wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

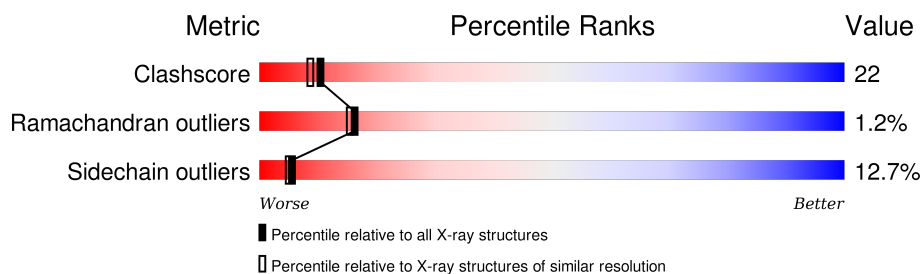|		
PDB ID	:	1DN0
Title	:	STRUCTURE OF THE FAB FRAGMENT FROM A HUMAN IGM COLD AGGLUTININ
Authors	:	Cauerhff, A.; Braden, B.; Carvalho, J.G.; Leoni, J.; Polikarpov, I.; Goldbaum, F.
Deposited on	:	1999-12-15
Resolution	:	2.28 Å(reported)

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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 2.28 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	Percentile Ranks	Value
Clashscore		22
Ramachandran outliers		1.2%
Sidechain outliers		12.7%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	215	59% / 32% / 8% •
1	C	215	65% / 25% / 10%
2	B	232	57% / 25% / 9% • 7%
2	D	232	62% / 24% / 7% 6%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7208 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 IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			
1	C	215	Total	C	N	O	S	0	0	0
			1638	1023	275	335	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	CYS	GLY	CONFLICT	PIR A23746
A	89	CYS	GLY	CONFLICT	PIR A23746
A	215	CYS	GLY	CONFLICT	PIR A23746
C	23	CYS	GLY	CONFLICT	PIR A23746
C	89	CYS	GLY	CONFLICT	PIR A23746
C	215	CYS	GLY	CONFLICT	PIR A23746

- Molecule 2 is a protein called IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1657	1052	279	321	5			
2	D	217	Total	C	N	O	S	0	0	0
			1661	1055	280	320	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLU	-	CONFLICT	PIR B23746
B	200	ALA	GLN	CONFLICT	PIR B23746
D	1	GLU	-	CONFLICT	PIR B23746
D	200	ALA	GLN	CONFLICT	PIR B23746

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	156	Total 156	O 156	0	0
3	C	149	Total 149	O 149	0	0
3	D	146	Total 146	O 146	0	0

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.
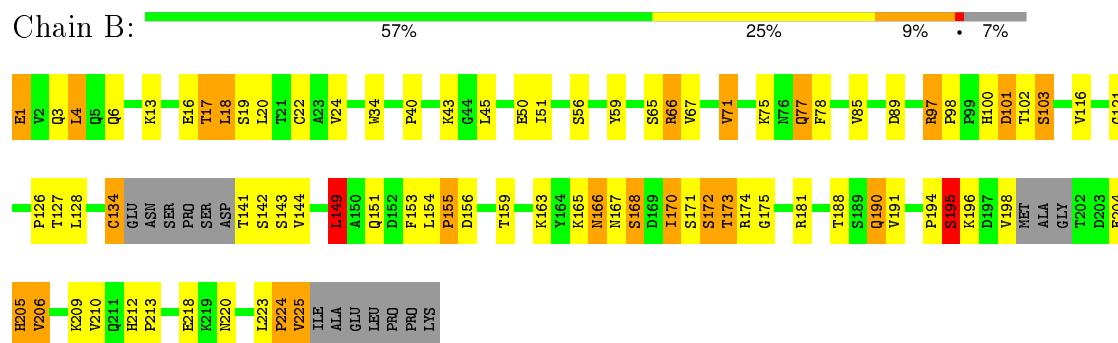
Note EDS was not executed.

- Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)
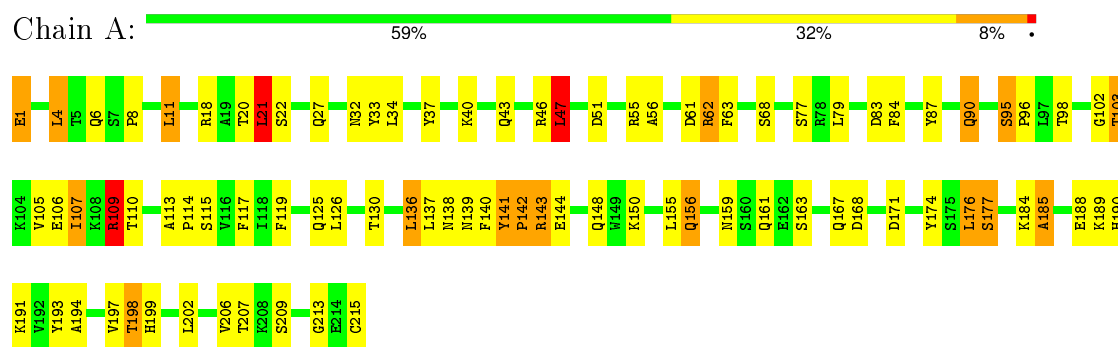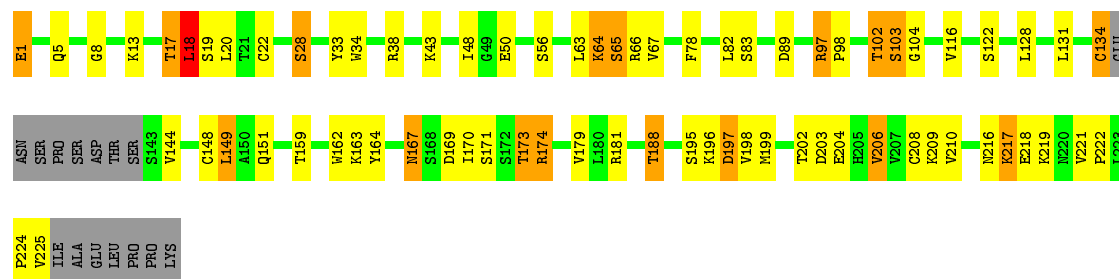

