



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2024 – 09:05 PM EDT

PDB ID : 6MEE
Title : Crystal structure of broadly neutralizing antibody HEPC74
Authors : Flyak, A.I.; Bjorkman, P.J.
Deposited on : 2018-09-06
Resolution : 1.36 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

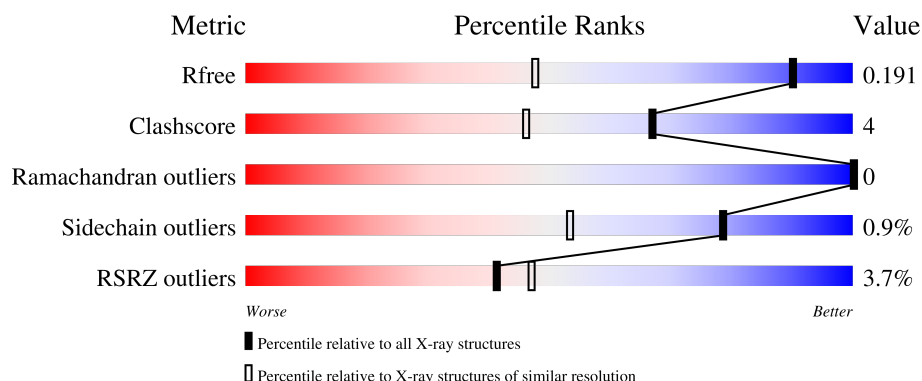
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	239	<div> <div>2%</div> <div>87%</div> <div>9%</div> </div>
1	C	239	<div> <div>9%</div> <div>87%</div> <div>8%</div> </div>
2	B	214	<div> <div>%</div> <div>94%</div> <div>5%</div> </div>
2	D	214	<div> <div>%</div> <div>91%</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14451 atoms, of which 6461 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 HEPC74 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	218	Total	C	H	N	O	S	0	0	0
			3205	1014	1592	271	320	8			
1	C	229	Total	C	H	N	O	S	0	0	0
			3362	1061	1671	284	338	8			

- Molecule 2 is a protein called antibody HEPC74 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	213	Total	C	H	N	O	S	0	0	0
			3243	1034	1599	274	331	5			
2	D	213	Total	C	H	N	O	S	0	0	0
			3243	1034	1599	274	331	5			

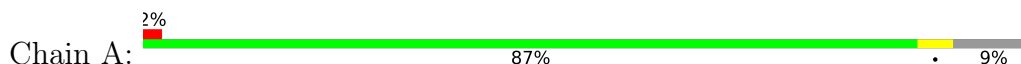
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	329	Total	O	0	0
			329	329		
3	B	398	Total	O	0	0
			398	398		
3	C	331	Total	O	0	0
			331	331		
3	D	340	Total	O	0	0
			340	340		

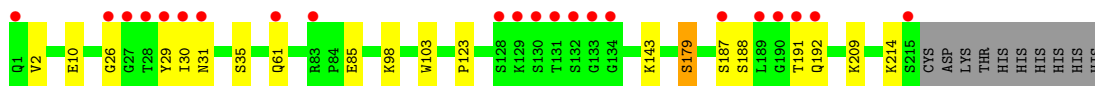
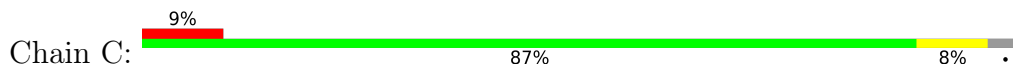
3 Residue-property plots [i](#)

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.

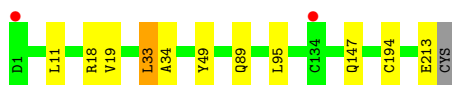
- Molecule 1: antibody HEPC74 Heavy Chain



