



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:44 PM UTC

PDB ID : 7FAU / pdb_00007fau
Title : Structure Determination of the NB1B11-RBD Complex
Authors : Shi, Z.Z.; Li, X.X.; Wang, L.; Sun, Z.C.; Zhang, H.W.; Chen, X.C.; Cui, Q.Q.;
Qiao, H.R.; Lan, Z.Y.; Zhang, X.
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

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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

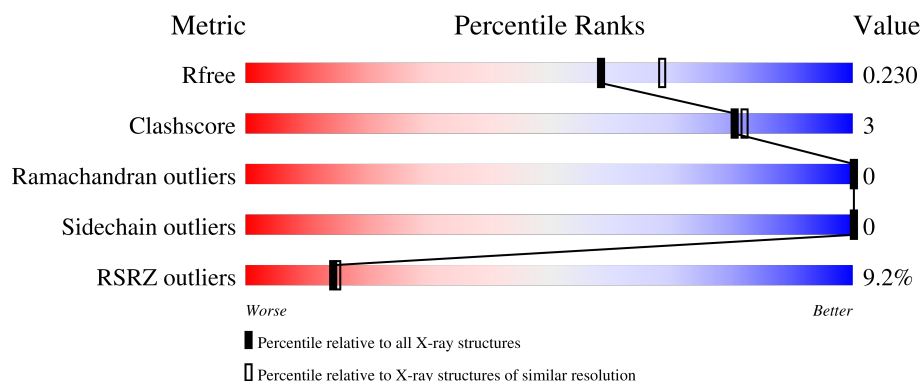
1 Overall quality at a glance

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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 ≥ 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	11% 72% 5% 22%
1	C	219	6% 82% • 16%
2	B	127	6% 88% 11% •
2	D	127	8% 90% 9% ••

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 (CCD ID: 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

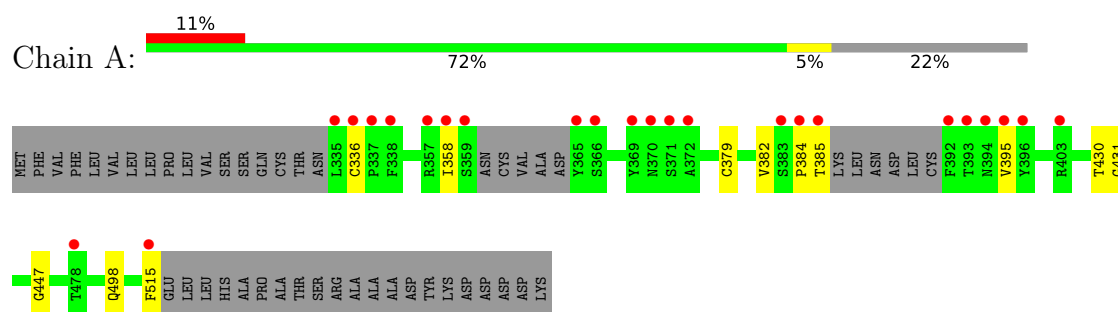
- Molecule 4 is water.

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

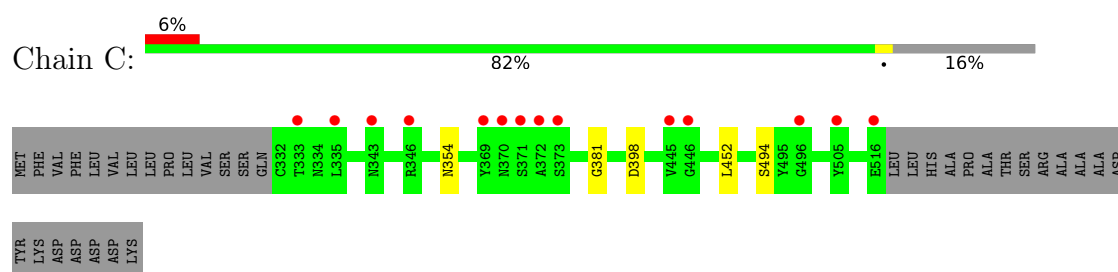
3 Residue-property plots [i](#)

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.

