wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:53 PM GMT

PDB ID	:	1HQ4
Title	:	STRUCTURE OF NATIVE CATALYTIC ANTIBODY HA5-19A4
Authors	:	Paschall, C.M.; Hasserodt, J.; Lerner, R.A.; Janda, K.D.; Christianson, D.W.
Deposited on	:	2000-12-14
Resolution	:	2.70 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 (i)) were used in the production of this report:

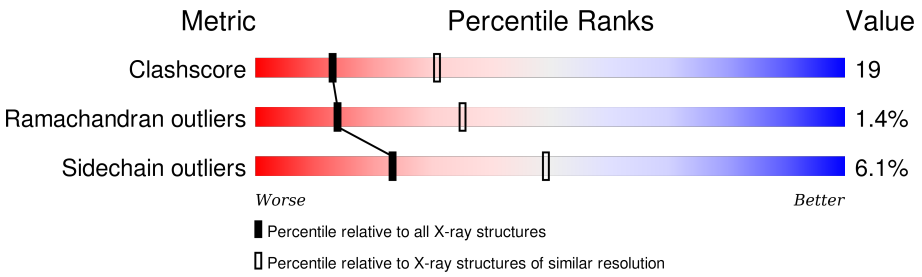
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	64% 33% •
1	C	215	66% 31% •
2	B	218	58% 36% 5% •
2	D	218	60% 33% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6617 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 ANTIBODY HA5-19A4 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	215	1650	1032	268	342	8	0	0	0
1	C	215	1650	1032	268	342	8	0	0	0

- Molecule 2 is a protein called ANTIBODY HA5-19A4 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	1633	1032	266	328	7	0	0	0
2	D	216	1633	1032	266	328	7	0	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	18	18	18	0	0
4	B	10	10	10	0	0
4	C	13	13	13	0	0
4	D	8	8	8	0	0

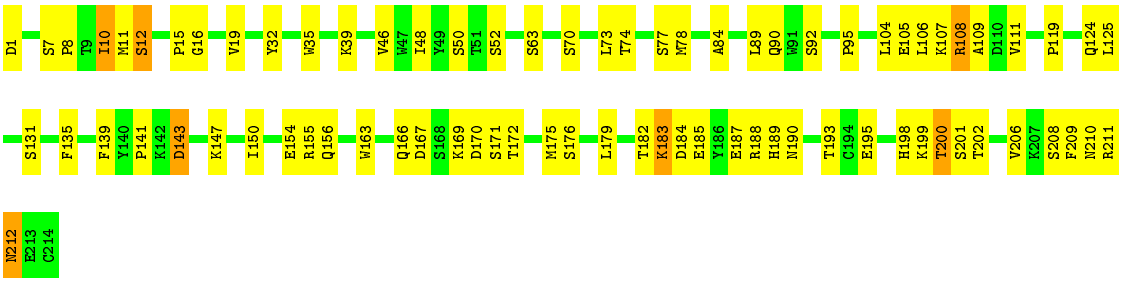
3 Residue-property plots (i)

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.

Note EDS was not executed.

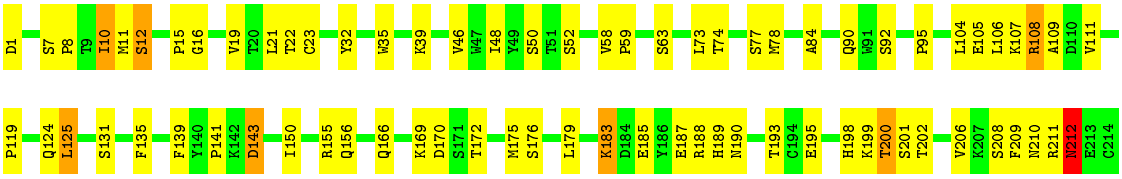
• Molecule 1: ANTIBODY HA5-19A4 FAB LIGHT CHAIN

Chain A:



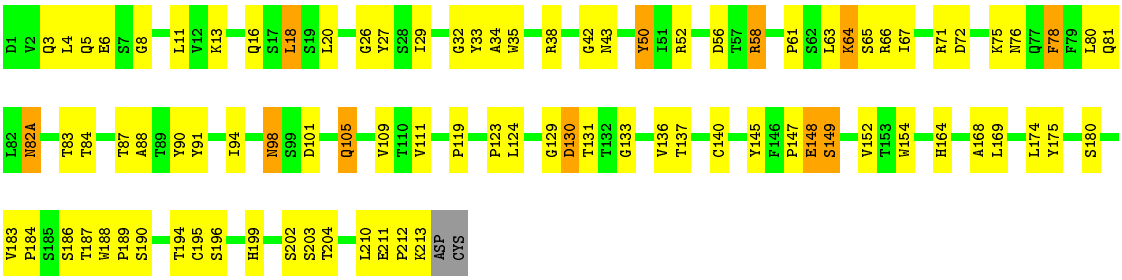
• Molecule 1: ANTIBODY HA5-19A4 FAB LIGHT CHAIN

Chain C:



