



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 9TH6 / pdb_00009th6
Title : nsp14 of SARS-CoV-2 in complex with a camelid nanobody
Authors : Gauffre, P.; Ferron, F.; Canard, B.
Deposited on : 2025-12-02
Resolution : 2.27 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

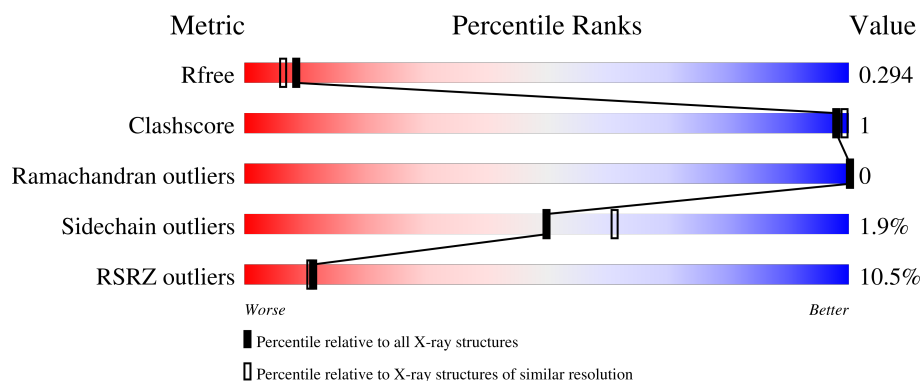
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	547	9% 79% 18%
2	B	132	8% 91% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9197 atoms, of which 4575 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 Guanine-N7 methyltransferase nsp14.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	448	Total	C	H	N	O	S	3460	0	0
			7040	2303	3460	605	638	34			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0DTD1
A	-18	GLY	-	expression tag	UNP P0DTD1
A	-17	GLY	-	expression tag	UNP P0DTD1
A	-16	SER	-	expression tag	UNP P0DTD1
A	-15	HIS	-	expression tag	UNP P0DTD1
A	-14	HIS	-	expression tag	UNP P0DTD1
A	-13	HIS	-	expression tag	UNP P0DTD1
A	-12	HIS	-	expression tag	UNP P0DTD1
A	-11	HIS	-	expression tag	UNP P0DTD1
A	-10	HIS	-	expression tag	UNP P0DTD1
A	-9	HIS	-	expression tag	UNP P0DTD1
A	-8	HIS	-	expression tag	UNP P0DTD1
A	-7	GLY	-	expression tag	UNP P0DTD1
A	-6	SER	-	expression tag	UNP P0DTD1
A	-5	GLU	-	expression tag	UNP P0DTD1
A	-4	ASN	-	expression tag	UNP P0DTD1
A	-3	LEU	-	expression tag	UNP P0DTD1
A	-2	TYR	-	expression tag	UNP P0DTD1
A	-1	PHE	-	expression tag	UNP P0DTD1
A	0	GLN	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called vhh anti-nsp14 of SARS-CoV-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	125	Total	C	H	N	O	S	875	0	0
			1794	573	875	159	182	5			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Zn 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	98	Total 294	H 196	O 98	196	0
4	B	22	Total 66	H 44	O 22	44	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.51Å 80.80Å 138.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.74 – 2.27 69.74 – 2.27	Depositor EDS
% Data completeness (in resolution range)	59.2 (69.74-2.27) 59.2 (69.74-2.27)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.233 , 0.290 (Not available) , 0.294	Depositor DCC
R_{free} test set	881 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9197	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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

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	0.77	0/3679	0.99	3/4994 (0.1%)
2	B	0.81	1/937 (0.1%)	0.93	0/1274
All	All	0.78	1/4616 (0.0%)	0.98	3/6268 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	103	ARG	CA-C	7.00	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TRP	N-CA-C	-7.13	98.98	109.11
1	A	423	LYS	N-CA-C	-5.72	105.97	113.12
1	A	344	ALA	N-CA-C	5.57	117.43	111.36

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	3580	3460	3440	5	0
2	B	919	875	874	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
4	A	98	196	0	1	0
4	B	22	44	0	0	0
All	All	4622	4575	4314	6	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 1.

