



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:51 PM EDT

PDB ID : 7L4I
Title : Crystal structure of a substrate-trapping variant of PPM1H phosphatase
Authors : Khan, A.R.; Waschbusch, D.
Deposited on : 2020-12-19
Resolution : 2.58 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

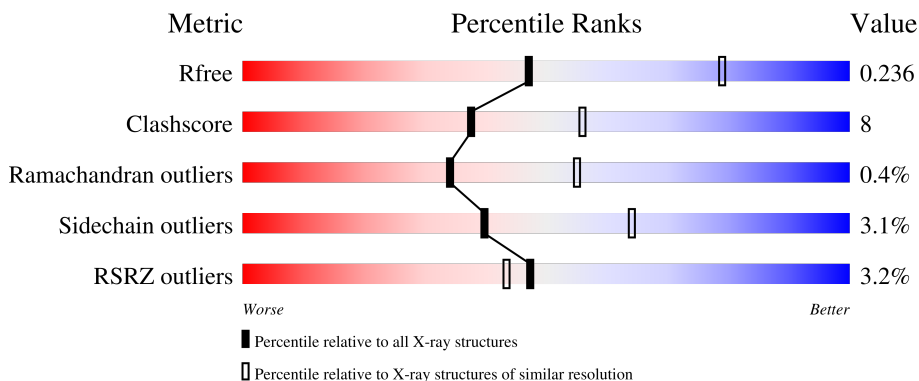
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	451	 4% 69% 17% 13%
1	B	451	 2% 73% 13% • 12%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6357 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 Protein phosphatase 1H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	394	3119	1976	546	583	14	0	0	0
1	B	396	3143	1996	547	587	13	0	1	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP Q9ULR3
A	30	SER	-	expression tag	UNP Q9ULR3
A	31	HIS	-	expression tag	UNP Q9ULR3
A	32	MET	-	expression tag	UNP Q9ULR3
A	56	ALA	CYS	engineered mutation	UNP Q9ULR3
A	223	GLY	-	linker	UNP Q9ULR3
A	224	SER	-	linker	UNP Q9ULR3
A	225	GLY	-	linker	UNP Q9ULR3
A	226	SER	-	linker	UNP Q9ULR3
A	288	ALA	ASP	engineered mutation	UNP Q9ULR3
B	29	GLY	-	expression tag	UNP Q9ULR3
B	30	SER	-	expression tag	UNP Q9ULR3
B	31	HIS	-	expression tag	UNP Q9ULR3
B	32	MET	-	expression tag	UNP Q9ULR3
B	56	ALA	CYS	engineered mutation	UNP Q9ULR3
B	223	GLY	-	linker	UNP Q9ULR3
B	224	SER	-	linker	UNP Q9ULR3
B	225	GLY	-	linker	UNP Q9ULR3
B	226	SER	-	linker	UNP Q9ULR3
B	288	ALA	ASP	engineered mutation	UNP Q9ULR3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	44	Total O 44 44	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.69Å 101.11Å 148.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.97 – 2.58 28.97 – 2.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.97-2.58) 99.6 (28.97-2.58)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.57Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.190 , 0.236 0.190 , 0.236	Depositor DCC
R_{free} test set	1708 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtrriage
Anisotropy	0.656	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: MG

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	0.30	0/3184	0.49	0/4310
1	B	0.28	0/3212	0.52	0/4347
All	All	0.29	0/6396	0.51	0/8657

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3119	0	3095	53	1
1	B	3143	0	3121	43	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	47	0	0	7	0
3	B	44	0	0	2	0
All	All	6357	0	6216	96	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 8.

