



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:45 PM UTC

PDB ID : 5F6I / pdb_00005f6i
Title : Crystal Structure of Tier 2 Neutralizing Antibody DH428 from a Rhesus Macaque
Authors : Fera, D.; Harrison, S.C.
Deposited on : 2015-12-06
Resolution : 2.32 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

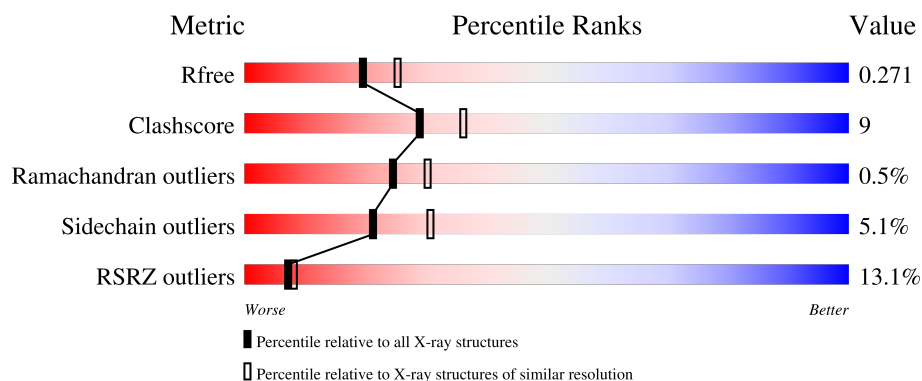
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 of 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 $\leq 5\%$. 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	B	227	11% 78% 14% 7%
2	C	216	14% 73% 21% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3225 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 DH428 Antibody Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	210	Total	C	N	O	S	0	0	0
			1575	1002	261	307	5			

- Molecule 2 is a protein called DH428 Antibody Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1567	973	264	325	5			

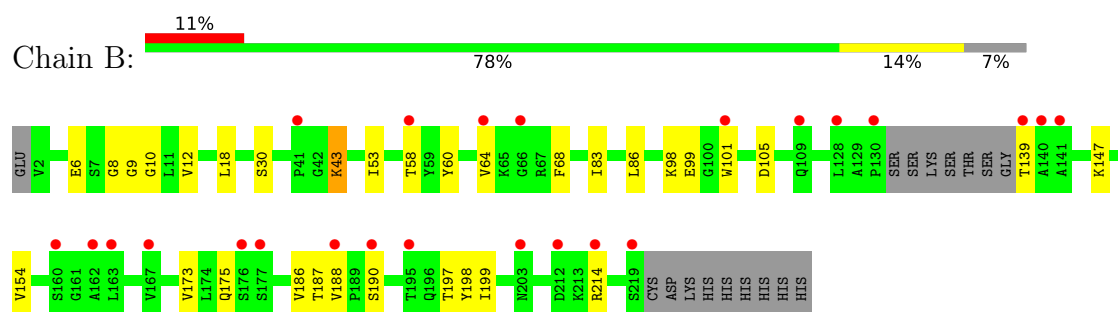
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	41	Total	O	0	0
			41	41		
3	C	42	Total	O	0	0
			42	42		

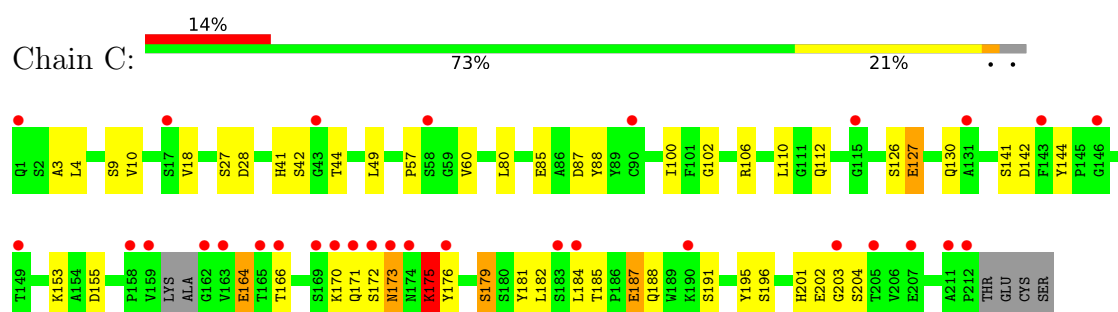
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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: DH428 Antibody Heavy Chain



