



wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 08:54 PM GMT

PDB ID : 3V6M
Title : Inhibition of caspase-6 activity by single mutation outside the active site
Authors : Cao, Q.; Wang, X.J.; Liu, D.F.; Li, L.F.; Su, X.D.
Deposited on : 2011-12-20
Resolution : 2.69 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

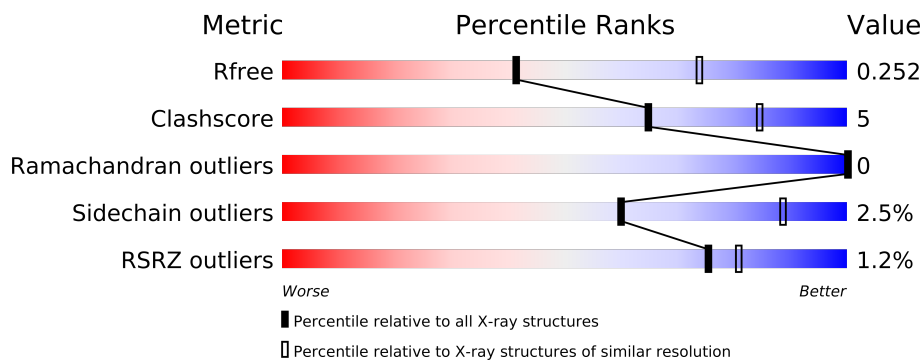
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.69 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. 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	279	
1	B	279	
1	C	279	
1	D	279	
1	F	279	
1	G	279	
1	I	279	
1	J	279	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12783 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1572	1013	265	281	13			
1	B	204	Total	C	N	O	S	0	0	0
			1597	1030	270	284	13			
1	C	205	Total	C	N	O	S	0	0	0
			1555	1002	261	279	13			
1	D	204	Total	C	N	O	S	0	0	0
			1595	1025	273	284	13			
1	F	203	Total	C	N	O	S	0	0	0
			1569	1012	265	279	13			
1	G	204	Total	C	N	O	S	0	0	0
			1616	1043	275	285	13			
1	I	204	Total	C	N	O	S	1	0	0
			1576	1017	263	283	13			
1	J	206	Total	C	N	O	S	0	0	0
			1638	1056	281	288	13			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP P55212
A	257	GLU	SER	SEE REMARK 999	UNP P55212
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	23	MET	-	EXPRESSION TAG	UNP P55212
B	257	GLU	SER	SEE REMARK 999	UNP P55212
B	294	LEU	-	EXPRESSION TAG	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	23	MET	-	EXPRESSION TAG	UNP P55212
C	257	GLU	SER	SEE REMARK 999	UNP P55212
C	294	LEU	-	EXPRESSION TAG	UNP P55212
C	295	GLU	-	EXPRESSION TAG	UNP P55212
C	296	HIS	-	EXPRESSION TAG	UNP P55212
C	297	HIS	-	EXPRESSION TAG	UNP P55212
C	298	HIS	-	EXPRESSION TAG	UNP P55212
C	299	HIS	-	EXPRESSION TAG	UNP P55212
C	300	HIS	-	EXPRESSION TAG	UNP P55212
C	301	HIS	-	EXPRESSION TAG	UNP P55212
D	23	MET	-	EXPRESSION TAG	UNP P55212
D	257	GLU	SER	SEE REMARK 999	UNP P55212
D	294	LEU	-	EXPRESSION TAG	UNP P55212
D	295	GLU	-	EXPRESSION TAG	UNP P55212
D	296	HIS	-	EXPRESSION TAG	UNP P55212
D	297	HIS	-	EXPRESSION TAG	UNP P55212
D	298	HIS	-	EXPRESSION TAG	UNP P55212
D	299	HIS	-	EXPRESSION TAG	UNP P55212
D	300	HIS	-	EXPRESSION TAG	UNP P55212
D	301	HIS	-	EXPRESSION TAG	UNP P55212
F	23	MET	-	EXPRESSION TAG	UNP P55212
F	257	GLU	SER	SEE REMARK 999	UNP P55212
F	294	LEU	-	EXPRESSION TAG	UNP P55212
F	295	GLU	-	EXPRESSION TAG	UNP P55212
F	296	HIS	-	EXPRESSION TAG	UNP P55212
F	297	HIS	-	EXPRESSION TAG	UNP P55212
F	298	HIS	-	EXPRESSION TAG	UNP P55212
F	299	HIS	-	EXPRESSION TAG	UNP P55212
F	300	HIS	-	EXPRESSION TAG	UNP P55212
F	301	HIS	-	EXPRESSION TAG	UNP P55212
G	23	MET	-	EXPRESSION TAG	UNP P55212
G	257	GLU	SER	SEE REMARK 999	UNP P55212
G	294	LEU	-	EXPRESSION TAG	UNP P55212
G	295	GLU	-	EXPRESSION TAG	UNP P55212
G	296	HIS	-	EXPRESSION TAG	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
G	297	HIS	-	EXPRESSION TAG	UNP P55212
G	298	HIS	-	EXPRESSION TAG	UNP P55212
G	299	HIS	-	EXPRESSION TAG	UNP P55212
G	300	HIS	-	EXPRESSION TAG	UNP P55212
G	301	HIS	-	EXPRESSION TAG	UNP P55212
I	23	MET	-	EXPRESSION TAG	UNP P55212
I	257	GLU	SER	SEE REMARK 999	UNP P55212
I	294	LEU	-	EXPRESSION TAG	UNP P55212
I	295	GLU	-	EXPRESSION TAG	UNP P55212
I	296	HIS	-	EXPRESSION TAG	UNP P55212
I	297	HIS	-	EXPRESSION TAG	UNP P55212
I	298	HIS	-	EXPRESSION TAG	UNP P55212
I	299	HIS	-	EXPRESSION TAG	UNP P55212
I	300	HIS	-	EXPRESSION TAG	UNP P55212
I	301	HIS	-	EXPRESSION TAG	UNP P55212
J	23	MET	-	EXPRESSION TAG	UNP P55212
J	257	GLU	SER	SEE REMARK 999	UNP P55212
J	294	LEU	-	EXPRESSION TAG	UNP P55212
J	295	GLU	-	EXPRESSION TAG	UNP P55212
J	296	HIS	-	EXPRESSION TAG	UNP P55212
J	297	HIS	-	EXPRESSION TAG	UNP P55212
J	298	HIS	-	EXPRESSION TAG	UNP P55212
J	299	HIS	-	EXPRESSION TAG	UNP P55212
J	300	HIS	-	EXPRESSION TAG	UNP P55212
J	301	HIS	-	EXPRESSION TAG	UNP P55212

