



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 05:23 am GMT

PDB ID : 2P2C  
Title : Inhibition of caspase-2 by a designed ankyrin repeat protein (DARPin)  
Authors : Roschitzki Voser, H.; Briand, C.; Capitani, G.; Gruetter, M.G.  
Deposited on : 2007-03-07  
Resolution : 3.24 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](mailto: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.

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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	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

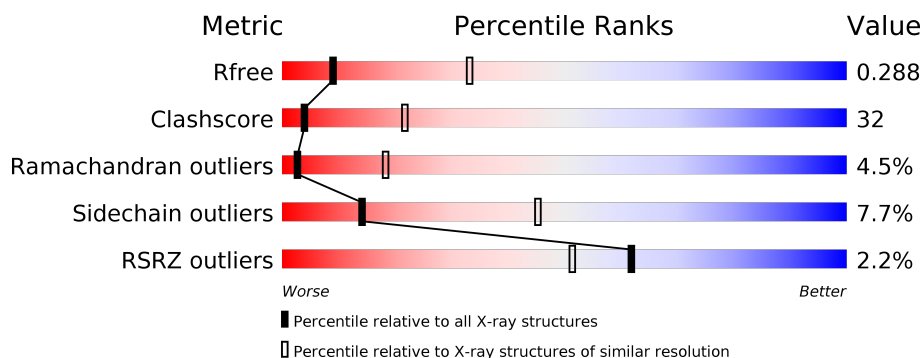
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.24 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))
$R_{free}$	111664	1379 (3.28-3.20)
Clashscore	122126	1510 (3.28-3.20)
Ramachandran outliers	120053	1485 (3.28-3.20)
Sidechain outliers	120020	1484 (3.28-3.20)
RSRZ outliers	108989	1331 (3.28-3.20)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	169	<div> <div>46%</div> <div>45%</div> <div>5%</div> <div>•</div> </div>
1	C	169	<div>2%</div> <div>45%</div> <div>43%</div> <div>6%</div> <div>5%</div> <div>•</div>

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Mol	Chain	Length	Quality of chain
2	B	106	<p>%</p> <p>57% 31% • 9%</p>
2	D	106	<p>%</p> <p>57% 34% • 8%</p>
2	F	106	<p>%</p> <p>56% 33% • 9%</p>
2	H	106	<p>%</p> <p>59% 29% • • 8%</p>
2	J	106	<p>3%</p> <p>55% 30% • 11%</p>
2	L	106	<p>%</p> <p>57% 27% • 13%</p>
3	P	169	<p>5%</p> <p>36% 49% 9% • 7%</p>
3	Q	169	<p>%</p> <p>43% 43% 7% • 7%</p>
3	R	169	<p>3%</p> <p>39% 43% 10% • 7%</p>
3	S	169	<p>2%</p> <p>38% 44% 8% 9%</p>
3	T	169	<p>8%</p> <p>40% 41% 8% • 10%</p>
3	U	169	<p>2%</p> <p>44% 40% 7% • 9%</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19285 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-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1284	810	223	243	8			
1	C	161	Total	C	N	O	S	0	0	0
			1276	804	222	242	8			
1	E	160	Total	C	N	O	S	0	0	0
			1267	800	221	238	8			
1	G	160	Total	C	N	O	S	0	0	0
			1267	800	221	238	8			
1	I	157	Total	C	N	O	S	0	0	0
			1244	786	217	234	7			
1	K	158	Total	C	N	O	S	0	0	0
			1252	792	218	235	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	CLONING ARTIFACT	UNP P42575
A	1	ALA	-	CLONING ARTIFACT	UNP P42575
A	7	LEU	VAL	VARIANT	UNP P42575
C	0	MET	-	CLONING ARTIFACT	UNP P42575
C	1	ALA	-	CLONING ARTIFACT	UNP P42575
C	7	LEU	VAL	VARIANT	UNP P42575
E	0	MET	-	CLONING ARTIFACT	UNP P42575
E	1	ALA	-	CLONING ARTIFACT	UNP P42575
E	7	LEU	VAL	VARIANT	UNP P42575
G	0	MET	-	CLONING ARTIFACT	UNP P42575
G	1	ALA	-	CLONING ARTIFACT	UNP P42575
G	7	LEU	VAL	VARIANT	UNP P42575
I	0	MET	-	CLONING ARTIFACT	UNP P42575
I	1	ALA	-	CLONING ARTIFACT	UNP P42575
I	7	LEU	VAL	VARIANT	UNP P42575
K	0	MET	-	CLONING ARTIFACT	UNP P42575
K	1	ALA	-	CLONING ARTIFACT	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
K	7	LEU	VAL	VARIANT	UNP P42575

