



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:37 PM GMT

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 : 1994-01-25
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
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

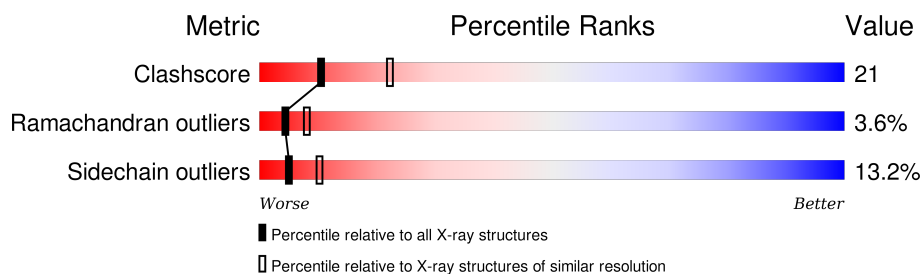
1 Overall quality at a glance

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	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)

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. 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:

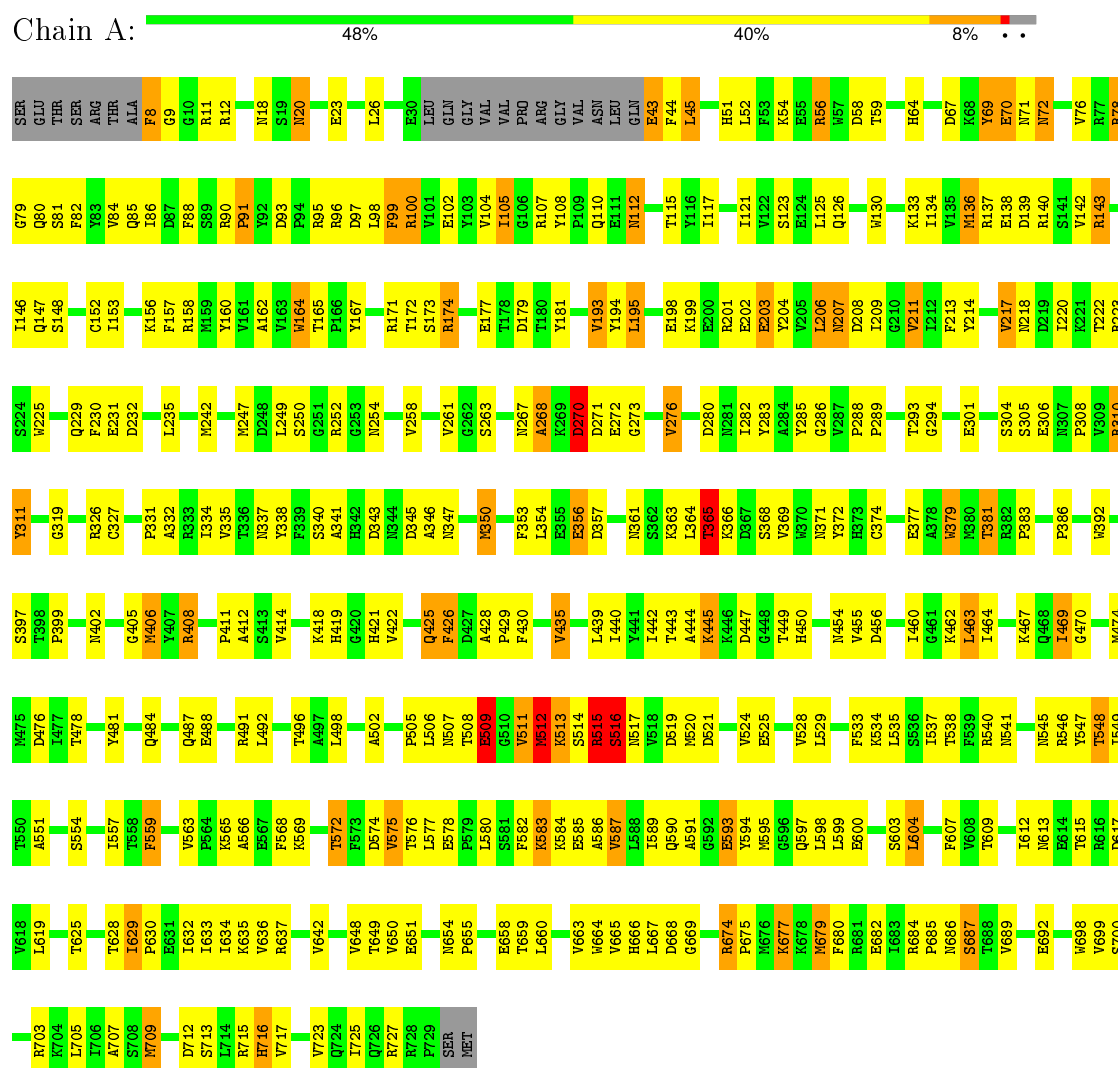
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	CONFLICT	UNP P00488
B	651	GLU	GLN	CONFLICT	UNP P00488

