

wwPDB X-ray Structure Validation Summary Report (i)

Aug 9, 2020 – 06:02 AM BST

PDB ID : 6JIV

Title : SspE crystal structure Authors : Bing, Y.Z.; Yang, H.G.

Deposited on : 2019-02-23

Resolution : 3.31 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 following versions of software and data (see references (1)) 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 : 2.13.1

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

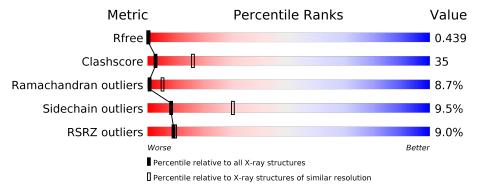
Validation Pipeline (wwPDB-VP) : 2.13.1

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 3.31 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	$egin{aligned} ext{Similar resolution} \ (\# ext{Entries, resolution range}(ext{Å})) \end{aligned}$
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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 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	A	771	44%	23%	5%	27%	-	
1	В	771	12%	23%	•	27%	_	
1	С	771	39%	27%	6%	28%	_	
1	D	771	43%	25%	5%	27%	_	



2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15028 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 SspE protein.

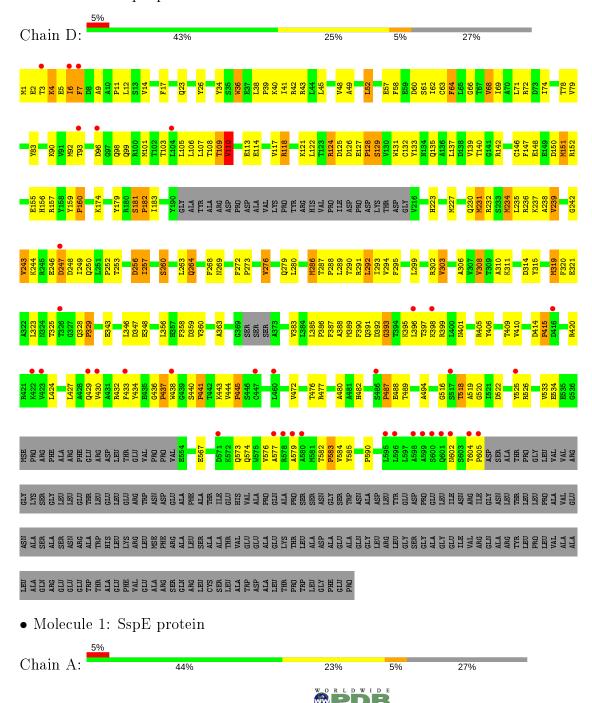
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	D	560	Total	С	N	О	S	Se	0	0	0
1	ש	300	3711	2310	674	713	3	11	U	U	0
1	Λ	560	Total	С	N	О	S	Se	0	0	0
1	A	300	3711	2310	674	713	3	11	U	U	0
1	В	560	Total	С	N	О	S	Se	0	0	0
1	Б	300	3711	2310	674	713	3	11	U	U	0
1	С	557	Total	С	N	О	S	Se	0	0	0
		997	3895	2439	697	743	4	12	U	U	U