- Molecule 2 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			760	477	137	134	12			
2	D	98	Total	C	N	O	S	0	0	0
			777	487	140	138	12			
2	F	96	Total	C	N	O	S	0	0	0
			760	477	137	134	12			
2	H	98	Total	C	N	O	S	0	0	0
			776	488	140	136	12			
2	J	94	Total	C	N	O	S	0	0	0
			746	467	135	132	12			
2	L	92	Total	C	N	O	S	0	0	0
			727	456	130	130	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	200	MET	-	CLONING ARTIFACT	UNP P42575
D	200	MET	-	CLONING ARTIFACT	UNP P42575
F	200	MET	-	CLONING ARTIFACT	UNP P42575
H	200	MET	-	CLONING ARTIFACT	UNP P42575
J	200	MET	-	CLONING ARTIFACT	UNP P42575
L	200	MET	-	CLONING ARTIFACT	UNP P42575

- Molecule 3 is a protein called Caspase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	158	Total	C	N	O	S	0	0	0
			1207	762	207	237	1			
3	Q	158	Total	C	N	O	S	0	0	0
			1209	764	205	239	1			
3	R	157	Total	C	N	O	S	0	0	0
			1198	757	205	235	1			
3	S	153	Total	C	N	O	S	0	0	0
			1168	740	197	230	1			
3	T	152	Total	C	N	O	S	0	0	0
			1161	735	197	228	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	U	154	Total	C	N	O	S	0	0	0
			1177	745	199	232	1			

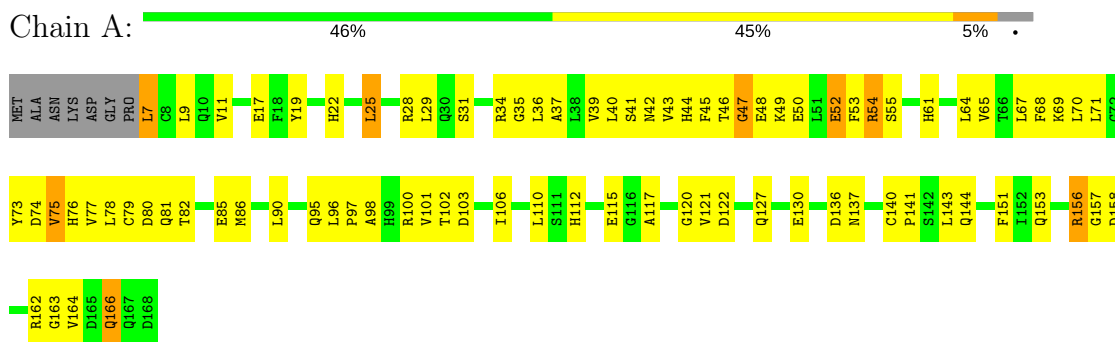
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	O	0	0
			4	4		
4	P	1	Total	O	0	0
			1	1		
4	C	5	Total	O	0	0
			5	5		
4	D	5	Total	O	0	0
			5	5		
4	Q	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	F	1	Total	O	0	0
			1	1		
4	R	1	Total	O	0	0
			1	1		
4	G	2	Total	O	0	0
			2	2		
4	H	4	Total	O	0	0
			4	4		
4	S	1	Total	O	0	0
			1	1		
4	I	1	Total	O	0	0
			1	1		
4	L	1	Total	O	0	0
			1	1		

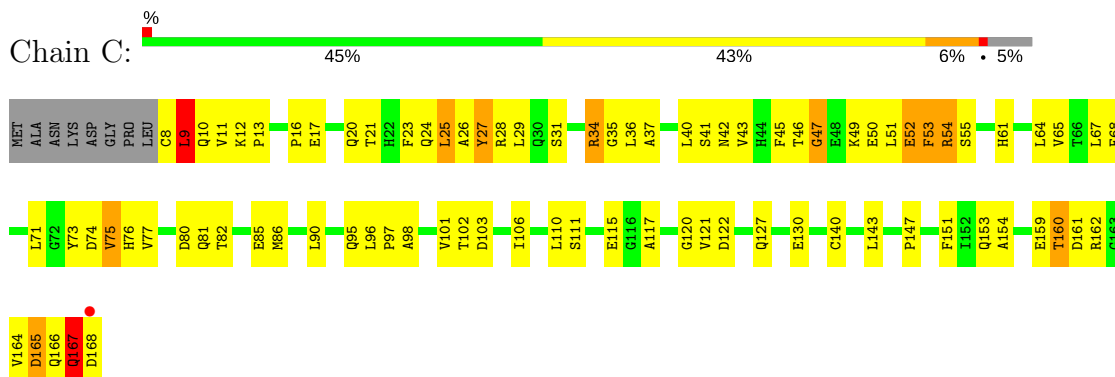
### 3 Residue-property plots [i](#)

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.

