wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	1FIE
Title	:	RECOMBINANT HUMAN COAGULATION FACTOR XIII
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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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

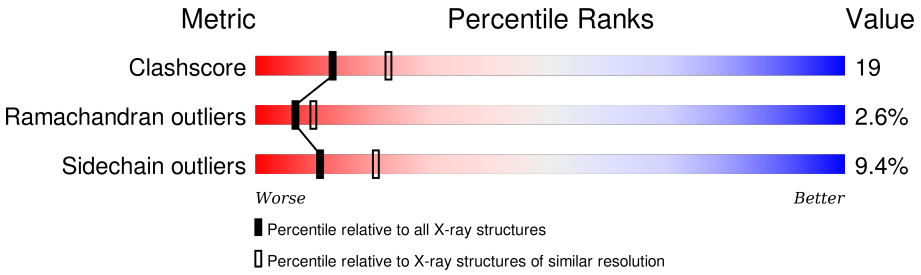
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (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. 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 <=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	56% 35% 5%
1	B	731	58% 36%

2 Entry composition (i)

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		

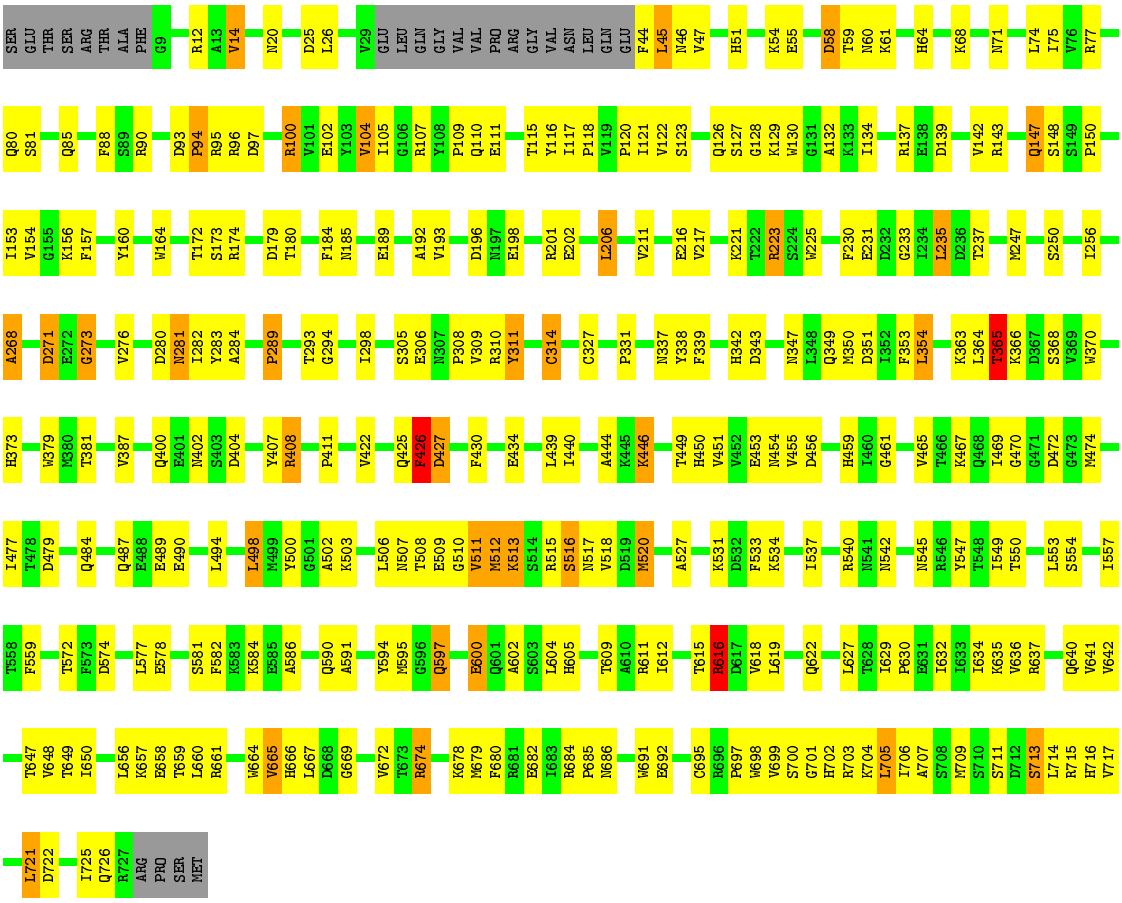
3 Residue-property plots (i)

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.