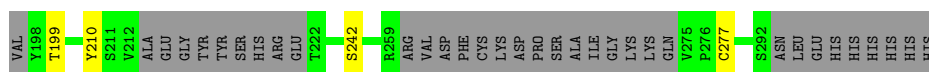
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	12	Total O 12 12	0	0
2	C	5	Total O 5 5	0	0
2	D	12	Total O 12 12	0	0
2	F	4	Total O 4 4	0	0
2	G	13	Total O 13 13	0	0
2	I	3	Total O 3 3	0	0

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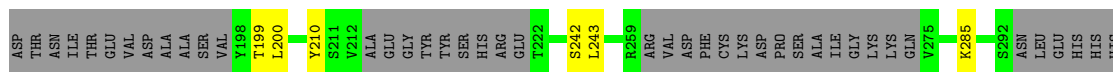
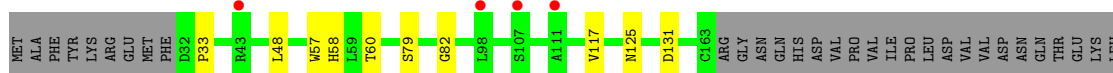
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	8	Total	O	0	0
			8	8		



• Molecule 1: Caspase-6

Chain F:



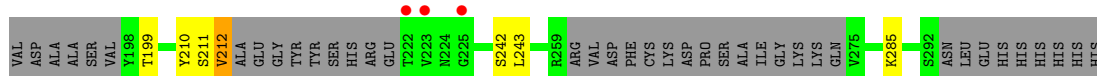
• Molecule 1: Caspase-6

Chain G:



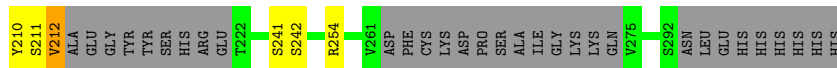
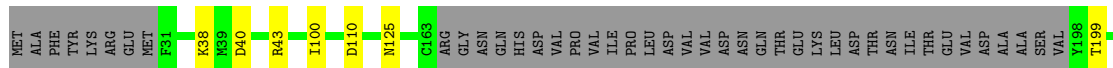
• Molecule 1: Caspase-6

Chain I:



