



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2021 – 10:16 AM EDT

PDB ID : 7M1B  
Title : SusE-like protein BT2857  
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Deposited on : 2021-03-12  
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

<https://www.wwpdb.org/validation/2017/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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
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) : 2.18

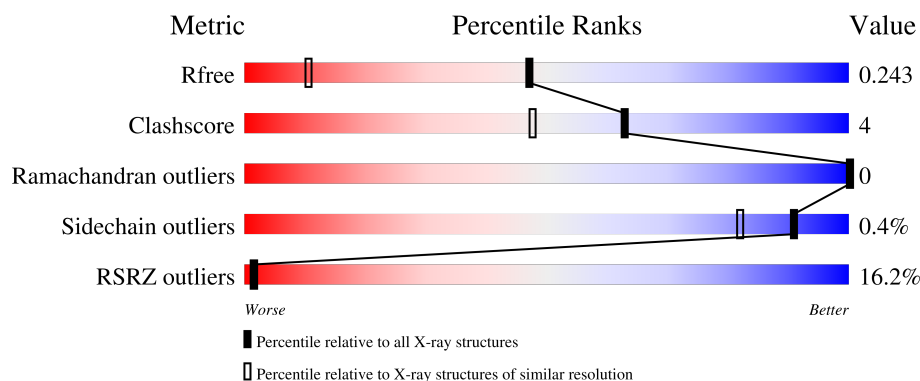
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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  $\geq 3$ , 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	AAA	382	<div> <div>11%</div> <div>63%</div> <div>6%</div> <div>30%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2393 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 Galactose-binding-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	266	Total	C	N	O	S	0	0	0
			2160	1389	349	417	5			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	AAA	1	Total	C	O	0	0
			4	2	2		

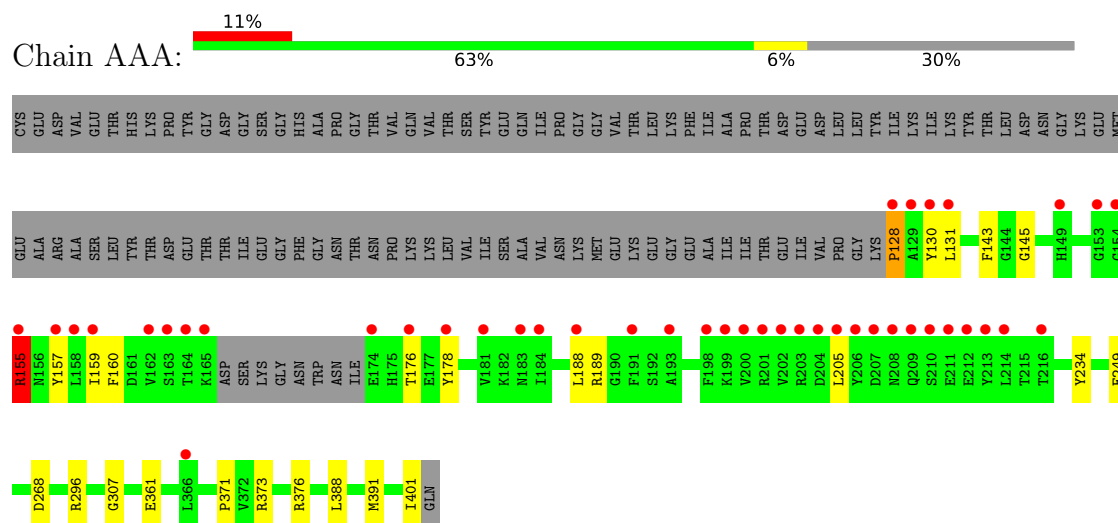
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	229	Total	O	0	0
			229	229		

### 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: Galactose-binding-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.65Å 48.79Å 112.66Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	40.49 – 1.50 40.49 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.49-1.50) 99.9 (40.49-1.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.201 , 0.237 0.205 , 0.243	Depositor DCC
$R_{free}$ test set	3163 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.17% 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

### 5.1 Standard geometry

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

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	AAA	0.86	4/2228 (0.2%)	1.04	7/3028 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	130	TYR	CZ-OH	7.40	1.50	1.37
1	AAA	155	ARG	C-O	5.97	1.34	1.23
1	AAA	361	GLU	CD-OE1	-5.91	1.19	1.25
1	AAA	128	PRO	N-CA	5.64	1.56	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	373	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	AAA	189	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	AAA	296	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	AAA	376	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	AAA	128	PRO	CA-N-CD	-5.42	103.91	111.50
1	AAA	143	PHE	CB-CG-CD2	5.22	124.45	120.80
1	AAA	234	TYR	CB-CG-CD2	-5.11	117.94	121.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-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 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	AAA	2160	0	2011	18	0
2	AAA	4	0	6	0	0
3	AAA	229	0	0	7	0
All	All	2393	0	2017	18	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 4.

