



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:36 AM GMT

PDB ID : 3R6L  
Title : Caspase-2 T380A bound with Ac-VDVAD-CHO  
Authors : Tang, Y.; Wells, J.; Arkin, M.  
Deposited on : 2011-03-21  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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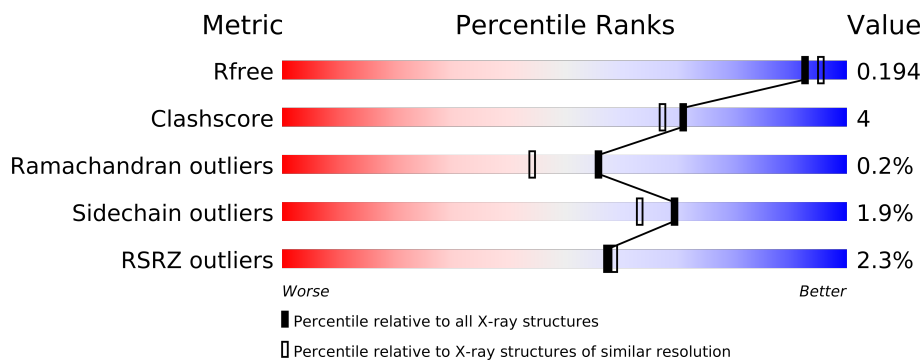
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	160	
1	C	160	
2	B	112	
2	D	112	
3	E	6	
3	F	6	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4489 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Caspase-2 subunit p18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	1	2	0
			1212	772	210	221	9			
1	C	160	Total	C	N	O	S	0	1	0
			1250	792	216	233	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	EXPRESSION TAG	UNP P42575
C	174	MET	-	EXPRESSION TAG	UNP P42575

- Molecule 2 is a protein called Caspase-2 subunit p12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	2	0
			762	480	137	131	14			
2	D	98	Total	C	N	O	S	2	3	0
			782	494	140	133	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	380	ALA	THR	ENGINEERED MUTATION	UNP P42575
B	453	LEU	-	EXPRESSION TAG	UNP P42575
B	454	GLU	-	EXPRESSION TAG	UNP P42575
B	455	HIS	-	EXPRESSION TAG	UNP P42575
B	456	HIS	-	EXPRESSION TAG	UNP P42575
B	457	HIS	-	EXPRESSION TAG	UNP P42575
B	458	HIS	-	EXPRESSION TAG	UNP P42575
B	459	HIS	-	EXPRESSION TAG	UNP P42575
B	460	HIS	-	EXPRESSION TAG	UNP P42575
D	380	ALA	THR	ENGINEERED MUTATION	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
D	453	LEU	-	EXPRESSION TAG	UNP P42575
D	454	GLU	-	EXPRESSION TAG	UNP P42575
D	455	HIS	-	EXPRESSION TAG	UNP P42575
D	456	HIS	-	EXPRESSION TAG	UNP P42575
D	457	HIS	-	EXPRESSION TAG	UNP P42575
D	458	HIS	-	EXPRESSION TAG	UNP P42575
D	459	HIS	-	EXPRESSION TAG	UNP P42575
D	460	HIS	-	EXPRESSION TAG	UNP P42575

- Molecule 3 is a protein called Peptide Inhibitor (ACE)VDVAD-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			38	23	5	10			
3	E	6	Total	C	N	O	0	0	0
			38	23	5	10			

- Molecule 4 is water.

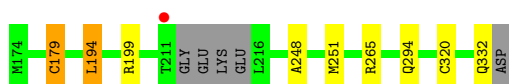
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	129	Total	O	0	0
			129	129		
4	B	59	Total	O	0	0
			59	59		
4	C	128	Total	O	0	0
			128	128		
4	D	86	Total	O	0	0
			86	86		
4	F	4	Total	O	0	0
			4	4		
4	E	1	Total	O	0	0
			1	1		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Caspase-2 subunit p18

Chain A: 



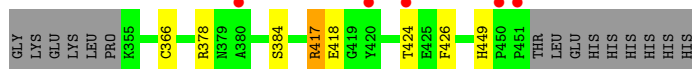
- Molecule 1: Caspase-2 subunit p18

Chain C: 



