



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 10, 2020 – 08:49 AM BST

PDB ID : 3UAJ
Title : Crystal structure of the envelope glycoprotein ectodomain from dengue virus serotype 4 in complex with the fab fragment of the chimpanzee monoclonal antibody 5H2
Authors : Cockburn, J.J.B.; Stura, E.A.; Navarro-Sanchez, M.E.; Rey, F.A.
Deposited on : 2011-10-21
Resolution : 3.23 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

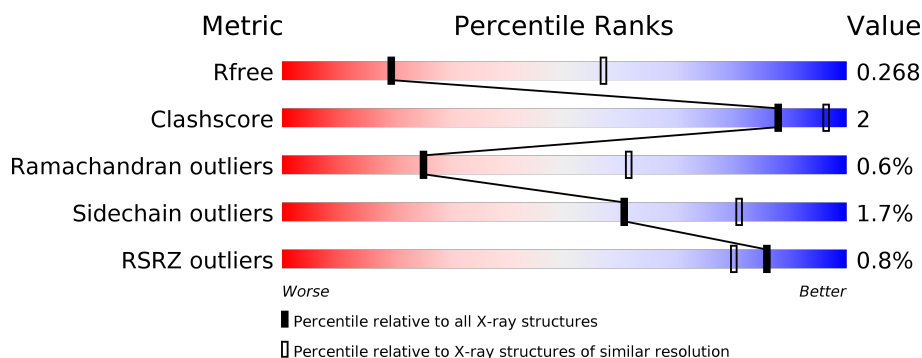
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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 $\leq 5\%$. 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	433	
1	B	433	
2	C	236	
2	H	236	
3	D	215	
3	L	215	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12314 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 envelope protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	371	Total	C	N	O	S	0	0	0
			2856	1801	493	537	25			
1	A	375	Total	C	N	O	S	0	0	0
			2882	1814	498	545	25			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	396	PRO	-	expression tag	UNP Q91AI1
B	397	PHE	-	expression tag	UNP Q91AI1
B	398	GLU	-	expression tag	UNP Q91AI1
B	399	ASP	-	expression tag	UNP Q91AI1
B	400	ASP	-	expression tag	UNP Q91AI1
B	401	ASP	-	expression tag	UNP Q91AI1
B	402	ASP	-	expression tag	UNP Q91AI1
B	403	LYS	-	expression tag	UNP Q91AI1
B	404	ALA	-	expression tag	UNP Q91AI1
B	405	GLY	-	expression tag	UNP Q91AI1
B	406	TRP	-	expression tag	UNP Q91AI1
B	407	SER	-	expression tag	UNP Q91AI1
B	408	HIS	-	expression tag	UNP Q91AI1
B	409	PRO	-	expression tag	UNP Q91AI1
B	410	GLN	-	expression tag	UNP Q91AI1
B	411	PHE	-	expression tag	UNP Q91AI1
B	412	GLU	-	expression tag	UNP Q91AI1
B	413	LYS	-	expression tag	UNP Q91AI1
B	414	GLY	-	expression tag	UNP Q91AI1
B	415	GLY	-	expression tag	UNP Q91AI1
B	416	GLY	-	expression tag	UNP Q91AI1
B	417	SER	-	expression tag	UNP Q91AI1
B	418	GLY	-	expression tag	UNP Q91AI1
B	419	GLY	-	expression tag	UNP Q91AI1
B	420	GLY	-	expression tag	UNP Q91AI1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	421	SER	-	expression tag	UNP Q91AI1
B	422	GLY	-	expression tag	UNP Q91AI1
B	423	GLY	-	expression tag	UNP Q91AI1
B	424	GLY	-	expression tag	UNP Q91AI1
B	425	SER	-	expression tag	UNP Q91AI1
B	426	TRP	-	expression tag	UNP Q91AI1
B	427	SER	-	expression tag	UNP Q91AI1
B	428	HIS	-	expression tag	UNP Q91AI1
B	429	PRO	-	expression tag	UNP Q91AI1
B	430	GLN	-	expression tag	UNP Q91AI1
B	431	PHE	-	expression tag	UNP Q91AI1
B	432	GLU	-	expression tag	UNP Q91AI1
B	433	LYS	-	expression tag	UNP Q91AI1
A	396	PRO	-	expression tag	UNP Q91AI1
A	397	PHE	-	expression tag	UNP Q91AI1
A	398	GLU	-	expression tag	UNP Q91AI1
A	399	ASP	-	expression tag	UNP Q91AI1
A	400	ASP	-	expression tag	UNP Q91AI1
A	401	ASP	-	expression tag	UNP Q91AI1
A	402	ASP	-	expression tag	UNP Q91AI1
A	403	LYS	-	expression tag	UNP Q91AI1
A	404	ALA	-	expression tag	UNP Q91AI1
A	405	GLY	-	expression tag	UNP Q91AI1
A	406	TRP	-	expression tag	UNP Q91AI1
A	407	SER	-	expression tag	UNP Q91AI1
A	408	HIS	-	expression tag	UNP Q91AI1
A	409	PRO	-	expression tag	UNP Q91AI1
A	410	GLN	-	expression tag	UNP Q91AI1
A	411	PHE	-	expression tag	UNP Q91AI1
A	412	GLU	-	expression tag	UNP Q91AI1
A	413	LYS	-	expression tag	UNP Q91AI1
A	414	GLY	-	expression tag	UNP Q91AI1
A	415	GLY	-	expression tag	UNP Q91AI1
A	416	GLY	-	expression tag	UNP Q91AI1
A	417	SER	-	expression tag	UNP Q91AI1
A	418	GLY	-	expression tag	UNP Q91AI1
A	419	GLY	-	expression tag	UNP Q91AI1
A	420	GLY	-	expression tag	UNP Q91AI1
A	421	SER	-	expression tag	UNP Q91AI1
A	422	GLY	-	expression tag	UNP Q91AI1
A	423	GLY	-	expression tag	UNP Q91AI1
A	424	GLY	-	expression tag	UNP Q91AI1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	425	SER	-	expression tag	UNP Q91AI1
A	426	TRP	-	expression tag	UNP Q91AI1
A	427	SER	-	expression tag	UNP Q91AI1
A	428	HIS	-	expression tag	UNP Q91AI1
A	429	PRO	-	expression tag	UNP Q91AI1
A	430	GLN	-	expression tag	UNP Q91AI1
A	431	PHE	-	expression tag	UNP Q91AI1
A	432	GLU	-	expression tag	UNP Q91AI1
A	433	LYS	-	expression tag	UNP Q91AI1