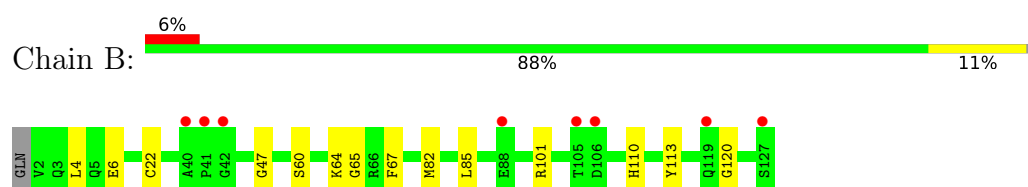
• Molecule 1: Spike protein S1



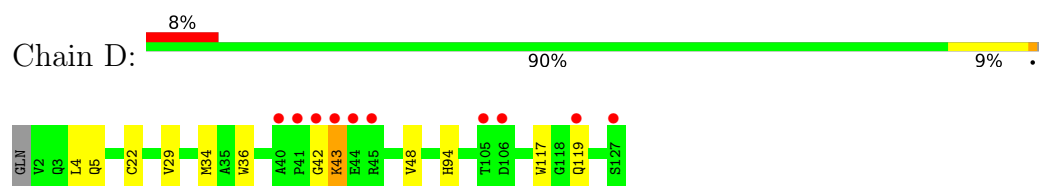
• Molecule 1: Spike protein S1



• Molecule 2: NB_1B11



• Molecule 2: NB_1B11



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.228 0.201 , 0.230	Depositor DCC
R_{free} test set	3187 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	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	0.95	EDS
Total number of atoms	4978	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.23	0/1388	0.45	0/1884
1	C	0.23	0/1516	0.47	0/2061
2	B	0.24	0/927	0.51	0/1251
2	D	0.33	0/927	0.63	1/1251 (0.1%)
All	All	0.26	0/4758	0.51	1/6447 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	43	LYS	CD-CE-NZ	-5.00	95.89	111.90

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	1351	0	1273	7	0
1	C	1475	0	1388	3	0
2	B	913	0	886	8	0
2	D	913	0	886	7	0
3	B	3	0	0	0	0
3	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	24	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 (24) 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:82:MET:HE2	2:B:85:LEU:HD21	1.73	0.70
2:B:110:HIS:NE2	4:B:301:HOH:O	2.25	0.69
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
2:B:67:PHE:CZ	2:B:82:MET:HE3	2.48	0.48
2:D:42:GLY:C	2:D:43:LYS:HD2	2.39	0.48
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
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
2:B:6:GLU:CD	2:B:120:GLY:H	2.30	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%)	161 (100%)	0	100	100
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%)	498 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	370	ASN
2	B	110	HIS
2	B	119	GLN
2	D	94	HIS

