wwPDB X-ray Structure Validation Summary Report (i)

Aug 29, 2023 – 08:23 PM EDT

PDB ID	:	3LVL
Title	:	Crystal Structure of E.coli IscS-IscU complex
Authors	:	Shi, R.; Proteau, A.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2010-02-22
Resolution	:	3.00 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:

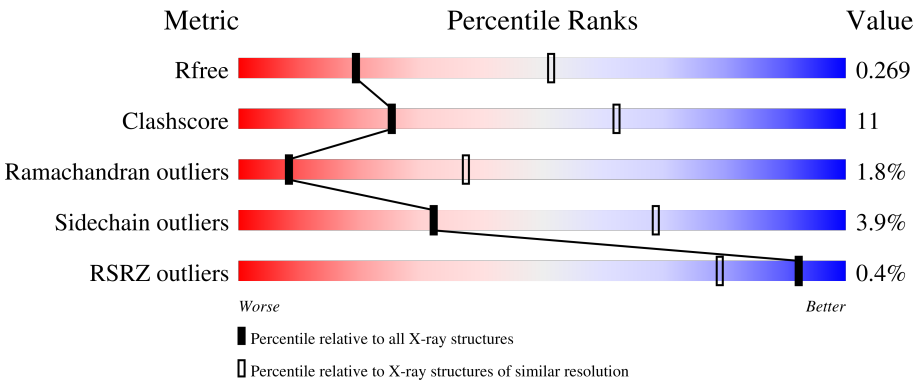
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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% 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	B	423	72% 18% • 8%
2	A	129	2% 56% 36% 5% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3966 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 Cysteine desulfurase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	388	3012	1888	535	572	17	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	MET	-	expression tag	UNP P0A6B9
B	-17	GLY	-	expression tag	UNP P0A6B9
B	-16	SER	-	expression tag	UNP P0A6B9
B	-15	SER	-	expression tag	UNP P0A6B9
B	-14	HIS	-	expression tag	UNP P0A6B9
B	-13	HIS	-	expression tag	UNP P0A6B9
B	-12	HIS	-	expression tag	UNP P0A6B9
B	-11	HIS	-	expression tag	UNP P0A6B9
B	-10	HIS	-	expression tag	UNP P0A6B9
B	-9	HIS	-	expression tag	UNP P0A6B9
B	-8	GLY	-	expression tag	UNP P0A6B9
B	-7	SER	-	expression tag	UNP P0A6B9
B	-6	MET	-	expression tag	UNP P0A6B9
B	-5	TYR	-	expression tag	UNP P0A6B9
B	-4	GLY	-	expression tag	UNP P0A6B9
B	-3	VAL	-	expression tag	UNP P0A6B9
B	-2	TYR	-	expression tag	UNP P0A6B9
B	-1	ARG	-	expression tag	UNP P0A6B9
B	0	ALA	-	expression tag	UNP P0A6B9

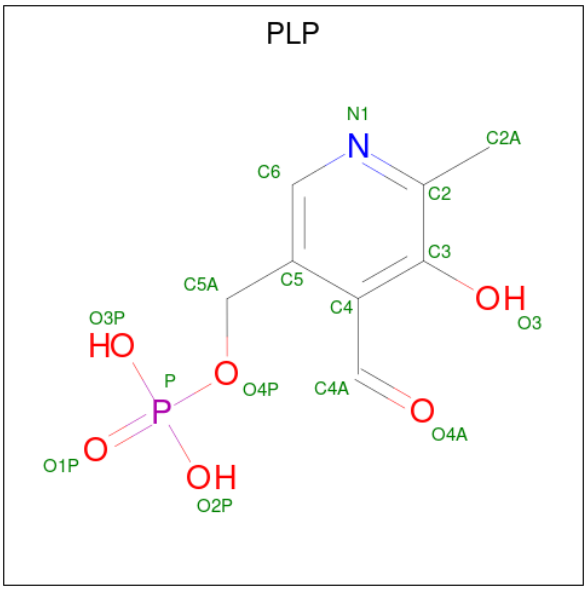
- Molecule 2 is a protein called NifU-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	125	926	574	156	191	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P0ACD6
A	1	SER	-	expression tag	UNP P0ACD6

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	15	8	1	5	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	B	12	12	12	0	0
			Total	O		
4	A	1	1	1	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 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: Cysteine desulfurase

Chain B: 72% 18% • 8%

MET GLY SER SER HIS HIS HIS HIS HIS HIS GLY GLY SER MET TYR GLY VAL TYR ARG ALA M1 K2 D8 T13 D16 P17 R18 H41 R42 F43 E49 I53 A54 R55 N56 Q57 L61 P66 R67 A75 L81 K94 F89 H104 K105 A106 T110

