



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 05:22 PM EDT

PDB ID : 9BB9 / pdb\_00009bb9  
Title : Structure of S1\_8A, a lambda-carrageenan specific sulfatase  
Authors : Hettle, J.A.; Vickers, C.; Boraston, A.B.  
Deposited on : 2024-04-05  
Resolution : 1.84 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

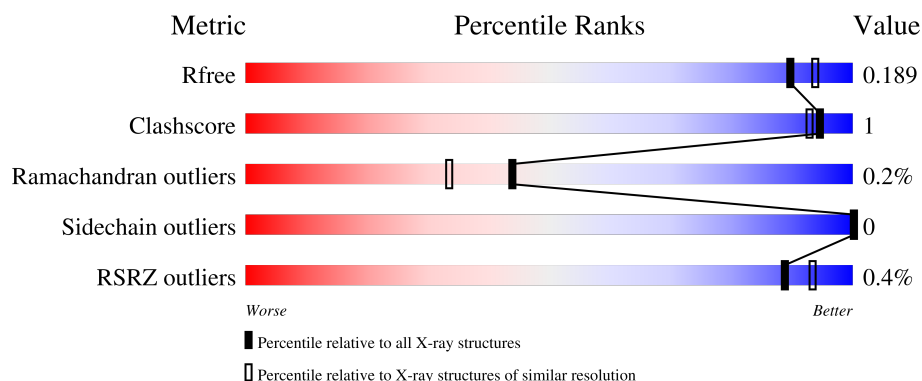
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 1.84 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))
$R_{free}$	164625	1150 (1.84-1.84)
Clashscore	180529	1248 (1.84-1.84)
Ramachandran outliers	177936	1240 (1.84-1.84)
Sidechain outliers	177891	1240 (1.84-1.84)
RSRZ outliers	164620	1149 (1.84-1.84)

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	A	514	 90% 8%
1	B	514	 88% 8%

## 2 Entry composition [i](#)

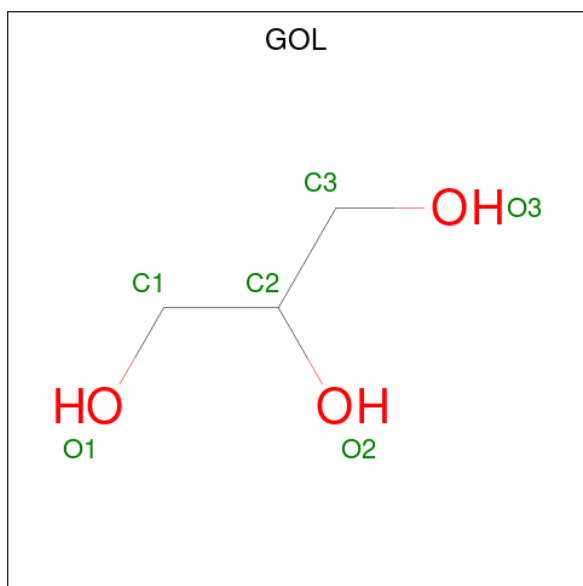
There are 5 unique types of molecules in this entry. The entry contains 8387 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S1\_8A sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3878	2487	656	723	12			
1	B	474	Total	C	N	O	S	1	2	0
			3847	2464	655	716	12			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		


- Molecule 5 is water.

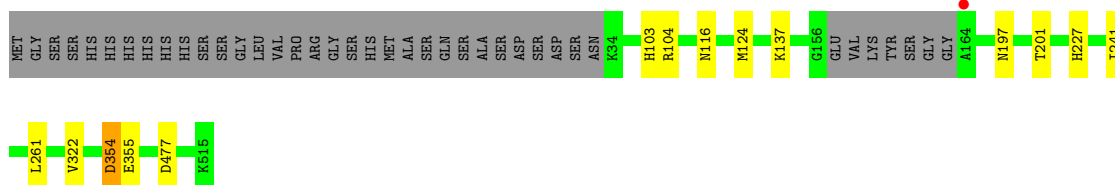
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	313	Total	O	0	0
			313	313		
5	B	313	Total	O	0	0
			313	313		

### 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.

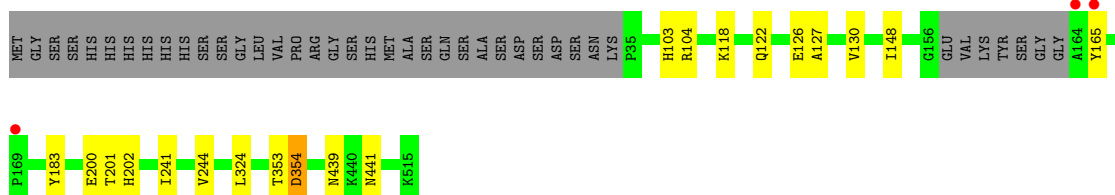
- Molecule 1: S1\_8A sulfatase

Chain A:  90% 8%



- Molecule 1: S1\_8A sulfatase

Chain B:  88% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.03Å 56.34Å 97.20Å 77.43° 76.36° 63.91°	Depositor
Resolution (Å)	29.28 – 1.84 29.28 – 1.84	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.28-1.84) 98.3 (29.28-1.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.158 , 0.190 0.159 , 0.189	Depositor DCC
$R_{free}$ test set	3890 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.117 for h,h-k,h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8387	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: GOL, EDO, CA

