



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:05 pm BST

PDB ID : 9H01 / pdb_00009h01
Title : nsp14 of SARS-CoV-2 in complex with a camelid nanobody
Authors : Gauffre, P.; Ferron, F.; Canard, B.
Deposited on : 2024-10-07
Resolution : 2.53 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	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

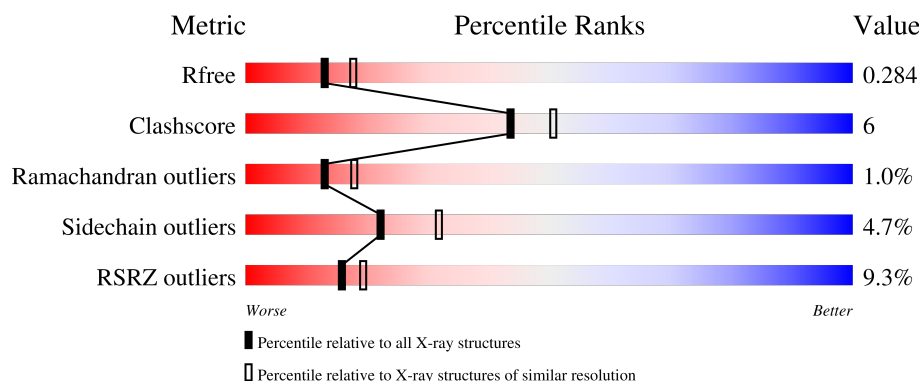
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	164625	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (2.54-2.54)

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	<div> <div>9%</div> <div>71%</div> <div>13%</div> <div>•</div> <div>15%</div> </div>
2	B	132	<div> <div>3%</div> <div>76%</div> <div>18%</div> <div>•</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4671 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 Guanine-N7 methyltransferase nsp14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3679	2361	622	662	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	N	O	S	0	0	0
			935	581	165	184	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

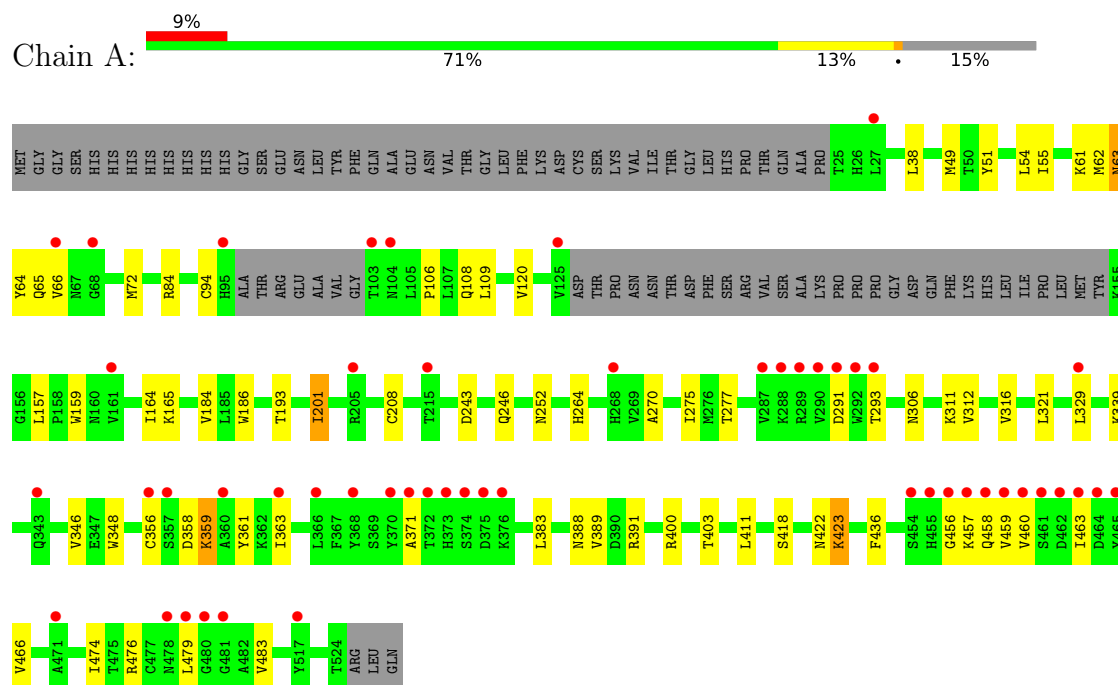
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	10	Total 10	O 10	0	0

