



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 02:06 pm BST

PDB ID : 3I78
Title : 35/99/170/186/220-loops of FXa in SGT
Authors : Page, M.J.; Di Cera, E.
Deposited on : 2009-07-08
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 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) : 2.11

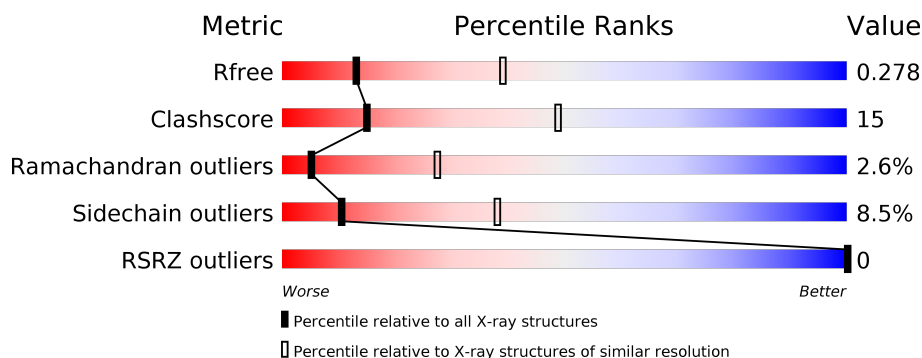
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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 $\leq 5\%$. 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	229	<div> <div style="width: 66%; background-color: green;"></div> <div style="width: 30%; background-color: yellow;"></div> <div style="width: 4%; background-color: orange;"></div> <div style="width: 0%; background-color: red;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <div>66% 30% .</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1728 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 Trypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1698	1058	295	336	9			

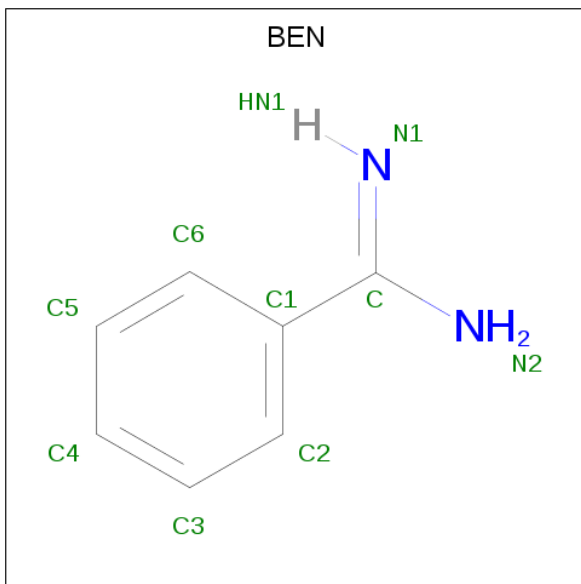
There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ILE	-	SEE REMARK 999	UNP P00775
A	35	ASN	-	SEE REMARK 999	UNP P00775
A	36	GLU	-	SEE REMARK 999	UNP P00775
A	37	GLU	-	SEE REMARK 999	UNP P00775
A	38	ASN	SER	SEE REMARK 999	UNP P00775
A	39	GLU	MET	SEE REMARK 999	UNP P00775
A	41	PHE	-	SEE REMARK 999	UNP P00775
A	94	PHE	-	SEE REMARK 999	UNP P00775
A	95	THR	TYR	SEE REMARK 999	UNP P00775
A	96	LYS	ASN	SEE REMARK 999	UNP P00775
A	97	GLU	GLY	SEE REMARK 999	UNP P00775
A	99	TYR	-	SEE REMARK 999	UNP P00775
A	171	SER	ALA	SEE REMARK 999	UNP P00775
A	172	SER	TYR	SEE REMARK 999	UNP P00775
A	173	SER	GLY	SEE REMARK 999	UNP P00775
A	174	PHE	ASN	SEE REMARK 999	UNP P00775
A	175	ILE	GLU	SEE REMARK 999	UNP P00775
A	180	MET	GLU	SEE REMARK 999	UNP P00775
A	?	-	PRO	SEE REMARK 999	UNP P00775
A	186	LYS	GLY	SEE REMARK 999	UNP P00775
A	187	GLN	GLY	SEE REMARK 999	UNP P00775
A	188	GLU	VAL	SEE REMARK 999	UNP P00775
A	208	VAL	ILE	SEE REMARK 999	UNP P00775
A	217	GLU	TYR	SEE REMARK 999	UNP P00775
A	223	LYS	PRO	SEE REMARK 999	UNP P00775
A	224	LYS	TYR	SEE REMARK 999	UNP P00775
A	225	TYR	PRO	SEE REMARK 999	UNP P00775

