



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:45 pm GMT

PDB ID : 1APY
Title : HUMAN ASPARTYLGLUCOSAMINIDASE
Authors : Rouvinen, J.; Oinonen, C.
Deposited on : 1995-06-14
Resolution : 2.00 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

<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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

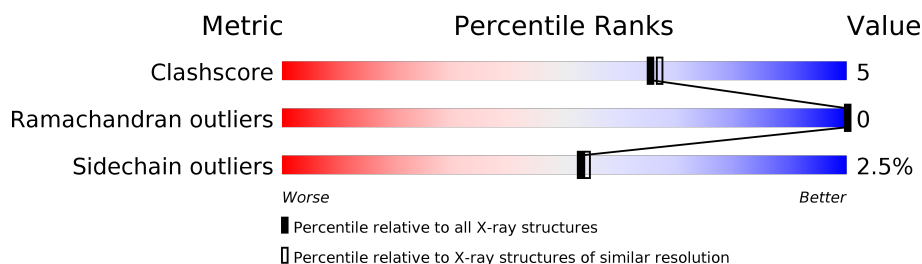
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	
1	C	162	
2	B	141	
2	D	141	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4838 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.

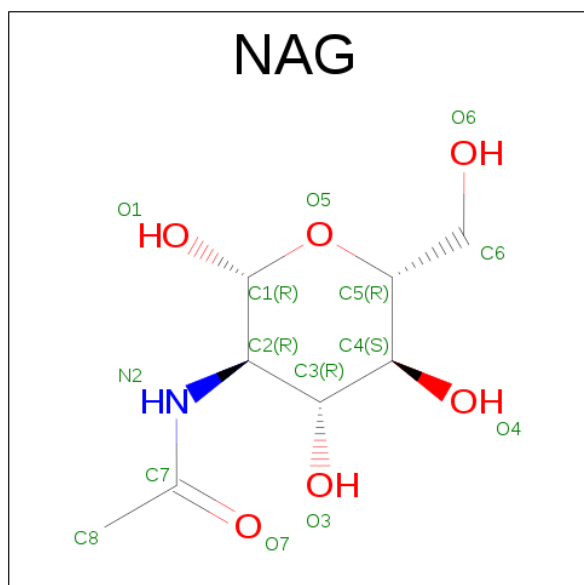
- Molecule 1 is a protein called ASPARTYLGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1203	746	208	239	10			
1	C	161	Total	C	N	O	S	0	0	0
			1203	746	208	239	10			

- Molecule 2 is a protein called ASPARTYLGLUCOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	141	Total	C	N	O	S	0	0	0
			1057	665	183	201	8			
2	D	141	Total	C	N	O	S	0	0	0
			1057	665	183	201	8			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is water.

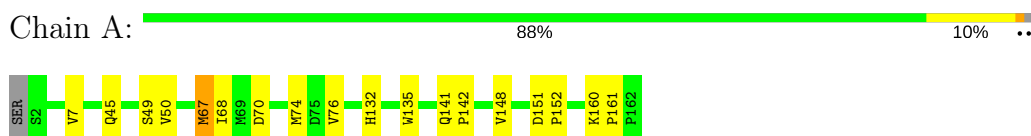
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	80	Total	O	0	0
			80	80		
5	B	47	Total	O	0	0
			47	47		
5	C	64	Total	O	0	0
			64	64		
5	D	46	Total	O	0	0
			46	46		

3 Residue-property plots [i](#)

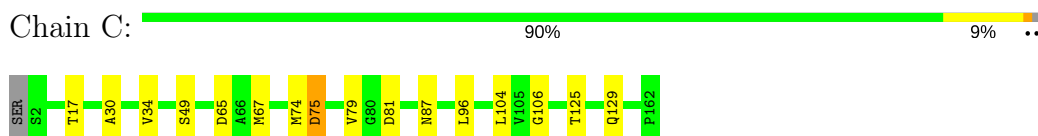
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($RSRZ > 2$). 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.

Note EDS was not executed.

