



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 18, 2018 – 11:04 pm GMT

PDB ID : 7API  
Title : THE S VARIANT OF HUMAN ALPHA1-ANTITRYPSIN, STRUCTURE  
AND IMPLICATIONS FOR FUNCTION AND METABOLISM  
Authors : Loebermann, H.; Tokuoka, R.; Deisenhofer, J.; Huber, R.  
Deposited on : 1988-09-08  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30686

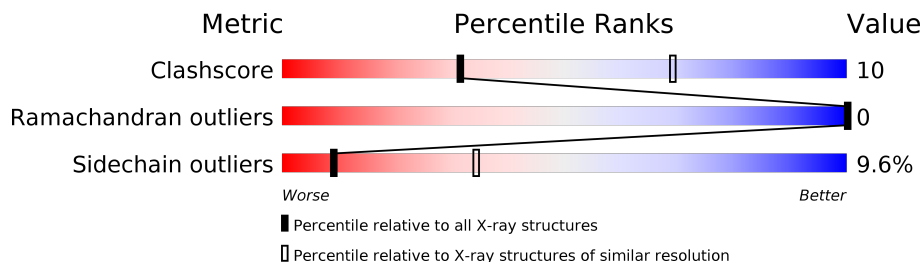
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	122078	2167 (3.00-3.00)
Ramachandran outliers	120005	2101 (3.00-3.00)
Sidechain outliers	119972	2104 (3.00-3.00)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	347	 61% 32% ...
2	B	36	 78% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	520	X	-	-	-
4	MAN	A	503	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3260 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.

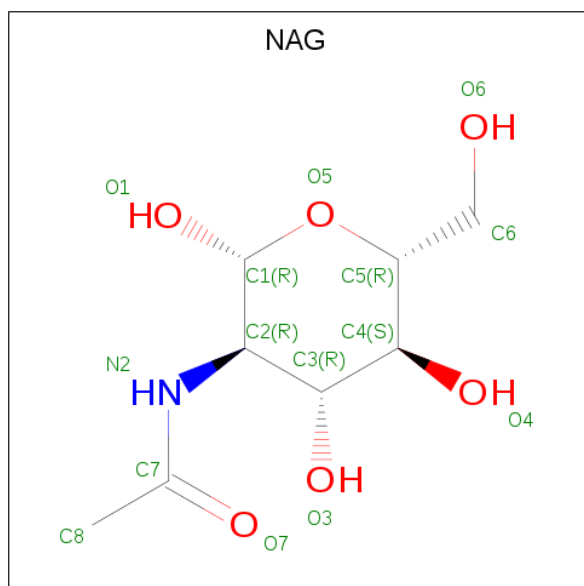
- Molecule 1 is a protein called ALPHA 1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	6	0	0
			2690	1726	441	515	8			

- Molecule 2 is a protein called ALPHA 1-ANTITRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	36	Total	C	N	O	S	4	0	0
			291	193	46	50	2			

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



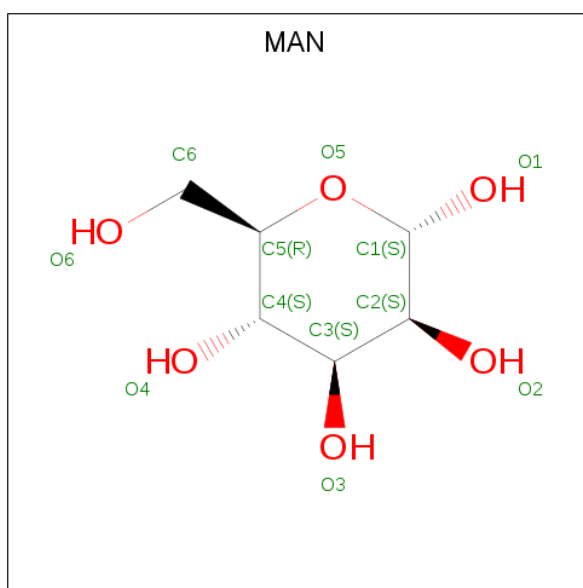
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		1	0
			14	8	1	5			
3	A	1	Total	C	N	O		6	0
			14	8	1	5			

