

Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 07:15 pm BST

PDB ID : 1JGV

Title : STRUCTURAL BASIS FOR DISFAVORED ELIMINATION REACTION IN

CATALYTIC ANTIBODY 1D4

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Deposited on : 2001-06-26

Resolution : 1.85 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 (1)) were used in the production of this report:

MolProbity : 4.02b-467 Xtriage (Phenix) : 1.13

EDS : 2.11

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac: 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

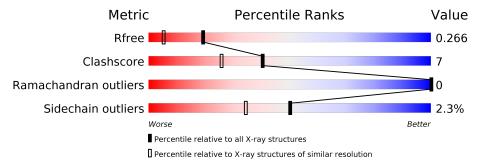
Validation Pipeline (wwPDB-VP) : 2.11

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 1.85 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{resolution range}(ext{Å}))$
R_{free}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)

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%

Mol	Chain	Length	Quality of chain	
1	L	220	85%	15%
2	Н	218	82%	17% •



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3611 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 Light Chain.

\mathbf{Mol}	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
1	L	220	Total 1701	C 1061	N 290	O 343	S 7	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	GLU	ASP	SEE REMARK 999	GB 522337
L	27B	LEU	ILE	SEE REMARK 999	GB 522337
L	34	HIS	GLU	SEE REMARK 999	GB 522337
L	87	PHE	TYR	SEE REMARK 999	GB 522337
L	89	SER	PHE	SEE REMARK 999	GB 522337
L	91	SER	GLY	SEE REMARK 999	GB 522337
L	97	THR	SER	SEE REMARK 999	GB 522337
L	96	LEU	_	SEE REMARK 999	GB 522337
L	100	ALA	GLY	SEE REMARK 999	GB 522337
L	103	LYS	ASN	SEE REMARK 999	GB 522337
L	106	LEU	ILE	SEE REMARK 999	GB 522337

• Molecule 2 is a protein called Antibody Heavy Chain.

Mol	Chain	Residues		\mathbf{At}	oms			ZeroOcc	AltConf	Trace
2	Н	218	Total 1664	C 1057	N 276	O 323	S 8	0	0	0

• Molecule 3 is water.

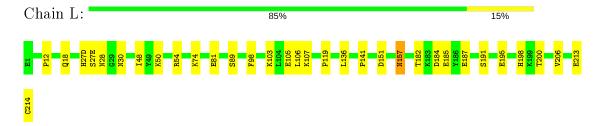
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	L	139	Total O 139 139	0	0
3	Н	107	Total O 107 107	0	0



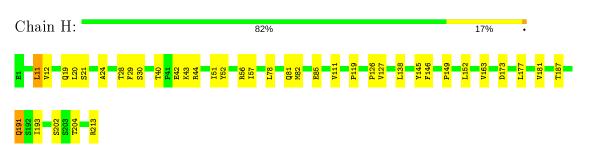
3 Residue-property plots (i)

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.

• Molecule 1: Antibody Light Chain



• Molecule 2: Antibody Heavy Chain





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	67.65Å 48.17Å 69.28Å	Depositor
a, b, c, α , β , γ	90.00° 106.20° 90.00°	Depositor
Resolution (Å)	20.00 - 1.85	Depositor
Resolution (A)	26.74 - 1.68	EDS
% Data completeness	(Not available) (20.00-1.85)	Depositor
(in resolution range)	91.4 (26.74-1.68)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	0.67 (at 1.68Å)	Xtriage
Refinement program	CNS	Depositor
D D.	0.206 , 0.247	Depositor
R, R_{free}	0.259 , 0.266	DCC
R_{free} test set	1947 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.38 , 43.9	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3611	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

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		
WIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5	
1	L	0.33	0/1740	0.63	0/2361	
2	Н	0.33	0/1707	0.64	0/2326	
All	All	0.33	0/3447	0.64	0/4687	

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	L	1701	0	1646	22	2
2	Н	1664	0	1630	27	0
3	Н	107	0	0	1	0
3	L	139	0	0	3	3
All	All	3611	0	3276	48	4

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 7.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} { m Clash} \\ { m overlap} \ ({ m \AA}) \end{array}$
1:L:27(D):HIS:HD2	1:L:28:ASN:H	1.15	0.93