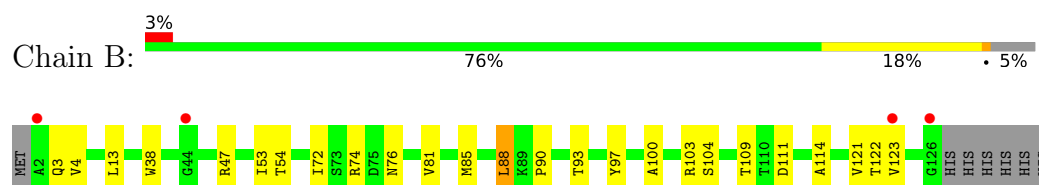
3 Residue-property plots

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: Guanine-N7 methyltransferase nsp14



- Molecule 2: vhh anti-nsp14 of SARS-CoV-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.53Å 80.83Å 138.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.52 – 2.53 51.52 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.52-2.53) 99.8 (51.52-2.53)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.243 , 0.289 0.236 , 0.284	Depositor DCC
R_{free} test set	1057 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4671	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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	0.70	0/3780	1.07	4/5137 (0.1%)
2	B	0.68	0/953	1.00	3/1293 (0.2%)
All	All	0.70	0/4733	1.06	7/6430 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	TRP	N-CA-C	-6.43	99.47	108.54
1	A	423	LYS	N-CA-C	-6.22	105.35	113.12
2	B	88	LEU	N-CA-C	5.99	117.77	109.15
2	B	54	THR	CA-C-N	5.52	127.94	120.38
2	B	54	THR	C-N-CA	5.52	127.94	120.38
1	A	456	GLY	CA-C-N	5.44	127.52	120.44
1	A	456	GLY	C-N-CA	5.44	127.52	120.44

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	3679	0	3530	37	0
2	B	935	0	900	18	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	44	0	0	0	0
4	B	10	0	0	0	0
All	All	4671	0	4430	54	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 6.

