



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 22, 2020 – 08:05 PM EST

PDB ID : 6XRJ
Title : Crystal structure of the disulfide linked DH717.1 Fab dimer, derived from a macaque HIV-1 vaccine-induced Env glycan-reactive neutralizing antibody B cell lineage
Authors : Manne, K.; Nicely, N.I.; Acharya, P.
Deposited on : 2020-07-13
Resolution : 3.15 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

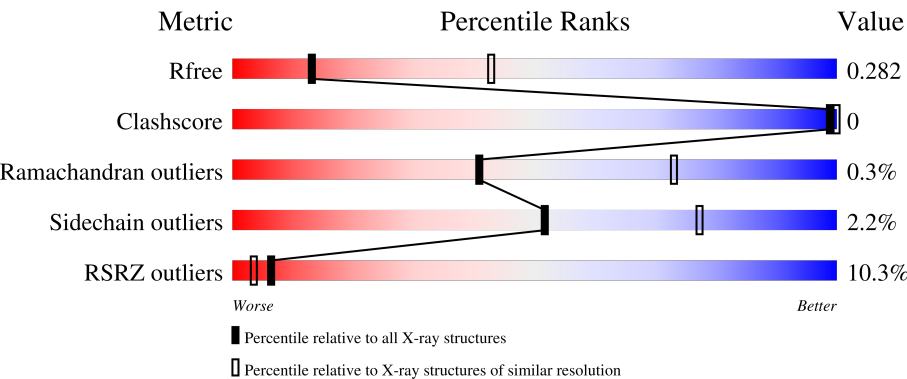
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	A	226	<div><div>5%</div><div>92%</div><div>...</div></div>
1	C	226	<div><div>19%</div><div>96%</div><div>.</div></div>
1	E	226	<div><div>19%</div><div>95%</div><div>5%</div></div>
1	H	226	<div><div>15%</div><div>92%</div><div>7%</div><div>.</div></div>
2	B	211	<div><div>%</div><div>96%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	D	211	<div><div></div><div>5%</div><div>95%</div><div>5%</div></div>
2	F	211	<div><div></div><div>9%</div><div>95%</div><div>5%</div></div>
2	L	211	<div><div></div><div>9%</div><div>91%</div><div>9%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25500 atoms, of which 12535 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 DH717.1 heavy chain Fab fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	0	0	0
			3257	1037	1615	278	321	6			
1	C	226	Total	C	H	N	O	S	0	0	0
			3362	1066	1668	289	333	6			
1	E	225	Total	C	H	N	O	S	0	0	0
			3348	1062	1661	288	331	6			
1	H	226	Total	C	H	N	O	S	0	0	0
			3362	1066	1668	289	333	6			

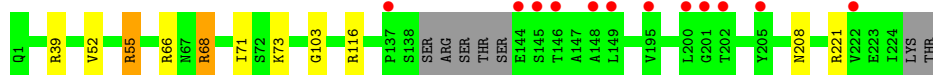
- Molecule 2 is a protein called DH717.1 light chain Fab fragment.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	211	Total	C	H	N	O	S	0	0	0
			3042	972	1480	260	325	5			
2	D	211	Total	C	H	N	O	S	0	0	0
			3044	972	1482	260	325	5			
2	F	211	Total	C	H	N	O	S	0	0	0
			3053	972	1491	260	325	5			
2	L	211	Total	C	H	N	O	S	0	0	0
			3032	972	1470	260	325	5			

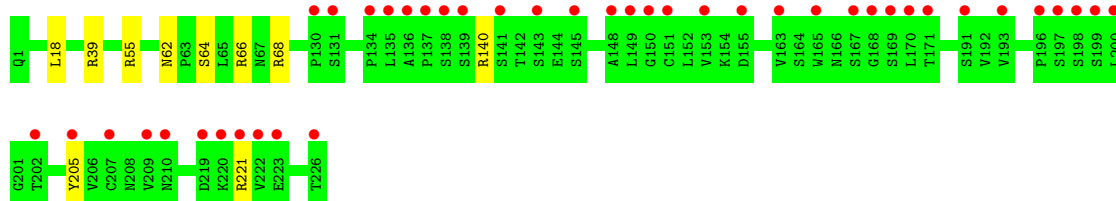
3 Residue-property plots [i](#)

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.