• Molecule 1: Caspase-6

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.15Å 162.63Å 89.15Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	19.99 – 2.69 39.24 – 2.69	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-2.69) 92.9 (39.24-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.80 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.215 , 0.259 0.211 , 0.252	Depositor DCC
R_{free} test set	2980 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 59159 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12783	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.72	0/1604	0.70	0/2161
1	B	0.69	0/1633	0.73	0/2199
1	C	0.70	0/1587	0.69	0/2141
1	D	0.69	1/1629 (0.1%)	0.75	0/2191
1	F	0.75	0/1604	0.72	0/2165
1	G	0.74	1/1653 (0.1%)	0.74	1/2224 (0.0%)
1	I	0.74	0/1610	0.67	0/2170
1	J	0.69	0/1676	0.73	0/2254
All	All	0.72	2/12996 (0.0%)	0.72	1/17505 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	148	CYS	CB-SG	-5.92	1.72	1.81
1	D	277	CYS	CB-SG	-5.14	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	77	ARG	NE-CZ-NH1	-5.40	117.60	120.30

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	1572	0	0	11	0
1	B	1597	0	0	8	0
1	C	1555	0	7	11	0
1	D	1595	0	0	6	1
1	F	1569	0	0	11	0
1	G	1616	0	0	10	1
1	I	1576	0	0	9	0
1	J	1638	0	0	5	0
2	A	8	0	0	1	0
2	B	12	0	0	2	0
2	C	5	0	0	1	0
2	D	12	0	0	3	0
2	F	4	0	0	0	0
2	G	13	0	0	0	0
2	I	3	0	0	1	0
2	J	8	0	0	0	0
All	All	12783	0	7	68	1

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 5.

The worst 5 of 68 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:274:GLN:O	1:A:275:VAL:CG2	2.31	0.77
1:J:43:ARG:NH2	1:J:110:ASP:OD1	2.23	0.71
1:B:57:TRP:CD1	1:B:58:HIS:CE1	2.78	0.71
1:A:76:ARG:NH1	1:G:72:ASP:OD2	2.23	0.71
1:G:57:TRP:CE3	1:G:58:HIS:CE1	2.80	0.69

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	Distance(Å)	Clash(Å)
1:D:107:SER:OG	1:G:105:THR:OG1[2_555]	2.17	0.03

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	197/279 (71%)	190 (96%)	7 (4%)	0	100	100
1	B	196/279 (70%)	191 (97%)	5 (3%)	0	100	100
1	C	197/279 (71%)	193 (98%)	4 (2%)	0	100	100
1	D	196/279 (70%)	188 (96%)	8 (4%)	0	100	100
1	F	195/279 (70%)	187 (96%)	8 (4%)	0	100	100
1	G	196/279 (70%)	189 (96%)	7 (4%)	0	100	100
1	I	196/279 (70%)	192 (98%)	4 (2%)	0	100	100
1	J	198/279 (71%)	190 (96%)	8 (4%)	0	100	100
All	All	1571/2232 (70%)	1520 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	158/247 (64%)	154 (98%)	4 (2%)	60	89
1	B	164/247 (66%)	159 (97%)	5 (3%)	53	84
1	C	156/247 (63%)	148 (95%)	8 (5%)	33	64
1	D	165/247 (67%)	164 (99%)	1 (1%)	92	98
1	F	159/247 (64%)	156 (98%)	3 (2%)	69	92
1	G	167/247 (68%)	163 (98%)	4 (2%)	61	89
1	I	162/247 (66%)	159 (98%)	3 (2%)	69	92
1	J	171/247 (69%)	166 (97%)	5 (3%)	55	85
All	All	1302/1976 (66%)	1269 (98%)	33 (2%)	60	89

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	242	SER
1	F	60	THR

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Mol	Chain	Res	Type
1	J	241	SER
1	C	243	LEU
1	C	277	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 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, 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	205/279 (73%)	-0.06	2 (0%) 79 83	36, 51, 79, 118	0
1	B	204/279 (73%)	-0.27	1 (0%) 88 92	29, 47, 78, 105	0
1	C	205/279 (73%)	-0.01	6 (2%) 49 55	36, 55, 80, 119	1 (0%)
1	D	204/279 (73%)	-0.15	1 (0%) 88 92	28, 47, 78, 105	0
1	F	203/279 (72%)	0.06	4 (1%) 62 68	40, 55, 80, 105	0
1	G	204/279 (73%)	-0.08	1 (0%) 88 92	26, 47, 79, 106	0
1	I	204/279 (73%)	0.01	4 (1%) 62 68	39, 57, 79, 106	1 (0%)
1	J	206/279 (73%)	-0.15	0 100 100	25, 46, 79, 123	0
All	All	1635/2232 (73%)	-0.08	19 (1%) 75 81	25, 51, 80, 123	2 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	VAL	5.4
1	A	42	ARG	3.0
1	I	225	GLY	2.9
1	C	225	GLY	2.9
1	A	199	THR	2.8

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

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

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.