



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 02:29 PM JST

PDB ID : 7FAU  
Title : Structure Determination of the NB1B11-RBD Complex  
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Deposited on : 2021-07-07  
Resolution : 2.08 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
buster-report : 1.1.7 (2018)  
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) : 2.28.1

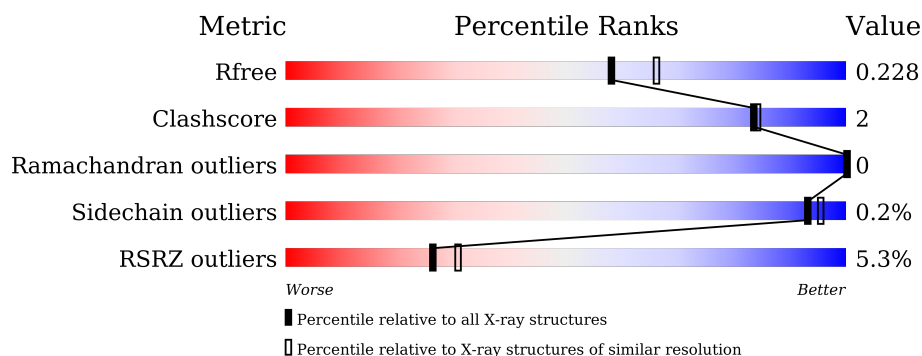
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 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	219	<div> <div>8%</div> <div>72% 5% 22%</div> </div>
1	C	219	<div> <div>3%</div> <div>82% 16%</div> </div>
2	B	127	<div> <div>3%</div> <div>91% 9%</div> </div>
2	D	127	<div> <div>3%</div> <div>89% 9%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4978 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1351	868	226	252	5			
1	C	185	Total	C	N	O	S	0	0	0
			1475	944	245	278	8			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MET	-	expression tag	UNP P0DTC2
A	319	PHE	-	expression tag	UNP P0DTC2
A	320	VAL	-	expression tag	UNP P0DTC2
A	321	PHE	-	expression tag	UNP P0DTC2
A	322	LEU	-	expression tag	UNP P0DTC2
A	323	VAL	-	expression tag	UNP P0DTC2
A	324	LEU	-	expression tag	UNP P0DTC2
A	325	LEU	-	expression tag	UNP P0DTC2
A	326	PRO	-	expression tag	UNP P0DTC2
A	327	LEU	-	expression tag	UNP P0DTC2
A	328	VAL	-	expression tag	UNP P0DTC2
A	329	SER	-	expression tag	UNP P0DTC2
A	330	SER	-	expression tag	UNP P0DTC2
A	331	GLN	-	expression tag	UNP P0DTC2
A	332	CYS	-	expression tag	UNP P0DTC2
A	524	SER	-	expression tag	UNP P0DTC2
A	525	ARG	-	expression tag	UNP P0DTC2
A	526	ALA	-	expression tag	UNP P0DTC2
A	527	ALA	-	expression tag	UNP P0DTC2
A	528	ALA	-	expression tag	UNP P0DTC2
A	529	ASP	-	expression tag	UNP P0DTC2
A	530	TYR	-	expression tag	UNP P0DTC2
A	531	LYS	-	expression tag	UNP P0DTC2
A	532	ASP	-	expression tag	UNP P0DTC2
A	533	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	534	ASP	-	expression tag	UNP P0DTC2
A	535	ASP	-	expression tag	UNP P0DTC2
A	536	LYS	-	expression tag	UNP P0DTC2
C	318	MET	-	expression tag	UNP P0DTC2
C	319	PHE	-	expression tag	UNP P0DTC2
C	320	VAL	-	expression tag	UNP P0DTC2
C	321	PHE	-	expression tag	UNP P0DTC2
C	322	LEU	-	expression tag	UNP P0DTC2
C	323	VAL	-	expression tag	UNP P0DTC2
C	324	LEU	-	expression tag	UNP P0DTC2
C	325	LEU	-	expression tag	UNP P0DTC2
C	326	PRO	-	expression tag	UNP P0DTC2
C	327	LEU	-	expression tag	UNP P0DTC2
C	328	VAL	-	expression tag	UNP P0DTC2
C	329	SER	-	expression tag	UNP P0DTC2
C	330	SER	-	expression tag	UNP P0DTC2
C	331	GLN	-	expression tag	UNP P0DTC2
C	332	CYS	-	expression tag	UNP P0DTC2
C	524	SER	-	expression tag	UNP P0DTC2
C	525	ARG	-	expression tag	UNP P0DTC2
C	526	ALA	-	expression tag	UNP P0DTC2
C	527	ALA	-	expression tag	UNP P0DTC2
C	528	ALA	-	expression tag	UNP P0DTC2
C	529	ASP	-	expression tag	UNP P0DTC2
C	530	TYR	-	expression tag	UNP P0DTC2
C	531	LYS	-	expression tag	UNP P0DTC2
C	532	ASP	-	expression tag	UNP P0DTC2
C	533	ASP	-	expression tag	UNP P0DTC2
C	534	ASP	-	expression tag	UNP P0DTC2
C	535	ASP	-	expression tag	UNP P0DTC2
C	536	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called NB\_1B11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	126	Total	C	N	O	S	0	0	0
			913	560	163	183	7			
2	D	126	Total	C	N	O	S	0	0	0
			913	560	163	183	7			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total 3	Zn 3	0	0
3	D	2	Total 2	Zn 2	0	0

