



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 10, 2018 – 02:29 PM EST

PDB ID : 5CRC  
Title : Structure of the SdeA DUB Domain  
Authors : Sheedlo, M.J.; Qiu, J.; Tan, Y.; Paul, L.N.; Luo, Z.Q.; Das, C.  
Deposited on : 2015-07-22  
Resolution : 2.85 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

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

with specific help available everywhere you see the ⓘ symbol.

---

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-20030736  
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-20030736

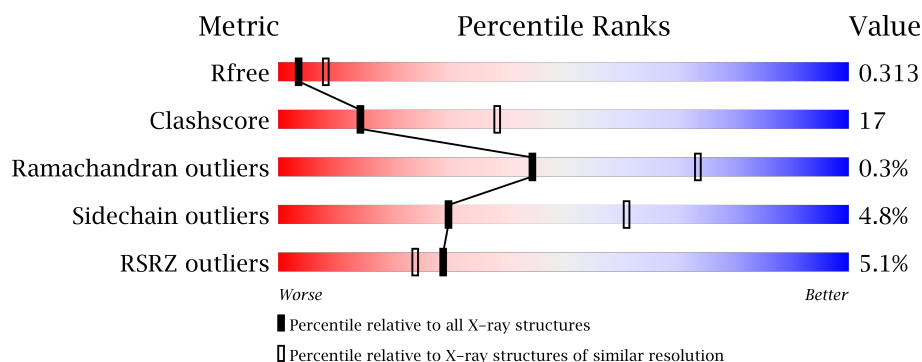
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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	193	<div> <div>4%</div> <div>48%</div> <div>28%</div> <div>•</div> <div>21%</div> </div>
1	B	193	<div> <div>4%</div> <div>48%</div> <div>29%</div> <div>••</div> <div>20%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2267 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.

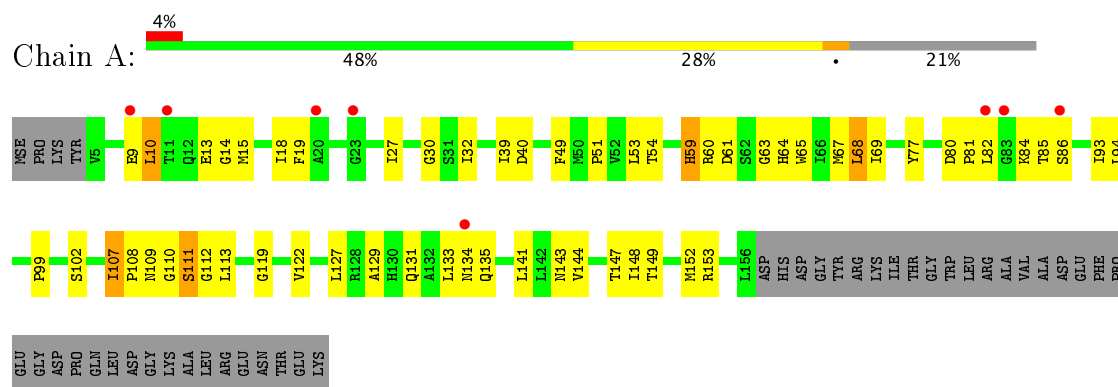
- Molecule 1 is a protein called SdeA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	Se	0	0	0
			1123	706	198	211	1	7			
1	B	155	Total	C	N	O	S	Se	0	1	0
			1144	722	198	216	1	7			

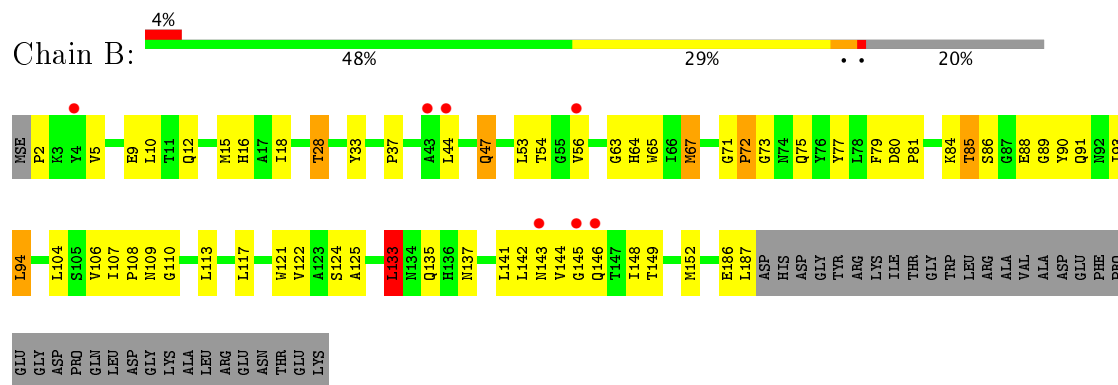
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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: SdeA



