



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:35 AM GMT

PDB ID : 1AE8
Title : HUMAN ALPHA-THROMBIN INHIBITION BY EOC-D-PHE-PRO-AZALYS-ONP
Authors : De Simone, G.; Balliano, G.; Milla, P.; Gallina, C.; Giordano, C.; Tarricone, C.; Rizzi, M.; Bolognesi, M.; Ascenzi, P.
Deposited on : 1997-03-06
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

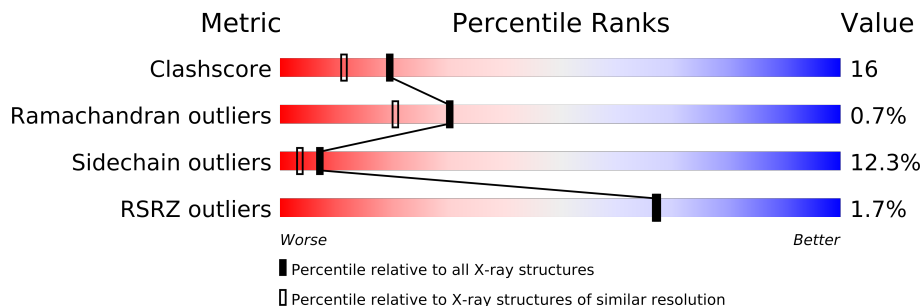
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	L	36	
2	H	259	
3	I	10	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2638 atoms, of which 0 are hydrogen and 0 are deuterium.

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-THROMBIN (SMALL SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	60	0	0
			287	177	48	61	1			

- Molecule 2 is a protein called ALPHA-THROMBIN (LARGE SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	253	Total	C	N	O	S	87	0	0
			2053	1310	362	367	14			

- Molecule 3 is a protein called HIRUGEN.

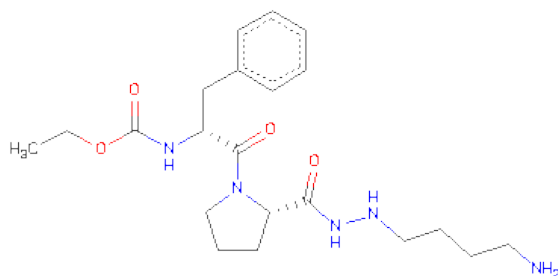
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	S	23	0	0
			95	59	10	25	1			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is 1-ETHOXYCARBONYL-D-PHE-PRO-2(4-AMINOBTYL)HYDRAZINE (three-letter code: AZL) (formula: $C_{21}H_{33}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	1	0
			30	21	5	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	137	Total 137	O 137	0	0
6	I	1	Total 1	O 1	0	0
6	L	21	Total 21	O 21	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.71Å 72.55Å 73.20Å 90.00° 100.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.00-2.00) 87.6 (19.84-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.26 (at 2.01Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	(Not available) , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 115.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21911 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2638	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: AZL, NAG, TYS

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	L	1.52	2/290 (0.7%)	1.14	2/384 (0.5%)
2	H	0.93	0/2107	1.01	6/2846 (0.2%)
3	I	2.00	1/79 (1.3%)	0.73	0/103
All	All	1.06	3/2476 (0.1%)	1.02	8/3333 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	15	ARG	C-OXT	18.08	1.57	1.23
3	I	64	LEU	C-OXT	16.35	1.54	1.23
1	L	8	GLU	CD-OE1	6.23	1.32	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	15	ARG	NE-CZ-NH1	8.82	124.71	120.30
2	H	77(A)	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	H	93	ARG	NE-CZ-NH1	6.17	123.38	120.30
2	H	206	ARG	NE-CZ-NH2	-5.87	117.37	120.30
2	H	148	TRP	N-CA-CB	-5.47	100.76	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	287	0	278	16	0
2	H	2053	0	2019	64	0
3	I	95	0	72	2	0
4	H	14	0	11	0	0
5	H	30	0	33	3	0
6	H	137	0	0	7	0
6	I	1	0	0	0	0
6	L	21	0	0	1	0
All	All	2638	0	2413	73	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

The worst 5 of 73 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:148:TRP:HE3	2:H:150:GLY:HA2	1.19	1.06
1:L:14(J):TYR:O	1:L:14(K):ILE:HG13	1.70	0.91
1:L:1(D):GLY:CA	2:H:123:LEU:H	1.95	0.79
2:H:148:TRP:CE3	2:H:150:GLY:HA2	2.12	0.78
1:L:1(F):GLY:HA2	2:H:235:LYS:CE	2.14	0.77

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	L	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	2	0
2	H	249/259 (96%)	234 (94%)	15 (6%)	0	100	100
3	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	290/305 (95%)	267 (92%)	21 (7%)	2 (1%)	30	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(L)	ASP
1	L	1(G)	PHE

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	L	31/31 (100%)	23 (74%)	8 (26%)	1	0
2	H	221/225 (98%)	198 (90%)	23 (10%)	10	5
3	I	9/9 (100%)	8 (89%)	1 (11%)	9	5
All	All	261/265 (98%)	229 (88%)	32 (12%)	7	3

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	87	LYS
2	H	126	ARG
2	H	241	VAL
2	H	109	LYS
2	H	127	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	78	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	TYS	I	63	3	16,16,17	4.78	3 (18%)	20,22,24	0.61	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
3	TYS	I	63	3	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	63	TYS	O-C	14.75	1.21	1.11
3	I	63	TYS	OH-S	-10.82	1.44	1.63
3	I	63	TYS	OH-CZ	-5.04	1.36	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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$
4	NAG	H	400	2	12,14,15	1.41	1 (8%)	15,19,21	5.54	12 (80%)
5	AZL	H	600	-	31,31,31	0.96	2 (6%)	39,39,39	2.10	6 (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	H	400	2	2/2/5/7	0/6/23/26	0/1/1/1
5	AZL	H	600	-	-	0/30/40/40	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	400	NAG	C2-N2	3.90	1.50	1.46
5	H	600	AZL	C8-N7	2.75	1.38	1.34
5	H	600	AZL	N7-N6	-2.34	1.37	1.42

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	400	NAG	O5-C5-C6	14.02	121.69	106.98
5	H	600	AZL	C24-O24-C23	8.52	132.64	116.09
4	H	400	NAG	C3-C2-N2	7.75	123.56	111.76
5	H	600	AZL	O23-C23-N9	-6.86	112.69	124.90
4	H	400	NAG	C3-C4-C5	5.99	120.90	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	H	400	NAG	C4
4	H	400	NAG	C2

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	L	34/36 (94%)	-0.27	4 (11%) 5 5	19, 32, 94, 100	11 (32%)
2	H	252/259 (97%)	-0.71	1 (0%) 90 91	16, 28, 55, 81	28 (11%)
3	I	10/10 (100%)	-0.09	0 100 100	44, 53, 61, 63	6 (60%)
All	All	296/305 (97%)	-0.64	5 (1%) 67 67	16, 29, 61, 100	45 (15%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	148	TRP	4.5
1	L	1(D)	GLY	2.8
1	L	1(E)	SER	2.6
1	L	1(F)	GLY	2.6
1	L	1(G)	PHE	2.5

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	TYS	I	63	16/17	0.15	-	30,48,72,77	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	H	400	14/15	-	-	55,55,55,55	14
5	AZL	H	600	30/30	0.07	-	19,29,56,94	1

6.5 Other polymers

There are no such residues in this entry.