



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:47 PM GMT

PDB ID : 1QMN
Title : Alpha1-antichymotrypsin serpin in the delta conformation (partial loop insertion)
Authors : Gooptu, B.; Hazes, B.; Lomas, D.A.
Deposited on : 1999-10-04
Resolution : 2.27 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

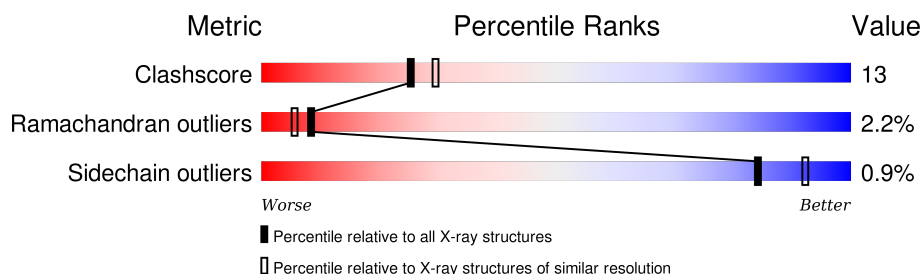
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)

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	401	<div> <div style="width: 71%;"></div> <div style="width: 18%;"></div> <div style="width: 9%;"></div> </div> <div>71% 18% • 9%</div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2897 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-ANTICHYMOTRYPSIN.

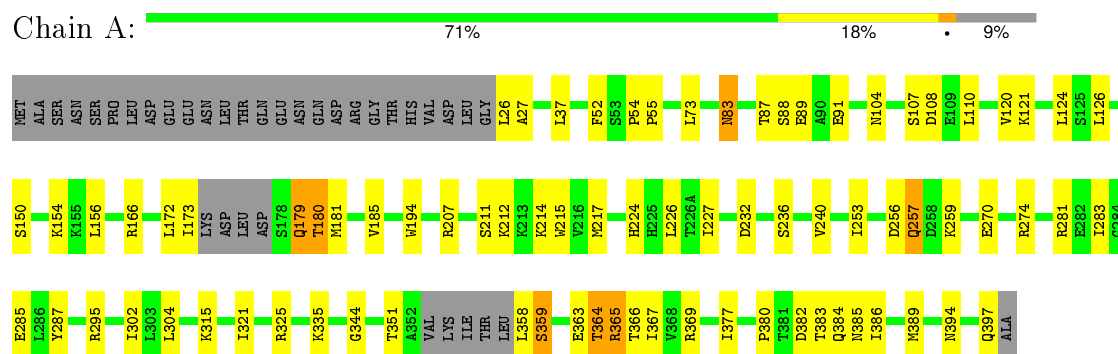
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2897	1859	478	547	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP P01011
A	1	ALA	-	EXPRESSION TAG	UNP P01011
A	2	SER	-	EXPRESSION TAG	UNP P01011
A	55	PRO	LEU	ENGINEERED MUTATION	UNP P01011

Note EDS was not executed.

- Molecule 1: ALPHA-1-ANTITRYPSIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.72 Å 122.09 Å 41.72 Å 90.00° 101.03° 90.00°	Depositor
Resolution (Å)	40.95 – 2.27	Depositor
% Data completeness (in resolution range)	60.0 (40.95-2.27)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNS 0.5	Depositor
R, R_{free}	0.197 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2897	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.37	0/2953	0.60	0/3994

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	2897	0	2889	73	0
All	All	2897	0	2889	73	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 13.

