wwPDB X-ray Structure Validation Summary Report (i)

Aug 16, 2023 – 07:31 PM EDT

PDB ID	:	2AR9
Title	:	Crystal structure of a dimeric caspase-9
Authors	:	Chao, Y.; Shiozaki, E.N.; Srinivassula, S.M.; Rigotti, D.J.; Fairman, R.; Shi, Y.
Deposited on	:	2005-08-19
Resolution	:	2.80 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 (i)) were used in the production of this report:

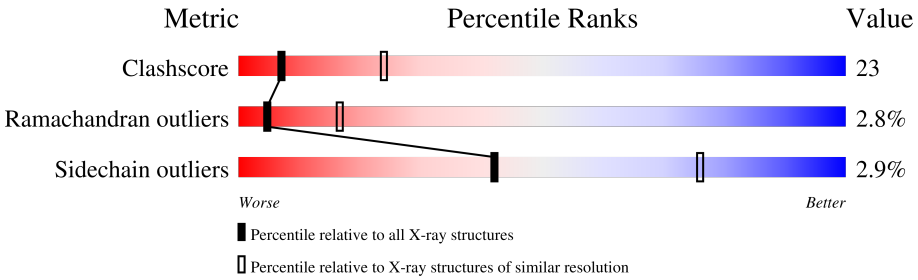
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	278	48% 32% · 17%
1	B	278	53% 28% · 17%
1	C	278	41% 37% 5% 17%
1	D	278	51% 30% · 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLT	A	668	X	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7286 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-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1783	1137	306	325	15			
1	B	232	Total	C	N	O	S	0	0	0
			1791	1141	308	327	15			
1	C	230	Total	C	N	O	S	0	0	0
			1783	1137	306	325	15			
1	D	231	Total	C	N	O	S	0	0	0
			1787	1139	307	326	15			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP P55211
A	287	SER	CYS	engineered mutation	UNP P55211
A	402	CYS	GLY	engineered mutation	UNP P55211
A	403	ILE	CYS	engineered mutation	UNP P55211
A	404	VAL	PHE	engineered mutation	UNP P55211
A	405	SER	ASN	engineered mutation	UNP P55211
A	406	MET	PHE	engineered mutation	UNP P55211
B	139	MET	-	initiating methionine	UNP P55211
B	287	SER	CYS	engineered mutation	UNP P55211
B	402	CYS	GLY	engineered mutation	UNP P55211
B	403	ILE	CYS	engineered mutation	UNP P55211
B	404	VAL	PHE	engineered mutation	UNP P55211
B	405	SER	ASN	engineered mutation	UNP P55211
B	406	MET	PHE	engineered mutation	UNP P55211
C	139	MET	-	initiating methionine	UNP P55211
C	287	SER	CYS	engineered mutation	UNP P55211
C	402	CYS	GLY	engineered mutation	UNP P55211
C	403	ILE	CYS	engineered mutation	UNP P55211
C	404	VAL	PHE	engineered mutation	UNP P55211
C	405	SER	ASN	engineered mutation	UNP P55211
C	406	MET	PHE	engineered mutation	UNP P55211

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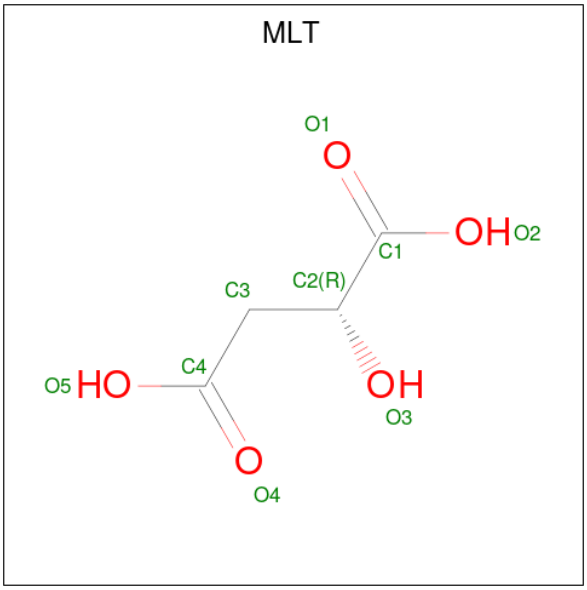
Chain	Residue	Modelled	Actual	Comment	Reference
D	139	MET	-	initiating methionine	UNP P55211
D	287	SER	CYS	engineered mutation	UNP P55211
D	402	CYS	GLY	engineered mutation	UNP P55211
D	403	ILE	CYS	engineered mutation	UNP P55211
D	404	VAL	PHE	engineered mutation	UNP P55211
D	405	SER	ASN	engineered mutation	UNP P55211
D	406	MET	PHE	engineered mutation	UNP P55211

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	45	Total O 45 45	0	0
3	B	34	Total O 34 34	0	0
3	C	24	Total O 24 24	0	0
3	D	30	Total O 30 30	0	0