- Molecule 2: Caspase-2 subunit p12

Chain B: 



- Molecule 2: Caspase-2 subunit p12

Chain D: 



- Molecule 3: Peptide Inhibitor (ACE)VDVAD-CHO

Chain F: 



- Molecule 3: Peptide Inhibitor (ACE)VDVAD-CHO

Chain E: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.91Å 97.06Å 98.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 46.51 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-1.90) 99.5 (46.51-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.85 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.168 , 0.194 0.169 , 0.194	Depositor DCC
$R_{free}$ test set	2408 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	16.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 32.5	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 47712 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4489	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.11% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/1242	0.65	0/1680
1	C	0.66	0/1278	0.72	3/1728 (0.2%)
2	B	0.70	0/786	0.75	2/1058 (0.2%)
2	D	0.79	2/810 (0.2%)	0.77	2/1088 (0.2%)
3	E	0.47	0/27	0.66	0/37
3	F	0.59	0/27	0.75	0/37
All	All	0.68	2/4170 (0.0%)	0.71	7/5628 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	440[A]	CYS	CB-SG	-7.63	1.69	1.82
2	D	440[B]	CYS	CB-SG	-7.63	1.69	1.82

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	ARG	NE-CZ-NH1	6.51	123.55	120.30
2	B	417	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	C	219	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	D	401[A]	MET	CG-SD-CE	5.30	108.69	100.20
2	D	401[B]	MET	CG-SD-CE	5.30	108.69	100.20
1	C	190	LEU	CA-CB-CG	5.14	127.13	115.30
1	C	301	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1212	0	1184	8	0
1	C	1250	0	1215	16	0
2	B	762	0	747	7	0
2	D	782	0	784	7	0
3	E	38	0	34	3	0
3	F	38	0	34	6	0
4	A	129	0	0	1	0
4	B	59	0	0	2	0
4	C	128	0	0	0	0
4	D	86	0	0	5	0
4	E	1	0	0	0	0
4	F	4	0	0	0	0
All	All	4489	0	3998	36	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (36) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:320:CYS:SG	3:F:406:ASA:C	2.21	1.29
2:D:366[A]:CYS:SG	4:D:580:HOH:O	1.98	1.21
1:A:320:CYS:SG	3:E:406:ASA:C	2.36	1.14
1:A:294:GLN:NE2	4:A:620:HOH:O	1.83	1.08
2:B:366[A]:CYS:SG	4:B:555:HOH:O	2.13	1.06
1:C:320:CYS:SG	3:F:406:ASA:HXT	2.03	0.98
1:C:187:HIS:O	1:C:190:LEU:HD22	1.82	0.79
1:A:194:LEU:HD22	1:A:199:ARG:HD2	1.70	0.72
1:C:325:THR:HG21	2:D:425:GLU:HG3	1.77	0.65
1:C:177:LYS:HD2	4:D:531:HOH:O	1.98	0.64
1:A:320:CYS:SG	3:E:406:ASA:HXT	2.34	0.63
2:D:354:PRO:O	2:D:355:LYS:HB3	2.00	0.62
4:D:584:HOH:O	3:F:401:ACE:H1	1.99	0.61
2:B:417:ARG:HD3	4:B:516:HOH:O	2.00	0.61
1:C:249:GLN:O	1:C:253:GLU:HG3	2.01	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:424:THR:HG23	2:B:426:PHE:H	1.66	0.60
1:C:248:ALA:HA	1:C:251:MET:HE2	1.87	0.57
1:A:320:CYS:SG	3:E:406:ASA:O	2.65	0.55
1:C:320:CYS:HG	3:F:406:ASA:HXT	1.75	0.52
1:C:306:PRO:HA	1:C:309:GLN:HG3	1.92	0.51
1:A:248:ALA:HA	1:A:251:MET:HE2	1.95	0.48
2:D:381:LYS:HG3	4:D:584:HOH:O	2.13	0.48
1:C:325:THR:HG21	2:D:425:GLU:CG	2.45	0.47
1:C:320:CYS:SG	3:F:406:ASA:O	2.67	0.45
1:A:179[B]:CYS:SG	2:B:449:HIS:HB2	2.57	0.45
2:B:417:ARG:HG2	2:B:418:GLU:N	2.31	0.45
1:C:205:LEU:HD23	1:C:243:LEU:HB2	1.98	0.45
1:C:200:GLY:HA2	1:C:267:THR:HB	2.00	0.44
2:B:417:ARG:HG2	2:B:418:GLU:H	1.83	0.43
1:C:320:CYS:SG	3:F:406:ASA:CA	3.00	0.43
1:C:205:LEU:HD23	1:C:243:LEU:CB	2.49	0.43
1:A:248:ALA:HA	1:A:251:MET:CE	2.47	0.43
2:D:396:GLU:CG	4:D:581:HOH:O	2.67	0.42
2:B:378:ARG:HA	2:B:384:SER:HA	2.02	0.41
1:C:248:ALA:HA	1:C:251:MET:CE	2.51	0.40
2:D:396:GLU:CG	2:D:397:ARG:HG2	2.51	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	153/160 (96%)	148 (97%)	5 (3%)	0	100	100
1	C	159/160 (99%)	155 (98%)	4 (2%)	0	100	100
2	B	97/112 (87%)	95 (98%)	2 (2%)	0	100	100
2	D	99/112 (88%)	97 (98%)	1 (1%)	1 (1%)	22	8
3	E	4/6 (67%)	4 (100%)	0	0	100	100
3	F	4/6 (67%)	4 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	516/556 (93%)	503 (98%)	12 (2%)	1 (0%)	56 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	355	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	131/140 (94%)	126 (96%)	5 (4%)	44 31
1	C	135/140 (96%)	133 (98%)	2 (2%)	76 73
2	B	80/95 (84%)	80 (100%)	0	100 100
2	D	84/95 (88%)	82 (98%)	2 (2%)	61 53
3	E	3/3 (100%)	3 (100%)	0	100 100
3	F	3/3 (100%)	3 (100%)	0	100 100
All	All	436/476 (92%)	427 (98%)	9 (2%)	69 59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179[A]	CYS
1	A	179[B]	CYS
1	A	194	LEU
1	A	265	ARG
1	A	332	GLN
1	C	190	LEU
1	C	325	THR
2	D	379	ASN
2	D	451	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	A	332	GLN
1	C	257	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ASA	E	406	3	7,7,7	1.80	1 (14%)	8,8,8	0.69	0
3	ASA	F	406	3	7,7,7	1.61	1 (14%)	8,8,8	0.79	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASA	E	406	3	-	1/5/6/6	0/0/0/0
3	ASA	F	406	3	-	1/5/6/6	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	406	ASA	CA-C	4.36	1.54	1.50
3	F	406	ASA	CA-C	3.76	1.54	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	406	ASA	O-C-CA-CB
3	F	406	ASA	O-C-CA-CB

