



wwPDB X-ray Structure Validation Summary Report

Apr 17, 2014 – 07:50 AM EDT

PDB ID : 4OII
Title : West Nile Virus NS1 in complex with neutralizing 22NS1 antibody Fab
Authors : Edeling, M.A.; Fremont, D.H.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-01-19
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

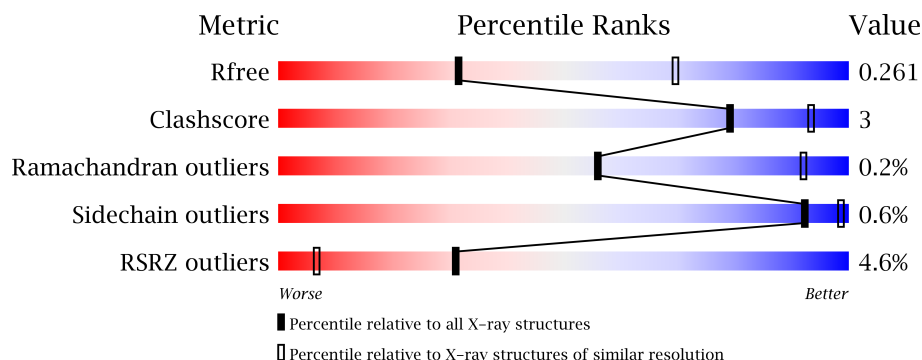
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	185	
1	B	185	
2	L	213	
2	M	213	
3	H	217	
3	I	217	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9455 atoms, of which 0 are hydrogen and 0 are deuterium.

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 NON-STRUCTURAL PROTEIN NS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1398	865	250	274	9			
1	B	177	Total	C	N	O	S	0	0	0
			1398	865	250	274	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	MET	-	EXPRESSION TAG	UNP U3N977
A	169	ALA	-	EXPRESSION TAG	UNP U3N977
A	170	SER	-	EXPRESSION TAG	UNP U3N977
A	171	MET	-	EXPRESSION TAG	UNP U3N977
B	168	MET	-	EXPRESSION TAG	UNP U3N977
B	169	ALA	-	EXPRESSION TAG	UNP U3N977
B	170	SER	-	EXPRESSION TAG	UNP U3N977
B	171	MET	-	EXPRESSION TAG	UNP U3N977

- Molecule 2 is a protein called Light Chain of Fab fragment of 22NS1 Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1655	1031	283	335	6			
2	M	213	Total	C	N	O	S	0	0	0
			1655	1031	283	335	6			

- Molecule 3 is a protein called Heavy Chain of Fab fragment of 22NS1 Antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	217	Total	C	N	O	S	0	0	0
			1641	1041	268	325	7			
3	I	217	Total	C	N	O	S	0	0	0
			1641	1041	268	325	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total 19	O 19	0	0
4	B	16	Total 16	O 16	0	0
4	L	15	Total 15	O 15	0	0
4	H	15	Total 15	O 15	0	0
4	M	1	Total 1	O 1	0	0
4	I	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: NON-STRUCTURAL PROTEIN NS1

Chain A: 



- Molecule 1: NON-STRUCTURAL PROTEIN NS1

Chain B: 



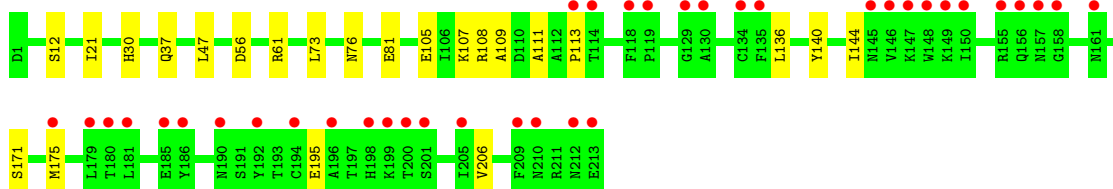
- Molecule 2: Light Chain of Fab fragment of 22NS1 Antibody

Chain L: 



- Molecule 2: Light Chain of Fab fragment of 22NS1 Antibody

Chain M: 



