



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:50 PM UTC

PDB ID : 7MPY / pdb_00007mpy
Title : Crystal structure of cytosolic HPPK-DHPS from A.thaliana
Authors : Vadlamani, G.; Bond, C.S.
Deposited on : 2021-05-05
Resolution : 2.30 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

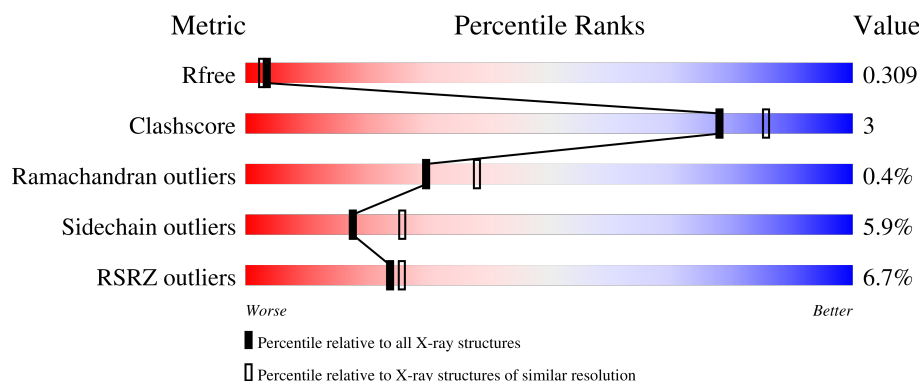
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	501	5% 76% 9% 16%
1	B	501	7% 73% 11% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6855 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 Folate synthesis bifunctional protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	1	0
			3323	2101	588	612	22			
1	B	430	Total	C	N	O	S	0	0	0
			3367	2127	597	621	22			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	MET	-	initiating methionine	UNP Q1ENB6
A	-15	ARG	-	expression tag	UNP Q1ENB6
A	-14	GLY	-	expression tag	UNP Q1ENB6
A	-13	SER	-	expression tag	UNP Q1ENB6
A	-12	HIS	-	expression tag	UNP Q1ENB6
A	-11	HIS	-	expression tag	UNP Q1ENB6
A	-10	HIS	-	expression tag	UNP Q1ENB6
A	-9	HIS	-	expression tag	UNP Q1ENB6
A	-8	HIS	-	expression tag	UNP Q1ENB6
A	-7	HIS	-	expression tag	UNP Q1ENB6
A	-6	GLY	-	expression tag	UNP Q1ENB6
A	-5	SER	-	expression tag	UNP Q1ENB6
A	-4	GLU	-	cloning artifact	UNP Q1ENB6
A	-3	ASN	-	cloning artifact	UNP Q1ENB6
A	-2	LEU	-	cloning artifact	UNP Q1ENB6
A	-1	TYR	-	cloning artifact	UNP Q1ENB6
A	0	PHE	-	cloning artifact	UNP Q1ENB6
A	1	GLN	-	cloning artifact	UNP Q1ENB6
B	-16	MET	-	initiating methionine	UNP Q1ENB6
B	-15	ARG	-	expression tag	UNP Q1ENB6
B	-14	GLY	-	expression tag	UNP Q1ENB6
B	-13	SER	-	expression tag	UNP Q1ENB6
B	-12	HIS	-	expression tag	UNP Q1ENB6
B	-11	HIS	-	expression tag	UNP Q1ENB6
B	-10	HIS	-	expression tag	UNP Q1ENB6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	HIS	-	expression tag	UNP Q1ENB6
B	-8	HIS	-	expression tag	UNP Q1ENB6
B	-7	HIS	-	expression tag	UNP Q1ENB6
B	-6	GLY	-	expression tag	UNP Q1ENB6
B	-5	SER	-	expression tag	UNP Q1ENB6
B	-4	GLU	-	cloning artifact	UNP Q1ENB6
B	-3	ASN	-	cloning artifact	UNP Q1ENB6
B	-2	LEU	-	cloning artifact	UNP Q1ENB6
B	-1	TYR	-	cloning artifact	UNP Q1ENB6
B	0	PHE	-	cloning artifact	UNP Q1ENB6
B	1	GLN	-	cloning artifact	UNP Q1ENB6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	86	Total O 86 86	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	66.68Å 240.15Å 148.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.46 – 2.30 93.46 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (93.46-2.30) 96.7 (93.46-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.238 , 0.300 0.253 , 0.309	Depositor DCC
R_{free} test set	3249 reflections (6.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6855	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.83% 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

