



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:55 AM UTC

PDB ID : 1GGT / pdb_00001ggt
Title : THREE-DIMENSIONAL STRUCTURE OF A TRANSGLUTAMINASE:
HUMAN BLOOD COAGULATION FACTOR XIII
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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

<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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

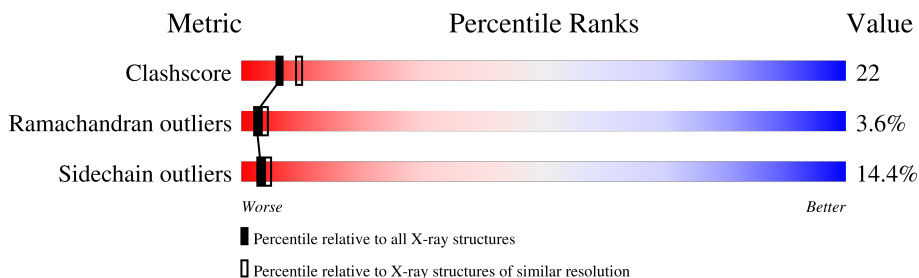
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

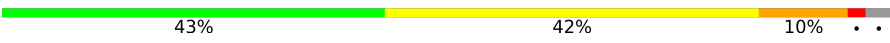
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)

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 $\leq 5\%$.

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:

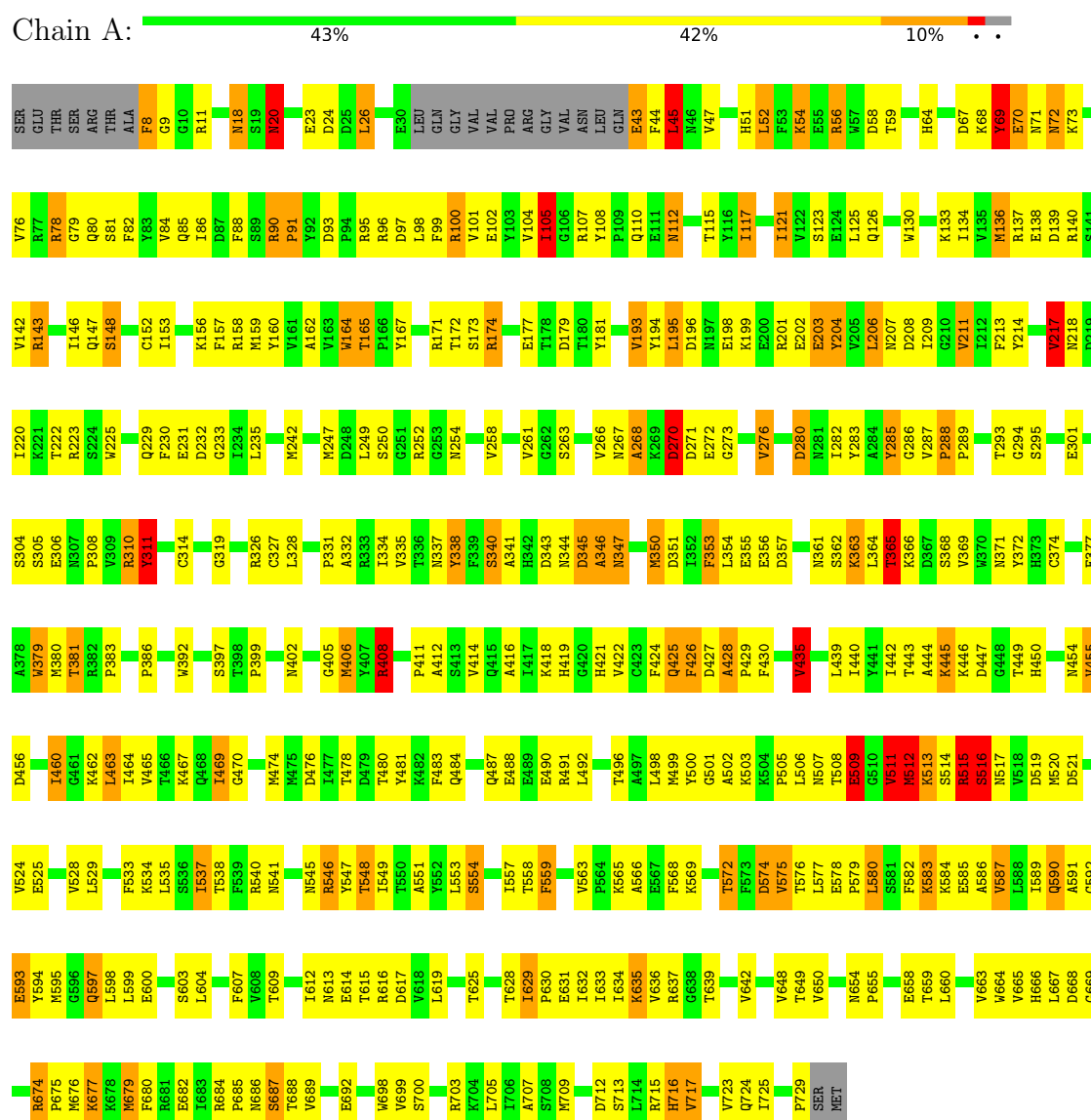
Chain	Residue	Modelled	Actual	Comment	Reference
A	651	GLU	GLN	conflict	UNP P00488
B	651	GLU	GLN	conflict	UNP P00488

3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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



