



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:11 AM UTC

PDB ID : 2A8J / pdb_00002a8j
Title : Crystal Structure of human Taspase1 (activated form)
Authors : Khan, J.A.; Dunn, B.M.; Tong, L.
Deposited on : 2005-07-08
Resolution : 1.90 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

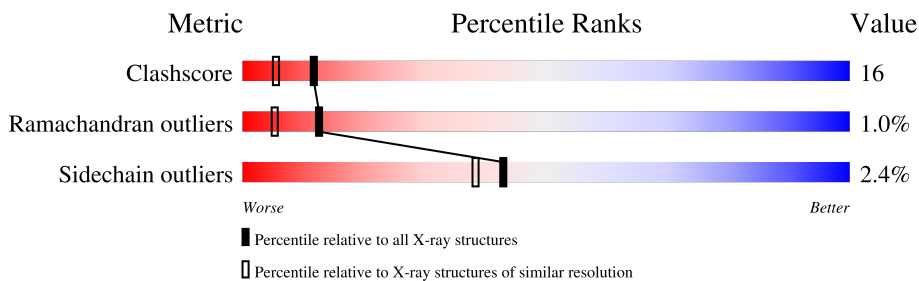
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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 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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4844 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	310	Total	C	N	O	S	0	0	0
			2247	1400	400	429	18			
1	B	313	Total	C	N	O	S	0	0	0
			2267	1410	404	434	19			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		
3	B	168	Total	O	0	0
			168	168		

M370	S371		S376	M377		M382	S383	A384	Q385		K388	A389		R395	L396		A407	I408	E409		R414	L415	E416	SER	PRO	VAL	ASN
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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, α , β , γ	60.57 Å 89.66 Å 104.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 1.90	Depositor
% Data completeness (in resolution range)	96.9 (29.71-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4844	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.39	0/2285	0.88	8/3090 (0.3%)
1	B	0.39	0/2304	0.87	8/3115 (0.3%)
All	All	0.39	0/4589	0.88	16/6205 (0.3%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	LEU	N-CA-C	9.13	121.24	111.28
1	A	160	ILE	CA-C-N	8.13	125.60	119.66
1	A	160	ILE	C-N-CA	8.13	125.60	119.66
1	B	282	ASN	CA-C-N	7.11	126.81	119.56
1	B	282	ASN	C-N-CA	7.11	126.81	119.56
1	A	302	LEU	N-CA-C	6.89	119.38	111.11
1	A	268	LEU	N-CA-C	6.44	119.22	108.73
1	A	68	ALA	N-CA-C	-5.97	104.85	111.36
1	B	57	LYS	N-CA-C	-5.87	105.00	114.09
1	B	268	LEU	N-CA-C	5.68	118.50	109.24
1	A	179	ILE	CA-C-N	5.57	126.80	119.84
1	A	179	ILE	C-N-CA	5.57	126.80	119.84
1	B	265	GLN	N-CA-C	5.23	117.73	111.71
1	A	255	LEU	N-CA-C	5.11	117.62	109.96
1	B	285	SER	N-CA-C	-5.05	101.07	109.46
1	B	325	ASN	N-CA-C	5.01	117.85	111.69

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	2247	0	2221	75	0
1	B	2267	0	2234	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	160	0	0	6	0
3	B	168	0	0	11	0
All	All	4844	0	4455	143	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 16.

