



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:57 AM UTC

PDB ID : 4LSZ / pdb_00004lsz
Title : Caspase-7 in Complex with DARPin D7.18
Authors : Fluetsch, A.; Lukarska, M.; Gruetter, M.G.
Deposited on : 2013-07-23
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

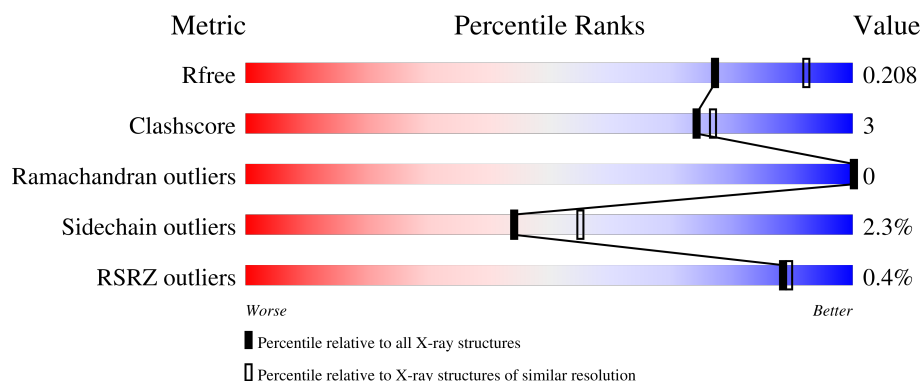
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	175	2% 74% 6% 20%
1	C	175	75% 5% 19%
2	B	105	86% 10%
2	D	105	2% 84% 6% 10%
3	E	169	83% 7% 9%

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Mol	Chain	Length	Quality of chain
3	F	169	79% 11% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6245 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-7 subunit p20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	1	0
			1106	695	189	211	11			
1	C	141	Total	C	N	O	S	0	0	0
			1105	694	189	211	11			

- Molecule 2 is a protein called Caspase-7 subunit p10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	0	0	0
			780	502	133	141	4			
2	D	95	Total	C	N	O	S	0	0	0
			787	507	134	142	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	304	LEU	-	expression tag	UNP P55210
B	305	GLU	-	expression tag	UNP P55210
B	306	HIS	-	expression tag	UNP P55210
B	307	HIS	-	expression tag	UNP P55210
B	308	HIS	-	expression tag	UNP P55210
B	309	HIS	-	expression tag	UNP P55210
B	310	HIS	-	expression tag	UNP P55210
B	311	HIS	-	expression tag	UNP P55210
D	304	LEU	-	expression tag	UNP P55210
D	305	GLU	-	expression tag	UNP P55210
D	306	HIS	-	expression tag	UNP P55210
D	307	HIS	-	expression tag	UNP P55210
D	308	HIS	-	expression tag	UNP P55210
D	309	HIS	-	expression tag	UNP P55210
D	310	HIS	-	expression tag	UNP P55210
D	311	HIS	-	expression tag	UNP P55210

- Molecule 3 is a protein called DARPin D7.18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	153	Total	C	N	O	S	0	1	0
			1163	724	199	238	2			
3	F	154	Total	C	N	O	S	0	0	0
			1163	726	197	238	2			

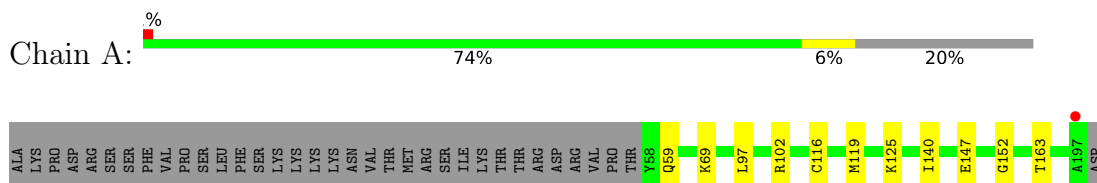
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	19	Total	O	0	0
			19	19		
4	C	25	Total	O	0	0
			25	25		
4	D	26	Total	O	0	0
			26	26		
4	E	17	Total	O	0	0
			17	17		
4	F	14	Total	O	0	0
			14	14		

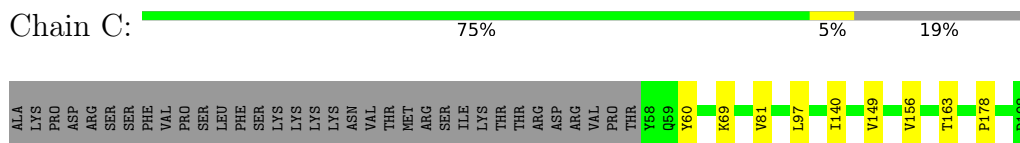
3 Residue-property plots [i](#)

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 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.

