



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1QRK
Title : HUMAN FACTOR XIII WITH STRONTIUM BOUND IN THE ION SITE
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Deposited on : 1999-06-14
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 ⓘ 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

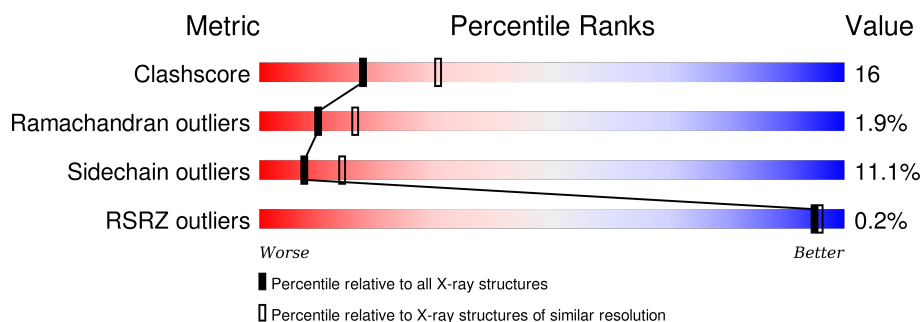
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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)
RSRZ outliers	91569	3562 (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 $\leq 5\%$. 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.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SR	A	732	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11492 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	700	Total	C	N	O	S	0	0	0
			5610	3557	966	1061	26			
1	B	705	Total	C	N	O	S	0	0	0
			5650	3583	973	1068	26			

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

- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

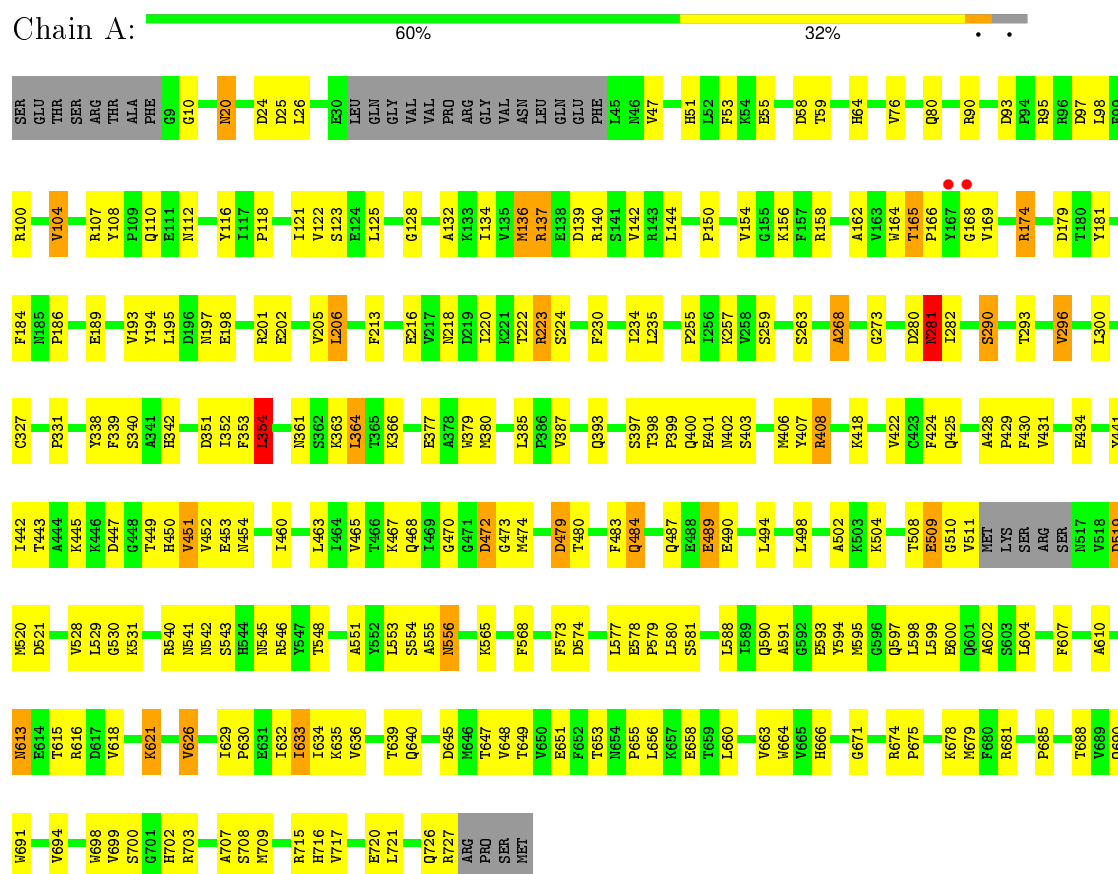
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	115	Total	O	0	0
			115	115		

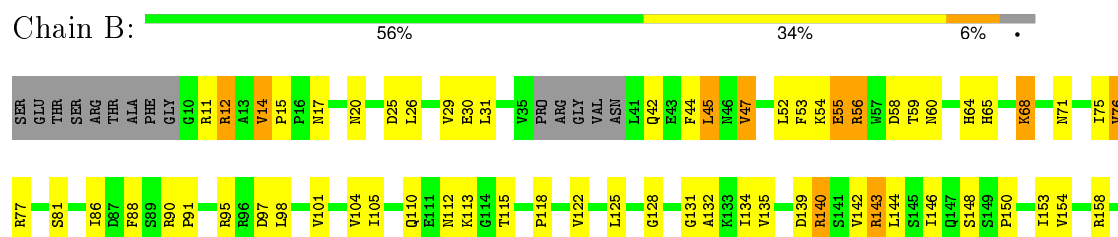
3 Residue-property plots

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.

• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



• Molecule 1: PROTEIN (COAGULATION FACTOR XIII)



D722	T639	I549	M474	K392	D271	V161
V723	Q640	Y552	I477	S397	E272	T165
Q724	V641	Y552	Q484	T398	L275	G168
I725	V642	A555	Q484	P399	M281	V169
Q726	G643	N556	Q487	Q400	P289	L170
R727	G643	I557	E488	E401	D297	A171
ARG	M646	T561	E489	M402	D404	T172
PRO	T647	Q565	E490	R491	G405	S173
SER	T647	K565	R491	L492	G405	R174
MET	T647	K565	L492	Y407	L300	
	T653	F568	E495	R408	E301	I182
	N654	K569	L498	C409	S305	L183
	P655	D574	L498	G410	E306	F184
	L656	L577	A502	P411	V309	W187
	R657	E578	P505	Q415	R310	C188
	T659	F579	L506	V422	Y311	E189
	L660	L580	N507	Q425	R326	A192
	R661	F581	THR	F426	C327	V193
	W664	F582	GLU	D427	I330	E198
	V665	K583	GLY	A428	T336	E202
	H666	K584	VAL	P429	N337	L206
	L667	E585	MET	F430	Y338	
	M676	L588	I589	V431	F339	V211
	M679	Q590	ARG	E434	S340	T212
	E682	A591	S516	V435	A341	F213
	T683	Y594	N517	R436	R342	
	R684	L599	V518	D437	N344	E216
	P685	E600	D520	D438	E217	
	N686	S603	M521	L439	N218	
	E693	L604	F522	I440	D219	
	V694	T609	E523	Y441	T220	
	C695	L604	V524	I442	K221	
	R696	W609	E525	T443	M350	
	P697	A610	N526	A444	L354	
	W698	R611	A527	K445	E355	
	V699	I612	W528	K446	E356	
	S700	M613	L529	V451	F230	
	R703	R616	F533	V452	N360	
	K704	D617	K534		L235	
	L705	V618	L535	V455	S362	
	I706	L619	S536	D456	K363	
	A707	A620	I537	H459	K366	
	S708	K621	T538	I460	W370	
	W709	T625	N541	G461	K260	
	S713	T625	M541	K462	Y261	
	L714	I632	S543	L463	E377	
	R715	I633	H544	I464	M380	
	H716	I634	N545	V465	T381	
	W717	K635	R546	T466	K269	
	E720	L721	Y547	K467	R382	
			T548		D270	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.90Å 72.32Å 135.03Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 72.32 – 2.20	Depositor EDS
% Data completeness (in resolution range)	78.5 (10.00-2.50) 62.6 (72.32-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , 0.275 0.182 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 60194 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11492	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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: SR

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	0.56	0/5741	0.79	1/7792 (0.0%)
1	B	0.60	0/5782	0.81	3/7847 (0.0%)
All	All	0.58	0/11523	0.80	4/15639 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	CA-CB-CG	5.76	128.56	115.30
1	B	170	LEU	N-CA-C	-5.73	95.53	111.00
1	B	588	LEU	CA-CB-CG	5.51	127.97	115.30
1	B	26	LEU	CA-CB-CG	5.05	126.91	115.30

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	5610	0	5467	166	0
1	B	5650	0	5495	189	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	115	0	0	4	0
All	All	11492	0	10962	353	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 16.

The worst 5 of 353 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	1.46	0.97
1:B:544:HIS:HA	1:B:579:PRO:HB3	1.52	0.90
1:B:44:PHE:O	1:B:45:LEU:HB2	1.73	0.87
1:A:709:MET:HB3	1:A:717:VAL:HB	1.58	0.85
1:B:591:ALA:HA	1:B:594:TYR:CE2	2.15	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	694/731 (95%)	631 (91%)	52 (8%)	11 (2%)	12	21
1	B	699/731 (96%)	613 (88%)	71 (10%)	15 (2%)	9	14
All	All	1393/1462 (95%)	1244 (89%)	123 (9%)	26 (2%)	10	16

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLU
1	A	281	ASN
1	B	45	LEU

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Mol	Chain	Res	Type
1	B	53	PHE
1	B	55	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	616/644 (96%)	559 (91%)	57 (9%)	11	21
1	B	619/644 (96%)	539 (87%)	80 (13%)	5	10
All	All	1235/1288 (96%)	1098 (89%)	137 (11%)	8	14

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	47	VAL
1	B	193	VAL
1	B	617	ASP
1	B	59	THR
1	B	140	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	726	GLN
1	B	46	ASN
1	B	468	GLN
1	A	686	ASN
1	A	716	HIS

5.3.3 RNA ⓘ

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](#)

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	700/731 (95%)	-0.69	2 (0%) 94 95	8, 31, 66, 83	0
1	B	705/731 (96%)	-0.68	1 (0%) 95 96	4, 28, 71, 85	0
All	All	1405/1462 (96%)	-0.68	3 (0%) 95 96	4, 29, 68, 85	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	LEU	2.9
1	A	168	GLY	2.6
1	A	167	TYR	2.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SR	A	732	1/1	0.99	0.17	2.07	51,51,51,51	0
2	SR	B	732	1/1	0.99	0.14	0.58	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.