



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 09:24 PM EDT

PDB ID : 3SIR / pdb_00003sir
Title : Crystal Structure of drICE
Authors : Li, X.; Wang, J.; Shi, Y.
Deposited on : 2011-06-20
Resolution : 2.68 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 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

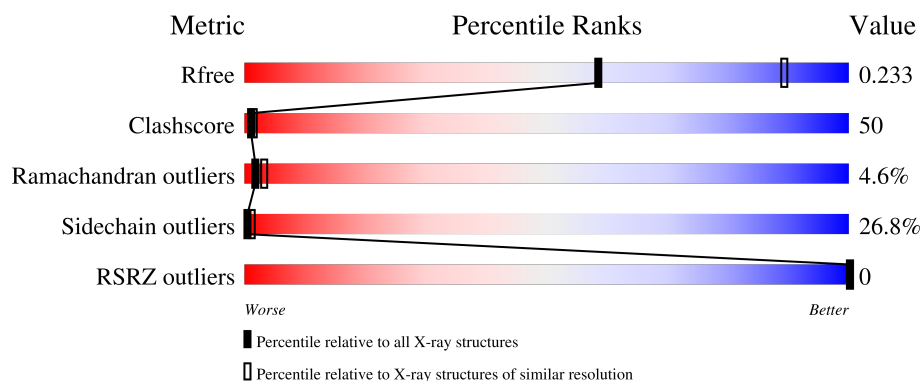
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	259	
1	B	259	
1	C	259	
1	D	259	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5766 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.

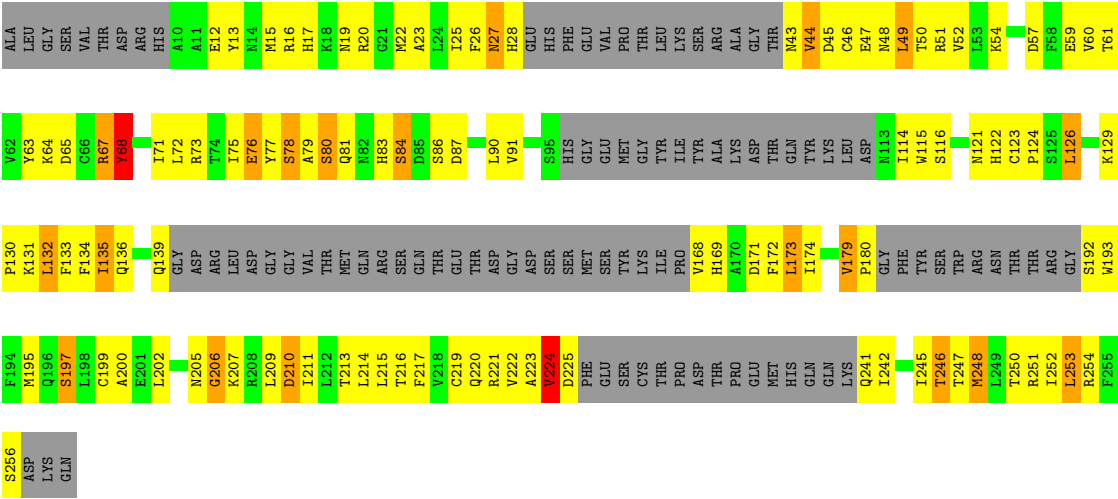
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1727	1102	300	312	13			
1	B	172	Total	C	N	O	S	0	0	0
			1377	882	236	246	13			
1	C	162	Total	C	N	O	S	0	0	0
			1298	830	224	232	12			
1	D	169	Total	C	N	O	S	0	0	0
			1361	873	234	244	10			

There are 20 discrepancies between the modelled and reference sequences:

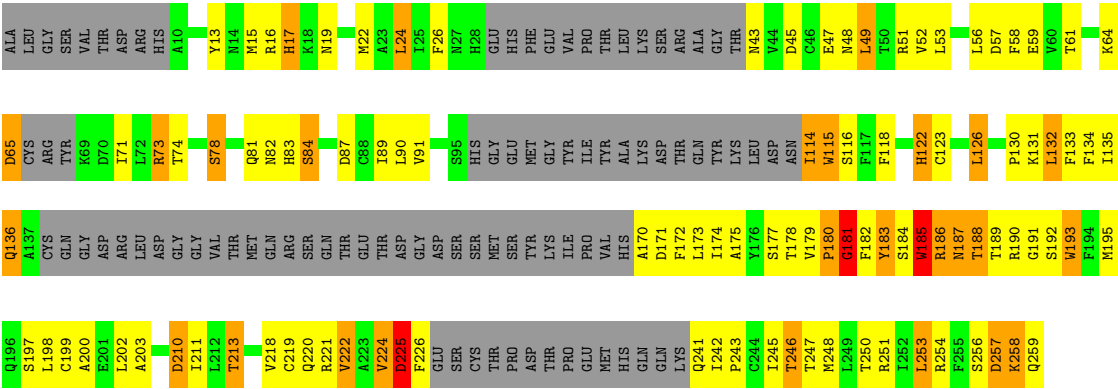
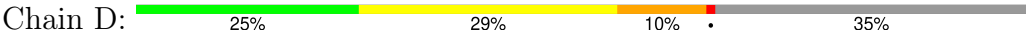
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	SEE REMARK 999	UNP O01382
A	2	LEU	-	SEE REMARK 999	UNP O01382
A	3	GLY	-	SEE REMARK 999	UNP O01382
A	4	SER	-	SEE REMARK 999	UNP O01382
A	78	SER	ALA	engineered mutation	UNP O01382
B	1	ALA	-	SEE REMARK 999	UNP O01382
B	2	LEU	-	SEE REMARK 999	UNP O01382
B	3	GLY	-	SEE REMARK 999	UNP O01382
B	4	SER	-	SEE REMARK 999	UNP O01382
B	78	SER	ALA	engineered mutation	UNP O01382
C	1	ALA	-	SEE REMARK 999	UNP O01382
C	2	LEU	-	SEE REMARK 999	UNP O01382
C	3	GLY	-	SEE REMARK 999	UNP O01382
C	4	SER	-	SEE REMARK 999	UNP O01382
C	78	SER	ALA	engineered mutation	UNP O01382
D	1	ALA	-	SEE REMARK 999	UNP O01382
D	2	LEU	-	SEE REMARK 999	UNP O01382
D	3	GLY	-	SEE REMARK 999	UNP O01382
D	4	SER	-	SEE REMARK 999	UNP O01382
D	78	SER	ALA	engineered mutation	UNP O01382

