



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2022 – 02:12 PM JST

PDB ID : 7VW5  
Title : Crystal structures of alphavirus nonstructural protein 4 (nsP4) reveal an intrinsically dynamic RNA-dependent RNA polymerase fold  
Authors : Tan, Y.B.; Luo, D.  
Deposited on : 2021-11-09  
Resolution : 2.30 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	:	2.26
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)	:	2.26

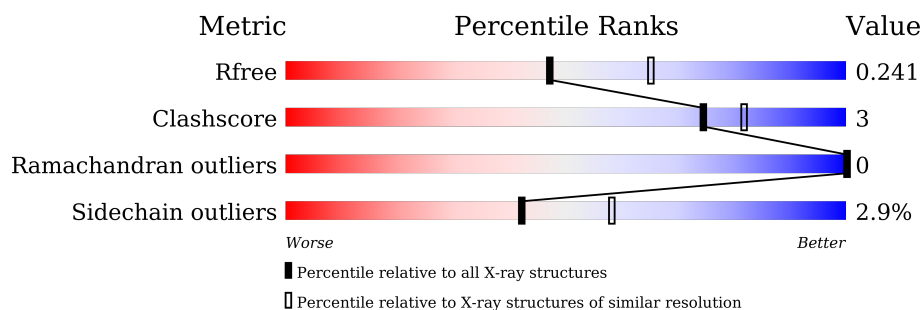
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	520	<div> <div style="width: 80%; background-color: green;"></div> <div style="width: 9%; background-color: yellow;"></div> <div style="width: 11%; background-color: grey;"></div> </div>
1	B	520	<div> <div style="width: 80%; background-color: green;"></div> <div style="width: 9%; background-color: yellow;"></div> <div style="width: 10%; background-color: grey;"></div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7615 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 RNA-directed RNA polymerase nsP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	464	Total	C	N	O	S	0	0	0
			3626	2302	611	689	24			
1	B	466	Total	C	N	O	S	0	0	0
			3641	2313	613	691	24			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	SER	CYS	engineered mutation	UNP P03317
B	164	SER	CYS	engineered mutation	UNP P03317

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	1	0
			1	1		
2	B	1	Total	Mg	1	0
			1	1		

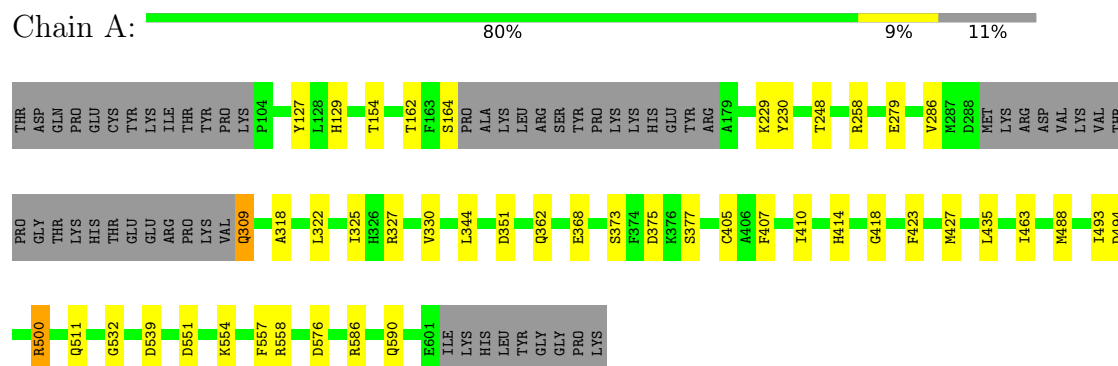
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	168	Total	O	0	0
			168	168		
3	B	178	Total	O	0	0
			178	178		