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

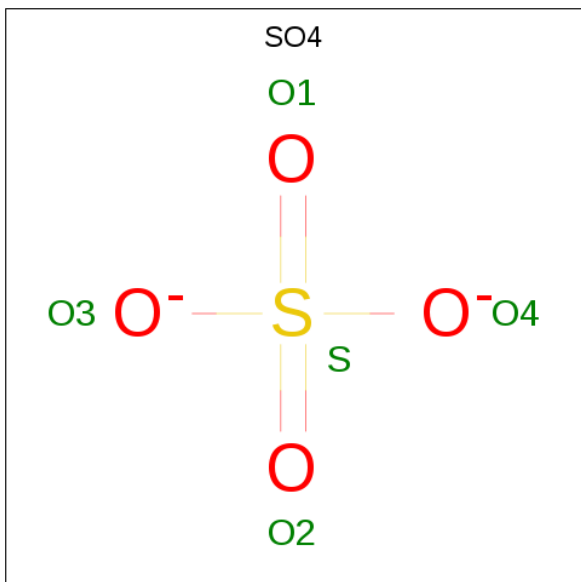
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			9	7	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

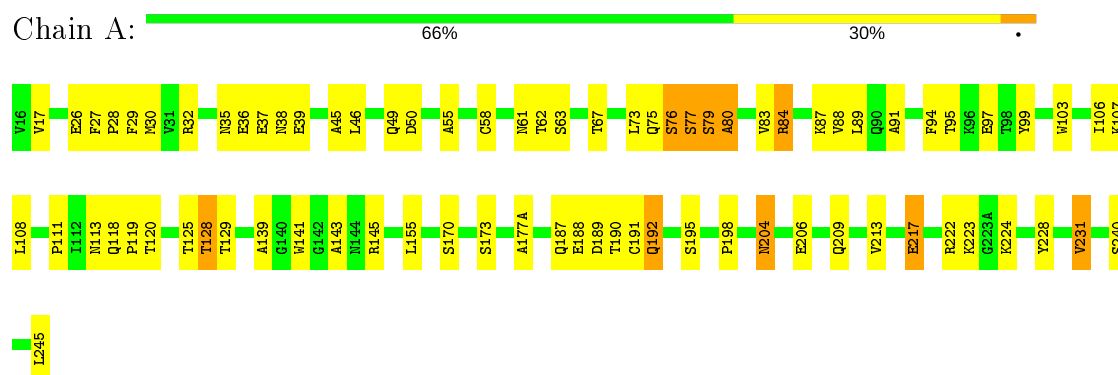


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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: Trypsin



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.71 Å 113.71 Å 52.62 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.94 – 3.00 35.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (35.94-3.00) 97.6 (35.95-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.208 , 0.275 0.210 , 0.278	Depositor DCC
R_{free} test set	359 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1728	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, BEN, SO4

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	0.77	0/1728	0.78	1/2341 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	125	THR	C-N-CA	5.12	134.51	121.70

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	1698	0	1649	51	0
2	A	1	0	0	0	0
3	A	9	0	7	0	0
4	A	20	0	0	0	0
All	All	1728	0	1656	51	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 15.

The worst 5 of 51 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:62:THR:O	1:A:84:ARG:NH1	2.24	0.70
1:A:35:ASN:ND2	1:A:38:ASN:OD1	2.29	0.65
1:A:38:ASN:O	1:A:39:GLU:HB2	1.95	0.65
1:A:35:ASN:O	1:A:37:GLU:N	2.30	0.64
1:A:128:THR:OG1	1:A:129:THR:N	2.30	0.63

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	Allowed	Outliers	Percentiles	
1	A	227/229 (99%)	204 (90%)	17 (8%)	6 (3%)	5	27

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	77	SER
1	A	177(A)	ALA
1	A	80	ALA
1	A	76	SER

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	Rotameric	Outliers	Percentiles	
1	A	176/176 (100%)	161 (92%)	15 (8%)	10	38

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ARG
1	A	170	SER
1	A	217	GLU
1	A	128	THR
1	A	206	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	159	ASN
1	A	204	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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	BEN	A	302	-	9,9,9	1.09	1 (11%)	7,11,11	1.12	1 (14%)
4	SO4	A	304	-	4,4,4	0.21	0	6,6,6	0.25	0
4	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.60	0
4	SO4	A	306	-	4,4,4	0.13	0	6,6,6	0.88	0
4	SO4	A	305	-	4,4,4	0.20	0	6,6,6	0.45	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	BEN	A	302	-	-	4/4/4/4	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	BEN	C1-C	-2.20	1.43	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	BEN	C1-C-N2	2.55	121.89	118.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	BEN	N2-C-C1-C2
3	A	302	BEN	N2-C-C1-C6
3	A	302	BEN	N1-C-C1-C2
3	A	302	BEN	N1-C-C1-C6

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, 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	229/229 (100%)	-0.55	0 100 100	42, 57, 69, 81	7 (3%)

There are no RSRZ outliers to report.

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](#)

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	304	5/5	0.89	0.17	107,107,107,108	0
2	NA	A	301	1/1	0.93	0.18	52,52,52,52	0
3	BEN	A	302	9/9	0.95	0.31	50,51,51,52	0
4	SO4	A	306	5/5	0.97	0.10	69,70,71,71	0
4	SO4	A	305	5/5	0.97	0.10	65,66,67,68	0
4	SO4	A	303	5/5	0.99	0.12	51,51,53,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.