



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 31, 2017 – 03:35 AM EDT

PDB ID : 3SDL  
Title : Crystal structure of human ISG15 in complex with NS1 N-terminal region from influenza B virus, Northeast Structural Genomics Consortium Target IDs HX6481, HR2873, and OR2  
Authors : Guan, R.; Ma, L.-C.; Krug, R.M.; Montelione, G.T.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : unknown  
Resolution : 2.29 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

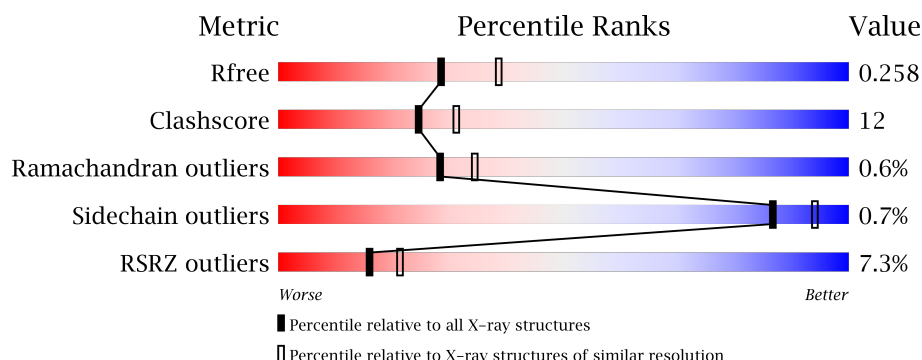
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	113	<div> <div>3%</div> <div>59%</div> <div>24%</div> <div>16%</div> </div>
1	B	113	<div> <div>12%</div> <div>57%</div> <div>27%</div> <div>14%</div> </div>
2	C	164	<div> <div>6%</div> <div>70%</div> <div>23%</div> <div>8%</div> </div>
2	D	164	<div> <div>6%</div> <div>73%</div> <div>19%</div> <div>8%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4018 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	1	0
			772	484	139	144	5			
1	B	97	Total	C	N	O	S	0	0	0
			786	494	141	146	5			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP P03502
A	-8	GLY	-	EXPRESSION TAG	UNP P03502
A	-7	HIS	-	EXPRESSION TAG	UNP P03502
A	-6	HIS	-	EXPRESSION TAG	UNP P03502
A	-5	HIS	-	EXPRESSION TAG	UNP P03502
A	-4	HIS	-	EXPRESSION TAG	UNP P03502
A	-3	HIS	-	EXPRESSION TAG	UNP P03502
A	-2	HIS	-	EXPRESSION TAG	UNP P03502
A	-1	SER	-	EXPRESSION TAG	UNP P03502
A	0	HIS	-	EXPRESSION TAG	UNP P03502
B	-9	MET	-	EXPRESSION TAG	UNP P03502
B	-8	GLY	-	EXPRESSION TAG	UNP P03502
B	-7	HIS	-	EXPRESSION TAG	UNP P03502
B	-6	HIS	-	EXPRESSION TAG	UNP P03502
B	-5	HIS	-	EXPRESSION TAG	UNP P03502
B	-4	HIS	-	EXPRESSION TAG	UNP P03502
B	-3	HIS	-	EXPRESSION TAG	UNP P03502
B	-2	HIS	-	EXPRESSION TAG	UNP P03502
B	-1	SER	-	EXPRESSION TAG	UNP P03502
B	0	HIS	-	EXPRESSION TAG	UNP P03502

- Molecule 2 is a protein called Ubiquitin-like protein ISG15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	151	Total 1159	C 734	N 200	O 221	S 4	0	0	0
2	D	151	Total 1159	C 734	N 200	O 221	S 4	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	SER	-	EXPRESSION TAG	UNP P05161
C	-5	HIS	-	EXPRESSION TAG	UNP P05161
C	-4	HIS	-	EXPRESSION TAG	UNP P05161
C	-3	HIS	-	EXPRESSION TAG	UNP P05161
C	-2	HIS	-	EXPRESSION TAG	UNP P05161
C	-1	HIS	-	EXPRESSION TAG	UNP P05161
C	0	HIS	-	EXPRESSION TAG	UNP P05161
D	-6	SER	-	EXPRESSION TAG	UNP P05161
D	-5	HIS	-	EXPRESSION TAG	UNP P05161
D	-4	HIS	-	EXPRESSION TAG	UNP P05161
D	-3	HIS	-	EXPRESSION TAG	UNP P05161
D	-2	HIS	-	EXPRESSION TAG	UNP P05161
D	-1	HIS	-	EXPRESSION TAG	UNP P05161
D	0	HIS	-	EXPRESSION TAG	UNP P05161

