



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2025 – 07:14 pm BST

PDB ID : 9I1M / pdb_00009i1m
Title : Structure of AauA, a sugar-binding protein with its substrate
Authors : Josts, I.; Cottam, C.; Connolly, J.P.R.
Deposited on : 2025-01-16
Resolution : 1.35 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

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>.

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 : 1.8.4, CSD as541be (2020)
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) : 2.44

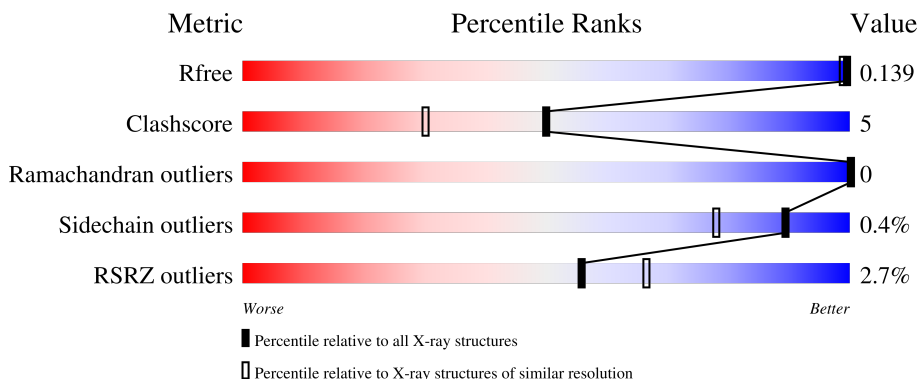
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 1.35 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	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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 ≥ 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	328	

2 Entry composition [i](#)

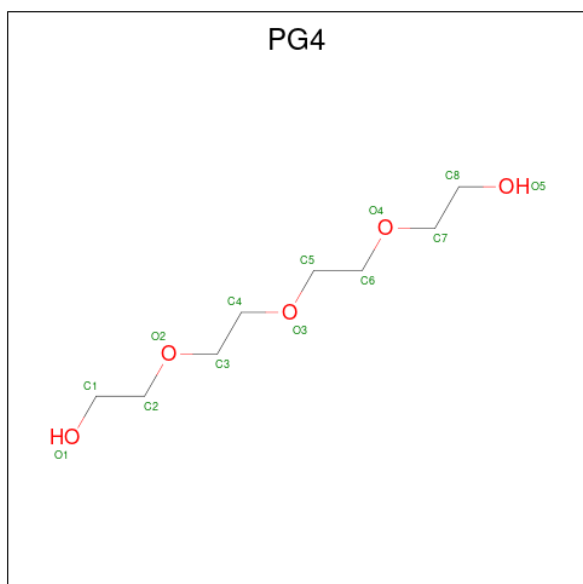
There are 4 unique types of molecules in this entry. The entry contains 2492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sugar-binding protein.

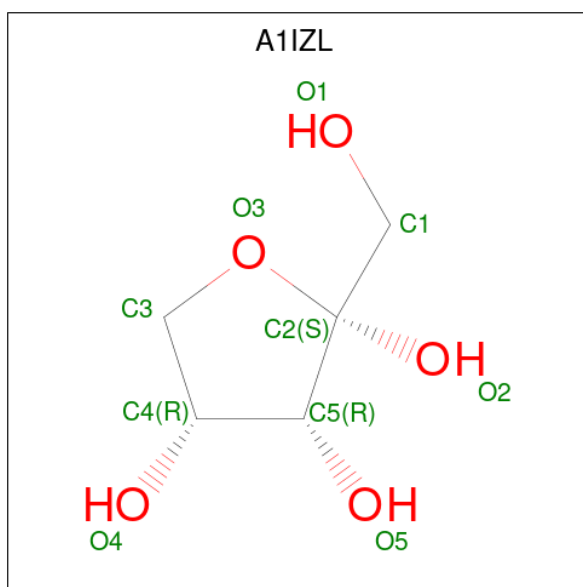
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2241	1418	387	426	10	0	1	0

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	13	8	5	0	0
2	A	1	13	8	5	0	0

- Molecule 3 is (2 {S},3 {R},4 {R})-2-(hydroxymethyl)oxolane-2,3,4-triol (CCD ID: A1IZL) (formula: C₅H₁₀O₅).

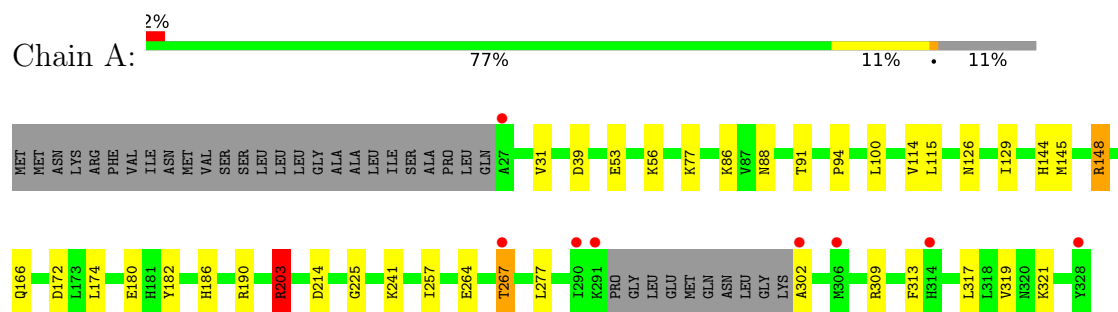


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		

- Molecule 1: Sugar-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.38Å 66.94Å 57.85Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	38.90 – 1.35 38.90 – 1.35	Depositor EDS
% Data completeness (in resolution range)	79.0 (38.90-1.35) 79.0 (38.90-1.35)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.40 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.126 , 0.143 0.137 , 0.139	Depositor DCC
R_{free} test set	3263 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	9.7	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2492	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: A1IZL, PG4