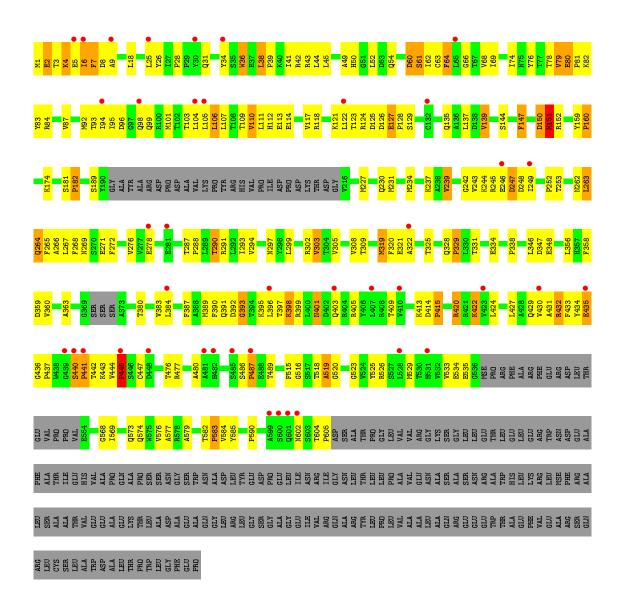


3 Residue-property plots (i)

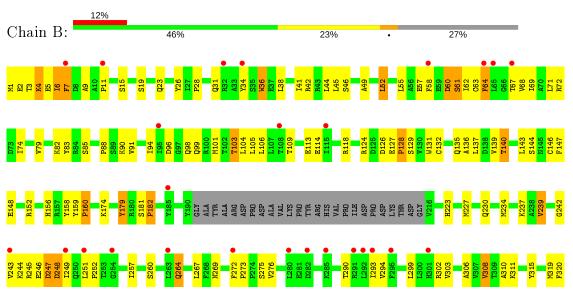
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.



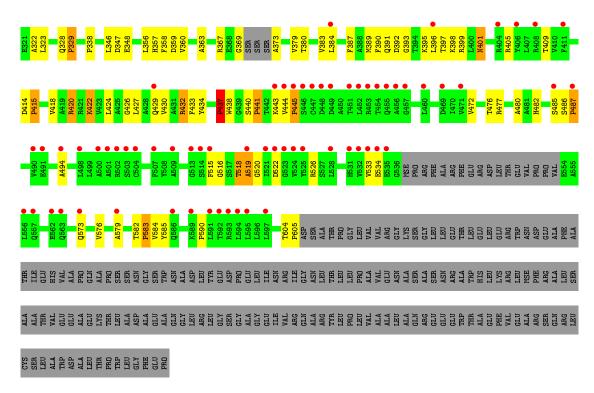




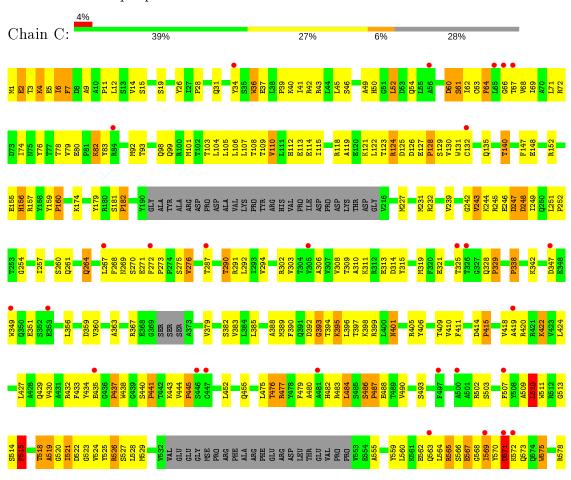
• Molecule 1: SspE protein



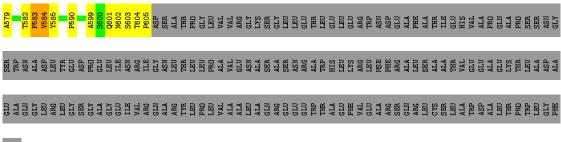




• Molecule 1: SspE protein











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	111.07Å 138.16Å 293.68Å	Donositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.33 - 3.31	Depositor
Resolution (A)	125.02 - 3.31	EDS
% Data completeness	99.5 (125.33-3.31)	Depositor
(in resolution range)	99.5 (125.02-3.31)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
D D	0.406 , 0.435	Depositor
R, R_{free}	0.407 , 0.439	DCC
R_{free} test set	3357 reflections $(4.96%)$	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.29 , 110.6	EDS
L-test for twinning ²	$ < L > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	15028	wwPDB-VP
Average B, all atoms $(Å^2)$	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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	Bo	nd lengths	Bond angles		
	RMSZ	# Z > 5	RMSZ	# Z >5		
1	A	0.60	0/3747	0.84	17/5100 (0.3%)	
1	В	0.52	0/3747	0.75	$16/5100 \; (0.3\%)$	
1	С	0.57	0/3943	0.82	$15/5351 \ (0.3\%)$	
1	D	0.73	5/3747~(0.1%)	0.90	$16/5100 \ (0.3\%)$	
All	All	0.61	5/15184 (0.0%)	0.83	$64/20651 \ (0.3\%)$	

