



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 09:14 am BST

PDB ID : 3P45
Title : Crystal structure of apo-caspase-6 at physiological pH
Authors : Mueller, I.; Lamers, M.B.A.C.; Ritchie, A.J.; Dominguez, C.; Munoz, I.; Mail-
lard, M.; Kiselyov, A.
Deposited on : 2010-10-06
Resolution : 2.53 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

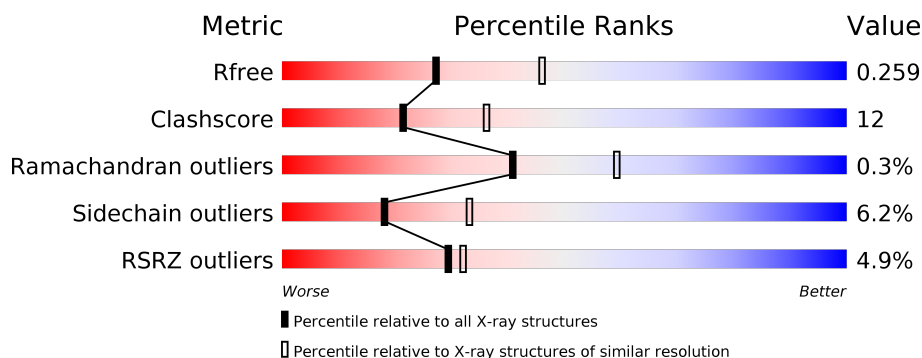
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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 on 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	179	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>13%</div> <div>•</div> <div>26%</div> </div> </div>
1	C	179	<div> <div>5%</div> <div> <div></div> <div>54%</div> <div>18%</div> <div>•</div> <div>26%</div> </div> </div>
1	E	179	<div> <div>2%</div> <div> <div></div> <div>55%</div> <div>16%</div> <div>•</div> <div>26%</div> </div> </div>
1	G	179	<div> <div>4%</div> <div> <div></div> <div>60%</div> <div>12%</div> <div>•</div> <div>27%</div> </div> </div>
1	I	179	<div> <div>0%</div> <div> <div></div> <div>58%</div> <div>13%</div> <div>•</div> <div>26%</div> </div> </div>
1	K	179	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>18%</div> <div>•</div> <div>26%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	M	179	
1	O	179	
2	B	108	
2	D	108	
2	F	108	
2	H	108	
2	J	108	
2	L	108	
2	N	108	
2	P	108	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12955 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	133	Total	C	N	O	S	0	0	0
			1058	678	183	190	7			
1	C	132	Total	C	N	O	S	0	0	0
			1054	676	184	188	6			
1	E	132	Total	C	N	O	S	0	0	0
			1058	679	186	187	6			
1	G	131	Total	C	N	O	S	0	0	0
			1040	666	180	188	6			
1	I	133	Total	C	N	O	S	0	0	0
			1063	681	185	190	7			
1	K	133	Total	C	N	O	S	0	0	0
			1037	665	181	184	7			
1	M	133	Total	C	N	O	S	0	0	0
			1055	677	183	188	7			
1	O	132	Total	C	N	O	S	0	0	0
			1043	670	179	188	6			

