



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 02:05 AM UTC

PDB ID : 4FXO / pdb_00004fxo
Title : Zinc-mediated allosteric inhibition of caspase-6
Authors : Velazquez-Delgado, E.M.; Hardy, J.A.
Deposited on : 2012-07-03
Resolution : 2.85 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
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

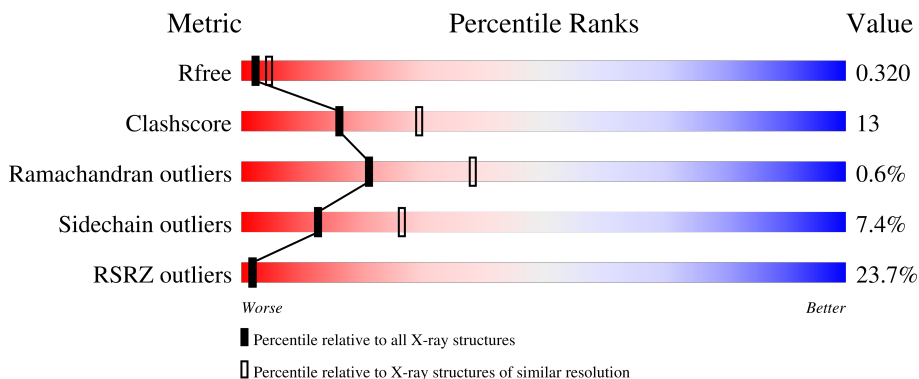
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	299	15% 54% 17% • 27%
1	B	299	19% 57% 16% • 24%
1	C	299	18% 49% 23% • 26%
1	D	299	18% 49% 22% • 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6781 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-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	1	0
			1692	1086	286	306	14			
1	B	227	Total	C	N	O	S	0	0	0
			1731	1106	300	311	14			
1	C	220	Total	C	N	O	S	0	0	0
			1680	1074	289	304	13			
1	D	220	Total	C	N	O	S	0	0	0
			1666	1064	286	303	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	294	HIS	-	expression tag	UNP P55212
A	295	HIS	-	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
B	294	HIS	-	expression tag	UNP P55212
B	295	HIS	-	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
C	294	HIS	-	expression tag	UNP P55212
C	295	HIS	-	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
D	294	HIS	-	expression tag	UNP P55212
D	295	HIS	-	expression tag	UNP P55212
D	296	HIS	-	expression tag	UNP P55212

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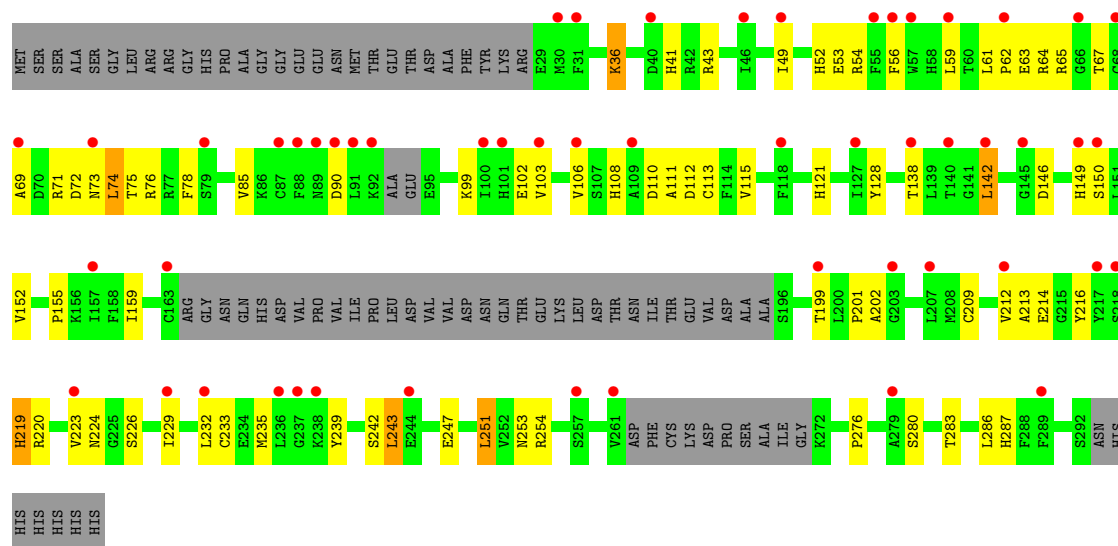
Chain	Residue	Modelled	Actual	Comment	Reference
D	297	HIS	-	expression tag	UNP P55212
D	298	HIS	-	expression tag	UNP P55212
D	299	HIS	-	expression tag	UNP P55212