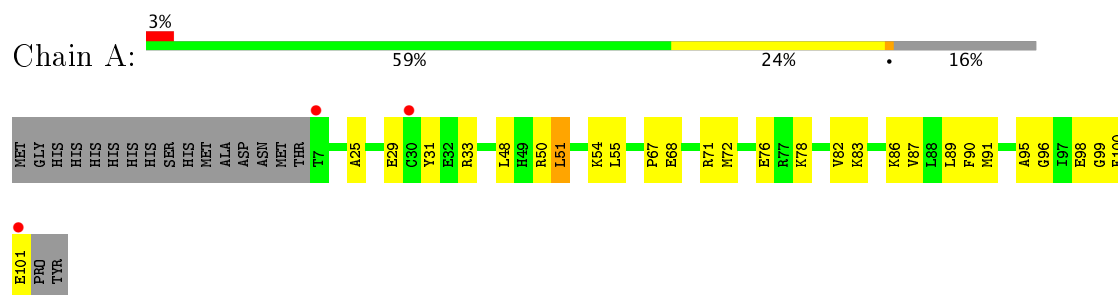
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total 33	O 33	0	0
3	B	17	Total 17	O 17	0	0
3	C	46	Total 46	O 46	0	0
3	D	46	Total 46	O 46	0	0

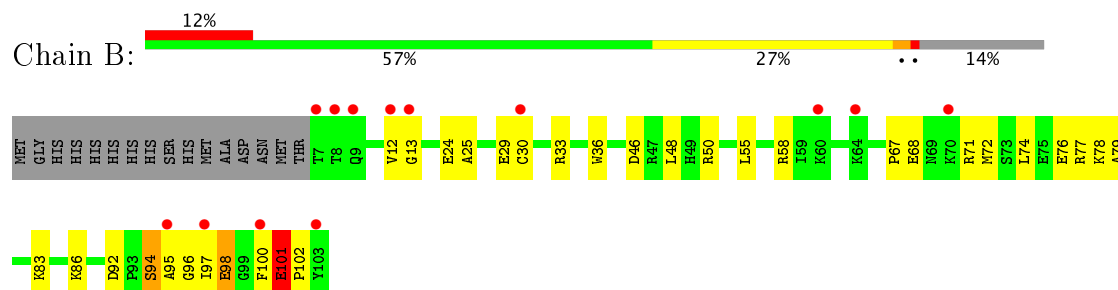
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