• Molecule 2: DH428 Antibody Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.11Å 74.63Å 102.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.36 – 2.32 60.36 – 2.32	Depositor EDS
% Data completeness (in resolution range)	91.7 (60.36-2.32) 85.0 (60.36-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.265 0.227 , 0.271	Depositor DCC
R_{free} test set	1214 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3225	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	B	0.65	1/1615 (0.1%)	0.93	1/2202 (0.0%)
2	C	0.52	0/1602	0.91	3/2184 (0.1%)
All	All	0.59	1/3217 (0.0%)	0.92	4/4386 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	10	GLY	C-O	-6.37	1.19	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	191	SER	N-CA-C	12.04	126.09	111.40
2	C	191	SER	CB-CA-C	-7.70	97.85	110.79
1	B	8	GLY	N-CA-C	-6.93	102.47	112.17
2	C	175	LYS	N-CA-C	5.42	117.50	109.69

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	B	1575	0	1539	22	0
2	C	1567	0	1509	34	0
3	B	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	42	0	0	1	0
All	All	3225	0	3048	54	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 9.

All (54) 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:C:201:HIS:ND1	2:C:202:GLU:OE1	2.05	0.89
2:C:202:GLU:HG2	2:C:203:GLY:H	1.45	0.82
1:B:64:VAL:HG13	1:B:68:PHE:CG	2.17	0.80
1:B:64:VAL:HG13	1:B:68:PHE:CD2	2.16	0.79
1:B:12:VAL:HG21	1:B:18:LEU:HG	1.68	0.75
2:C:87:ASP:OD1	2:C:106:ARG:NE	2.18	0.75
2:C:141:SER:HB2	2:C:171:GLN:NE2	2.03	0.73
1:B:64:VAL:CG1	1:B:68:PHE:CD2	2.73	0.72
2:C:170:LYS:HB3	2:C:172:SER:HB2	1.72	0.69
2:C:141:SER:HB2	2:C:171:GLN:HE22	1.56	0.67
2:C:166:THR:HG22	2:C:179:SER:H	1.61	0.66
2:C:202:GLU:HG2	2:C:203:GLY:N	2.11	0.65
1:B:58:THR:HG22	1:B:60:TYR:CE2	2.35	0.62
1:B:64:VAL:CG1	1:B:68:PHE:CG	2.82	0.62
2:C:188:GLN:O	2:C:195:TYR:OH	2.18	0.61
2:C:42:SER:H	2:C:170:LYS:HD2	1.66	0.60
2:C:110:LEU:O	2:C:144:TYR:OH	2.17	0.59
2:C:185:THR:OG1	2:C:187:GLU:OE1	2.21	0.57
1:B:139:THR:N	1:B:190:SER:HG	2.04	0.54
2:C:187:GLU:OE1	2:C:188:GLN:N	2.41	0.54
2:C:182:LEU:HG	2:C:184:LEU:CD1	2.38	0.53
1:B:98:LYS:HE2	1:B:105:ASP:OD1	2.08	0.53
2:C:85:GLU:OE2	2:C:176:TYR:OH	2.28	0.51
1:B:173:VAL:HG21	2:C:181:TYR:CE1	2.46	0.51
1:B:43:LYS:HB2	3:B:329:HOH:O	2.11	0.50
1:B:18:LEU:HD22	3:B:308:HOH:O	2.11	0.50
2:C:142:ASP:HA	2:C:175:LYS:HG3	1.94	0.50
1:B:64:VAL:HG12	1:B:68:PHE:HB2	1.94	0.49
2:C:3:ALA:HA	2:C:100:ILE:HD11	1.95	0.49
2:C:112:GLN:HB2	2:C:144:TYR:CZ	2.48	0.48
1:B:30:SER:O	1:B:53:ILE:HG23	2.14	0.47
2:C:153:LYS:HB2	2:C:196:SER:HB2	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:HE3	1:B:99:GLU:O	2.16	0.46
2:C:171:GLN:N	2:C:172:SER:HA	2.31	0.45
2:C:127:GLU:H	2:C:127:GLU:CD	2.24	0.44
2:C:41:HIS:HA	2:C:170:LYS:NZ	2.32	0.44
2:C:10:VAL:HG11	2:C:18:VAL:HG21	2.00	0.43
2:C:41:HIS:HA	2:C:170:LYS:HZ3	1.84	0.43
2:C:172:SER:O	2:C:173:ASN:C	2.62	0.43
2:C:57:PRO:HG2	2:C:60:VAL:HG21	2.00	0.42
1:B:64:VAL:HG11	1:B:68:PHE:CD2	2.53	0.42
1:B:173:VAL:HG11	2:C:164:GLU:HB2	2.01	0.42
2:C:44:THR:HG23	3:C:311:HOH:O	2.20	0.42
1:B:83:ILE:HG13	1:B:86:LEU:HD11	2.02	0.42
1:B:188:VAL:HG11	1:B:198:TYR:CE1	2.56	0.41
2:C:49:LEU:HD11	2:C:88:TYR:HE2	1.86	0.41
2:C:49:LEU:HD11	2:C:88:TYR:CE2	2.56	0.41
1:B:9:GLY:HA2	1:B:18:LEU:HD13	2.02	0.41
1:B:58:THR:HG22	1:B:60:TYR:HE2	1.84	0.41
1:B:199:ILE:HG12	1:B:214:ARG:HG2	2.03	0.41
1:B:147:LYS:HE3	1:B:147:LYS:HB2	1.71	0.40
2:C:126:SER:O	2:C:130:GLN:HG3	2.22	0.40
2:C:4:LEU:HB2	2:C:102:GLY:HA2	2.03	0.40
2:C:184:LEU:HD21	2:C:195:TYR:CZ	2.57	0.40