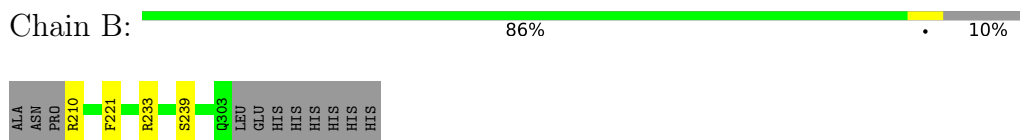
- Molecule 1: Caspase-7 subunit p20



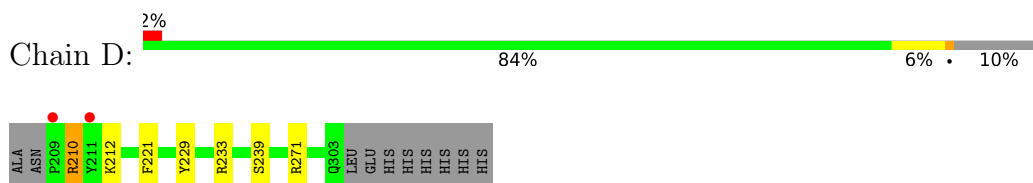
- Molecule 1: Caspase-7 subunit p20



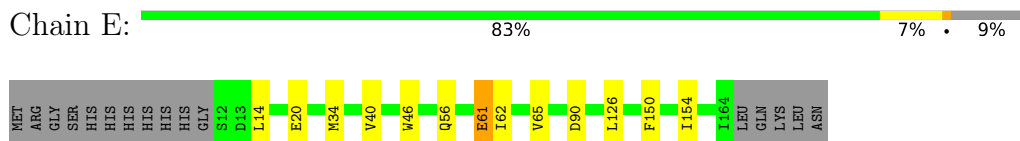
- Molecule 2: Caspase-7 subunit p10



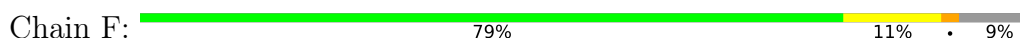
- Molecule 2: Caspase-7 subunit p10



- Molecule 3: DARPin D7.18



- Molecule 3: DARPin D7.18



MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	D13	L14	A24	G25	Q26	V30	M34	A42	W46	P50	E61	I62	V65	K68	D90	V129	D143	K144	E159	D160	L161	A162	E163	Q166	LYS	LEU	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.84Å 82.31Å 95.08Å 90.00° 91.86° 90.00°	Depositor
Resolution (Å)	12.93 – 2.26 12.93 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.5 (12.93-2.26) 99.2 (12.93-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.78 (at 2.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.175 , 0.208 0.176 , 0.208	Depositor DCC
R_{free} test set	1719 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6245	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1025e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.50	0/1123	0.75	1/1505 (0.1%)
1	C	0.53	0/1122	0.75	0/1504
2	B	0.50	0/803	0.81	0/1086
2	D	0.56	0/811	0.81	1/1097 (0.1%)
3	E	0.50	0/1180	0.75	0/1606
3	F	0.53	0/1180	0.81	1/1607 (0.1%)
All	All	0.52	0/6219	0.78	3/8405 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLY	N-CA-C	-5.70	103.86	112.41
2	D	229	TYR	N-CA-C	5.31	118.38	110.14
3	F	14	LEU	N-CA-C	-5.17	105.33	111.69

There are no chirality outliers.

There are no planarity outliers.

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	1106	0	1089	9	0
1	C	1105	0	1088	4	0
2	B	780	0	753	2	0
2	D	787	0	761	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1163	0	1118	8	0
3	F	1163	0	1120	13	0
4	A	40	0	0	3	0
4	B	19	0	0	0	0
4	C	25	0	0	0	0
4	D	26	0	0	1	0
4	E	17	0	0	1	0
4	F	14	0	0	1	0
All	All	6245	0	5929	37	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 3.