All (54) 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:306:ASN:HD21	1:A:422:ASN:HD21	1.12	0.97
2:B:3:GLN:HG2	2:B:4:VAL:H	1.42	0.84
2:B:74:ARG:HE	2:B:76:ASN:HD21	1.26	0.81
1:A:306:ASN:HD21	1:A:422:ASN:ND2	1.79	0.79
1:A:306:ASN:ND2	1:A:422:ASN:HD21	1.81	0.77
1:A:363:ILE:HD11	1:A:389:VAL:HG21	1.69	0.74
2:B:3:GLN:HG2	2:B:4:VAL:N	2.05	0.70
1:A:109:LEU:HD11	1:A:159:TRP:CH2	2.27	0.69
1:A:84:ARG:HG2	1:A:411:LEU:HD11	1.78	0.66
1:A:306:ASN:HD22	1:A:423:LYS:NZ	1.92	0.66
1:A:306:ASN:HD22	1:A:423:LYS:HZ2	1.46	0.63
2:B:74:ARG:HE	2:B:76:ASN:ND2	1.97	0.62
1:A:361:TYR:HB2	1:A:389:VAL:HG12	1.82	0.61
1:A:363:ILE:HD11	1:A:389:VAL:CG2	2.34	0.54
2:B:103:ARG:NH1	2:B:111:ASP:O	2.40	0.54
2:B:74:ARG:NE	2:B:76:ASN:HD21	2.00	0.54
1:A:363:ILE:HG13	1:A:391:ARG:O	2.08	0.54
2:B:100:ALA:HB3	2:B:114:ALA:HB3	1.91	0.52
1:A:63:ASN:O	1:A:65:GLN:HG2	2.10	0.52
1:A:403:THR:HB	1:A:418:SER:HB3	1.91	0.52
1:A:329:LEU:HD11	1:A:383:LEU:HB2	1.92	0.52
1:A:356:CYS:SG	1:A:388:ASN:HB2	2.49	0.51
1:A:94:CYS:HB3	1:A:106:PRO:HG2	1.93	0.51
2:B:47:ARG:NH2	2:B:97:TYR:CD1	2.79	0.50
1:A:339:LYS:NZ	1:A:348:TRP:HB2	2.27	0.50
2:B:93:THR:HG23	2:B:122:THR:HA	1.95	0.49
1:A:358:ASP:O	1:A:359:LYS:O	2.32	0.48
2:B:85:MET:HE1	2:B:121:VAL:HG11	1.96	0.47
1:A:243:ASP:HB3	1:A:246:GLN:HG2	1.97	0.47
1:A:321:LEU:HD22	1:A:346:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:NZ	1:A:63:ASN:HA	2.30	0.46
2:B:38:TRP:HE1	2:B:81:VAL:HG12	1.80	0.46
1:A:184:VAL:HG12	1:A:277:THR:HG22	1.98	0.46
1:A:312:VAL:O	1:A:316:VAL:HG23	2.16	0.46
2:B:3:GLN:CG	2:B:4:VAL:H	2.22	0.46
2:B:90:PRO:HA	2:B:123:VAL:HB	1.98	0.46
1:A:61:LYS:HZ1	1:A:63:ASN:HA	1.81	0.46
1:A:339:LYS:NZ	1:A:348:TRP:CB	2.79	0.45
1:A:49:MET:HE1	1:A:54:LEU:HD13	2.01	0.43
1:A:51:TYR:O	1:A:55:ILE:HG12	2.19	0.43
2:B:38:TRP:HD1	2:B:72:ILE:HD12	1.85	0.42
2:B:3:GLN:CG	2:B:4:VAL:N	2.80	0.42
1:A:264:HIS:CD2	1:A:275:ILE:CG2	3.02	0.42
1:A:72:MET:HE3	1:A:201:ILE:HD11	2.02	0.42
1:A:363:ILE:CD1	1:A:389:VAL:HG21	2.45	0.42
1:A:108:GLN:NE2	1:A:270:ALA:H	2.17	0.42
1:A:208:CYS:HA	2:B:104:SER:HA	2.02	0.42
1:A:400:ARG:HG2	1:A:436:PHE:HZ	1.85	0.42
1:A:264:HIS:CD2	1:A:275:ILE:HG21	2.55	0.41
2:B:85:MET:HB3	2:B:88:LEU:HD21	2.01	0.41
1:A:109:LEU:HD11	1:A:159:TRP:HH2	1.84	0.41
1:A:306:ASN:ND2	1:A:423:LYS:HZ2	2.16	0.40
1:A:358:ASP:O	1:A:359:LYS:C	2.65	0.40
2:B:53:ILE:HD13	2:B:74:ARG:HB2	2.03	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	458/547 (84%)	423 (92%)	29 (6%)	6 (1%)	10 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	123/132 (93%)	120 (98%)	3 (2%)	0	100	100
All	All	581/679 (86%)	543 (94%)	32 (6%)	6 (1%)	13	18

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	LYS
1	A	291	ASP
1	A	459	VAL
1	A	371	ALA
1	A	63	ASN
1	A	64	TYR

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	399/479 (83%)	378 (95%)	21 (5%)	19	26
2	B	94/101 (93%)	92 (98%)	2 (2%)	48	66
All	All	493/580 (85%)	470 (95%)	23 (5%)	22	32

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	62	MET
1	A	66	VAL
1	A	120	VAL
1	A	157	LEU
1	A	164	ILE
1	A	165	LYS
1	A	193	THR
1	A	201	ILE
1	A	252	ASN

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Mol	Chain	Res	Type
1	A	293	THR
1	A	311	LYS
1	A	457	LYS
1	A	458	GLN
1	A	460	VAL
1	A	463	ILE
1	A	466	VAL
1	A	474	ILE
1	A	476	ARG
1	A	479	LEU
1	A	483	VAL
2	B	13	LEU
2	B	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	108	GLN
1	A	256	ASN
1	A	306	ASN
1	A	422	ASN
1	A	455	HIS
1	A	518	ASN
2	B	15	GLN
2	B	76	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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