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	1.08	0/3375	1.50	12/4548 (0.3%)
1	B	1.09	2/3421 (0.1%)	1.50	8/4611 (0.2%)
All	All	1.08	2/6796 (0.0%)	1.50	20/9159 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	421	SER	C-O	6.19	1.31	1.23
1	B	370	ILE	N-CA	5.11	1.50	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	ILE	O-C-N	6.90	127.09	121.85
1	B	303	ILE	CA-C-O	-6.62	115.08	120.70
1	B	265	LEU	CA-C-N	5.78	123.88	120.24
1	B	265	LEU	C-N-CA	5.78	123.88	120.24
1	B	60	GLN	CB-CA-C	5.75	116.25	109.47
1	B	119	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	206	GLY	CA-C-O	-5.51	116.33	121.18
1	A	134	VAL	N-CA-C	-5.45	106.87	111.56
1	A	165	GLY	CA-C-N	5.25	127.66	120.46
1	A	165	GLY	C-N-CA	5.25	127.66	120.46
1	A	260	GLU	CA-C-N	5.22	127.71	120.29
1	A	260	GLU	C-N-CA	5.22	127.71	120.29
1	A	356	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	29	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	477	THR	CA-CB-OG1	-5.10	101.95	109.60
1	B	302	ASP	CA-C-N	-5.02	118.05	122.97
1	B	302	ASP	C-N-CA	-5.02	118.05	122.97
1	A	37	LYS	CA-C-N	5.01	127.00	120.28
1	A	37	LYS	C-N-CA	5.01	127.00	120.28
1	A	145	GLU	CB-CA-C	5.01	120.39	110.42

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	3323	0	3400	14	0
1	B	3367	0	3433	24	0
2	A	79	0	0	1	0
2	B	86	0	0	0	0
All	All	6855	0	6833	38	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.

All (38) 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:265:LEU:HD12	1:B:265:LEU:O	1.96	0.64
1:B:265:LEU:HD12	1:B:265:LEU:C	2.22	0.64
1:B:262:ILE:HG22	1:B:292:VAL:HG22	1.85	0.57
1:B:418:ILE:HD12	1:B:420:PRO:HD3	1.87	0.56
1:A:68:ILE:C	1:A:68:ILE:HD12	2.33	0.54
1:A:64:LEU:HD21	1:A:195:LEU:HD11	1.90	0.53
1:B:417:LEU:C	1:B:417:LEU:HD23	2.36	0.51
1:B:135:LEU:HD12	1:B:173:LEU:HD12	1.93	0.51
1:B:224:VAL:HG13	1:B:271:VAL:HG11	1.93	0.50
1:A:136:ALA:HB2	1:A:170:TRP:CH2	2.46	0.49
1:A:43:VAL:HG12	1:A:68:ILE:HD13	1.94	0.48
1:A:235:ILE:HD11	1:A:278:MET:SD	2.54	0.48
1:A:401:ARG:CZ	1:A:416:ILE:HD12	2.44	0.47
1:B:43:VAL:HG12	1:B:68:ILE:HD13	1.96	0.47
1:A:417:LEU:C	1:A:417:LEU:HD23	2.41	0.46
1:A:80:LEU:HD22	1:A:121:LEU:HD13	1.99	0.45
1:B:261:GLU:O	1:B:261:GLU:HG3	2.16	0.44
1:B:184:ILE:HG22	1:B:184:ILE:O	2.17	0.44
1:A:387:ILE:HG23	1:A:429:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD23	1:B:108:ILE:CD1	2.48	0.44
1:B:265:LEU:HD21	1:B:285:VAL:CG2	2.48	0.44
1:A:328:MET:HE3	1:A:376:MET:HE3	2.00	0.42
1:A:320:VAL:O	1:A:374:ARG:NH2	2.53	0.42
1:B:28:ASN:HA	1:B:90:MET:HE2	2.02	0.42
1:B:265:LEU:HD21	1:B:285:VAL:HG23	2.01	0.42
1:B:153:VAL:HG22	1:B:157:HIS:CD2	2.54	0.41
1:B:307:VAL:C	1:B:308:SER:OG	2.62	0.41
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.87	0.41
1:B:76:PRO:HD3	1:B:111:TYR:CZ	2.55	0.41
1:B:331:HIS:CE1	1:B:354:VAL:HG22	2.55	0.41
1:B:136:ALA:HB2	1:B:170:TRP:CH2	2.54	0.41
1:A:323:SER:O	1:A:374:ARG:NH2	2.53	0.41
1:A:401:ARG:HD2	2:A:532:HOH:O	2.20	0.41
1:B:198:PHE:O	1:B:455:ASN:HB3	2.20	0.41
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.82	0.41
1:B:45:ARG:NH1	1:B:359:TYR:OH	2.54	0.40
1:B:184:ILE:O	1:B:184:ILE:CG2	2.70	0.40
1:B:356:THR:O	1:B:360:GLU:HG2	2.21	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	412/501 (82%)	394 (96%)	17 (4%)	1 (0%)	43	55
1	B	420/501 (84%)	385 (92%)	33 (8%)	2 (0%)	24	31
All	All	832/1002 (83%)	779 (94%)	50 (6%)	3 (0%)	30	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	260	GLU
1	A	192	GLY
1	B	192	GLY

