

Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 05:42 PM EDT

PDB ID : 3SQE

Title: Crystal structure of prethrombin-2 mutant S195A in the alternative form

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Deposited on : 2011-07-05

Resolution : 1.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.35

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

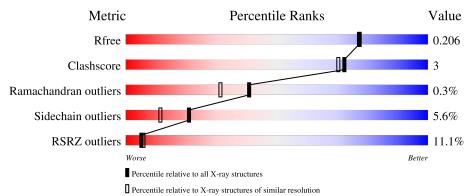
Validation Pipeline (wwPDB-VP) : 2.35

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 1.90 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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		
			11%		
1	${ m E}$	290	90%	8%	•



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2582 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.

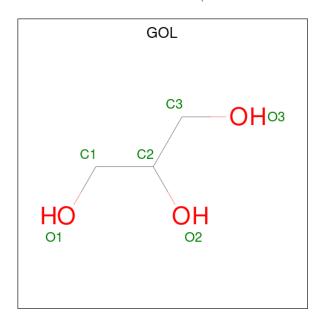
• Molecule 1 is a protein called Thrombin light chain, heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	E	289	Total 2360	C 1498	N 416	O 427	S 19	0	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Е	195	ALA	SER	engineered mutation	UNP P00734

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Е	1	Total C O 6 3 3	0	0
2	Е	1	Total C O 6 3 3	0	0

• Molecule 3 is water.



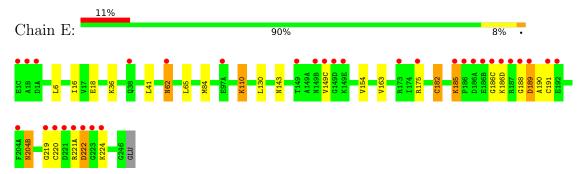
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	210	Total O 210 210	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Thrombin light chain, heavy chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	44.38Å 58.05Å 52.88Å	Donositor
a, b, c, α , β , γ	90.00° 98.24° 90.00°	Depositor
Resolution (Å)	25.38 - 1.90	Depositor
Resolution (A)	25.38 - 1.90	EDS
% Data completeness	95.6 (25.38-1.90)	Depositor
(in resolution range)	95.6 (25.38-1.90)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	6.62 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
D D.	0.171 , 0.206	Depositor
R, R_{free}	0.172 , 0.206	DCC
R_{free} test set	1046 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36, 49.4	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2582	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.13% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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: GOL

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Е	0.52	0/2418	0.64	0/3265	

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	Е	2360	0	2322	16	0
2	Е	12	0	16	0	0
3	Е	210	0	0	2	0
All	All	2582	0	2338	16	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 3.

All (16) 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:E:36:LYS:HE2	1:E:62:ASN:O	2.00	0.62	

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Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:E:222:ASP:HB3	1:E:224:LYS:HG2	1.83	0.60
1:E:190:ALA:HB1	3:E:342:HOH:O	2.04	0.57
1:E:16:ILE:O	1:E:186(D):LYS:HG3	2.05	0.56
1:E:16:ILE:HG23	1:E:186(C):GLY:O	2.09	0.51
1:E:163:VAL:HB	1:E:182[A]:CYS:SG	2.52	0.50
1:E:18:GLU:HB2	1:E:188:GLY:HA3	1.97	0.45
1:E:189:ASP:OD2	1:E:191[A]:CYS:SG	2.75	0.45
1:E:204(B):ASN:C	1:E:204(B):ASN:HD22	2.21	0.44
1:E:36:LYS:HG2	1:E:65:LEU:HG	2.00	0.43
1:E:110:LYS:HE3	1:E:110:LYS:HA	2.01	0.43
1:E:219:GLY:HA3	3:E:380:HOH:O	2.17	0.43
1:E:65:LEU:CD2	1:E:84:MET:SD	3.07	0.42
1:E:224:LYS:HD3	1:E:224:LYS:HA	1.48	0.42
1:E:220[A]:CYS:O	1:E:220[A]:CYS:SG	2.78	0.41
1:E:185:LYS:H	1:E:185:LYS:HD3	1.85	0.41

There are no symmetry-related clashes.

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	voured Allowed		Percentiles	
1	E	291/290 (100%)	278 (96%)	12 (4%)	1 (0%)	41	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Ε	222	ASP



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	Analysed Rotameric		Percentiles		
1	E	255/252 (101%)	240 (94%)	15 (6%)	19 10		

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Е	6	LEU
1	Е	41	LEU
1	Е	62	ASN
1	Е	110	LYS
1	Е	130	LEU
1	Е	143	ASN
1	Е	149(C)	VAL
1	Е	154	VAL
1	Е	175	ARG
1	Е	182[A]	CYS
1	Е	182[B]	CYS
1	Е	185	LYS
1	Е	189	ASP
1	Е	204(B)	ASN
1	Е	221(A)	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type	
1	Е	156	GLN	
1	Е	204(B)	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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).

Mal	Mol Type Chain Res I		Tiple	B	Bond lengths			Bond angles		
MIOI TY	Type	Chain	Res	Link	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	GOL	Е	301	-	5,5,5	0.38	0	5,5,5	0.51	0
2	GOL	Е	302	-	5,5,5	0.53	0	5,5,5	0.21	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
2	GOL	Е	301	-	-	1/4/4/4	-
2	GOL	Е	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	\mathbf{E}	301	GOL	C1-C2-C3-O3



There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$OWAB(Å^2)$	Q<0.9
1	Е	289/290 (99%)	0.38	32 (11%)	5 6	17, 28, 57, 72	1 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	223	GLY	7.7
1	Е	186(A)	ASP	6.7
1	Е	222	ASP	6.1
1	Е	186(C)	GLY	5.6
1	Е	149	THR	5.5
1	Е	149(E)	LYS	5.3
1	Е	149(C)	VAL	4.5
1	Е	221(A)	ARG	4.2
1	Е	220[A]	CYS	3.9
1	Е	149(D)	GLY	3.9
1	Е	186	PRO	3.5
1	Е	219	GLY	3.5
1	Е	173	ARG	3.4
1	Е	97(A)	GLU	3.1
1	Е	221	ASP	3.0
1	Е	1(B)	ALA	3.0
1	Е	192	GLU	3.0
1	Е	188	GLY	2.8
1	Е	62	ASN	2.8
1	Е	224	LYS	2.7
1	Е	204(A)	PHE	2.5
1	Е	189	ASP	2.4
1	Е	149(B)	ASN	2.4
1	Е	191[A]	CYS	2.4
1	Е	1(C)	GLU	2.3
1	Е	38	GLN	2.2
1	Е	185	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	Е	186(D)	LYS	2.2
1	Е	186(B)	GLU	2.1
1	Е	1(A)	ASP	2.1
1	Е	175	ARG	2.0
1	Е	187	ARG	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	GOL	Ε	301	6/6	0.92	0.16	24,28,30,35	0
2	GOL	Ε	302	6/6	0.92	0.20	31,32,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.