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 oligosaccharides 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, 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	170/219 (77%)	0.68	24 (14%) 6 6	29, 40, 82, 92	0
1	C	185/219 (84%)	0.35	14 (7%) 20 21	26, 38, 55, 72	0
2	B	126/127 (99%)	0.16	8 (6%) 26 27	26, 33, 54, 74	0
2	D	126/127 (99%)	0.13	10 (7%) 18 20	24, 32, 54, 75	0
All	All	607/692 (87%)	0.36	56 (9%) 14 15	24, 36, 64, 92	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	LEU	6.2
1	A	365	TYR	6.2
1	A	392	PHE	5.3
1	A	383	SER	5.0
1	A	385	THR	4.6
1	A	369	TYR	4.4
1	A	384	PRO	4.1
1	A	358	ILE	4.0
2	D	42	GLY	4.0
2	D	45	ARG	3.9
1	C	372	ALA	3.7
1	A	393	THR	3.7
2	B	41	PRO	3.7
2	B	106	ASP	3.5
1	A	478	THR	3.4
2	B	42	GLY	3.3
1	C	371	SER	3.2
1	A	338	PHE	3.1
1	A	394	ASN	3.1
1	A	336	CYS	3.1
1	C	445	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	43	LYS	3.0
2	D	44	GLU	3.0
2	D	41	PRO	3.0
1	C	369	TYR	3.0
2	D	127	SER	2.9
2	D	105	THR	2.9
2	B	88	GLU	2.9
1	A	515	PHE	2.9
1	A	337	PRO	2.8
1	C	446	GLY	2.8
1	C	496	GLY	2.8
2	B	40	ALA	2.7
2	B	105	THR	2.7
1	C	516	GLU	2.6
1	C	343	ASN	2.6
1	A	359	SER	2.6
2	B	127	SER	2.6
1	A	370	ASN	2.5
1	A	366	SER	2.4
1	C	373	SER	2.4
2	B	119	GLN	2.3
1	A	396	TYR	2.3
2	D	106	ASP	2.3
1	C	505	TYR	2.3
1	C	346	ARG	2.3
1	A	372	ALA	2.3
1	C	333	THR	2.2
1	A	371	SER	2.2
1	A	357	ARG	2.2
1	A	395	VAL	2.2
2	D	119	GLN	2.2
1	C	370	ASN	2.2
2	D	40	ALA	2.1
1	C	335	LEU	2.0
1	A	403	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

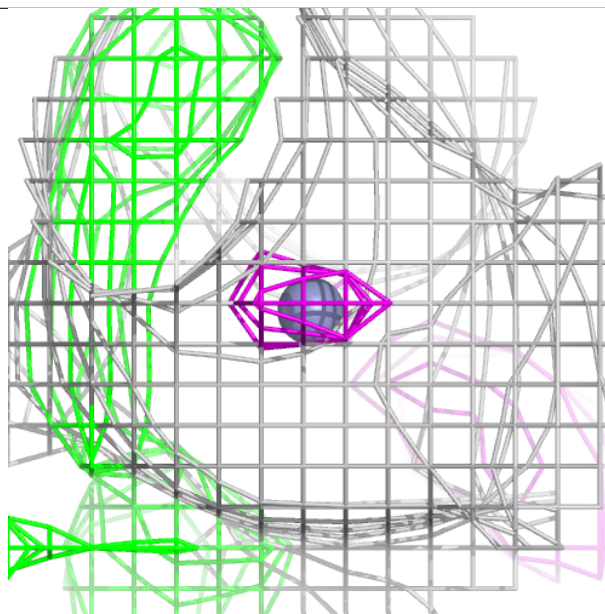
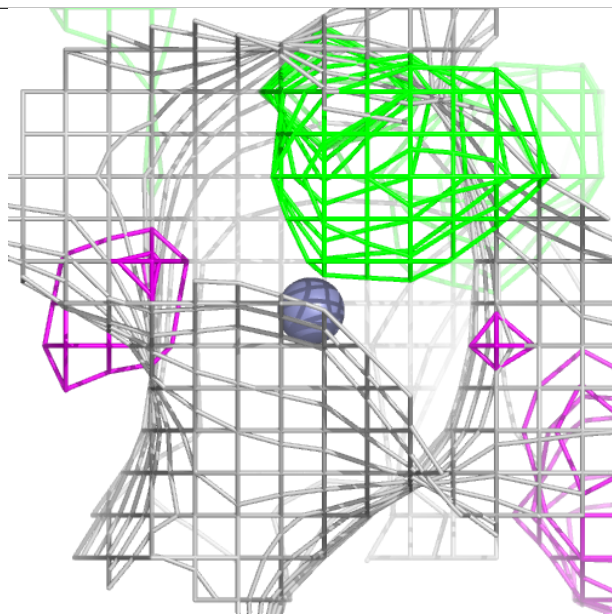
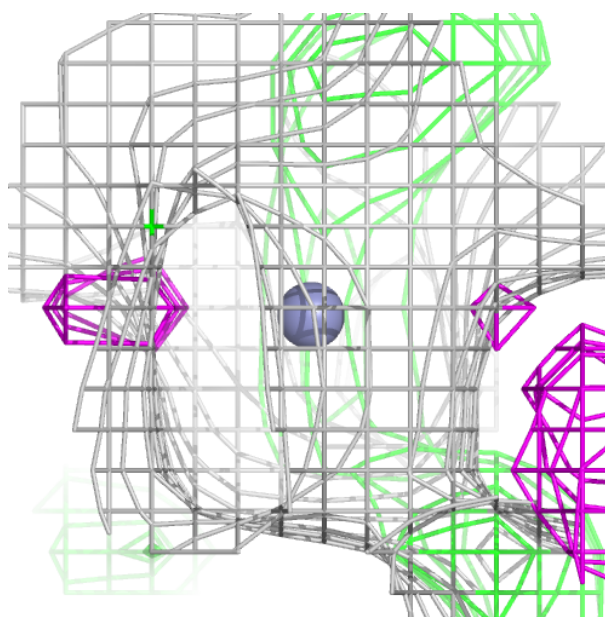
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ZN	B	203	1/1	0.90	0.10	78,78,78,78	0
3	ZN	D	201	1/1	0.92	0.08	52,52,52,52	0
3	ZN	B	201	1/1	0.97	0.06	46,46,46,46	0
3	ZN	D	202	1/1	0.99	0.04	41,41,41,41	0
3	ZN	B	202	1/1	1.00	0.03	38,38,38,38	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.