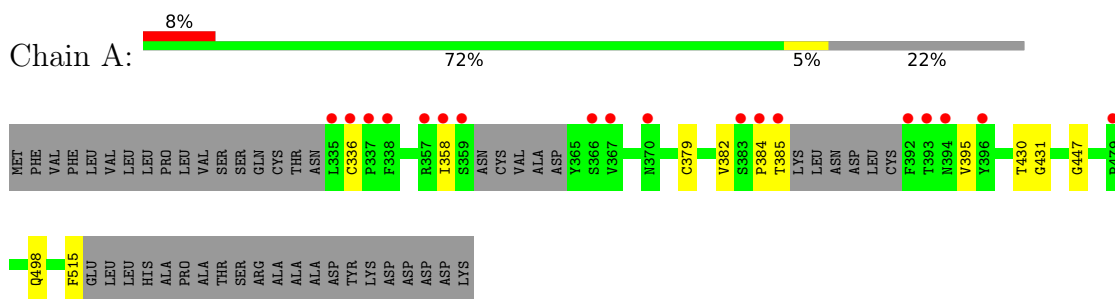
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total 91	O 91	0	0
4	B	74	Total 74	O 74	0	0
4	C	87	Total 87	O 87	0	0
4	D	69	Total 69	O 69	0	0

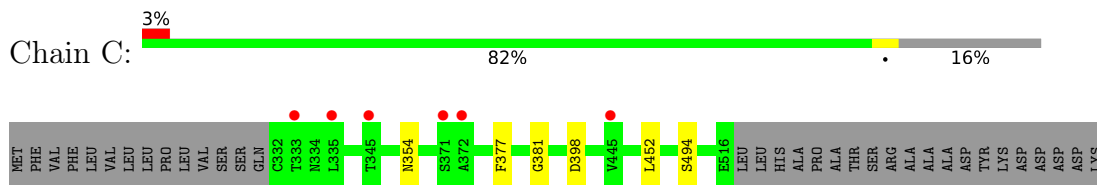
### 3 Residue-property plots

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.

