



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 19, 2024 – 01:02 pm GMT

PDB ID : 8OS5  
Title : Crystal structure of the Factor XII heavy chain reveals an interlocking dimer with a FnII to kringle domain interaction  
Authors : Li, C.; Saleem, M.; Kaira, B.G.; Brown, A.; Wilson, C.; Philippou, H.; Emsley, J.  
Deposited on : 2023-04-18  
Resolution : 3.40 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](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

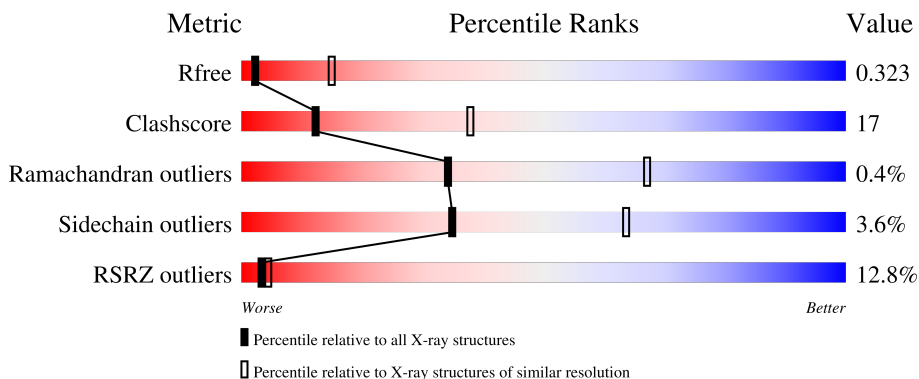
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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))
$R_{free}$	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	295	
1	B	295	
1	C	295	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5690 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.

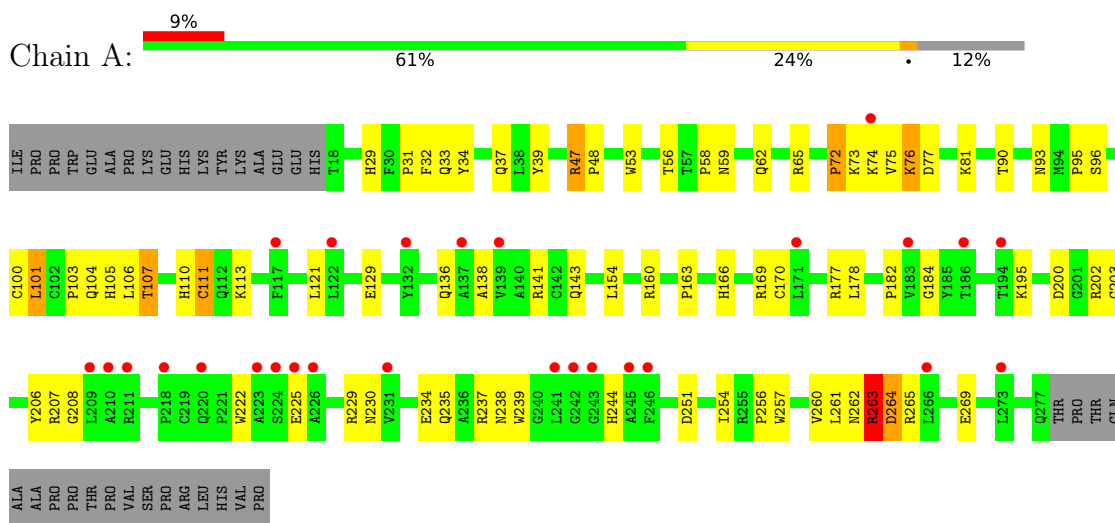
- Molecule 1 is a protein called Coagulation factor XII-Mie.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	Total 2063	C 1278	N 393	O 365	S 27	2	0	0
1	B	201	Total 1573	C 963	N 304	O 283	S 23	1	0	0
1	C	259	Total 2054	C 1273	N 391	O 363	S 27	3	0	0

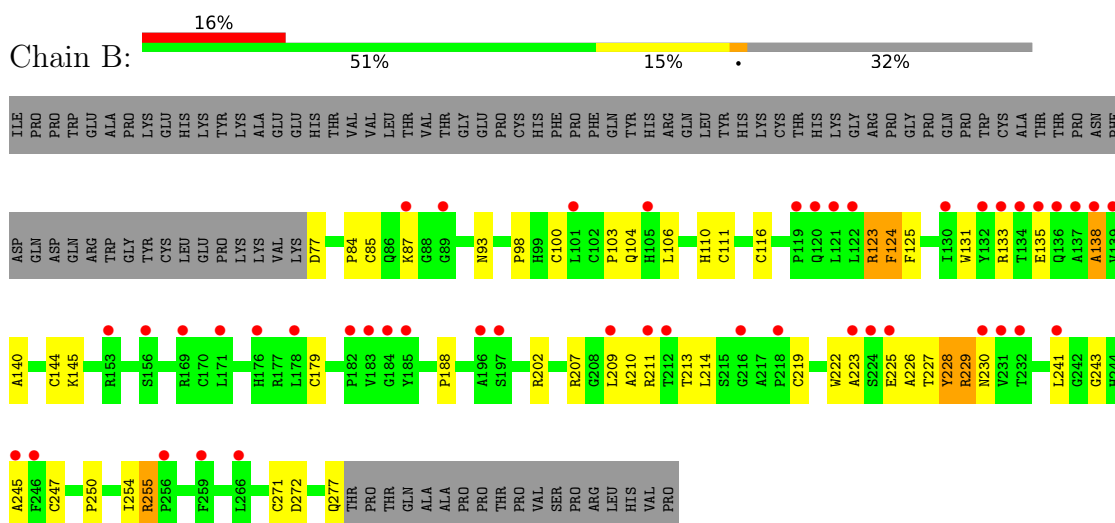
### 3 Residue-property plots i

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 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: Coagulation factor XII-Mie