All (143) 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:50:ALA:HB2	1:B:377:MET:HE3	1.43	1.00
1:A:159:ARG:HD2	1:B:255:LEU:HD21	1.54	0.90
1:A:383:SER:HB3	1:A:386:ASP:HB2	1.54	0.89
1:B:290:THR:HG22	1:B:343:VAL:HG12	1.59	0.84
1:A:50:ALA:HB2	1:A:377:MET:HE3	1.65	0.78
1:B:382:MET:HE3	1:B:389:ALA:N	1.98	0.78
1:B:414:ARG:HD2	3:B:516:HOH:O	1.84	0.77
1:A:414:ARG:HH11	1:A:414:ARG:HB2	1.49	0.77
1:B:295:GLU:HG2	3:B:499:HOH:O	1.87	0.75
1:A:59:LYS:HA	1:A:59:LYS:HE3	1.67	0.74
1:B:278:THR:HG21	3:B:446:HOH:O	1.88	0.73
1:A:414:ARG:HB2	1:A:414:ARG:NH1	2.03	0.73
1:B:83:THR:HG23	1:B:119:ILE:HD11	1.71	0.71
1:B:49:GLY:N	3:B:429:HOH:O	2.24	0.70
1:B:126:ASN:HD22	1:B:127:PHE:H	1.42	0.67
1:A:290:THR:HG22	1:A:343:VAL:HG12	1.77	0.67
1:A:299:ARG:HH22	1:B:126:ASN:HD21	1.41	0.66
1:A:390:LYS:N	1:A:390:LYS:HD2	2.12	0.64
1:A:70:GLN:HA	1:A:382:MET:HE1	1.81	0.63
1:B:385:GLN:NE2	1:B:416:GLU:H	1.96	0.62
1:B:385:GLN:HE22	1:B:416:GLU:N	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ALA:O	1:B:93:LEU:HD22	1.99	0.62
1:A:396:LEU:HD23	1:A:407:ALA:HB2	1.83	0.60
1:B:160:ILE:HG22	3:B:459:HOH:O	2.01	0.60
1:A:73:ILE:CG1	1:A:382:MET:HE3	2.32	0.59
1:B:388:LYS:HE3	3:B:582:HOH:O	2.01	0.59
1:B:346:LEU:C	1:B:346:LEU:HD12	2.27	0.59
1:B:83:THR:HG23	1:B:119:ILE:CD1	2.32	0.58
1:B:265:GLN:HG2	1:B:297:LEU:HD12	1.85	0.58
1:A:389:ALA:C	1:A:390:LYS:HD2	2.29	0.58
1:B:349:CYS:HA	3:B:446:HOH:O	2.03	0.58
1:B:265:GLN:HG2	1:B:294:GLY:HA2	1.86	0.57
1:A:73:ILE:HG12	1:A:382:MET:HE3	1.86	0.57
1:A:107:LEU:HD12	1:A:107:LEU:N	2.20	0.57
1:B:147:LEU:HD23	1:B:147:LEU:C	2.30	0.57
1:A:299:ARG:HH22	1:B:126:ASN:ND2	2.04	0.56
1:B:382:MET:HE3	1:B:389:ALA:H	1.69	0.56
1:B:126:ASN:ND2	1:B:127:PHE:H	2.04	0.56
1:B:113:ILE:O	1:B:134:SER:HB3	2.05	0.56
1:A:155:LEU:HD12	1:A:155:LEU:N	2.21	0.56
1:B:100:ASN:ND2	1:B:106:ASN:H	2.04	0.55
1:A:299:ARG:HH12	1:B:126:ASN:ND2	2.05	0.55
1:B:385:GLN:NE2	1:B:416:GLU:N	2.54	0.55
1:A:299:ARG:HD2	3:B:437:HOH:O	2.06	0.55
1:B:76:LEU:HD13	1:B:85:ALA:HB2	1.89	0.54
1:B:86:VAL:O	1:B:90:LEU:HD23	2.08	0.54
1:A:172:ARG:HH11	1:A:172:ARG:HB3	1.72	0.54
1:A:295:GLU:O	1:A:299:ARG:HG2	2.07	0.54
1:B:376:SER:HB3	1:B:395:ARG:HD2	1.90	0.53
1:B:370:TRP:NE1	1:B:409:GLU:HB2	2.24	0.53
1:A:295:GLU:CB	1:B:160:ILE:HD13	2.37	0.53
1:A:90:LEU:O	1:A:94:GLU:HG3	2.07	0.53
1:B:265:GLN:NE2	1:B:272:GLY:HA2	2.23	0.53
1:A:301:ILE:HD12	1:B:304:ARG:HD2	1.90	0.52
1:B:314:ASP:OD2	1:B:317:GLN:HB2	2.09	0.52