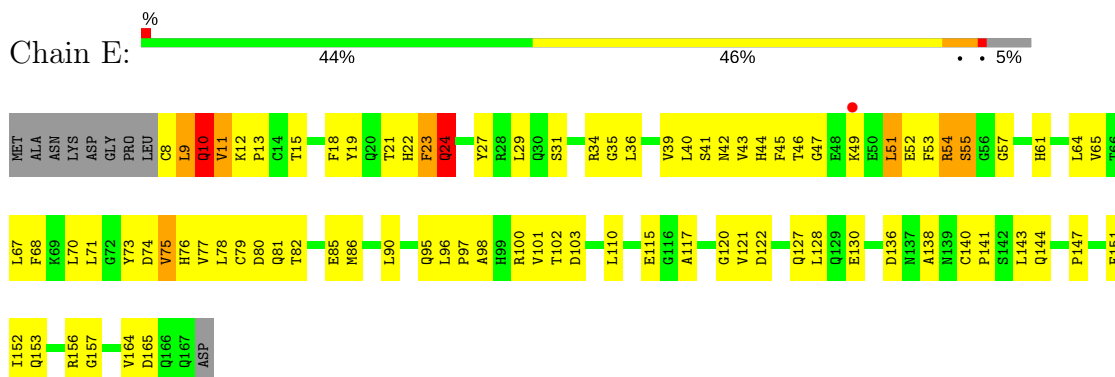
#### • Molecule 1: Caspase-2



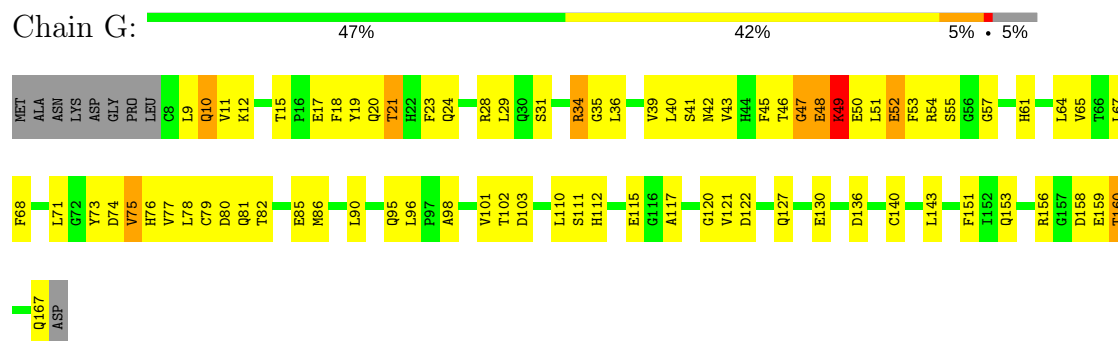
#### • Molecule 1: Caspase-2



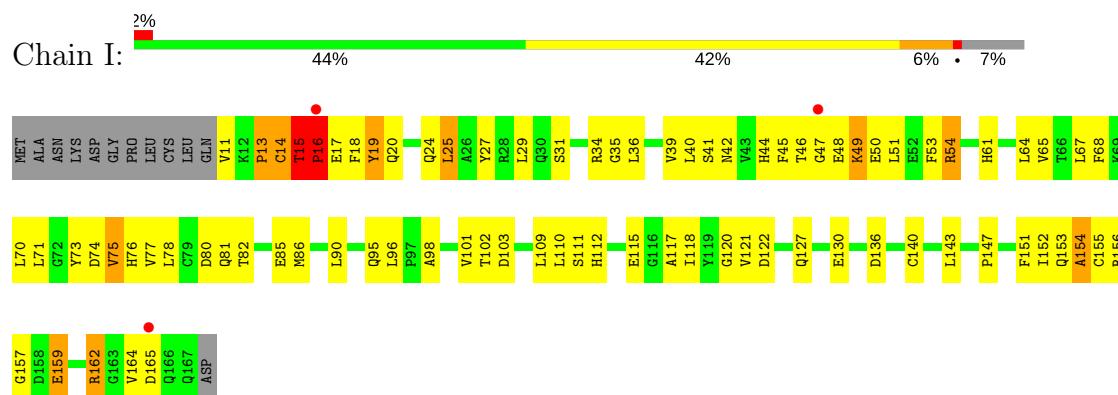