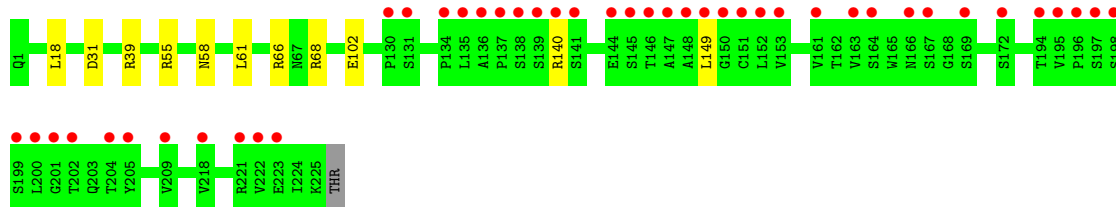
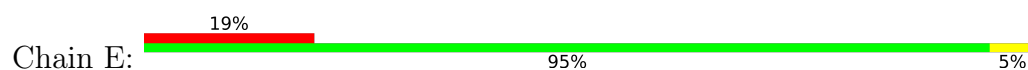
- Molecule 1: DH717.1 heavy chain Fab fragment



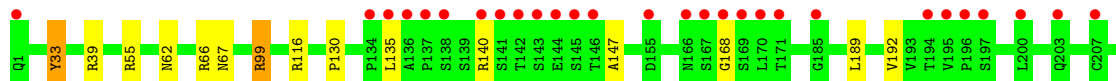
- Molecule 1: DH717.1 heavy chain Fab fragment

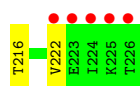


- Molecule 1: DH717.1 heavy chain Fab fragment



- Molecule 1: DH717.1 heavy chain Fab fragment





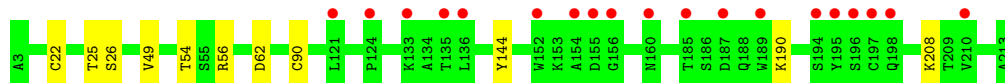
- Molecule 2: DH717.1 light chain Fab fragment



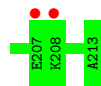
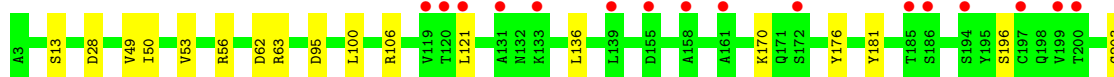
- Molecule 2: DH717.1 light chain Fab fragment



- Molecule 2: DH717.1 light chain Fab fragment



- Molecule 2: DH717.1 light chain Fab fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	201.59Å 201.59Å 154.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.71 – 3.15 41.71 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.71-3.15) 99.8 (41.71-3.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.245 , 0.282 0.243 , 0.282	Depositor DCC
R_{free} test set	1999 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 81.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	25500	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.42% 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

5.1 Standard geometry

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	0.61	0/1679	1.06	6/2290 (0.3%)
1	C	0.63	0/1732	1.04	5/2362 (0.2%)
1	E	0.65	0/1725	1.07	5/2352 (0.2%)
1	H	0.65	0/1732	1.13	6/2362 (0.3%)
2	B	0.59	0/1598	1.02	2/2180 (0.1%)
2	D	0.60	0/1598	1.00	2/2180 (0.1%)
2	F	0.61	0/1598	0.99	1/2180 (0.0%)
2	L	0.60	0/1598	1.07	3/2180 (0.1%)
All	All	0.62	0/13260	1.05	30/18086 (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
1	A	0	1
1	C	0	1
1	H	0	1
2	F	0	1
All	All	0	4

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	68	ARG	NE-CZ-NH1	8.65	124.63	120.30
2	L	56	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	55	ARG	NE-CZ-NH1	7.86	124.23	120.30
2	D	56	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	66	ARG	NE-CZ-NH1	7.33	123.97	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ARG	Sidechain
1	C	205	TYR	Sidechain
2	F	144	TYR	Sidechain
1	H	33	TYR	Sidechain

5.2 Too-close contacts ⓘ

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	1642	1615	1616	1	1
1	C	1694	1668	1670	0	4
1	E	1687	1661	1663	0	6
1	H	1694	1668	1670	3	0
2	B	1562	1480	1504	1	0
2	D	1562	1482	1504	2	3
2	F	1562	1491	1504	2	2
2	L	1562	1470	1504	2	3
All	All	12965	12535	12635	11	11

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 0.

