



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2017 – 11:57 AM EST

PDB ID : 1GGT  
Title : THREE-DIMENSIONAL STRUCTURE OF A TRANSGLUTAMINASE:  
HUMAN BLOOD COAGULATION FACTOR XIII  
Authors : Yee, V.C.; Pedersen, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller,  
D.C.  
Deposited on : unknown  
Resolution : 2.65 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](mailto: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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

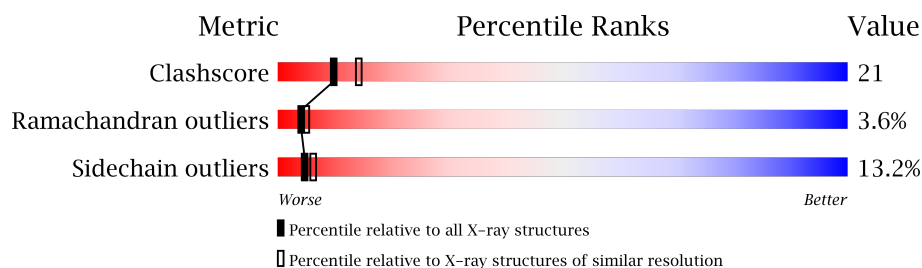
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	731	
1	B	731	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 11382 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 COAGULATION FACTOR XIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	710	Total	C	N	O	S	0	0	0
			5700	3614	983	1076	27			
1	B	708	Total	C	N	O	S	0	0	0
			5682	3603	978	1074	27			

There are 2 discrepancies between the modelled and reference sequences:

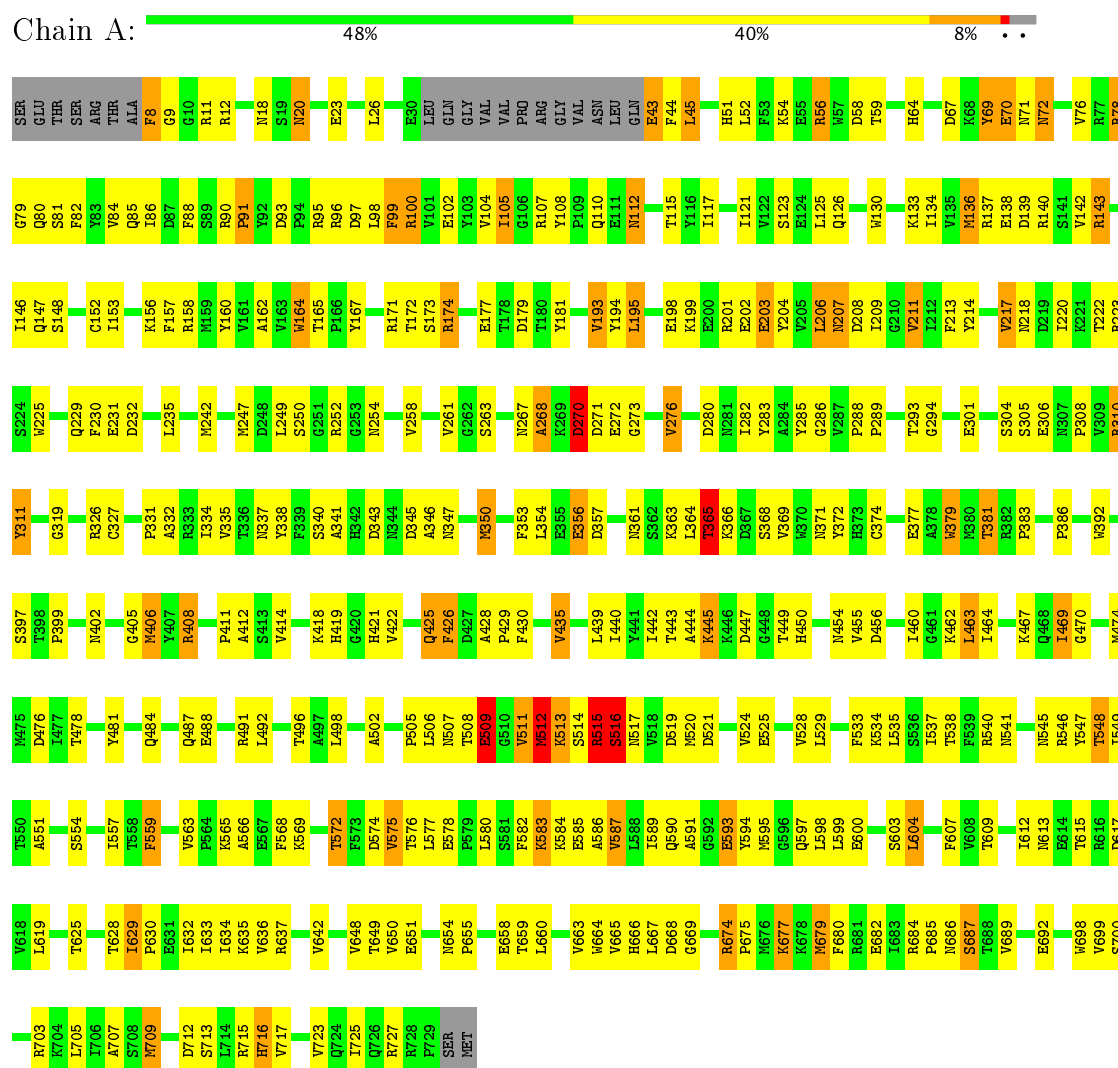
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	CONFLICT	UNP P00488
B	651	GLU	GLN	CONFLICT	UNP P00488

### 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 ( $RSRZ > 2$ ). 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.

Note EDS was not executed.