#### • Molecule 1: Caspase-2



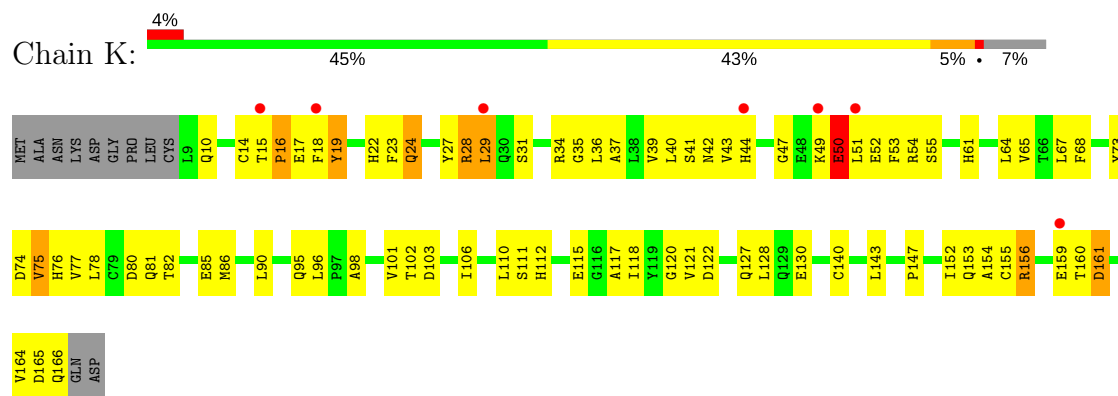
- Molecule 1: Caspase-2



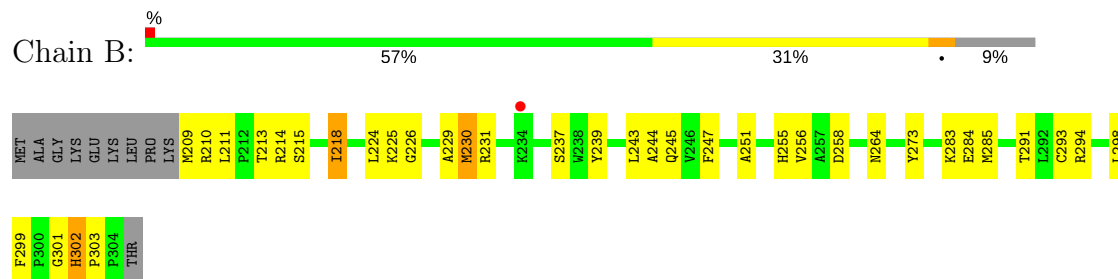
- Molecule 1: Caspase-2



- Molecule 1: Caspase-2

