wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 9, 2024 – 04:05 PM EST

PDB ID	:	1OAK
Title	:	CRYSTAL STRUCTURE OF THE VON WILLEBRAND FACTOR (VWF) A1 DOMAIN IN COMPLEX WITH THE FUNCTION BLOCKING NMC-4 FAB
Authors	:	Celikel, R.; Varughese, K.I.
Deposited on	:	1997-12-18
Resolution	:	2.20 Å(reported)

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

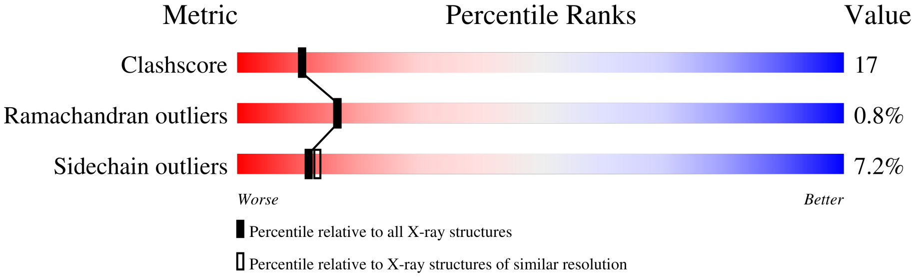
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.20 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	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	212	
2	H	223	
3	A	196	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5240 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 NMC-4 IGG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	212	1650	1029	274	341	6	0	0	0

- Molecule 2 is a protein called NMC-4 IGG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	1648	1040	268	333	7	0	0	0

- Molecule 3 is a protein called VON WILLEBRAND FACTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	196	1576	1004	279	286	7	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	115	115	115	0	0
			Total	O		
4	H	137	137	137	0	0
			Total	O		
4	A	114	114	114	0	0

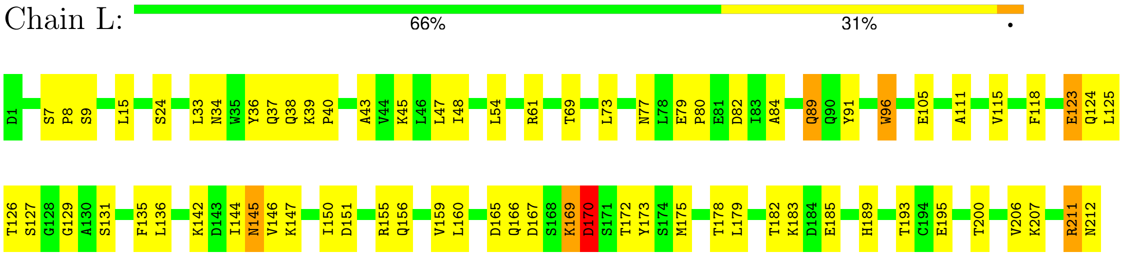
3 Residue-property plots ⓘ

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. 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.

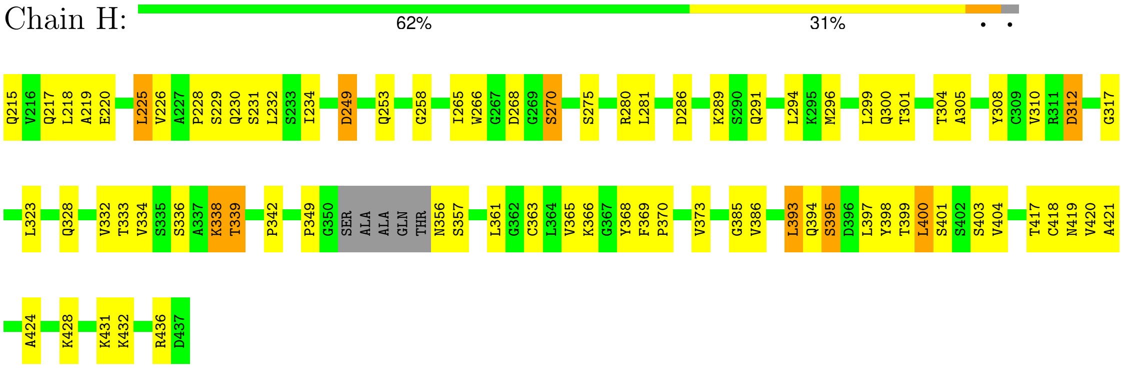
- Molecule 1: NMC-4 IGG1

Chain L:



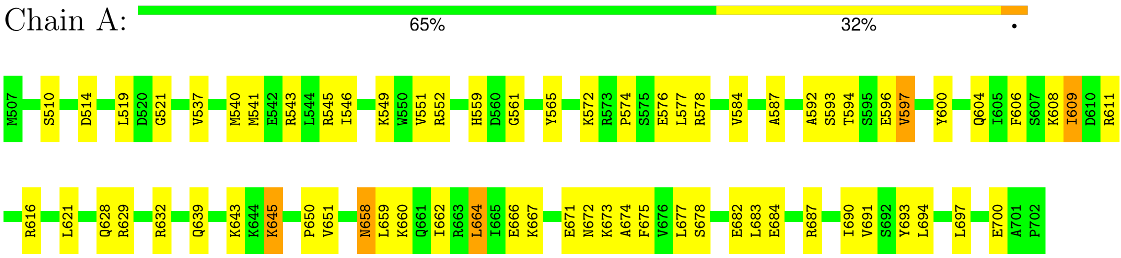
- Molecule 2: NMC-4 IGG1

Chain H:



- Molecule 3: VON WILLEBRAND FACTOR

Chain A:



4 Data and refinement statistics ⓘ

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.20Å 61.90Å 72.90Å 90.00° 108.60° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	99.0 (50.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.201 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5240	wwPDB-VP
Average B, all atoms (Å^2)	37.0	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	L	0.36	0/1688	0.65	0/2292
2	H	0.39	0/1691	0.68	0/2315
3	A	0.40	0/1602	0.63	0/2155
All	All	0.38	0/4981	0.65	0/6762

There are no bond length outliers.

There are no bond angle outliers.

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	L	1650	0	1575	51	0
2	H	1648	0	1591	67	0
3	A	1576	0	1632	48	0
4	A	114	0	0	5	1
4	H	137	0	0	2	0
4	L	115	0	0	1	0
All	All	5240	0	4798	160	1

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 160 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)
2:H:338:LYS:H	2:H:338:LYS:HD2	1.04	1.13
2:H:338:LYS:HD2	2:H:338:LYS:N	1.78	0.96
1:L:169:LYS:O	1:L:170:ASP:HB3	1.68	0.90
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.54	0.87
2:H:394:GLN:HG3	2:H:399:THR:OG1	1.79	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:916:HOH:O	4:A:916:HOH:O[2_657]	2.07	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	L	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	25	28
2	H	214/223 (96%)	199 (93%)	12 (6%)	3 (1%)	9	7
3	A	194/196 (99%)	182 (94%)	11 (6%)	1 (0%)	25	28
All	All	618/631 (98%)	578 (94%)	35 (6%)	5 (1%)	16	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	170	ASP
2	H	339	THR
2	H	349	PRO
2	H	395	SER
3	A	658	ASN

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	L	190/190 (100%)	176 (93%)	14 (7%)	11	12
2	H	190/193 (98%)	174 (92%)	16 (8%)	9	9
3	A	174/174 (100%)	164 (94%)	10 (6%)	17	21
All	All	554/557 (100%)	514 (93%)	40 (7%)	12	13

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	418	CYS
3	A	611	ARG
2	H	419	ASN
3	A	597	VAL
3	A	645	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	A	590	GLN
3	A	625	GLN
1	L	156	GLN
2	H	328	GLN
2	H	356	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 ⓘ

There are no oligosaccharides 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 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.