



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2017 – 05:03 PM EDT

PDB ID : 2A8L  
Title : Crystal structure of Human Taspase1 (T234A mutant)  
Authors : Khan, J.A.; Dunn, B.M.; Tong, L.  
Deposited on : unknown  
Resolution : 2.00 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

<http://wwpdb.org/validation/2016/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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

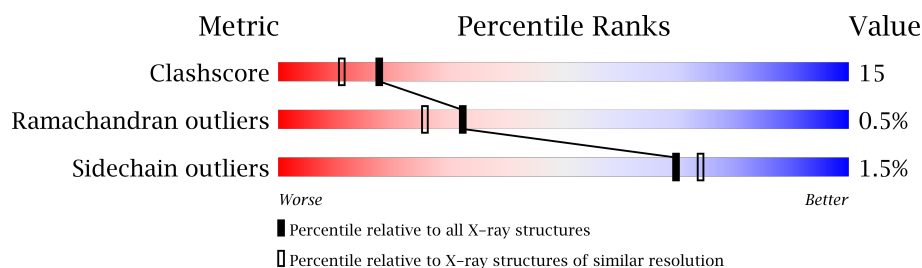
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	420	
1	B	420	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4732 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 Threonine aspartase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2221	1382	396	425	18			
1	B	310	Total	C	N	O	S	0	0	0
			2245	1399	400	428	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	THR	ENGINEERED	UNP Q9H6P5
B	234	ALA	THR	ENGINEERED	UNP Q9H6P5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	116	Total	O	0	0
			116	116		



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.20 Å 85.75 Å 104.56 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.46 – 2.00	Depositor
% Data completeness (in resolution range)	96.8 (28.46-2.00)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.205 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4732	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 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	0.33	0/2258	0.57	0/3053
1	B	0.31	0/2283	0.56	0/3087
All	All	0.32	0/4541	0.57	0/6140

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

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	2221	0	2188	66	0
1	B	2245	0	2219	79	0
2	A	150	0	0	5	0
2	B	116	0	0	4	0
All	All	4732	0	4407	136	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 15.