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	1
1	С	0	2
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(\mathbf{\mathring{A}})$	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	146	CYS	CB-SG	-10.19	1.65	1.82
1	D	110	VAL	CB-CG1	-5.86	1.40	1.52
1	D	133	TYR	CE1-CZ	-5.46	1.31	1.38
1	D	260	SER	CA-CB	-5.23	1.45	1.52
1	D	68	VAL	CB-CG1	-5.01	1.42	1.52

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\mathbf{Ideal}(^o)$
1	С	484	LEU	CB-CG-CD1	-9.98	94.03	111.00
1	D	160	PRO	N-CA-CB	9.37	114.54	103.30
1	A	160	PRO	N-CA-CB	8.07	112.98	103.30
1	A	329	PRO	N-CA-CB	7.82	112.69	103.30
1	В	329	PRO	N-CA-CB	7.54	112.35	103.30



There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLU	Peptide
1	С	477	ARG	Peptide
1	С	584	VAL	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	3711	0	3036	217	0
1	В	3711	0	3038	219	0
1	С	3895	0	3376	323	0
1	D	3711	0	3038	246	0
All	All	15028	0	12488	970	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 35.

The worst 5 of 970 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} \ (ext{Å}) \end{aligned}$	$egin{array}{c} { m Clash} \ { m overlap} \ ({ m \AA}) \end{array}$
1:C:515:PHE:CZ	1:C:578:ARG:HD3	1.32	1.63
1:D:356:LEU:CA	1:D:427:LEU:HD11	1.17	1.59
1:A:356:LEU:CA	1:A:427:LEU:HD11	1.16	1.59
1:D:356:LEU:HA	1:D:427:LEU:CD1	1.30	1.55
1:D:395:LYS:CE	1:D:526:ARG:HD3	1.37	1.55

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	552/771 (72%)	429 (78%)	73 (13%)	50 (9%)	1 5
1	В	552/771 (72%)	437 (79%)	70 (13%)	45 (8%)	1 6
1	С	549/771 (71%)	423 (77%)	80 (15%)	46 (8%)	1 6
1	D	552/771 (72%)	427 (77%)	75 (14%)	50 (9%)	1 5
All	All	2205/3084~(72%)	1716 (78%)	298 (14%)	191 (9%)	1 5

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	GLU
1	D	4	LYS
1	D	6	ILE
1	D	61	SER
1	D	129	SER

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	$268/637 \; (42\%)$	241 (90%)	27 (10%)	7	28
1	В	$268/637 \; (42\%)$	245 (91%)	23 (9%)	10	36
1	С	$322/637\ (50\%)$	293 (91%)	29 (9%)	9	33
1	D	268/637 (42%)	240 (90%)	28 (10%)	7	26
All	All	1126/2548 (44%)	1019 (90%)	107 (10%)	8	30



5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	VAL
1	В	67	THR
1	С	515	PHE
1	A	358	PHE
1	A	525	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	391	GLN
1	В	156	HIS
1	В	429	GLN
1	A	156	HIS
1	В	391	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)

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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	A	548/771 (71%)	0.30	41 (7%) 14 14	53, 109, 176, 219	0
1	В	548/771 (71%)	0.87	92 (16%) 1 1	62, 120, 274, 329	0
1	С	545/771 (70%)	0.37	28 (5%) 28 27	30, 104, 136, 171	0
1	D	548/771 (71%)	0.36	36 (6%) 18 19	37, 91, 169, 223	0
All	All	$2189/3084 \ (70\%)$	0.47	197 (8%) 9 10	30, 106, 216, 329	0

The worst 5 of 197 RSRZ outliers are listed below:

Mol	Chain	${f Res}$	Type	RSRZ
1	В	446	SER	14.8
1	В	448	ASP	12.9
1	В	533	VAL	10.3
1	В	522	ASP	9.0
1	В	532	VAL	8.3

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)

There are no ligands in this entry.



6.5 Other polymers (i)

There are no such residues in this entry.