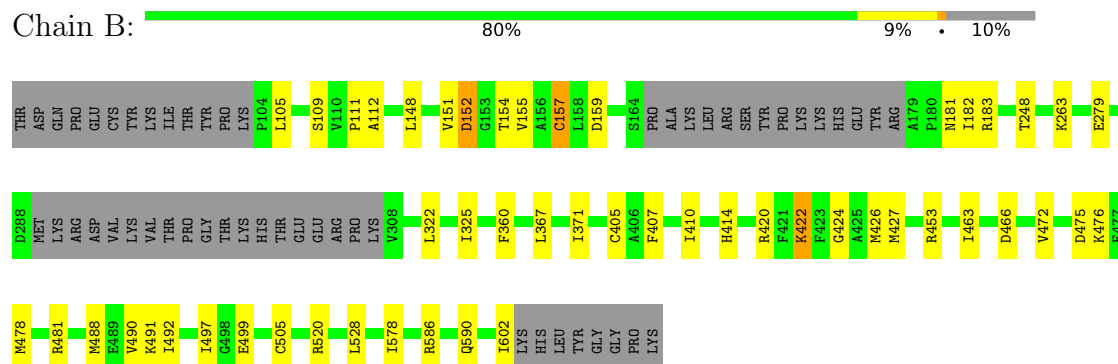
### 3 Residue-property plots

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. 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. 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: RNA-directed RNA polymerase nsP4



- Molecule 1: RNA-directed RNA polymerase nsP4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.45Å 68.94Å 71.42Å 116.31° 107.05° 95.10°	Depositor
Resolution (Å)	36.27 – 2.30 40.59 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.4 (36.27-2.30) 85.2 (40.59-1.91)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 1.91Å)	Xtriage
Refinement program	PHENIX 1.19.2	Depositor
R, $R_{free}$	0.197 , 0.240 0.196 , 0.241	Depositor DCC
$R_{free}$ test set	2000 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.03% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.24	0/3695	0.46	0/5020
1	B	0.24	0/3710	0.45	0/5041
All	All	0.24	0/7405	0.46	0/10061

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	3626	0	3607	25	0
1	B	3641	0	3627	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	168	0	0	0	0
3	B	178	0	0	0	0
All	All	7615	0	7234	46	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 (46) 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:286:VAL:HB	1:A:309:GLN:HG3	1.76	0.67
1:A:554:LYS:HG2	1:A:586:ARG:HH12	1.60	0.66
1:A:164:SER:HB3	1:A:330:VAL:HG11	1.78	0.66
1:A:322:LEU:HA	1:A:325:ILE:HD12	1.76	0.66
1:B:488:MET:O	1:B:491:LYS:NZ	2.32	0.62
1:B:155:VAL:HG22	1:B:463:ILE:HG12	1.83	0.61
1:A:407:PHE:HD1	1:A:410:ILE:HD11	1.67	0.58
1:B:151:VAL:HG21	1:B:157:CYS:HB2	1.85	0.57
1:B:152:ASP:HB3	1:B:183:ARG:HB3	1.87	0.56
1:A:154:THR:HG23	1:A:435:LEU:HD13	1.88	0.55
1:B:586:ARG:HH21	1:B:590:GLN:HE22	1.53	0.55
1:B:155:VAL:HB	1:B:182:ILE:HD11	1.90	0.54
1:A:418:GLY:HA2	1:B:602:ILE:HD11	1.93	0.51
1:B:371:ILE:HA	1:B:490:VAL:HG22	1.93	0.50
1:A:248:THR:HA	1:A:279:GLU:HA	1.93	0.49
1:B:586:ARG:NE	1:B:590:GLN:OE1	2.45	0.49
1:A:407:PHE:CD1	1:A:410:ILE:HD11	2.46	0.49
1:A:414:HIS:HE1	1:B:528:LEU:O	1.97	0.48
1:A:423:PHE:HA	1:A:427:MET:HE2	1.96	0.48
1:B:478:MET:HG2	1:B:492:ILE:HD13	1.96	0.48
1:A:375:ASP:OD1	1:A:377:SER:OG	2.30	0.47
1:B:499:GLU:N	1:B:499:GLU:OE1	2.48	0.47
1:A:344:LEU:HB2	1:A:463:ILE:HB	1.96	0.47
1:B:360:PHE:HD2	1:B:497:ILE:HD11	1.79	0.46
1:A:586:ARG:NE	1:A:590:GLN:OE1	2.49	0.45
1:B:248:THR:HA	1:B:279:GLU:HA	1.98	0.45
1:B:367:LEU:HD13	1:B:472:VAL:HG12	1.98	0.45
1:B:505:CYS:O	1:B:520:ARG:NH2	2.42	0.45
1:B:322:LEU:HD23	1:B:325:ILE:HD12	1.98	0.45
1:A:127:TYR:CZ	1:B:578:ILE:HD12	2.52	0.44
1:B:148:LEU:HD22	1:B:154:THR:HA	1.99	0.44
1:A:558:ARG:HA	1:B:109:SER:HA	1.99	0.43
1:A:532:GLY:HA3	1:B:414:HIS:CE1	2.53	0.43
1:B:453:ARG:HH22	1:B:481:ARG:HH22	1.65	0.43
1:B:105:LEU:HD12	1:B:105:LEU:HA	1.89	0.42
1:A:494:ASP:O	1:A:500:ARG:NH1	2.52	0.42
1:A:258:ARG:HA	1:A:258:ARG:HD3	1.76	0.42
1:A:362:GLN:HB2	1:A:511:GLN:OE1	2.20	0.42
1:A:229:LYS:HD2	1:A:230:TYR:CZ	2.55	0.42
1:B:109:SER:O	1:B:111:PRO:HD3	2.19	0.42
1:B:422:LYS:HD2	1:B:424:GLY:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:O	1:A:322:LEU:HD12	2.21	0.41
1:A:557:PHE:CE1	1:B:112:ALA:HB3	2.56	0.41
1:A:162:THR:HB	1:A:327:ARG:NH1	2.36	0.41
1:B:407:PHE:HA	1:B:410:ILE:HG12	2.03	0.40
1:A:368:GLU:HB3	1:A:493:ILE:HB	2.02	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	458/520 (88%)	442 (96%)	16 (4%)	0	100	100
1	B	460/520 (88%)	449 (98%)	11 (2%)	0	100	100
All	All	918/1040 (88%)	891 (97%)	27 (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	394/446 (88%)	384 (98%)	10 (2%)	47	65
1	B	396/446 (89%)	383 (97%)	13 (3%)	38	53
All	All	790/892 (89%)	767 (97%)	23 (3%)	42	58



