



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:43 pm BST

PDB ID : 5Y8U  
Title : Crystal structure of the C276S mutant of MAP2K7  
Authors : Kinoshita, T.  
Deposited on : 2017-08-21  
Resolution : 2.92 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](mailto: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.

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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	:	2.11
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)	:	2.11

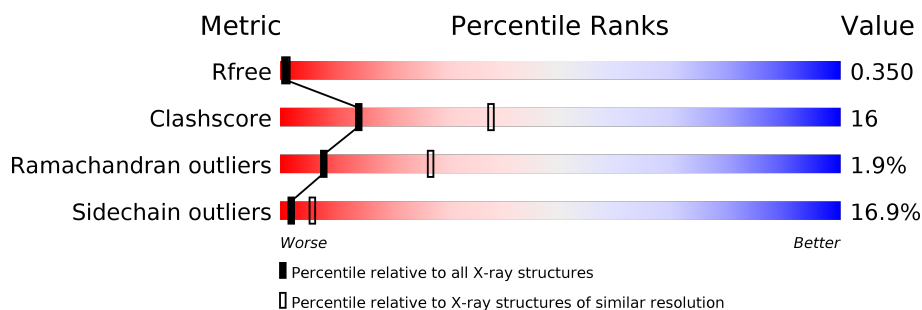
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	323	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2137 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 Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2117	1350	366	384	17			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	SER	CYS	engineered mutation	UNP O14733
A	436	HIS	-	expression tag	UNP O14733
A	437	HIS	-	expression tag	UNP O14733
A	438	HIS	-	expression tag	UNP O14733
A	439	HIS	-	expression tag	UNP O14733
A	440	HIS	-	expression tag	UNP O14733
A	441	HIS	-	expression tag	UNP O14733

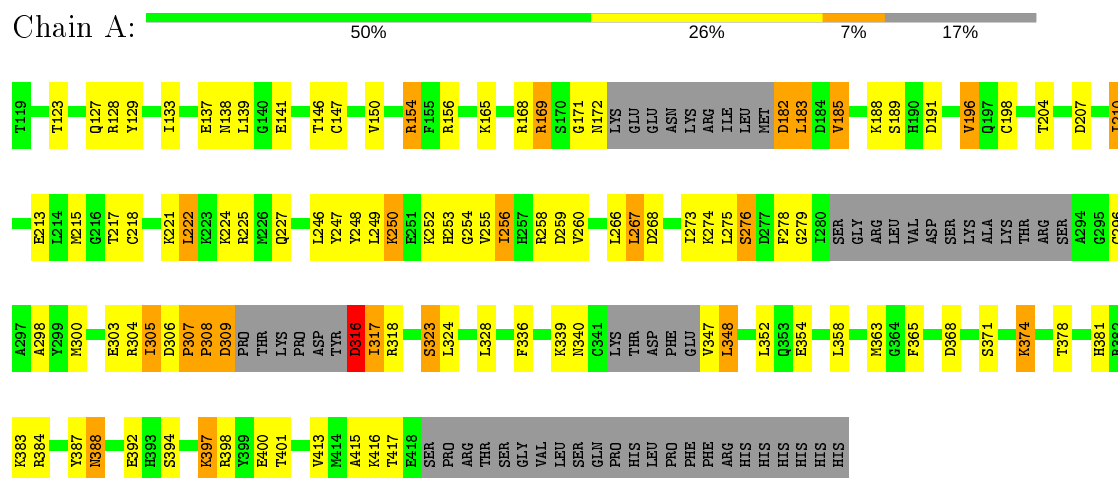
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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. 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. 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: Dual specificity mitogen-activated protein kinase kinase 7



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.53 Å 71.53 Å 262.31 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.95 – 2.92 45.03 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (61.95-2.92) 99.9 (45.03-2.92)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.88 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.8.0069	Depositor
R, $R_{free}$	0.230 , 0.299 0.282 , 0.350	Depositor DCC
$R_{free}$ test set	467 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.0	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2137	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.64	1/2157 (0.0%)	0.89	4/2899 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	PRO	N-CD	5.11	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	ASP	CB-CA-C	-6.59	97.23	110.40
1	A	306	ASP	C-N-CD	6.05	141.10	128.40
1	A	340	ASN	CB-CA-C	-5.63	99.13	110.40
1	A	307	PRO	C-N-CD	5.34	139.61	128.40

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	2117	0	2141	67	1
2	A	20	0	0	2	0
All	All	2137	0	2141	67	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 16.

