



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 11:07 PM UTC

PDB ID : 2H5J / pdb_00002h5j
Title : Crystal structure of caspase-3 with inhibitor Ac-DMQD-Cho
Authors : Fang, B.; Boross, P.I.; Tozser, J.; Weber, I.T.
Deposited on : 2006-05-26
Resolution : 2.00 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

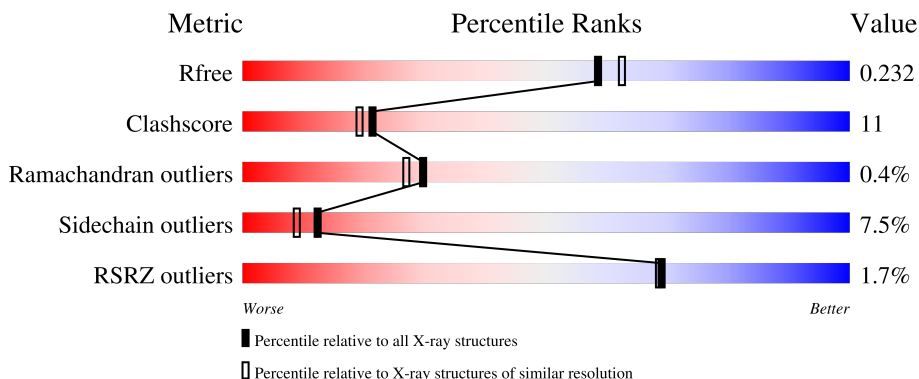
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	146	2% 75% 16% 5% ••
1	C	146	66% 24% 5% •
2	B	95	4% 80% 17% ••
2	D	95	• 78% 19% ••
3	E	5	80% 20%

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Mol	Chain	Length	Quality of chain
3	F	5	 60%40%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4359 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, p17 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	1	0
			1124	694	203	218	9			
1	C	140	Total	C	N	O	S	0	1	0
			1116	692	201	214	9			

- Molecule 2 is a protein called caspase-3, p12 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	95	Total	C	N	O	S	0	1	0
			800	524	132	138	6			
2	D	93	Total	C	N	O	S	0	2	0
			787	518	126	138	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	278	HIS	-	expression tag	UNP P42574
D	278	HIS	-	expression tag	UNP P42574

- Molecule 3 is a protein called Ac-DMQD-Cho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	5	Total	C	N	O	S	0	0	0
			36	20	5	10	1			
3	F	5	Total	C	N	O	S	0	0	0
			36	20	5	10	1			

- Molecule 4 is water.

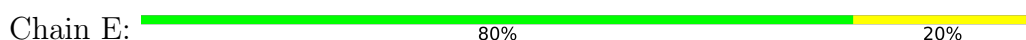
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	83	Total 83	O 83	0	0
4	C	128	Total 128	O 128	0	0
4	D	77	Total 77	O 77	0	0
4	E	12	Total 12	O 12	0	0
4	F	5	Total 5	O 5	0	0

- Molecule 1: caspase-3, p17 subunit





- Molecule 3: Ac-DMQD-Cho

Chain F:  60% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.15Å 69.34Å 94.09Å 90.00° 102.37° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00 10.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (10.00-2.00) 90.0 (10.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.179 , 0.269 0.176 , 0.232	Depositor DCC
R_{free} test set	2010 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.5	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 90.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4359	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.26% 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: ACE, ASJ

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	0.42	0/1143	1.34	8/1531 (0.5%)
1	C	0.38	0/1135	1.29	2/1520 (0.1%)
2	B	0.40	0/830	1.30	3/1120 (0.3%)
2	D	0.40	0/820	1.27	0/1106
3	E	0.32	0/25	1.33	0/32
3	F	0.25	0/25	0.80	0/32
All	All	0.40	0/3978	1.30	13/5341 (0.2%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	262	ILE	CA-C-O	-12.49	111.77	119.51
1	A	57	LYS	CA-C-N	8.20	137.20	121.54
1	A	57	LYS	C-N-CA	8.20	137.20	121.54
2	B	261	GLN	CA-C-N	-6.34	117.81	123.33
2	B	261	GLN	C-N-CA	-6.34	117.81	123.33

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	1124	0	1115	24	0
1	C	1116	0	1116	39	0
2	B	800	0	775	13	0
2	D	787	0	765	14	0
3	E	36	0	28	0	0
3	F	36	0	28	2	0
4	A	155	0	0	4	0
4	B	83	0	0	3	0
4	C	128	0	0	8	0
4	D	77	0	0	3	0
4	E	12	0	0	0	0
4	F	5	0	0	1	0
All	All	4359	0	3827	84	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 11.