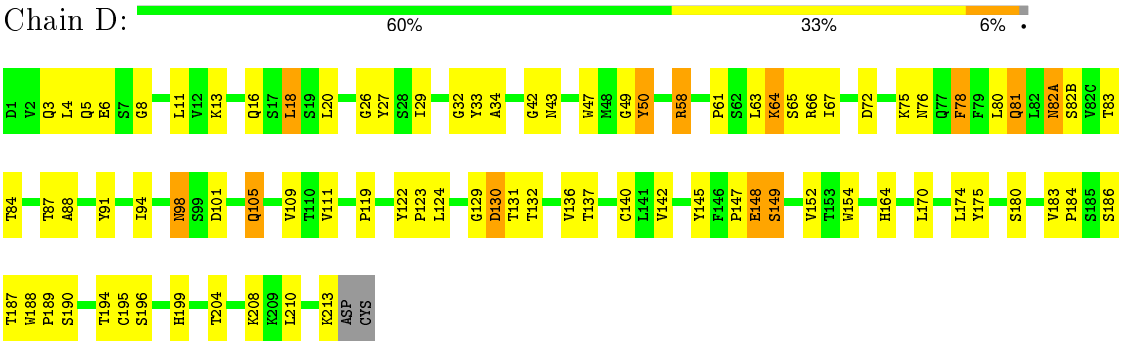
• Molecule 2: ANTIBODY HA5-19A4 FAB HEAVY CHAIN

Chain B:



• Molecule 2: ANTIBODY HA5-19A4 FAB HEAVY CHAIN

Chain D:


60%
33%
6%
D1 V2 Q3 L4 Q5 E6 S7 G8 L11 V12 K13 Q16 S17 L18 S19 L20 G26 Y27 S28 I29 G32 Y33 A34 G42 N43 W47 M48 G49 Y50 R58 P61 S62 L63 K64 S65 R66 I67 D72 K75 N76 Q77 F78 F79 L80 Q81 L82 N82A S82B V82C T83
T84 T87 A88 Y91 I94 N98 S99 D101 Q105 V109 T110 V111 P119 Y122 P123 L124 G129 D130 T131 T132 V136 T137 C140 L141 V142 Y145 F146 P147 E148 S149 V152 T153 W154 H164 L170 L174 Y175 S180 V183 P184 S185 S186
T187 W188 P189 S190 T194 C195 S196 H199 T204 K208 K209 I210 K213 ASP CYS

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 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.90Å 88.70Å 72.90Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	92.6 (20.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6617	wwPDB-VP
Average B, all atoms ($Å^2$)	32.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD

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	0/1691	0.64	0/2300
1	C	0.41	0/1691	0.65	0/2300
2	B	0.41	0/1677	0.70	0/2297
2	D	0.40	0/1677	0.70	0/2297
All	All	0.41	0/6736	0.67	0/9194

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 (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	1650	0	1570	58	1
1	C	1650	0	1570	54	1
2	B	1633	0	1584	71	0
2	D	1633	0	1584	69	0
3	A	1	0	0	0	1
3	C	1	0	0	0	1
4	A	18	0	0	2	0
4	B	10	0	0	1	0
4	C	13	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	8	0	0	1	0
All	All	6617	0	6308	244	2

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 19.

The worst 5 of 244 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:D:105:GLN:H	2:D:105:GLN:NE2	1.77	0.82
2:B:105:GLN:H	2:B:105:GLN:NE2	1.78	0.81
1:A:119:PRO:HG2	2:B:213:LYS:HE3	1.66	0.76
2:B:64:LYS:NZ	2:B:65:SER:HB3	2.02	0.74
2:D:64:LYS:NZ	2:D:65:SER:HB3	2.03	0.73

All (2) 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)
1:A:185:GLU:OE1	3:A:2001:CD:CD[2_545]	2.10	0.10
1:C:185:GLU:OE1	3:C:2002:CD:CD[2_645]	2.13	0.07

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	213/215 (99%)	202 (95%)	10 (5%)	1 (0%)	34 63
1	C	213/215 (99%)	201 (94%)	10 (5%)	2 (1%)	21 49
2	B	214/218 (98%)	191 (89%)	18 (8%)	5 (2%)	8 20
2	D	214/218 (98%)	190 (89%)	20 (9%)	4 (2%)	10 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	854/866 (99%)	784 (92%)	58 (7%)	12 (1%)	14 35

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	130	ASP
2	B	149	SER
1	C	212	ASN
2	D	130	ASP
2	D	149	SER

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	192/192 (100%)	183 (95%)	9 (5%)	32 63
1	C	192/192 (100%)	183 (95%)	9 (5%)	32 63
2	B	188/190 (99%)	174 (93%)	14 (7%)	17 39
2	D	188/190 (99%)	174 (93%)	14 (7%)	17 39
All	All	760/764 (100%)	714 (94%)	46 (6%)	23 49

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	174	LEU
1	C	63	SER
2	D	148	GLU
2	B	186	SER
1	C	10	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	105	GLN
1	C	53	ASN
2	D	105	GLN
1	C	37	GLN
1	C	157	ASN

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.