



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 07:38 pm BST

PDB ID : 6KMT
Title : P32 of caspase-11 mutant C254A
Authors : Ding, J.; Sun, Q.
Deposited on : 2019-08-01
Resolution : 2.60 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 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

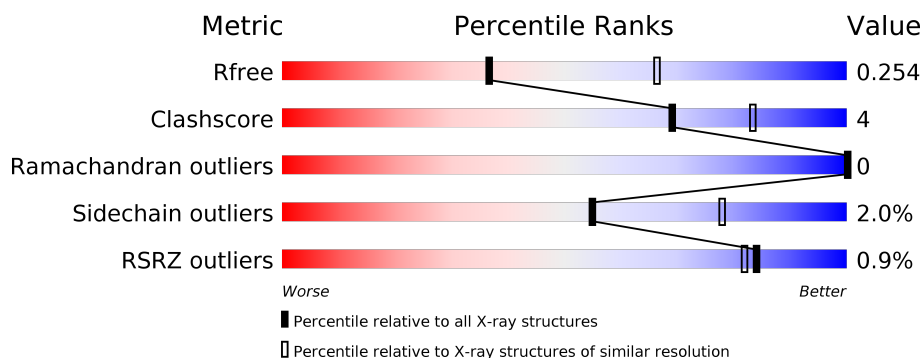
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	273	<div> <div>79%</div> <div>6%</div> <div>14%</div> </div>
1	B	273	<div> <div>74%</div> <div>11%</div> <div>14%</div> </div>
1	C	273	<div> <div>%</div> <div>74%</div> <div>11%</div> <div>14%</div> </div>
1	D	273	<div> <div>%</div> <div>74%</div> <div>11%</div> <div>15%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7523 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.

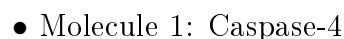
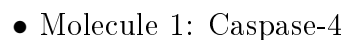
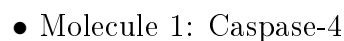
- Molecule 1 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1882	1198	320	349	15			
1	B	234	Total	C	N	O	S	0	0	0
			1882	1198	320	349	15			
1	C	234	Total	C	N	O	S	0	0	0
			1882	1198	320	349	15			
1	D	233	Total	C	N	O	S	0	0	0
			1877	1195	319	348	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	CYS	engineered mutation	UNP P70343
B	254	ALA	CYS	engineered mutation	UNP P70343
C	254	ALA	CYS	engineered mutation	UNP P70343
D	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 1: Caspase-4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.51Å 86.47Å 93.23Å 90.00° 123.15° 90.00°	Depositor
Resolution (Å)	46.55 – 2.60 46.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.55-2.60) 94.9 (46.55-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.202 , 0.254 0.202 , 0.254	Depositor DCC
R_{free} test set	1989 reflections (6.14%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.680	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.004 for $1/2^*h-3/2^*k,-1/2^*h-1/2^*k,-1/2^*h+1/2^*k-l$ 0.014 for $1/2^*h+3/2^*k,1/2^*h-1/2^*k,-1/2^*h-1/2^*k-l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7523	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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	0.26	0/1922	0.45	0/2586
1	B	0.30	0/1922	0.45	0/2586
1	C	0.30	0/1922	0.49	0/2586
1	D	0.25	0/1917	0.43	0/2579
All	All	0.28	0/7683	0.46	0/10337

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	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	310	ARG	Sidechain
1	C	310	ARG	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	1882	0	1861	10	0
1	B	1882	0	1861	20	0
1	C	1882	0	1861	16	0
1	D	1877	0	1856	15	0
All	All	7523	0	7439	55	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 4.