- Molecule 2 is a protein called caspase-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	S	0	0	0
			579	377	94	102	6			
2	D	70	Total	C	N	O	S	0	0	0
			554	361	89	98	6			
2	F	68	Total	C	N	O	S	0	0	0
			535	348	86	95	6			
2	H	68	Total	C	N	O	S	0	0	0
			545	356	89	94	6			
2	J	70	Total	C	N	O	S	0	0	0
			543	353	87	97	6			
2	L	66	Total	C	N	O	S	0	0	0
			521	339	84	92	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	67	Total	C	N	O	S	0	0	0
			531	345	85	95	6			
2	P	68	Total	C	N	O	S	0	0	0
			538	349	87	96	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	ARG	-	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
B	300	HIS	-	EXPRESSION TAG	UNP P55212
D	294	ARG	-	EXPRESSION TAG	UNP P55212
D	295	HIS	-	EXPRESSION TAG	UNP P55212
D	296	HIS	-	EXPRESSION TAG	UNP P55212
D	297	HIS	-	EXPRESSION TAG	UNP P55212
D	298	HIS	-	EXPRESSION TAG	UNP P55212
D	299	HIS	-	EXPRESSION TAG	UNP P55212
D	300	HIS	-	EXPRESSION TAG	UNP P55212
F	294	ARG	-	EXPRESSION TAG	UNP P55212
F	295	HIS	-	EXPRESSION TAG	UNP P55212
F	296	HIS	-	EXPRESSION TAG	UNP P55212
F	297	HIS	-	EXPRESSION TAG	UNP P55212
F	298	HIS	-	EXPRESSION TAG	UNP P55212
F	299	HIS	-	EXPRESSION TAG	UNP P55212
F	300	HIS	-	EXPRESSION TAG	UNP P55212
H	294	ARG	-	EXPRESSION TAG	UNP P55212
H	295	HIS	-	EXPRESSION TAG	UNP P55212
H	296	HIS	-	EXPRESSION TAG	UNP P55212
H	297	HIS	-	EXPRESSION TAG	UNP P55212
H	298	HIS	-	EXPRESSION TAG	UNP P55212
H	299	HIS	-	EXPRESSION TAG	UNP P55212
H	300	HIS	-	EXPRESSION TAG	UNP P55212
J	294	ARG	-	EXPRESSION TAG	UNP P55212
J	295	HIS	-	EXPRESSION TAG	UNP P55212
J	296	HIS	-	EXPRESSION TAG	UNP P55212
J	297	HIS	-	EXPRESSION TAG	UNP P55212
J	298	HIS	-	EXPRESSION TAG	UNP P55212
J	299	HIS	-	EXPRESSION TAG	UNP P55212

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Chain	Residue	Modelled	Actual	Comment	Reference
J	300	HIS	-	EXPRESSION TAG	UNP P55212
L	294	ARG	-	EXPRESSION TAG	UNP P55212
L	295	HIS	-	EXPRESSION TAG	UNP P55212
L	296	HIS	-	EXPRESSION TAG	UNP P55212
L	297	HIS	-	EXPRESSION TAG	UNP P55212
L	298	HIS	-	EXPRESSION TAG	UNP P55212
L	299	HIS	-	EXPRESSION TAG	UNP P55212
L	300	HIS	-	EXPRESSION TAG	UNP P55212
N	294	ARG	-	EXPRESSION TAG	UNP P55212
N	295	HIS	-	EXPRESSION TAG	UNP P55212
N	296	HIS	-	EXPRESSION TAG	UNP P55212
N	297	HIS	-	EXPRESSION TAG	UNP P55212
N	298	HIS	-	EXPRESSION TAG	UNP P55212
N	299	HIS	-	EXPRESSION TAG	UNP P55212
N	300	HIS	-	EXPRESSION TAG	UNP P55212
P	294	ARG	-	EXPRESSION TAG	UNP P55212
P	295	HIS	-	EXPRESSION TAG	UNP P55212
P	296	HIS	-	EXPRESSION TAG	UNP P55212
P	297	HIS	-	EXPRESSION TAG	UNP P55212
P	298	HIS	-	EXPRESSION TAG	UNP P55212
P	299	HIS	-	EXPRESSION TAG	UNP P55212
P	300	HIS	-	EXPRESSION TAG	UNP P55212

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	24	Total O 24 24	0	0
3	B	7	Total O 7 7	0	0
3	C	8	Total O 8 8	0	0
3	D	8	Total O 8 8	0	0
3	E	30	Total O 30 30	0	0
3	F	11	Total O 11 11	0	0
3	G	8	Total O 8 8	0	0
3	H	7	Total O 7 7	0	0

