wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 03:27 AM GMT

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

1   Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.234
Clashscore		47
Ramachandran outliers		4.6%
Sidechain outliers		24.3%
RSRZ outliers		0.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

⟦ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

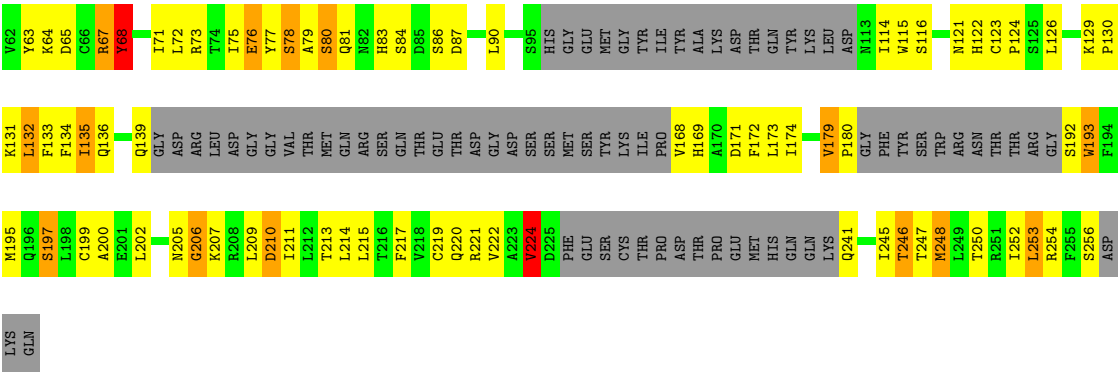- Molecule 1 is a protein called Caspase.

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
			Total	O		
2	A	3	3	3	0	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A:

- Molecule 1: Caspase

Chain B:

- Molecule 1: Caspase

Chain C:

V62 Y63 K64 D65 C66 R67 Y68 I71 L72 R73 T74 I75 E76 Y77 S78 A79 S80 Q81 N82 H83 S84 D85 S86 D87 L90 S95 HIS GLY GLU MET GLY TYR ILE PRO TYR ALA LYS ASP THR GLN TYR LYS LEU ASP N113 I114 W115 S116 N121 H122 C123 P124 S125 L126 K129 P130

K131 L132 F133 F134 I135 Q136 Q139 GLY ASP ARG LEU ASP GLY GLY VAL THR MET GLN ARG SER GLN THR GLU ASP GLY ASP SER MET SER TYR LYS ILE PRO V168 H169 A170 D171 F172 L173 I174 V179 P180 GLY PHE TYR SER ARG ASN THR THR ARG GLY S192 W193 F194

M195 Q196 S197 L198 C199 A200 E201 L202 N205 G206 K207 R208 L209 D210 I211 L212 T213 L214 L215 T216 F217 V218 C219 Q220 R221 V222 A223 V224 D225 PHE GLU SER CYS THR PRO ASP THR PRO GLU MET HIS GLN GLN LYS Q241 I245 T246 T247 M248 L249 T250 R251 I252 L253 R254 F255 S256 ASP

LYS GLN

• Molecule 1: Caspase

Chain D:

ALA LEU GLY SER VAL THR ASP ARG HIS A10 Y13 R16 H17 K18 N19 M22 A23 L24 I25 F26 N27 H28 GLU HIS PHE GLU VAL PRO THR LEU TYR LEU LYS SER ARG ALA GLY THR N43 V44 D45 C46 E47 N48 L49 T50 R51 V52 L53 L56 D57 F58 E59 V60 T61 K64 D65

CYS ARG TYR K69 D70 I71 L72 R73 T74 S78 Q81 N82 H83 S84 D87 C88 I89 L90 V91 S95 HIS GLY GLU MET GLY TYR ILE TYR ALA LYS ASP THR GLN TYR LYS LEU ASP ASN I114 W115 S116 F117 F118 H122 C123 L126 P130 K131 L132 F133 F134 I135 Q136

A137 CYS GLN GLY ASP ARG LEU ASP GLY GLY VAL THR MET GLN ARG SER GLN THR GLU THR ASP GLY ASP SER SER MET SER TYR LYS ILE PRO VAL HIS A170 D171 F172 L173 I174 A175 Y176 S177 T178 V179 P180 G181 F182 Y183 S184 W185 R186 N187 T188 T189 R190 G191 S192 W193 F194 M195 Q196

S197 L198 C199 L202 A203 D210 I211 L212 T213 V218 C219 Q220 R221 V222 A223 V224 D225 F226 GLU SER CYS THR PRO ASP THR PRO GLU MET HIS GLN GLN LYS Q241 I242 P243 C244 I245 T246 T247 M248 L249 T250 L253 R254 F255 S256 D257 K258 Q259

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
$< I/\sigma(I) >$ [1]	2.15 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.165 , 0.235 0.164 , 0.234	Depositor DCC
R_{free} test set	1400 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 18.2	EDS
Estimated 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 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
L-test for twinning	$< |L| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 27934 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

---

[1]Intensities estimated from amplitudes.

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	0/1765	0.45	0/2384
1	B	0.25	0/1402	0.43	0/1891
1	C	0.25	0/1320	0.42	0/1781
1	D	0.24	0/1386	0.42	0/1869
All	All	0.25	0/5873	0.43	0/7925

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.

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Peptide
1	A	183	TYR	Peptide
1	A	2	LEU	Peptide
1	A	65	ASP	Peptide
1	A	97	GLY	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1727	0	1694	221	0
1	B	1377	0	1375	126	0
1	C	1298	0	1296	106	0
1	D	1361	0	1353	114	0
2	A	3	0	0	0	0
All	All	5766	0	5718	545	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 47.

The worst 5 of 545 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:A:111:LEU:O	1:A:114:ILE:CD1	1.80	1.28

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	206/259 (80%)	162 (79%)	32 (16%)	12 (6%)	3	3
1	B	160/259 (62%)	135 (84%)	20 (12%)	5 (3%)	7	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	150/259 (58%)	130 (87%)	15 (10%)	5 (3%)	6	12
1	D	157/259 (61%)	137 (87%)	11 (7%)	9 (6%)	3	4
All	All	673/1036 (65%)	564 (84%)	78 (12%)	31 (5%)	4	6

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 (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	188/229 (82%)	138 (73%)	50 (27%)	1	2
1	B	154/229 (67%)	115 (75%)	39 (25%)	1	2
1	C	145/229 (63%)	113 (78%)	32 (22%)	1	3
1	D	150/229 (66%)	116 (77%)	34 (23%)	1	3
All	All	637/916 (70%)	482 (76%)	155 (24%)	1	2

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	ILE
1	B	248	MET
1	D	210	ASP
1	B	165	LYS
1	B	210	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	GLN
1	C	48	ASN
1	D	83	HIS
1	B	136	GLN
1	D	122	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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(Å²)	Q<0.9
1	A	214/259 (82%)	-0.27	0	100	100	2, 41, 55, 63	0
1	B	172/259 (66%)	-0.25	0	100	100	28, 43, 60, 73	0
1	C	162/259 (62%)	-0.26	0	100	100	27, 42, 57, 65	0
1	D	169/259 (65%)	-0.27	1 (0%)	86	90	24, 44, 62, 73	0
All	All	717/1036 (69%)	-0.26	1 (0%)	93	96	2, 42, 60, 73	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	TYR	3.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.