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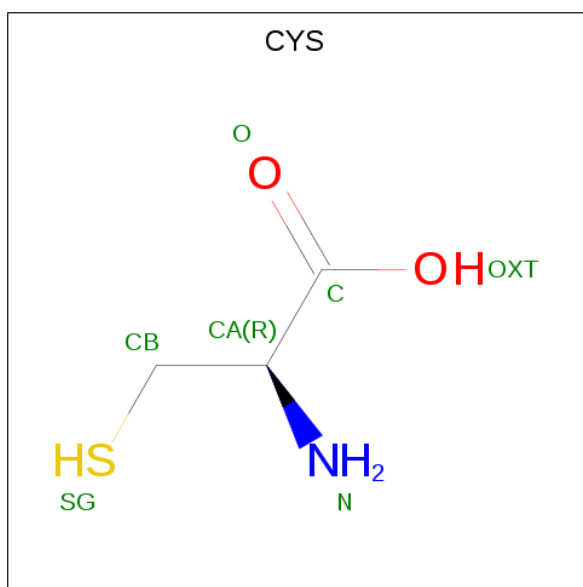
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	8	0
			14	8	1	5		
3	A	1	Total	C	N	O	4	0
			14	8	1	5		
3	A	1	Total	C	N	O	14	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	5	0
			14	8	1	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	2	0
			11	6	5		
4	A	1	Total	C	O	4	0
			11	6	5		
4	A	1	Total	C	O	4	0
			11	6	5		

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

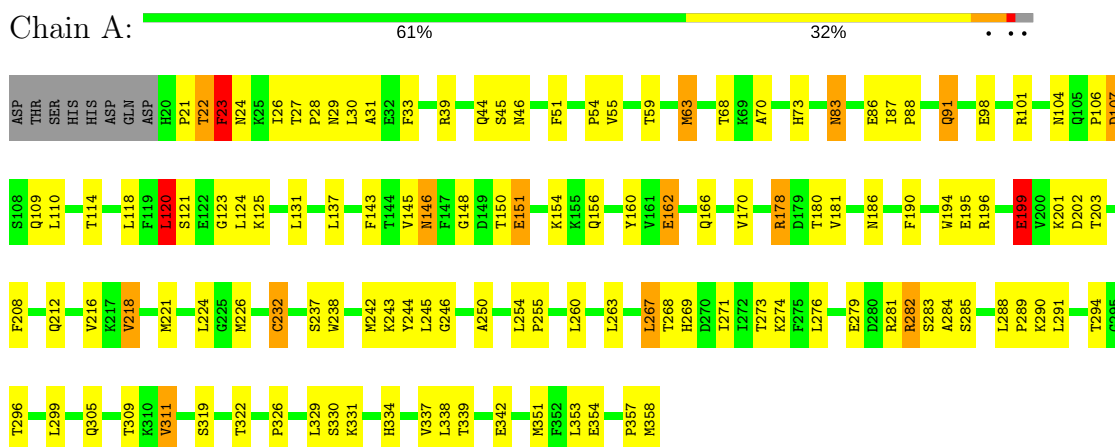
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	13	Total	O	0	0
			13	13		

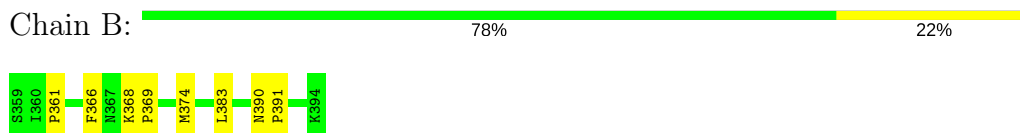


Note EDS was not executed.

- Molecule 1: ALPHA 1-ANTITRYPSIN



• Molecule 2: ALPHA 1-ANTITRYPSIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.50Å 120.50Å 113.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	EREF	Depositor
R, $R_{free}$	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3260	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.93	3/2744 (0.1%)	1.41	10/3707 (0.3%)
2	B	0.83	0/299	1.30	0/402
All	All	0.92	3/3043 (0.1%)	1.40	10/4109 (0.2%)

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	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	TRP	NE1-CE2	-8.08	1.27	1.37
1	A	194	TRP	NE1-CE2	-7.84	1.27	1.37
1	A	123	GLY	CA-C	6.28	1.61	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	CYS	CB-CA-C	-8.49	93.41	110.40
1	A	101	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	216	VAL	CA-CB-CG1	6.05	119.98	110.90
1	A	21	PRO	CA-C-N	-6.04	103.91	117.20
1	A	178	ARG	NE-CZ-NH2	5.52	123.06	120.30

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASN	Mainchain
1	A	23	PHE	Mainchain
1	A	63	MET	Mainchain
1	A	70	ALA	Mainchain
1	A	83	ASN	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	2690	0	2685	57	1
2	B	291	0	306	6	0
3	A	98	0	87	3	0
4	A	33	0	27	0	0
5	A	7	0	3	0	0
6	A	128	0	0	0	4
6	B	13	0	0	0	0
All	All	3260	0	3108	59	4

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 10.