All (37) 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:A:102:ARG:HH12	3:E:20:GLU:CD	2.00	0.69
2:D:210:ARG:HH21	2:D:210:ARG:CG	2.11	0.64
2:D:210:ARG:HH21	2:D:210:ARG:HG2	1.66	0.60
3:F:25:GLY:HA2	3:F:62:ILE:HD12	1.84	0.59
3:E:34:MET:HE1	3:E:40:VAL:HB	1.86	0.57
1:A:59:GLN:CG	4:A:202:HOH:O	2.52	0.56
2:D:271:ARG:NH2	4:D:414:HOH:O	2.38	0.56
1:A:163:THR:HG21	2:B:221:PHE:HE1	1.71	0.55
1:A:97:LEU:HD13	1:A:140:ILE:HG21	1.87	0.55
3:E:61:GLU:H	3:E:61:GLU:CD	2.13	0.55
3:F:24:ALA:HB3	3:F:26:GLN:HG2	1.90	0.54
3:E:150:PHE:CE2	3:E:154:ILE:HD11	2.43	0.53
1:C:97:LEU:HD13	1:C:140:ILE:HG21	1.90	0.53
3:F:61:GLU:H	3:F:61:GLU:CD	2.17	0.53
1:C:163:THR:HG21	2:D:221:PHE:HE1	1.74	0.53
3:E:56:GLN:NE2	4:E:209:HOH:O	2.26	0.51
1:C:69:LYS:HD3	3:F:46:TRP:CH2	2.45	0.51
3:F:42:ALA:O	3:F:50:PRO:HD3	2.11	0.51
3:F:13:ASP:OD1	3:F:13:ASP:N	2.44	0.50
3:F:30:VAL:O	3:F:34:MET:HG2	2.12	0.50
3:F:62:ILE:HA	3:F:65:VAL:HG12	1.92	0.50
2:D:210:ARG:CZ	2:D:212:LYS:HD3	2.41	0.50
3:F:68:LYS:NZ	4:F:212:HOH:O	2.38	0.49
2:D:210:ARG:CG	2:D:210:ARG:NH2	2.72	0.49
2:D:233:ARG:HA	2:D:239:SER:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:159:GLU:O	3:F:163:GLU:HG3	2.12	0.48
2:B:233:ARG:HA	2:B:239:SER:HA	1.94	0.48
1:C:60:TYR:CD1	1:C:178:PRO:HD3	2.50	0.47
3:F:24:ALA:CB	3:F:26:GLN:HG2	2.44	0.47
3:F:143:ASP:O	3:F:144:LYS:C	2.57	0.47
3:F:129:VAL:HG21	3:F:161:LEU:HD11	1.97	0.46
1:A:102:ARG:NH1	3:E:20:GLU:OE1	2.48	0.45
1:A:59:GLN:HG2	4:A:202:HOH:O	2.17	0.44
3:E:62:ILE:HA	3:E:65:VAL:HG12	1.99	0.43
1:A:59:GLN:HG3	4:A:202:HOH:O	2.14	0.42
1:A:116:CYS:HA	1:A:119:MET:HE2	2.00	0.42
1:A:69:LYS:HD3	3:E:46:TRP:CH2	2.57	0.40

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	139/175 (79%)	138 (99%)	1 (1%)	0	100	100
1	C	139/175 (79%)	138 (99%)	1 (1%)	0	100	100
2	B	92/105 (88%)	92 (100%)	0	0	100	100
2	D	93/105 (89%)	93 (100%)	0	0	100	100
3	E	152/169 (90%)	149 (98%)	3 (2%)	0	100	100
3	F	152/169 (90%)	148 (97%)	4 (3%)	0	100	100
All	All	767/898 (85%)	758 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	120/153 (78%)	117 (98%)	3 (2%)	42	52
1	C	120/153 (78%)	117 (98%)	3 (2%)	42	52
2	B	86/96 (90%)	85 (99%)	1 (1%)	63	74
2	D	87/96 (91%)	86 (99%)	1 (1%)	65	75
3	E	119/132 (90%)	115 (97%)	4 (3%)	32	40
3	F	119/132 (90%)	115 (97%)	4 (3%)	32	40
All	All	651/762 (85%)	635 (98%)	16 (2%)	44	52

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	LYS
1	A	147[A]	GLU
1	A	147[B]	GLU
2	B	210	ARG
1	C	81	VAL
1	C	149	VAL
1	C	156	VAL
2	D	210	ARG
3	E	14	LEU
3	E	61	GLU
3	E	90	ASP
3	E	126	LEU
3	F	14	LEU
3	F	61	GLU
3	F	90	ASP
3	F	143	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	GLN

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Mol	Chain	Res	Type
2	B	252	HIS
1	C	120	GLN
1	C	165	HIS
2	D	303	GLN
3	E	48	GLN
3	E	59	HIS
3	E	118	ASN
3	F	48	GLN

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](#)

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	140/175 (80%)	-0.71	1 (0%) 84 85	25, 50, 71, 100	1 (0%)
1	C	141/175 (80%)	-0.67	0 100 100	39, 50, 70, 110	0
2	B	94/105 (89%)	-0.70	0 100 100	34, 46, 76, 114	0
2	D	95/105 (90%)	-0.63	2 (2%) 63 64	35, 47, 74, 125	0
3	E	153/169 (90%)	-0.30	0 100 100	30, 63, 110, 124	1 (0%)
3	F	154/169 (91%)	-0.39	0 100 100	45, 64, 97, 112	0
All	All	777/898 (86%)	-0.55	3 (0%) 88 89	25, 54, 94, 125	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	209	PRO	2.8
2	D	211	TYR	2.2
1	A	197	ALA	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.