All (67) 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:267:LEU:HD13	1:A:273:ILE:HG12	1.66	0.77
1:A:317:ILE:HD12	1:A:317:ILE:H	1.54	0.71
1:A:305:ILE:O	1:A:305:ILE:HG22	1.92	0.70
1:A:378:THR:O	1:A:384:ARG:NH1	2.25	0.70
1:A:304:ARG:O	1:A:305:ILE:HD13	1.91	0.69
1:A:256:ILE:HD13	1:A:258:ARG:HD2	1.78	0.66
1:A:317:ILE:HD13	1:A:318:ARG:HD3	1.78	0.65
1:A:168:ARG:HG3	2:A:517:HOH:O	1.97	0.64
1:A:127:GLN:HG2	2:A:509:HOH:O	1.97	0.64
1:A:256:ILE:HG21	1:A:316:ASP:O	1.99	0.62
1:A:371:SER:HA	1:A:374:LYS:HE2	1.83	0.60
1:A:317:ILE:N	1:A:317:ILE:HD12	2.16	0.59
1:A:398:ARG:O	1:A:401:THR:HG22	2.01	0.59
1:A:123:THR:HG22	1:A:128:ARG:HA	1.85	0.57
1:A:298:ALA:HB2	1:A:348:LEU:HD13	1.88	0.55
1:A:182:ASP:OD1	1:A:182:ASP:N	2.39	0.55
1:A:185:VAL:O	1:A:185:VAL:HG12	2.07	0.54
1:A:249:LEU:HB3	1:A:255:VAL:HB	1.88	0.54
1:A:123:THR:HG22	1:A:128:ARG:CB	2.37	0.54
1:A:260:VAL:HB	1:A:323:SER:HB2	1.90	0.53
1:A:224:LYS:O	1:A:227:GLN:HG2	2.09	0.52
1:A:303:GLU:OE2	1:A:384:ARG:NH2	2.42	0.52
1:A:169:ARG:NE	1:A:204:THR:O	2.37	0.52
1:A:146:THR:HG21	1:A:278:PHE:CD1	2.45	0.52
1:A:317:ILE:CD1	1:A:317:ILE:H	2.18	0.52
1:A:397:LYS:NZ	1:A:400:GLU:OE1	2.43	0.52
1:A:218:CYS:HB2	1:A:221:LYS:H	1.76	0.51
1:A:368:ASP:OD2	1:A:398:ARG:NH2	2.43	0.51
1:A:225:ARG:HG2	1:A:416:LYS:NZ	2.27	0.49
1:A:196:VAL:HG23	1:A:213:GLU:HG2	1.95	0.49
1:A:267:LEU:CD2	1:A:267:LEU:N	2.76	0.49
1:A:318:ARG:NH2	1:A:381:HIS:O	2.46	0.48
1:A:137:GLU:OE2	1:A:154:ARG:NH1	2.47	0.47
1:A:185:VAL:HG13	1:A:188:LYS:HE3	1.97	0.47
1:A:303:GLU:CD	1:A:381:HIS:HB3	2.35	0.47
1:A:415:ALA:O	1:A:416:LYS:HG3	2.14	0.47
1:A:268:ASP:OD1	1:A:268:ASP:C	2.52	0.47
1:A:307:PRO:CB	1:A:308:PRO:HA	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASP:N	1:A:309:ASP:OD1	2.33	0.46
1:A:317:ILE:HB	1:A:318:ARG:CD	2.46	0.46
1:A:123:THR:HG22	1:A:128:ARG:CA	2.46	0.45
1:A:256:ILE:HD12	1:A:256:ILE:H	1.81	0.45
1:A:127:GLN:O	1:A:129:TYR:CE1	2.70	0.45
1:A:215:MET:HE1	1:A:274:LYS:HE3	1.99	0.44
1:A:147:CYS:HB3	1:A:165:LYS:HE3	1.98	0.44
1:A:256:ILE:O	1:A:258:ARG:HG3	2.18	0.44
1:A:387:TYR:O	1:A:388:ASN:C	2.56	0.44
1:A:183:LEU:HD21	1:A:279:GLY:HA3	2.00	0.44
1:A:358:LEU:CD2	1:A:374:LYS:HA	2.47	0.43
1:A:347:VAL:HG23	1:A:348:LEU:HD12	1.99	0.43
1:A:171:GLY:O	1:A:172:ASN:CG	2.57	0.43
1:A:305:ILE:CG2	1:A:305:ILE:O	2.63	0.43
1:A:191:ASP:HB2	1:A:248:TYR:OH	2.18	0.43
1:A:246:LEU:HB3	1:A:387:TYR:CZ	2.54	0.42
1:A:250:LYS:O	1:A:254:GLY:HA2	2.18	0.42
1:A:253:HIS:O	1:A:255:VAL:HG23	2.19	0.42
1:A:347:VAL:O	1:A:348:LEU:HD12	2.20	0.42
1:A:374:LYS:HE2	1:A:374:LYS:HB3	1.88	0.42
1:A:413:VAL:O	1:A:413:VAL:HG12	2.20	0.42
1:A:392:GLU:HA	1:A:397:LYS:HD3	2.02	0.41
1:A:196:VAL:HG13	1:A:276:SER:HA	2.02	0.41
1:A:317:ILE:HB	1:A:318:ARG:HD2	2.02	0.41
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.87	0.40
1:A:198:CYS:SG	1:A:210:ILE:CD1	3.09	0.40
1:A:255:VAL:HG12	1:A:256:ILE:N	2.37	0.40
1:A:221:LYS:O	1:A:222:LEU:C	2.60	0.40
1:A:363:MET:HB3	1:A:365:PHE:CE2	2.56	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:247:TYR:OH	1:A:247:TYR:OH[10_444]	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	257/323 (80%)	226 (88%)	26 (10%)	5 (2%)	8 27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ARG
1	A	185	VAL
1	A	259	ASP
1	A	305	ILE
1	A	133	ILE

### 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	231/284 (81%)	192 (83%)	39 (17%)	2 6

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	139	LEU
1	A	141	GLU
1	A	150	VAL
1	A	154	ARG
1	A	169	ARG

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Mol	Chain	Res	Type
1	A	182	ASP
1	A	183	LEU
1	A	189	SER
1	A	196	VAL
1	A	207	ASP
1	A	210	ILE
1	A	217	THR
1	A	222	LEU
1	A	250	LYS
1	A	252	LYS
1	A	256	ILE
1	A	266	LEU
1	A	267	LEU
1	A	275	LEU
1	A	276	SER
1	A	296	CYS
1	A	300	MET
1	A	309	ASP
1	A	316	ASP
1	A	317	ILE
1	A	323	SER
1	A	324	LEU
1	A	336	PHE
1	A	339	LYS
1	A	348	LEU
1	A	352	LEU
1	A	354	GLU
1	A	374	LYS
1	A	383	LYS
1	A	388	ASN
1	A	394	SER
1	A	397	LYS
1	A	417	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN

### 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 carbohydrates 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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.