- Molecule 1: antibody HEPC74 Heavy Chain



- Molecule 2: antibody HEPC74 Light Chain



- Molecule 2: antibody HEPC74 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.13Å 63.59Å 73.76Å 80.31° 74.11° 83.73°	Depositor
Resolution (Å)	35.10 – 1.36 35.10 – 1.36	Depositor EDS
% Data completeness (in resolution range)	93.7 (35.10-1.36) 93.7 (35.10-1.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 1.36Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.167 , 0.191 0.167 , 0.191	Depositor DCC
R_{free} test set	9561 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	14451	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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	0.45	0/1649	0.66	1/2249 (0.0%)
1	C	0.48	0/1730	0.65	0/2361
2	B	0.54	1/1682 (0.1%)	0.69	1/2286 (0.0%)
2	D	0.53	1/1682 (0.1%)	0.69	1/2286 (0.0%)
All	All	0.50	2/6743 (0.0%)	0.67	3/9182 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	194	CYS	CB-SG	-5.52	1.72	1.81
2	D	194	CYS	CB-SG	-5.40	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	LEU	CA-CB-CG	6.84	131.03	115.30
2	D	33	LEU	CA-CB-CG	-6.40	100.57	115.30
2	B	33	LEU	CA-CB-CG	-5.91	101.71	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1613	1592	1590	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1691	1671	1671	18	0
2	B	1644	1599	1599	12	0
2	D	1644	1599	1599	16	0
3	A	329	0	0	5	3
3	B	398	0	0	5	3
3	C	331	0	0	13	5
3	D	340	0	0	10	1
All	All	7990	6461	6459	51	6

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 4.

All (51) 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:143:GLU:OE2	3:D:301:HOH:O	1.90	0.88
1:C:85:GLU:OE2	3:C:302:HOH:O	1.99	0.80
2:B:213:GLU:OE2	3:B:301:HOH:O	2.06	0.74
2:D:1:ASP:HB2	3:D:534:HOH:O	1.87	0.74
1:A:156:SER:OG	3:A:301:HOH:O	2.05	0.73
2:B:147:GLN:NE2	3:B:302:HOH:O	2.08	0.71
1:A:83:ARG:NH1	3:A:304:HOH:O	2.19	0.70
1:A:64:GLN:O	3:A:303:HOH:O	2.10	0.70
2:D:123:GLU:OE1	3:D:302:HOH:O	2.13	0.67
1:C:10:GLU:OE1	3:C:304:HOH:O	2.12	0.66
1:C:30:ILE:N	3:C:303:HOH:O	2.10	0.65
1:C:61:GLN:HG3	3:C:486:HOH:O	1.96	0.64
2:D:167:ASP:OD1	3:D:303:HOH:O	2.16	0.62
1:C:31:ASN:ND2	3:C:305:HOH:O	2.15	0.59
2:D:162:SER:HB3	3:D:305:HOH:O	2.03	0.59
1:C:98:LYS:NZ	3:C:311:HOH:O	2.37	0.57
1:A:100(H):LEU:HD21	2:B:49:TYR:CB	2.37	0.54
2:B:11:LEU:CD2	2:B:19:VAL:HG13	2.38	0.53
1:C:143:LYS:HE3	3:C:372:HOH:O	2.09	0.53
1:A:151:THR:HG23	3:A:393:HOH:O	2.08	0.53
3:B:335:HOH:O	2:D:11:LEU:HD12	2.11	0.51
2:D:142:ARG:NH2	2:D:163:VAL:HG11	2.25	0.51
2:D:33:LEU:HG	2:D:34:ALA:N	2.26	0.50
1:A:68:THR:HG21	3:A:590:HOH:O	2.11	0.50
2:D:24:ARG:NE	2:D:70:GLU:OE2	2.46	0.49
1:A:100(H):LEU:HD21	2:B:49:TYR:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:187:GLU:OE1	3:D:304:HOH:O	2.20	0.48
1:A:100(H):LEU:HD21	2:B:49:TYR:HB2	1.96	0.48
2:B:18:ARG:NE	3:B:304:HOH:O	2.22	0.47
1:C:29:TYR:HB3	3:C:303:HOH:O	2.14	0.47
1:A:80:MET:HE2	1:A:82:LEU:HB2	1.97	0.46
2:D:48:ILE:HD12	2:D:73:LEU:CD1	2.45	0.46
2:D:142:ARG:CZ	3:D:316:HOH:O	2.63	0.46
1:C:123:PRO:HD3	1:C:209:LYS:HE2	1.97	0.46
2:B:18:ARG:NH2	3:B:304:HOH:O	2.40	0.46
1:A:100(H):LEU:CD2	2:B:49:TYR:HB3	2.47	0.45
1:C:179:SER:HB2	3:D:338:HOH:O	2.17	0.44
1:C:85:GLU:CG	3:C:456:HOH:O	2.66	0.44
2:D:142:ARG:HH21	2:D:163:VAL:HG11	1.82	0.44
2:B:33:LEU:HG	2:B:34:ALA:N	2.32	0.44
2:D:27:GLN:HG3	3:D:361:HOH:O	2.18	0.44
1:C:187:SER:OG	3:C:306:HOH:O	2.21	0.43
1:C:85:GLU:HG2	3:C:456:HOH:O	2.17	0.42
1:C:103:TRP:CZ2	2:D:44:PRO:HG2	2.54	0.42
2:D:142:ARG:NH2	3:D:316:HOH:O	2.51	0.42
2:B:11:LEU:HD21	2:B:19:VAL:HG13	2.02	0.42
1:C:214:LYS:NZ	3:C:301:HOH:O	1.98	0.41
1:C:209:LYS:HD3	3:C:307:HOH:O	2.19	0.41
1:C:188:SER:HB2	1:C:192:GLN:CD	2.40	0.41
2:B:95:LEU:HD12	2:B:95:LEU:C	2.41	0.41
1:C:2:VAL:HG12	1:C:26:GLY:O	2.21	0.41