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	B	206/227 (91%)	199 (97%)	7 (3%)	0	100	100
2	C	206/216 (95%)	193 (94%)	11 (5%)	2 (1%)	12	14
All	All	412/443 (93%)	392 (95%)	18 (4%)	2 (0%)	24	30

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	155	ASP
2	C	173	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	B	176/192 (92%)	168 (96%)	8 (4%)	24	36
2	C	178/183 (97%)	168 (94%)	10 (6%)	19	27
All	All	354/375 (94%)	336 (95%)	18 (5%)	21	31

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	GLU
1	B	43	LYS
1	B	101	TRP
1	B	154	VAL
1	B	175	GLN
1	B	186	VAL
1	B	187	THR
1	B	197	THR
2	C	9	SER
2	C	27	SER
2	C	28	ASP
2	C	80	LEU
2	C	127	GLU
2	C	164	GLU
2	C	175	LYS
2	C	179	SER
2	C	187	GLU
2	C	204	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	168	HIS
2	C	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 oligosaccharides 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

6.1 Protein, DNA and RNA chains

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	B	210/227 (92%)	0.80	24 (11%)	10 11	26, 43, 79, 94	0
2	C	210/216 (97%)	0.87	31 (14%)	5 6	26, 47, 87, 99	0
All	All	420/443 (94%)	0.83	55 (13%)	7 8	26, 45, 83, 99	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	174	ASN	4.3
2	C	203	GLY	4.1
1	B	195	THR	4.0
2	C	172	SER	4.0
1	B	190	SER	3.9
1	B	109	GLN	3.8
2	C	166	THR	3.7
1	B	64	VAL	3.5
1	B	101	TRP	3.5
2	C	170	LYS	3.4
2	C	212	PRO	3.3
2	C	205	THR	3.3
1	B	58	THR	3.0
2	C	159	VAL	3.0
1	B	139	THR	2.9
1	B	41	PRO	2.8
2	C	173	ASN	2.8
1	B	219	SER	2.7
2	C	190	LYS	2.7
1	B	140	ALA	2.6
2	C	90	CYS	2.6
1	B	162	ALA	2.6
1	B	141	ALA	2.6
2	C	131	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	162	GLY	2.6
1	B	176	SER	2.5
2	C	115	GLY	2.5
2	C	1	GLN	2.5
2	C	58	SER	2.5
2	C	207	GLU	2.5
1	B	188	VAL	2.5
1	B	163	LEU	2.5
2	C	17	SER	2.4
1	B	167	VAL	2.4
2	C	143	PHE	2.4
2	C	211	ALA	2.4
1	B	66	GLY	2.4
1	B	212	ASP	2.4
2	C	163	VAL	2.4
2	C	183	SER	2.4
2	C	165	THR	2.3
1	B	203	ASN	2.3
1	B	177	SER	2.2
2	C	184	LEU	2.2
2	C	158	PRO	2.2
2	C	169	SER	2.1
2	C	176	TYR	2.1
2	C	43	GLY	2.1
1	B	214	ARG	2.1
2	C	146	GLY	2.1
2	C	149	THR	2.1
2	C	171	GLN	2.1
1	B	160	SER	2.0
1	B	128	LEU	2.0
1	B	130	PRO	2.0

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 oligosaccharides 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.