- Molecule 1: IGM-KAPPA COLD AGGLUTININ (LIGHT CHAIN)
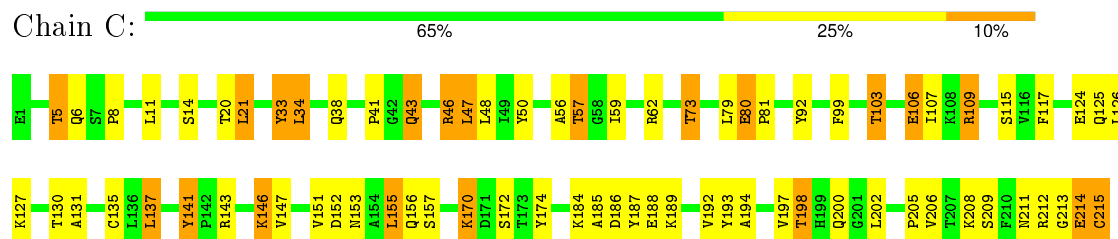
- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)

- Molecule 2: IGM-KAPPA COLD AGGLUTININ (HEAVY CHAIN)

Chain D:

62%   24%   7%   6%

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.88Å 110.88Å 170.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.28	Depositor
% Data completeness (in resolution range)	(Not available) (100.00-2.28)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.180 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7208	wwPDB-VP
Average B, all atoms (Å²)	31.0	wwPDB-VP

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	1.09	0/1673	1.20	14/2273 (0.6%)
1	C	1.12	3/1673 (0.2%)	1.27	11/2273 (0.5%)
2	B	1.05	1/1703 (0.1%)	1.12	8/2325 (0.3%)
2	D	1.10	0/1708	1.09	3/2332 (0.1%)
All	All	1.09	4/6757 (0.1%)	1.17	36/9203 (0.4%)

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	2
1	C	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	VAL	CA-CB	5.71	1.66	1.54
1	C	50	TYR	CE2-CZ	5.63	1.45	1.38
1	C	99	PHE	CE2-CZ	5.33	1.47	1.37
1	C	215	CYS	CB-SG	-5.12	1.73	1.81

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	ARG	NE-CZ-NH2	-16.46	112.07	120.30
1	A	46	ARG	NE-CZ-NH2	-13.63	113.48	120.30
1	C	62	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	C	62	ARG	NE-CZ-NH2	-10.25	115.18	120.30
1	C	46	ARG	NE-CZ-NH1	9.73	125.17	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	141	TYR	Sidechain
1	A	33	TYR	Sidechain
1	C	141	TYR	Sidechain
1	C	33	TYR	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	1638	0	1587	78	0
1	C	1638	0	1587	69	0
2	B	1657	0	1601	72	0
2	D	1661	0	1607	71	0
3	A	163	0	0	12	0
3	B	156	0	0	2	1
3	C	149	0	0	9	0
3	D	146	0	0	6	0
All	All	7208	0	6382	277	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 22.

The worst 5 of 277 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:B:1:GLU:OE1	2:B:1:GLU:N	1.75	1.19
1:C:198:THR:HG22	3:C:2200:HOH:O	1.55	1.04
1:C:215:CYS:HB3	2:D:134:CYS:HB2	1.38	1.04
2:D:1:GLU:N	2:D:1:GLU:OE1	1.91	1.03
2:D:181:ARG:HH11	2:D:181:ARG:HB3	1.32	0.94

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)
3:B:2132:HOH:O	3:B:2132:HOH:O[6_555]	2.17	0.03

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	A	213/215 (99%)	203 (95%)	9 (4%)	1 (0%)	34	39
1	C	213/215 (99%)	199 (93%)	13 (6%)	1 (0%)	34	39
2	B	210/232 (90%)	194 (92%)	12 (6%)	4 (2%)	10	7
2	D	213/232 (92%)	198 (93%)	11 (5%)	4 (2%)	10	7
All	All	849/894 (95%)	794 (94%)	45 (5%)	10 (1%)	16	15

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	172	SER
1	C	214	GLU
2	D	64	LYS
2	D	103	SER
2	D	167	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	A	185/185 (100%)	165 (89%)	20 (11%)	8	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	C	185/185 (100%)	166 (90%)	19 (10%)	9	9	
2	B	187/200 (94%)	158 (84%)	29 (16%)	3	3	
2	D	186/200 (93%)	160 (86%)	26 (14%)	4	3	
All	All	743/770 (96%)	649 (87%)	94 (13%)	5	5	

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	173	THR
1	C	34	LEU
2	D	196	LYS
2	B	190	GLN
2	B	205	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	214	ASN
1	C	43	GLN
2	D	205	HIS
2	B	190	GLN
2	D	151	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.