C111 R112 Q113 L114 E115 R116 V121 Q127 D133 E138 H152 V153 N154 I157 M169 C170 R171 A172 R173 A181 V185 D198 F202 S203 I207 Y208 V224 R225 I226 M230 H231 G232 R237 P245 Q248 A259 M263 R271 R274

W278 N279 K282 D283 L289 L293 F305 N306 Y307 Y308 E309 G310 E311 S312 L313 I314 M315 A321 S324 A327 CYS THR SER ALA SER L333 S336 L339 L344 S351 R374 R379 L383 G393 VAL ASP LEU ASN SER ILE GLU TRP ALA HIS

HIS

- Molecule 2: NifU-like protein

Chain A: 2% 56% 36% 5% •

GLY SER A2 Y3 S4 I8 D9 H10 Y11 R15 N16 V17 N23 D24 E25 N26 V27 G28 S29 G30 M31 A34 P35 A36 V40 K41 K42 L43 Q44 I45 K46 V47 N48 D49 E50 G51 I52 I53 E54 D55 A56 R57 F58 K59 T60 Y61 G62 C63 I67 A68 S69 S70 S71 L72

V73 T74 S81 E84 A85 I88 K89 N90 T91 E96 L97 S107 Y121 K124 R125 E126 ALA LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	77.65Å 77.65Å 355.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.49 – 3.00 44.49 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.8 (44.49-3.00) 83.9 (44.49-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.90 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.225 , 0.269 0.221 , 0.269	Depositor DCC
R_{free} test set	555 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	56.4	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 24.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3966	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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)

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

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	B	0.22	0/3063	0.41	0/4133
2	A	0.22	0/939	0.45	0/1272
All	All	0.22	0/4002	0.42	0/5405

There are no bond length outliers.

There are no bond angle outliers.

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	B	3012	0	2982	48	0
2	A	926	0	885	39	0
3	B	15	0	7	1	0
4	A	1	0	0	0	0
4	B	12	0	0	0	0
All	All	3966	0	3874	84	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 11.

The worst 5 of 84 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)
2:A:125:ARG:H	2:A:126:GLU:HA	1.09	1.14
2:A:125:ARG:N	2:A:126:GLU:HA	1.76	0.92
1:B:173:ARG:HG2	1:B:173:ARG:HH11	1.41	0.86
2:A:48:ASN:HB3	2:A:52:ILE:HG23	1.61	0.81
1:B:54:ALA:HA	1:B:57:GLN:HE21	1.45	0.78

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	B	384/423 (91%)	363 (94%)	18 (5%)	3 (1%)	19 57
2	A	123/129 (95%)	104 (85%)	13 (11%)	6 (5%)	2 13
All	All	507/552 (92%)	467 (92%)	31 (6%)	9 (2%)	8 37

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	LYS
2	A	36	ALA
2	A	125	ARG
2	A	50	GLU
1	B	152	HIS

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	B	316/352 (90%)	306 (97%)	10 (3%)	39	74
2	A	97/104 (93%)	91 (94%)	6 (6%)	18	52
All	All	413/456 (91%)	397 (96%)	16 (4%)	32	69

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	63	CYS
2	A	57	ARG
1	B	313	LEU
2	A	52	ILE
1	B	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	16	ASN
1	B	275	ASN
1	B	154	ASN
1	B	127	GLN
1	B	194	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 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	$\#\|Z\| > 2$
3	PLP	B	764	1	15,15,16	2.30	2 (13%)	20,22,23	1.27	2 (10%)

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
3	PLP	B	764	1	-	0/6/6/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	764	PLP	P-O4P	7.96	1.85	1.60
3	B	764	PLP	O4P-C5A	-2.65	1.35	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	764	PLP	O3P-P-O4P	-2.96	98.86	106.73
3	B	764	PLP	O2P-P-O4P	-2.31	100.58	106.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	764	PLP	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 (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	B	388/423 (91%)	-0.45	0 100 100	45, 60, 80, 97	0
2	A	125/129 (96%)	0.03	2 (1%) 72 44	62, 75, 104, 122	0
All	All	513/552 (92%)	-0.33	2 (0%) 92 79	45, 65, 90, 122	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	23	ASN	2.1
2	A	34	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PLP	B	764	15/16	0.96	0.11	60,60,60,60	0

6.5 Other polymers (i)

There are no such residues in this entry.