



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:24 am BST

PDB ID : 1FIE
Title : RECOMBINANT HUMAN COAGULATION FACTOR XIII
Authors : Yee, V.C.; Teller, D.C.
Deposited on : 1996-08-24
Resolution : 2.50 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

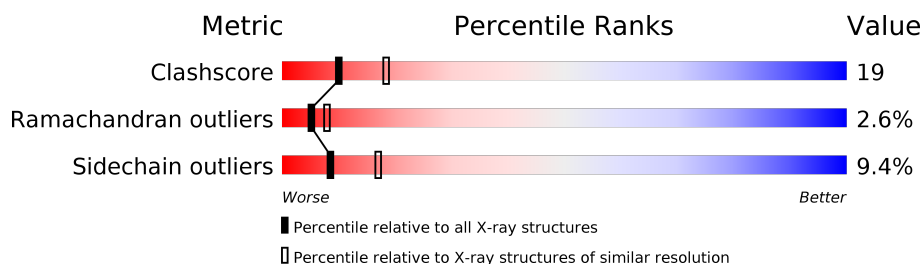
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11928 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	705	Total	C	N	O	S	0	0	0
			5651	3584	976	1064	27			
1	B	715	Total	C	N	O	S	0	0	0
			5720	3626	986	1081	27			

- Molecule 2 is water.

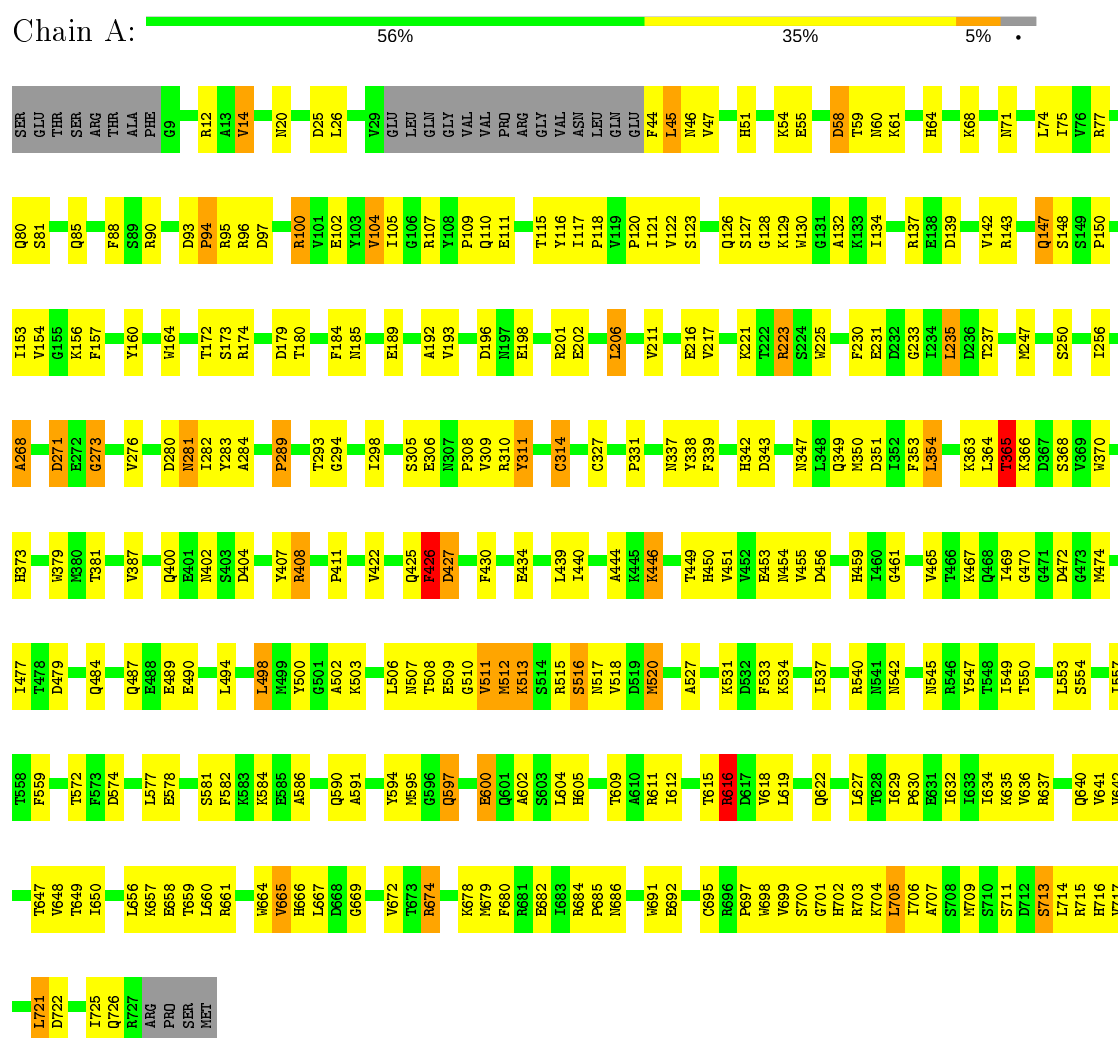
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	270	Total	O	0	0
			270	270		
2	B	287	Total	O	0	0
			287	287		