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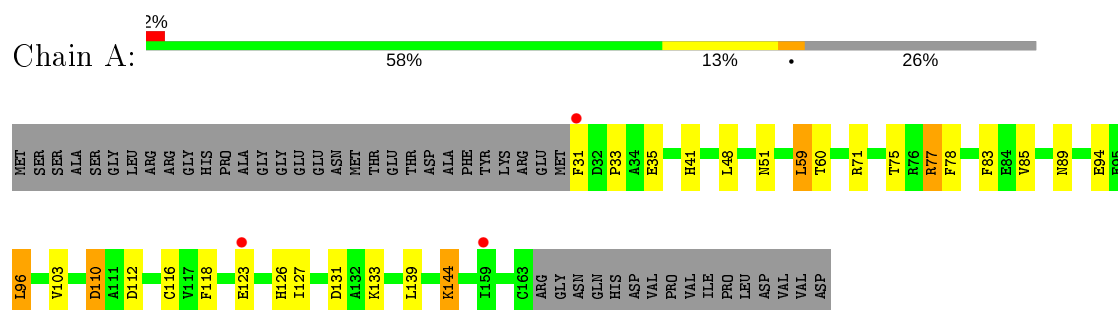
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	21	Total 21	O 21	0	0
3	J	10	Total 10	O 10	0	0
3	K	14	Total 14	O 14	0	0
3	L	6	Total 6	O 6	0	0
3	M	29	Total 29	O 29	0	0
3	N	4	Total 4	O 4	0	0
3	O	8	Total 8	O 8	0	0
3	P	6	Total 6	O 6	0	0

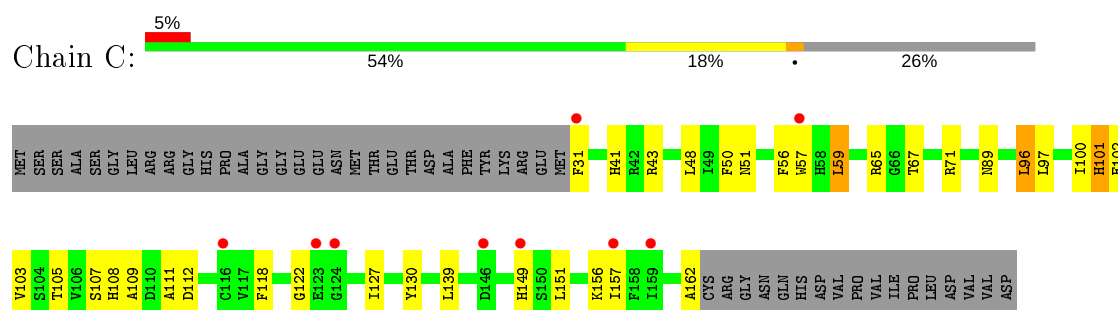
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