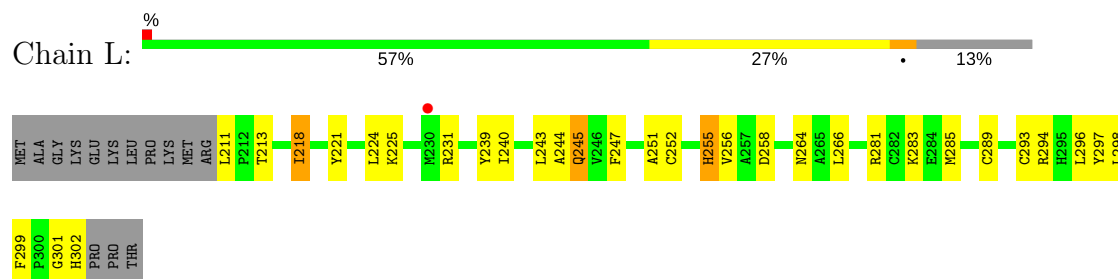
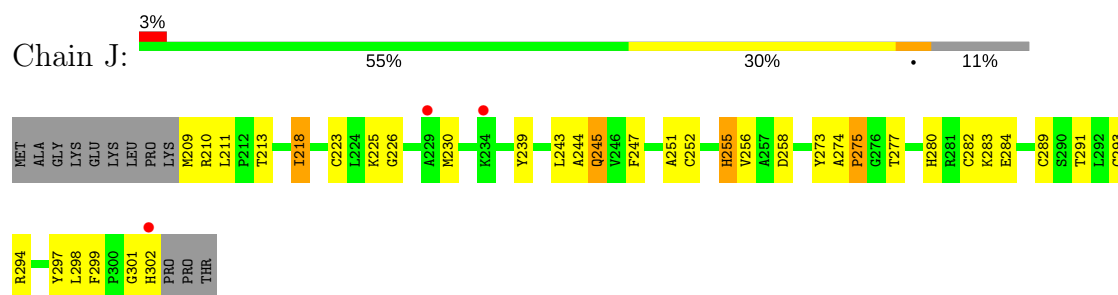
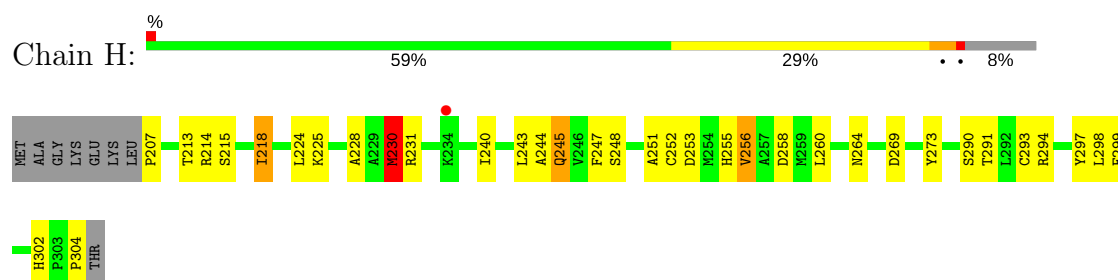
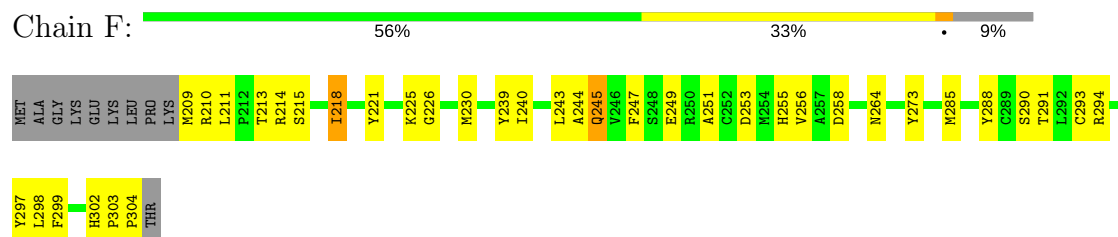
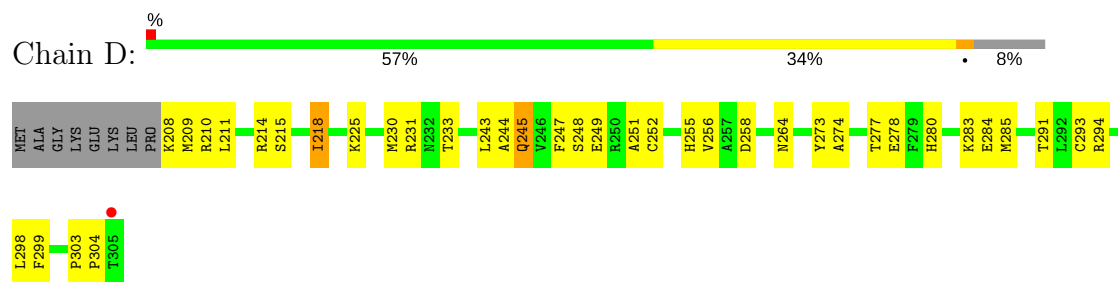