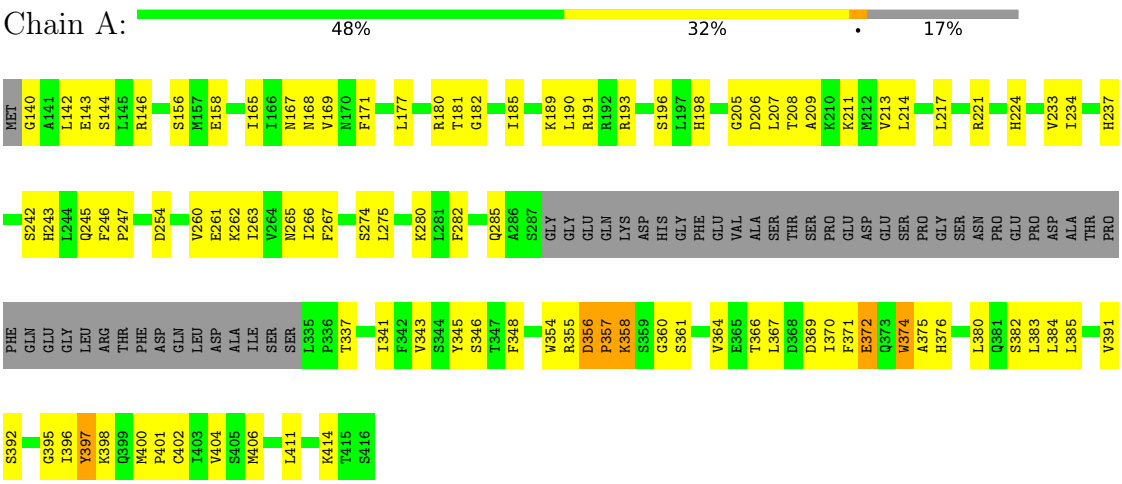
3 Residue-property plots (i)

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.

Note EDS was not executed.

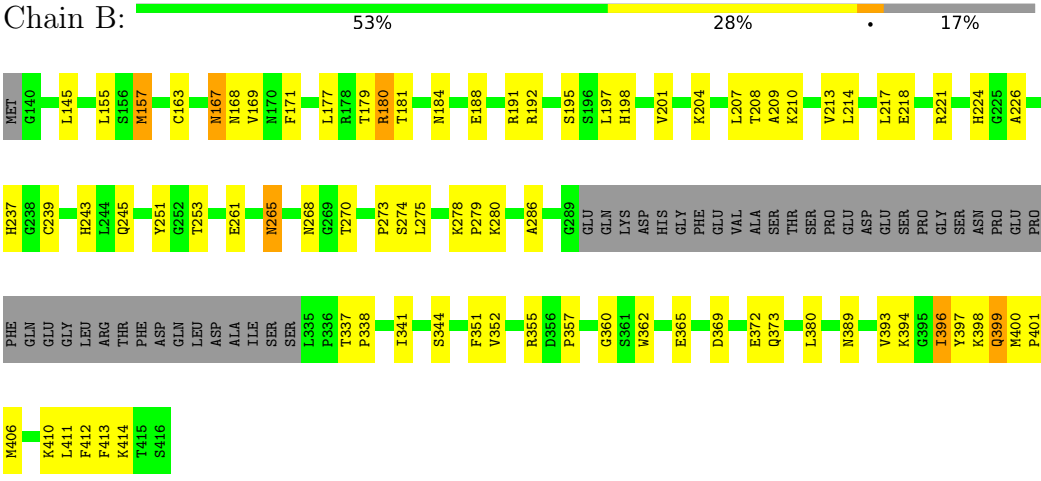
• Molecule 1: Caspase-9

Chain A:



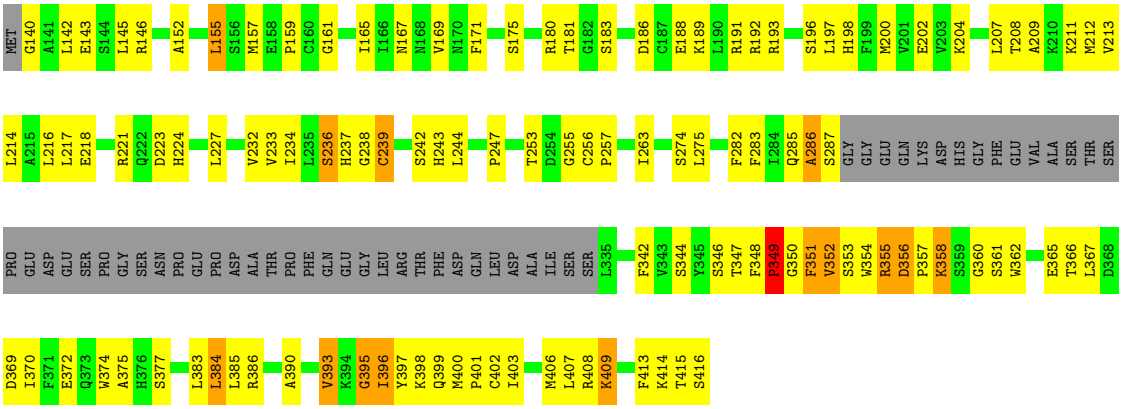
• Molecule 1: Caspase-9

Chain B:



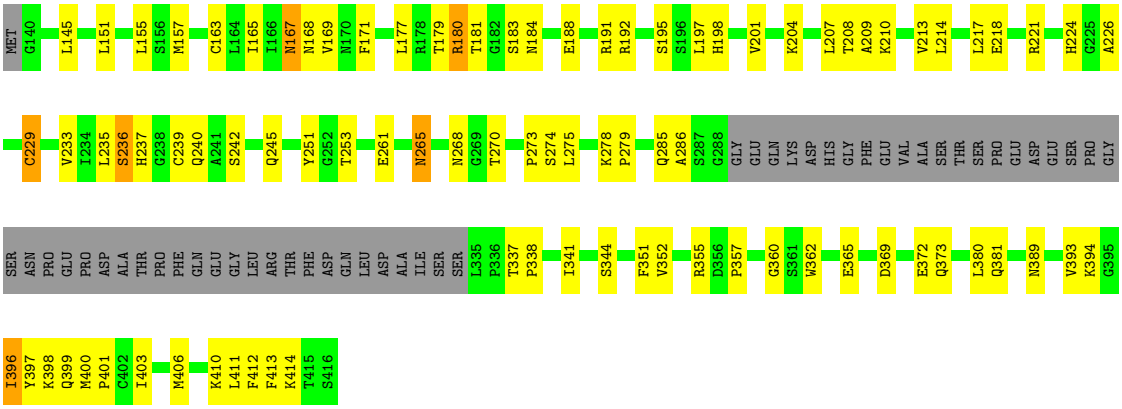
• Molecule 1: Caspase-9

Chain C:



- Molecule 1: Caspase-9

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.70Å 78.06Å 125.96Å 90.00° 112.50° 90.00°	Depositor
Resolution (Å)	11.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (11.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLT

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	0.48	0/1821	0.73	1/2459 (0.0%)
1	B	0.41	0/1829	0.63	0/2469
1	C	0.45	0/1821	0.67	0/2459
1	D	0.40	0/1825	0.63	0/2464
All	All	0.44	0/7296	0.66	1/9851 (0.0%)

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	A	374	TRP	N-CA-C	5.62	126.18	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1783	0	1791	81	0
1	B	1791	0	1797	74	0
1	C	1783	0	1791	114	0
1	D	1787	0	1794	80	0
2	A	9	0	4	1	0
3	A	45	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	1	0
3	C	24	0	0	0	0
3	D	30	0	0	0	0
All	All	7286	0	7177	326	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 23.

The worst 5 of 326 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:352:VAL:HG12	1:D:352:VAL:HG12	1.13	1.07
1:B:352:VAL:HG12	1:D:352:VAL:CG1	1.96	0.95
1:B:352:VAL:CG1	1:D:352:VAL:HG12	1.96	0.93
1:C:347:THR:CG2	1:C:353:SER:HB2	2.02	0.90
1:C:355:ARG:NH1	1:C:355:ARG:H	1.72	0.87

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	226/278 (81%)	203 (90%)	16 (7%)	7 (3%)	4 14
1	B	228/278 (82%)	207 (91%)	18 (8%)	3 (1%)	12 36
1	C	226/278 (81%)	183 (81%)	31 (14%)	12 (5%)	2 6
1	D	227/278 (82%)	208 (92%)	16 (7%)	3 (1%)	12 36
All	All	907/1112 (82%)	801 (88%)	81 (9%)	25 (3%)	5 17

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	357	PRO
1	A	358	LYS
1	B	399	GLN
1	C	157	MET
1	C	351	PHE

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	200/240 (83%)	197 (98%)	3 (2%)	65	89
1	B	200/240 (83%)	195 (98%)	5 (2%)	47	80
1	C	200/240 (83%)	190 (95%)	10 (5%)	24	56
1	D	200/240 (83%)	195 (98%)	5 (2%)	47	80
All	All	800/960 (83%)	777 (97%)	23 (3%)	42	76

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	355	ARG
1	C	409	LYS
1	C	408	ARG
1	D	167	ASN
1	B	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	162	HIS
1	D	240	GLN
1	D	376	HIS
1	D	265	ASN
1	D	184	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MLT	A	668	-	8,8,8	2.46	2 (25%)	10,10,10	2.59	6 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLT	A	668	-	1/1/3/3	6/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	668	MLT	O3-C2	6.04	1.55	1.42
2	A	668	MLT	O4-C4	2.56	1.30	1.22

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	668	MLT	C2-C3-C4	4.00	122.04	112.13
2	A	668	MLT	O3-C2-C1	-3.76	100.34	110.36
2	A	668	MLT	C3-C2-C1	3.28	118.08	110.33
2	A	668	MLT	O2-C1-C2	2.69	118.63	112.72
2	A	668	MLT	O1-C1-C2	-2.64	117.38	122.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	668	MLT	C2

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	668	MLT	O1-C1-C2-O3
2	A	668	MLT	O2-C1-C2-O3
2	A	668	MLT	O1-C1-C2-C3
2	A	668	MLT	C2-C3-C4-O5
2	A	668	MLT	C2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	668	MLT	1	0

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.