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	155/160 (96%)	-0.20	1 (0%) 86 88	8, 17, 28, 33	4 (2%)
1	C	160/160 (100%)	-0.16	1 (0%) 86 88	7, 17, 30, 38	2 (1%)
2	B	97/112 (86%)	0.29	5 (5%) 26 26	6, 14, 36, 41	0
2	D	98/112 (87%)	0.13	4 (4%) 35 36	6, 14, 28, 43	1 (1%)
3	E	6/6 (100%)	0.99	1 (16%) 2 2	28, 33, 34, 37	0
3	F	6/6 (100%)	-0.15	0 100 100	20, 23, 27, 30	0
All	All	522/556 (93%)	-0.02	12 (2%) 57 59	6, 16, 32, 43	7 (1%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	354	PRO	5.5
1	A	211	THR	4.0
1	C	333	ASP	3.2
2	D	451	PRO	3.0
2	B	380	ALA	3.0
3	E	402	VAL	2.7
2	B	451	PRO	2.7
2	D	355	LYS	2.6
2	B	420	TYR	2.4
2	B	450	PRO	2.4
2	D	436	CYS	2.0
2	B	424	THR	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ASA	E	406	8/8	0.19	4.11	33,33,33,34	0
3	ASA	F	406	8/8	0.10	1.84	22,23,24,25	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.