#### • Molecule 1: SdeA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.54Å 63.34Å 136.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.95 – 2.85 36.96 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.9 (36.95-2.85) 90.9 (36.96-2.85)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.33 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.280 , 0.296 0.289 , 0.313	Depositor DCC
$R_{free}$ test set	318 reflections (4.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	2267	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.76 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0858e-04.*

<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

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	0.31	0/1142	0.72	0/1541
1	B	0.31	0/1167	0.62	2/1578 (0.1%)
All	All	0.31	0/2309	0.67	2/3119 (0.1%)

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	4
1	B	0	4
All	All	0	8

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	LEU	CA-CB-CG	-6.50	100.35	115.30
1	B	2	PRO	N-CA-CB	5.89	110.37	103.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LEU	Peptide
1	A	111	SER	Peptide
1	A	40	ASP	Peptide
1	A	81	PRO	Peptide
1	B	133	LEU	Peptide
1	B	47	GLN	Peptide
1	B	5	VAL	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	B	72	PRO	Peptide

## 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	A	1123	0	1082	46	0
1	B	1144	0	1094	47	0
All	All	2267	0	2176	77	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 17.

All (77) 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:A:67:MSE:HB2	1:B:122:VAL:HG13	1.51	0.92
1:A:32:ILE:HD11	1:A:94:LEU:HD21	1.65	0.77
1:A:30:GLY:HA3	1:A:39:ILE:HG22	1.70	0.73
1:A:122:VAL:HG13	1:B:67:MSE:HB2	1.73	0.70
1:B:75:GLN:NE2	1:B:77:TYR:OH	2.23	0.69
1:A:82:LEU:O	1:A:86:SER:OG	2.13	0.67
1:A:61:ASP:HB2	1:B:85:THR:HG21	1.78	0.66
1:B:28:THR:H	1:B:44:LEU:HD22	1.61	0.66
1:B:91:GLN:HG3	1:B:104:LEU:HD12	1.78	0.65
1:B:15:MSE:HE3	1:B:65:TRP:CD2	2.33	0.64
1:B:143:ASN:OD1	1:B:144:VAL:N	2.32	0.62
1:B:144:VAL:HA	1:B:148:ILE:HG23	1.81	0.62
1:A:15:MSE:HE3	1:A:19:PHE:HE2	1.63	0.61
1:A:110:GLY:H	1:B:149:THR:HG22	1.66	0.60
1:A:59:HIS:ND1	1:A:60:ARG:HG3	2.16	0.60
1:A:99:PRO:O	1:A:102:SER:OG	2.16	0.58
1:A:82:LEU:HD13	1:A:111:SER:HB2	1.86	0.57
1:B:15:MSE:HE3	1:B:65:TRP:CE2	2.40	0.57
1:B:9:GLU:HG3	1:B:63:GLY:O	2.04	0.57
1:A:53:LEU:HD11	1:A:63:GLY:HA3	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HG3	1:A:85:THR:HG23	1.86	0.56
1:A:27:ILE:HD13	1:A:51:PRO:HD2	1.90	0.54
1:A:69:ILE:HB	1:A:77:TYR:HB2	1.90	0.54
1:B:84:LYS:HG2	1:B:108:PRO:HA	1.90	0.53
1:A:15:MSE:HE3	1:A:19:PHE:CE2	2.42	0.53
1:B:93:ILE:HG23	1:B:94:LEU:HD13	1.91	0.52
1:A:112:GLY:HA2	1:B:152:MSE:HG2	1.92	0.52
1:A:49:PHE:HB2	1:A:67:MSE:SE	2.60	0.51
1:A:108:PRO:HG2	1:B:141:LEU:HD12	1.92	0.51
1:B:144:VAL:O	1:B:148:ILE:N	2.41	0.51
1:A:148:ILE:HG22	1:A:152:MSE:HE2	1.93	0.51
1:A:84:LYS:HG3	1:A:85:THR:H	1.75	0.51
1:A:144:VAL:O	1:A:147:THR:OG1	2.27	0.50
1:B:121:TRP:CE2	1:B:152:MSE:HG3	2.47	0.50
1:A:64:HIS:NE2	1:A:80:ASP:OD1	2.44	0.49
1:A:149:THR:OG1	1:B:110:GLY:N	2.44	0.49
1:A:143:ASN:O	1:A:147:THR:HG23	2.13	0.49
1:B:124:SER:OG	1:B:125:ALA:N	2.45	0.47
1:A:152:MSE:HE1	1:B:109:ASN:HD22	1.79	0.47
1:B:88:GLU:HA	1:B:91:GLN:HB2	1.98	0.46
1:B:12:GLN:O	1:B:16:HIS:ND1	2.32	0.46
1:A:82:LEU:HB2	1:A:111:SER:HB2	1.97	0.45
1:A:109:ASN:HA	1:B:145:GLY:HA2	1.98	0.45
1:B:80:ASP:HA	1:B:81:PRO:HD2	1.80	0.45
1:A:77:TYR:CE2	1:B:133:LEU:HD13	2.52	0.45
1:A:93:ILE:H	1:A:93:ILE:HD12	1.81	0.45
1:B:37:PRO:HD3	1:B:93:ILE:HD11	2.00	0.44
1:A:134:ASN:HA	1:A:135:GLN:HA	1.45	0.44
1:A:60:ARG:HG2	1:B:89:GLY:HA3	1.98	0.44
1:A:64:HIS:HE2	1:A:80:ASP:CG	2.20	0.44
1:A:54:THR:OG1	1:A:64:HIS:HB3	2.17	0.44
1:B:142:LEU:HA	1:B:146:GLN:HG2	2.00	0.44
1:B:53:LEU:HG	1:B:56:VAL:HG21	2.00	0.44
1:B:72:PRO:HA	1:B:73:GLY:HA2	1.64	0.44
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.84	0.43
1:A:119:GLY:HA3	1:B:15:MSE:HE1	2.00	0.43
1:A:113:LEU:HD21	1:B:117:LEU:HD22	1.99	0.43
1:B:54:THR:O	1:B:63:GLY:HA3	2.19	0.43
1:A:107:ILE:HA	1:A:108:PRO:HD3	1.74	0.43
1:B:33:TYR:HA	1:B:56:VAL:O	2.18	0.43
1:A:129:ALA:O	1:A:133:LEU:HD23	2.18	0.43