3 Residue-property plots

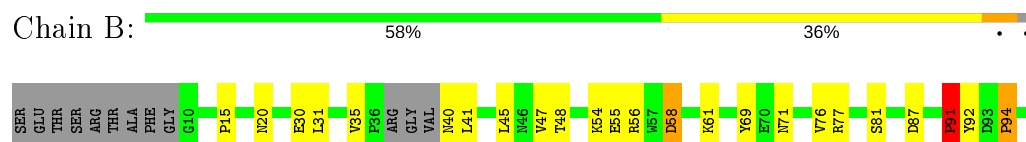
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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



V665	G596	D519	K418	G312	M197	Y108
R666	Q597	M520	F424	A318	N197	N112
L667	L598	D521	Q425	A318	R201	K113
P670	L599	F522	F426	N322	L206	G114
T673	G601	E523	D427	R326	I209	T115
	A602	E525	A428	I330	G210	Y116
R678	S603	M526	P429	P331	V211	P120
	L604	A527	F430	V335	V122	I121
R681	H605	V528	V431	V335	Y214	V122
E682	F606	L529	E434	F339	Y217	S123
I683	T609	G530	V435	S340	K221	Q126
R684	A610	K531	Y441	A341	R223	S127
P685	E611	F533	I442	H342	S224	G128
S686	M612	M534	K446	L354	W225	W130
T688	N613	L535	V452	E355	S226	G131
V689	G614	T538	E453	E356	Y227	A132
Q690	T615	F539	V455	N361	L235	I134
W691	R616	R540	I460	L364	E137	R137
E692	D617	M541	L463	E365	E138	E138
E693	V618	N542	I464	R366	D139	D139
V694	L619	S543	V465	R370	S141	S141
C695	Q622	H544	L466	W371	I146	I146
R696	K623	M545	I467	Y372	Q147	Q147
P697	V626	R546	K467	H373	S148	S148
R703	I629	I549	G470	C374	S149	S149
S708	L632	T550	D471	E377	P150	P150
W709	I633	A551	D472	A378	I153	I153
S710	I634	F552	G473	W379	R158	R158
S713	K635	S554	M474	M380	W164	W164
V717	V636	I557	E485	T381	Y167	Y167
	R637	T558	Q487	R382	G168	G168
L721	G638	F559	E488	D396	R171	R171
D722	T639	Y560	E489	S397	T172	T172
V723	Q640	K565	E490	T398	S173	S173
Q724	G643	V575	R491	P399	R174	R174
I725	S644	L577	L494	Q400	M175	M175
Q726	D645	L577	N507	M406	D179	D179
R727	R646	E578	T508	Y407	T180	T180
ARG	T647	P579	F581	R408	Y181	Y181
PRO	I650	L580	F582	C409	M185	M185
SER	T653	K581	K583	G410	P186	P186
MET	M654	K584	G510	P411	W187	W187
	L656	L588	V511	A416	V193	V193
	K657	I589	R512	I417	Y194	Y194
	E658	Q590	K513			
	T659	A591	S514			
	L660	Y594	R515			
	R661	M595	S516			
	N662		N517			

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	101.10 Å 73.13 Å 134.70 Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50	Depositor
% Data completeness (in resolution range)	77.0 (10.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/5784	0.83	2/7848 (0.0%)
1	B	0.61	0/5853	0.84	3/7941 (0.0%)
All	All	0.60	0/11637	0.83	5/15789 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	THR	N-CA-C	-7.06	91.95	111.00
1	A	426	PHE	CB-CA-C	5.36	121.13	110.40
1	B	425	GLN	N-CA-C	5.33	125.39	111.00
1	B	518	VAL	N-CA-C	-5.28	96.76	111.00
1	B	460	ILE	N-CA-C	5.21	125.06	111.00

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	5651	0	5518	214	0
1	B	5720	0	5566	216	0
2	A	270	0	0	14	0
2	B	287	0	0	17	0
All	All	11928	0	11084	427	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 19.

The worst 5 of 427 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:538:THR:HG22	1:B:584:LYS:HG3	1.37	1.06
1:B:528:VAL:HB	1:B:531:LYS:HD3	1.44	0.97
1:A:650:ILE:HB	1:A:691:TRP:HB3	1.50	0.90
1:B:509:GLU:HB2	1:B:511:VAL:O	1.76	0.85
1:A:331:PRO:HB2	1:A:379:TRP:HB3	1.59	0.84

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	701/731 (96%)	617 (88%)	63 (9%)	21 (3%)	4	6
1	B	710/731 (97%)	626 (88%)	69 (10%)	15 (2%)	7	11
All	All	1411/1462 (96%)	1243 (88%)	132 (9%)	36 (3%)	5	8

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	511	VAL
1	B	426	PHE
1	B	613	ASN
1	B	616	ARG

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	620/644 (96%)	561 (90%)	59 (10%)	8	17
1	B	626/644 (97%)	568 (91%)	58 (9%)	9	17
All	All	1246/1288 (97%)	1129 (91%)	117 (9%)	8	17

5 of 117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	665	VAL
1	B	98	LEU
1	B	604	LEU
1	A	705	LEU
1	B	20	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	ASN
1	A	726	GLN
1	B	613	ASN
1	A	545	ASN
1	B	662	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.