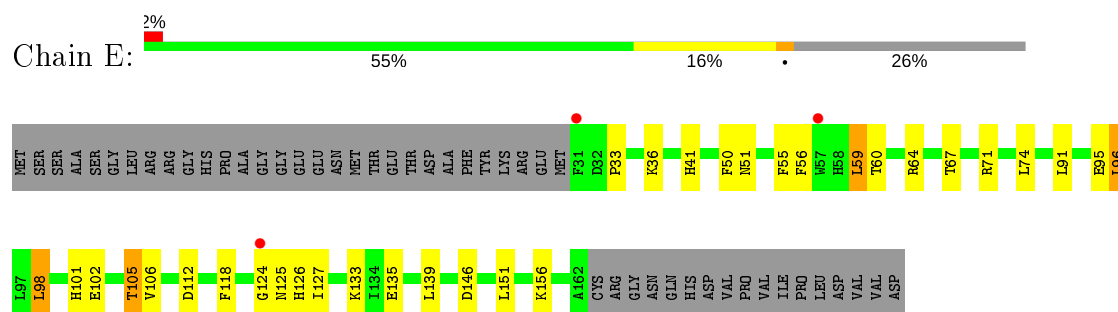
- Molecule 1: caspase-6



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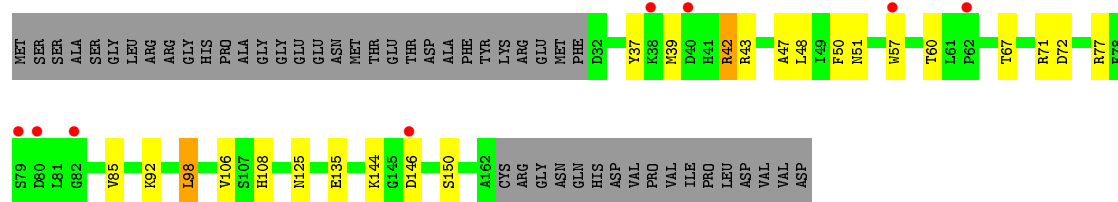


