



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U0N
Title : The ternary von Willebrand Factor A1-glycoprotein Ibalphabotrocetin complex
Authors : Fukuda, K.; Liddington, R.C.
Deposited on : 2004-07-13
Resolution : 2.95 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) : **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

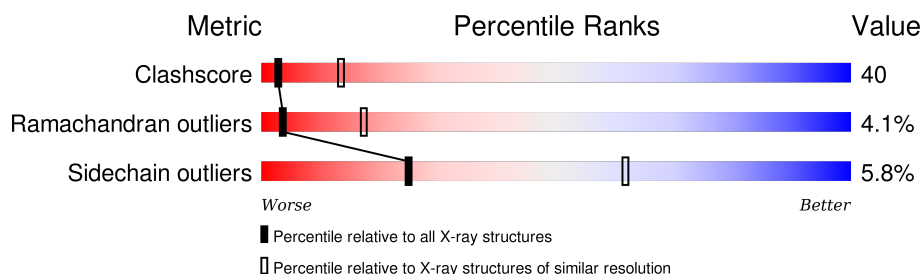
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	208	
2	B	133	
3	C	125	
4	D	265	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5864 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 Von Willebrand factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	1
			1664	1062	293	303	6			

- Molecule 2 is a protein called Botrocetin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1066	679	175	204	8			

- Molecule 3 is a protein called Botrocetin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			1060	682	166	202	10			

- Molecule 4 is a protein called Platelet glycoprotein Ib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	265	Total	C	N	O	S	0	0	0
			2074	1334	344	387	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	21	GLN	ASN	ENGINEERED	UNP P07359
D	159	GLN	ASN	ENGINEERED	UNP P07359

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.

Note EDS was not executed.

• Molecule 1: Von Willebrand factor



H1	K69	T138	I213
P2	L70	L139	F216
I3	Q71	P140	R217
C4	V72	L143	L220
E5	D73	L144	Q221
V6	G74	T145	D222
S7	T75	P146	N223
K8	V78	L150	N226
V9	L79	E151	V227
H12	G80	K152	W230
L13	T81	L153	K231
E14	L82	S154	Q232
V15	D83	L155	G233
M16	L84	A156	V234
C17	S85	N157	D235
D18	H86	N158	V236
K19	L89	Q159	K237
R20	L92	L160	A238
Q21	P93	T161	N239
L22	L94	P164	V243
L25	L95	A165	A244
P26	L96	G166	S245
L29	T98	L167	V246
P30	L99	L168	Q247
T34	P100	E172	C248
I35	A101	N173	D249
L38	L102	L174	N250
S39	T103	D175	S251
L42	V104	T176	D252
L43	L105	L177	K253
Y44	V107	L178	F254
L47	R111	L179	P255
S47	L115	Q180	V256
L48	P116	E181	Y259
A49	L117	N182	P260
T50	G118	S183	Q261
L51	A119	F192	K262
P52	L120	G193	P265
P53	A121	S194	
V54	H195	L196	
T55	G122	L197	
B56	L123	P198	
L57	G124	F199	
T58	E125	A200	
Q59	L126	L202	
L60	Q127	E203	
B61	E128	W207	
L62	L129	L208	
L63	Y130	C209	
D63	L131	N210	
B64	K132	C211	
G65	L136	E212	
B66	L137		
L67			
T68			

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	108.31Å 108.31Å 221.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.95	Depositor
% Data completeness (in resolution range)	94.5 (6.00-2.95)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.213 , 0.276	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5864	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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	0.41	0/1696	0.68	0/2290
2	B	0.41	0/1094	0.66	0/1476
3	C	0.38	0/1098	0.56	1/1490 (0.1%)
4	D	0.36	0/2121	0.67	0/2895
All	All	0.39	0/6009	0.65	1/8151 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2067	GLY	N-CA-C	5.29	126.32	113.10

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	1664	0	1708	152	0
2	B	1066	0	1009	82	0
3	C	1060	0	937	96	0
4	D	2074	0	2112	191	0
All	All	5864	0	5766	461	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 40.

The worst 5 of 461 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)
4:D:75:THR:HA	4:D:98:THR:HG23	1.43	1.01
4:D:47:SER:HA	4:D:71:GLN:HB2	1.39	1.00
2:B:1074:GLU:HB2	3:C:2078:GLU:HG2	1.42	1.00
4:D:232:GLN:NE2	4:D:233:GLY:H	1.59	0.99
4:D:232:GLN:HE21	4:D:233:GLY:N	1.60	0.99

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	206/208 (99%)	183 (89%)	19 (9%)	4 (2%)	10	40
2	B	131/133 (98%)	107 (82%)	18 (14%)	6 (5%)	3	15
3	C	123/125 (98%)	94 (76%)	20 (16%)	9 (7%)	1	5
4	D	263/265 (99%)	216 (82%)	36 (14%)	11 (4%)	3	17
All	All	723/731 (99%)	600 (83%)	93 (13%)	30 (4%)	3	17

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1061	GLN
3	C	2055	THR
3	C	2057	GLU
3	C	2067	GLY
4	D	43	LEU

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	185/186 (100%)	174 (94%)	11 (6%)	24	61
2	B	118/119 (99%)	108 (92%)	10 (8%)	13	42
3	C	114/114 (100%)	111 (97%)	3 (3%)	54	84
4	D	238/238 (100%)	224 (94%)	14 (6%)	24	61
All	All	655/657 (100%)	617 (94%)	38 (6%)	25	62

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1083	GLU
3	C	2081	ASP
4	D	232	GLN
2	B	1099	THR
3	C	2093	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	1075	ASN
2	B	1094	ASN
4	D	86	HIS
2	B	1061	GLN
4	D	159	GLN

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 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 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.