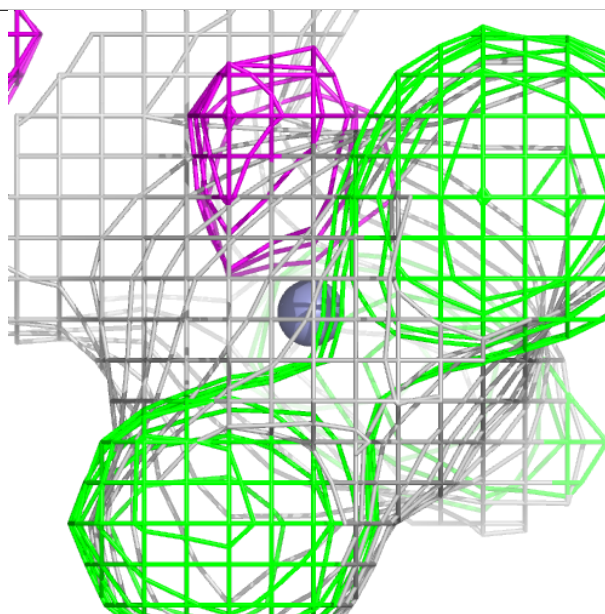
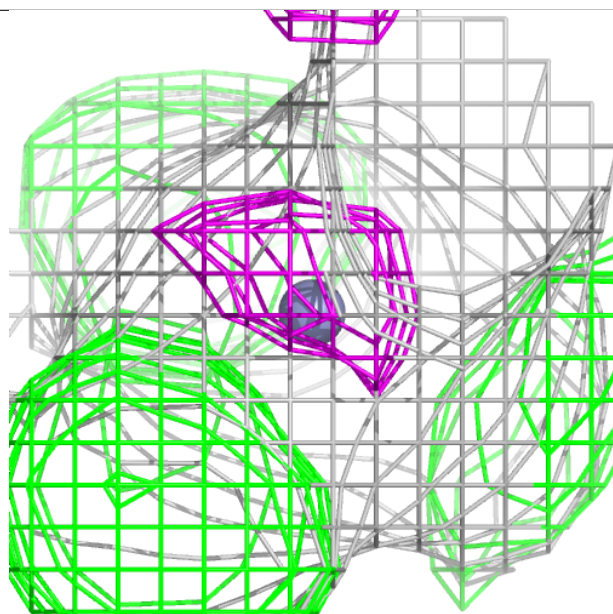
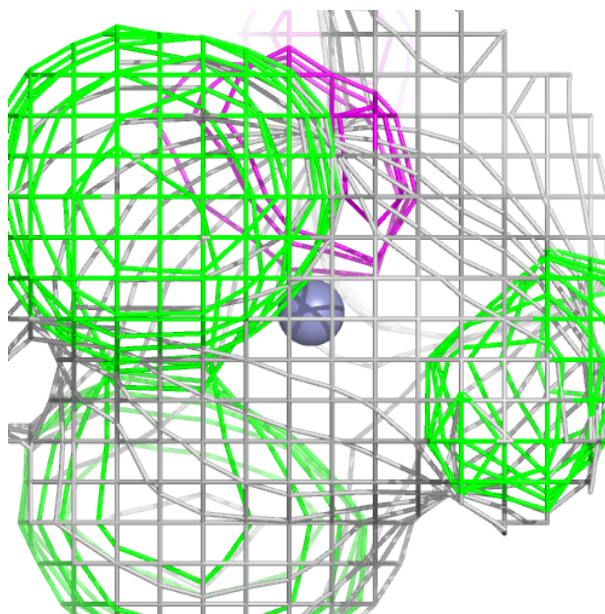
Electron density around ZN B 203:

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



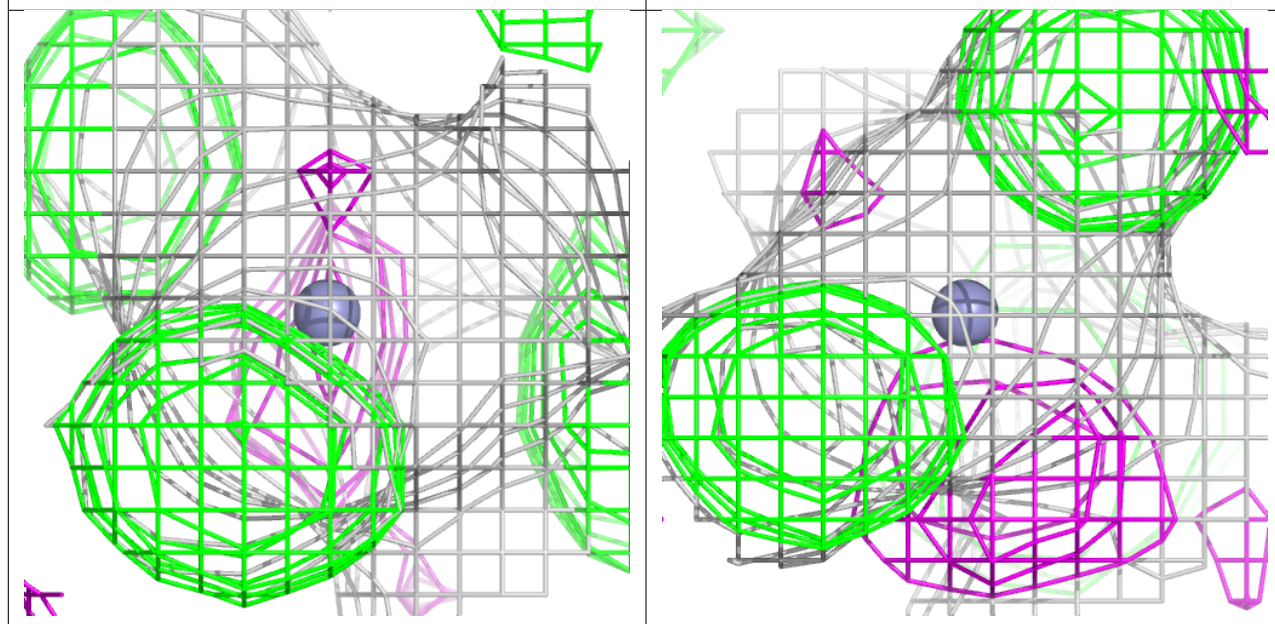
Electron density around ZN D 201:

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



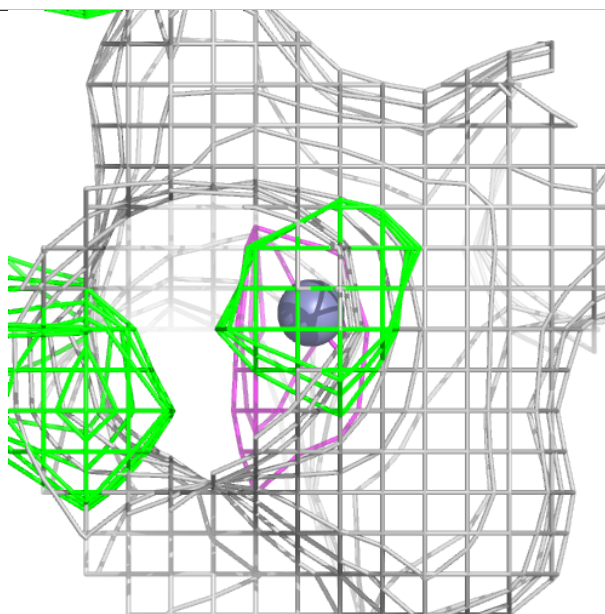
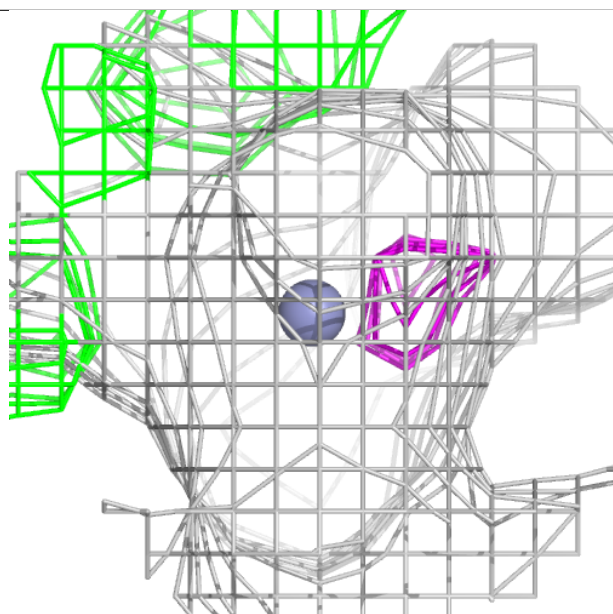
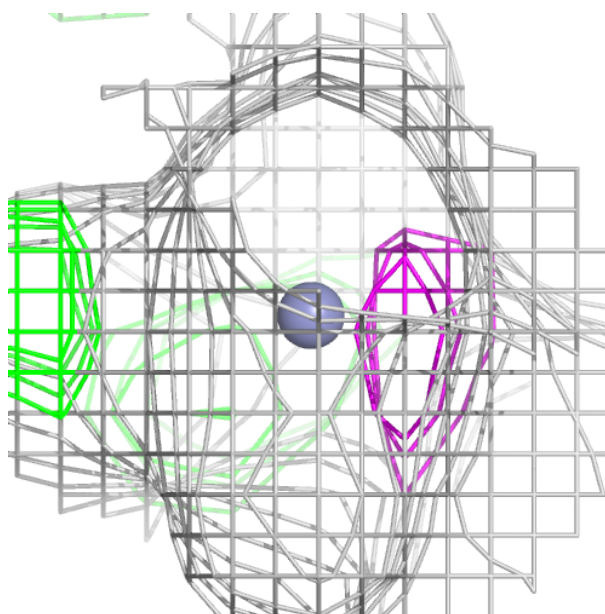
Electron density around ZN B 201:

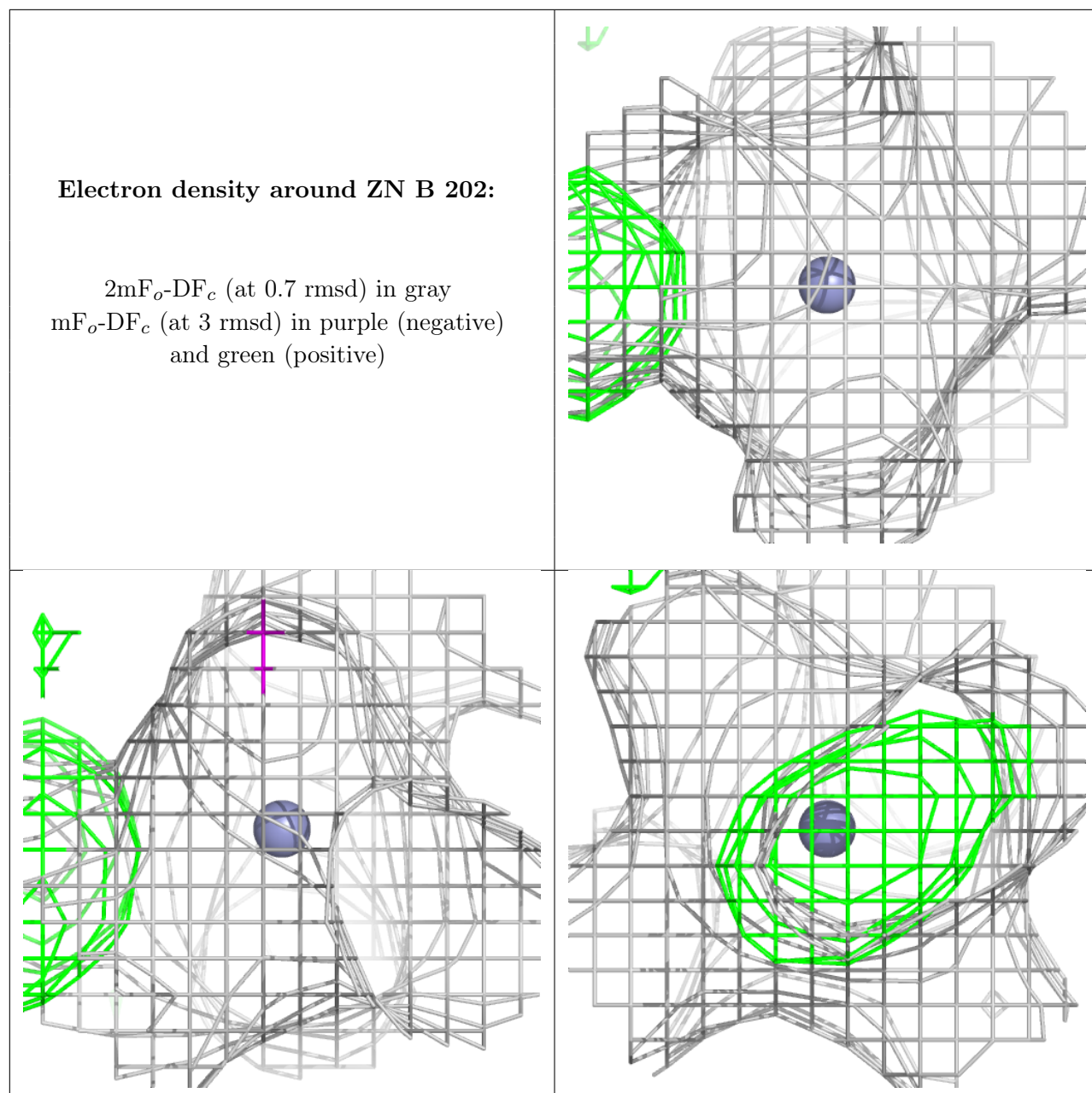
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 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.