The worst 5 of 11 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:F:22:CYS:HG	2:F:90:CYS:HG	1.42	0.67
2:D:22:CYS:HG	2:D:90:CYS:HG	1.55	0.54
2:F:22:CYS:SG	2:F:90:CYS:SG	3.01	0.51
1:A:52:VAL:CG2	1:A:71:ILE:HG22	2.44	0.47
2:L:170:LYS:HE3	2:L:176:TYR:CE1	2.51	0.46

The worst 5 of 11 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:E:31:ASP:O	1:E:31:ASP:OD1[7_554]	1.33	0.87
2:F:190:LYS:NZ	2:F:190:LYS:NZ[5_555]	1.42	0.78
1:C:55:ARG:NH2	1:E:58:ASN:HD22[7_554]	1.03	0.57
2:D:11:SER:H	2:L:13:SER:HG[3_454]	1.16	0.44
1:A:103:GLY:HA3	2:F:54:THR:HG21[7_554]	1.21	0.39

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	215/226 (95%)	202 (94%)	13 (6%)	0	100	100
1	C	224/226 (99%)	209 (93%)	15 (7%)	0	100	100
1	E	223/226 (99%)	210 (94%)	13 (6%)	0	100	100
1	H	224/226 (99%)	203 (91%)	19 (8%)	2 (1%)	17	53
2	B	209/211 (99%)	204 (98%)	5 (2%)	0	100	100
2	D	209/211 (99%)	196 (94%)	12 (6%)	1 (0%)	29	65
2	F	209/211 (99%)	196 (94%)	12 (6%)	1 (0%)	29	65
2	L	209/211 (99%)	188 (90%)	19 (9%)	2 (1%)	15	51
All	All	1722/1748 (98%)	1608 (93%)	108 (6%)	6 (0%)	41	73

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	95	ASP
1	H	147	ALA
2	F	26	SER
1	H	168	GLY
2	D	53	VAL

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	186/193 (96%)	183 (98%)	3 (2%)	62	83
1	C	193/193 (100%)	190 (98%)	3 (2%)	62	83
1	E	192/193 (100%)	189 (98%)	3 (2%)	62	83
1	H	193/193 (100%)	189 (98%)	4 (2%)	53	78
2	B	176/176 (100%)	172 (98%)	4 (2%)	50	76
2	D	176/176 (100%)	173 (98%)	3 (2%)	60	82
2	F	176/176 (100%)	172 (98%)	4 (2%)	50	76
2	L	176/176 (100%)	167 (95%)	9 (5%)	24	56
All	All	1468/1476 (100%)	1435 (98%)	33 (2%)	52	77

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	61	LEU
2	F	62	ASP
2	L	136	LEU
1	E	149	LEU
2	F	25	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

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	A	219/226 (96%)	0.32	12 (5%) 25 13	48, 86, 157, 198	0
1	C	226/226 (100%)	0.86	42 (18%) 1 0	47, 104, 221, 244	0
1	E	225/226 (99%)	0.98	43 (19%) 1 0	35, 76, 213, 229	0
1	H	226/226 (100%)	0.78	33 (14%) 2 1	48, 97, 175, 214	0
2	B	211/211 (100%)	0.21	2 (0%) 84 75	72, 111, 148, 164	0
2	D	211/211 (100%)	0.46	11 (5%) 27 14	67, 125, 203, 220	0
2	F	211/211 (100%)	0.43	19 (9%) 9 5	52, 109, 192, 206	0
2	L	211/211 (100%)	0.49	18 (8%) 10 5	70, 119, 173, 190	0
All	All	1740/1748 (99%)	0.57	180 (10%) 6 3	35, 108, 195, 244	0

The worst 5 of 180 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	137	PRO	16.0
1	H	135	LEU	8.3
1	H	137	PRO	8.2
1	C	138	SER	7.4
1	E	205	TYR	7.2

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 monosaccharides 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.