



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5IBC
Title : Caspase 3 V266I
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Deposited on : 2016-02-22
Resolution : 1.66 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

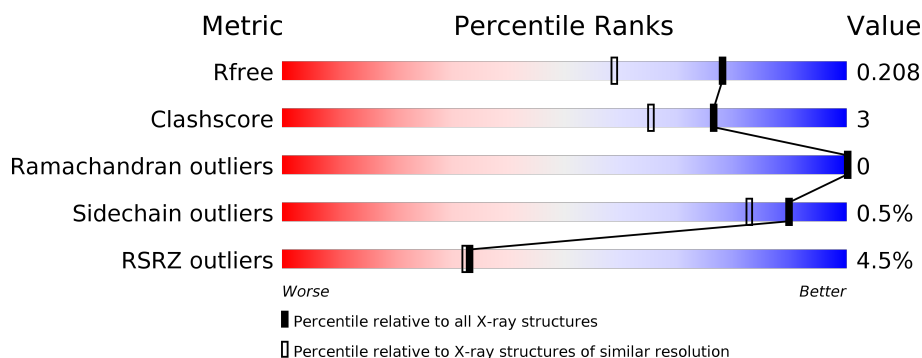
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.66 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}	111664	1521 (1.66-1.66)
Clashscore	122126	1616 (1.66-1.66)
Ramachandran outliers	120053	1584 (1.66-1.66)
Sidechain outliers	120020	1584 (1.66-1.66)
RSRZ outliers	108989	1487 (1.66-1.66)

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. 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	279	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>14%</div> </div> </div>
2	B	6	<div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2266 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	9	0
			1972	1257	337	362	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ILE	VAL	engineered mutation	UNP P42574
A	278	LEU	-	expression tag	UNP P42574
A	279	HIS	-	expression tag	UNP P42574

- Molecule 2 is a protein called ACE-ASP-GLU-VAL-ASK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	6	Total	C	Cl	N	O	0	0	1
			37	21	1	4	11			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	B	12	Total	O	0	0
			12	12		

i

- Molecule 1: Caspase-3



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	68.59Å 84.33Å 96.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.98 – 1.66 23.98 – 1.66	Depositor EDS
% Data completeness (in resolution range)	93.9 (23.98-1.66) 90.8 (23.98-1.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.12 (at 1.66Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.172 , 0.208 0.173 , 0.208	Depositor DCC
R_{free} test set	2000 reflections (6.34%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2266	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 5.42% 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: NA, OQE, 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	0.35	0/2038	0.56	0/2738
2	B	0.54	0/32	1.11	0/43
All	All	0.35	0/2070	0.57	0/2781

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	1972	0	1969	12	0
2	B	37	0	26	2	0
3	A	1	0	0	0	0
4	A	244	0	0	4	0
4	B	12	0	0	1	0
All	All	2266	0	1995	13	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 3.

All (13) 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)
2:B:994:OQE:CL1	4:B:1109:HOH:O	2.40	0.76
1:A:163:CYS:SG	2:B:993:ASP:C	2.75	0.65
1:A:185:HIS:N	4:A:401:HOH:O	2.30	0.65
1:A:207:ARG:HA	1:A:213:SER:HA	1.89	0.54
1:A:220:CYS:O	1:A:224:LYS:HD3	2.08	0.54
1:A:75[A]:ARG:NH2	4:A:407:HOH:O	2.42	0.53
1:A:74:LEU:HD13	1:A:117:VAL:HG11	1.94	0.50
1:A:228:ASP:OD1	1:A:229:LYS:NZ	2.45	0.49
1:A:242[A]:LYS:NZ	4:A:413:HOH:O	2.51	0.43
1:A:195:TYR:HB2	1:A:266:ILE:HB	2.00	0.42
1:A:88:LYS:HE3	1:A:88:LYS:HB3	1.89	0.42
1:A:149:ARG:HG2	4:A:563:HOH:O	2.19	0.41
1:A:120:SER:HB3	1:A:127[B]:ILE:HD11	2.03	0.41

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	246/279 (88%)	243 (99%)	3 (1%)	0	100	100
2	B	3/6 (50%)	3 (100%)	0	0	100	100
All	All	249/285 (87%)	246 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	219/251 (87%)	217 (99%)	2 (1%)	81	67
2	B	4/4 (100%)	4 (100%)	0	100	100
All	All	223/255 (88%)	221 (99%)	2 (1%)	90	67

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268[A]	MET
1	A	268[B]	MET

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

5.3.3 RNA [i](#)

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](#)

Of 1 ligands modelled in this entry, 1 is 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 [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	241/279 (86%)	0.10	11 (4%) 32 31	11, 16, 31, 59	0
2	B	4/6 (66%)	0.04	0 100 100	14, 15, 15, 16	0
All	All	245/285 (85%)	0.10	11 (4%) 33 32	11, 16, 31, 59	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	174	THR	6.7
1	A	185	HIS	6.5
1	A	172	ILE	4.9
1	A	170	CYS	4.8
1	A	32	SER	4.7
1	A	31	ILE	3.7
1	A	29	SER	3.7
1	A	33	LEU	3.6
1	A	278	LEU	3.6
1	A	279	HIS	3.2
1	A	30	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

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	NA	A	301	1/1	0.98	0.05	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.