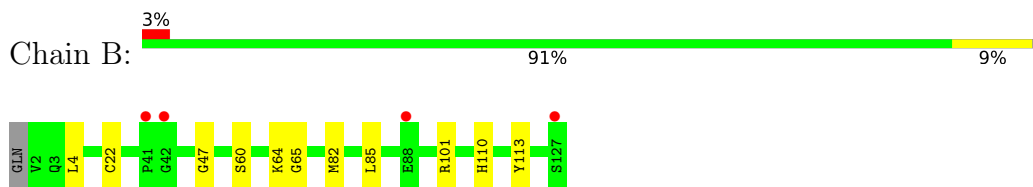
#### • Molecule 1: Spike protein S1



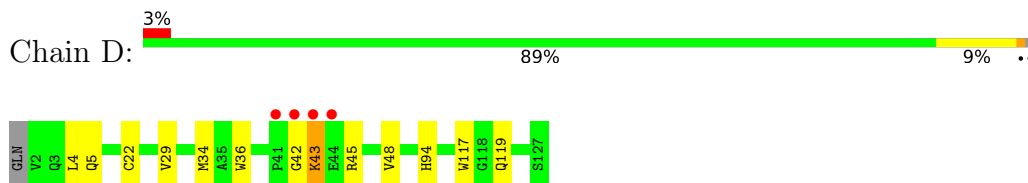
#### • Molecule 1: Spike protein S1



#### • Molecule 2: NB\_1B11



#### • Molecule 2: NB\_1B11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.51Å 88.83Å 190.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.53 – 2.08 47.53 – 2.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.53-2.08) 100.0 (47.53-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.198 , 0.228 0.198 , 0.228	Depositor DCC
$R_{free}$ test set	3187 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.2	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.34	0/1388	0.51	0/1884
1	C	0.33	0/1516	0.55	0/2061
2	B	0.32	0/927	0.56	0/1251
2	D	0.39	0/927	0.73	3/1251 (0.2%)
All	All	0.34	0/4758	0.58	3/6447 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	45	ARG	NE-CZ-NH2	-8.82	115.89	120.30
2	D	43	LYS	CD-CE-NZ	-6.88	95.89	111.70
2	D	45	ARG	NE-CZ-NH1	6.66	123.63	120.30

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	1351	0	1273	7	0
1	C	1475	0	1388	3	0
2	B	913	0	886	6	0
2	D	913	0	886	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	D	2	0	0	0	0
4	A	91	0	0	0	0
4	B	74	0	0	1	0
4	C	87	0	0	0	0
4	D	69	0	0	0	0
All	All	4978	0	4433	22	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.

All (22) 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:B:110:HIS:NE2	4:B:301:HOH:O	2.25	0.69
2:B:82:MET:HE2	2:B:85:LEU:HD21	1.76	0.68
2:D:94:HIS:CD2	2:D:117:TRP:HE3	2.13	0.66
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.79	0.64
1:A:379:CYS:HB2	1:A:384:PRO:HG3	1.85	0.59
1:A:385:THR:HG23	1:C:381:GLY:HA2	1.85	0.58
2:D:4:LEU:HB3	2:D:22:CYS:SG	2.46	0.56
2:B:4:LEU:HB3	2:B:22:CYS:SG	2.46	0.55
2:D:5:GLN:HA	2:D:119:GLN:HE22	1.75	0.50
1:A:382:VAL:HG13	1:A:430:THR:HG23	1.95	0.47
1:A:431:GLY:HA2	1:A:515:PHE:CE2	2.49	0.47
2:B:64:LYS:HD2	2:B:65:GLY:H	1.80	0.46
2:D:36:TRP:O	2:D:48:VAL:HG22	2.15	0.46
1:A:447:GLY:HA2	1:A:498:GLN:HG2	1.97	0.46
2:D:29:VAL:HG13	2:D:34:MET:SD	2.56	0.45
1:C:354:ASN:O	1:C:398:ASP:HA	2.18	0.44
2:D:42:GLY:C	2:D:43:LYS:HD2	2.39	0.43
1:C:452:LEU:HD23	1:C:494:SER:HA	2.00	0.42
2:D:94:HIS:CD2	2:D:117:TRP:CE3	3.01	0.42
2:B:101:ARG:HD3	2:B:113:TYR:CE2	2.55	0.42
1:A:336:CYS:HB3	1:A:358:ILE:HG21	2.03	0.41
2:B:47:GLY:O	2:B:60:SER:HB3	2.21	0.40