The worst 5 of 84 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:C:36:SER:HB3	2:D:272[A]:GLU:HB2	1.61	0.82
1:A:97:VAL:HG22	1:A:138:LYS:HD2	1.64	0.79
2:B:213:SER:O	2:B:217:GLN:HG2	1.83	0.79
1:A:170:CYS:HB2	4:A:762:HOH:O	1.83	0.78
1:A:56:HIS:HB3	4:A:614:HOH:O	1.89	0.73

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	140/146 (96%)	135 (96%)	4 (3%)	1 (1%)	18 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	139/146 (95%)	134 (96%)	5 (4%)	0	100	100
2	B	94/95 (99%)	92 (98%)	1 (1%)	1 (1%)	11	7
2	D	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
3	E	3/5 (60%)	3 (100%)	0	0	100	100
3	F	3/5 (60%)	3 (100%)	0	0	100	100
All	All	472/492 (96%)	458 (97%)	12 (2%)	2 (0%)	30	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	SER
2	B	229	LYS

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	128/131 (98%)	116 (91%)	12 (9%)	8	5
1	C	127/131 (97%)	116 (91%)	11 (9%)	9	6
2	B	86/85 (101%)	82 (95%)	4 (5%)	23	22
2	D	85/85 (100%)	79 (93%)	6 (7%)	13	10
3	E	3/3 (100%)	3 (100%)	0	100	100
3	F	3/3 (100%)	3 (100%)	0	100	100
All	All	432/438 (99%)	399 (92%)	33 (8%)	12	9

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

Mol	Chain	Res	Type
2	D	209	SER
2	D	224	LYS
2	D	277	HIS
2	B	210	LYS

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Mol	Chain	Res	Type
1	A	173	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	234	HIS
2	D	185	HIS
1	C	80	ASN
1	C	35	ASN
1	C	89	ASN

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	$\# Z > 2$
3	ASJ	F	5	1,3	7,7,7	0.89	0	5,8,8	1.86	2 (40%)
3	ASJ	E	5	1,3	7,7,7	0.94	0	5,8,8	2.11	2 (40%)

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	ASJ	F	5	1,3	-	4/6/6/6	-
3	ASJ	E	5	1,3	-	4/6/6/6	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	5	ASJ	O-C-CA	3.10	123.47	111.52
3	F	5	ASJ	O-C-CA	3.09	123.39	111.52
3	E	5	ASJ	CB-CA-C	-2.81	107.12	112.21
3	F	5	ASJ	CB-CA-C	-2.21	108.21	112.21

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	5	ASJ	C-CA-CB-CG
3	E	5	ASJ	N-CA-CB-CG
3	F	5	ASJ	O-C-CA-N
3	F	5	ASJ	N-CA-CB-CG
3	E	5	ASJ	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 [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	141/146 (96%)	-0.49	3 (2%) 63 63	10, 20, 44, 62	1 (0%)
1	C	140/146 (95%)	-0.30	0 100 100	11, 25, 46, 59	1 (0%)
2	B	95/95 (100%)	-0.57	4 (4%) 40 39	8, 17, 34, 90	1 (1%)
2	D	93/95 (97%)	-0.57	1 (1%) 78 77	11, 20, 37, 78	2 (2%)
3	E	3/5 (60%)	-0.62	0 100 100	22, 22, 22, 23	0
3	F	3/5 (60%)	-0.47	0 100 100	26, 26, 27, 28	0
All	All	475/492 (96%)	-0.47	8 (1%) 69 68	8, 21, 45, 90	5 (1%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	277	HIS	3.4
1	A	56	HIS	3.3
1	A	58	SER	3.0
2	D	277	HIS	2.9
2	B	278	HIS	2.8

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
3	ASJ	E	5	8/8	0.94	0.06	17,18,22,23	0
3	ASJ	F	5	8/8	0.96	0.05	20,22,24,31	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.