All (73) 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:256:ASP:HB2	1:A:259:LYS:HD2	1.42	0.99
1:A:83:ASN:H	1:A:83:ASN:HD22	1.26	0.83
1:A:224:HIS:HB3	1:A:285:GLU:OE2	1.81	0.80
1:A:172:LEU:HD23	1:A:173:ILE:N	2.02	0.75
1:A:26:LEU:HG	1:A:27:ALA:H	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASN:ND2	1:A:83:ASN:H	1.86	0.73
1:A:394:ASN:HD22	1:A:397:GLN:HB2	1.53	0.73
1:A:394:ASN:ND2	1:A:397:GLN:HB2	2.05	0.71
1:A:315:LYS:HD2	1:A:315:LYS:N	2.05	0.71
1:A:256:ASP:HB2	1:A:259:LYS:CD	2.20	0.70
1:A:179:GLN:HG3	1:A:180:THR:H	1.54	0.70
1:A:83:ASN:N	1:A:83:ASN:HD22	1.88	0.69
1:A:73:LEU:HD21	1:A:89:GLU:OE1	1.94	0.66
1:A:365:ARG:HG2	1:A:366:THR:H	1.61	0.65
1:A:257:GLN:CD	1:A:257:GLN:H	1.99	0.65
1:A:52:PHE:CE2	1:A:54:PRO:HG3	2.32	0.64
1:A:365:ARG:HG2	1:A:366:THR:N	2.13	0.62
1:A:377:ILE:HG23	1:A:386:ILE:HD12	1.81	0.62
1:A:363:GLU:O	1:A:363:GLU:HG3	2.01	0.60
1:A:88:SER:OG	1:A:91:GLU:HG2	2.02	0.59
1:A:232:ASP:OD2	1:A:274:ARG:NH2	2.35	0.59
1:A:108:ASP:C	1:A:110:LEU:H	2.07	0.58
1:A:365:ARG:HG2	1:A:366:THR:HG23	1.86	0.57
1:A:295:ARG:O	1:A:335:LYS:HD2	2.04	0.57
1:A:37:LEU:HD23	1:A:52:PHE:CE2	2.40	0.57
1:A:83:ASN:O	1:A:87:THR:HG22	2.04	0.56
1:A:358:LEU:O	1:A:359:SER:CB	2.53	0.56
1:A:120:VAL:HG13	1:A:124:LEU:HD23	1.88	0.54
1:A:285:GLU:HB3	1:A:287:TYR:CE1	2.43	0.53
1:A:315:LYS:HD2	1:A:315:LYS:H	1.72	0.53
1:A:236:SER:HB2	1:A:259:LYS:HD3	1.91	0.52
1:A:194:TRP:CD1	1:A:344:GLY:HA2	2.44	0.52
1:A:285:GLU:HB3	1:A:287:TYR:HE1	1.75	0.51
1:A:382:ASP:O	1:A:383:THR:OG1	2.26	0.51
1:A:156:LEU:HD23	1:A:156:LEU:O	2.10	0.50
1:A:26:LEU:CG	1:A:27:ALA:H	2.24	0.50
1:A:285:GLU:HB2	1:A:367:ILE:HG12	1.93	0.50
1:A:166:ARG:CG	1:A:185:VAL:HG12	2.42	0.49
1:A:120:VAL:CG1	1:A:124:LEU:HD23	2.43	0.49
1:A:150:SER:O	1:A:154:LYS:HG3	2.13	0.49
1:A:226:LEU:H	1:A:226:LEU:HD23	1.78	0.48
1:A:270:GLU:H	1:A:270:GLU:CD	2.16	0.48
1:A:281:ARG:NH1	1:A:283:ILE:HD13	2.29	0.48
1:A:367:ILE:HG21	1:A:369:ARG:NH2	2.29	0.48
1:A:380:PRO:HD2	1:A:385:ASN:O	2.14	0.47
1:A:365:ARG:CG	1:A:366:THR:H	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD12	1:A:325:ARG:O	2.13	0.47
1:A:363:GLU:O	1:A:363:GLU:CG	2.63	0.47
1:A:253:ILE:HD12	1:A:253:ILE:N	2.30	0.46
1:A:364:THR:O	1:A:365:ARG:O	2.34	0.45
1:A:227:ILE:HD12	1:A:240:VAL:CG1	2.46	0.45
1:A:211:SER:OG	1:A:214:LYS:HB3	2.17	0.45
1:A:226:LEU:HD23	1:A:226:LEU:N	2.32	0.45
1:A:156:LEU:C	1:A:156:LEU:HD23	2.37	0.45
1:A:150:SER:HB2	1:A:154:LYS:HE3	1.99	0.45
1:A:304:LEU:O	1:A:304:LEU:HD23	2.17	0.45
1:A:383:THR:HG22	1:A:384:GLN:N	2.32	0.44
1:A:121:LYS:HG2	1:A:124:LEU:HD22	1.98	0.44
1:A:386:ILE:HD11	1:A:389:MET:HB2	1.99	0.43
1:A:126:LEU:HD22	1:A:321:ILE:HG22	2.01	0.42
1:A:236:SER:CB	1:A:259:LYS:HD3	2.48	0.42
1:A:126:LEU:CD2	1:A:321:ILE:HG22	2.49	0.42
1:A:179:GLN:HG3	1:A:180:THR:N	2.29	0.42
1:A:325:ARG:O	1:A:325:ARG:HG3	2.19	0.41
1:A:302:ILE:N	1:A:302:ILE:HD12	2.35	0.41
1:A:52:PHE:HE2	1:A:54:PRO:HG3	1.79	0.41
1:A:121:LYS:HE2	1:A:181:MET:CE	2.51	0.41
1:A:215:TRP:HZ3	1:A:217:MET:SD	2.45	0.41
1:A:54:PRO:N	1:A:55:PRO:HD2	2.36	0.40
1:A:207:ARG:HG2	1:A:215:TRP:CZ3	2.56	0.40
1:A:108:ASP:C	1:A:110:LEU:N	2.74	0.40
1:A:227:ILE:HD12	1:A:240:VAL:HG13	2.02	0.40
1:A:215:TRP:CD1	1:A:215:TRP:N	2.90	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	359/401 (90%)	327 (91%)	24 (7%)	8 (2%)	8 5

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	180	THR
1	A	359	SER
1	A	365	ARG
1	A	104	ASN
1	A	107	SER
1	A	351	THR
1	A	364	THR

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	318/356 (89%)	315 (99%)	3 (1%)	84 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	212	LYS
1	A	257	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	69	HIS
1	A	83	ASN
1	A	97	GLN
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	394	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](#)

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](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.