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	164/219 (75%)	158 (96%)	6 (4%)	0	100	100
1	C	183/219 (84%)	176 (96%)	7 (4%)	0	100	100
2	B	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
2	D	124/127 (98%)	122 (98%)	2 (2%)	0	100	100
All	All	595/692 (86%)	577 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	145/190 (76%)	145 (100%)	0	100	100
1	C	161/190 (85%)	160 (99%)	1 (1%)	86	89
2	B	96/97 (99%)	96 (100%)	0	100	100
2	D	96/97 (99%)	96 (100%)	0	100	100
All	All	498/574 (87%)	497 (100%)	1 (0%)	93	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	377	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such

sidechains are listed below:

Mol	Chain	Res	Type
2	B	119	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](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

### 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	170/219 (77%)	0.30	18 (10%) 6 7	29, 40, 82, 92	0
1	C	185/219 (84%)	-0.04	6 (3%) 47 53	26, 38, 55, 72	0
2	B	126/127 (99%)	0.09	4 (3%) 47 53	26, 33, 54, 74	0
2	D	126/127 (99%)	0.00	4 (3%) 47 53	24, 32, 54, 75	0
All	All	607/692 (87%)	0.09	32 (5%) 26 31	24, 36, 64, 92	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	42	GLY	6.9
1	A	393	THR	6.8
1	A	383	SER	5.3
2	B	41	PRO	5.0
1	A	394	ASN	4.8
1	A	385	THR	4.7
1	A	359	SER	4.5
1	A	338	PHE	4.1
2	D	42	GLY	3.9
1	C	445	VAL	3.9
2	D	44	GLU	3.7
1	A	357	ARG	3.6
1	A	392	PHE	3.6
1	A	335	LEU	3.4
2	D	41	PRO	3.2
1	A	336	CYS	3.0
1	A	367	VAL	2.9
1	A	370	ASN	2.9
1	C	372	ALA	2.7
1	A	337	PRO	2.7
1	C	333	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	43	LYS	2.6
1	C	335	LEU	2.6
1	A	366	SER	2.3
2	B	88	GLU	2.3
1	A	384	PRO	2.3
1	C	371	SER	2.3
1	A	479	PRO	2.2
1	C	345	THR	2.1
1	A	396	TYR	2.1
1	A	358	ILE	2.0
2	B	127	SER	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](#)