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	0.78	1/2280 (0.0%)	1.09	11/3086 (0.4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	HIS	CE1-NE2	-5.13	1.27	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLY	O-C-N	-7.11	118.51	121.07
1	A	39	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	166	GLN	N-CA-CB	6.64	119.99	110.16
1	A	267	THR	CB-CA-C	-6.45	97.59	110.42
1	A	145	MET	CG-SD-CE	-6.30	87.05	100.90
1	A	203	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	203	ARG	NE-CZ-NH1	5.49	126.99	121.50
1	A	182	TYR	O-C-N	-5.46	116.35	121.32
1	A	214	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	172	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	180	GLU	CG-CD-OE2	-5.07	106.74	118.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	203	ARG	Sidechain
1	A	309	ARG	Sidechain

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	2241	0	2271	23	0
2	A	26	0	36	3	0
3	A	10	0	0	0	0
4	A	215	0	0	7	0
All	All	2492	0	2307	24	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 5.

All (24) 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:53:GLU:HG3	4:A:612:HOH:O	1.87	0.74
1:A:203:ARG:HG3	4:A:503:HOH:O	1.87	0.74
1:A:31:VAL:H	1:A:88:ASN:HD22	1.40	0.70
1:A:86:LYS:HA	2:A:403:PG4:H81	1.78	0.65
1:A:267:THR:O	1:A:317:LEU:HB3	1.99	0.61
1:A:56:LYS:HG3	4:A:510:HOH:O	2.04	0.57
1:A:241:LYS:NZ	4:A:504:HOH:O	2.37	0.56
1:A:321:LYS:HG3	4:A:621:HOH:O	2.05	0.56
1:A:144:HIS:HD2	1:A:264:GLU:OE1	1.90	0.55
1:A:31:VAL:H	1:A:88:ASN:ND2	2.05	0.55
1:A:257:ILE:HD13	1:A:319:VAL:HG12	1.90	0.53
1:A:114:VAL:H	1:A:126:ASN:ND2	2.08	0.52
1:A:321:LYS:CG	4:A:621:HOH:O	2.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HD3	2:A:403:PG4:H22	1.93	0.51
1:A:77:LYS:HE3	4:A:525:HOH:O	2.11	0.50
1:A:302:ALA:HB2	1:A:313:PHE:CE1	2.48	0.49
1:A:94:PRO:HB3	1:A:100:LEU:HD12	1.94	0.49
2:A:401:PG4:H32	2:A:401:PG4:H52	1.55	0.48
1:A:129:ILE:HD12	1:A:277:LEU:HA	1.97	0.47
1:A:129:ILE:HD12	1:A:277:LEU:HD23	2.00	0.43
1:A:114:VAL:H	1:A:126:ASN:HD22	1.67	0.41
1:A:267:THR:O	1:A:317:LEU:O	2.38	0.41
1:A:91:THR:HA	1:A:115:LEU:O	2.20	0.41
1:A:174:LEU:C	1:A:174:LEU:HD23	2.46	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	289/328 (88%)	281 (97%)	8 (3%)	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	A	240/269 (89%)	239 (100%)	1 (0%)	89 78

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

Mol	Chain	Res	Type
1	A	148	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	64	GLN
1	A	88	ASN
1	A	126	ASN
1	A	144	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are 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	PG4	A	401	-	12,12,12	0.13	0	11,11,11	0.15	0
2	PG4	A	403	-	12,12,12	0.15	0	11,11,11	0.13	0
3	A1IZL	A	402	-	9,10,10	0.66	0	8,15,15	0.75	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	PG4	A	401	-	-	4/10/10/10	-
2	PG4	A	403	-	-	2/10/10/10	-
3	A1IZL	A	402	-	-	1/3/19/19	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PG4	O3-C5-C6-O4
2	A	401	PG4	C3-C4-O3-C5
2	A	403	PG4	O3-C5-C6-O4
2	A	401	PG4	C6-C5-O3-C4
3	A	402	A1IZL	O1-C1-C2-C5
2	A	403	PG4	O2-C3-C4-O3
2	A	401	PG4	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PG4	1	0
2	A	403	PG4	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th 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 ²)	Q<0.9
1	A	292/328 (89%)	-0.24	8 (2%) 56 66	6, 10, 25, 55	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	LYS	5.1
1	A	290	ILE	4.0
1	A	328	TYR	3.6
1	A	267	THR	3.6
1	A	306	MET	3.1
1	A	314	HIS	2.6
1	A	27	ALA	2.5
1	A	302	ALA	2.2

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, 95th 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(\AA^2)	Q<0.9
2	PG4	A	403	13/13	0.53	0.21	31,35,38,44	0
2	PG4	A	401	13/13	0.87	0.15	16,27,41,45	0
3	A1IZL	A	402	10/10	0.98	0.04	5,6,7,7	0

6.5 Other polymers [i](#)

There are no such residues in this entry.