All (6) 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:A:84:ARG:HD3	4:A:1113:HOH:O	2.05	0.55
1:A:264:HIS:CD2	1:A:275:ILE:HG21	2.48	0.48
1:A:84:ARG:HG2	1:A:411:LEU:HD11	1.97	0.46
2:B:32:THR:O	2:B:55:TRP:HB2	2.17	0.45
1:A:51:TYR:O	1:A:55:ILE:HG12	2.20	0.41
1:A:257:HIS:HD2	1:A:258:ASP:OD1	2.03	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	436/547 (80%)	412 (94%)	24 (6%)	0	100	100
2	B	123/132 (93%)	120 (98%)	3 (2%)	0	100	100
All	All	559/679 (82%)	532 (95%)	27 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	389/479 (81%)	382 (98%)	7 (2%)	51	63
2	B	91/101 (90%)	89 (98%)	2 (2%)	45	56
All	All	480/580 (83%)	471 (98%)	9 (2%)	50	61

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	268	HIS
1	A	289	ARG
1	A	329	LEU
1	A	354	GLN
1	A	363	ILE
1	A	389	VAL
2	B	3	GLN
2	B	123	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	108	GLN
1	A	245	GLN
1	A	257	HIS
1	A	283	HIS
1	A	343	GLN
2	B	41	GLN

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 3 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	448/547 (81%)	0.84	50 (11%) 10 9	15, 25, 40, 53	0
2	B	125/132 (94%)	0.84	10 (8%) 18 16	15, 26, 37, 48	0
All	All	573/679 (84%)	0.84	60 (10%) 11 11	15, 25, 40, 53	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	CYS	5.5
2	B	2	ALA	5.0
1	A	463	ILE	4.7
1	A	93	GLY	4.4
1	A	524	THR	4.4
1	A	66	VAL	4.1
1	A	482	ALA	4.0
1	A	367	PHE	4.0
1	A	481	GLY	3.8
1	A	95	HIS	3.8
1	A	289	ARG	3.7
1	A	454	SER	3.7
1	A	290	VAL	3.6
1	A	370	TYR	3.6
1	A	480	GLY	3.6
1	A	462	ASP	3.6
1	A	287	VAL	3.5
1	A	63	ASN	3.5
1	A	250	THR	3.4
1	A	357	SER	3.4
2	B	46	GLU	3.3
1	A	455	HIS	3.3
1	A	465	TYR	3.3
1	A	123	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	3.2
1	A	479	LEU	3.1
1	A	67	ASN	2.9
1	A	368	TYR	2.8
2	B	90	PRO	2.8
1	A	461	SER	2.8
1	A	124	TYR	2.8
2	B	126	GLY	2.8
2	B	123	VAL	2.8
1	A	37	GLY	2.7
1	A	464	ASP	2.7
1	A	345	ASP	2.7
2	B	43	PRO	2.7
1	A	335	PRO	2.7
1	A	267	ALA	2.6
1	A	517	TYR	2.6
1	A	337	ALA	2.6
1	A	61	LYS	2.6
1	A	155	LYS	2.5
1	A	268	HIS	2.5
1	A	94	CYS	2.5
1	A	336	LYS	2.5
1	A	344	ALA	2.4
2	B	42	ALA	2.4
2	B	50	ILE	2.3
2	B	44	GLY	2.3
1	A	260	TYR	2.2
1	A	25	THR	2.2
1	A	105	LEU	2.1
1	A	346	VAL	2.1
1	A	377	PHE	2.1
1	A	492	ARG	2.1
1	A	294	ILE	2.1
1	A	523	PHE	2.1
1	A	288	LYS	2.0
2	B	124	SER	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](#)

