



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:19 PM GMT

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

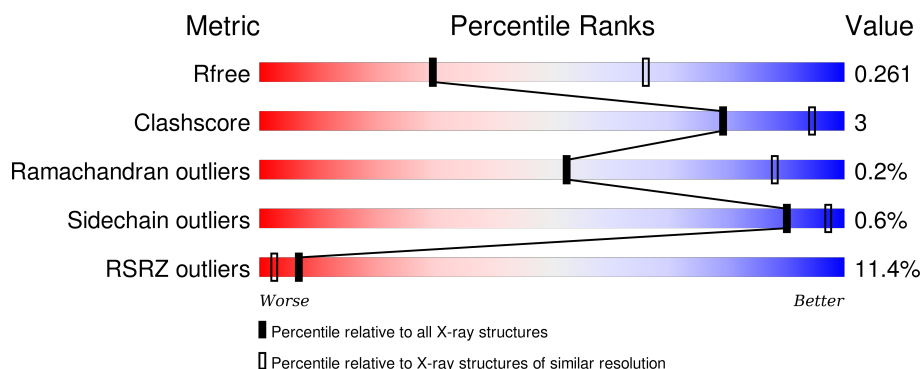
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	185	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div>.</div> </div> </div>
1	B	185	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>.</div> </div> </div>
2	L	213	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
2	M	213	<div> <div>32%</div> <div> <div></div> <div>89%</div> <div>11%</div> </div> </div>
3	H	217	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	I	217	<div> <div>28%</div> <div>90%</div> <div>10%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9455 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 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			

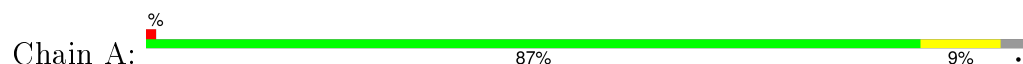
- Molecule 4 is water.

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

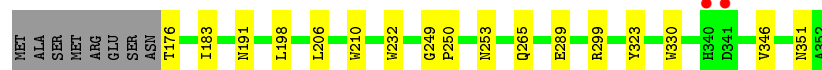
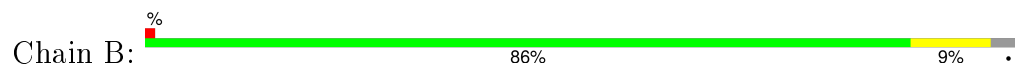
### 3 Residue-property plots [i](#)

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.

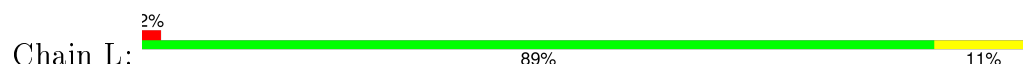
- Molecule 1: NON-STRUCTURAL PROTEIN NS1



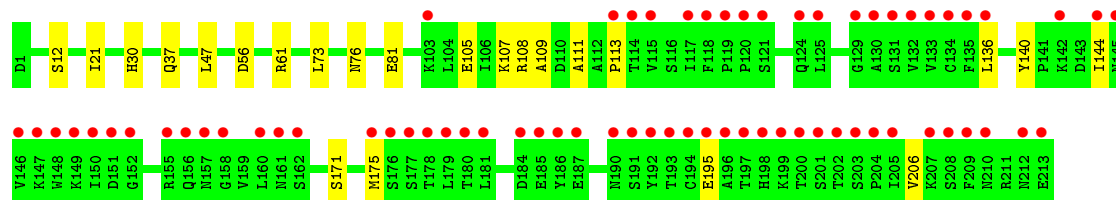
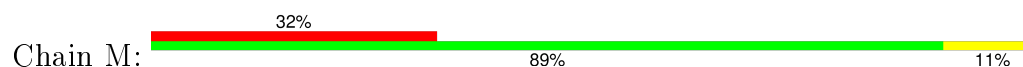
- Molecule 1: NON-STRUCTURAL PROTEIN NS1



