



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 28, 2020 – 02:39 PM EST

PDB ID : 7KKM
Title : Structure of the catalytic domain of tankyrase 1
Authors : Gajiwala, K.S.; Ryan, K.
Deposited on : 2020-10-27
Resolution : 1.58 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 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 : 2.16
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) : 2.16

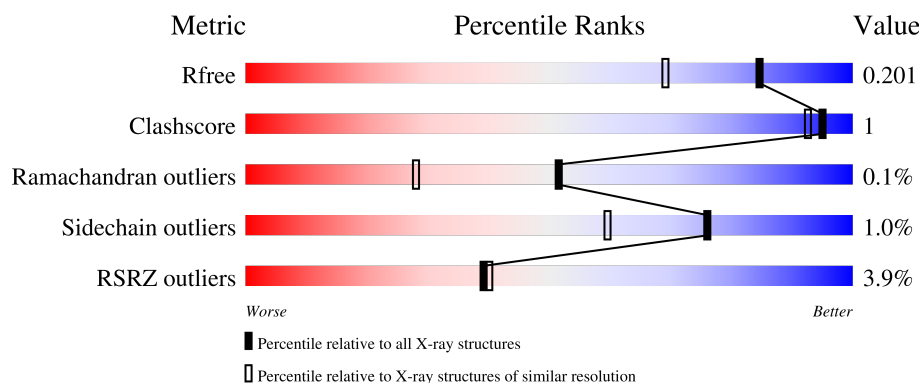
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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	213	<div> <div>3%</div> <div>94%</div> <div>• •</div> </div>
1	B	213	<div> <div>%</div> <div>90%</div> <div>• 7%</div> </div>
1	C	213	<div> <div>5%</div> <div>89%</div> <div>5% 6%</div> </div>
1	D	213	<div> <div>5%</div> <div>85%</div> <div>6% 9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7235 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 Poly [ADP-ribose] polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	1	0
			1668	1048	307	301	12			
1	B	199	Total	C	N	O	S	0	0	0
			1613	1014	297	292	10			
1	C	201	Total	C	N	O	S	0	0	0
			1630	1026	299	294	11			
1	D	193	Total	C	N	O	S	0	0	0
			1567	987	287	283	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1102	GLY	-	expression tag	UNP Q59FX0
A	1103	SER	-	expression tag	UNP Q59FX0
B	1102	GLY	-	expression tag	UNP Q59FX0
B	1103	SER	-	expression tag	UNP Q59FX0
C	1102	GLY	-	expression tag	UNP Q59FX0
C	1103	SER	-	expression tag	UNP Q59FX0
D	1102	GLY	-	expression tag	UNP Q59FX0
D	1103	SER	-	expression tag	UNP Q59FX0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

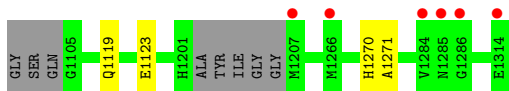
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total 218	O 218	0	0
3	B	204	Total 204	O 204	0	0
3	C	173	Total 173	O 173	0	0
3	D	158	Total 158	O 158	0	0

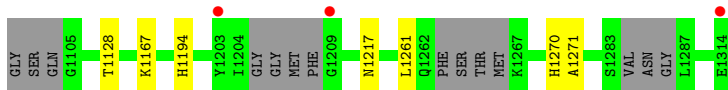
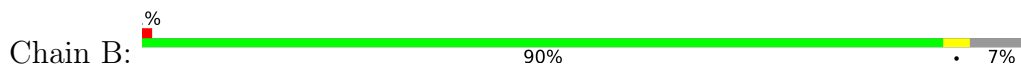
3 Residue-property plots

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.

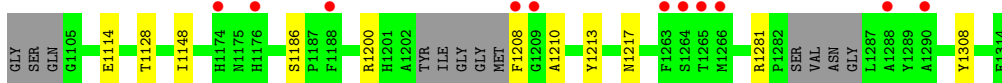
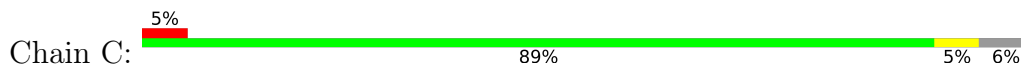
- Molecule 1: Poly [ADP-ribose] polymerase



