wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2DKO
Title	:	Extended substrate recognition in caspase-3 revealed by high resolution X-ray structure analysis
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Deposited on	:	2006-04-12
Resolution	:	1.06 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 (i) 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 (1)) were used in the production of this report:

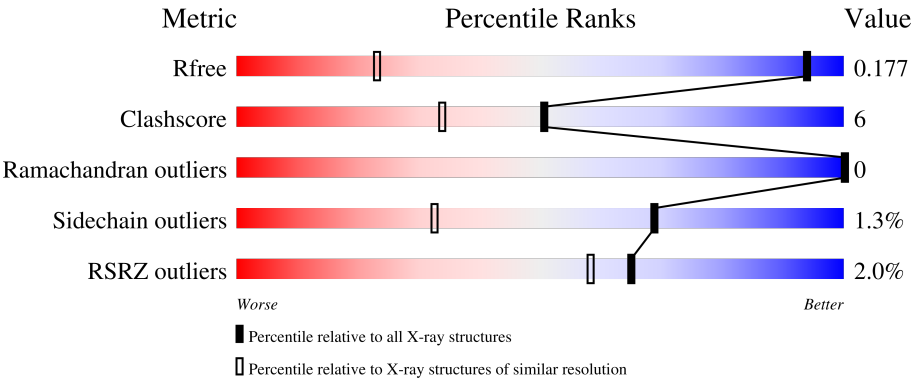
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

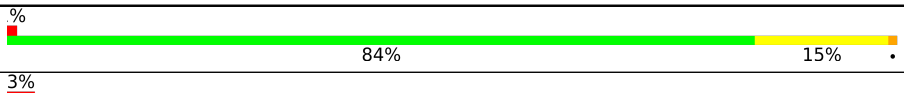
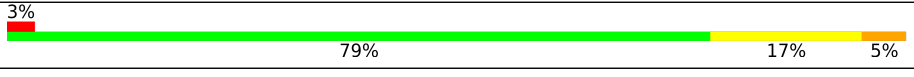
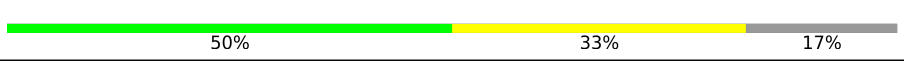
The reported resolution of this entry is 1.06 Å.

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	1202 (1.10-1.02)
Clashscore	141614	1252 (1.10-1.02)
Ramachandran outliers	138981	1204 (1.10-1.02)
Sidechain outliers	138945	1202 (1.10-1.02)
RSRZ outliers	127900	1178 (1.10-1.02)

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 <=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	146	
2	B	103	
3	I	6	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2427 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	146	Total	C	N	O	S	0	11	0
			1186	739	207	229	11			

- Molecule 2 is a protein called Caspase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	103	Total	C	N	O	S	0	9	0
			873	570	136	158	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	ALA	ASP	engineered mutation	UNP P42574

- Molecule 3 is a protein called PHQ-ASP-GLU-VAL-ASP-CHLOROMETHYLKETONE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	5	Total	C	N	O	0	0	1
			33	19	4	10			

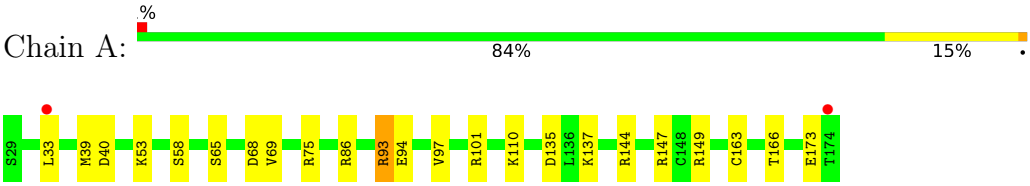
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	219	Total	O	0	0
			219	219		
4	B	109	Total	O	0	0
			109	109		
4	I	7	Total	O	0	0
			7	7		