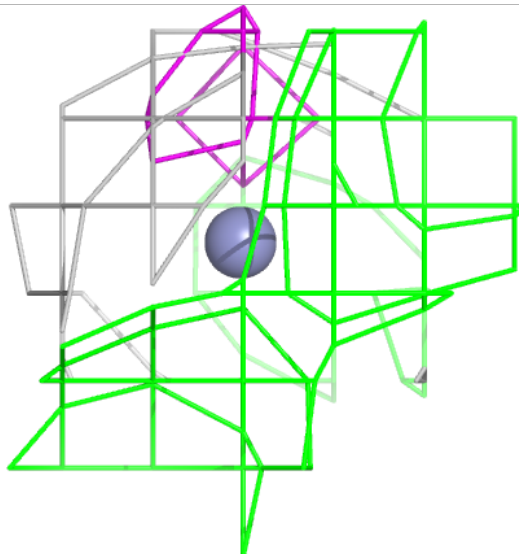
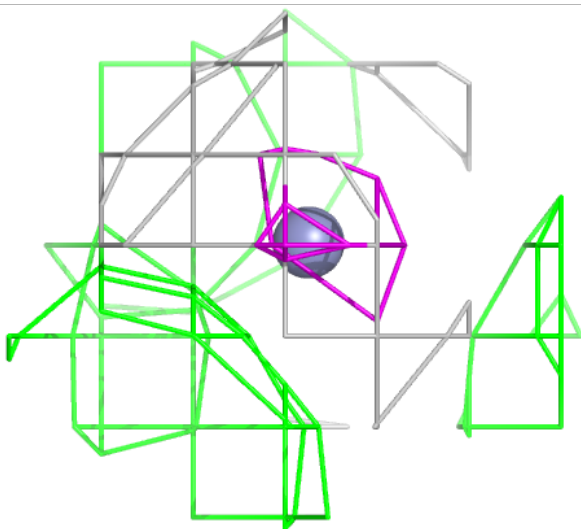
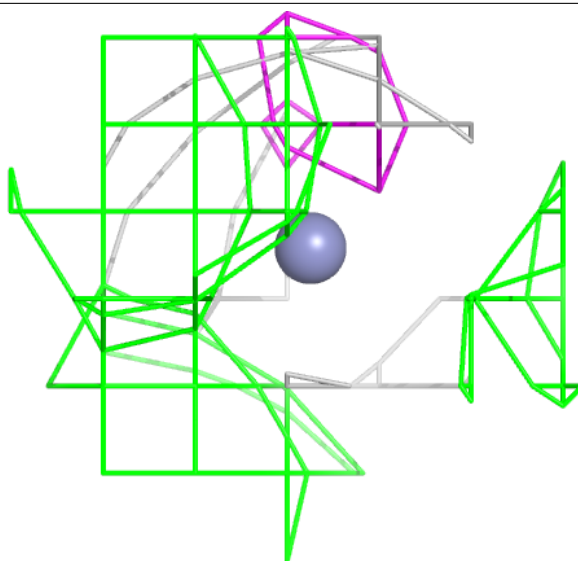
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ZN	D	201	1/1	0.87	0.10	52,52,52,52	0
3	ZN	B	203	1/1	0.92	0.05	78,78,78,78	0
3	ZN	B	201	1/1	0.96	0.07	46,46,46,46	0
3	ZN	B	202	1/1	0.99	0.10	38,38,38,38	0
3	ZN	D	202	1/1	0.99	0.07	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

