wwPDB X-ray Structure Validation Summary Report (i)

Sep 6, 2023 – 02:26 PM EDT

PDB ID	:	4FXO
Title	:	Zinc-mediated allosteric inhibiton 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 (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:

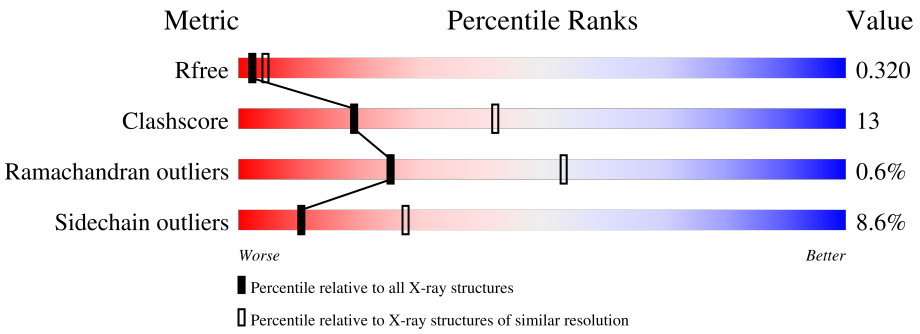
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)

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%

Mol	Chain	Length	Quality of chain
1	A	299	53% 18% • 27%
1	B	299	57% 17% • 24%
1	C	299	48% 23% • 26%
1	D	299	49% 21% • 26%

2 Entry composition (i)

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

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

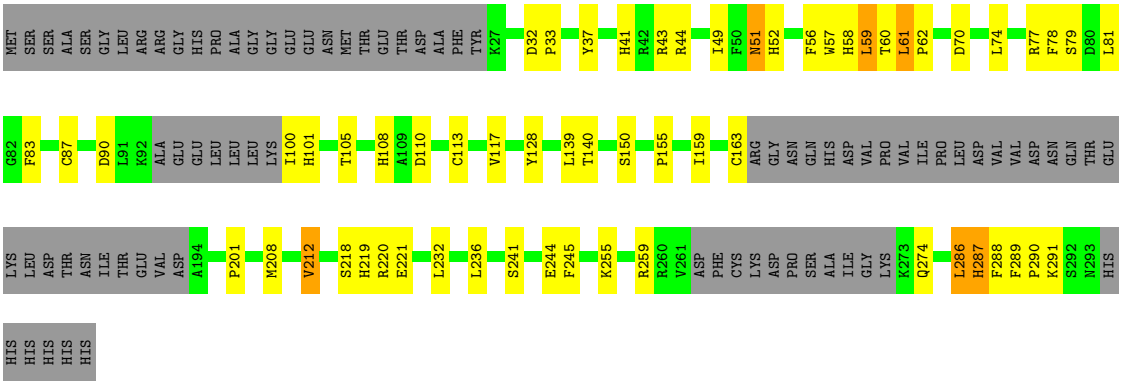
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

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. 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. 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.

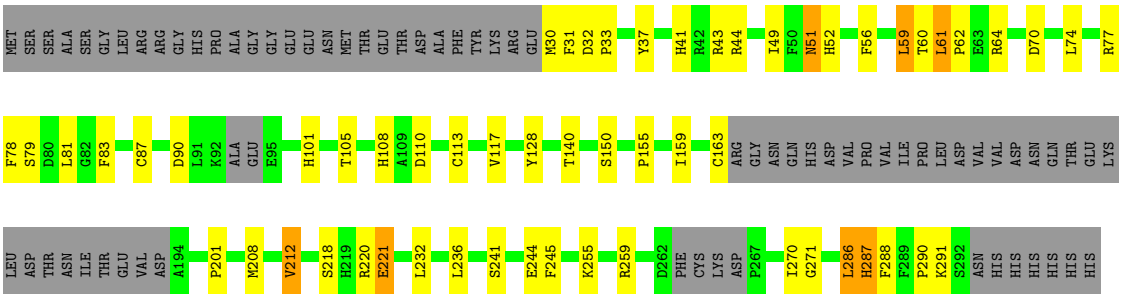
- Molecule 1: Caspase-6

Chain A:



