



wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 08:54 pm BST

PDB ID : 3OD5
Title : Crystal structure of active caspase-6 bound with Ac-VEID-CHO
Authors : Wang, X.-J.; Liu, X.; Wang, K.-T.; Cao, Q.; Su, X.-D.
Deposited on : 2010-08-11
Resolution : 1.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
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

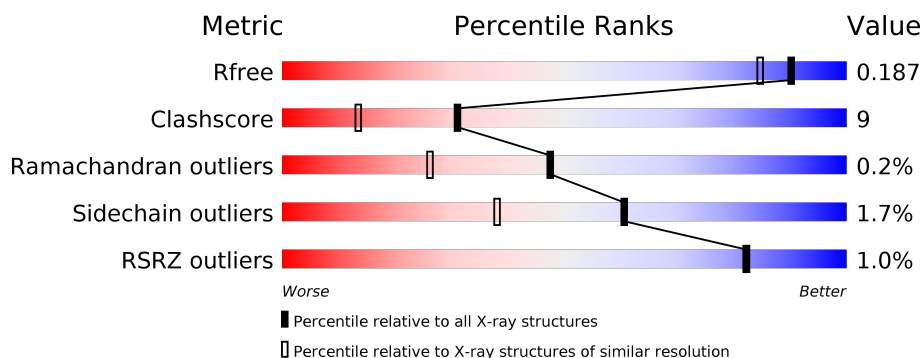
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 ≥ 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	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 9%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 76% 9% 14% </div> </div>
1	B	278	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 76%, yellow 9%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> % 76% 9% 14% </div> </div>
2	C	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 60%, yellow 40%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 60% 40% </div> </div>
2	D	5	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 60%, yellow 20%, orange 20%);"></div> <div style="display: flex; justify-content: space-between; padding: 0 5px;"> 60% 20% 20% </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASA	C	304	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4688 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 Caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1916	1232	329	341	14			
1	B	240	Total	C	N	O	S	0	0	0
			1915	1229	330	342	14			

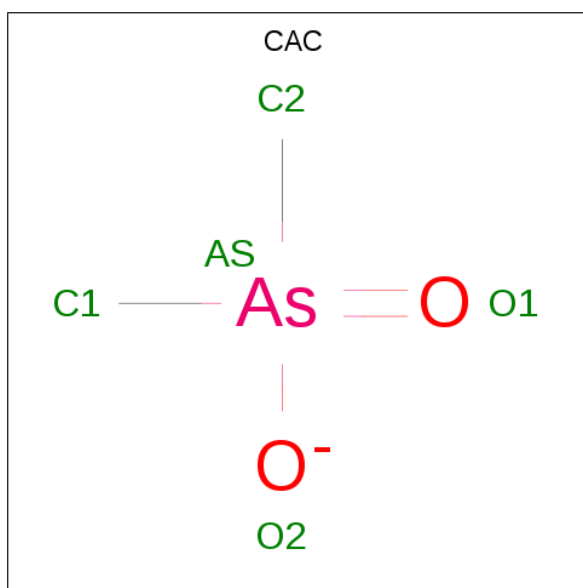
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	LEU	-	EXPRESSION TAG	UNP P55212
A	295	GLU	-	EXPRESSION TAG	UNP P55212
A	296	HIS	-	EXPRESSION TAG	UNP P55212
A	297	HIS	-	EXPRESSION TAG	UNP P55212
A	298	HIS	-	EXPRESSION TAG	UNP P55212
A	299	HIS	-	EXPRESSION TAG	UNP P55212
A	300	HIS	-	EXPRESSION TAG	UNP P55212
A	301	HIS	-	EXPRESSION TAG	UNP P55212
B	294	LEU	-	EXPRESSION TAG	UNP P55212
B	295	GLU	-	EXPRESSION TAG	UNP P55212
B	296	HIS	-	EXPRESSION TAG	UNP P55212
B	297	HIS	-	EXPRESSION TAG	UNP P55212
B	298	HIS	-	EXPRESSION TAG	UNP P55212
B	299	HIS	-	EXPRESSION TAG	UNP P55212
B	300	HIS	-	EXPRESSION TAG	UNP P55212
B	301	HIS	-	EXPRESSION TAG	UNP P55212

- Molecule 2 is a protein called peptide aldehyde inhibitor AC-VEID-CHO.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	0
			35	22	4	9			
2	D	5	Total	C	N	O	0	0	0
			35	22	4	9			

- Molecule 3 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	As	C	0	0
			3	1	2		
3	A	1	Total	As	C	0	0
			3	1	2		
3	A	1	Total	As	C	0	0
			3	1	2		
3	A	1	Total	As	C	0	0
			3	1	2		
3	B	1	Total	As	C	0	0
			3	1	2		
3	B	1	Total	As	C	0	0
			3	1	2		
3	B	1	Total	As	C	0	0
			3	1	2		

- Molecule 4 is water.

