Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 – 11:07 pm BST

PDB ID	:	1UM5
Title	:	Catalytic Antibody 21H3 with alcohol substrate
Authors	:	Beuscher IV, A.E.; Reuter, J.; Olson, A.J.; Romesberg, F.E.; Schultz, P.G.; Wirsching, P.; Janda, K.D.; Lerner, R.A.; Stevens, R.C.
Deposited on	:	2003-09-23
Resolution	:	1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/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:

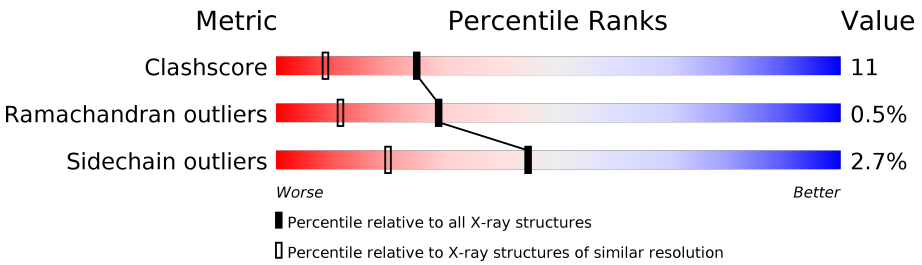
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.60 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	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)

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 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	219	82% 15% ••
2	H	217	83% 15% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3682 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.

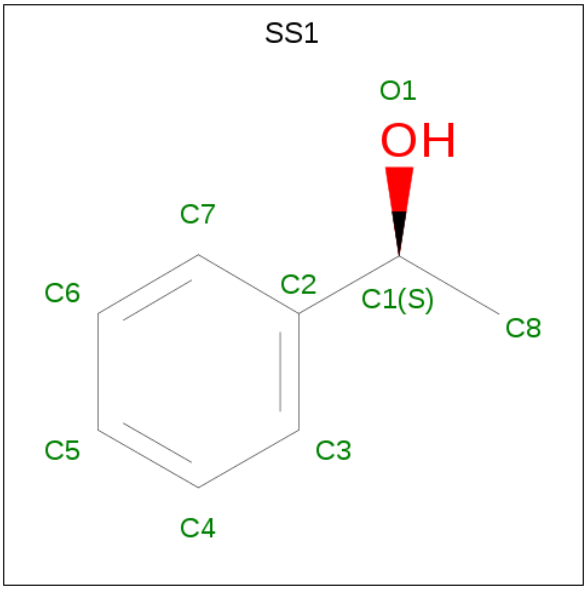
- Molecule 1 is a protein called Antibody 21H3 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	1659	1034	279	341	5	0	0	0

- Molecule 2 is a protein called Antibody 21H3 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1616	1020	265	325	6	0	0	0

- Molecule 3 is 1-PHENYLETHANOL (three-letter code: SS1) (formula: $C_8H_{10}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	H	1	9	8	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	L	206	206	206	0	0
			Total	O		
4	H	192	192	192	0	0

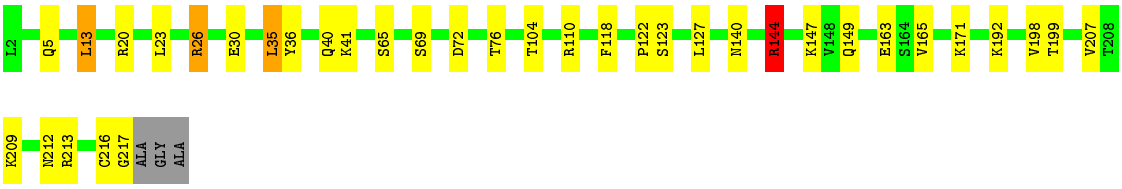
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

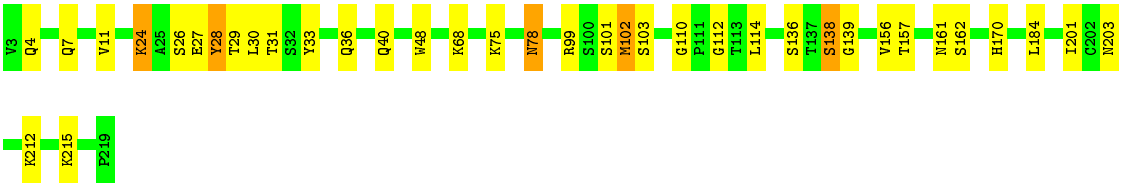
- Molecule 1: Antibody 21H3 L chain

Chain L:



- Molecule 2: Antibody 21H3 H chain

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	47.13Å 64.71Å 138.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 1.60	Depositor
% Data completeness (in resolution range)	98.2 (19.96-1.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3682	wwPDB-VP
Average B, all atoms (Å^2)	17.0	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: SS1

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	1.02	0/1692	1.14	7/2290 (0.3%)
2	H	1.11	0/1656	1.06	1/2255 (0.0%)
All	All	1.07	0/3348	1.11	8/4545 (0.2%)

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
2	H	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	144	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	L	144	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	L	35	LEU	CA-CB-CG	-6.60	100.13	115.30
2	H	68	LYS	CD-CE-NZ	6.05	125.62	111.70
1	L	217	GLY	N-CA-C	-5.91	98.34	113.10
1	L	13	LEU	CA-CB-CG	5.90	128.87	115.30
1	L	213	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	L	110	ARG	NE-CZ-NH2	-5.43	117.58	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	28	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	L	1659	0	1600	35	0
2	H	1616	0	1583	39	0
3	H	9	0	10	0	0
4	H	192	0	0	4	0
4	L	206	0	0	5	1
All	All	3682	0	3193	70	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 11.

All (70) 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:L:123:SER:O	1:L:127:LEU:HD13	1.61	0.99
1:L:192:LYS:HG2	1:L:212:ASN:OD1	1.63	0.98
1:L:40:GLN:HE22	2:H:40:GLN:HE22	1.18	0.88
2:H:162:SER:H	2:H:203:ASN:HD21	1.18	0.88
2:H:138:SER:OG	2:H:139:GLY:N	2.02	0.86
1:L:122:PRO:HB2	1:L:127:LEU:HD11	1.60	0.84
1:L:163:GLU:HG3	4:L:392:HOH:O	1.82	0.80
2:H:29:THR:HG22	2:H:31:THR:H	1.46	0.80
1:L:192:LYS:CG	1:L:212:ASN:OD1	2.32	0.77
1:L:147:LYS:HB3	1:L:199:THR:OG1	1.88	0.72
1:L:20:ARG:HB2	1:L:20:ARG:NH1	2.05	0.71
1:L:26:ARG:HG2	1:L:72:ASP:OD2	1.92	0.70
2:H:24:LYS:NZ	2:H:24:LYS:HB2	2.08	0.68
1:L:149:GLN:HG2	4:L:354:HOH:O	1.94	0.68
1:L:171:LYS:N	1:L:171:LYS:HD2	2.09	0.67
4:L:363:HOH:O	2:H:170:HIS:HD2	1.77	0.66
1:L:140:ASN:HD21	2:H:170:HIS:HE1	1.45	0.65
2:H:36:GLN:NE2	2:H:48:TRP:HE1	1.95	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:29:THR:O	2:H:30:LEU:HB2	2.00	0.61
1:L:127:LEU:N	1:L:127:LEU:HD12	2.16	0.60
2:H:162:SER:H	2:H:203:ASN:ND2	1.97	0.59
2:H:27:GLU:OE2	2:H:27:GLU:N	2.32	0.59
2:H:33:TYR:CE1	2:H:101:SER:OG	2.57	0.57
1:L:198:VAL:HB	1:L:207:VAL:HG13	1.86	0.57
1:L:199:THR:HG23	4:L:316:HOH:O	2.05	0.56
1:L:23:LEU:HD22	1:L:104:THR:HG21	1.87	0.56
2:H:7:GLN:HE21	2:H:110:GLY:HA3	1.71	0.56
2:H:102:MET:O	2:H:103:SER:HB2	2.07	0.55
2:H:215:LYS:NZ	4:H:1134:HOH:O	2.39	0.55
2:H:24:LYS:HB2	2:H:24:LYS:HZ1	1.71	0.55
2:H:36:GLN:HE21	2:H:48:TRP:HE1	1.55	0.55
2:H:29:THR:HG21	2:H:33:TYR:HE2	1.72	0.54
1:L:123:SER:O	1:L:127:LEU:CD1	2.46	0.54
2:H:33:TYR:CE2	2:H:99:ARG:NH1	2.75	0.54
2:H:29:THR:HG21	2:H:33:TYR:CE2	2.42	0.54
2:H:11:VAL:HG21	4:H:1139:HOH:O	2.07	0.54
1:L:140:ASN:HD21	2:H:170:HIS:CE1	2.25	0.53
2:H:24:LYS:NZ	2:H:24:LYS:CB	2.72	0.53
1:L:35:LEU:HG	1:L:36:TYR:N	2.23	0.53
2:H:114:LEU:C	2:H:114:LEU:HD23	2.30	0.53
2:H:28:TYR:CD2	2:H:28:TYR:N	2.75	0.52
1:L:198:VAL:HB	1:L:207:VAL:CG1	2.40	0.51
1:L:118:PHE:HD1	2:H:136:SER:HA	1.78	0.49
1:L:147:LYS:HE2	1:L:149:GLN:CG	2.43	0.49
1:L:147:LYS:HE2	1:L:149:GLN:HG3	1.94	0.48
1:L:127:LEU:CD1	1:L:127:LEU:N	2.76	0.48
2:H:78:ASN:N	2:H:78:ASN:HD22	2.13	0.47
1:L:147:LYS:HE2	1:L:149:GLN:CD	2.35	0.46
1:L:20:ARG:CB	1:L:20:ARG:HH11	2.28	0.46
1:L:144:ARG:NH1	1:L:165:VAL:HG21	2.31	0.46
2:H:161:ASN:ND2	2:H:201:ILE:H	2.14	0.46
1:L:20:ARG:HB2	1:L:20:ARG:HH11	1.80	0.46
2:H:33:TYR:CG	2:H:99:ARG:HD2	2.51	0.45
1:L:20:ARG:CB	1:L:20:ARG:NH1	2.78	0.45
2:H:156:VAL:HG12	2:H:157:THR:N	2.31	0.45
2:H:33:TYR:CD1	2:H:101:SER:OG	2.70	0.45
2:H:4:GLN:HA	4:H:1144:HOH:O	2.17	0.44
1:L:13:LEU:HD23	1:L:23:LEU:HD21	1.99	0.44
2:H:156:VAL:CG1	2:H:157:THR:N	2.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:GLN:HG2	2:H:26:SER:HB3	2.00	0.43
2:H:7:GLN:NE2	2:H:112:GLY:H	2.16	0.43
2:H:75:LYS:O	2:H:78:ASN:ND2	2.52	0.43
1:L:26:ARG:CG	1:L:72:ASP:OD2	2.65	0.43
1:L:207:VAL:HG13	1:L:207:VAL:O	2.19	0.42
2:H:114:LEU:HD22	4:H:1006:HOH:O	2.20	0.42
1:L:65:SER:OG	1:L:76:THR:CG2	2.68	0.42
2:H:114:LEU:C	2:H:114:LEU:CD2	2.88	0.42
2:H:184:LEU:HD12	2:H:184:LEU:C	2.40	0.41
1:L:163:GLU:CG	4:L:392:HOH:O	2.55	0.41
1:L:5:GLN:HE21	1:L:5:GLN:HB3	1.63	0.41