All (96) 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:386:ILE:HD11	1:B:406:ILE:CG2	1.51	1.38
1:B:386:ILE:CD1	1:B:406:ILE:HG21	1.59	1.31
1:B:344:LEU:HD11	1:B:368:LEU:HD11	1.53	0.90
1:A:31:HIS:HD2	1:A:33:SER:H	1.19	0.87
1:B:308:PRO:HG3	1:B:382:VAL:HG23	1.62	0.79
1:A:307:THR:H	1:A:310:THR:HG22	1.49	0.76
1:A:31:HIS:CD2	1:A:33:SER:H	2.02	0.75
1:B:43:ARG:NH2	1:B:94:ASP:O	2.22	0.72
1:A:103:VAL:HB	1:A:142:VAL:HG22	1.72	0.72
1:B:386:ILE:CD1	1:B:406:ILE:CG2	2.40	0.71
1:B:348:MET:HG2	1:B:363:ILE:HD11	1.73	0.70
1:A:32:MET:HG2	1:A:264:ASN:HA	1.77	0.66
3:A:745:HOH:O	1:B:239:CYS:SG	2.54	0.66
1:B:69:LYS:HE3	1:B:72:ARG:HD2	1.78	0.65
1:A:447:GLU:OE2	3:A:701:HOH:O	2.15	0.65
1:B:270:THR:HB	1:B:287:GLY:HA3	1.80	0.64
1:B:513:LEU:HD22	1:B:513:LEU:O	1.98	0.63
1:A:308:PRO:HG3	1:A:382:VAL:HG23	1.82	0.62
1:A:459:CYS:HB2	1:A:466:ARG:HG3	1.80	0.62
1:B:479:ARG:NH1	1:B:480:GLY:O	2.33	0.62
1:B:482:LEU:HG	1:B:487:TRP:CE2	2.34	0.62
1:A:43:ARG:NH2	1:A:94:ASP:O	2.27	0.61
1:A:352:ASP:OD2	3:A:702:HOH:O	2.16	0.61
1:A:82:GLU:OE1	3:A:703:HOH:O	2.17	0.58
1:B:442:VAL:HG23	1:B:443:LEU:HD13	1.84	0.58
1:A:239:CYS:SG	3:B:742:HOH:O	2.57	0.58
1:B:315:LEU:HD11	1:B:389:THR:HG21	1.85	0.58
1:B:308:PRO:HB3	1:B:373:ILE:HD12	1.84	0.58
1:A:473:ASP:OD1	1:A:477:ARG:NH1	2.37	0.57
1:A:257:GLU:HB2	1:A:395:HIS:CE1	2.39	0.57
1:A:364:GLU:O	1:A:366:GLU:N	2.36	0.56
1:A:253:ASP:O	1:A:254:LEU:HB2	2.08	0.54
1:A:274:VAL:HA	1:A:282:TYR:O	2.08	0.54
1:B:60:HIS:ND1	1:B:87:GLY:HA2	2.22	0.54
1:A:305:GLU:O	1:A:310:THR:HG21	2.08	0.54
1:B:398:LYS:HD2	1:B:403:ASN:HA	1.90	0.53
1:B:83:VAL:HG21	1:B:479:ARG:HD3	1.90	0.53
1:A:395:HIS:HD2	3:A:737:HOH:O	1.91	0.53
1:B:343:GLU:O	1:B:346:LYS:HB2	2.10	0.52
1:A:83:VAL:HG21	1:A:479:ARG:HD3	1.92	0.51
1:B:242:ILE:HD11	1:B:418:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:HIS:NE2	1:A:255:GLN:OE1	2.35	0.50
1:A:372:LEU:HD12	1:A:383:MET:HG2	1.94	0.49
1:B:484:ASP:OD1	3:B:701:HOH:O	2.20	0.49
1:A:382:VAL:HB	1:A:386:ILE:HG13	1.95	0.49
1:B:347:LYS:HD2	1:B:362:THR:HA	1.95	0.49
1:A:363:ILE:HG23	1:A:367:ASP:HB2	1.95	0.49
1:B:158:ALA:N	1:B:266:SER:O	2.44	0.49
1:B:161:VAL:HG13	1:B:165:LEU:HD12	1.94	0.48
1:A:83:VAL:HG12	1:A:500:ILE:HB	1.95	0.48
1:A:337:ARG:NH1	1:A:343:GLU:OE1	2.29	0.48
1:A:483:LYS:CD	1:A:484:ASP:H	2.26	0.48
1:A:180:ILE:HG22	1:A:180:ILE:O	2.14	0.47
1:A:344:LEU:HD11	1:A:365:ASP:H	1.78	0.47
1:A:344:LEU:HD13	1:A:368:LEU:HD11	1.97	0.47
1:B:145:HIS:O	1:B:275:ILE:HA	2.15	0.46
1:B:63:ARG:HD3	1:B:487:TRP:CZ2	2.50	0.46
1:A:371:PRO:HG2	1:A:374:TYR:HB2	1.96	0.46
1:A:270:THR:HB	1:A:287:GLY:HA3	1.99	0.45
1:A:483:LYS:HD3	1:A:484:ASP:H	1.81	0.45
1:B:386:ILE:HD11	1:B:406:ILE:HG21	0.62	0.45
1:A:395:HIS:CD2	3:A:737:HOH:O	2.67	0.45
1:B:341:ARG:HG3	1:B:341:ARG:HH11	1.82	0.45
1:A:57:SER:CB	1:A:66:LEU:HD11	2.47	0.44
1:A:281:LEU:HG	1:A:421:LEU:HD11	1.99	0.44
1:A:50:SER:OG	1:A:53:GLU:HG3	2.18	0.44
1:A:145:HIS:O	1:A:275:ILE:HA	2.17	0.44
1:A:399:VAL:HG22	1:A:406:ILE:HD11	2.00	0.44
1:A:377:GLY:O	1:A:379:LYS:N	2.51	0.43
1:A:455:PHE:HZ	1:A:469:LEU:HB3	1.83	0.43
1:A:463:ASP:O	1:A:466:ARG:HB2	2.17	0.43
1:A:57:SER:HB2	1:A:66:LEU:HD11	2.00	0.43
1:B:281:LEU:HD13	1:B:421:LEU:HD11	2.00	0.43
1:B:233:LYS:HE2	1:B:233:LYS:HB2	1.82	0.43
1:B:345:GLY:HA2	1:B:362:THR:CG2	2.49	0.43
1:B:339:VAL:HG12	1:B:368:LEU:HD23	2.00	0.43
1:A:362:THR:O	1:A:364:GLU:HG2	2.19	0.42
1:B:467:TYR:CE1	1:B:506:PRO:HB3	2.54	0.42
1:A:316:GLN:HG2	1:A:332:HIS:O	2.19	0.42
1:B:386:ILE:H	1:B:386:ILE:HG13	1.70	0.42
1:B:347:LYS:HA	1:B:361:LYS:O	2.20	0.42
1:A:476:MET:SD	1:A:479:ARG:NH2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:HB2	1:B:66:LEU:HD11	2.01	0.42
1:B:57:SER:CB	1:B:66:LEU:HD11	2.50	0.41
1:A:464:PRO:O	3:A:705:HOH:O	2.22	0.41
1:B:467:TYR:CZ	1:B:506:PRO:HB3	2.55	0.41
1:B:41:TYR:CZ	1:B:91:HIS:HB3	2.55	0.41
1:A:456:LEU:O	1:A:466:ARG:NH1	2.54	0.41
1:A:252:MET:C	1:A:253:ASP:O	2.58	0.41
1:B:479:ARG:NH1	1:B:487:TRP:HZ3	2.19	0.41
1:B:35:LEU:N	1:B:36:PRO:HD2	2.35	0.41
1:A:455:PHE:CZ	1:A:469:LEU:HB3	2.56	0.41
1:A:31:HIS:CD2	1:A:32:MET:N	2.89	0.41
1:A:459:CYS:HB2	1:A:466:ARG:CG	2.48	0.41
1:A:290:ARG:HB3	1:A:440:TRP:CE2	2.57	0.40
1:B:291:ALA:H	1:B:303:SER:HB3	1.86	0.40