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



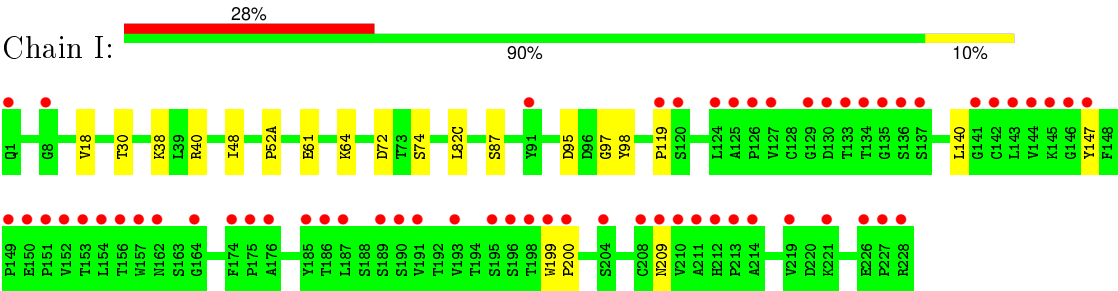
- Molecule 2: Light Chain of Fab fragment of 22NS1 Antibody



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	1425 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.3	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.22	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 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	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
4	H	15	0	0	0	0
4	I	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	15	0	0	0	0
4	M	1	0	0	0	0
All	All	9455	0	9026	64	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 3.

All (64) 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: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
2:M:37:GLN:HB2	2:M:47:LEU:HD11	1.82	0.59
2:M:108:ARG:HD2	2:M:171:SER:HB2	1.84	0.59
2:L:108:ARG:HD2	2:L:171:SER:HB2	1.84	0.59
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.83	0.59
2:M:195:GLU:HG2	2:M:206:VAL:HG22	1.90	0.54
2:L:195:GLU:HG2	2:L:206:VAL:HG22	1.90	0.54
2:L:136:LEU:HB2	2:L:175:MET:HG3	1.92	0.52
2:L:108:ARG:HH12	2:L:111:ALA:HB2	1.75	0.52
2:M:136:LEU:HB2	2:M:175:MET:HG3	1.92	0.52
2:L:136:LEU:HD23	2:L:144:ILE:HD13	1.92	0.51
2:M:136:LEU:HD23	2:M:144:ILE:HD13	1.91	0.51
1:B:232:TRP:CD2	1:B:253:ASN:HB2	2.46	0.51
2:M:108:ARG:HH12	2:M:111:ALA:HB2	1.76	0.50
1:A:232:TRP:CD2	1:A:253:ASN:HB2	2.46	0.50
3:I:199:TRP:CG	3:I:200:PRO:HA	2.47	0.50
2:L:61:ARG:HB2	2:L:76:ASN:O	2.12	0.50
2:M:12:SER:HA	2:M:105:GLU:HB2	1.94	0.49
2:M:61:ARG:HB2	2:M:76:ASN:O	2.12	0.49
1:A:206:LEU:HB2	1:A:210:TRP:CE2	2.48	0.49
1:B:206:LEU:HB2	1:B:210:TRP:CE2	2.48	0.49
2:L:12:SER:HA	2:L:105:GLU:HB2	1.95	0.49
3:I:119:PRO:HB3	3:I:147:TYR:HB3	1.94	0.48
3:H:119:PRO:HB3	3:H:147:TYR:HB3	1.94	0.48
3:H:38:LYS:HB2	3:H:48:ILE:HD11	1.96	0.48
3:I:38:LYS:HB2	3:I:48:ILE:HD11	1.96	0.48
2:M:108:ARG:NH1	2:M:109:ALA:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:95:ASP:OD1	3:H:98:TYR:N	2.48	0.46
3:H:56:GLY:HA2	3:H:57:PRO:HD3	1.80	0.46
3:I:95:ASP:OD1	3:I:98:TYR:N	2.48	0.46
2:L:108:ARG:NH1	2:L:109:ALA:O	2.49	0.46
3:H:30:THR:HA	3:H:52(A):PRO:HB2	1.99	0.45
3:I:30:THR:HA	3:I:52(A):PRO:HB2	1.98	0.45
3:I:140:LEU:HD11	3:I:199:TRP:CD1	2.52	0.45
2:L:108:ARG:NH2	2:L:109:ALA:HB3	2.32	0.45
3:H:61:GLU:HA	3:H:64:LYS:HG3	2.00	0.44
1:A:183:ILE:HB	1:A:198:LEU:HD13	2.00	0.44
3:I:61:GLU:HA	3:I:64:LYS:HG3	2.00	0.43
3:H:18:VAL:HG12	3:H:82(C):LEU:HD11	2.01	0.43
2:M:113:PRO:HG3	2:M:144:ILE:HD11	2.00	0.43
3:H:40:ARG:NH1	3:H:87:SER:O	2.52	0.43
1:B:183:ILE:HB	1:B:198:LEU:HD13	2.00	0.43
2:L:113:PRO:HG3	2:L:144:ILE:HD11	2.00	0.43
3:I:18:VAL:HG12	3:I:82(C):LEU:HD11	2.01	0.43
1:B:249:GLY:HA2	1:B:250:PRO:HD3	1.91	0.42
2:M:107:LYS:HA	2:M:140:TYR:OH	2.20	0.42
1:A:299:ARG:NH2	1:A:346:VAL:HG21	2.34	0.42
1:B:299:ARG:NH2	1:B:346:VAL:HG21	2.34	0.42
3:I:40:ARG:NH1	3:I:87:SER:O	2.52	0.42
1:B:191:ASN:OD1	1:B:191:ASN:N	2.53	0.42
1:A:265:GLN:HE21	1:A:351:ASN:ND2	2.18	0.42
1:B:232:TRP:CH2	2:M:30:HIS:HE1	2.38	0.42
3:I:72:ASP:OD2	3:I:74:SER:OG	2.34	0.41
2:L:107:LYS:HA	2:L:140:TYR:OH	2.20	0.41
1:B:289:GLU:HG3	2:M:56:ASP:HB2	2.03	0.41
3:H:199:TRP:CG	3:H:200:PRO:HA	2.55	0.41
3:H:12:VAL:HG11	3:H:82(C):LEU:HD13	2.03	0.40
2:L:28:ASN:OD1	2:L:30:HIS:HD2	2.04	0.40
1:B:265:GLN:HE21	1:B:351:ASN:ND2	2.18	0.40
1:A:191:ASN:OD1	1:A:191:ASN:N	2.54	0.40

