/4	0.93	0.09	16,16,17,21	0
3	ACY	A	501	4/4	0.96	0.07	15,16,17,17	0
2	NA	A	505	1/1	0.99	0.03	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.