- Molecule 1: caspase-6

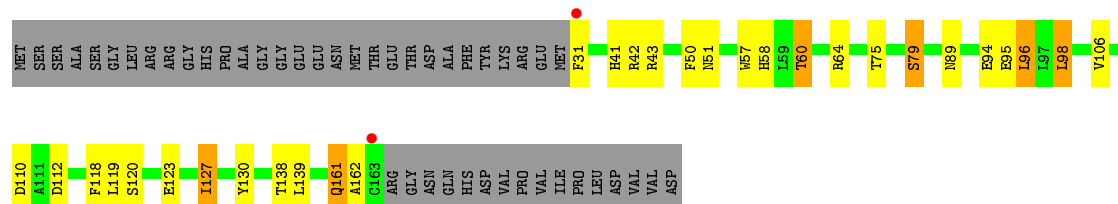


- Molecule 1: caspase-6

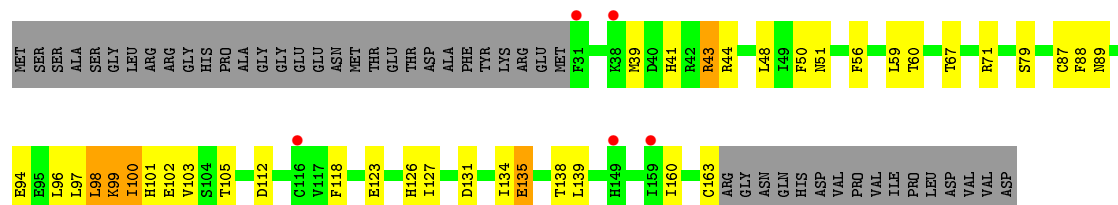




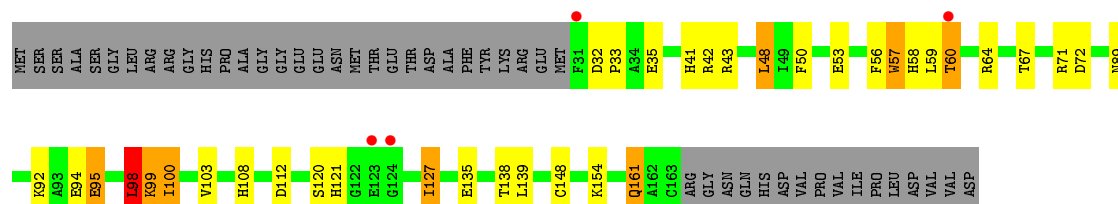
• Molecule 1: caspase-6



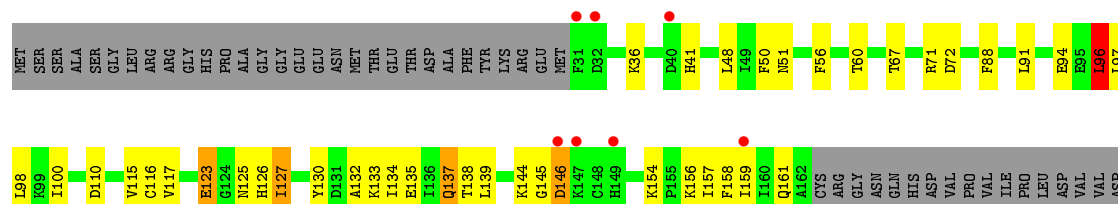
• Molecule 1: caspase-6



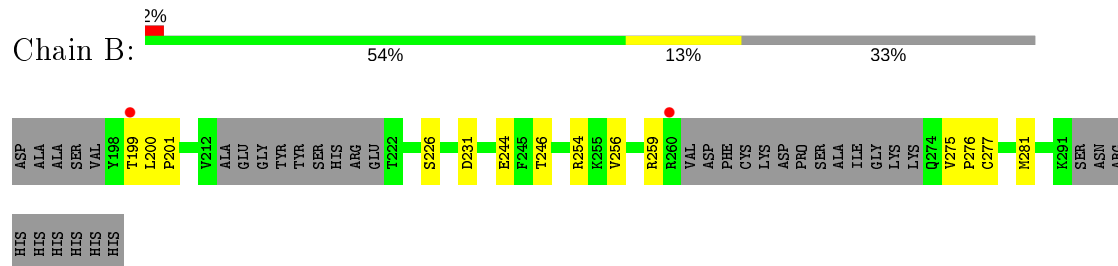
• Molecule 1: caspase-6



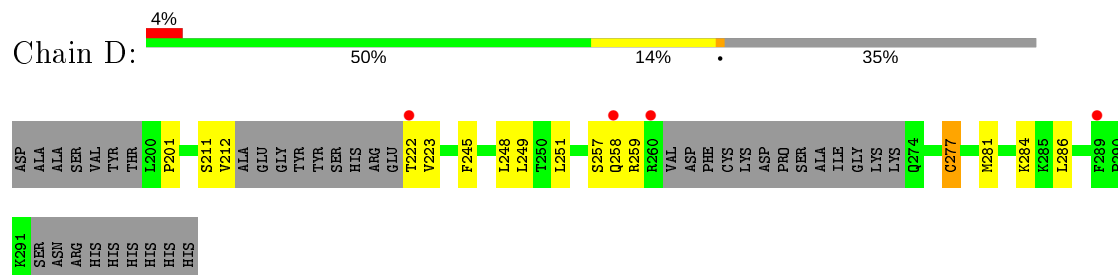
• Molecule 1: caspase-6



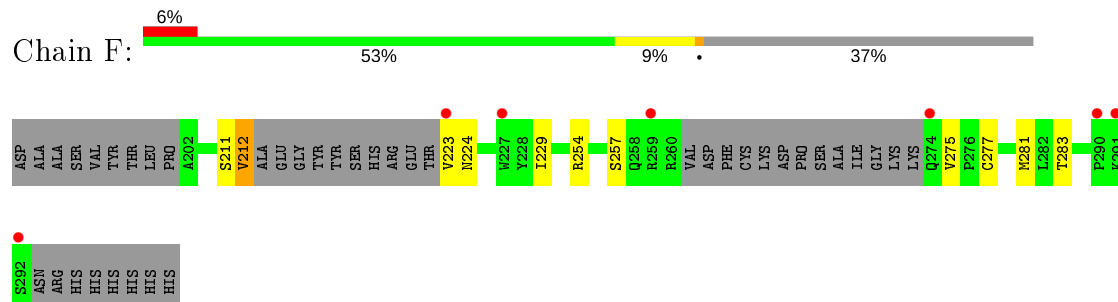
- Molecule 2: caspase-6



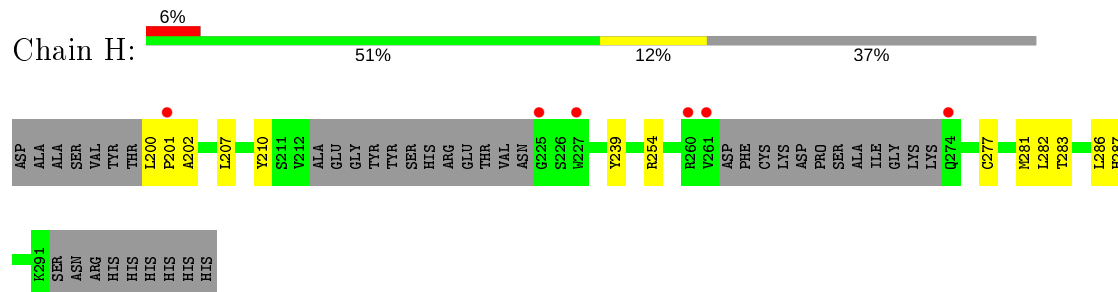
- Molecule 2: caspase-6



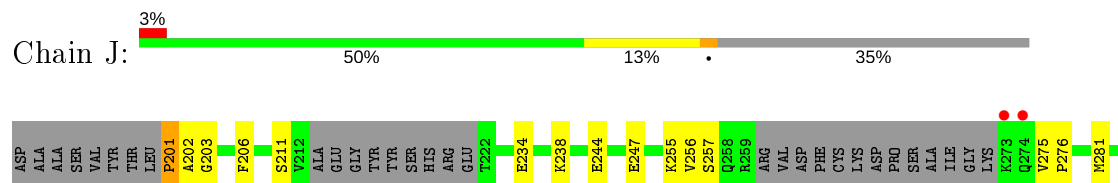
- Molecule 2: caspase-6

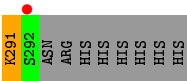


- Molecule 2: caspase-6

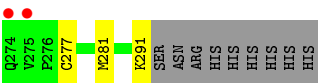
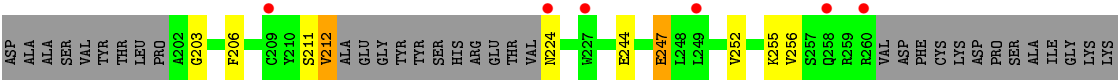


- Molecule 2: caspase-6





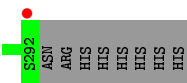
• Molecule 2: caspase-6



• Molecule 2: caspase-6



• Molecule 2: 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	81.23Å 161.24Å 88.92Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	29.96 – 2.53 29.96 