- Molecule 2 is a protein called Heavy chain, monoclonal antibody 5H2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1627	1030	268	325	4			
2	C	220	Total	C	N	O	S	0	0	0
			1636	1036	270	326	4			

- Molecule 3 is a protein called Light chain, monoclonal antibody 5H2.

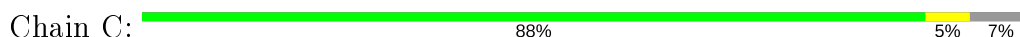
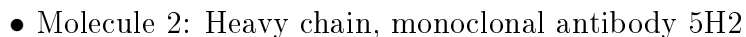
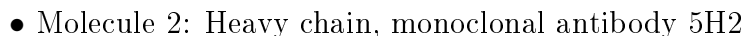
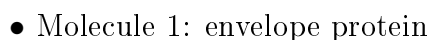
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1639	1024	275	335	5			
3	D	214	Total	C	N	O	S	0	0	0
			1646	1027	276	337	6			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



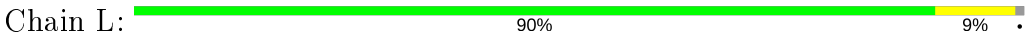
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 1: envelope protein

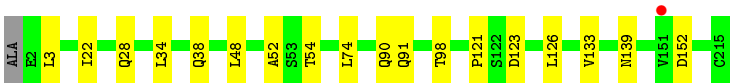
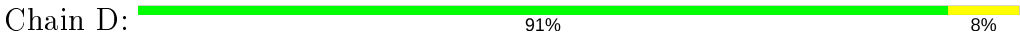




- Molecule 3: Light chain, monoclonal antibody 5H2



- Molecule 3: Light chain, monoclonal antibody 5H2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.11Å 134.75Å 106.08Å 90.00° 106.70° 90.00°	Depositor
Resolution (Å)	47.74 – 3.23 47.74 – 3.23	Depositor EDS
% Data completeness (in resolution range)	96.9 (47.74-3.23) 97.1 (47.74-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.25Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.3, BUSTER 2.9.3	Depositor
R, R_{free}	0.241 , 0.246 0.260 , 0.268	Depositor DCC
R_{free} test set	1986 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 12.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12314	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.35	0/2936	0.53	0/3967
1	B	0.35	0/2911	0.53	0/3934
2	C	0.34	0/1674	0.54	0/2285
2	H	0.35	0/1665	0.55	0/2274
3	D	0.35	0/1680	0.56	0/2278
3	L	0.35	0/1673	0.55	0/2270
All	All	0.35	0/12539	0.54	0/17008