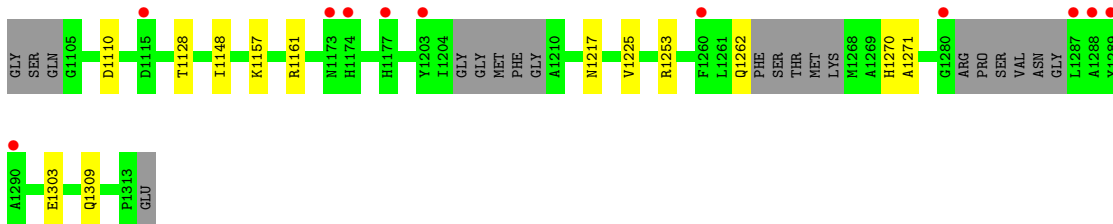
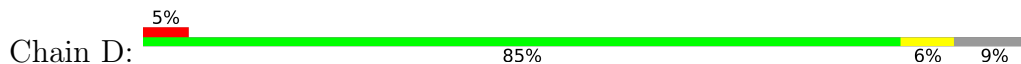
- Molecule 1: Poly [ADP-ribose] polymerase



- Molecule 1: Poly [ADP-ribose] polymerase



- Molecule 1: Poly [ADP-ribose] polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.03Å 114.93Å 80.52Å 90.00° 91.48° 90.00°	Depositor
Resolution (Å)	22.82 – 1.58 80.49 – 1.58	Depositor EDS
% Data completeness (in resolution range)	74.7 (22.82-1.58) 74.7 (80.49-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 1.58Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.195 , 0.233 0.201 , 0.201	Depositor DCC
R_{free} test set	4726 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7235	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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	0.53	0/1710	0.63	0/2297
1	B	0.53	0/1651	0.64	0/2216
1	C	0.52	0/1670	0.64	0/2242
1	D	0.50	0/1604	0.63	0/2154
All	All	0.52	0/6635	0.63	0/8909

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	1668	0	1600	3	0
1	B	1613	0	1551	3	0
1	C	1630	0	1566	4	0
1	D	1567	0	1504	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	218	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	204	0	0	1	0
3	C	173	0	0	0	0
3	D	158	0	0	1	0
All	All	7235	0	6221	15	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 (15) 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:C:1208:PHE:N	1:C:1213:TYR:HH	2.00	0.58
1:B:1270:HIS:HD2	1:B:1271:ALA:O	1.90	0.55
1:C:1148:ILE:HD12	1:C:1308:TYR:HA	1.88	0.54
1:A:1119:GLN:O	1:A:1123:GLU:HB2	2.16	0.46
1:A:1270[B]:HIS:HD2	1:A:1271:ALA:O	2.00	0.44
1:A:1270[B]:HIS:CD2	1:C:1200:ARG:HA	2.53	0.44
1:D:1270:HIS:HD2	1:D:1271:ALA:O	2.01	0.43
1:D:1253:ARG:HG3	1:D:1303:GLU:HG3	2.01	0.42
1:B:1128:THR:HB	1:B:1217:ASN:HA	2.02	0.41
1:B:1194:HIS:HD2	3:B:9191:HOH:O	2.03	0.41
1:D:1148:ILE:HD11	1:D:1309:GLN:HG3	2.02	0.41
1:C:1128:THR:HB	1:C:1217:ASN:HA	2.02	0.41
1:D:1157:LYS:HD3	1:D:1161:ARG:HH21	1.85	0.41
1:D:1225:VAL:HG22	3:D:9122:HOH:O	2.21	0.41
1:D:1128:THR:HB	1:D:1217:ASN:HA	2.04	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	202/213 (95%)	198 (98%)	4 (2%)	0	100	100
1	B	191/213 (90%)	190 (100%)	1 (0%)	0	100	100
1	C	195/213 (92%)	193 (99%)	1 (0%)	1 (0%)	29	10
1	D	185/213 (87%)	183 (99%)	2 (1%)	0	100	100
All	All	773/852 (91%)	764 (99%)	8 (1%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1210	ALA

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	177/180 (98%)	177 (100%)	0	100	100
1	B	170/180 (94%)	168 (99%)	2 (1%)	71	52
1	C	172/180 (96%)	169 (98%)	3 (2%)	60	36
1	D	165/180 (92%)	163 (99%)	2 (1%)	71	52
All	All	684/720 (95%)	677 (99%)	7 (1%)	76	59

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1167	LYS
1	B	1261	LEU
1	C	1114	GLU
1	C	1186	SER
1	C	1281	ARG
1	D	1110	ASP
1	D	1262	GLN