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ILE:HG21	1:B:79:PHE:CE1	2.54	0.42
1:B:137:ASN:OD1	1:B:137:ASN:N	2.46	0.42
1:B:135[A]:GLN:H	1:B:135[A]:GLN:HG2	1.46	0.42
1:A:10:LEU:HD21	1:A:65:TRP:N	2.35	0.41
1:A:49:PHE:HA	1:A:68:LEU:O	2.19	0.41
1:B:186:GLU:O	1:B:187:LEU:HB2	2.19	0.41
1:A:134:ASN:CB	1:B:71:GLY:HA2	2.50	0.41
1:A:27:ILE:HG13	1:A:27:ILE:H	1.69	0.41
1:B:88:GLU:HG3	1:B:106:VAL:HG11	2.03	0.41
1:B:10:LEU:HD21	1:B:18:ILE:HD12	2.02	0.41
1:B:64:HIS:HD2	1:B:90:TYR:CE2	2.39	0.41
1:A:141:LEU:HG	1:B:108:PRO:HD3	2.03	0.41
1:A:127:LEU:O	1:A:131:GLN:HB2	2.21	0.40
1:B:79:PHE:HB2	1:B:107:ILE:HD12	2.03	0.40
1:A:14:GLY:O	1:A:18:ILE:HG23	2.21	0.40
1:B:86:SER:O	1:B:89:GLY:N	2.50	0.40

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	150/193 (78%)	127 (85%)	22 (15%)	1 (1%)	25	56
1	B	154/193 (80%)	143 (93%)	11 (7%)	0	100	100
All	All	304/386 (79%)	270 (89%)	33 (11%)	1 (0%)	44	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	GLU

### 5.3.2 Protein sidechains ⓘ

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	115/146 (79%)	110 (96%)	5 (4%)	33	65
1	B	117/146 (80%)	111 (95%)	6 (5%)	28	58
All	All	232/292 (80%)	221 (95%)	11 (5%)	30	62

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	59	HIS
1	A	68	LEU
1	A	107	ILE
1	A	153	ARG
1	B	28	THR
1	B	47	GLN
1	B	67	MSE
1	B	85	THR
1	B	94	LEU
1	B	113	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	109	ASN

### 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 [i](#)

There are no carbohydrates 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<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	145/193 (75%)	0.53	8 (5%) 26 21	9, 14, 24, 34	0
1	B	148/193 (76%)	0.47	7 (4%) 32 27	10, 13, 21, 29	0
All	All	293/386 (75%)	0.50	15 (5%) 29 24	9, 14, 24, 34	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	ASN	4.4
1	B	4	TYR	3.5
1	B	44	LEU	3.4
1	A	86	SER	3.3
1	B	43	ALA	3.3
1	B	143	ASN	3.2
1	A	82	LEU	3.2
1	A	9	GLU	3.1
1	B	146	GLN	3.0
1	A	83	GLY	2.9
1	B	145	GLY	2.8
1	A	11	THR	2.3
1	A	23	GLY	2.3
1	B	56	VAL	2.2
1	A	20	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 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.