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%)	34	76
3	I	215/217 (99%)	210 (98%)	4 (2%)	1 (0%)	34	76
All	All	1202/1230 (98%)	1148 (96%)	52 (4%)	2 (0%)	52	88

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%)	76	93
1	B	157/164 (96%)	156 (99%)	1 (1%)	90	97
2	L	187/187 (100%)	186 (100%)	1 (0%)	92	98
2	M	187/187 (100%)	186 (100%)	1 (0%)	92	98
3	H	186/186 (100%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	186/186 (100%)	185 (100%)	1 (0%)	92	98
All	All	1060/1074 (99%)	1054 (99%)	6 (1%)	90	97

All (6) residues with a non-rotameric sidechain are listed below:

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

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 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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	177/185 (95%)	-0.27	1 (0%) 90 73	27, 44, 81, 133	0
1	B	177/185 (95%)	-0.16	2 (1%) 82 58	29, 52, 97, 172	0
2	L	213/213 (100%)	-0.02	4 (1%) 70 41	30, 62, 126, 152	0
2	M	213/213 (100%)	1.74	69 (32%) 1 0	52, 134, 183, 196	0
3	H	217/217 (100%)	-0.10	2 (0%) 85 64	38, 61, 91, 158	0
3	I	217/217 (100%)	1.38	61 (28%) 1 0	54, 117, 176, 190	0
All	All	1214/1230 (98%)	0.47	139 (11%) 7 2	27, 69, 167, 196	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	155	ARG	12.6
2	M	209	PHE	9.1
2	M	194	CYS	8.4
2	M	157	ASN	8.4
2	M	200	THR	8.4
3	I	144	VAL	8.0
2	M	146	VAL	7.9
2	M	212	ASN	7.1
2	M	145	ASN	7.1
3	I	133	THR	6.8
2	M	150	ILE	6.8
3	I	204	SER	6.6
2	M	156	GLN	6.6
2	M	149	LYS	6.1
2	M	201	SER	6.0
2	M	161	ASN	5.6
3	I	142	CYS	5.6
2	M	119	PRO	5.5
3	I	189	SER	5.5