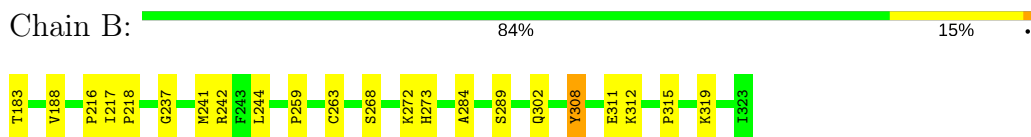
• Molecule 1: ASPARTYLGLUCOSAMINIDASE



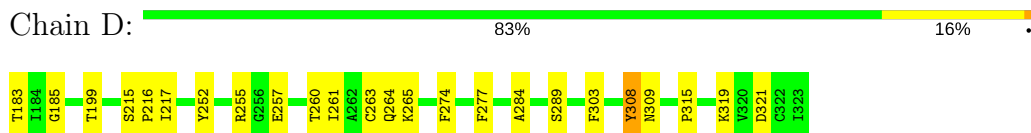
• Molecule 1: ASPARTYLGLUCOSAMINIDASE



• Molecule 2: ASPARTYLGLUCOSAMINIDASE



• Molecule 2: ASPARTYLGLUCOSAMINIDASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	98.40 Å 98.40 Å 134.50 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.169 , 0.224	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4838	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.35	0/1230	0.66	0/1674
1	C	0.35	0/1230	0.66	0/1674
2	B	0.35	0/1079	0.61	0/1457
2	D	0.34	0/1079	0.61	0/1457
All	All	0.35	0/4618	0.64	0/6262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1203	0	1148	14	0
1	C	1203	0	1148	12	0
2	B	1057	0	1030	14	0
2	D	1057	0	1030	13	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
3	C	14	0	13	0	0
4	D	39	0	34	0	0
5	A	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	47	0	0	0	0
5	C	64	0	0	0	0
5	D	46	0	0	0	0
All	All	4838	0	4429	42	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 (42) 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:160:LYS:HG2	1:A:161:PRO:HD2	1.74	0.69
2:B:302:GLN:NE2	2:B:319:LYS:HD3	2.14	0.62
2:D:252:TYR:HB3	2:D:257:GLU:HG3	1.82	0.61
1:C:67:MET:HB3	2:D:216:PRO:HA	1.83	0.60
2:B:237:GLY:O	2:B:241:MET:HB2	2.01	0.60
1:C:49:SER:HG	2:D:183:THR:N	1.99	0.59
1:C:65:ASP:HB3	2:D:216:PRO:HD3	1.86	0.57
1:A:160:LYS:HG2	1:A:161:PRO:CD	2.34	0.57
1:C:81:ASP:O	1:C:106:GLY:HA2	2.05	0.56
1:C:75:ASP:HB3	1:C:96:LEU:CD1	2.36	0.56
2:B:268:SER:O	2:B:272:LYS:HG2	2.05	0.55
2:B:217:ILE:HD12	2:D:217:ILE:HD12	1.90	0.54
2:B:273:HIS:CE1	1:C:74:MET:SD	3.01	0.53
1:A:76:VAL:HG11	2:B:218:PRO:HG3	1.92	0.52
1:C:75:ASP:HB3	1:C:96:LEU:HD11	1.94	0.49
1:A:49:SER:HG	2:B:183:THR:N	2.11	0.48
1:A:132:HIS:O	1:A:135:TRP:HB3	2.14	0.48
2:D:185:GLY:HA2	2:D:199:THR:HG22	1.96	0.48
1:A:67:MET:HB2	2:B:216:PRO:HA	1.96	0.47
1:A:67:MET:HG2	1:A:68:ILE:N	2.29	0.47
2:B:311:GLU:HG3	2:B:312:LYS:N	2.29	0.47
2:D:308:TYR:CE2	2:D:315:PRO:HD3	2.49	0.47
1:A:7:VAL:HG22	2:B:188:VAL:HG22	1.97	0.47
2:D:284:ALA:HA	2:D:289:SER:O	2.15	0.47
1:A:148:VAL:CG2	1:A:152:PRO:HG3	2.45	0.46
2:D:261:ILE:O	2:D:265:LYS:HG3	2.17	0.45
1:A:70:ASP:O	1:A:74:MET:HA	2.17	0.44
2:B:284:ALA:HA	2:B:289:SER:O	2.17	0.43
2:B:308:TYR:CE2	2:B:315:PRO:HG3	2.52	0.43
2:D:274:PHE:O	2:D:277:PHE:HD1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:VAL:HG23	1:A:152:PRO:HG3	2.01	0.43
2:D:303:PHE:O	2:D:319:LYS:HA	2.19	0.42
1:C:125:THR:O	1:C:129:GLN:HG3	2.20	0.42
2:B:242:ARG:HD3	1:C:74:MET:O	2.19	0.42
1:C:67:MET:HG2	2:D:215:SER:O	2.19	0.42
2:D:260:THR:O	2:D:264:GLN:HG3	2.20	0.41
1:C:79:VAL:HA	1:C:104:LEU:O	2.20	0.41
1:A:45:GLN:HA	1:A:50:VAL:O	2.20	0.41
1:A:141:GLN:HA	1:A:142:PRO:HA	1.83	0.41
2:B:244:LEU:HD22	2:B:244:LEU:N	2.35	0.41
1:C:30:ALA:O	1:C:34:VAL:HG23	2.20	0.40
1:A:151:ASP:HA	1:A:152:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	159/162 (98%)	152 (96%)	7 (4%)	0	100	100
1	C	159/162 (98%)	154 (97%)	5 (3%)	0	100	100
2	B	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
2	D	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
All	All	596/606 (98%)	574 (96%)	22 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	129/130 (99%)	128 (99%)	1 (1%)	85	88
1	C	129/130 (99%)	126 (98%)	3 (2%)	56	58
2	B	110/110 (100%)	107 (97%)	3 (3%)	50	51
2	D	110/110 (100%)	105 (96%)	5 (4%)	32	27
All	All	478/480 (100%)	466 (98%)	12 (2%)	53	54