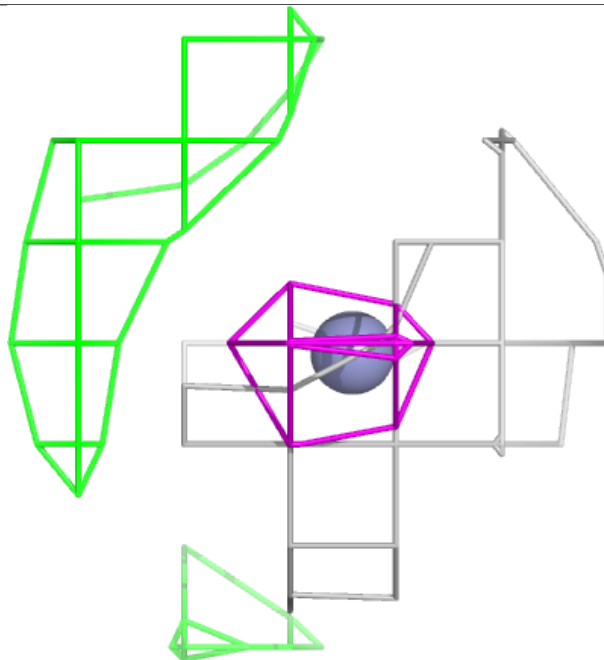
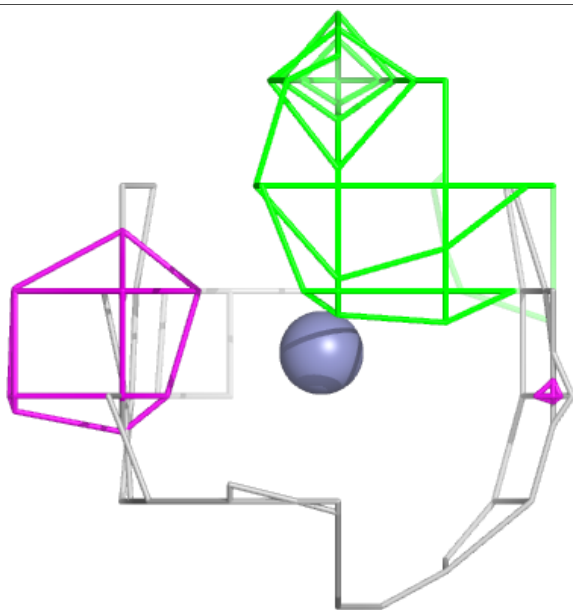
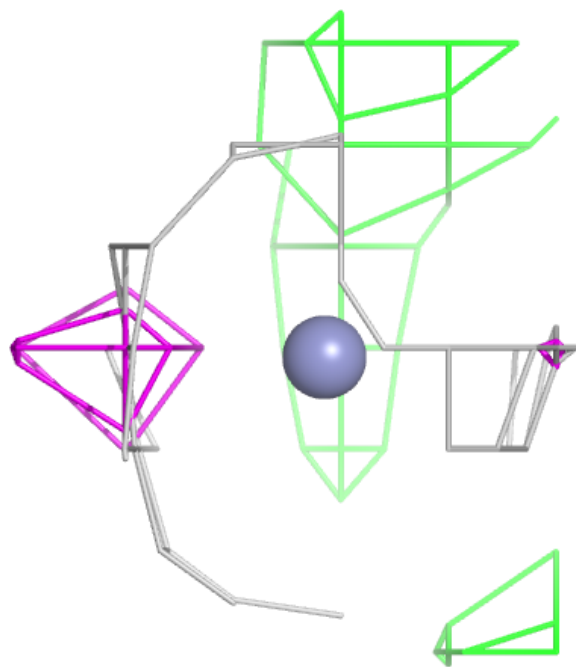
**Electron density around ZN D 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



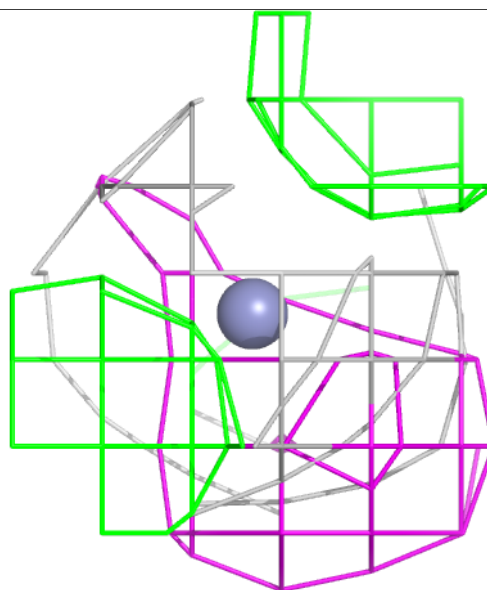
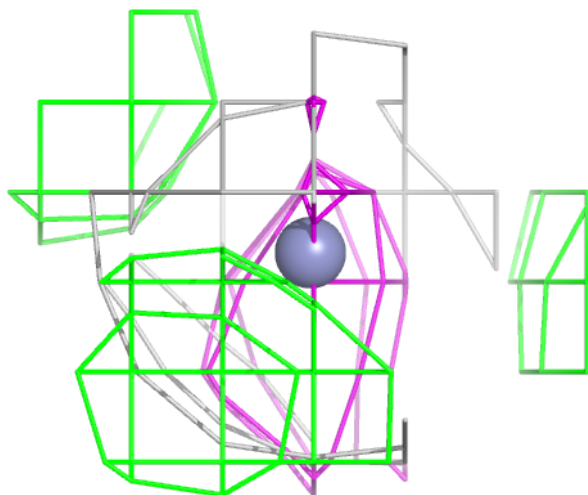
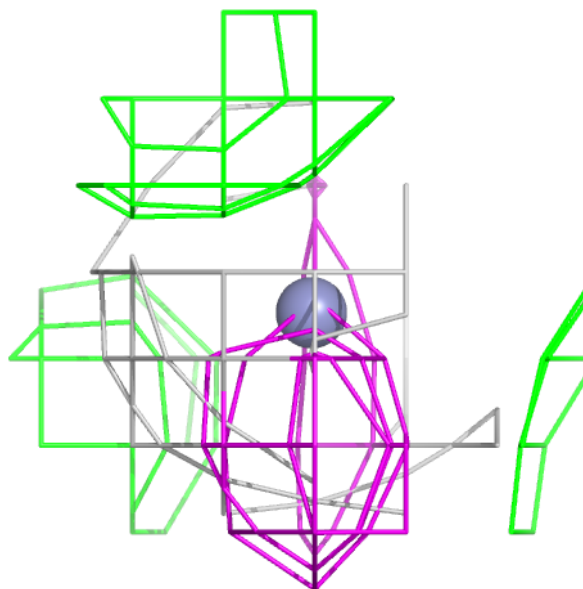
**Electron density around ZN B 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