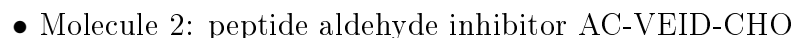
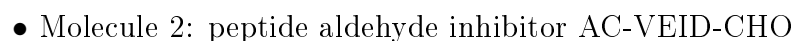
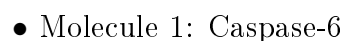
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	357	Total	O	0	0
			357	357		
4	C	14	Total	O	0	0
			14	14		
4	B	381	Total	O	0	0
			381	381		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	11	Total	O	0	0
			11	11		

- Molecule 1: Caspase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.46Å 89.59Å 61.15Å 90.00° 111.67° 90.00°	Depositor
Resolution (Å)	35.18 – 1.60 35.18 – 1.59	Depositor EDS
% Data completeness (in resolution range)	93.0 (35.18-1.60) 92.1 (35.18-1.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.59Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.155 , 0.189 0.152 , 0.187	Depositor DCC
R_{free} test set	3000 reflections (4.09%)	wwPDB-VP
Wilson B-factor (Å ²)	10.6	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4688	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.82% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CAC, 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	0.67	0/1964	0.78	2/2650 (0.1%)
1	B	0.73	0/1963	0.82	2/2651 (0.1%)
2	C	2.26	1/24 (4.2%)	1.12	0/32
2	D	1.80	1/24 (4.2%)	0.82	0/32
All	All	0.74	2/3975 (0.1%)	0.80	4/5365 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	300	ACE	C-N	10.62	1.58	1.34
2	D	300	ACE	C-N	7.35	1.50	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	65	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	65	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	71	ARG	NE-CZ-NH1	-5.82	117.39	120.30

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	1916	0	1867	35	0
1	B	1915	0	1858	31	0
2	C	35	0	33	4	0
2	D	35	0	32	3	0
3	A	12	0	0	1	0
3	B	12	0	0	1	0
4	A	357	0	0	16	1
4	B	381	0	0	18	1
4	C	14	0	0	0	0
4	D	11	0	0	1	0
All	All	4688	0	3790	68	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 9.

The worst 5 of 68 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:163:CYS:SG	2:C:304:ASA:HXT	1.79	1.17
1:B:138:THR:HB	4:B:729:HOH:O	1.49	1.12
1:B:101:HIS:O	1:B:105:THR:HG23	1.80	0.82
1:A:68:CYS:HB3	4:A:820:HOH:O	1.79	0.80
1:B:105:THR:HG22	4:B:695:HOH:O	1.81	0.80

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)
4:A:817:HOH:O	4:B:408:HOH:O[1_554]	2.17	0.03

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	236/278 (85%)	229 (97%)	6 (2%)	1 (0%)	34	15
1	B	236/278 (85%)	232 (98%)	4 (2%)	0	100	100
2	C	3/5 (60%)	3 (100%)	0	0	100	100
2	D	3/5 (60%)	3 (100%)	0	0	100	100
All	All	478/566 (84%)	467 (98%)	10 (2%)	1 (0%)	47	26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	TYR

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	205/246 (83%)	200 (98%)	5 (2%)	49	24
1	B	205/246 (83%)	203 (99%)	2 (1%)	76	61
2	C	3/3 (100%)	3 (100%)	0	100	100
2	D	3/3 (100%)	3 (100%)	0	100	100
All	All	416/498 (84%)	409 (98%)	7 (2%)	60	38

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	LEU
1	B	97	LEU
1	A	166	ASN
1	A	97	LEU
1	B	75	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	B	51	ASN
1	B	126	HIS
1	A	230	GLN
1	B	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	$\# Z > 2$
2	ASA	D	304	1,2	3,7,7	1.62	1 (33%)	1,8,8	1.64	0
2	ASA	C	304	1,2	3,7,7	0.94	0	1,8,8	1.13	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
2	ASA	D	304	1,2	-	2/3/6/6	-
2	ASA	C	304	1,2	-	3/3/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	ASA	O-C	2.73	1.30	1.19

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	304	ASA	C-CA-CB-CG
2	C	304	ASA	O-C-CA-CB
2	C	304	ASA	C-CA-CB-CG
2	D	304	ASA	N-CA-CB-CG
2	C	304	ASA	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	304	ASA	2	0
2	C	304	ASA	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands 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	CAC	A	7	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	A	3	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	A	8	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	B	6	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	B	2	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	B	5	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	A	1	1	0,2,4	0.00	-	0,1,6	0.00	-
3	CAC	B	4	1	0,2,4	0.00	-	0,1,6	0.00	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	8	CAC	1	0
3	B	5	CAC	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	240/278 (86%)	-0.53	2 (0%) 86 86	10, 16, 30, 58	0
1	B	240/278 (86%)	-0.41	3 (1%) 77 77	10, 14, 27, 67	0
2	C	3/5 (60%)	-0.56	0 100 100	17, 17, 17, 19	0
2	D	3/5 (60%)	-0.64	0 100 100	17, 17, 18, 18	0
All	All	486/566 (85%)	-0.47	5 (1%) 82 82	10, 15, 29, 67	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	VAL	7.4
1	A	197	VAL	4.3
1	A	198	TYR	3.7
1	B	198	TYR	3.5
1	B	175	LEU	2.5

6.2 Non-standard residues in protein, DNA, RNA chains [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	ASA	D	304	8/8	0.97	0.06	11,13,16,19	0
2	ASA	C	304	8/8	0.97	0.06	12,15,17,18	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
3	CAC	A	8	3/5	0.98	0.19	27,27,31,32	0
3	CAC	A	7	3/5	0.99	0.07	13,13,19,21	0
3	CAC	B	6	3/5	0.99	0.06	20,20,20,25	0
3	CAC	B	4	3/5	0.99	0.10	21,21,21,25	0
3	CAC	B	2	3/5	1.00	0.04	17,17,18,21	0
3	CAC	B	5	3/5	1.00	0.05	17,17,18,21	0
3	CAC	A	1	3/5	1.00	0.04	17,17,21,21	0
3	CAC	A	3	3/5	1.00	0.05	18,18,21,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.