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.96-2.53) 99.9 (29.96-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.54Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.264 0.207 , 0.259	Depositor DCC
R_{free} test set	3815 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12955	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 16.57% 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](#)

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	1.00	1/1083 (0.1%)	0.99	4/1460 (0.3%)
1	C	0.88	0/1080	0.87	0/1457
1	E	0.95	0/1083	0.92	0/1458
1	G	0.82	0/1065	0.82	0/1437
1	I	0.97	1/1089 (0.1%)	0.90	1/1468 (0.1%)
1	K	0.77	0/1061	0.84	0/1431
1	M	0.96	2/1080 (0.2%)	0.93	1/1456 (0.1%)
1	O	0.79	0/1068	0.88	1/1442 (0.1%)
2	B	0.90	1/591 (0.2%)	0.85	0/794
2	D	0.91	0/565	0.83	1/759 (0.1%)
2	F	1.00	1/545 (0.2%)	0.85	0/730
2	H	0.86	1/556 (0.2%)	0.85	0/745
2	J	0.99	1/554 (0.2%)	0.88	0/743
2	L	0.91	2/531 (0.4%)	0.81	0/711
2	N	0.95	1/541 (0.2%)	0.94	2/725 (0.3%)
2	P	0.92	1/549 (0.2%)	0.82	1/735 (0.1%)
All	All	0.91	12/13041 (0.1%)	0.88	11/17551 (0.1%)