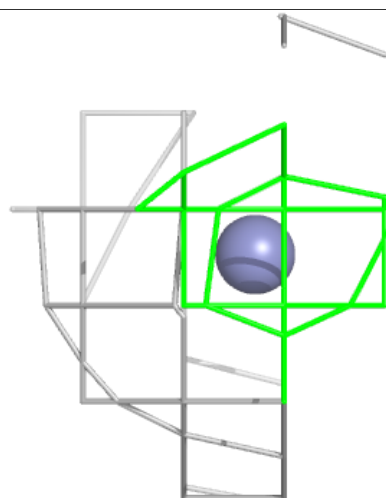
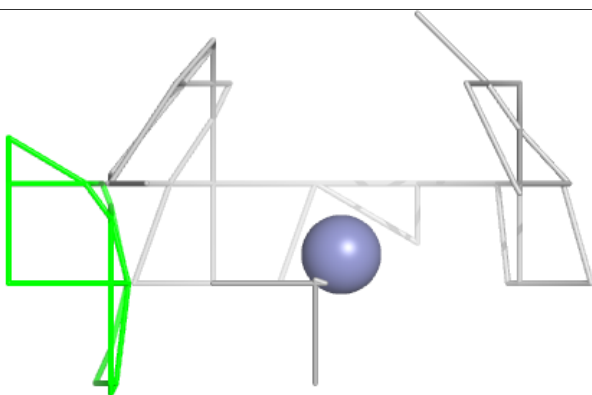
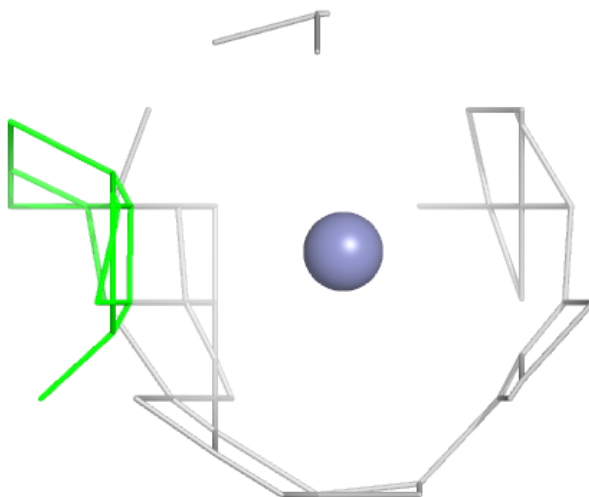
**Electron density around ZN B 201:**