All (136) 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:385:GLN:HE22	1:B:416:GLU:H	1.14	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:HA	1:B:59:LYS:HE3	1.55	0.87
1:A:234:ALA:HB3	1:A:251:SER:O	1.76	0.85
1:A:59:LYS:HE3	1:A:59:LYS:HA	1.66	0.78
1:B:382:MET:CE	1:B:389:ALA:HB2	2.14	0.77
1:B:414:ARG:NH1	1:B:414:ARG:HB2	2.00	0.75
1:B:396:LEU:HD23	1:B:407:ALA:HB2	1.73	0.70
1:B:66:LYS:O	1:B:70:GLN:HG3	1.91	0.70
1:A:290:THR:HG22	1:A:343:VAL:HG12	1.73	0.70
1:B:382:MET:HE1	1:B:389:ALA:HB2	1.73	0.69
1:A:337:ASP:H	1:B:154:LYS:NZ	1.92	0.68
1:B:66:LYS:HG3	1:B:389:ALA:HB3	1.76	0.67
1:A:100:ASN:O	1:A:234:ALA:HB1	1.96	0.66
1:B:364:LEU:HB3	1:B:415:LEU:HB2	1.77	0.65
1:B:395:ARG:HD2	2:B:454:HOH:O	1.97	0.64
1:B:310:LEU:HD11	1:B:345:VAL:HG11	1.80	0.63
1:B:145:ARG:NH1	1:B:177:HIS:HB3	2.14	0.63
1:B:310:LEU:CD1	1:B:345:VAL:HG11	2.28	0.63
1:B:414:ARG:HH11	1:B:414:ARG:HB2	1.62	0.62
1:B:70:GLN:O	1:B:74:GLU:HG3	1.99	0.61
1:B:286:THR:HG22	1:B:347:ARG:HG3	1.84	0.59
1:B:383:SER:HB3	1:B:386:ASP:CG	2.22	0.59
1:B:172:ARG:HG2	1:B:172:ARG:HH11	1.66	0.59
1:B:323:MET:O	1:B:327:PHE:HB3	2.02	0.59
1:A:364:LEU:HB2	1:A:415:LEU:HB2	1.84	0.58
1:B:75:LYS:HE3	1:B:88:ALA:HB2	1.85	0.58
1:A:160:ILE:HD11	1:B:336:GLU:OE1	2.04	0.57
1:B:90:LEU:O	1:B:94:GLU:HG3	2.04	0.57
1:A:304:ARG:HD3	2:A:474:HOH:O	2.04	0.56
1:B:100:ASN:ND2	1:B:106:ASN:H	2.02	0.56
1:A:262:ARG:HH21	1:A:295:GLU:CD	2.09	0.56
1:A:337:ASP:H	1:B:154:LYS:HZ2	1.51	0.56
1:A:100:ASN:O	1:A:234:ALA:CB	2.53	0.56
1:B:382:MET:HE2	1:B:389:ALA:HB2	1.87	0.56
1:A:246:VAL:H	1:A:277:ASN:HD21	1.52	0.55
1:B:241:ASP:OD2	1:B:245:ASN:HB2	2.06	0.55
1:A:301:ILE:HD12	1:B:304:ARG:NH1	2.22	0.55
1:A:234:ALA:CB	1:A:252:SER:HA	2.37	0.54
1:B:73:ILE:HG13	1:B:382:MET:SD	2.46	0.54
2:A:443:HOH:O	1:B:299:ARG:HD2	2.08	0.54
1:B:246:VAL:H	1:B:277:ASN:HD21	1.55	0.53
1:A:126:ASN:CB	1:A:151:GLN:HE22	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:HIS:CE1	1:B:291:SER:HB2	2.44	0.53
2:A:548:HOH:O	1:B:154:LYS:HG3	2.08	0.53
1:A:126:ASN:HB2	1:A:151:GLN:HE22	1.73	0.52
1:A:69:CYS:C	1:A:382:MET:HE1	2.30	0.52
1:A:288:VAL:HG22	1:A:345:VAL:HG22	1.90	0.52
1:B:385:GLN:HE22	1:B:416:GLU:N	1.96	0.51
1:B:107:LEU:N	1:B:107:LEU:HD12	2.26	0.51
1:B:142:VAL:HA	1:B:179:ILE:HD13	1.92	0.51
1:B:62:LYS:HE3	1:B:393:ILE:HG12	1.93	0.50
1:B:116:ASP:HB3	1:B:267:ALA:HB2	1.94	0.50
1:B:295:GLU:O	1:B:299:ARG:HG2	2.11	0.50
1:B:66:LYS:HB3	1:B:66:LYS:NZ	2.27	0.50
1:B:66:LYS:HZ3	1:B:66:LYS:HB3	1.76	0.50
1:A:415:LEU:HD12	1:A:415:LEU:N	2.27	0.49
1:B:63:HIS:HB2	2:B:493:HOH:O	2.11	0.49
1:B:339:VAL:O	1:B:403:GLY:HA2	2.13	0.49
1:A:100:ASN:ND2	1:A:106:ASN:H	2.11	0.49
1:A:286:THR:CG2	1:A:311:GLN:HE22	2.25	0.49
1:A:73:ILE:CG1	1:A:382:MET:HE2	2.43	0.49
1:B:73:ILE:O	1:B:77:GLN:HG3	2.11	0.49
1:B:242:HIS:CE1	1:B:243:GLU:HG3	2.48	0.49
1:A:169:GLY:HA3	1:B:260:PRO:O	2.12	0.49
1:B:67:ARG:HG3	1:B:92:GLU:CG	2.42	0.49
1:B:242:HIS:ND1	1:B:243:GLU:HG3	2.27	0.48
1:A:168:GLU:O	1:A:172:ARG:HG3	2.13	0.48
1:B:239:VAL:HG12	1:B:240:VAL:N	2.29	0.48
1:A:381:TYR:CE2	1:A:390:LYS:HD2	2.48	0.48
1:B:168:GLU:O	1:B:172:ARG:HG3	2.14	0.48
1:A:159:ARG:HH21	1:B:262:ARG:HH11	1.60	0.48
1:A:137:LYS:HE2	2:A:450:HOH:O	2.13	0.48
1:A:59:LYS:CE	1:A:59:LYS:HA	2.41	0.47
1:A:310:LEU:CD1	1:A:345:VAL:HG11	2.44	0.47
1:A:401:VAL:HB	1:A:404:GLN:HB2	1.95	0.47
1:A:73:ILE:HB	1:A:382:MET:HE3	1.97	0.47
1:B:174:ALA:HA	1:B:179:ILE:HD12	1.96	0.46
1:B:386:ASP:OD2	1:B:387:GLY:N	2.48	0.46