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	I	0	1
1	O	0	1
2	J	0	1
2	N	0	2
All	All	0	7

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	277	CYS	CB-SG	-8.36	1.68	1.82
2	P	277	CYS	CB-SG	-7.90	1.68	1.82
1	I	95	GLU	CG-CD	6.80	1.62	1.51
2	L	247	GLU	CG-CD	6.73	1.62	1.51
2	N	247	GLU	CG-CD	6.47	1.61	1.51

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	98	LEU	CB-CG-CD1	-7.32	98.56	111.00
1	O	96	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	110	ASP	CB-CA-C	-6.67	97.06	110.40
2	N	203	GLY	N-CA-C	-5.91	98.33	113.10
2	P	254	ARG	NE-CZ-NH2	5.86	123.23	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	130	TYR	Peptide
1	C	31	PHE	Peptide
1	I	130	TYR	Peptide
2	J	201	PRO	Peptide
2	N	202	ALA	Mainchain

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	1058	0	1020	25	0
1	C	1054	0	1013	28	0
1	E	1058	0	1033	40	0
1	G	1040	0	1000	19	0
1	I	1063	0	1025	35	0
1	K	1037	0	996	32	0
1	M	1055	0	1018	37	0
1	O	1043	0	997	38	0
2	B	579	0	582	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	554	0	555	14	0
2	F	535	0	531	7	0
2	H	545	0	553	13	0
2	J	543	0	533	14	0
2	L	521	0	515	13	0
2	N	531	0	532	12	0
2	P	538	0	534	16	0
3	A	24	0	0	1	0
3	B	7	0	0	1	0
3	C	8	0	0	0	0
3	D	8	0	0	0	0
3	E	30	0	0	3	0
3	F	11	0	0	0	0
3	G	8	0	0	0	0
3	H	7	0	0	1	0
3	I	21	0	0	0	0
3	J	10	0	0	0	0
3	K	14	0	0	4	0
3	L	6	0	0	0	0
3	M	29	0	0	1	0
3	N	4	0	0	0	0
3	O	8	0	0	0	0
3	P	6	0	0	0	0
All	All	12955	0	12437	301	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 12.

The worst 5 of 301 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:H:201:PRO:HB2	2:H:281:MET:SD	1.77	1.24
1:O:88:PHE:HB3	1:O:91:LEU:HD21	1.34	1.09
1:I:161:GLN:HE21	1:I:161:GLN:HA	1.12	1.09
2:B:201:PRO:HB2	2:B:281:MET:SD	1.97	1.03
1:I:127:ILE:HD12	1:I:127:ILE:O	1.60	1.01

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	131/179 (73%)	126 (96%)	4 (3%)	1 (1%)	19	33
1	C	130/179 (73%)	123 (95%)	6 (5%)	1 (1%)	19	33
1	E	130/179 (73%)	120 (92%)	9 (7%)	1 (1%)	19	33
1	G	129/179 (72%)	120 (93%)	9 (7%)	0	100	100
1	I	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	K	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	M	131/179 (73%)	127 (97%)	4 (3%)	0	100	100
1	O	130/179 (73%)	122 (94%)	6 (5%)	2 (2%)	10	17
2	B	66/108 (61%)	62 (94%)	4 (6%)	0	100	100
2	D	64/108 (59%)	62 (97%)	2 (3%)	0	100	100
2	F	62/108 (57%)	57 (92%)	5 (8%)	0	100	100
2	H	62/108 (57%)	59 (95%)	3 (5%)	0	100	100
2	J	64/108 (59%)	61 (95%)	3 (5%)	0	100	100
2	L	60/108 (56%)	57 (95%)	3 (5%)	0	100	100
2	N	61/108 (56%)	57 (93%)	4 (7%)	0	100	100
2	P	62/108 (57%)	60 (97%)	2 (3%)	0	100	100
All	All	1544/2296 (67%)	1467 (95%)	72 (5%)	5 (0%)	41	59

