



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2025 – 04:34 PM EST

PDB ID : 9BDI
Title : Crystal structure of HIV-1 MPER scaffold in complex with antibody Fab Ab45.2
Authors : Lee, C.C.D.; Wilson, I.A.
Deposited on : 2024-04-11
Resolution : 2.07 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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

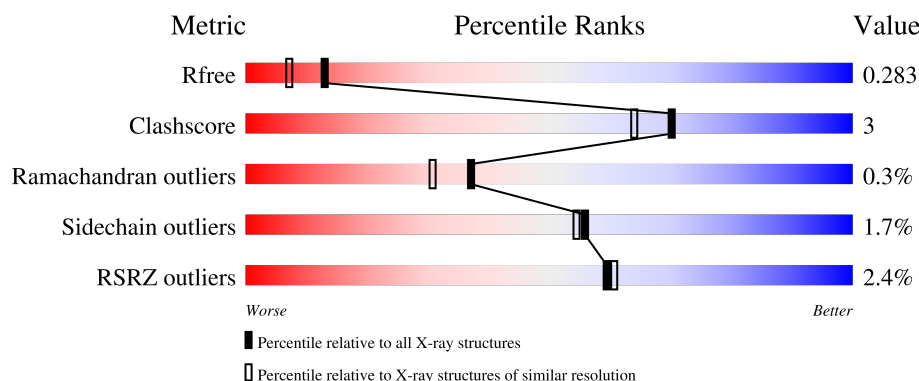
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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}	164625	3436 (2.08-2.04)
Clashscore	180529	3661 (2.08-2.04)
Ramachandran outliers	177936	3649 (2.08-2.04)
Sidechain outliers	177891	3649 (2.08-2.04)
RSRZ outliers	164620	3436 (2.08-2.04)

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	153	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	B	153	<div> <div>4%</div> <div> <div></div> <div>84%</div> <div>15%</div> </div> </div>
2	C	234	<div> <div>%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> </div>
2	H	234	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
3	D	214	<div> <div>3%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	L	214	<div><div></div><div>2%</div><div>91%</div><div>9%</div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9996 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 GT10.2 glycan KO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	1	0
			1243	798	212	229	4			
1	B	153	Total	C	N	O	S	0	1	0
			1243	798	212	229	4			

- Molecule 2 is a protein called Fab 45.2 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	234	Total	C	N	O	S	0	0	0
			1760	1112	295	345	8			
2	H	234	Total	C	N	O	S	0	0	0
			1760	1112	295	345	8			

- Molecule 3 is a protein called Fab 45.2 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	214	Total	C	N	O	S	0	0	0
			1649	1035	276	332	6			
3	L	214	Total	C	N	O	S	0	0	0
			1649	1035	276	332	6			

- Molecule 4 is water.

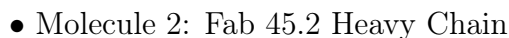
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	72	Total	O	0	0
			72	72		
4	C	150	Total	O	0	0
			150	150		
4	D	125	Total	O	0	0
			125	125		

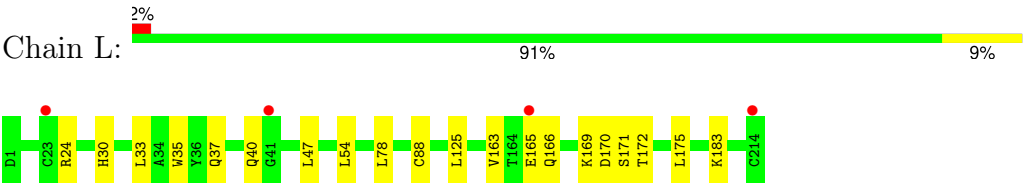
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	141	Total 141	O 141	0	0
4	L	130	Total 130	O 130	0	0

- Molecule 1: GT10.2 glycan KO





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	37.62Å 46.64Å 178.35Å 86.67° 86.76° 77.04°	Depositor
Resolution (Å)	44.47 – 2.07 44.47 – 2.07	Depositor EDS
% Data completeness (in resolution range)	85.8 (44.47-2.07) 87.5 (44.47-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, R_{free}	0.235 , 0.283 0.237 , 0.283	Depositor DCC
R_{free} test set	3507 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9996	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 99.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1104e-12. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.26	0/1272	0.52	0/1724
1	B	0.27	0/1272	0.51	0/1724
2	C	0.27	0/1805	0.52	0/2456
2	H	0.28	0/1805	0.52	0/2456
3	D	0.27	0/1686	0.50	0/2289
3	L	0.28	0/1686	0.50	0/2289
All	All	0.27	0/9526	0.51	0/12938

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	A	1243	0	1258	11	2
1	B	1243	0	1258	13	1
2	C	1760	0	1714	12	0
2	H	1760	0	1714	8	1
3	D	1649	0	1597	8	1
3	L	1649	0	1597	9	1
4	A	74	0	0	2	0
4	B	72	0	0	2	0
4	C	150	0	0	2	0
4	D	125	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	141	0	0	2	0
4	L	130	0	0	0	0
All	All	9996	0	9138	60	3

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 3.