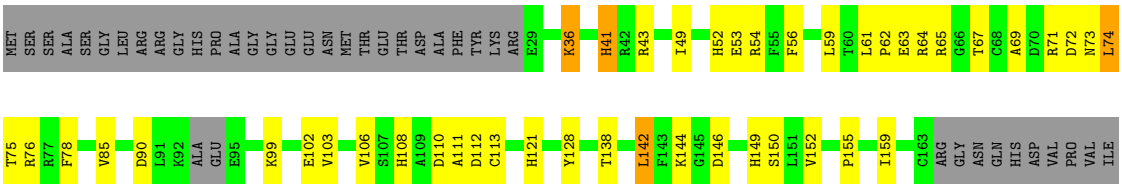
- Molecule 1: Caspase-6

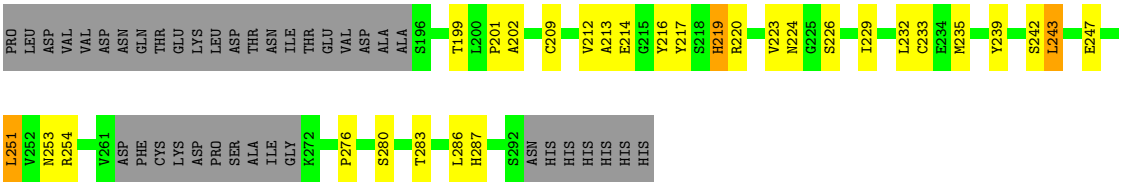
Chain B:



- Molecule 1: Caspase-6

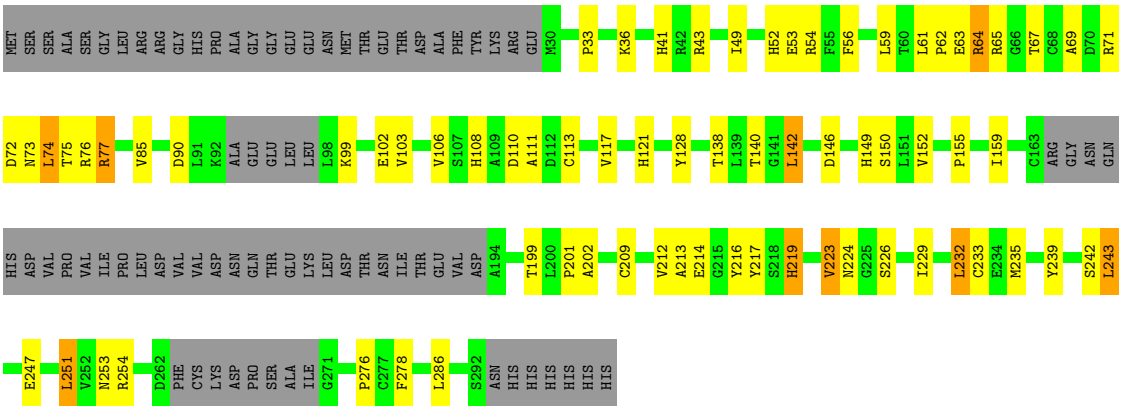
Chain C:





- Molecule 1: Caspase-6

Chain D:



4 Data and refinement statistics (i)

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 40.14 – 2.70	Depositor EDS
% Data completeness (in resolution range)	84.2 (30.00-2.85) 87.5 (40.14-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [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	1184 reflections (5.04%)	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 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.36$	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.31	0/1734	0.40	0/2343
1	B	0.31	0/1770	0.41	0/2389
1	C	0.34	0/1717	0.46	0/2317
1	D	0.35	0/1704	0.45	1/2304 (0.0%)
All	All	0.33	0/6925	0.43	1/9353 (0.0%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	232	LEU	CA-CB-CG	5.52	128.00	115.30

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

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Mol	Chain	Res	Type	Group
1	D	65	ARG	Peptide

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	1692	0	1584	37	0
1	B	1731	0	1619	34	0
1	C	1680	0	1561	55	0
1	D	1666	0	1529	53	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	170	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 170 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 (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	212/299 (71%)	203 (96%)	8 (4%)	1 (0%)	29	57
1	B	219/299 (73%)	211 (96%)	7 (3%)	1 (0%)	29	57
1	C	212/299 (71%)	200 (94%)	11 (5%)	1 (0%)	29	57
1	D	212/299 (71%)	200 (94%)	10 (5%)	2 (1%)	17	43
All	All	855/1196 (72%)	814 (95%)	36 (4%)	5 (1%)	25	53

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 (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	172/261 (66%)	161 (94%)	11 (6%)	17	41
1	B	173/261 (66%)	161 (93%)	12 (7%)	15	38
1	C	168/261 (64%)	151 (90%)	17 (10%)	7	20
1	D	164/261 (63%)	146 (89%)	18 (11%)	6	17
All	All	677/1044 (65%)	619 (91%)	58 (9%)	10	27

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	142	LEU
1	D	243	LEU
1	C	232	LEU
1	D	235	MET
1	D	146	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	258	GLN
1	D	121	HIS
1	D	258	GLN
1	D	219	HIS
1	B	52	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)

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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.