



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6P9U / pdb_00006p9u
Title : Crystal structure of human thrombin mutant W215A
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Deposited on : 2019-06-10
Resolution : 3.30 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

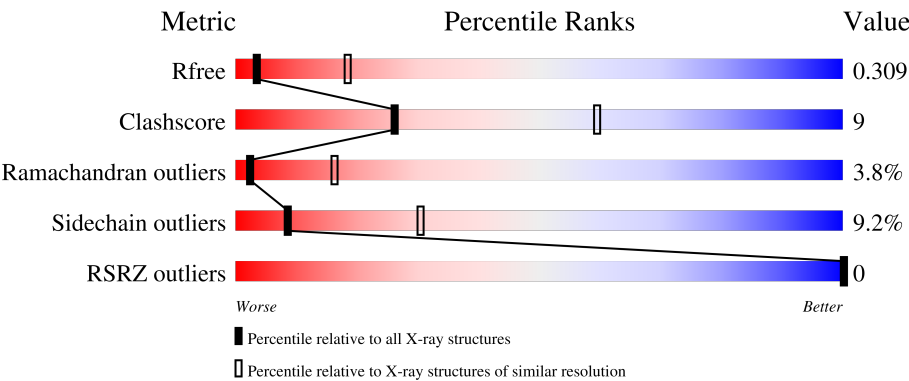
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	136.32Å 44.23Å 136.19Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	32.59 – 3.30 32.59 – 3.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (32.59-3.30) 89.6 (32.59-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.225 , 0.308 0.225 , 0.309	Depositor DCC
R_{free} test set	1087 reflections (4.30%)	wwPDB-VP
Wilson B-factor (Å ²)	61.0	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.369 for -l,k,h 0.052 for -h,-k,l 0.054 for l,-k,h	Xtriage
Reported twinning fraction	0.534 for H, K, L 0.466 for L, K, -H	Depositor
Outliers	13 of 22632 reflections (0.057%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9011	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3112e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

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

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	0.88	0/245	0.94	0/326
1	C	0.95	0/256	1.09	0/340
1	E	1.00	0/256	1.06	1/340 (0.3%)
1	G	1.18	0/256	1.07	0/340
2	B	1.03	1/2022 (0.0%)	1.15	5/2730 (0.2%)
2	D	0.92	1/2017 (0.0%)	1.11	7/2724 (0.3%)
2	F	0.98	3/2048 (0.1%)	1.07	3/2766 (0.1%)
2	H	0.97	0/2047	1.14	10/2764 (0.4%)
All	All	0.98	5/9147 (0.1%)	1.11	26/12330 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	41	LEU	C-O	-6.47	1.15	1.24
2	D	248	TYR	N-CA	5.91	1.53	1.46
2	F	42	CYS	C-O	-5.73	1.16	1.24
2	F	124	PRO	CA-C	-5.38	1.47	1.53
2	F	43	GLY	N-CA	-5.01	1.40	1.44

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	36	LYS	N-CA-C	7.65	119.41	111.14
2	B	60(F)	LYS	N-CA-C	7.64	122.48	108.58
2	H	27	SER	CA-C-N	7.48	127.15	119.82
2	H	27	SER	C-N-CA	7.48	127.15	119.82
2	B	154	VAL	N-CA-C	6.60	118.44	108.80

There are no chirality outliers.

There are no planarity outliers.

3.2 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	243	0	238	11	0
1	C	254	0	251	6	0
1	E	254	0	251	5	0
1	G	254	0	251	2	0
2	B	1973	0	1953	38	0
2	D	1968	0	1939	37	0
2	F	1998	0	1976	39	0
2	H	1997	0	1970	41	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	F	14	0	13	0	0
4	H	14	0	13	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	H	2	0	0	0	0
All	All	9011	0	8881	168	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 9.

The worst 5 of 168 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)
2:B:42:CYS:HB3	2:B:195:SER:O	1.79	0.81
2:F:100:ASP:OD1	2:F:177:THR:HG21	1.82	0.80
2:H:250:GLU:N	2:H:250:GLU:OE1	2.15	0.80
2:B:33:LEU:O	2:B:41:LEU:HB2	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14(D):ARG:NH2	2:H:97(A):GLU:O	2.28	0.67

There are no symmetry-related clashes.

3.3 Torsion angles [i](#)

3.3.1 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	28/31 (90%)	22 (79%)	4 (14%)	2 (7%)	1	6
1	C	29/31 (94%)	21 (72%)	6 (21%)	2 (7%)	1	7
1	E	29/31 (94%)	24 (83%)	3 (10%)	2 (7%)	1	7
1	G	29/31 (94%)	25 (86%)	4 (14%)	0	100	100
2	B	239/273 (88%)	196 (82%)	35 (15%)	8 (3%)	3	19
2	D	238/273 (87%)	202 (85%)	29 (12%)	7 (3%)	3	21
2	F	241/273 (88%)	197 (82%)	33 (14%)	11 (5%)	2	13
2	H	242/273 (89%)	205 (85%)	28 (12%)	9 (4%)	2	17
All	All	1075/1216 (88%)	892 (83%)	142 (13%)	41 (4%)	2	16

5 of 41 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	217	GLU
1	E	14(L)	ASP
2	F	247	GLU
2	H	247	GLU
1	A	14(K)	ILE

3.3.2 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	27/28 (96%)	26 (96%)	1 (4%)	30	58
1	C	28/28 (100%)	28 (100%)	0	100	100
1	E	28/28 (100%)	27 (96%)	1 (4%)	31	58
1	G	28/28 (100%)	27 (96%)	1 (4%)	31	58
2	B	213/237 (90%)	186 (87%)	27 (13%)	4	18
2	D	212/237 (90%)	190 (90%)	22 (10%)	7	25
2	F	216/237 (91%)	201 (93%)	15 (7%)	14	41
2	H	215/237 (91%)	193 (90%)	22 (10%)	7	26
All	All	967/1060 (91%)	878 (91%)	89 (9%)	8	30

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	131	GLN
2	H	110	LYS
2	F	170	ASP
2	F	240	LYS
2	H	129(C)	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	91	HIS
2	D	205	ASN
2	D	230	HIS
2	B	151	GLN
2	B	143	ASN

3.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

3.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

3.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

3.7 Other polymers [i](#)

There are no such residues in this entry.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 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	30/31 (96%)	-1.34	0 100 100	52, 67, 82, 87	0
1	C	31/31 (100%)	-1.42	0 100 100	55, 67, 81, 90	0
1	E	31/31 (100%)	-1.29	0 100 100	55, 70, 84, 87	0
1	G	31/31 (100%)	-1.31	0 100 100	62, 70, 83, 89	0
2	B	245/273 (89%)	-1.31	0 100 100	45, 68, 90, 109	0
2	D	244/273 (89%)	-1.31	0 100 100	45, 66, 87, 107	0
2	F	247/273 (90%)	-1.27	0 100 100	49, 66, 88, 103	0
2	H	248/273 (90%)	-1.31	0 100 100	49, 67, 88, 111	0
All	All	1107/1216 (91%)	-1.30	0 100 100	45, 67, 88, 111	0

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

4.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

LIGAND-RSR INFOmissingINFO

4.4 Other polymers [i](#)

There are no such residues in this entry.