All (18) 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:AAA:371:PRO:HB3	1:AAA:401:ILE:CD1	2.11	0.80
1:AAA:391:MET:HG3	3:AAA:822:HOH:O	1.83	0.77
1:AAA:371:PRO:HB3	1:AAA:401:ILE:HD12	1.72	0.71
1:AAA:159:ILE:HD12	1:AAA:178:TYR:CD2	2.32	0.65
1:AAA:249:GLU:OE2	3:AAA:601:HOH:O	2.16	0.61
1:AAA:157:TYR:CE2	1:AAA:159:ILE:HD11	2.36	0.61
1:AAA:205:LEU:HB2	3:AAA:614:HOH:O	2.02	0.59
1:AAA:159:ILE:HD12	1:AAA:178:TYR:HD2	1.68	0.58
1:AAA:268:ASP:OD2	3:AAA:602:HOH:O	2.18	0.53
1:AAA:160:PHE:O	1:AAA:176:THR:HA	2.09	0.52
1:AAA:128:PRO:HG2	1:AAA:131:LEU:HD12	1.92	0.52
1:AAA:371:PRO:CB	1:AAA:401:ILE:CD1	2.88	0.49
1:AAA:145:GLY:HA3	1:AAA:188:LEU:O	2.13	0.49
1:AAA:391:MET:CG	3:AAA:822:HOH:O	2.51	0.48
1:AAA:155:ARG:HE	1:AAA:155:ARG:HB3	1.26	0.43
1:AAA:155:ARG:NH1	3:AAA:604:HOH:O	2.34	0.43
1:AAA:128:PRO:HD3	3:AAA:786:HOH:O	2.17	0.43
1:AAA:307:GLY:HA2	1:AAA:388:LEU:O	2.20	0.42

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	AAA	262/382 (69%)	252 (96%)	10 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	AAA	230/328 (70%)	229 (100%)	1 (0%)	91	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	155	ARG

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

### 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	$\# Z  > 2$
2	EDO	AAA	501	-	3,3,3	0.51	0	2,2,2	0.59	0

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
2	EDO	AAA	501	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 ⓘ

### 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, 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	AAA	266/382 (69%)	0.81	43 (16%) <b>1</b> <b>1</b>	16, 23, 52, 78	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	131	LEU	7.0
1	AAA	366	LEU	5.3
1	AAA	178	TYR	5.3
1	AAA	211	GLU	5.1
1	AAA	205	LEU	4.9
1	AAA	201	ARG	4.8
1	AAA	130	TYR	4.7
1	AAA	159	ILE	4.4
1	AAA	165	LYS	4.3
1	AAA	158	LEU	4.2
1	AAA	209	GLN	4.1
1	AAA	163	SER	4.1
1	AAA	214	LEU	4.1
1	AAA	200	VAL	4.0
1	AAA	202	VAL	4.0
1	AAA	213	TYR	4.0
1	AAA	155	ARG	3.8
1	AAA	207	ASP	3.8
1	AAA	164	THR	3.6
1	AAA	154	GLY	3.5
1	AAA	193	ALA	3.5
1	AAA	191	PHE	3.4
1	AAA	128	PRO	3.4
1	AAA	129	ALA	3.3
1	AAA	176	THR	3.1
1	AAA	206	TYR	3.0
1	AAA	162	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	AAA	157	TYR	2.8
1	AAA	199	LYS	2.8
1	AAA	153	GLY	2.7
1	AAA	210	SER	2.7
1	AAA	181	VAL	2.6
1	AAA	212	GLU	2.6
1	AAA	184	ILE	2.5
1	AAA	198	PHE	2.4
1	AAA	183	ASN	2.4
1	AAA	188	LEU	2.3
1	AAA	208	ASN	2.3
1	AAA	149	HIS	2.2
1	AAA	204	ASP	2.1
1	AAA	216	THR	2.1
1	AAA	174	GLU	2.1
1	AAA	203	ARG	2.0

## 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	EDO	AAA	501	4/4	0.89	0.12	28,30,32,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.