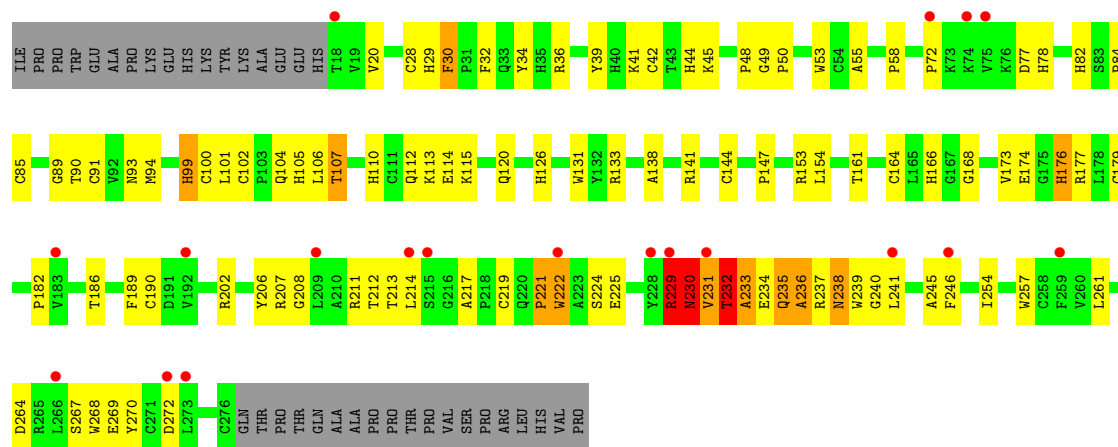


- Molecule 1: Coagulation factor XII-Mie



- Molecule 1: Coagulation factor XII-Mie





## 4 Data and refinement statistics i

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.54Å 144.59Å 155.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.97 – 3.40 77.97 – 3.39	Depositor EDS
% Data completeness (in resolution range)	61.2 (77.97-3.40) 61.0 (77.97-3.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 3.41Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.255 , 0.319 0.271 , 0.323	Depositor DCC
$R_{free}$ test set	1416 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	118.9	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.074 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	5690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	117.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 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	0.62	0/2129	0.98	4/2891 (0.1%)
1	B	0.55	0/1618	0.95	6/2193 (0.3%)
1	C	0.67	0/2120	1.01	9/2879 (0.3%)
All	All	0.62	0/5867	0.98	19/7963 (0.2%)

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	4
1	B	0	4
1	C	0	3
All	All	0	11

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PRO	N-CA-C	-6.97	93.98	112.10
1	C	236	ALA	CB-CA-C	6.74	120.21	110.10
1	C	230	ASN	N-CA-C	-6.60	93.19	111.00
1	A	138	ALA	N-CA-CB	6.17	118.74	110.10
1	C	238	ASN	N-CA-CB	5.95	121.31	110.60

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	263	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	47	ARG	Sidechain
1	A	65	ARG	Sidechain
1	B	123	ARG	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	2063	0	1917	59	0
1	B	1573	0	1452	38	0
1	C	2054	0	1909	89	0
All	All	5690	0	5278	186	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 17.

The worst 5 of 186 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:C:231:VAL:HA	1:C:235:GLN:HE22	1.20	1.01
1:C:231:VAL:HA	1:C:235:GLN:NE2	1.79	0.96
1:A:29:HIS:CE1	1:A:58:PRO:HG3	2.05	0.92
1:C:36:ARG:HH11	1:C:36:ARG:HG2	1.37	0.89
1:C:106:LEU:HA	1:C:113:LYS:O	1.75	0.86

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	258/295 (88%)	239 (93%)	18 (7%)	1 (0%)	34	67
1	B	199/295 (68%)	182 (92%)	16 (8%)	1 (0%)	29	61
1	C	257/295 (87%)	233 (91%)	23 (9%)	1 (0%)	34	67
All	All	714/885 (81%)	654 (92%)	57 (8%)	3 (0%)	34	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	72	PRO
1	A	72	PRO
1	B	103	PRO

### 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	223/254 (88%)	214 (96%)	9 (4%)	31	60
1	B	169/254 (66%)	168 (99%)	1 (1%)	86	94
1	C	222/254 (87%)	210 (95%)	12 (5%)	22	52
All	All	614/762 (81%)	592 (96%)	22 (4%)	35	63

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	221	PRO
1	C	230	ASN
1	C	229	ARG
1	C	231	VAL
1	A	200	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	HIS
1	C	99	HIS

### 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 monosaccharides 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](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	260/295 (88%)	0.71	27 (10%) 6 8	76, 108, 146, 168	2 (0%)
1	B	201/295 (68%)	1.10	46 (22%) 0 1	105, 133, 158, 167	0
1	C	259/295 (87%)	0.55	19 (7%) 15 17	81, 110, 142, 162	1 (0%)
All	All	720/885 (81%)	0.76	92 (12%) 3 4	76, 116, 153, 168	3 (0%)

The worst 5 of 92 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	74	LYS	9.8
1	B	138	ALA	9.3
1	B	223	ALA	8.0
1	B	225	GLU	7.5
1	B	137	ALA	5.8

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.