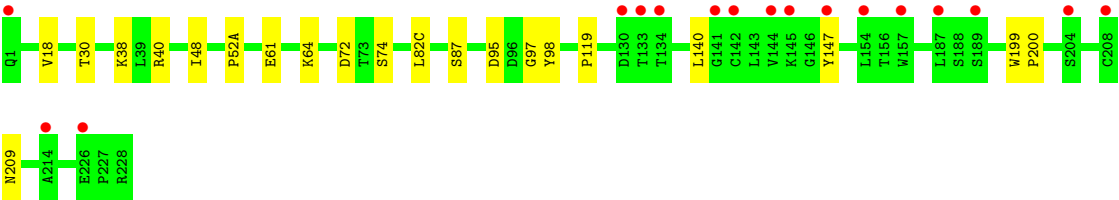
- Molecule 3: Heavy Chain of Fab fragment of 22NS1 Antibody

Chain H: 



- Molecule 3: Heavy Chain of Fab fragment of 22NS1 Antibody

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.87Å 49.55Å 130.07Å 90.00° 91.21° 90.00°	Depositor
Resolution (Å)	49.47 – 3.00 49.47 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.47-3.00) 99.9 (49.47-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.214 , 0.265 0.210 , 0.261	Depositor DCC
R_{free} test set	1428 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.0	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28187 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9455	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.22	0/1432	0.42	0/1952
1	B	0.21	0/1432	0.42	0/1952
2	L	0.24	0/1694	0.42	0/2300
2	M	0.24	0/1694	0.42	0/2300
3	H	0.22	0/1686	0.41	0/2306
3	I	0.22	0/1686	0.41	0/2306
All	All	0.22	0/9624	0.42	0/13116

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1398	0	1335	8	0
1	B	1398	0	1335	10	0
2	L	1655	0	1582	15	0
2	M	1655	0	1582	14	0
3	H	1641	0	1596	10	0
3	I	1641	0	1596	10	0
4	A	19	0	0	0	0
4	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	15	0	0	0	0
4	I	1	0	0	0	0
4	L	15	0	0	0	0
4	M	1	0	0	0	0
All	All	9455	0	9026	64	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 64 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:323:TYR:HB2	1:B:330:TRP:HB2	1.68	0.75
1:A:323:TYR:HB2	1:A:330:TRP:HB2	1.68	0.74
2:M:21:ILE:HD11	2:M:73:LEU:HD23	1.77	0.67
2:L:21:ILE:HD11	2:L:73:LEU:HD23	1.77	0.67
1:A:289:GLU:HG3	2:L:56:ASP:HB2	1.83	0.61

There are no symmetry-related clashes.

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	175/185 (95%)	161 (92%)	14 (8%)	0	100	100
1	B	175/185 (95%)	160 (91%)	15 (9%)	0	100	100
2	L	211/213 (99%)	204 (97%)	7 (3%)	0	100	100
2	M	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
3	H	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	38	84
3	I	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	38	84
All	All	1202/1230 (98%)	1148 (96%)	52 (4%)	2 (0%)	56	92

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	97	GLY
3	I	97	GLY

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	157/164 (96%)	155 (99%)	2 (1%)	80	96
1	B	157/164 (96%)	156 (99%)	1 (1%)	92	98
2	L	187/187 (100%)	186 (100%)	1 (0%)	94	99
2	M	187/187 (100%)	186 (100%)	1 (0%)	94	99
3	H	186/186 (100%)	186 (100%)	0	100	100
3	I	186/186 (100%)	185 (100%)	1 (0%)	94	99
All	All	1060/1074 (99%)	1054 (99%)	6 (1%)	92	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	176	THR
3	I	209	ASN
2	L	81	GLU
1	A	269	ASP
2	M	81	GLU

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

Mol	Chain	Res	Type
1	A	265	GLN
1	B	265	GLN
2	L	30	HIS
2	M	30	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	177/185 (95%)	-0.23	0	100 100	27, 44, 81, 133	0
1	B	177/185 (95%)	-0.16	0	100 100	29, 52, 97, 172	0
2	L	213/213 (100%)	-0.11	1 (0%)	88 36	30, 62, 126, 152	0
2	M	213/213 (100%)	0.87	38 (17%)	2 1	52, 134, 183, 196	0
3	H	217/217 (100%)	-0.11	0	100 100	38, 61, 91, 158	0
3	I	217/217 (100%)	0.64	17 (7%)	13 3	54, 117, 176, 190	0
All	All	1214/1230 (98%)	0.17	56 (4%)	31 7	27, 69, 167, 196	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	155	ARG	8.7
2	M	200	THR	5.1
2	M	194	CYS	5.0
2	M	157	ASN	4.3
2	M	156	GLN	4.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.