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

Mol	Chain	Res	Type
1	B	1143	ASN
1	B	1270	HIS
1	C	1164	HIS
1	D	1270	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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	205/213 (96%)	0.05	6 (2%) 51 53	14, 21, 40, 58	0
1	B	199/213 (93%)	-0.02	3 (1%) 73 75	15, 21, 41, 88	0
1	C	201/213 (94%)	0.14	11 (5%) 25 25	16, 24, 46, 58	0
1	D	193/213 (90%)	0.30	11 (5%) 23 23	17, 27, 51, 62	0
All	All	798/852 (93%)	0.12	31 (3%) 39 40	14, 23, 46, 88	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1284	VAL	6.8
1	D	1287	LEU	5.2
1	C	1263	PHE	3.7
1	B	1209	GLY	3.6
1	D	1289	TYR	3.5
1	C	1265	THR	3.4
1	B	1314	GLU	3.3
1	D	1288	ALA	3.3
1	A	1207	MET	3.1
1	D	1260	PHE	3.1
1	A	1285	ASN	3.0
1	C	1188	PHE	2.9
1	C	1208	PHE	2.8
1	A	1286	GLY	2.8
1	D	1174	HIS	2.8
1	D	1203	TYR	2.8
1	C	1174	HIS	2.7
1	C	1288	ALA	2.4
1	D	1290	ALA	2.4
1	C	1209	GLY	2.3
1	D	1115	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1266	MET	2.3
1	A	1314	GLU	2.3
1	D	1173	ASN	2.2
1	D	1177	HIS	2.2
1	B	1203	TYR	2.2
1	C	1290	ALA	2.1
1	C	1266	MET	2.1
1	C	1264	SER	2.1
1	D	1280	GLY	2.1
1	C	1176	HIS	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](#)

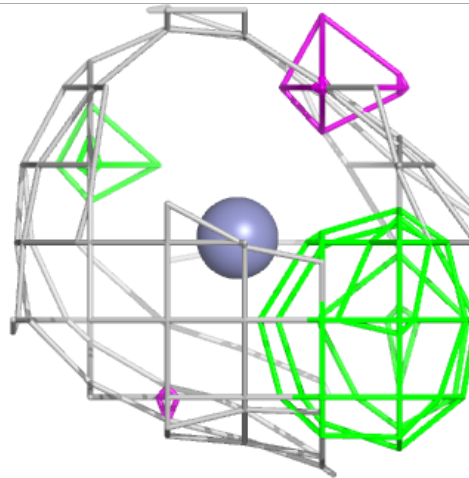
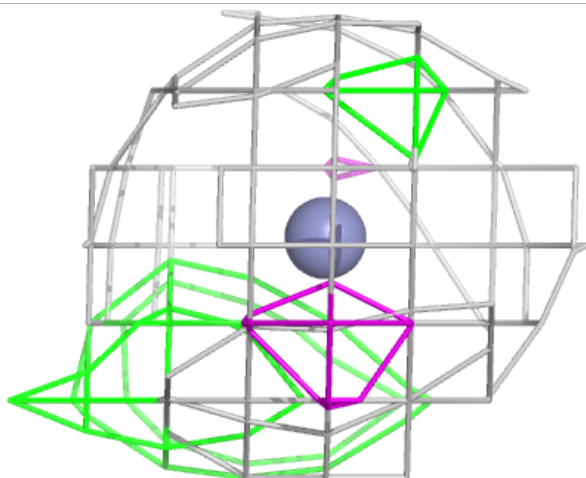
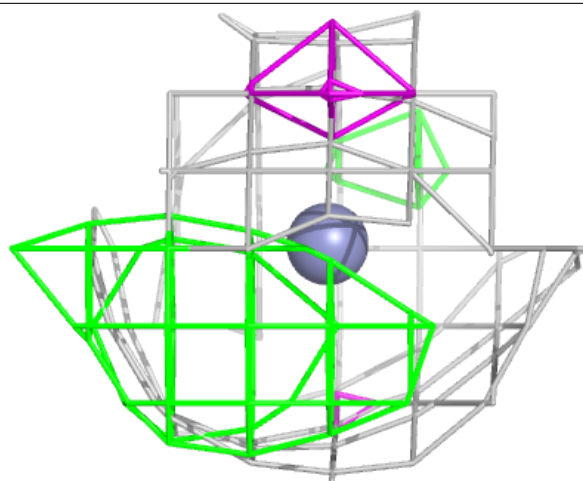
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	D	9001	1/1	0.97	0.09	27,27,27,27	0
2	ZN	B	9001	1/1	0.98	0.10	22,22,22,22	0
2	ZN	A	9001	1/1	1.00	0.09	20,20,20,20	0
2	ZN	C	9001	1/1	1.00	0.08	20,20,20,20	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.