#### • Molecule 1: COAGULATION FACTOR XIII



#### • Molecule 1: COAGULATION FACTOR XIII



I706	T615	N542	R382	V258	R158	Q80	SER
A707	R616	S543	P383	S263	A162	S81	GLU
S708	D617	L463	D384	S263	A162	F82	THR
M709	V618	R546	L385	K269	H164	Q85	ARG
S713	L619	Y547	P386	D270	T165	I86	THR
L714	A620	T548	V387	D271	D165	D87	ALA
R715	K621	I549	S397	E272	L170	D87	F8
V717	S824	L553	M474	G273	R171	R90	G9
L721	L627	S554	T480	V276	T172	D93	N17
	D722	F559	F483	S403	F184	P94	N20
V723	E631	V563	D404	D280	N185	R95	D24
Q724	I632	P564	Q487	R281	P186	R96	
T725	I633	P564	E488	I282	H187	D87	D25
L726	I634	K565	E489	A283	C188	L98	L26
Q727	K635	A566	R408	A284	E189	F99	T28
ARG	V636	E567	L494	G285	R100	R100	
PRO	T639	F568	Q410	Z286	V101	V101	V29
	Q640	K569	P411	V287	E102	E102	E30
SER	V641	K570	A412	W292	Y104	Y103	LEU
MET	V642	E571	S413	E301	R201	I105	GLN
	M646	T572	Y500	E301	E202	G106	GLY
T649		V573	K504	Y302	R107	R107	VAL
	V646	V575	P505	R303	L206	Y108	VAL
T649	V650	T576	H419	P109	P109	P109	PRO
	E651	L577	E422	Q110	Q110	Q110	ARG
N654	L578	E578	Q423	Y311	F213	E111	GLY
	P579	P579	F424	C314	F213	T115	ASN
P655	L580	V511	Q425	P331	V217	I116	LEU
L656	P655	S581	F426	P331	P331	I117	GLN
K657	L656	F582	D427	N337	T220	P118	E43
E585	K583	K583	A428	Y338	R221	V119	F44
T659	E585	K584	P429	T222	T222	P120	L45
V663	V587	E586	F430	F339	R223	I121	T48
	L586	A586	V431	S340	R223	V122	
H666	L588	D519	E434	A341	F230	S123	H51
	L589	D520	V435	H342	E231	I123	
L667	Q590	D521	V436	D232	D232	G128	L52
D668	A591	F522	S437	N947	G233	F53	F53
G669	E592	E523	D438	L234	L234	K133	K54
P670	E593	V524	I439	M350	L235	I134	E55
M676	Y594	E525	T440	F353	D236	V135	D68
	M595	N526	T441	T237	M136	M136	
M679	G596	A527	L364	Y240	D139	D139	K61
	Q597	V528	L364	N359	N247	R143	H64
R684	L598	T443	K445	V360	T248	L144	H65
P685	L599	T443	K446	N361	L249	S145	T66
N686	H605	D447	D447	S362	G250	I146	N71
P697	F606	K334	K334	R363	S250	I146	
W698	F607	L335	L335	L364	G251	P150	I75
V699	V608	S536	V451	T365	R252	K151	V76
R703	I612	T537	V452	Y372	G253	C152	V77
	N613	T538	E453	W379	N254	I153	R78
K704	F539	E453	D456		L256	F157	G79
L705	R540	R540	D456	K257			

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.20 Å   182.70 Å   93.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.65	Depositor
% Data completeness (in resolution range)	97.6 (10.00-2.65)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.216 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11382	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.66	1/5835 (0.0%)	0.90	9/7917 (0.1%)
1	B	0.69	3/5816 (0.1%)	0.92	11/7891 (0.1%)
All	All	0.67	4/11651 (0.0%)	0.91	20/15808 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	651	GLU	CD-OE2	8.44	1.34	1.25
1	A	651	GLU	CD-OE2	6.95	1.33	1.25
1	B	188	CYS	CB-SG	-6.20	1.71	1.82
1	B	152	CYS	CB-SG	-5.07	1.73	1.81

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-9.94	84.15	111.00
1	B	460	ILE	N-CA-C	8.19	133.12	111.00
1	B	365	THR	N-CA-C	-7.38	91.07	111.00
1	B	425	GLN	N-CA-C	7.01	129.94	111.00
1	B	553	LEU	CA-CB-CG	6.34	129.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	TYR	Sidechain

## 5.2 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	5700	0	5557	252	0
1	B	5682	0	5537	229	0
All	All	11382	0	11094	480	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 21.

The worst 5 of 480 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:B:659:THR:HG22	1:B:685:PRO:HD3	1.43	0.98
1:A:538:THR:HG22	1:A:584:LYS:HG2	1.50	0.92
1:A:100:ARG:HD2	1:A:164:TRP:HZ3	1.34	0.91
1:A:381:THR:HG23	1:A:383:PRO:HD3	1.51	0.91
1:B:527:ALA:HB2	1:B:533:PHE:HB3	1.55	0.88

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	A	706/731 (97%)	633 (90%)	49 (7%)	24 (3%)	<b>4</b> <b>5</b>

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	4 4
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	4 5

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	91	PRO
1	A	139	ASP
1	A	426	PHE
1	A	509	GLU

### 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	626/644 (97%)	536 (86%)	90 (14%)	4 4
1	B	624/644 (97%)	549 (88%)	75 (12%)	6 8
All	All	1250/1288 (97%)	1085 (87%)	165 (13%)	5 6

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	604	LEU
1	B	28	THR
1	B	583	LYS
1	A	625	THR
1	A	677	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	HIS
1	A	526	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	322	ASN
1	A	347	ASN
1	B	337	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](#)

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.