All (55) 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:B:154:ASP:OD2	1:B:309:TYR:OH	1.84	0.94
1:B:309:TYR:CE1	1:B:316:SER:HB3	2.23	0.73
1:B:228:ASP:OD1	1:B:360:ARG:NH1	2.23	0.71
1:A:228:ASP:OD1	1:A:360:ARG:NH1	2.24	0.70
1:C:228:ASP:OD1	1:C:360:ARG:NH1	2.25	0.69
1:B:103:LYS:HE2	1:B:328:LYS:HA	1.75	0.68
1:B:309:TYR:CZ	1:B:316:SER:HB3	2.30	0.67
1:D:228:ASP:OD1	1:D:360:ARG:NH1	2.30	0.65
1:B:303:THR:HA	1:B:354:GLN:OE1	1.96	0.65
1:B:153:PHE:CZ	1:B:313:THR:O	2.51	0.63
1:D:172:LYS:HG3	1:D:183:GLU:HG2	1.84	0.60
1:A:358:ILE:HB	1:B:361:ALA:HB3	1.86	0.57
1:D:303:THR:HG22	1:D:354:GLN:HB3	1.87	0.55
1:D:242:LEU:HA	1:D:245:LYS:HD2	1.88	0.55
1:D:133:LYS:NZ	1:D:168:ASP:OD2	2.38	0.53
1:C:207:GLY:HA3	1:C:253:ALA:HB1	1.91	0.53
1:B:131:THR:OG1	1:B:195:THR:HG23	2.09	0.53
1:B:207:GLY:HA3	1:B:253:ALA:HB1	1.90	0.52
1:C:240:PRO:HA	1:C:243:ARG:HG3	1.92	0.52
1:C:205:SER:HB3	1:C:212:ILE:HD11	1.90	0.52
1:A:242:LEU:HA	1:A:245:LYS:HD2	1.92	0.52
1:A:361:ALA:HB3	1:B:358:ILE:HB	1.92	0.51
1:C:361:ALA:HB3	1:D:358:ILE:HB	1.91	0.51
1:A:141:GLU:HG2	1:A:147:LEU:HD12	1.93	0.49
1:B:172:LYS:HB3	1:B:175:LEU:HD11	1.94	0.49
1:C:191:SER:O	1:C:194:GLN:HG2	2.14	0.48
1:C:358:ILE:HB	1:D:361:ALA:HB3	1.95	0.48
1:C:159:LYS:NZ	1:C:163:GLU:OE2	2.34	0.47
1:C:133:LYS:NZ	1:C:168:ASP:OD2	2.35	0.47
1:B:310:ARG:HB2	1:B:317:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HB3	1:A:167:TYR:CD2	2.49	0.47
1:C:137:ILE:HB	1:C:203:LEU:HD23	1.95	0.47
1:B:136:ILE:HG12	1:B:202:VAL:HB	1.97	0.47
1:B:329:HIS:CE1	1:B:341:LYS:HD3	2.49	0.47
1:A:293:GLU:OE2	1:A:360:ARG:NH2	2.49	0.46
1:B:195:THR:OG1	1:B:195:THR:O	2.34	0.46
1:D:132:ARG:HB3	1:D:167:TYR:CD2	2.49	0.46
1:D:207:GLY:HA3	1:D:253:ALA:HB1	1.98	0.46
1:D:236:ASN:O	1:D:243:ARG:NE	2.32	0.45
1:B:205:SER:HB3	1:B:212:ILE:HD11	1.99	0.45
1:C:145:LEU:HD11	1:C:217:HIS:HD2	1.81	0.45
1:C:364:THR:O	1:D:344:GLN:HG2	2.17	0.45
1:C:114:CYS:O	1:C:118:THR:OG1	2.27	0.44
1:A:131:THR:OG1	1:A:195:THR:HG23	2.17	0.44
1:B:153:PHE:CE2	1:B:313:THR:O	2.71	0.44
1:D:136:ILE:HG12	1:D:202:VAL:HB	1.98	0.44
1:D:131:THR:OG1	1:D:195:THR:HG23	2.18	0.43
1:B:102:LEU:HD12	1:B:327:ARG:HA	2.02	0.42
1:A:159:LYS:HE3	1:A:159:LYS:HB2	1.78	0.42
1:C:299:PHE:HD1	1:C:299:PHE:HA	1.78	0.41
1:B:122:TYR:CD2	1:B:365:ARG:HB2	2.55	0.41
1:D:330:ALA:HA	1:D:338:ILE:HD11	2.03	0.41
1:C:132:ARG:HB3	1:C:167:TYR:CD2	2.56	0.41
1:A:145:LEU:O	1:C:172:LYS:NZ	2.42	0.41
1:D:240:PRO:HA	1:D:243:ARG:HG3	2.04	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	228/273 (84%)	221 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	228/273 (84%)	219 (96%)	9 (4%)	0	100	100
1	C	228/273 (84%)	217 (95%)	11 (5%)	0	100	100
1	D	227/273 (83%)	219 (96%)	8 (4%)	0	100	100
All	All	911/1092 (83%)	876 (96%)	35 (4%)	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	209/242 (86%)	206 (99%)	3 (1%)	67	85
1	B	209/242 (86%)	206 (99%)	3 (1%)	67	85
1	C	209/242 (86%)	203 (97%)	6 (3%)	42	68
1	D	209/242 (86%)	204 (98%)	5 (2%)	49	74
All	All	836/968 (86%)	819 (98%)	17 (2%)	55	78

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	THR
1	A	299	PHE
1	A	359	ASP
1	B	195	THR
1	B	299	PHE
1	B	313	THR
1	C	124	ILE
1	C	195	THR
1	C	299	PHE
1	C	310	ARG
1	C	311	ASP
1	C	313	THR
1	D	195	THR

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Mol	Chain	Res	Type
1	D	299	PHE
1	D	313	THR
1	D	355	MET
1	D	359	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [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	234/273 (85%)	-0.12	0 100 100	39, 55, 79, 108	0
1	B	234/273 (85%)	-0.02	1 (0%) 92 91	39, 59, 99, 117	0
1	C	234/273 (85%)	-0.07	3 (1%) 77 73	40, 57, 92, 116	0
1	D	233/273 (85%)	0.03	4 (1%) 70 66	45, 68, 97, 119	0
All	All	935/1092 (85%)	-0.05	8 (0%) 84 82	39, 60, 96, 119	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	354	GLN	3.4
1	B	354	GLN	3.2
1	D	126	GLU	2.8
1	D	106	SER	2.7
1	D	336	PHE	2.5
1	C	349	ALA	2.2
1	C	115	ARG	2.1
1	C	209	LEU	2.0

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.