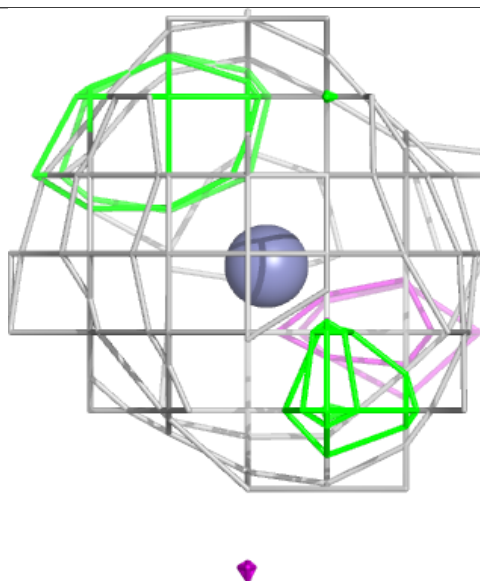
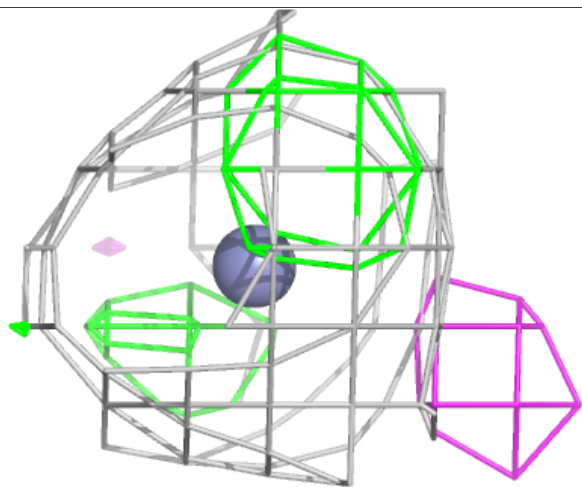
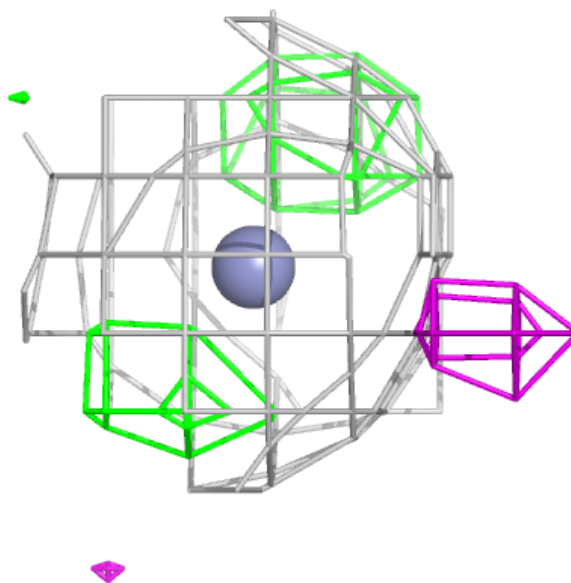
Electron density around ZN D 9001:

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



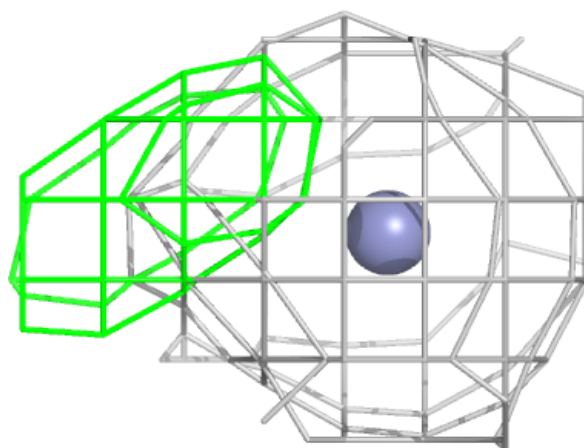
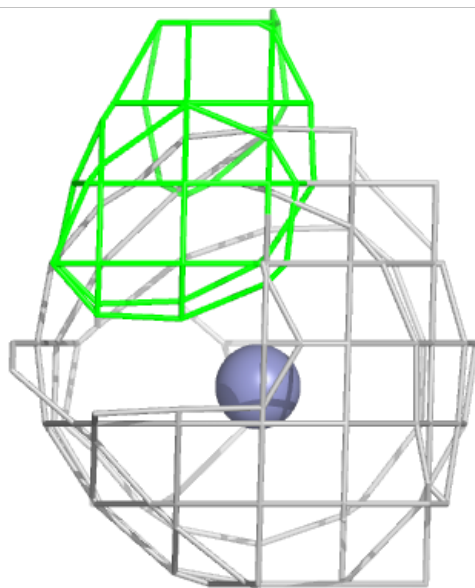
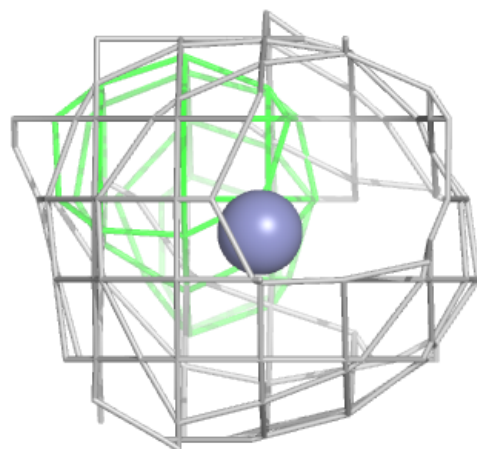
Electron density around ZN B 9001:

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



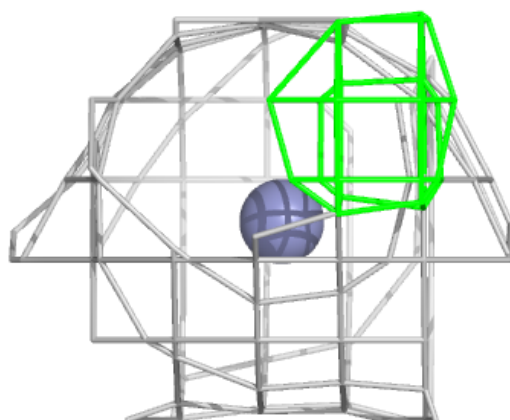
Electron density around ZN A 9001:

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

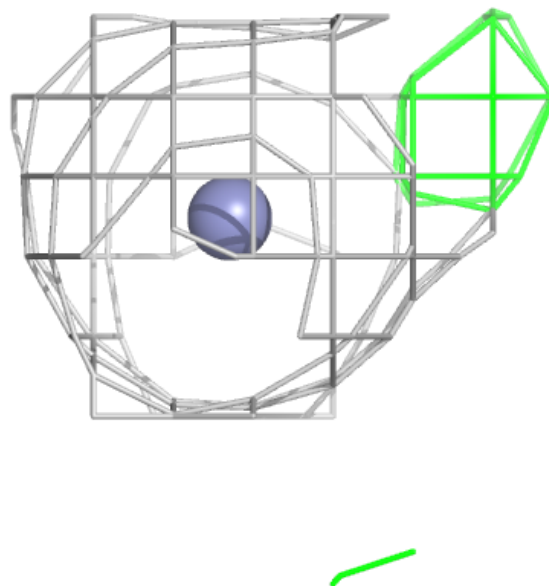
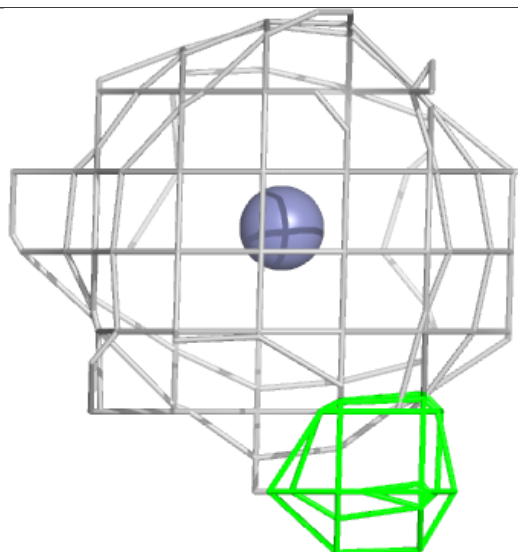


Electron density around ZN C 9001:

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



1



1

6.5 Other polymers [i](#)

There are no such residues in this entry.