All (60) 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:A:29:GLU:OE2	4:A:201:HOH:O	2.09	0.70
3:D:33:LEU:HD11	3:D:88:CYS:HB2	1.73	0.69
1:B:29:GLU:OE2	4:B:201:HOH:O	2.10	0.68
2:C:135:LYS:NZ	4:C:302:HOH:O	2.30	0.65
1:B:142:GLN:HG2	1:B:143:LEU:HD12	1.80	0.64
2:C:64:ALA:HA	2:C:67:LYS:HG2	1.79	0.63
3:L:33:LEU:HD11	3:L:88:CYS:HB2	1.81	0.62
1:A:142:GLN:HG2	1:A:143:LEU:HD12	1.85	0.58
1:B:34[A]:ARG:HH21	1:B:55:LEU:HD11	1.70	0.57
1:B:28:ALA:O	1:B:32:ILE:HG12	2.07	0.53
2:H:166:GLU:OE1	4:H:301:HOH:O	2.19	0.53
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.91	0.52
1:B:98:TRP:O	1:B:102:VAL:HG23	2.10	0.51
1:A:45:LYS:HD3	1:A:115:GLU:HG3	1.93	0.50
2:C:189:GLN:HE21	3:D:160:GLN:HE22	1.57	0.50
3:L:165:GLU:N	3:L:165:GLU:OE1	2.44	0.50
3:D:145:LYS:HB3	3:D:197:THR:HB	1.94	0.50
3:D:123:GLU:OE2	4:D:301:HOH:O	2.20	0.49
1:B:71:LYS:HG3	1:B:72:PRO:HD2	1.94	0.48
3:D:120:PRO:HD3	3:D:132:VAL:HG22	1.95	0.48
1:A:71:LYS:HG3	1:A:72:PRO:HD2	1.96	0.48
1:A:98:TRP:O	1:A:102:VAL:HG23	2.14	0.48
1:A:34[A]:ARG:HH21	1:A:55:LEU:HD11	1.80	0.47
2:H:43:LYS:HB3	2:H:43:LYS:HE2	1.71	0.47
1:A:115:GLU:O	1:A:119:LYS:HG2	2.14	0.47
2:C:34:MET:HB3	2:C:81:LEU:HD22	1.96	0.47
2:H:91:GLU:OE1	2:H:91:GLU:N	2.41	0.47
1:B:53:HIS:HB3	1:B:93:LEU:HB2	1.98	0.45
2:H:159:LEU:CD1	2:H:161:LYS:HB2	2.47	0.45
1:A:156:LEU:OXT	4:A:202:HOH:O	2.20	0.44
2:C:13:LYS:HD2	2:C:13:LYS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LEU:O	1:B:145:GLY:N	2.50	0.44
1:A:5:THR:O	1:A:9:ILE:HG12	2.18	0.43
3:L:125:LEU:HB3	3:L:183:LYS:HE2	2.00	0.43
1:A:39:PRO:HB3	1:A:76:GLU:HB3	2.00	0.43
1:B:115:GLU:O	1:B:119:LYS:HG2	2.18	0.43
2:C:159:LEU:CD1	2:C:161:LYS:HB2	2.48	0.43
2:H:135:LYS:NZ	4:H:310:HOH:O	2.51	0.43
1:A:143:LEU:O	1:A:145:GLY:N	2.52	0.43
2:C:6:GLU:OE2	2:C:122:GLY:HA3	2.18	0.43
3:L:166:GLN:HG2	3:L:171:SER:HA	2.01	0.42
1:B:34[B]:ARG:NH2	4:B:211:HOH:O	2.52	0.42
1:B:151:GLU:OE1	1:B:151:GLU:N	2.34	0.42
1:B:33:ALA:O	1:B:37:ARG:HG3	2.20	0.42
2:C:91:GLU:OE1	2:C:91:GLU:N	2.48	0.42
2:C:143:ALA:HB3	2:C:232:LYS:HE2	2.01	0.42
1:B:34[A]:ARG:NH1	1:B:38:SER:OG	2.53	0.42
3:D:90:TYR:CZ	3:D:92:TRP:HB3	2.55	0.42
2:H:6:GLU:OE2	2:H:122:GLY:HA3	2.20	0.42
2:H:140:PHE:HD2	2:H:159:LEU:HD12	1.85	0.41
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.56	0.41
2:C:12:VAL:HG11	2:C:88:LEU:HD13	2.03	0.41
2:C:140:PHE:HD2	2:C:159:LEU:HD12	1.86	0.41
2:C:189:GLN:HB3	4:C:333:HOH:O	2.20	0.41
3:D:166:GLN:HG2	3:D:171:SER:HA	2.03	0.41
3:D:140:TYR:CG	3:D:141:PRO:HA	2.56	0.41
2:H:34:MET:HB3	2:H:81:LEU:HD22	2.02	0.41
3:L:37:GLN:HB2	3:L:47:LEU:HD11	2.02	0.40
3:L:170:ASP:OD2	3:L:172:THR:OG1	2.28	0.40
3:L:54:LEU:HD12	3:L:54:LEU:HA	1.87	0.40