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:L:364:HOH:O	4:L:365:HOH:O[4_466]	2.11	0.09

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	L	214/219 (98%)	209 (98%)	4 (2%)	1 (0%)	29 11
2	H	215/217 (99%)	208 (97%)	6 (3%)	1 (0%)	29 11
All	All	429/436 (98%)	417 (97%)	10 (2%)	2 (0%)	29 11

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	216	CYS
2	H	138	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	L	187/189 (99%)	181 (97%)	6 (3%)	39	15
2	H	184/185 (100%)	180 (98%)	4 (2%)	52	27
All	All	371/374 (99%)	361 (97%)	10 (3%)	44	20

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	26	ARG
1	L	30	GLU
1	L	41	LYS
1	L	69	SER
1	L	144	ARG
1	L	209	LYS
2	H	24	LYS
2	H	78	ASN
2	H	102	MET
2	H	212	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	5	GLN
1	L	8	GLN
1	L	29	GLN
1	L	139	ASN
1	L	140	ASN
2	H	7	GLN
2	H	36	GLN
2	H	40	GLN
2	H	78	ASN
2	H	161	ASN
2	H	170	HIS
2	H	203	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	205	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)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SS1	H	1001	-	9,9,9	1.86	2 (22%)	11,11,11	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SS1	H	1001	-	-	2/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	1001	SS1	C7-C2	4.37	1.46	1.39
3	H	1001	SS1	C5-C4	2.10	1.43	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	1001	SS1	C8-C1-C2-C3
3	H	1001	SS1	C8-C1-C2-C7

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.