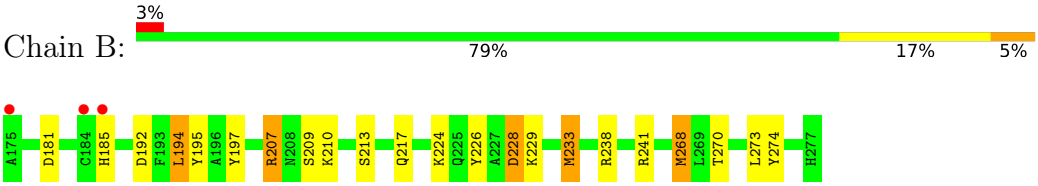
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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-3



• Molecule 2: Caspase-3



• Molecule 3: PHQ-ASP-GLU-VAL-ASP-CHLOROMETHYLKETONE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	67.65Å 83.89Å 96.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.06 13.48 – 1.06	Depositor EDS
% Data completeness (in resolution range)	89.9 (20.00-1.06) 91.6 (13.48-1.06)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 1.06Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.142 , 0.175 0.143 , 0.177	Depositor DCC
R_{free} test set	2054 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å^2)	10.3	Xtriage
Anisotropy	0.396	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 708.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2427	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7791e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 0QE

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	0.80	0/1246	1.39	18/1668 (1.1%)
2	B	0.90	0/934	1.52	20/1261 (1.6%)
3	I	1.02	0/31	1.40	0/41
All	All	0.84	0/2211	1.45	38/2970 (1.3%)

There are no bond length outliers.

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	238	ARG	NE-CZ-NH1	14.02	127.31	120.30
2	B	185	HIS	CA-CB-CG	12.32	134.55	113.60
1	A	75	ARG	NE-CZ-NH1	12.05	126.33	120.30
1	A	40	ASP	CB-CG-OD2	10.54	127.79	118.30
1	A	101	ARG	CD-NE-CZ	10.21	137.89	123.60

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	1186	0	1189	16	0
2	B	873	0	843	9	0
3	I	33	0	22	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	219	0	0	10	0
4	B	109	0	0	3	0
4	I	7	0	0	0	0
All	All	2427	0	2054	23	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 6.

The worst 5 of 23 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:228:ASP:OD1	2:B:229:LYS:HG3	1.90	0.72
1:A:163:CYS:SG	3:I:6:0QE:C1	2.79	0.70
1:A:110:LYS:HE2	4:A:337:HOH:O	1.91	0.69
1:A:166[B]:THR:HG23	4:A:200:HOH:O	1.98	0.62
1:A:163:CYS:SG	3:I:5:ASP:CA	2.87	0.62

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	155/146 (106%)	153 (99%)	2 (1%)	0	100	100
2	B	110/103 (107%)	109 (99%)	1 (1%)	0	100	100
3	I	2/6 (33%)	2 (100%)	0	0	100	100
All	All	267/255 (105%)	264 (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	142/131 (108%)	142 (100%)	0	100 100
2	B	99/90 (110%)	94 (95%)	5 (5%)	24 2
3	I	4/4 (100%)	4 (100%)	0	100 100
All	All	245/225 (109%)	240 (98%)	5 (2%)	69 17

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	194[A]	LEU
2	B	194[B]	LEU
2	B	210	LYS
2	B	268[A]	MET
2	B	268[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
2	B	234	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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^{th} 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	146/146 (100%)	0.39	2 (1%) 75 69	11, 16, 29, 38	1 (0%)
2	B	103/103 (100%)	0.49	3 (2%) 51 47	9, 14, 30, 42	0
3	I	4/6 (66%)	0.30	0 100 100	18, 19, 20, 21	0
All	All	253/255 (99%)	0.43	5 (1%) 65 58	9, 15, 30, 42	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	ALA	3.8
1	A	33	LEU	2.8
1	A	174	THR	2.7
2	B	184[A]	CYS	2.4
2	B	185	HIS	2.3

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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.