wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VL5
Title	:	STRUCTURE OF ANTI-COLLAGEN TYPE II FAB CIIC1
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Deposited on	:	2008-01-08
Resolution	:	2.10 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 (1)) were used in the production of this report:

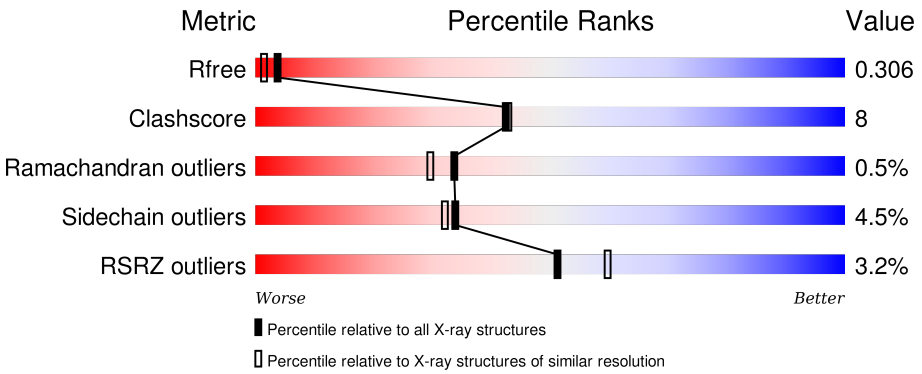
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	218	3% 83% 16% •
1	C	218	2% 81% 15% •
2	B	218	4% 82% 15% •
2	D	218	4% 79% 19% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7164 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 CIIC1 ANTICOLLAGEN FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	218	1646	1044	270	324	8	0	0	0
1	C	218	1646	1044	270	324	8	0	0	0

- Molecule 2 is a protein called CIIC1 ANTICOLLAGEN FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	217	1683	1045	285	347	6	0	0	0
2	D	216	1667	1036	281	344	6	0	0	0

- Molecule 3 is water.

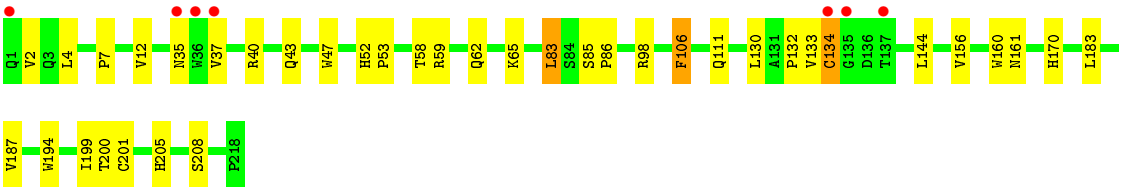
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	117	117	117	0	0
3	B	124	124	124	0	0
3	C	136	136	136	0	0
3	D	145	145	145	0	0

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.

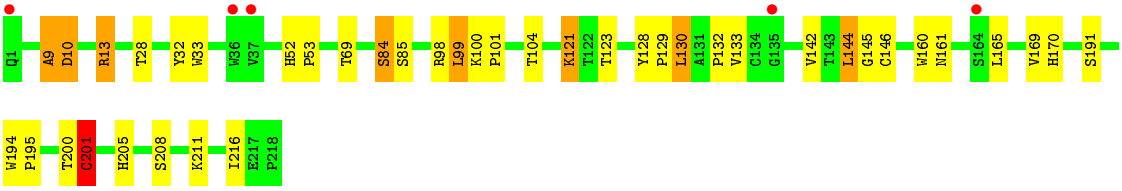
- Molecule 1: CIIC1 ANTICOLLAGEN FAB

Chain A:



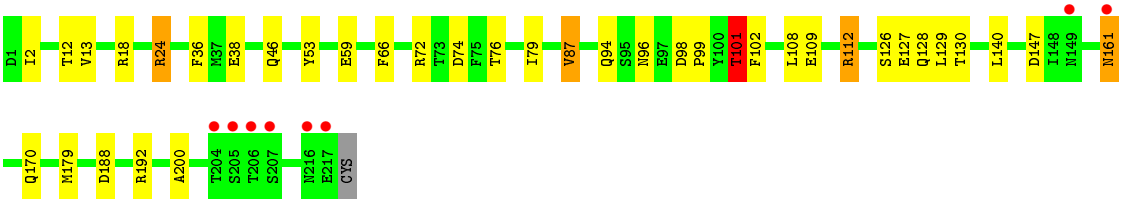
- Molecule 1: CIIC1 ANTICOLLAGEN FAB

Chain C:



- Molecule 2: CIIC1 ANTICOLLAGEN FAB

Chain B:



- Molecule 2: CIIC1 ANTICOLLAGEN FAB

Chain D:

I154
D155
R159
Q160
L164
M179
S180
T186
H193
T197
K203
T206
S207
N214
R215
N216
GLU
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	60.60Å 78.00Å 99.50Å 90.00° 83.10° 90.00°	Depositor
Resolution (Å)	24.42 – 2.10 24.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.42-2.10) 98.8 (24.42-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.212 , 0.289 0.231 , 0.306	Depositor DCC
R_{free} test set	2659 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	25.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 53177 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7164	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.74	0/1691	0.79	1/2312 (0.0%)
1	C	0.83	1/1691 (0.1%)	0.80	0/2312
2	B	0.72	0/1720	0.82	2/2337 (0.1%)
2	D	0.81	0/1704	0.84	1/2316 (0.0%)
All	All	0.78	1/6806 (0.0%)	0.81	4/9277 (0.0%)

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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	CYS	CB-SG	-7.71	1.69	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	164	LEU	CA-CB-CG	6.90	131.17	115.30
2	B	101	THR	N-CA-CB	-5.16	100.49	110.30
2	B	112	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	83	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	9	ALA	Peptide

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	1646	0	1618	27	0
1	C	1646	0	1618	34	0
2	B	1683	0	1610	26	0
2	D	1667	0	1592	25	0
3	A	117	0	0	7	0
3	B	124	0	0	6	0
3	C	136	0	0	7	0
3	D	145	0	0	5	0
All	All	7164	0	6438	108	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 8.

The worst 5 of 108 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:104:THR:HG22	2:D:54:ARG:HH21	1.17	1.08
2:B:2:ILE:O	2:B:101:THR:HG21	1.67	0.95
2:B:161:ASN:HB2	3:B:2100:HOH:O	1.69	0.93
3:A:2076:HOH:O	2:B:46:GLN:HG2	1.71	0.90
3:A:2039:HOH:O	2:B:102:PHE:CE2	2.25	0.88

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	216/218 (99%)	208 (96%)	8 (4%)	0	100	100
1	C	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
2	B	215/218 (99%)	204 (95%)	9 (4%)	2 (1%)	21	15
2	D	214/218 (98%)	205 (96%)	7 (3%)	2 (1%)	21	15
All	All	861/872 (99%)	826 (96%)	31 (4%)	4 (0%)	34	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	129	LEU
2	B	72	ARG
2	D	72	ARG
2	D	155	ASP

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	188/188 (100%)	179 (95%)	9 (5%)	31	29
1	C	188/188 (100%)	177 (94%)	11 (6%)	24	20
2	B	192/193 (100%)	183 (95%)	9 (5%)	32	30
2	D	190/193 (98%)	185 (97%)	5 (3%)	54	58
All	All	758/762 (100%)	724 (96%)	34 (4%)	34	32

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	147	ASP
1	C	13	ARG
2	D	130	THR
2	B	179	MET
1	A	106	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	214	ASN
1	C	62	GLN
2	D	57	ASN
2	B	194	ASN
2	D	193	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 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 (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	218/218 (100%)	0.35	7 (3%)	51	60	24, 30, 42, 47	1 (0%)
1	C	218/218 (100%)	0.21	5 (2%)	64	70	23, 31, 42, 45	1 (0%)
2	B	217/218 (99%)	0.27	8 (3%)	45	54	24, 31, 38, 49	0
2	D	216/218 (99%)	0.18	8 (3%)	45	54	23, 30, 38, 46	0
All	All	869/872 (99%)	0.25	28 (3%)	51	60	23, 31, 40, 49	2 (0%)

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	216	ASN	5.0
2	B	206	THR	4.6
1	C	135	GLY	3.7
1	A	134	CYS	3.3
1	C	1	GLN	3.2

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.