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	MET
2	B	259	PRO
2	B	263	CYS
2	B	308	TYR
1	C	17	THR
1	C	75	ASP
1	C	87	ASN
2	D	255	ARG
2	D	263	CYS
2	D	308	TYR
2	D	309	ASN
2	D	321	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
2	B	264	GLN
2	B	273	HIS
2	B	302	GLN
1	C	87	ASN
1	C	129	GLN
2	D	264	GLN
2	D	309	ASN
2	D	314	GLN

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 ⓘ

3 carbohydrates 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$
4	NAG	D	531	2,4	14,14,15	0.80	1 (7%)	15,19,21	1.25	1 (6%)
4	NAG	D	532	4	14,14,15	0.88	0	15,19,21	1.31	2 (13%)
4	BMA	D	533	4	11,11,12	1.23	2 (18%)	13,15,17	2.11	2 (15%)

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
4	NAG	D	531	2,4	-	0/6/23/26	0/1/1/1
4	NAG	D	532	4	-	0/6/23/26	0/1/1/1
4	BMA	D	533	4	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	533	BMA	C2-C3	2.14	1.55	1.52
4	D	531	NAG	C1-C2	2.19	1.55	1.52
4	D	533	BMA	C4-C5	2.30	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	533	BMA	C1-C2-C3	-4.69	103.71	109.65
4	D	533	BMA	O5-C1-C2	-4.34	103.98	110.79
4	D	532	NAG	O4-C4-C3	-3.27	103.25	110.36
4	D	531	NAG	O7-C7-C8	-2.33	117.82	122.06
4	D	532	NAG	C1-O5-C5	2.12	115.09	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	NAG	A	501	1	14,14,15	1.20	3 (21%)	15,19,21	1.70	4 (26%)
3	NAG	B	511	2	14,14,15	0.61	0	15,19,21	1.62	2 (13%)
3	NAG	C	521	1	14,14,15	0.94	1 (7%)	15,19,21	2.08	1 (6%)

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
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	B	511	2	-	0/6/23/26	0/1/1/1
3	NAG	C	521	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	NAG	C3-C2	2.06	1.57	1.52
3	A	501	NAG	C4-C3	2.06	1.57	1.52
3	C	521	NAG	C1-C2	2.12	1.55	1.52
3	A	501	NAG	C4-C5	2.35	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-C2-N2	-3.79	104.01	110.49
3	B	511	NAG	O5-C1-C2	-2.06	108.61	111.47
3	A	501	NAG	C1-O5-C5	2.07	115.03	112.17
3	A	501	NAG	C6-C5-C4	2.53	118.93	113.00
3	A	501	NAG	O5-C1-C2	3.52	116.37	111.47
3	B	511	NAG	C1-O5-C5	4.01	117.69	112.17
3	C	521	NAG	C1-O5-C5	7.26	122.17	112.17

There are no chirality outliers.

There are no torsion outliers.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.