



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 3GJR / pdb_00003gjr
Title : Caspase-3 Binds Diverse P4 Residues in Peptides
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Deposited on : 2009-03-09
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

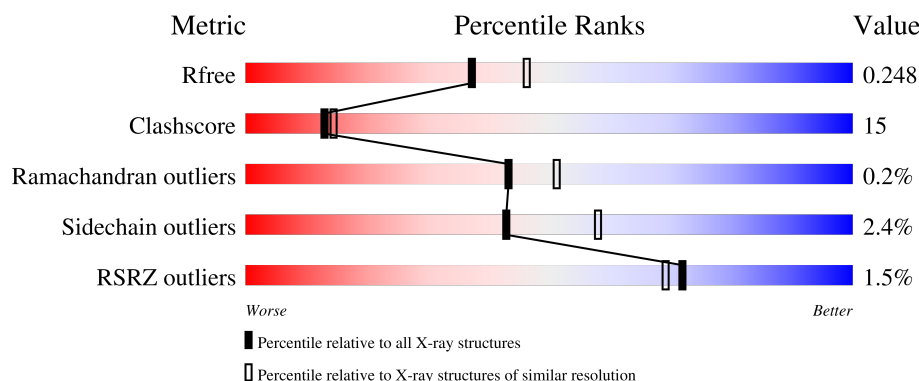
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 $\leq 5\%$. 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	147	 73% 22% .
1	C	147	 3% 61% 33% .. .
2	B	108	 % 65% 17% . . 15%
2	D	108	 % 63% 22% 15%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DZE	A	1	-	-	X	-
3	DZE	C	2	-	-	X	-
4	GOL	B	284	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3994 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 subunit p17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1120	692	202	217	9			
1	C	141	Total	C	N	O	S	0	0	0
			1120	692	202	217	9			

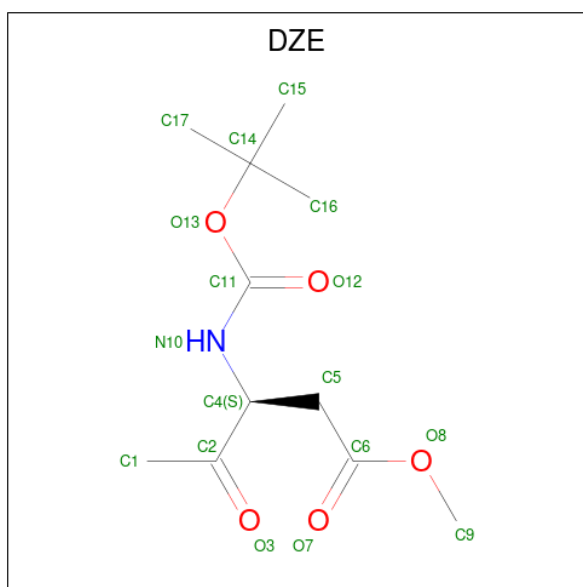
- Molecule 2 is a protein called Caspase-3 subunit p12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	92	Total	C	N	O	S	0	0	0
			767	505	122	135	5			
2	D	92	Total	C	N	O	S	0	0	0
			767	505	122	135	5			

There are 12 discrepancies between the modelled and reference sequences:

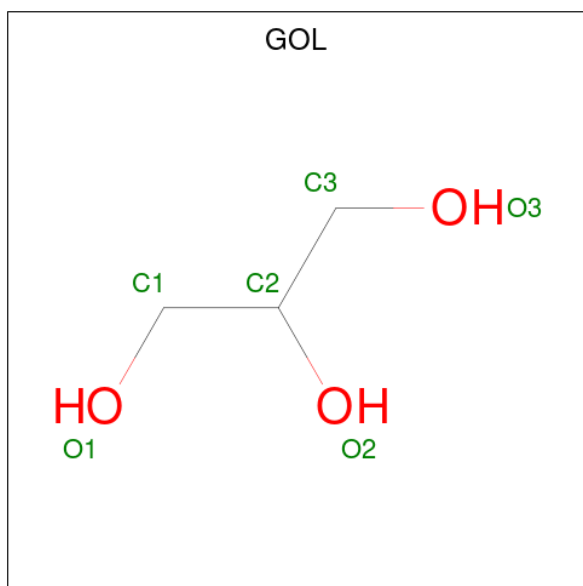
Chain	Residue	Modelled	Actual	Comment	Reference
B	278	HIS	-	expression tag	UNP P42574
B	279	HIS	-	expression tag	UNP P42574
B	280	HIS	-	expression tag	UNP P42574
B	281	HIS	-	expression tag	UNP P42574
B	282	HIS	-	expression tag	UNP P42574
B	283	HIS	-	expression tag	UNP P42574
D	278	HIS	-	expression tag	UNP P42574
D	279	HIS	-	expression tag	UNP P42574
D	280	HIS	-	expression tag	UNP P42574
D	281	HIS	-	expression tag	UNP P42574
D	282	HIS	-	expression tag	UNP P42574
D	283	HIS	-	expression tag	UNP P42574

- Molecule 3 is methyl (3S)-3-[(tert-butoxycarbonyl)amino]-4-oxopentanoate (CCD ID: DZE) (formula: C₁₁H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	11	1	5		
3	C	1	Total	C	N	O	0	0
			17	11	1	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	61	Total 61	O 61	0	0
5	B	39	Total 39	O 39	0	0
5	C	47	Total 47	O 47	0	0
5	D	27	Total 27	O 27	0	0