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	0.50	0/3980	0.70	0/5404
1	B	0.50	0/3952	0.69	2/5372 (0.0%)
All	All	0.50	0/7932	0.70	2/10776 (0.0%)

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	B	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	353	THR	CA-C-N	5.03	131.14	121.54
1	B	353	THR	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	ASP	Mainchain
1	B	354	ASP	Mainchain

## 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	3878	0	3730	8	0
1	B	3847	0	3672	10	0
2	A	12	0	15	0	0
2	B	6	0	8	0	0
3	A	12	0	18	1	0
3	B	4	0	6	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	313	0	0	0	0
5	B	313	0	0	0	0
All	All	8387	0	7449	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 1.

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:A:124:MET:HE1	1:A:322:VAL:HG11	1.81	0.62
1:A:355:GLU:HB2	1:A:477:ASP:HA	1.85	0.57
1:A:227:HIS:HE2	3:A:605:EDO:H11	1.69	0.57
1:B:201:THR:HG21	1:B:241:ILE:HG12	1.94	0.48
1:B:200:GLU:HA	1:B:201:THR:HA	1.68	0.47
1:B:439:ASN:OD1	1:B:441:ASN:HB2	2.15	0.46
1:B:130:VAL:HG11	1:B:183:TYR:CD1	2.51	0.46
1:A:116:ASN:OD1	1:A:116:ASN:N	2.43	0.44
1:B:122:GLN:CD	1:B:148:ILE:HD11	2.43	0.44
1:A:201:THR:HG21	1:A:241:ILE:HG12	2.00	0.43
1:B:127:ALA:HB2	1:B:324:LEU:HD21	2.00	0.43
1:B:165:TYR:CB	1:B:202[B]:HIS:CE1	3.01	0.43
1:A:137:LYS:HB3	1:A:197:ASN:HB3	2.01	0.42
1:B:103:HIS:HA	1:B:104:ARG:HA	1.88	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.84	0.42
1:A:103:HIS:HA	1:A:104:ARG:HA	1.90	0.41
1:B:118:LYS:NZ	1:B:126:GLU:OE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLU:HB2	1:B:244:VAL:HB	2.02	0.41

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	471/514 (92%)	457 (97%)	13 (3%)	1 (0%)	44	33
1	B	472/514 (92%)	456 (97%)	15 (3%)	1 (0%)	44	33
All	All	943/1028 (92%)	913 (97%)	28 (3%)	2 (0%)	44	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	ASP
1	B	354	ASP

### 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	410/455 (90%)	410 (100%)	0	100	100
1	B	404/455 (89%)	404 (100%)	0	100	100
All	All	814/910 (90%)	814 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	GLN
1	A	373	ASN
1	A	408	HIS
1	A	454	GLN
1	A	487	GLN
1	B	373	ASN
1	B	408	HIS

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	GOL	A	602	-	5,5,5	1.37	1 (20%)	5,5,5	0.88	0
2	GOL	A	601	-	5,5,5	1.77	1 (20%)	5,5,5	1.22	0
3	EDO	B	602	-	3,3,3	0.42	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	B	601	-	5,5,5	1.39	1 (20%)	5,5,5	1.28	1 (20%)
3	EDO	A	605	-	3,3,3	0.67	0	2,2,2	0.16	0
3	EDO	A	606	-	3,3,3	0.71	0	2,2,2	0.13	0
3	EDO	A	603	-	3,3,3	0.35	0	2,2,2	0.57	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	GOL	A	602	-	-	0/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-
3	EDO	B	602	-	-	1/1/1/1	-
2	GOL	B	601	-	-	0/4/4/4	-
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	GOL	C1-C2	3.25	1.64	1.51
2	B	601	GOL	C3-C2	2.76	1.62	1.51
2	A	602	GOL	O2-C2	-2.38	1.36	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	GOL	C3-C2-C1	-2.44	102.84	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	EDO	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	EDO	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, 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	475/514 (92%)	-0.69	1 (0%) 92 95	11, 18, 31, 42	1 (0%)
1	B	474/514 (92%)	-0.64	3 (0%) 85 91	11, 18, 31, 44	8 (1%)
All	All	949/1028 (92%)	-0.66	4 (0%) 89 93	11, 18, 31, 44	9 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	ALA	3.1
1	B	165	TYR	2.4
1	B	164	ALA	2.2
1	B	169	PRO	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	EDO	A	605	4/4	0.68	0.15	35,38,41,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	EDO	A	606	4/4	0.72	0.14	24,30,36,41	0
3	EDO	B	602	4/4	0.85	0.11	23,27,28,30	0
2	GOL	B	601	6/6	0.89	0.09	19,22,25,33	0
2	GOL	A	601	6/6	0.92	0.09	17,24,25,34	0
2	GOL	A	602	6/6	0.95	0.08	22,26,28,28	0
3	EDO	A	603	4/4	0.96	0.06	24,25,26,27	0
4	CA	A	604	1/1	1.00	0.01	14,14,14,14	0
4	CA	B	603	1/1	1.00	0.02	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.