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	366/433 (84%)	352 (96%)	14 (4%)	29	44
1	B	368/433 (85%)	339 (92%)	29 (8%)	11	15
All	All	734/866 (85%)	691 (94%)	43 (6%)	18	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	62	ARG
1	A	113	LYS
1	A	127	ARG
1	A	147	ILE
1	A	150	ASP
1	A	185	ILE
1	A	210	LEU
1	A	239	VAL
1	A	268	VAL
1	A	315	ASN
1	A	349	GLU
1	A	412	SER
1	A	446	VAL
1	B	15	VAL
1	B	45	ARG
1	B	51	GLU
1	B	64	LEU
1	B	69	ARG
1	B	76	PRO
1	B	94	GLU

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Mol	Chain	Res	Type
1	B	102	ARG
1	B	119	ASP
1	B	131	ARG
1	B	144	THR
1	B	179	LEU
1	B	228	VAL
1	B	234	MET
1	B	239	VAL
1	B	259	GLN
1	B	260	GLU
1	B	261	GLU
1	B	262	ILE
1	B	263	ASP
1	B	265	LEU
1	B	271	VAL
1	B	277	GLU
1	B	290	SER
1	B	317	HIS
1	B	407	LYS
1	B	420	PRO
1	B	446	VAL
1	B	479	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	289	ASN
1	A	331	HIS
1	B	81	ASN
1	B	114	HIS
1	B	162	HIS
1	B	209	ASN
1	B	289	ASN
1	B	348	ASN
1	B	465	ASN

5.3.3 RNA ⓘ

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](#)

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 [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	423/501 (84%)	0.33	24 (5%)	29 31	19, 63, 117, 144	1 (0%)
1	B	430/501 (85%)	0.54	33 (7%)	19 21	26, 71, 127, 158	4 (0%)
All	All	853/1002 (85%)	0.44	57 (6%)	24 26	19, 67, 122, 158	5 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	GLU	7.2
1	A	246	ALA	4.7
1	A	256	ILE	4.6
1	B	246	ALA	4.2
1	A	184	ILE	4.0
1	B	332	MET	3.1
1	B	143	GLY	3.0
1	B	350	ILE	3.0
1	B	13	GLU	2.9
1	A	369	GLY	2.9
1	A	212	PRO	2.9
1	A	307	VAL	2.9
1	B	120	LYS	2.8
1	A	332	MET	2.8
1	A	121	LEU	2.6
1	B	268	VAL	2.6
1	B	310	GLY	2.6
1	B	260	GLU	2.5
1	B	288	PHE	2.5
1	B	222	GLN	2.5
1	A	117	ILE	2.5
1	B	71	VAL	2.5
1	A	359	TYR	2.4
1	A	103	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	10	THR	2.4
1	A	147	ILE	2.4
1	B	142	LEU	2.4
1	B	349	GLU	2.4
1	B	73	LYS	2.3
1	B	110	PHE	2.3
1	B	116	ILE	2.3
1	B	259	GLN	2.3
1	A	122	ILE	2.3
1	B	303	ILE	2.3
1	B	307	VAL	2.3
1	B	146	ASP	2.2
1	B	19	GLY	2.2
1	B	373	TRP	2.2
1	B	184	ILE	2.2
1	A	120	LYS	2.2
1	B	158	SER	2.2
1	B	161	MET	2.1
1	B	152	ILE	2.1
1	B	210	LEU	2.1
1	A	368	SER	2.1
1	B	405	ALA	2.1
1	B	327	TYR	2.1
1	A	389	HIS	2.1
1	A	329	ILE	2.1
1	A	327	TYR	2.1
1	A	385	LYS	2.0
1	A	143	GLY	2.0
1	A	373	TRP	2.0
1	A	163	SER	2.0
1	B	145	GLU	2.0
1	B	148	ASP	2.0
1	A	166	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.