The worst 5 of 59 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:27:THR:HA	1:A:30:LEU:HD12	1.61	0.80
1:A:83:ASN:HD22	1:A:86:GLU:HG3	1.53	0.74
1:A:331:LYS:HB2	1:A:354:GLU:HG2	1.70	0.72
1:A:26:ILE:HA	1:A:29:ASN:HD22	1.56	0.70
1:A:110:LEU:HD11	1:A:190:PHE:HE1	1.58	0.69

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:728:HOH:O	6:A:728:HOH:O[8_666]	0.38	1.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:750:HOH:O	6:A:750:HOH:O[7_556]	1.50	0.70
6:A:698:HOH:O	6:A:698:HOH:O[7_556]	1.78	0.42
1:A:319:SER:OG	6:A:608:HOH:O[4_555]	2.11	0.09

## 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	337/347 (97%)	315 (94%)	22 (6%)	0	100	100
2	B	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
All	All	371/383 (97%)	347 (94%)	24 (6%)	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	297/305 (97%)	267 (90%)	30 (10%)	8	31
2	B	35/35 (100%)	34 (97%)	1 (3%)	45	80
All	All	332/340 (98%)	301 (91%)	31 (9%)	9	36

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	201	LYS
1	A	311	VAL
1	A	186	ASN
1	A	202	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
2	B	377	GLN
1	A	212	GLN
1	A	139	HIS
1	A	186	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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
5	CYS	A	395	1	2,6,6	2.45	1 (50%)	1,7,7	0.27	0
3	NAG	A	501	1,3	14,14,15	0.84	0	17,19,21	1.75	4 (23%)
3	NAG	A	502	3,4	14,14,15	1.19	2 (14%)	17,19,21	2.91	2 (11%)
4	MAN	A	503	3,4	11,11,12	0.91	0	15,15,17	1.30	2 (13%)
4	MAN	A	504	3,4	11,11,12	0.93	0	15,15,17	2.13	3 (20%)
3	NAG	A	505	4	14,14,15	1.00	1 (7%)	17,19,21	1.96	3 (17%)
4	MAN	A	506	4	11,11,12	1.11	1 (9%)	15,15,17	2.10	2 (13%)
3	NAG	A	510	1,3	14,14,15	0.92	0	17,19,21	1.75	3 (17%)
3	NAG	A	511	3	14,14,15	0.65	0	17,19,21	1.51	2 (11%)
3	NAG	A	520	1,3	14,14,15	1.37	1 (7%)	17,19,21	2.07	7 (41%)
3	NAG	A	521	3	14,14,15	0.89	1 (7%)	17,19,21	2.02	4 (23%)

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
5	CYS	A	395	1	-	0/2/6/6	0/0/0/0
3	NAG	A	501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	502	3,4	-	0/6/23/26	0/1/1/1
4	MAN	A	503	3,4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	A	504	3,4	-	0/2/19/22	0/1/1/1
3	NAG	A	505	4	-	0/6/23/26	0/1/1/1
4	MAN	A	506	4	-	0/2/19/22	0/1/1/1
3	NAG	A	510	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	511	3	-	0/6/23/26	0/1/1/1
3	NAG	A	520	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	521	3	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	521	NAG	C1-C2	2.03	1.55	1.52
3	A	502	NAG	C4-C5	2.11	1.57	1.53
4	A	506	MAN	C2-C3	2.12	1.55	1.52
3	A	505	NAG	C1-C2	2.39	1.55	1.52
3	A	502	NAG	C1-C2	2.80	1.56	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	O5-C5-C6	-5.67	98.17	107.15
3	A	520	NAG	O5-C1-C2	-4.25	105.65	111.52
3	A	501	NAG	O5-C1-C2	-4.00	105.99	111.52
3	A	505	NAG	O5-C1-C2	-3.89	106.15	111.52
3	A	521	NAG	O5-C1-C2	-3.02	107.35	111.52

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	520	NAG	C1
4	A	503	MAN	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	NAG	1	0
3	A	520	NAG	2	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

### 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.