1:A:299:ARG:HH12	1:B:126:ASN:HD22	1.57	0.52
1:B:246:VAL:H	1:B:277:ASN:HD21	1.56	0.52
1:A:69:CYS:HB3	1:A:382:MET:HE2	1.91	0.52
1:B:395:ARG:HG3	1:B:395:ARG:HH11	1.75	0.51
1:A:172:ARG:HH11	1:A:172:ARG:CB	2.24	0.51
1:B:284:TYR:HB3	1:B:347:ARG:HG3	1.92	0.51
1:A:113:ILE:O	1:A:134:SER:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ARG:HE	1:B:308:HIS:CE1	2.28	0.50
1:A:302:LEU:HD13	1:A:343:VAL:HG11	1.94	0.50
1:A:242:HIS:CE1	1:A:243:GLU:HG3	2.47	0.50
1:B:292:GLY:HA3	1:B:341:GLY:HA2	1.93	0.50
1:B:388:LYS:HA	3:B:577:HOH:O	2.12	0.49
1:B:278:THR:HG22	1:B:284:TYR:C	2.37	0.49
1:A:153:GLY:C	1:A:155:LEU:H	2.20	0.49
1:A:168:GLU:O	1:A:172:ARG:HG3	2.12	0.49
1:B:124:SER:O	1:B:125:LEU:HB2	2.13	0.49
1:B:365:LEU:C	1:B:365:LEU:HD13	2.37	0.49
1:A:56:SER:N	3:A:504:HOH:O	2.44	0.48
1:A:103:MET:HE2	1:A:137:LYS:HE3	1.94	0.48
1:B:382:MET:HE3	1:B:389:ALA:HB2	1.96	0.48
1:A:246:VAL:H	1:A:277:ASN:HD21	1.60	0.48
1:A:414:ARG:HH11	1:A:414:ARG:CB	2.23	0.47
1:A:62:LYS:O	1:A:391:THR:HG21	2.14	0.47
1:A:147:LEU:C	1:A:147:LEU:HD23	2.40	0.47
1:A:346:LEU:C	1:A:346:LEU:HD23	2.40	0.47
1:A:300:THR:O	1:A:301:ILE:C	2.58	0.47
1:A:47:HIS:CE1	1:A:291:SER:HB2	2.49	0.47
1:B:116:ASP:HB3	1:B:267:ALA:HB2	1.98	0.46
1:B:295:GLU:OE1	1:B:295:GLU:HA	2.16	0.46
1:A:109:LEU:HD23	1:B:172:ARG:HH12	1.80	0.46
1:A:327:PHE:CE2	1:A:339:VAL:HG12	2.50	0.46
1:B:64:VAL:HG21	1:B:96:SER:HB2	1.98	0.46
1:A:73:ILE:HG13	1:A:382:MET:HG2	1.98	0.46
1:A:313:GLU:HG2	3:A:489:HOH:O	2.15	0.46
1:B:90:LEU:O	1:B:94:GLU:HG3	2.16	0.46
1:B:278:THR:HG22	1:B:284:TYR:CA	2.45	0.46
1:B:290:THR:HG22	1:B:343:VAL:CG1	2.40	0.46
1:A:44:VAL:HG23	1:A:239:VAL:HG22	1.98	0.45
1:A:54:SER:C	1:A:56:SER:H	2.25	0.45
1:B:317:GLN:O	1:B:321:GLU:HG3	2.15	0.45
1:A:159:ARG:CD	1:B:255:LEU:HD21	2.36	0.45
1:A:348:SER:HA	1:A:365:LEU:O	2.18	0.44
1:B:337:ASP:CG	1:B:337:ASP:O	2.61	0.44
1:B:83:THR:HG22	1:B:144:ASN:OD1	2.17	0.44
1:A:246:VAL:HG22	1:A:277:ASN:HD22	1.83	0.44
1:A:70:GLN:O	1:A:74:GLU:HG3	2.17	0.43
1:B:371:SER:HA	1:B:407:ALA:O	2.18	0.43
1:A:335:SER:HB2	3:A:532:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:382:MET:HB2	1:B:389:ALA:HA	1.99	0.43
1:A:59:LYS:HA	1:A:59:LYS:CE	2.43	0.43
1:A:116:ASP:HB3	1:A:267:ALA:HB2	2.01	0.43
1:A:234:THR:HG23	1:A:252:SER:HB2	2.00	0.43
1:A:240:VAL:HA	1:A:245:ASN:O	2.17	0.43
1:A:63:HIS:O	1:A:66:LYS:HB3	2.19	0.43
1:B:300:THR:O	1:B:301:ILE:C	2.61	0.43
1:A:100:ASN:ND2	1:A:106:ASN:H	2.16	0.42
1:B:47:HIS:CE1	1:B:291:SER:HB2	2.54	0.42