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Continued from prev		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	${ m overlap}({ m \AA})$
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.59	0.85
1:L:191:SER:HB2	3:L:334:HOH:O	1.75	0.84
2:H:40:THR:OG1	2:H:44:ARG:HG2	1.77	0.83
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.64	0.79
1:L:27(D):HIS:CD2	1:L:28:ASN:H	2.03	0.73
1:L:12:PRO:HB2	1:L:107:LYS:HG2	1.75	0.67
2:H:11:LEU:HD11	2:H:146:PHE:HE2	1.60	0.66
1:L:213:GLU:O	1:L:214:CYS:HB2	1.96	0.65
1:L:81:GLU:HG2	3:L:304:HOH:O	1.99	0.62
2:H:24:ALA:HB2	2:H:29:PHE:CE1	2.33	0.62
2:H:213:ARG:HG3	2:H:213:ARG:O	2.00	0.62
2:H:51:ILE:HG13	2:H:57:ILE:CD1	2.31	0.60
1:L:27(D):HIS:HD2	1:L:28:ASN:N	1.95	0.58
2:H:28:THR:HG23	3:H:283:HOH:O	2.05	0.56
1:L:213:GLU:O	1:L:214:CYS:CB	2.57	0.52
1:L:12:PRO:HB2	1:L:107:LYS:CG	2.40	0.51
1:L:119:PRO:HD3	2:H:127:VAL:HG12	1.93	0.51
2:H:85:GLU:H	2:H:85:GLU:CD	2.14	0.51
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.94	0.50
2:H:24:ALA:HB2	2:H:29:PHE:HE1	1.74	0.50
1:L:182:THR:OG1	1:L:185:GLU:HG3	2.12	0.49
2:H:51:ILE:HG13	2:H:57:ILE:HD13	1.93	0.49
1:L:103:LYS:HG2	1:L:105:GLU:HG3	1.95	0.48
2:H:52:TYR:HB3	2:H:56:ARG:HB3	1.96	0.48
2:H:138:LEU:HD12	2:H:193:ILE:HG21	1.95	0.47
2:H:11:LEU:HD11	2:H:146:PHE:CE2	2.46	0.47
1:L:157:ASN:N	1:L:157:ASN:HD22	2.13	0.46
2:H:12:VAL:O	2:H:111:VAL:HA	2.15	0.45
1:L:48:ILE:HD13	1:L:54:ARG:HA	1.98	0.45
2:H:202:SER:O	2:H:204:THR:HG23	2.17	0.45
2:H:152:LEU:HD23	2:H:152:LEU:C	2.37	0.45
1:L:151:ASP:HA	1:L:191:SER:HB3	1.99	0.45
2:H:42:GLU:O	2:H:43:LYS:HB2	2.16	0.44
1:L:141:PRO:O	1:L:198:HIS:HE1	2.00	0.44
1:L:89:SER:HB2	1:L:98:PHE:CD2	2.52	0.44
2:H:20:LEU:HG	2:H:82:MET:CE	2.47	0.44
2:H:126:PRO:HD3	2:H:138:LEU:CD2	2.48	0.43
2:H:19:GLN:HB2	2:H:81:GLN:NE2	2.33	0.43
2:H:126:PRO:HD3	2:H:138:LEU:HD22	1.99	0.43
2:H:21:SER:HA	2:H:78:LEU:O	2.18	0.43
2:H:187:THR:O	2:H:191:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic	Clash
		$\operatorname{distance}\left(\mathrm{\AA}\right)$	overlap(A)
2:H:40:THR:HG21	2:H:44:ARG:CZ	2.49	0.42
1:L:27(D):HIS:CD2	1:L:27(E):SER:N	2.88	0.42
1:L:74:LYS:HG3	3:L:248:HOH:O	2.20	0.42
2:H:163:VAL:HG22	2:H:181:VAL:HG23	2.03	0.41
1:L:136:LEU:N	1:L:136:LEU:HD12	2.36	0.40
2:H:28:THR:HG22	2:H:30:SER:H	1.87	0.40

All (4) 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	$egin{array}{c} ext{Interatomic} \ ext{distance } (ext{Å}) \end{array}$	$egin{array}{c} ext{Clash} \ ext{overlap } (ext{Å}) \end{array}$
1:L:30:ASN:OD1	3:L:216:HOH:O[1_556]	2.03	0.17
3:L:289:HOH:O	3:L:301:HOH:O[1_556]	2.04	0.16
3:L:220:HOH:O	3:L:252:HOH:O[1_554]	2.11	0.09
1:L:50:LYS:NZ	1:L:187:GLU:OE1[1_556]	2.18	0.02

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	Perce	\mathbf{ntiles}
1	L	218/220 (99%)	215 (99%)	3 (1%)	0	100	100
2	Н	216/218 (99%)	209 (97%)	7 (3%)	0	100	100
All	All	434/438 (99%)	424 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	198/198 (100%)	194 (98%)	4 (2%)	55 40
2	Н	186/186 (100%)	181 (97%)	5 (3%)	44 29
All	All	384/384 (100%)	375 (98%)	9 (2%)	50 34

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	18	GLN
1	L	106	LEU
1	L	157	ASN
1	L	184	ASP
2	Н	11	LEU
2	Н	149	PRO
2	Н	173	ASP
2	Н	177	LEU
2	Н	191	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27(D)	HIS
1	L	42	GLN
1	L	157	ASN
1	L	161	ASN
1	L	189	HIS
1	L	198	HIS
2	Н	19	GLN
2	Н	81	GLN
2	Н	171	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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