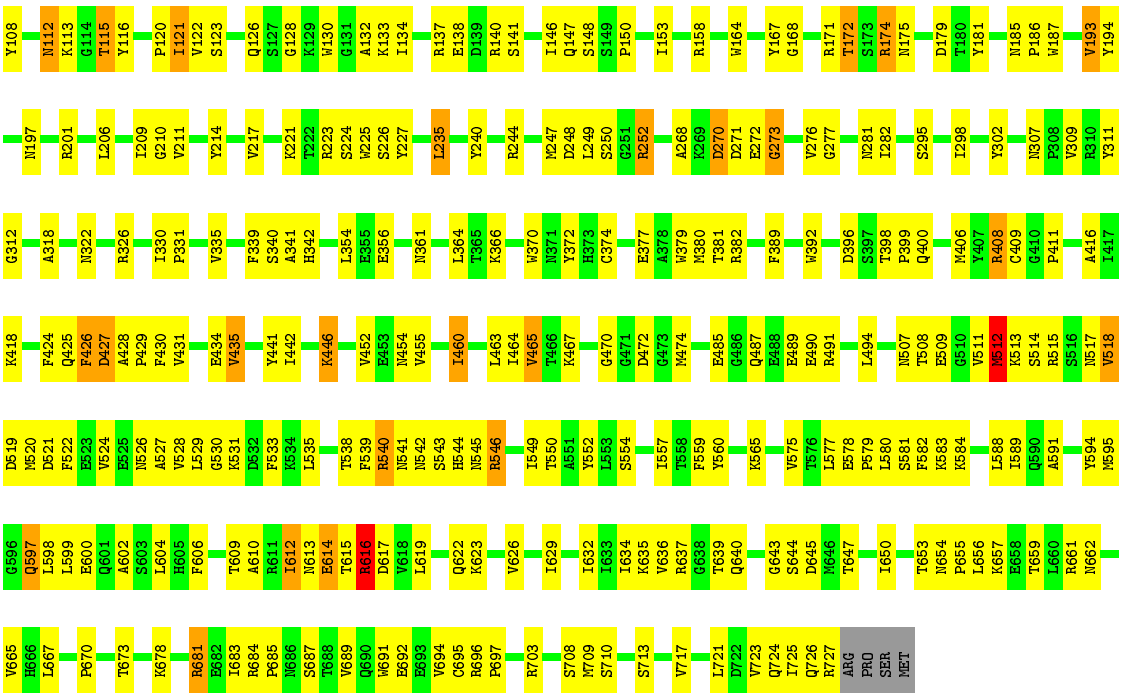
- Molecule 1: COAGULATION FACTOR XIII

Chain A:



- Molecule 1: COAGULATION FACTOR XIII

Chain B:


Y108 N112 K113 G114 T115 Y116 P120 I121 V122 S123 Q126 S127 G128 K129 W130 G131 A132 K133 I134 R137 E138 D139 R140 S141 I146 Q147 S148 S149 P150 I153 R158 W164 Y167 G168 R171 T172 S173 R174 N175 D179 T180 Y181 N185 P186 W187 V193 Y194
N197 R201 L206 I209 G210 V211 Y214 V217 K221 T222 R223 S224 W225 S226 Y227 L235 Y240 R244 M247 D248 L249 S250 G251 R252 A268 K269 D270 D271 E272 G273 V276 G277 N281 I282 S296 I298 Y302 N307 P308 V309 R310 Y311
G312 A318 N322 R326 I330 P331 V335 F339 S340 A341 H342 L354 E355 E356 N361 L364 T365 K366 W370 N371 Y372 H373 C374 E377 A378 W379 M380 T381 R382 F389 W392 D396 S397 T398 P399 Q400 M406 Y407 R408 C409 G410 P411 A416 I417
K418 F424 Q425 F426 D427 A428 P429 F430 V431 E434 V435 Y441 I442 K446 V452 E453 N454 V455 I460 L463 I464 V465 T466 K467 G470 G471 D472 G473 M474 E485 G486 Q487 E488 E489 E490 R491 L494 N507 T508 E509 G510 V511 M512 K513 S514 R515 S516 N517 V518
D519 M520 D521 F522 E523 V524 E525 N526 A527 V528 L529 G530 K531 D532 F533 K534 L535 T538 F539 R540 N541 N542 S543 H544 N545 R546 I549 T550 A551 Y552 L553 S554 I557 T558 F559 Y560 K565 V575 T576 L577 E578 P579 L580 S581 F582 K583 K584 L588 I589 Q590 A591 Y594 M595
G596 Q597 L598 L599 E600 Q601 A602 S603 L604 H605 F606 T609 A610 R611 I612 N613 E614 T615 R616 D617 V618 L619 Q622 K623 V626 I629 I632 I633 I634 K635 V636 R637 G638 T639 Q640 G643 S644 D645 M646 T647 I650 T653 N654 P655 L656 K657 E658 T659 L660 R661 N662
V665 H666 L667 P670 T673 K678 R681 E682 I683 R684 P685 N686 S687 T688 V689 Q690 W691 E692 E693 V694 C695 R696 P697 R703 S708 M709 S710 S713 V717 L721 D722 V723 Q724 I725 Q726 R727 ARG PRO SER MET

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.10Å 73.13Å 134.70Å 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

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	0.58	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(^{o})	Ideal(^{o})
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

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%)	5 7
1	B	710/731 (97%)	626 (88%)	69 (10%)	15 (2%)	9 14
All	All	1411/1462 (96%)	1243 (88%)	132 (9%)	36 (3%)	7 10

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 (i)

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%)	11	20
1	B	626/644 (97%)	568 (91%)	58 (9%)	11	21
All	All	1246/1288 (97%)	1129 (91%)	117 (9%)	11	20

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 (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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.