



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:54 PM UTC

PDB ID : 1GGU / pdb_00001ggu
Title : HUMAN FACTOR XIII WITH CALCIUM BOUND IN THE ION SITE
Authors : Fox, B.A.; Yee, V.C.; Pederson, L.C.; Trong, I.L.; Bishop, P.D.; Stenkamp, R.E.; Teller, D.C.
Deposited on : 1998-07-22
Resolution : 2.10 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

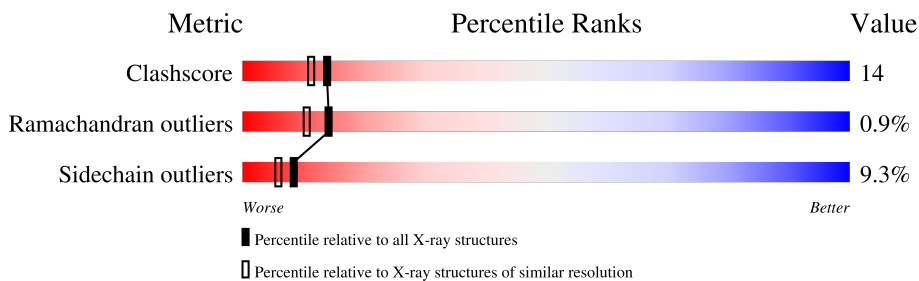
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	 58% 30% 7% . .
1	B	731	 62% 28% 5% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12297 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 PROTEIN (COAGULATION FACTOR XIII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	701	Total	C	N	O	S	0	0	0
			5627	3571	967	1063	26			
1	B	707	Total	C	N	O	S	0	0	0
			5667	3595	975	1071	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLU	GLN	conflict	UNP P00488
B	567	GLU	GLN	conflict	UNP P00488

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

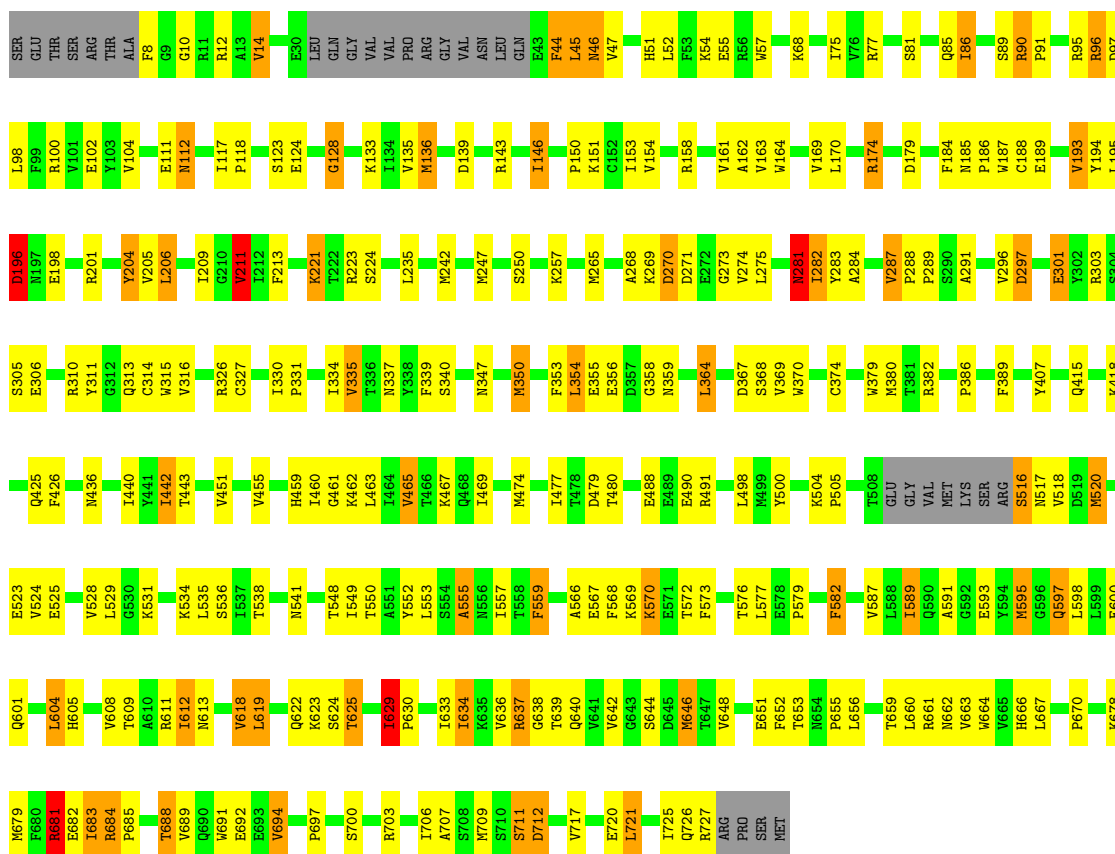
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