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 errors 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	A620	Y547	P386	K269	H164	Q85	THR	
L714	K621	T548	V387	D270	T165	I86	ALA	
R715	S824	I549	S397	D271	D87	D87	F8	
V717		L553	M474	E272	L170	R90	G9	
L721	L627	S554	E401	G273	R171	R90	N17	
	E631	F559	H402	V276	T172	D93		N20
D722	T632	F483	S403	D280	F184	P94	D24	
Q724	I633	V563	D404	I282	N185	R95		D25
I725	S634	P564	G405	I282	H187	R96	L26	
Q726	L635	E566	H406	L282	C188	D87	T27	
R727	V636	A566	Y407	A284	E189	F99	ARG	
	T639	E567	R408	Z285	G189	R100	PRO	
PRO	Q640	F568	G409	G286	V193	V101	GLN	
SER	V641	F568	P411	V287	H194	E102	GLY	
MET	V642	E570	G410	W292	L195	Y103	ASN	
	V646	E571	A412	W292	L195	Y103	LEU	
		T572	S413	E301	R201	I105	I117	GLN
		F573	I417	Y302	E202	G106	I117	E43
	V649	D574	K418	R303	L206	P109	V119	F44
		V575	H419	R303	L206	P109	V119	L45
	T649	T576	V422	R310	V211	T115	T48	
	V650	P579	C423	Y311	T212	I115	H51	
	E651	L580	F424	Y311	F213	I116		L52
	N654	S581	G425	C314	F213	I116	F53	
	P655	F582	F426	P331	V217	K133	K54	
	L656	K583	D427	N337	T220	L134	E55	
	R657	R584	A428	Y338	T221	V135	D68	
	E658	E585	P429	Y338	T222	M136		K61
	T659	S585	S516	F430	T222	L134	H64	
	V663	A586	N517	V431	R223	V122	H65	
		V587	V518	V431	R223	V122	H65	T66
H666	L588	D519	E434	F230	S123	N71		
L667	L589	M520	H436	E231	S123	I75		
D668	A591	D521	H436	H342	G128	V76		
G669	G592	F522	S437	N947	L144	R77		
P670	E593	E523	D438	T234	S145	G79		
M676	V594	V524	L439	M350	L134	H61		
	M595	E526	I440	M350	V135		L52	
M679	M679	H596	T440	F353	T237	L52		
		G596	L354	F353	T237	L52	L52	
R684	P685	Q597	T442	L354	D139	H65		
M686	P685	L598	T443	L354	D139		H65	
P697	P697	L599	K445	N359	R247	L144	T66	
		E600	K445	N359	R247	L144	L146	
W698	W698	F606	K446	N361	T248	P150	N71	
V699	V699	V608	D447	S362	L249	P150		I75
R703	R703	N614	K448	R363	S250	C151	V76	
			H605	R363	S250	C151	C152	R77
L704	L704	L612	V451	T365	G251	I153	G79	
W705	W705	H614	V452	Y372	R252	L256	F79	
			D456	W379	K257			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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:381:THR:HG23	1:A:383:PRO:HD3	1.51	0.91
1:A:100:ARG:HD2	1:A:164:TRP:HZ3	1.34	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%)	5 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	4 7
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	4 8

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 8
1	B	624/644 (97%)	549 (88%)	75 (12%)	6 13
All	All	1250/1288 (97%)	1085 (87%)	165 (13%)	5 10

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

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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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.