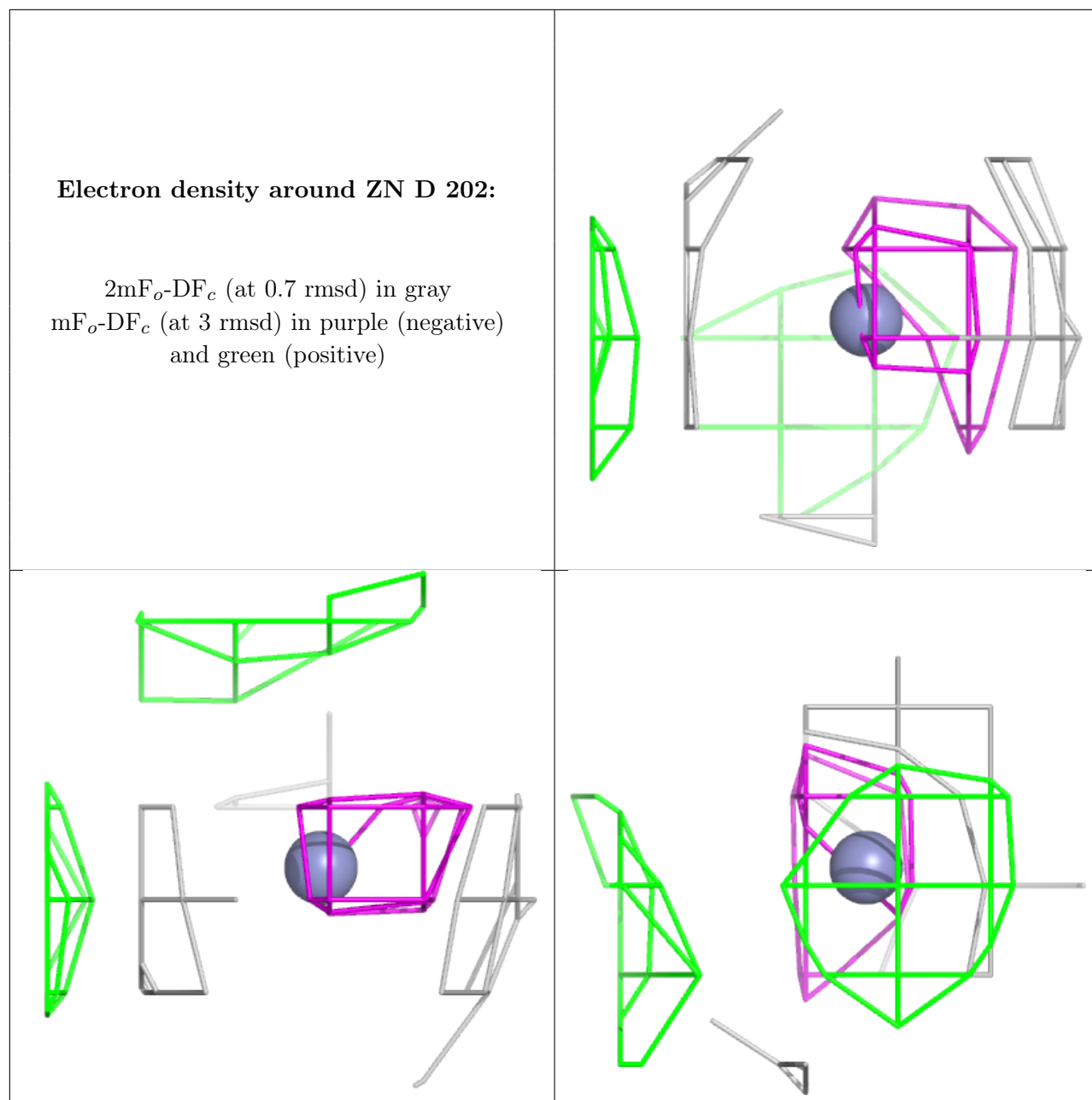
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around ZN B 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.