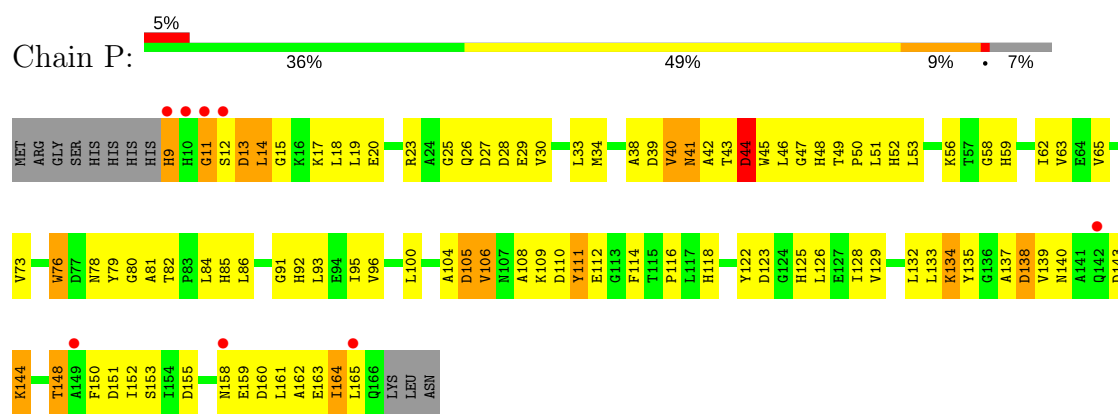
- Molecule 2: Caspase-2



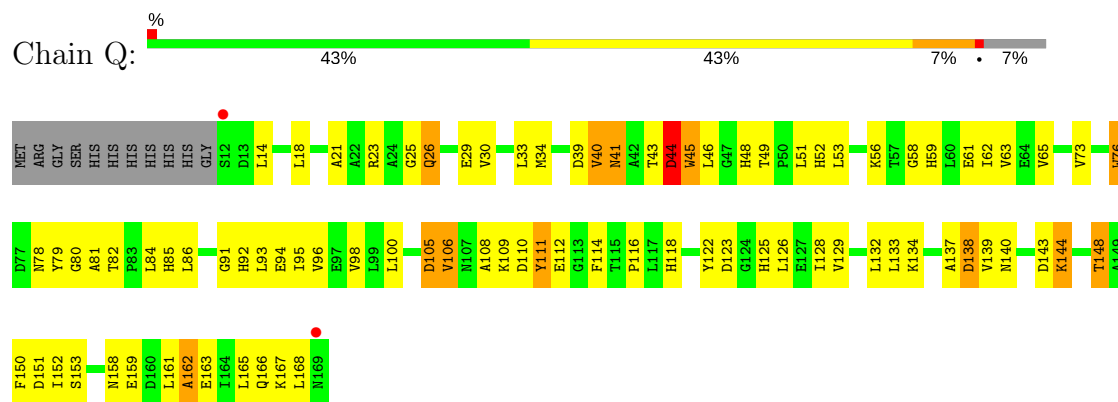
- Molecule 2: Caspase-2



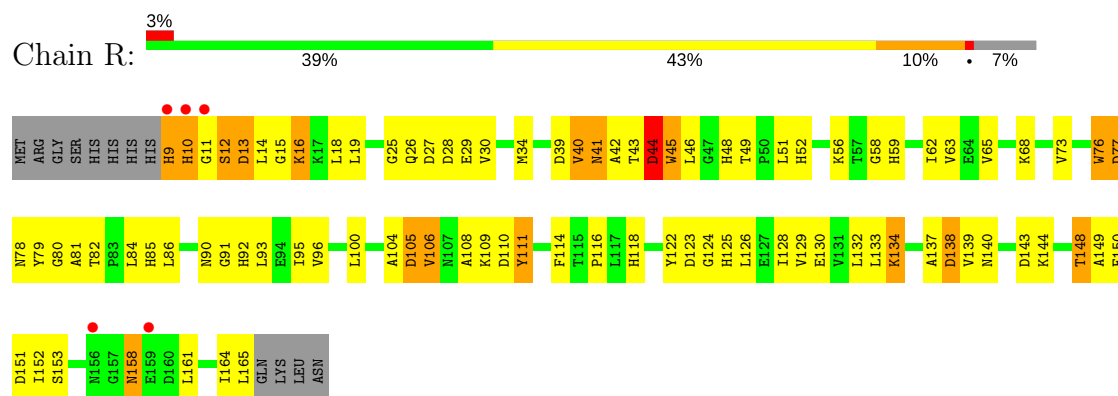




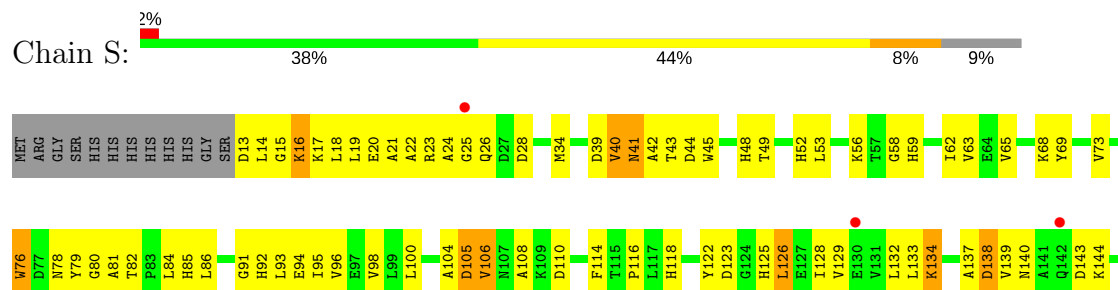
• Molecule 3: Caspase-2



• Molecule 3: Caspase-2

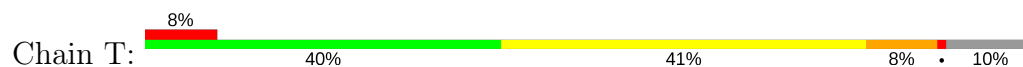


• Molecule 3: Caspase-2

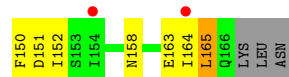
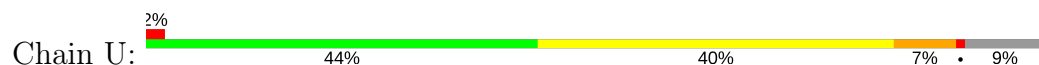