Q724	T639	K570	K504	F424	N337	L235	L144	V76	SER
I725	Q640	E571	P505	Q425	Y338	D236	S145	R77	GLU
Q726	V641	T572	L506	F426	F339	T237	I146	R78	THR
	V642	F573	N507	D427	S340	C238	Q147	G79	SER
		D574	T508	A428	A341	L239	S148	Q80	ARG
	M646	V575	E509	P429	H342	Y240	S149	S81	THR
		T576	G510	F430	D343		P150	F82	ALA
	T649	L577	V511	V431	N344	M247			F8
	V650	E578	M512			D248	I153	Q85	G9
	E651	P579	K513	E434	N347	L249	I86	I86	G10
		L580	S514	V435		S250	F157	D87	R11
	M654	S581	S515	V435	N350	R251	R158		M17
	P655	F582	S516	S437	D351	G252	A162	R90	N18
	L656	K583	N517	D438	F352	G253	V163	P91	N19
	K657	V518	V518	L439	L353	N254	P163	Y92	S19
	E658	E585	D519	I440	F354	P255	W164	D93	N20
	T659	A586	M520	Y441		I256	T165	P94	
		V587	D521	I442	N359	K257	L170	R95	D24
	V663	L588	F522	T443	V360	V258	R171	R96	D25
		T589	E523	A444	N361		T172	D97	L26
	H666	Q590	V524	K445	S362	S263	I171	L98	P27
	L667	A591	E525	K446	K363		S173	F99	T28
	D668	G592	N526	D447	L364	A268	R174	R100	V29
	G669	E593	A527	G448	T365	K269	F184	V101	E30
	P670	Y594	V528		K366	D270	M185	E102	LEU
		M595	L529	V451		D271	P186	Y103	GLN
	R674	G596	G530	V452	Y372	E272	W187	V104	GLY
	P675	Q597	K531	E453		G273	C188	I105	VAL
	M676	L598	D532	N454	W379	V274	E189	G106	VAL
		L599	F533	V455	M380	L275		R107	PRO
	M679	E600	K534	D456	T381	V276	V193	Y108	ARG
			L535		R382		Y194	P109	GLY
	E682	L604	S536	T460	P383	D280	L195	Q110	VAL
	T683	H605	T537		D384	N281		E111	ASN
	R684	P606	T538	L463	L385	I282			LEU
	P685	F607	F539	I464	P386	Y283	R201	T115	GLN
	N686	V608	R540		V387	A284	E202	Y116	E43
			N541	K467		Y285	E203	I117	P44
		I612	R542		S397	G286	Y204	P118	L45
		M613	S543	D472		V287	L206	V119	
	E614	T615		G473	E401	P288		P120	T48
	R616	Y547	R546	M474	M402	W292	V211	I121	H51
	P617	T548	T548	T480	D404		T212	V122	L52
	V618	L549			G405	I298	F213	S123	F53
	L619		L553	F483	Y407	E301	V217	E124	K54
	A620	K621	S554	Q487	R408	Y302		S127	E55
				E488	G409	R303	K221	G128	R56
	S624		I557	E489	G410		I220	K133	W57
			T586		P411	R310	K221	I134	D58
			F599	L494	A412	Y311	T222	V135	K61
				E495	S413	G312	R223	M136	
			V563	L498	I417	Q313	Y227	R137	H64
			P564	M499	K418	G314		E138	H65
			K565	Y500	H419	T323	F230	D139	T66
			A566	G501	V422	D232	E231	R140	
			E567	A502		G233	V142	S141	N71
			F568	K503	C423	I234		V142	I75

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, α , β , γ	101.20Å 182.70Å 93.40Å 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	0.79	2/5835 (0.0%)	1.24	69/7917 (0.9%)
1	B	0.83	3/5816 (0.1%)	1.26	71/7891 (0.9%)
All	All	0.81	5/11651 (0.0%)	1.25	140/15808 (0.9%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	460	ILE	CA-CB	-6.75	1.45	1.54
1	A	266	VAL	CA-CB	-5.57	1.47	1.54
1	B	380	MET	SD-CE	-5.25	1.66	1.79
1	A	424	PHE	CA-C	-5.06	1.46	1.52
1	B	651	GLU	CD-OE2	5.04	1.34	1.25

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-12.51	84.15	110.80
1	B	460	ILE	N-CA-C	11.44	133.12	109.34
1	B	363	LYS	N-CA-C	-10.45	99.43	111.03
1	A	310	ARG	N-CA-C	9.98	124.59	108.63
1	B	44	PHE	N-CA-C	9.31	123.66	109.23

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 [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	5700	0	5557	263	0
1	B	5682	0	5537	237	0
All	All	11382	0	11094	499	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 22.

The worst 5 of 499 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 [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	706/731 (97%)	633 (90%)	49 (7%)	24 (3%)	3 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	704/731 (96%)	607 (86%)	70 (10%)	27 (4%)	2	3
All	All	1410/1462 (96%)	1240 (88%)	119 (8%)	51 (4%)	2	4

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%)	521 (83%)	105 (17%)	2	2
1	B	624/644 (97%)	549 (88%)	75 (12%)	5	7
All	All	1250/1288 (97%)	1070 (86%)	180 (14%)	3	4

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	135	VAL
1	B	460	ILE
1	B	172	THR
1	B	301	GLU
1	B	499	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	666	HIS
1	B	313	GLN

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Mol	Chain	Res	Type
1	B	545	ASN
1	B	71	ASN
1	B	322	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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.