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	464/547 (84%)	1.03	51 (10%) 12 14	25, 67, 91, 108	22 (4%)
2	B	125/132 (94%)	0.37	4 (3%) 50 56	38, 69, 89, 99	1 (0%)
All	All	589/679 (86%)	0.89	55 (9%) 16 19	25, 68, 91, 108	23 (3%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	VAL	18.7
1	A	463	ILE	18.0
1	A	460	VAL	17.5
1	A	456	GLY	16.7
1	A	455	HIS	16.2
1	A	373	HIS	16.0
1	A	374	SER	15.3
1	A	458	GLN	15.0
1	A	462	ASP	14.0
1	A	375	ASP	14.0
1	A	372	THR	13.8
1	A	461	SER	13.6
1	A	371	ALA	12.7
1	A	479	LEU	12.3
1	A	457	LYS	11.9
1	A	480	GLY	10.1
1	A	370	TYR	9.3
1	A	376	LYS	8.7
1	A	454	SER	7.3
1	A	481	GLY	6.6
2	B	2	ALA	6.4
1	A	104	ASN	4.7
1	A	288	LYS	4.4
1	A	125	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	366	LEU	3.9
2	B	126	GLY	3.8
1	A	290	VAL	3.7
1	A	287	VAL	3.4
1	A	356	CYS	3.4
2	B	44	GLY	3.3
1	A	465	TYR	3.2
1	A	357	SER	3.2
1	A	363	ILE	3.1
1	A	27	LEU	3.1
1	A	517	TYR	3.1
1	A	291	ASP	3.0
1	A	292	TRP	2.9
1	A	268	HIS	2.8
1	A	161	VAL	2.8
1	A	464	ASP	2.8
1	A	289	ARG	2.7
1	A	343	GLN	2.6
1	A	360	ALA	2.6
1	A	103	THR	2.4
1	A	205	ARG	2.4
1	A	368	TYR	2.4
1	A	478	ASN	2.3
1	A	215	THR	2.2
1	A	66	VAL	2.2
1	A	293	THR	2.2
1	A	95	HIS	2.1
2	B	123	VAL	2.1
1	A	68	GLY	2.1
1	A	329	LEU	2.0
1	A	471	ALA	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 oligosaccharides in this entry.

6.4 Ligands

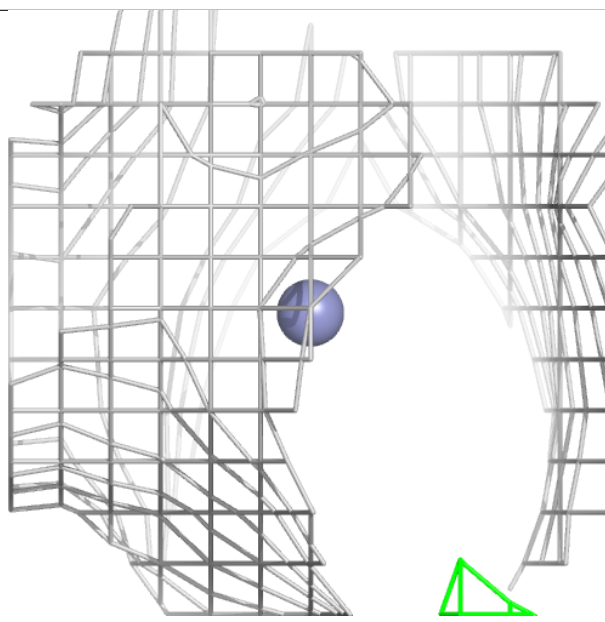
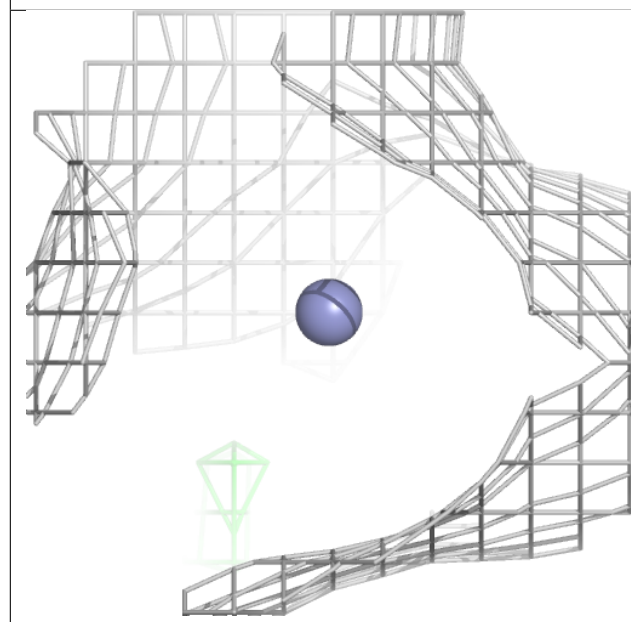
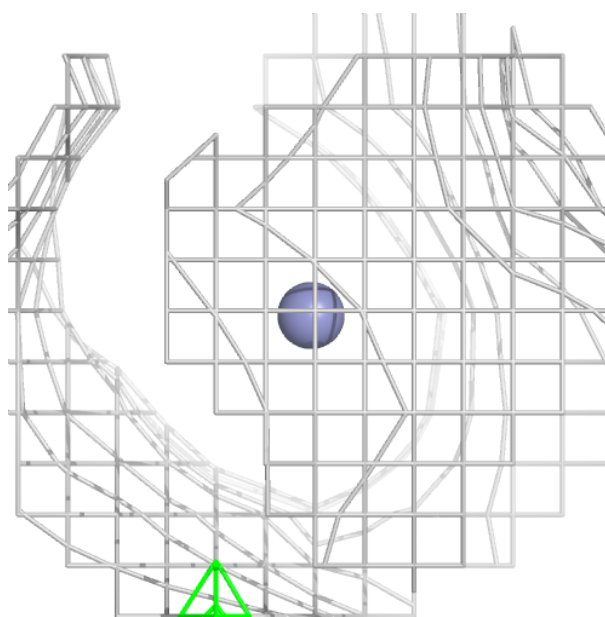
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	A	1002	1/1	0.99	0.04	70,70,70,70	0
3	ZN	A	1001	1/1	1.00	0.06	61,61,61,61	0
3	ZN	A	1003	1/1	1.00	0.04	60,60,60,60	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.