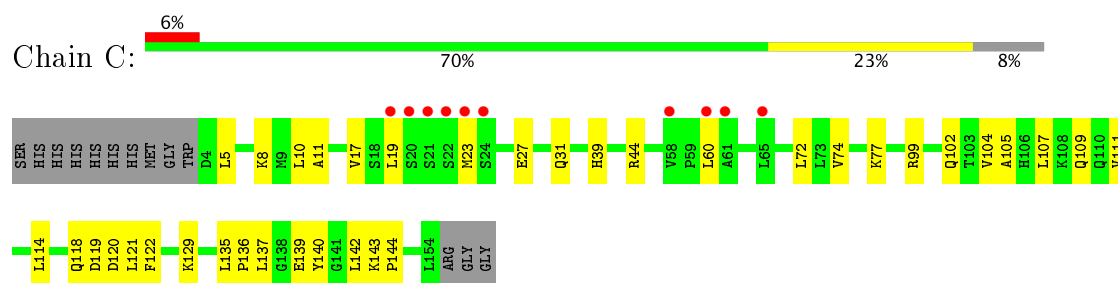
- Molecule 1: Non-structural protein 1



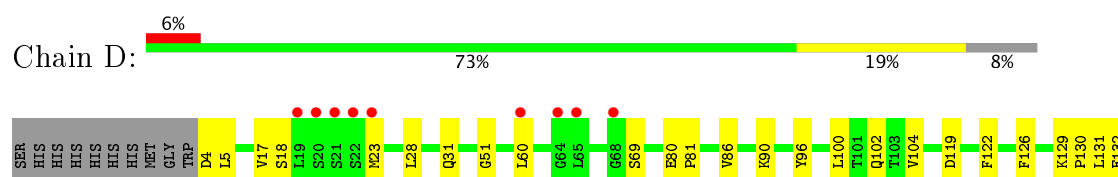
- Molecule 1: Non-structural protein 1



- Molecule 2: Ubiquitin-like protein ISG15



- Molecule 2: Ubiquitin-like protein ISG15



L137	K143	L154	ARG
G138	P144	GLY	GLY
E139	L146	GLY	GLY
S146			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.01Å 56.14Å 74.02Å 70.59° 84.24° 83.91°	Depositor
Resolution (Å)	36.72 – 2.29 36.71 – 2.29	Depositor EDS
% Data completeness (in resolution range)	86.1 (36.72-2.29) 78.2 (36.71-2.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.222 , 0.261 0.215 , 0.258	Depositor DCC
$R_{free}$ test set	1079 reflections (4.74%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4018	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.23	0/788	0.37	0/1054
1	B	0.23	0/801	0.40	0/1072
2	C	0.22	0/1177	0.41	0/1594
2	D	0.23	0/1177	0.40	0/1594
All	All	0.23	0/3943	0.40	0/5314

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	A	772	0	778	30	0
1	B	786	0	788	27	0
2	C	1159	0	1190	28	0
2	D	1159	0	1190	21	0
3	A	33	0	0	0	0
3	B	17	0	0	0	0
3	C	46	0	0	1	0
3	D	46	0	0	2	0
All	All	4018	0	3946	96	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 12.



The worst 5 of 96 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:C:17:VAL:HG13	2:C:31:GLN:HG2	1.56	0.87
2:C:136:PRO:HG2	2:C:139:GLU:HG2	1.72	0.72
1:B:12:VAL:HG23	1:B:13:GLY:H	1.57	0.70
1:A:95:ALA:N	1:A:96:GLY:HA3	2.07	0.69
1:A:25:ALA:HA	1:A:55:LEU:HD21	1.73	0.69

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	94/113 (83%)	90 (96%)	4 (4%)	0	100	100
1	B	95/113 (84%)	86 (90%)	6 (6%)	3 (3%)	5	3
2	C	149/164 (91%)	146 (98%)	3 (2%)	0	100	100
2	D	149/164 (91%)	146 (98%)	3 (2%)	0	100	100
All	All	487/554 (88%)	468 (96%)	16 (3%)	3 (1%)	28	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101	GLU
1	B	94	SER
1	B	98	GLU

### 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	83/98 (85%)	82 (99%)	1 (1%)	75	87
1	B	84/98 (86%)	82 (98%)	2 (2%)	54	72
2	C	132/142 (93%)	132 (100%)	0	100	100
2	D	132/142 (93%)	132 (100%)	0	100	100
All	All	431/480 (90%)	428 (99%)	3 (1%)	87	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	B	97	ILE
1	B	101	GLU

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

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	95/113 (84%)	0.40	3 (3%) 48 55	36, 64, 113, 125	0
1	B	97/113 (85%)	0.87	13 (13%) 4 5	37, 64, 142, 160	0
2	C	151/164 (92%)	0.49	10 (6%) 19 25	40, 60, 109, 156	0
2	D	151/164 (92%)	0.47	10 (6%) 19 25	38, 64, 102, 145	0
All	All	494/554 (89%)	0.54	36 (7%) 16 21	36, 63, 120, 160	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	100	PHE	8.5
2	D	20	SER	7.3
2	C	19	LEU	6.4
1	B	97	ILE	5.6
2	C	20	SER	5.5

### 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.