1:A:161:PRO:HA	1:A:162:PRO:HD3	1.81	0.42
1:A:367:GLU:HG2	1:A:412:VAL:HG12	2.01	0.42
1:B:384:ALA:HB3	3:B:565:HOH:O	2.18	0.42
1:A:66:LYS:O	1:A:70:GLN:HG3	2.19	0.42
1:A:103:MET:CE	1:A:137:LYS:HE3	2.49	0.42
1:B:73:ILE:HG13	1:B:382:MET:SD	2.60	0.42
1:B:278:THR:HG23	1:B:285:SER:OG	2.20	0.42
1:A:55:GLU:C	3:A:504:HOH:O	2.63	0.41
1:A:73:ILE:HG13	1:A:382:MET:HE3	2.02	0.41
1:A:370:TRP:CE2	1:A:409:GLU:HB2	2.56	0.41
1:A:370:TRP:NE1	1:A:409:GLU:HB2	2.35	0.41
1:B:72:ALA:HB2	1:B:89:ALA:HB2	2.02	0.41
1:A:46:VAL:HG12	1:A:237:ALA:CB	2.51	0.41
1:A:304:ARG:NH1	1:B:301:ILE:HD12	2.35	0.41
1:A:127:PHE:CZ	1:A:129:ALA:HB2	2.55	0.41
1:B:76:LEU:HD13	1:B:85:ALA:CB	2.51	0.41
1:B:126:ASN:HD22	1:B:127:PHE:N	2.12	0.41
1:A:47:HIS:HB3	1:A:344:ILE:HG21	2.02	0.41
1:A:146:LEU:HD23	1:A:173:TRP:CZ2	2.55	0.41
1:A:383:SER:O	1:A:386:ASP:HB3	2.19	0.41
1:B:66:LYS:HE2	1:B:70:GLN:OE1	2.20	0.41
1:B:239:VAL:CG1	1:B:240:VAL:N	2.83	0.41
1:B:370:TRP:CE2	1:B:409:GLU:HB2	2.56	0.41
1:A:313:GLU:HB2	3:A:535:HOH:O	2.21	0.41
1:A:380:GLY:HA2	1:A:390:LYS:O	2.21	0.41
1:B:323:MET:O	1:B:327:PHE:HB3	2.21	0.41
1:B:145:ARG:NH2	1:B:149:GLU:OE2	2.55	0.40
1:A:67:ARG:NH2	3:A:496:HOH:O	2.54	0.40
1:B:396:LEU:HD23	1:B:407:ALA:HB2	2.03	0.40
1:B:49:GLY:N	3:B:561:HOH:O	2.53	0.40
1:B:287:ALA:HB3	1:B:346:LEU:HG	2.04	0.40

There are no symmetry-related clashes.

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	302/420 (72%)	291 (96%)	7 (2%)	4 (1%)	9	3
1	B	305/420 (73%)	296 (97%)	7 (2%)	2 (1%)	18	10
All	All	607/840 (72%)	587 (97%)	14 (2%)	6 (1%)	12	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	SER
1	A	154	LYS
1	A	387	GLY
1	A	388	LYS
1	B	49	GLY
1	A	180	PRO

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	233/331 (70%)	227 (97%)	6 (3%)	40	35
1	B	235/331 (71%)	230 (98%)	5 (2%)	47	44
All	All	468/662 (71%)	457 (98%)	11 (2%)	43	38

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LYS
1	A	107	LEU
1	A	172	ARG
1	A	265	GLN
1	A	302	LEU
1	A	390	LYS
1	B	76	LEU
1	B	93	LEU
1	B	265	GLN
1	B	313	GLU
1	B	346	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	144	ASN
1	A	277	ASN
1	A	282	ASN
1	A	385	GLN
1	B	77	GLN
1	B	100	ASN
1	B	126	ASN
1	B	151	GLN
1	B	265	GLN
1	B	277	ASN
1	B	308	HIS
1	B	311	GLN
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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

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

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.