



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 07:47 pm GMT

PDB ID : 3DRU
Title : Crystal Structure of Gly117Phe Alpha1-Antitrypsin
Authors : Gooptu, B.; Nobeli, I.; Purkiss, A.; Phillips, R.L.; Mallya, M.; Lomas, D.A.; Barrett, T.E.
Deposited on : 2008-07-11
Resolution : 3.20 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

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

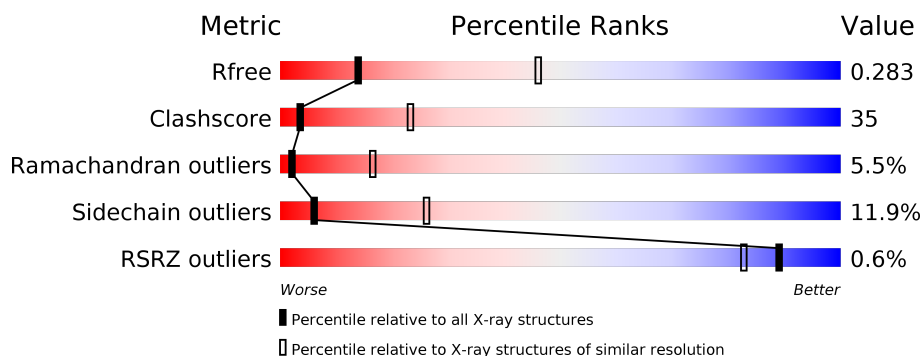
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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.

Mol	Chain	Length	Quality of chain
1	A	404	
1	B	404	
1	C	404	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8560 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	363	Total	C	N	O	S	0	0	0
			2861	1845	466	541	9			
1	B	362	Total	C	N	O	S	0	0	0
			2867	1849	467	542	9			
1	C	360	Total	C	N	O	S	0	0	0
			2832	1825	462	537	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	EXPRESSION TAG	UNP P01009
A	-8	ARG	-	EXPRESSION TAG	UNP P01009
A	-7	GLY	-	EXPRESSION TAG	UNP P01009
A	-6	SER	-	EXPRESSION TAG	UNP P01009
A	-5	HIS	-	EXPRESSION TAG	UNP P01009
A	-4	HIS	-	EXPRESSION TAG	UNP P01009
A	-3	HIS	-	EXPRESSION TAG	UNP P01009
A	-2	HIS	-	EXPRESSION TAG	UNP P01009
A	-1	HIS	-	EXPRESSION TAG	UNP P01009
A	0	HIS	-	EXPRESSION TAG	UNP P01009
A	1	THR	-	EXPRESSION TAG	UNP P01009
A	117	PHE	GLY	ENGINEERED	UNP P01009
B	-9	MET	-	EXPRESSION TAG	UNP P01009
B	-8	ARG	-	EXPRESSION TAG	UNP P01009
B	-7	GLY	-	EXPRESSION TAG	UNP P01009
B	-6	SER	-	EXPRESSION TAG	UNP P01009
B	-5	HIS	-	EXPRESSION TAG	UNP P01009
B	-4	HIS	-	EXPRESSION TAG	UNP P01009
B	-3	HIS	-	EXPRESSION TAG	UNP P01009
B	-2	HIS	-	EXPRESSION TAG	UNP P01009
B	-1	HIS	-	EXPRESSION TAG	UNP P01009
B	0	HIS	-	EXPRESSION TAG	UNP P01009
B	1	THR	-	EXPRESSION TAG	UNP P01009