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Mol	Chain	Res	Type	RSRZ
2	M	148	TRP	5.5
2	M	190	ASN	5.5
2	M	208	SER	5.3
2	M	113	PRO	5.2
2	M	179	LEU	5.1
3	I	141	GLY	4.9
2	M	210	ASN	4.9
2	M	134	CYS	4.8
2	L	202	THR	4.7
2	M	151	ASP	4.7
2	M	198	HIS	4.7
2	M	197	THR	4.7
2	M	186	TYR	4.7
3	I	130	ASP	4.6
3	I	187	LEU	4.6
2	M	130	ALA	4.6
2	M	180	THR	4.4
2	M	135	PHE	4.3
2	M	118	PHE	4.3
3	I	157	TRP	4.2
2	M	178	THR	4.2
2	M	196	ALA	4.2
3	I	154	LEU	4.2
3	I	208	CYS	4.1
2	M	147	LYS	4.1
2	M	181	LEU	4.1
2	M	205	ILE	4.0
2	M	152	GLY	4.0
3	I	134	THR	4.0
3	I	226	GLU	4.0
2	M	192	TYR	4.0
2	M	132	VAL	4.0
3	I	143	LEU	4.0
2	M	129	GLY	3.9
3	I	213	PRO	3.9
2	M	207	LYS	3.9
3	I	214	ALA	3.8
2	L	200	THR	3.8
3	I	129	GLY	3.8
2	M	193	THR	3.8
3	I	147	TYR	3.7
2	M	185	GLU	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	I	145	LYS	3.6
3	I	199	TRP	3.6
2	M	199	LYS	3.6
3	I	152	VAL	3.5
2	M	114	THR	3.4
2	M	158	GLY	3.4
3	I	198	THR	3.4
2	M	133	VAL	3.4
3	I	190	SER	3.4
2	M	144	ILE	3.3
3	I	149	PRO	3.3
3	H	134	THR	3.3
3	I	126	PRO	3.3
2	M	131	SER	3.3
2	M	175	MET	3.3
2	M	162	SER	3.3
3	I	150	GLU	3.3
2	M	125	LEU	3.2
2	M	184	ASP	3.1
1	B	340	HIS	3.1
3	I	162	ASN	3.1
2	M	136	LEU	3.1
3	I	219	VAL	3.1
2	M	204	PRO	3.0
1	A	340	HIS	3.0
3	I	127	VAL	3.0
2	L	157	ASN	3.0
3	I	1	GLN	3.0
3	I	151	PRO	2.9
3	I	120	SER	2.9
2	M	213	GLU	2.9
3	I	153	THR	2.9
2	M	124	GLN	2.9
2	M	176	SER	2.9
3	I	135	GLY	2.8
3	I	175	PRO	2.8
3	I	193	VAL	2.8
3	I	156	THR	2.8
2	M	195	GLU	2.7
2	M	177	SER	2.7
2	M	203	SER	2.7
2	M	120	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
3	I	211	ALA	2.7
1	B	341	ASP	2.6
3	I	8	GLY	2.6
2	M	187	GLU	2.6
3	I	176	ALA	2.5
3	I	164	GLY	2.5
2	M	115	VAL	2.5
2	M	160	LEU	2.5
3	I	146	GLY	2.5
3	H	133	THR	2.5
2	M	121	SER	2.4
3	I	174	PHE	2.4
3	I	185	TYR	2.4
3	I	228	ARG	2.4
3	I	124	LEU	2.3
3	I	212	HIS	2.3
3	I	136	SER	2.3
2	M	191	SER	2.3
3	I	227	PRO	2.3
3	I	195	SER	2.2
2	M	103	LYS	2.2
3	I	91	TYR	2.2
2	L	198	HIS	2.2
3	I	200	PRO	2.2
3	I	221	LYS	2.2
3	I	210	VAL	2.2
3	I	196	SER	2.1
3	I	125	ALA	2.1
2	M	117	ILE	2.1
3	I	137	SER	2.1
2	M	202	THR	2.1
3	I	209	ASN	2.1
2	M	142	LYS	2.1
3	I	119	PRO	2.0
3	I	191	VAL	2.0
3	I	186	THR	2.0

## 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 [i](#)

There are no carbohydrates 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.