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

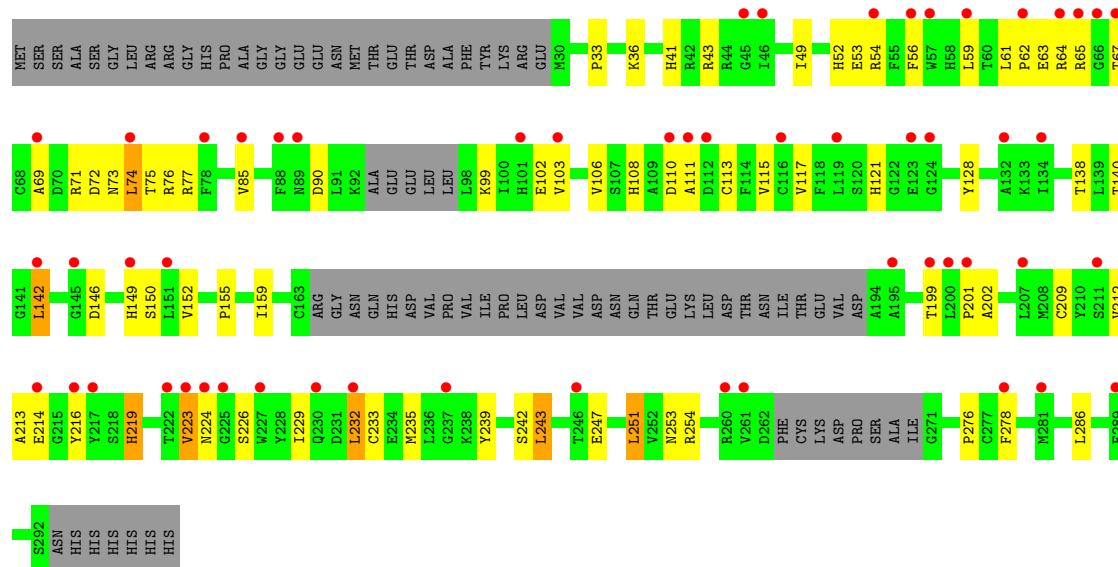
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		



● Molecule 1: Caspase-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.70Å 90.86Å 85.76Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	84.2 (30.00-2.85) 99.2 (30.00-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.215 , 0.233 0.302 , 0.320	Depositor DCC
R_{free} test set	4395 reflections (16.47%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.080 for h,-k,-l	Xtriage
Reported twinning fraction	0.401 for H, K, L 0.363 for -h,-k,l 0.119 for -H, -L, -K 0.117 for -H, L, K	Depositor
Outliers	0 of 23471 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	6781	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: ZN

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	0.37	0/1734	0.71	0/2343
1	B	0.37	0/1770	0.71	0/2389
1	C	0.41	0/1717	0.72	0/2317
1	D	0.41	0/1704	0.72	0/2304
All	All	0.39	0/6925	0.71	0/9353

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	VAL	Peptide
1	C	65	ARG	Peptide
1	D	223	VAL	Peptide
1	D	65	ARG	Peptide

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	1692	0	1584	37	0
1	B	1731	0	1619	34	0
1	C	1680	0	1561	54	0
1	D	1666	0	1529	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	6781	0	6293	171	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 13.

The worst 5 of 171 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:D:74:LEU:HD12	1:D:233:CYS:SG	1.93	1.08
1:C:67:THR:OG1	1:C:121:HIS:HE1	1.39	1.06
1:D:71:ARG:O	1:D:75:THR:HG22	1.57	1.05
1:C:71:ARG:O	1:C:75:THR:HG22	1.57	1.04
1:D:67:THR:OG1	1:D:121:HIS:HE1	1.42	0.99

There are no symmetry-related clashes.

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	212/299 (71%)	203 (96%)	8 (4%)	1 (0%)	24	42
1	B	219/299 (73%)	211 (96%)	7 (3%)	1 (0%)	24	42
1	C	212/299 (71%)	200 (94%)	11 (5%)	1 (0%)	24	42
1	D	212/299 (71%)	200 (94%)	10 (5%)	2 (1%)	14	28
All	All	855/1196 (72%)	814 (95%)	36 (4%)	5 (1%)	21	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	201	PRO
1	D	201	PRO
1	D	223	VAL
1	A	201	PRO
1	B	201	PRO

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	172/261 (66%)	163 (95%)	9 (5%)	21	43
1	B	173/261 (66%)	163 (94%)	10 (6%)	18	38
1	C	168/261 (64%)	153 (91%)	15 (9%)	9	20
1	D	164/261 (63%)	148 (90%)	16 (10%)	7	16
All	All	677/1044 (65%)	627 (93%)	50 (7%)	13	26

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	220	ARG
1	D	41	HIS
1	D	286	LEU

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Mol	Chain	Res	Type
1	C	232	LEU
1	C	251	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	GLN
1	D	219	HIS
1	D	258	GLN
1	D	121	HIS
1	B	89	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](#)

Of 4 ligands modelled in this entry, 4 are 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 [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	219/299 (73%)	1.43	45 (20%)	2 2	13, 28, 38, 40	1 (0%)
1	B	227/299 (75%)	1.56	57 (25%)	1 1	19, 29, 38, 40	0
1	C	220/299 (73%)	1.62	53 (24%)	2 1	29, 35, 42, 44	0
1	D	220/299 (73%)	1.56	55 (25%)	2 1	29, 35, 42, 44	0
All	All	886/1196 (74%)	1.54	210 (23%)	2 2	13, 32, 40, 44	1 (0%)

The worst 5 of 210 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	PHE	6.5
1	B	292	SER	6.2
1	A	104	SER	6.1
1	B	215	GLY	5.4
1	A	105	THR	5.4

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
2	ZN	A	301	1/1	0.67	0.10	21,21,21,21	0
2	ZN	D	301	1/1	0.78	0.23	28,28,28,28	0
2	ZN	C	301	1/1	0.83	0.16	34,34,34,34	0
2	ZN	B	301	1/1	0.94	0.08	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.