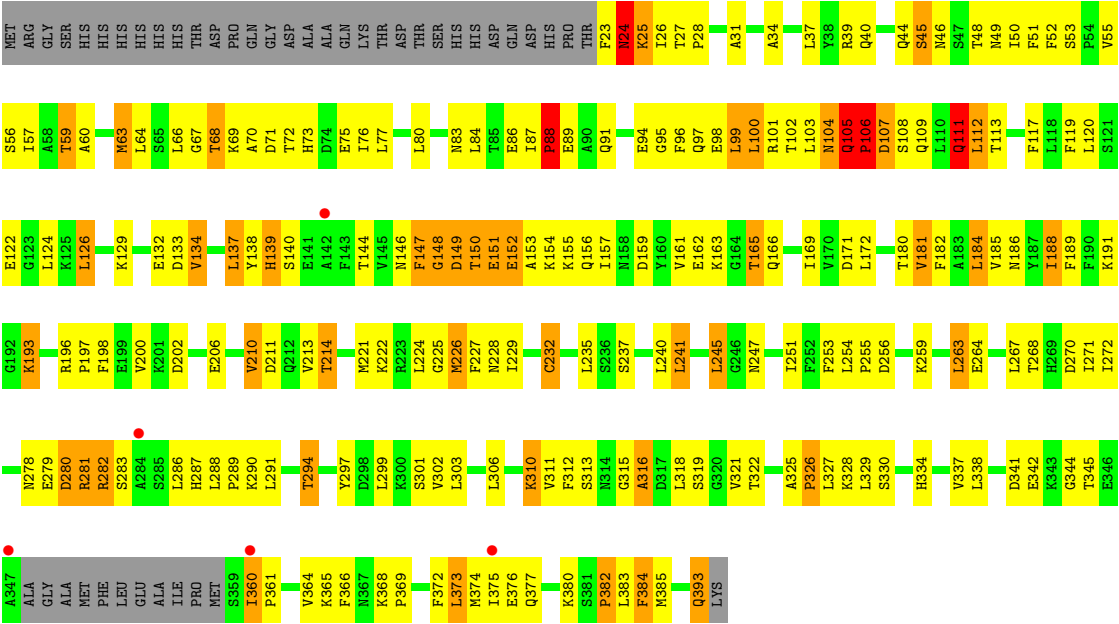
Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	117	PHE	GLY	ENGINEERED	UNP P01009
C	-9	MET	-	EXPRESSION TAG	UNP P01009
C	-8	ARG	-	EXPRESSION TAG	UNP P01009
C	-7	GLY	-	EXPRESSION TAG	UNP P01009
C	-6	SER	-	EXPRESSION TAG	UNP P01009
C	-5	HIS	-	EXPRESSION TAG	UNP P01009
C	-4	HIS	-	EXPRESSION TAG	UNP P01009
C	-3	HIS	-	EXPRESSION TAG	UNP P01009
C	-2	HIS	-	EXPRESSION TAG	UNP P01009
C	-1	HIS	-	EXPRESSION TAG	UNP P01009
C	0	HIS	-	EXPRESSION TAG	UNP P01009
C	1	THR	-	EXPRESSION TAG	UNP P01009
C	117	PHE	GLY	ENGINEERED	UNP P01009



● Molecule 1: Alpha-1-antitrypsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.84Å 149.30Å 77.29Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	55.00 – 3.20 77.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (55.00-3.20) 99.7 (77.09-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.242 , 0.290 0.238 , 0.283	Depositor DCC
R_{free} test set	1116 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	72.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8560	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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 [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	0.51	0/2920	0.73	0/3948
1	B	0.53	0/2926	0.79	4/3955 (0.1%)
1	C	0.46	0/2890	0.75	4/3911 (0.1%)
All	All	0.50	0/8736	0.76	8/11814 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	GLU	N-CA-C	-9.51	85.34	111.00
1	C	105	GLN	N-CA-C	-6.62	93.11	111.00
1	C	279	GLU	N-CA-C	-6.58	93.24	111.00
1	B	110	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	101	ARG	N-CA-C	-5.60	95.87	111.00

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	2861	0	2858	171	3
1	B	2867	0	2874	207	2
1	C	2832	0	2814	219	0
All	All	8560	0	8546	595	3

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 35.

The worst 5 of 595 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:C:100:LEU:H	1:C:100:LEU:HD12	1.13	1.12
1:B:294:THR:HG22	1:B:337:VAL:HG13	1.25	1.10
1:A:348:ALA:HB2	1:C:98:GLU:HG3	1.16	1.10
1:A:288:LEU:HD12	1:A:289:PRO:HD2	1.35	1.09
1:B:109:GLN:O	1:B:110:LEU:HB3	1.54	1.06

All (3) 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)
1:A:358:MET:N	1:B:224:LEU:N[1_455]	1.73	0.47
1:A:357:PRO:N	1:B:223:ARG:O[1_455]	1.82	0.38
1:A:160:TYR:OH	1:A:233:LYS:NZ[1_655]	1.98	0.22

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	359/404 (89%)	284 (79%)	60 (17%)	15 (4%)	3	23
1	B	358/404 (89%)	277 (77%)	59 (16%)	22 (6%)	2	13
1	C	356/404 (88%)	277 (78%)	57 (16%)	22 (6%)	2	13
All	All	1073/1212 (88%)	838 (78%)	176 (16%)	59 (6%)	2	16

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	SER
1	A	109	GLN
1	A	281	ARG
1	A	316	ALA

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	316/358 (88%)	283 (90%)	33 (10%)	8	33
1	B	319/358 (89%)	286 (90%)	33 (10%)	8	33
1	C	312/358 (87%)	265 (85%)	47 (15%)	3	16
All	All	947/1074 (88%)	834 (88%)	113 (12%)	6	26

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	245	LEU
1	B	383	LEU
1	C	301	SER
1	B	263	LEU
1	B	282	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	ASN
1	B	166	GLN
1	C	265	ASN
1	B	83	ASN
1	B	91	GLN

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](#)

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	363/404 (89%)	-0.21	2 (0%) 89 83	28, 57, 94, 109	0
1	B	362/404 (89%)	-0.22	0 100 100	27, 59, 92, 108	0
1	C	360/404 (89%)	-0.04	5 (1%) 75 63	53, 85, 117, 141	0
All	All	1085/1212 (89%)	-0.15	7 (0%) 89 83	27, 67, 105, 141	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	347	ALA	5.2
1	A	394	LYS	2.9
1	C	360	ILE	2.8
1	C	284	ALA	2.7
1	C	142	ALA	2.5

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.