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	2882	0	2865	13	0
1	B	2856	0	2845	11	0
2	C	1636	0	1621	6	0
2	H	1627	0	1608	7	0
3	D	1646	0	1594	6	0
3	L	1639	0	1589	8	0
4	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
All	All	12314	0	12148	48	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 2.

The worst 5 of 48 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)
3:L:38:GLN:HB2	3:L:48:LEU:HD11	1.79	0.65
3:D:38:GLN:HB2	3:D:48:LEU:HD11	1.79	0.64
2:H:14:PRO:HD2	2:H:123:LEU:HG	1.87	0.56
2:C:14:PRO:HD2	2:C:123:LEU:HG	1.88	0.56
1:B:140:VAL:HG22	1:B:161:THR:HG22	1.89	0.54

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	A	367/433 (85%)	350 (95%)	15 (4%)	2 (0%)	29	64
1	B	363/433 (84%)	348 (96%)	12 (3%)	3 (1%)	19	55
2	C	216/236 (92%)	205 (95%)	11 (5%)	0	100	100
2	H	215/236 (91%)	202 (94%)	12 (6%)	1 (0%)	29	64
3	D	212/215 (99%)	199 (94%)	11 (5%)	2 (1%)	17	52
3	L	211/215 (98%)	197 (93%)	12 (6%)	2 (1%)	17	52
All	All	1584/1768 (90%)	1501 (95%)	73 (5%)	10 (1%)	25	61

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	139	ASN
3	D	139	ASN
1	B	202	LYS
1	A	202	LYS
1	B	67	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	A	317/360 (88%)	310 (98%)	7 (2%)	52	76
1	B	315/360 (88%)	310 (98%)	5 (2%)	62	82
2	C	187/203 (92%)	185 (99%)	2 (1%)	73	87
2	H	186/203 (92%)	183 (98%)	3 (2%)	62	82
3	D	188/188 (100%)	184 (98%)	4 (2%)	53	77
3	L	187/188 (100%)	184 (98%)	3 (2%)	62	82
All	All	1380/1502 (92%)	1356 (98%)	24 (2%)	60	81

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	152	ASP
1	A	70	THR
3	D	90	GLN
1	A	23	LEU
1	A	55	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	134	ASN
3	L	93	ASN
3	L	138	ASN
3	L	172	ASN

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Mol	Chain	Res	Type
3	D	28	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1001	1	14,14,15	1.26	1 (7%)	17,19,21	1.01	2 (11%)
4	NAG	B	1001	1	14,14,15	1.20	1 (7%)	17,19,21	0.82	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1001	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAG	C1-C2	3.40	1.57	1.52
4	B	1001	NAG	C1-C2	2.96	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C2-N2-C7	2.17	125.99	122.90
4	A	1001	NAG	C4-C3-C2	2.06	114.03	111.02
4	B	1001	NAG	C4-C3-C2	2.02	113.98	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	375/433 (86%)	0.28	2 (0%) 91 87	57, 73, 87, 111	0
1	B	371/433 (85%)	0.30	9 (2%) 59 47	53, 80, 99, 111	0
2	C	220/236 (93%)	0.03	0 100 100	45, 58, 79, 95	0
2	H	219/236 (92%)	0.10	1 (0%) 91 87	45, 59, 75, 94	0
3	D	214/215 (99%)	0.09	1 (0%) 91 87	49, 62, 79, 86	0
3	L	213/215 (99%)	0.11	0 100 100	51, 64, 77, 85	0
All	All	1612/1768 (91%)	0.18	13 (0%) 86 80	45, 67, 90, 111	0

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	THR	3.4
2	H	143	GLY	3.1
1	B	276	ASN	2.5
1	B	88	GLN	2.4
1	B	240	PHE	2.4

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	1001	14/15	0.79	0.34	93,96,99,99	0
4	NAG	B	1001	14/15	0.87	0.32	102,106,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.