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:A:73:ARG:NH2	1:B:232:GLU:OE1[3_556]	2.01	0.19

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	388/451 (86%)	375 (97%)	11 (3%)	2 (0%)	29 50
1	B	391/451 (87%)	377 (96%)	13 (3%)	1 (0%)	41 62
All	All	779/902 (86%)	752 (96%)	24 (3%)	3 (0%)	34 55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	LYS
1	B	363	ILE
1	A	253	ASP

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	337/384 (88%)	330 (98%)	7 (2%)	53	75
1	B	339/384 (88%)	325 (96%)	14 (4%)	30	54
All	All	676/768 (88%)	655 (97%)	21 (3%)	40	64

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	182	LYS
1	A	253	ASP
1	A	378	LYS
1	A	381	ARG
1	A	398	LYS
1	A	512	LYS
1	B	232	GLU
1	B	233	LYS
1	B	303	SER
1	B	342	LYS
1	B	344	LEU
1	B	346	LYS
1	B	348	MET
1	B	365	ASP
1	B	376	GLU
1	B	378	LYS
1	B	386	ILE
1	B	466	ARG
1	B	482	LEU
1	B	513	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	95	GLN
1	A	173	GLN
1	A	296	ASN
1	A	458	ASN
1	B	173	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 monosaccharides 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 [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

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	394/451 (87%)	0.15	16 (4%) 37 33	36, 54, 87, 108	0
1	B	396/451 (87%)	0.08	9 (2%) 60 57	35, 53, 86, 108	0
All	All	790/902 (87%)	0.11	25 (3%) 47 43	35, 54, 87, 108	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	231	THR	3.6
1	A	52	ASP	3.4
1	A	491	ASN	3.1
1	A	273	ILE	3.1
1	B	491	ASN	3.0
1	A	179	ASP	2.9
1	A	379	LYS	2.9
1	A	180	ILE	2.8
1	A	104	LYS	2.6
1	A	378	LYS	2.6
1	B	513	LEU	2.5
1	B	376	GLU	2.4
1	B	148	SER	2.4
1	A	148	SER	2.4
1	A	485	ARG	2.4
1	B	273	ILE	2.3
1	A	50	SER	2.3
1	A	400	HIS	2.2
1	A	149	LEU	2.2
1	B	505	ILE	2.2
1	B	149	LEU	2.1
1	A	271	ALA	2.1
1	A	503	TYR	2.1
1	B	344	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	490	SER	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 monosaccharides 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(Å ²)	Q<0.9
2	MG	B	600	1/1	0.93	0.41	66,66,66,66	0
2	MG	A	601	1/1	0.94	0.07	56,56,56,56	0
2	MG	B	601	1/1	0.94	0.18	47,47,47,47	0
2	MG	A	600	1/1	0.95	0.08	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.