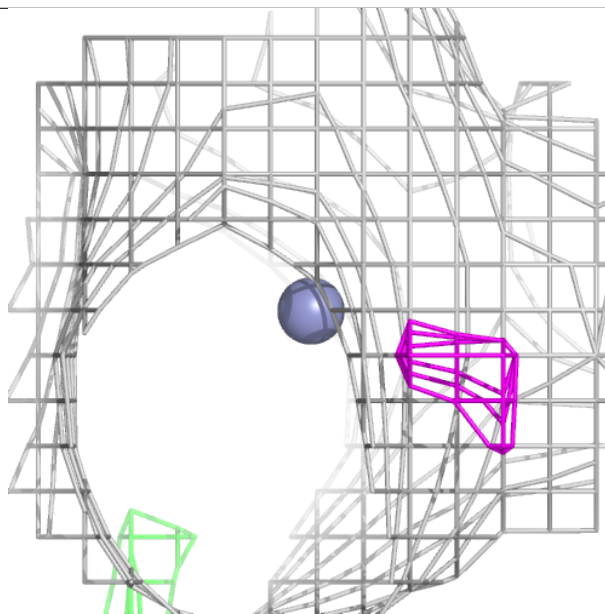
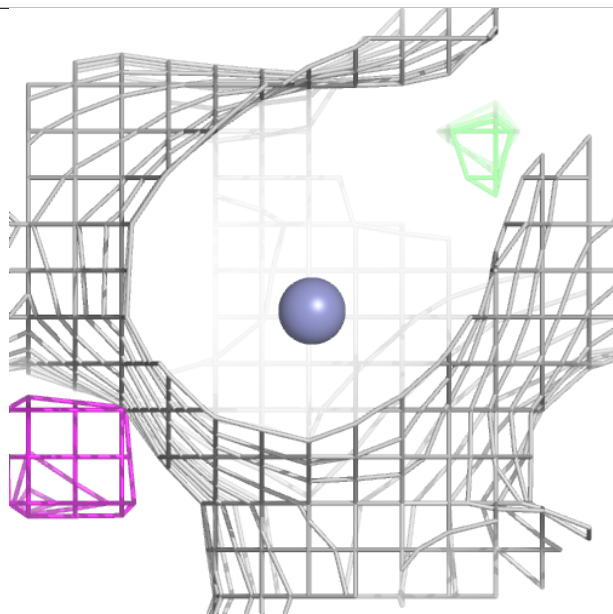
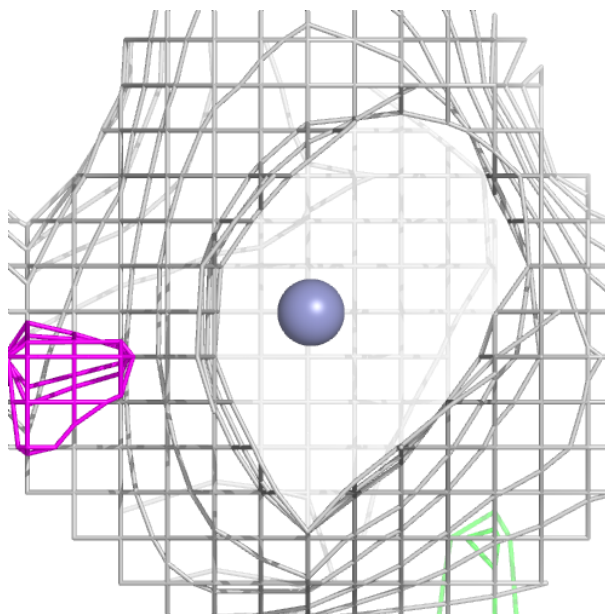
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	1002	1/1	0.98	0.04	51,51,51,51	0
3	ZN	A	1001	1/1	0.99	0.05	45,45,45,45	0
3	ZN	A	1003	1/1	1.00	0.03	42,42,42,42	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.

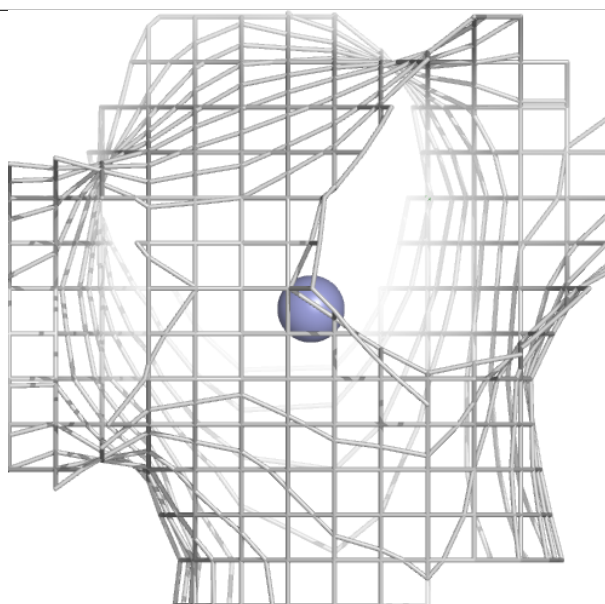
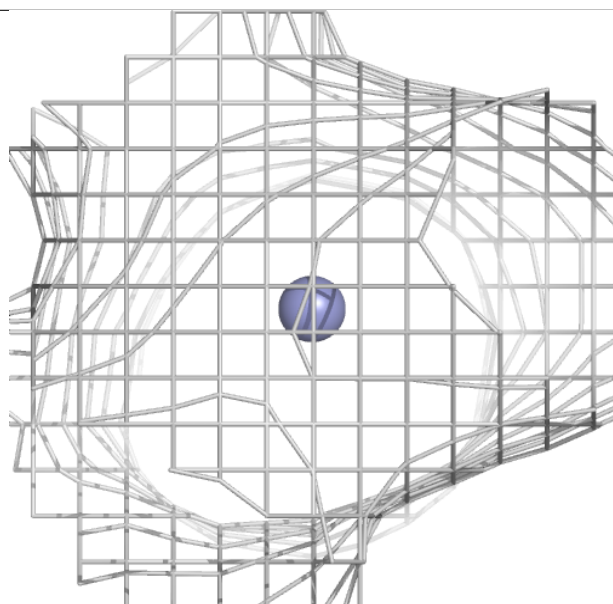
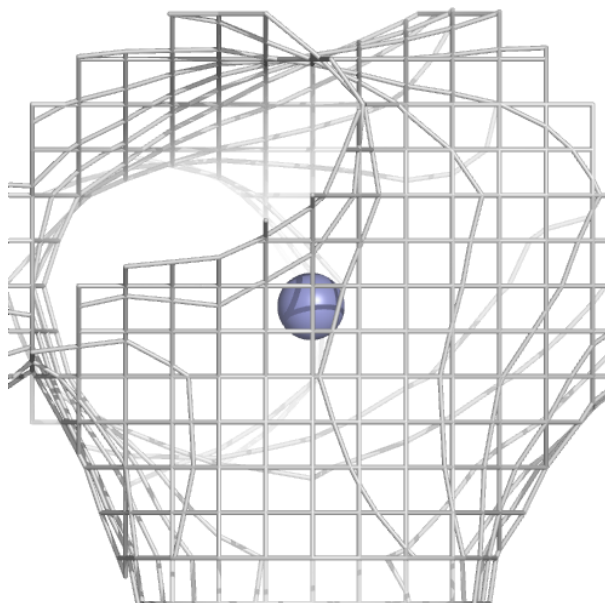
Electron density around ZN A 1002:

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



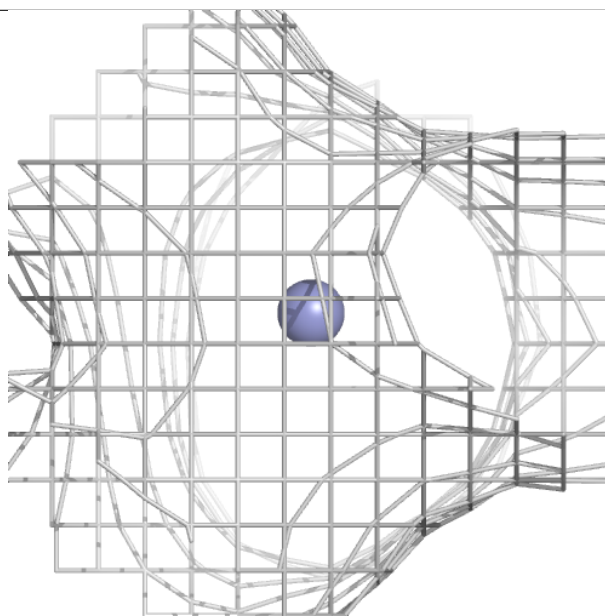
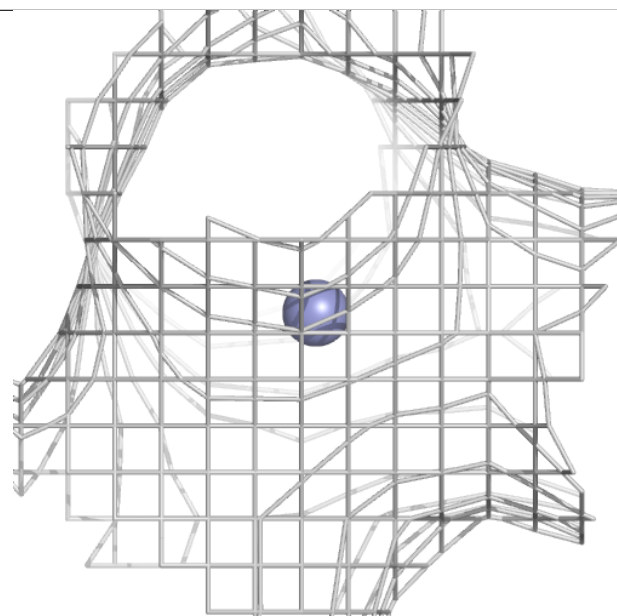
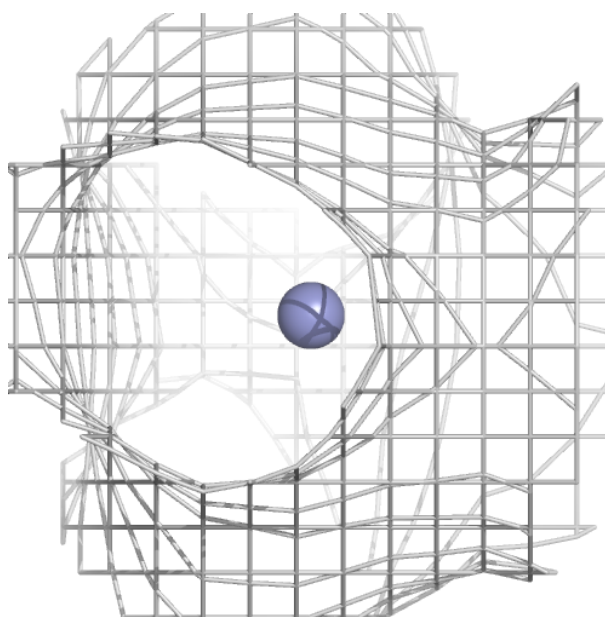
Electron density around ZN A 1001:

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



Electron density around ZN A 1003:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.