All (6) 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)
3:A:496:HOH:O	3:D:410:HOH:O[1_546]	1.64	0.56
3:B:538:HOH:O	3:C:576:HOH:O[1_456]	1.76	0.44
3:A:466:HOH:O	3:C:551:HOH:O[1_556]	2.08	0.12
3:B:516:HOH:O	3:C:607:HOH:O[1_456]	2.10	0.10
3:A:609:HOH:O	3:C:603:HOH:O[1_446]	2.17	0.03
3:B:635:HOH:O	3:C:555:HOH:O[1_456]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	212/239 (89%)	209 (99%)	3 (1%)	0	100	100
1	C	227/239 (95%)	222 (98%)	5 (2%)	0	100	100
2	B	211/214 (99%)	207 (98%)	4 (2%)	0	100	100
2	D	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
All	All	861/906 (95%)	843 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	185/204 (91%)	183 (99%)	2 (1%)	73	45
1	C	194/204 (95%)	191 (98%)	3 (2%)	65	33
2	B	188/189 (100%)	187 (100%)	1 (0%)	88	74
2	D	188/189 (100%)	187 (100%)	1 (0%)	88	74
All	All	755/786 (96%)	748 (99%)	7 (1%)	78	53

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	178	LEU

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Mol	Chain	Res	Type
2	B	89	GLN
1	C	35	SER
1	C	179	SER
1	C	191	THR
2	D	42	ARG

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

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 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

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	A	218/239 (91%)	0.06	5 (2%) 60 66	13, 23, 51, 70	0
1	C	229/239 (95%)	0.40	22 (9%) 8 10	15, 23, 61, 81	0
2	B	213/214 (99%)	-0.09	2 (0%) 84 87	11, 17, 36, 61	0
2	D	213/214 (99%)	-0.06	3 (1%) 75 80	14, 22, 41, 68	0
All	All	873/906 (96%)	0.08	32 (3%) 41 47	11, 21, 49, 81	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	132	SER	12.2
1	C	27	GLY	9.5
1	C	29	TYR	9.3
1	C	131	THR	9.2
1	C	133	GLY	7.2
1	C	28	THR	7.1
1	C	30	ILE	5.9
1	C	129	LYS	5.7
1	A	26	GLY	5.3
1	C	130	SER	4.8
1	A	215	SER	4.5
1	C	134	GLY	4.2
1	C	190	GLY	4.2
2	D	1	ASP	3.9
1	C	128	SER	3.8
2	B	134	CYS	3.6
2	B	1	ASP	3.5
1	C	191	THR	3.0
1	C	187	SER	3.0
1	C	26	GLY	2.8
1	C	215	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	61	GLN	2.6
1	C	31	ASN	2.5
1	C	83	ARG	2.5
2	D	88	CYS	2.3
1	C	1	GLN	2.2
1	A	191	THR	2.2
1	C	192	GLN	2.2
1	A	214	LYS	2.2
1	C	189	LEU	2.1
1	A	31	ASN	2.1
2	D	194	CYS	2.1

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.