• Molecule 3: Caspase-2



• Molecule 3: Caspase-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.02Å 229.21Å 114.93Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.00 – 3.24 29.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	98.2 (20.00-3.24) 97.6 (29.51-3.24)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	5.90	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.262 , 0.305 0.256 , 0.288	Depositor DCC
$R_{free}$ test set	1026 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	97.7	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 24.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.235 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	1/1309 (0.1%)	0.64	0/1769
1	C	0.38	0/1301	0.63	1/1758 (0.1%)
1	E	0.48	0/1292	0.68	2/1747 (0.1%)
1	G	0.42	0/1292	0.63	0/1747
1	I	0.38	0/1269	0.62	0/1716
1	K	0.39	0/1277	0.62	0/1727
2	B	0.41	0/778	0.63	0/1047
2	D	0.38	0/795	0.63	0/1068
2	F	0.39	0/778	0.65	0/1047
2	H	0.40	0/795	0.66	0/1069
2	J	0.38	0/762	0.64	0/1023
2	L	0.37	0/743	0.59	0/999
3	P	0.54	1/1231 (0.1%)	0.76	2/1674 (0.1%)
3	Q	0.50	0/1231	0.70	1/1672 (0.1%)
3	R	0.51	0/1222	0.73	2/1662 (0.1%)
3	S	0.61	3/1190 (0.3%)	0.78	3/1619 (0.2%)
3	T	0.51	0/1183	0.78	4/1609 (0.2%)
3	U	0.52	2/1199 (0.2%)	0.73	3/1631 (0.2%)
All	All	0.46	7/19647 (0.0%)	0.68	18/26584 (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
2	F	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	106	VAL	CB-CG1	-8.08	1.35	1.52
3	P	12	SER	CB-OG	7.92	1.52	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	127	GLU	CD-OE1	-7.16	1.17	1.25
1	A	69	LYS	CE-NZ	-7.09	1.31	1.49
3	S	106	VAL	CB-CG2	-6.92	1.38	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	126	LEU	CA-CB-CG	9.13	136.29	115.30
3	S	106	VAL	CG1-CB-CG2	-7.89	98.27	110.90
3	T	105	ASP	CB-CG-OD1	7.72	125.25	118.30
3	S	126	LEU	CB-CG-CD1	6.77	122.50	111.00
3	T	105	ASP	OD1-CG-OD2	-6.44	111.06	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	288	TYR	Sidechain

## 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	1284	0	1256	95	0
1	C	1276	0	1245	89	0
1	E	1267	0	1241	104	0
1	G	1267	0	1241	93	0
1	I	1244	0	1217	99	0
1	K	1252	0	1228	99	0
2	B	760	0	748	46	0
2	D	777	0	768	48	0
2	F	760	0	748	35	0
2	H	776	0	769	39	0
2	J	746	0	734	47	0
2	L	727	0	712	51	0
3	P	1207	0	1162	95	0
3	Q	1209	0	1175	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1198	0	1154	89	0
3	S	1168	0	1132	88	0
3	T	1161	0	1125	99	0
3	U	1177	0	1140	86	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	H	4	0	0	1	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
All	All	19285	0	18795	1225	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 32.

The worst 5 of 1225 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)
3:T:25:GLY:HA2	3:T:59:HIS:CD2	1.74	1.21
2:J:255:HIS:HE1	2:J:258:ASP:OD2	1.24	1.17
2:L:255:HIS:HE1	2:L:258:ASP:OD2	1.27	1.16
2:D:255:HIS:HE1	2:D:258:ASP:OD2	1.33	1.12
2:H:255:HIS:HE1	2:H:258:ASP:OD2	1.35	1.10

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	160/169 (95%)	135 (84%)	21 (13%)	4 (2%)	6	33
1	C	159/169 (94%)	128 (80%)	26 (16%)	5 (3%)	4	27
1	E	158/169 (94%)	127 (80%)	26 (16%)	5 (3%)	4	26
1	G	158/169 (94%)	128 (81%)	24 (15%)	6 (4%)	3	22
1	I	155/169 (92%)	120 (77%)	28 (18%)	7 (4%)	3	18
1	K	156/169 (92%)	125 (80%)	21 (14%)	10 (6%)	1	10
2	B	94/106 (89%)	83 (88%)	7 (7%)	4 (4%)	3	20
2	D	96/106 (91%)	89 (93%)	5 (5%)	2 (2%)	8	37
2	F	94/106 (89%)	88 (94%)	4 (4%)	2 (2%)	8	37
2	H	96/106 (91%)	85 (88%)	8 (8%)	3 (3%)	4	27
2	J	92/106 (87%)	83 (90%)	5 (5%)	4 (4%)	3	20
2	L	90/106 (85%)	80 (89%)	7 (8%)	3 (3%)	4	25
3	P	156/169 (92%)	117 (75%)	26 (17%)	13 (8%)	1	5
3	Q	156/169 (92%)	121 (78%)	26 (17%)	9 (6%)	2	13
3	R	155/169 (92%)	124 (80%)	21 (14%)	10 (6%)	1	10
3	S	151/169 (89%)	117 (78%)	27 (18%)	7 (5%)	2	18
3	T	150/169 (89%)	113 (75%)	28 (19%)	9 (6%)	2	12
3	U	152/169 (90%)	119 (78%)	27 (18%)	6 (4%)	3	21
All	All	2428/2664 (91%)	1982 (82%)	337 (14%)	109 (4%)	3	18