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	123	GLU
1	E	146	ASP
1	O	146	ASP
1	A	144	LYS
1	C	149	HIS

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	111/154 (72%)	103 (93%)	8 (7%)	14	26
1	C	110/154 (71%)	105 (96%)	5 (4%)	27	48
1	E	111/154 (72%)	105 (95%)	6 (5%)	22	40
1	G	109/154 (71%)	101 (93%)	8 (7%)	14	26
1	I	112/154 (73%)	103 (92%)	9 (8%)	12	22
1	K	107/154 (70%)	96 (90%)	11 (10%)	7	13
1	M	110/154 (71%)	99 (90%)	11 (10%)	7	14
1	O	108/154 (70%)	100 (93%)	8 (7%)	13	25
2	B	65/95 (68%)	63 (97%)	2 (3%)	40	65
2	D	62/95 (65%)	58 (94%)	4 (6%)	17	31
2	F	59/95 (62%)	56 (95%)	3 (5%)	24	43
2	H	61/95 (64%)	61 (100%)	0	100	100
2	J	59/95 (62%)	57 (97%)	2 (3%)	37	61
2	L	57/95 (60%)	56 (98%)	1 (2%)	59	80
2	N	60/95 (63%)	57 (95%)	3 (5%)	24	44
2	P	60/95 (63%)	57 (95%)	3 (5%)	24	44
All	All	1361/1992 (68%)	1277 (94%)	84 (6%)	18	33

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	60	THR
1	K	43	ARG
1	O	98	LEU
1	I	96	LEU
1	I	123	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	125	ASN
1	I	161	GLN
1	O	58	HIS
1	I	41	HIS
1	I	51	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 carbohydrates 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, 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	133/179 (74%)	-0.02	3 (2%) 60 64	13, 22, 41, 55	0
1	C	132/179 (73%)	0.18	9 (6%) 17 18	17, 34, 58, 66	0
1	E	132/179 (73%)	-0.14	3 (2%) 60 64	12, 23, 40, 56	0
1	G	131/179 (73%)	0.17	8 (6%) 21 22	20, 35, 52, 67	0
1	I	133/179 (74%)	-0.09	2 (1%) 73 76	11, 20, 41, 61	0
1	K	133/179 (74%)	0.34	5 (3%) 40 44	23, 38, 53, 62	0
1	M	133/179 (74%)	-0.08	4 (3%) 50 54	12, 23, 44, 60	0
1	O	132/179 (73%)	0.26	7 (5%) 26 28	23, 37, 68, 77	0
2	B	72/108 (66%)	0.34	2 (2%) 53 57	17, 27, 48, 67	0
2	D	70/108 (64%)	0.30	4 (5%) 23 25	19, 33, 53, 62	0
2	F	68/108 (62%)	0.37	7 (10%) 6 6	13, 28, 56, 72	0
2	H	68/108 (62%)	0.62	6 (8%) 10 10	18, 34, 53, 74	0
2	J	70/108 (64%)	0.16	3 (4%) 35 39	14, 27, 44, 52	0
2	L	66/108 (61%)	0.37	8 (12%) 4 4	21, 36, 52, 64	0
2	N	67/108 (62%)	0.29	4 (5%) 21 23	16, 31, 51, 55	0
2	P	68/108 (62%)	0.34	4 (5%) 22 23	23, 35, 53, 78	0
All	All	1608/2296 (70%)	0.17	79 (4%) 29 32	11, 30, 54, 78	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	261	VAL	6.2
2	H	260	ARG	5.9
2	B	260	ARG	5.2
1	O	31	PHE	4.8
2	P	292	SER	4.5

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 carbohydrates 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.