1:B:105:SER:HB3	1:B:253:GLY:HA3	1.98	0.46
1:A:376:SER:HB3	1:A:395:ARG:HD2	1.97	0.46
1:A:73:ILE:HG13	1:A:382:MET:HE2	1.97	0.46
1:B:142:VAL:HG22	1:B:179:ILE:HD13	1.97	0.45
1:B:302:LEU:HD22	1:B:306:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HD11	1:A:345:VAL:HG11	1.97	0.45
1:B:300:THR:O	1:B:301:ILE:C	2.55	0.45
1:B:86:VAL:O	1:B:90:LEU:HD23	2.17	0.45
1:A:63:HIS:NE2	1:A:67:ARG:HD3	2.31	0.45
1:A:286:THR:HG23	2:A:569:HOH:O	2.17	0.45
1:A:67:ARG:O	1:A:71:LYS:HG2	2.16	0.45
1:A:345:VAL:CG1	1:A:346:LEU:N	2.79	0.45
1:B:172:ARG:NH1	1:B:172:ARG:HG2	2.29	0.45
1:A:53:HIS:HB2	1:A:395:ARG:NH1	2.31	0.44
1:A:47:HIS:CE1	1:A:291:SER:HB2	2.53	0.44
1:B:127:PHE:CZ	1:B:129:ALA:HB2	2.53	0.44
1:B:234:ALA:HB2	1:B:252:SER:HB2	2.00	0.44
1:B:239:VAL:CG1	1:B:240:VAL:N	2.80	0.44
1:A:317:GLN:O	1:A:321:GLU:HG3	2.18	0.43
1:A:90:LEU:CD1	1:A:235:VAL:HG23	2.48	0.43
1:B:369:LEU:N	1:B:369:LEU:HD12	2.34	0.43
1:B:310:LEU:HD13	1:B:345:VAL:HG11	1.99	0.43
1:B:414:ARG:CB	1:B:414:ARG:HH11	2.28	0.43
1:A:286:THR:HG21	1:A:311:GLN:HE22	1.83	0.43
1:B:304:ARG:NE	1:B:308:HIS:CE1	2.87	0.43
1:A:234:ALA:HB3	1:A:252:SER:HA	2.00	0.43
1:B:161:PRO:HA	1:B:162:PRO:HD3	1.81	0.43
1:A:239:VAL:CG1	1:A:240:VAL:N	2.81	0.43
1:B:100:ASN:HD22	1:B:105:SER:HA	1.83	0.43
1:B:292:GLY:HA3	1:B:341:GLY:HA2	2.00	0.43
1:A:64:VAL:HA	1:A:67:ARG:HE	1.84	0.42
1:A:260:PRO:O	1:B:169:GLY:HA3	2.19	0.42
1:A:70:GLN:N	1:A:382:MET:HE1	2.35	0.42
1:B:288:VAL:HG22	1:B:345:VAL:HG22	2.02	0.42
1:A:124:SER:O	1:A:125:LEU:HB2	2.20	0.42
1:A:41:GLY:HA3	1:A:242:HIS:HB3	2.02	0.42
1:A:246:VAL:HG22	1:A:277:ASN:HD22	1.83	0.42
1:A:286:THR:HG21	1:A:311:GLN:NE2	2.35	0.42
1:A:368:PHE:C	1:A:369:LEU:HD12	2.40	0.42
1:A:396:LEU:HD23	1:A:407:ALA:HB2	2.01	0.42
1:A:246:VAL:HG22	1:A:277:ASN:ND2	2.35	0.42
1:A:337:ASP:H	1:B:154:LYS:HZ1	1.67	0.42
1:B:64:VAL:HG22	1:B:93:LEU:HD23	2.02	0.42
1:A:147:LEU:C	1:A:147:LEU:HD23	2.41	0.41
1:A:86:VAL:O	1:A:90:LEU:HD23	2.20	0.41
1:B:67:ARG:O	1:B:71:LYS:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLY:HA3	2:B:470:HOH:O	2.19	0.41
1:B:295:GLU:HG2	2:B:529:HOH:O	2.19	0.41
1:A:130:VAL:HA	1:A:165:LEU:O	2.19	0.41
1:A:239:VAL:HG12	1:A:240:VAL:N	2.35	0.41
1:B:401:VAL:CG1	1:B:404:GLN:HG3	2.51	0.41
1:A:317:GLN:HA	1:A:317:GLN:OE1	2.21	0.41
1:A:278:THR:HA	1:A:282:ASN:O	2.21	0.41
1:A:142:VAL:HA	1:A:179:ILE:HD13	2.03	0.40
1:B:368:PHE:C	1:B:369:LEU:HD12	2.42	0.40
1:A:304:ARG:NH1	1:B:301:ILE:HD12	2.37	0.40
1:A:306:CYS:O	1:A:310:LEU:HG	2.22	0.40
1:A:370:TRP:CE2	1:A:409:GLU:HB2	2.57	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	299/420 (71%)	291 (97%)	6 (2%)	2 (1%)	25	18
1	B	302/420 (72%)	292 (97%)	9 (3%)	1 (0%)	44	40
All	All	601/840 (72%)	583 (97%)	15 (2%)	3 (0%)	32	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	ASP
1	B	388	LYS
1	A	388	LYS

### 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	229/330 (69%)	226 (99%)	3 (1%)	73	78
1	B	232/330 (70%)	228 (98%)	4 (2%)	66	70
All	All	461/660 (70%)	454 (98%)	7 (2%)	70	74

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	302	LEU
1	A	317	GLN
1	B	59	LYS
1	B	302	LEU
1	B	313	GLU
1	B	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	151	GLN
1	A	277	ASN
1	A	324	GLN
1	B	100	ASN
1	B	106	ASN
1	B	277	ASN
1	B	385	GLN

### 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 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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.