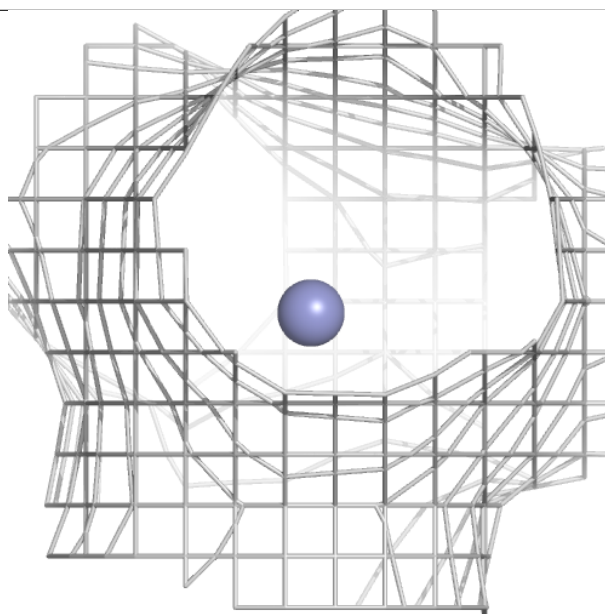
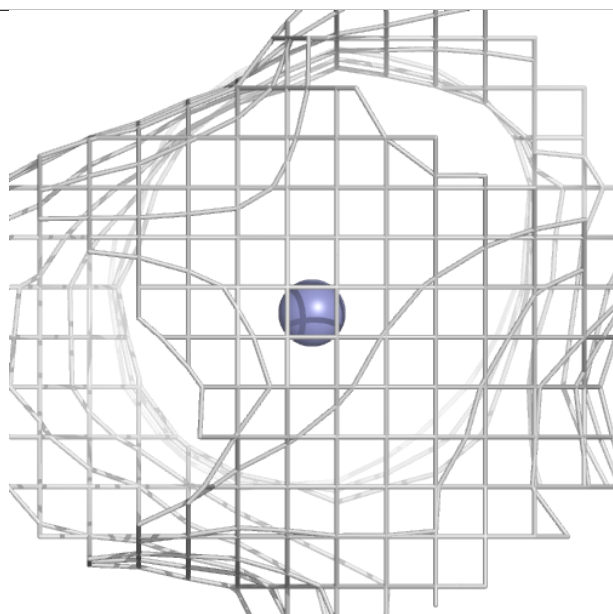
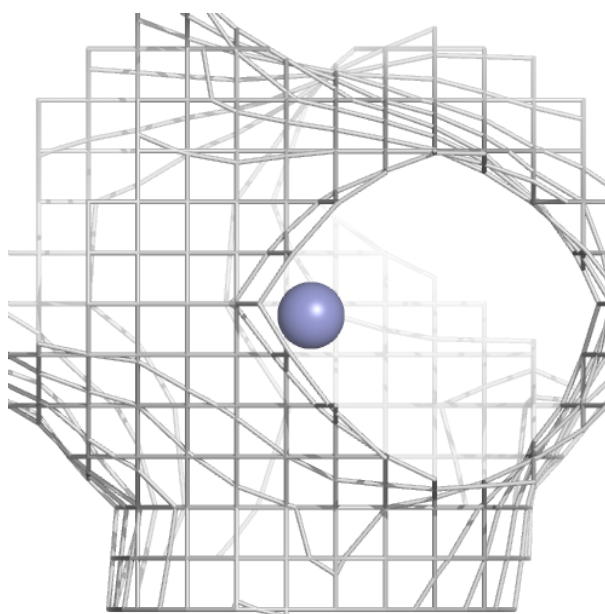
Electron density around ZN A 1002:

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



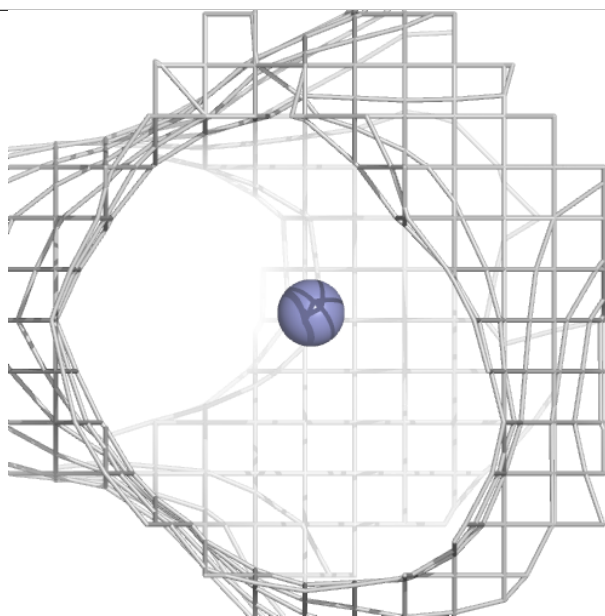
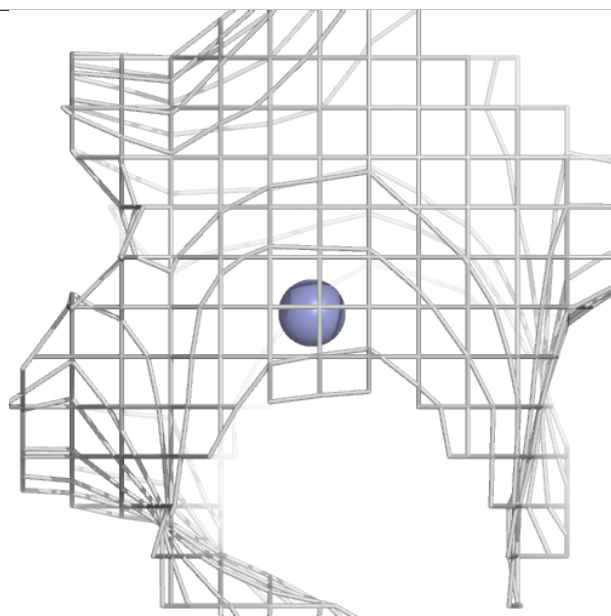
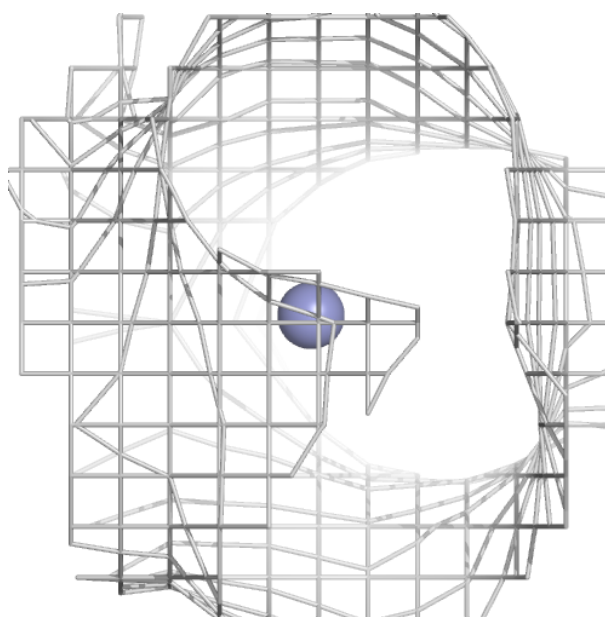
Electron density around ZN A 1001:

$2mF_o-DF_c$ (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.