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	O	0	0
			3	3		



● Molecule 1: Caspase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	56.02Å 56.02Å 287.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.97 – 2.68 45.97 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.97-2.68) 98.8 (45.97-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.235 0.163 , 0.233	Depositor DCC
R_{free} test set	1400 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 26.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l 0.417 for h,-h-k,-l 0.416 for -k,-h,-l	Xtriage
Reported twinning fraction	0.294 for H, K, L 0.213 for -H, H+K, -L 0.214 for K, H, -L 0.279 for -h,-k,l	Depositor
Outliers	0 of 27934 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5766	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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

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	0.29	0/1765	0.70	0/2384
1	B	0.28	0/1402	0.68	2/1891 (0.1%)
1	C	0.27	0/1320	0.70	0/1781
1	D	0.27	0/1386	0.68	2/1869 (0.1%)
All	All	0.28	0/5873	0.69	4/7925 (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	A	0	8
1	B	0	7
1	C	0	2
1	D	0	4
All	All	0	21

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	CYS	CB-CA-C	-5.57	110.14	116.54
1	B	251	ARG	N-CA-C	5.22	115.42	108.38
1	D	179	VAL	CA-C-N	5.04	126.14	119.84
1	D	179	VAL	C-N-CA	5.04	126.14	119.84

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	183	TYR	Peptide
1	A	2	LEU	Peptide
1	A	65	ASP	Peptide
1	A	97	GLY	Peptide

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	1727	0	1694	235	0
1	B	1377	0	1375	127	0
1	C	1298	0	1296	107	0
1	D	1361	0	1353	122	0
2	A	3	0	0	0	0
All	All	5766	0	5718	569	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 50.

The worst 5 of 569 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:111:LEU:CA	1:A:114:ILE:HD11	1.52	1.36
1:A:109:TYR:CA	1:A:112:ASP:OD2	1.74	1.35
1:A:7:ASP:O	1:A:9:HIS:N	1.60	1.34
1:D:210:ASP:OD2	1:D:213:THR:HG23	1.19	1.32
1:D:22:MET:HE3	1:D:83:HIS:CE1	1.63	1.31

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	206/259 (80%)	162 (79%)	32 (16%)	12 (6%)	1	2
1	B	160/259 (62%)	135 (84%)	20 (12%)	5 (3%)	3	7
1	C	150/259 (58%)	130 (87%)	15 (10%)	5 (3%)	3	6
1	D	157/259 (61%)	137 (87%)	11 (7%)	9 (6%)	1	2
All	All	673/1036 (65%)	564 (84%)	78 (12%)	31 (5%)	2	3

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	HIS
1	A	57	ASP
1	A	97	GLY
1	B	68	TYR

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	188/229 (82%)	136 (72%)	52 (28%)	0	1
1	B	154/229 (67%)	108 (70%)	46 (30%)	0	1
1	C	145/229 (63%)	108 (74%)	37 (26%)	0	1
1	D	150/229 (66%)	114 (76%)	36 (24%)	1	2
All	All	637/916 (70%)	466 (73%)	171 (27%)	0	1

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	126	LEU
1	D	78	SER

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Mol	Chain	Res	Type
1	C	169	HIS
1	C	246	THR
1	D	177	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	83	HIS
1	D	81	GLN
1	C	139	GLN
1	D	83	HIS
1	A	136	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	214/259 (82%)	-1.49	0 100 100	2, 41, 55, 63	0
1	B	172/259 (66%)	-1.44	0 100 100	28, 43, 60, 73	0
1	C	162/259 (62%)	-1.48	0 100 100	27, 42, 57, 65	0
1	D	169/259 (65%)	-1.47	0 100 100	24, 44, 62, 73	0
All	All	717/1036 (69%)	-1.47	0 100 100	2, 42, 60, 73	0

There are no RSRZ outliers to report.

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.