- Molecule 1: Caspase-3 subunit p17



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.40Å 69.68Å 93.40Å 90.00° 102.22° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.20) 89.2 (10.00-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.36Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.253 0.211 , 0.248	Depositor DCC
R_{free} test set	1209 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 45.0	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	0.92	EDS
Total number of atoms	3994	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/1135	0.87	3/1520 (0.2%)
1	C	0.43	0/1135	0.88	6/1520 (0.4%)
2	B	0.45	0/791	0.92	3/1068 (0.3%)
2	D	0.44	0/791	0.94	4/1068 (0.4%)
All	All	0.44	0/3852	0.90	16/5176 (0.3%)

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	267	SER	N-CA-C	6.61	119.29	108.52
2	D	252	PHE	N-CA-C	-6.37	104.99	112.89
1	C	129	GLY	N-CA-C	-6.21	102.84	112.85
2	D	268	MET	N-CA-C	-5.97	104.64	112.41
1	C	126	ILE	N-CA-C	5.79	117.02	108.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1120	0	1113	34	0
1	C	1120	0	1113	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	767	0	747	23	0
2	D	767	0	747	16	0
3	A	17	0	19	15	0
3	C	17	0	18	8	0
4	B	6	0	8	4	0
4	D	6	0	8	0	0
5	A	61	0	0	1	0
5	B	39	0	0	1	0
5	C	47	0	0	2	0
5	D	27	0	0	2	0
All	All	3994	0	3773	114	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 15.

The worst 5 of 114 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	3:A:1:DZE:C2	2.04	1.44
1:A:163:CYS:SG	3:A:1:DZE:C1	2.10	1.40
1:A:163:CYS:SG	3:A:1:DZE:H1B	1.70	1.31
2:D:194:LEU:HD12	2:D:269:LEU:HD11	1.44	0.99
1:C:170:CYS:HB2	5:C:209:HOH:O	1.62	0.98

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	139/147 (95%)	134 (96%)	5 (4%)	0	100	100
1	C	139/147 (95%)	132 (95%)	6 (4%)	1 (1%)	18	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	90/108 (83%)	87 (97%)	3 (3%)	0	100	100
2	D	90/108 (83%)	88 (98%)	2 (2%)	0	100	100
All	All	458/510 (90%)	441 (96%)	16 (4%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	90	ASP

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	127/132 (96%)	125 (98%)	2 (2%)	55	71
1	C	127/132 (96%)	124 (98%)	3 (2%)	43	58
2	B	82/96 (85%)	79 (96%)	3 (4%)	30	41
2	D	82/96 (85%)	80 (98%)	2 (2%)	43	58
All	All	418/456 (92%)	408 (98%)	10 (2%)	43	58

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	173	GLU
2	D	204	TYR
2	D	273	LEU
2	B	268	MET
2	B	273	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	56	HIS

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Mol	Chain	Res	Type
1	C	89	ASN
1	C	161	GLN
1	A	89	ASN
1	A	35	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	DZE	A	1	-	15,16,16	1.43	2 (13%)	18,22,22	2.17	4 (22%)
4	GOL	D	284	-	5,5,5	0.34	0	5,5,5	0.36	0
4	GOL	B	284	-	5,5,5	0.32	0	5,5,5	0.31	0
3	DZE	C	2	-	15,16,16	1.43	2 (13%)	18,22,22	2.19	4 (22%)

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	DZE	A	1	-	-	5/19/19/19	-
4	GOL	D	284	-	-	0/4/4/4	-
4	GOL	B	284	-	-	0/4/4/4	-
3	DZE	C	2	-	-	4/19/19/19	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	DZE	O8-C6	3.50	1.43	1.33
3	A	1	DZE	O8-C6	3.34	1.43	1.33
3	A	1	DZE	O13-C14	-2.34	1.44	1.48
3	C	2	DZE	O13-C14	-2.16	1.44	1.48

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	DZE	C14-O13-C11	-4.90	113.54	120.97
3	A	1	DZE	O13-C11-N10	4.89	118.04	110.03
3	C	2	DZE	O13-C11-N10	4.86	117.99	110.03
3	C	2	DZE	C14-O13-C11	-4.75	113.77	120.97
3	C	2	DZE	O7-C6-C5	-4.38	114.47	124.65

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	DZE	C2-C4-C5-C6
3	A	1	DZE	C5-C6-O8-C9
3	C	2	DZE	C5-C6-O8-C9
3	A	1	DZE	O7-C6-O8-C9
3	C	2	DZE	O7-C6-O8-C9

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	DZE	15	0
4	B	284	GOL	4	0
3	C	2	DZE	8	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	141/147 (95%)	-0.25	0 100 100	9, 19, 35, 48	0
1	C	141/147 (95%)	-0.02	5 (3%) 47 44	11, 23, 43, 58	0
2	B	92/108 (85%)	-0.41	1 (1%) 78 76	6, 15, 24, 45	0
2	D	92/108 (85%)	-0.30	1 (1%) 78 76	9, 17, 31, 55	0
All	All	466/510 (91%)	-0.22	7 (1%) 72 69	6, 19, 36, 58	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	CYS	3.6
2	D	277	HIS	2.8
1	C	126	ILE	2.8
2	B	277	HIS	2.2
1	C	34	ASP	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	GOL	D	284	6/6	0.78	0.16	42,44,45,45	0
3	DZE	C	2	17/17	0.79	0.16	35,40,46,46	0
3	DZE	A	1	17/17	0.81	0.17	29,33,40,40	0
4	GOL	B	284	6/6	0.84	0.12	21,26,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.