- Molecule 3 is water.

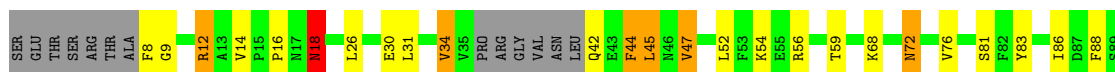
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total	O	0	0
			437	437		
3	B	564	Total	O	0	0
			564	564		

Note EDS was not executed.

Chain A: 58% 30% 7% . .



Chain B: 62% 28% 5% . .





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.17Å 70.76Å 133.82Å 90.00° 106.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.9 (20.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.227 , 0.313	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12297	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: CA

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	1.01	9/5760 (0.2%)	1.26	59/7817 (0.8%)
1	B	1.05	8/5800 (0.1%)	1.27	47/7871 (0.6%)
All	All	1.03	17/11560 (0.1%)	1.27	106/15688 (0.7%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	VAL	CA-CB	8.86	1.61	1.54
1	B	387	VAL	CA-CB	7.05	1.61	1.54
1	A	629	ILE	CA-CB	6.89	1.63	1.54
1	B	629	ILE	CA-CB	6.71	1.60	1.53
1	B	47	VAL	CA-CB	6.46	1.62	1.54

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	LEU	N-CA-C	-11.68	91.74	110.32
1	B	382	ARG	CA-C-N	9.47	129.12	119.56
1	B	382	ARG	C-N-CA	9.47	129.12	119.56
1	B	314	CYS	N-CA-C	9.22	122.17	111.11
1	B	196	ASP	N-CA-C	9.10	126.30	111.37

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	5627	0	5478	170	0
1	B	5667	0	5512	159	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	437	0	0	14	0
3	B	564	0	0	14	0
All	All	12297	0	10990	320	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 14.

The worst 5 of 320 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:331:PRO:HG2	1:A:379:TRP:HB3	1.26	1.13
1:A:633:ILE:HB	1:A:651:GLU:HB3	1.51	0.89
1:B:44:PHE:O	1:B:45:LEU:HB2	1.74	0.86
1:A:520:MET:HB2	1:A:619:LEU:HD13	1.59	0.83
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.44	0.82

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	695/731 (95%)	644 (93%)	44 (6%)	7 (1%)	12	9
1	B	701/731 (96%)	662 (94%)	34 (5%)	5 (1%)	18	15
All	All	1396/1462 (96%)	1306 (94%)	78 (6%)	12 (1%)	14	10

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	B	45	LEU
1	A	281	ASN
1	A	270	ASP
1	A	196	ASP

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	618/644 (96%)	563 (91%)	55 (9%)	9	6
1	B	621/644 (96%)	561 (90%)	60 (10%)	8	5
All	All	1239/1288 (96%)	1124 (91%)	115 (9%)	8	6

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	18	ASN
1	B	650	VAL
1	B	176	PRO
1	B	639	THR
1	B	557	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	GLN
1	B	613	ASN
1	B	126	GLN
1	B	484	GLN
1	B	112	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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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

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.