All (3) 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:A:80:GLN:NE2	3:L:30:HIS:O[1_655]	2.10	0.10
1:A:106:LYS:NZ	2:H:105:TYR:OH[1_655]	2.12	0.08
1:B:80:GLN:NE2	3:D:30:HIS:O[1_655]	2.16	0.04

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	152/153 (99%)	149 (98%)	1 (1%)	2 (1%)	10	3
1	B	152/153 (99%)	150 (99%)	1 (1%)	1 (1%)	19	10
2	C	232/234 (99%)	229 (99%)	3 (1%)	0	100	100
2	H	232/234 (99%)	228 (98%)	4 (2%)	0	100	100
3	D	212/214 (99%)	207 (98%)	4 (2%)	1 (0%)	25	17
3	L	212/214 (99%)	209 (99%)	3 (1%)	0	100	100
All	All	1192/1202 (99%)	1172 (98%)	16 (1%)	4 (0%)	37	31

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	B	144	SER
3	D	213	GLU
1	A	83	ASP

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	136/135 (101%)	136 (100%)	0	100	100
1	B	136/135 (101%)	133 (98%)	3 (2%)	47	43
2	C	196/196 (100%)	193 (98%)	3 (2%)	60	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	196/196 (100%)	191 (97%)	5 (3%)	41	37
3	D	186/186 (100%)	183 (98%)	3 (2%)	58	57
3	L	186/186 (100%)	182 (98%)	4 (2%)	47	43
All	All	1036/1034 (100%)	1018 (98%)	18 (2%)	56	54

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

Mol	Chain	Res	Type
1	B	73	VAL
1	B	119	LYS
1	B	154	ARG
2	C	13	LYS
2	C	150	SER
2	C	187	VAL
3	D	24	ARG
3	D	78	LEU
3	D	169	LYS
2	H	13	LYS
2	H	45	LEU
2	H	153	THR
2	H	187	VAL
2	H	201	THR
3	L	24	ARG
3	L	40	GLN
3	L	78	LEU
3	L	169	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	119	GLN
2	C	189	GLN
3	D	160	GLN
2	H	119	GLN

5.3.3 RNA ⓘ

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	A	153/153 (100%)	0.17	9 (5%)	29	30	17, 29, 51, 72	1 (0%)
1	B	153/153 (100%)	0.16	6 (3%)	44	45	17, 29, 49, 57	1 (0%)
2	C	234/234 (100%)	-0.09	2 (0%)	81	83	18, 26, 39, 79	0
2	H	234/234 (100%)	-0.09	2 (0%)	81	83	16, 26, 37, 76	0
3	D	214/214 (100%)	-0.04	6 (2%)	55	56	17, 25, 44, 59	0
3	L	214/214 (100%)	-0.07	4 (1%)	66	68	17, 25, 42, 56	0
All	All	1202/1202 (100%)	-0.01	29 (2%)	59	61	16, 26, 43, 79	2 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	234	CYS	8.9
2	H	234	CYS	7.9
1	B	56	GLY	5.1
3	L	23	CYS	5.0
1	A	56	GLY	4.7
3	D	23	CYS	4.6
3	L	214	CYS	4.1
3	D	214	CYS	4.1
1	A	143	LEU	4.0
3	L	41	GLY	3.5
1	B	143	LEU	3.5
1	A	106	LYS	3.5
1	B	82	PRO	3.2
3	D	41	GLY	3.2
1	A	82	PRO	3.1
1	A	83	ASP	3.1
3	L	165	GLU	2.9
1	A	4	VAL	2.8
1	B	46	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	165	GLU	2.5
1	A	46	GLY	2.3
1	A	98	TRP	2.3
1	B	116	GLU	2.3
1	B	45	LYS	2.3
2	C	208	GLY	2.2
2	H	208	GLY	2.1
3	D	42	LYS	2.1
3	D	56	ASP	2.0
1	A	36	ASP	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 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.