5 of 109 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	52	GLU
3	P	27	ASP
3	P	126	LEU
3	P	162	ALA

### 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	142/147 (97%)	132 (93%)	10 (7%)	16	50
1	C	141/147 (96%)	130 (92%)	11 (8%)	14	44
1	E	140/147 (95%)	131 (94%)	9 (6%)	19	54
1	G	140/147 (95%)	133 (95%)	7 (5%)	27	62
1	I	137/147 (93%)	126 (92%)	11 (8%)	13	44
1	K	138/147 (94%)	131 (95%)	7 (5%)	26	61
2	B	81/89 (91%)	79 (98%)	2 (2%)	50	78
2	D	83/89 (93%)	80 (96%)	3 (4%)	38	70
2	F	81/89 (91%)	76 (94%)	5 (6%)	20	55
2	H	83/89 (93%)	78 (94%)	5 (6%)	21	56
2	J	79/89 (89%)	77 (98%)	2 (2%)	50	78
2	L	77/89 (86%)	75 (97%)	2 (3%)	49	77
3	P	122/132 (92%)	107 (88%)	15 (12%)	5	23
3	Q	123/132 (93%)	112 (91%)	11 (9%)	11	37
3	R	121/132 (92%)	103 (85%)	18 (15%)	3	15
3	S	118/132 (89%)	103 (87%)	15 (13%)	5	21
3	T	117/132 (89%)	105 (90%)	12 (10%)	8	30
3	U	119/132 (90%)	106 (89%)	13 (11%)	7	28
All	All	2042/2208 (92%)	1884 (92%)	158 (8%)	14	45

5 of 158 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	44	ASP
1	G	52	GLU
3	U	27	ASP
3	R	68	LYS
3	R	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
3	R	90	ASN

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Mol	Chain	Res	Type
2	H	245	GLN
2	L	302	HIS
3	R	118	HIS
1	G	76	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	162/169 (95%)	-0.12	0 <span>100</span> <span>100</span>	41, 83, 113, 125	0
1	C	161/169 (95%)	-0.09	1 (0%) <span>89</span> <span>85</span>	37, 81, 105, 121	0
1	E	160/169 (94%)	-0.09	1 (0%) <span>89</span> <span>85</span>	49, 88, 122, 142	0
1	G	160/169 (94%)	-0.07	0 <span>100</span> <span>100</span>	36, 78, 105, 121	0
1	I	157/169 (92%)	-0.08	3 (1%) <span>66</span> <span>56</span>	52, 91, 142, 160	0
1	K	158/169 (93%)	0.09	7 (4%) <span>34</span> <span>24</span>	55, 92, 156, 176	0
2	B	96/106 (90%)	-0.04	1 (1%) <span>82</span> <span>75</span>	31, 72, 128, 136	0
2	D	98/106 (92%)	-0.05	1 (1%) <span>82</span> <span>75</span>	35, 71, 125, 135	0
2	F	96/106 (90%)	-0.16	0 <span>100</span> <span>100</span>	29, 73, 127, 136	0
2	H	98/106 (92%)	-0.02	1 (1%) <span>82</span> <span>75</span>	33, 71, 126, 136	0
2	J	94/106 (88%)	-0.05	3 (3%) <span>47</span> <span>35</span>	50, 75, 129, 136	0
2	L	92/106 (86%)	-0.14	1 (1%) <span>80</span> <span>72</span>	49, 74, 122, 137	0
3	P	158/169 (93%)	0.25	8 (5%) <span>28</span> <span>18</span>	57, 106, 181, 191	0
3	Q	158/169 (93%)	0.03	2 (1%) <span>77</span> <span>68</span>	64, 106, 177, 186	0
3	R	157/169 (92%)	0.10	5 (3%) <span>47</span> <span>35</span>	63, 107, 178, 186	0
3	S	153/169 (90%)	0.13	4 (2%) <span>56</span> <span>44</span>	67, 110, 177, 186	0
3	T	152/169 (89%)	0.39	14 (9%) <span>9</span> <span>7</span>	70, 112, 183, 191	0
3	U	154/169 (91%)	0.11	3 (1%) <span>66</span> <span>56</span>	66, 110, 182, 196	0
All	All	2464/2664 (92%)	0.02	55 (2%) <span>62</span> <span>51</span>	29, 91, 168, 196	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	12	SER	7.5
3	Q	169	ASN	6.3
3	R	10	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
3	S	25	GLY	4.7
3	P	11	GLY	4.2

## 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.