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

Mol	Chain	Res	Type
1	A	129	HIS
1	A	309	GLN
1	A	351	ASP
1	A	373	SER
1	A	405	CYS
1	A	488	MET
1	A	500	ARG
1	A	539	ASP
1	A	551	ASP
1	A	576	ASP
1	B	152	ASP
1	B	157	CYS
1	B	159	ASP
1	B	181	ASN
1	B	263	LYS
1	B	405	CYS
1	B	420	ARG
1	B	422	LYS
1	B	426	MET
1	B	427	MET
1	B	466	ASP
1	B	475	ASP
1	B	476	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	414	HIS
1	A	596	GLN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

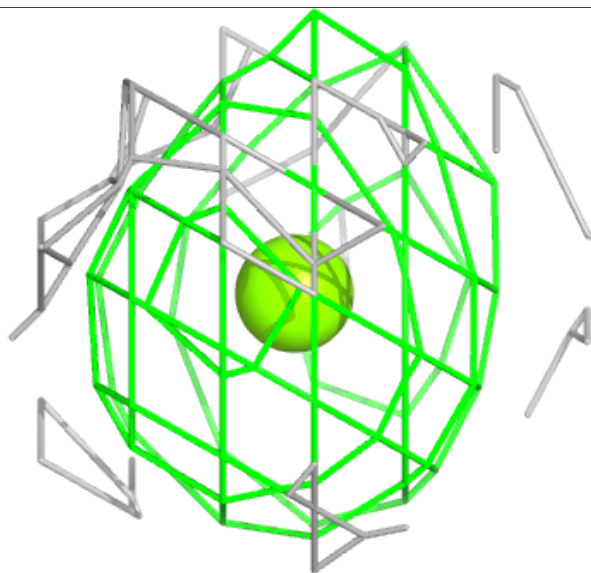
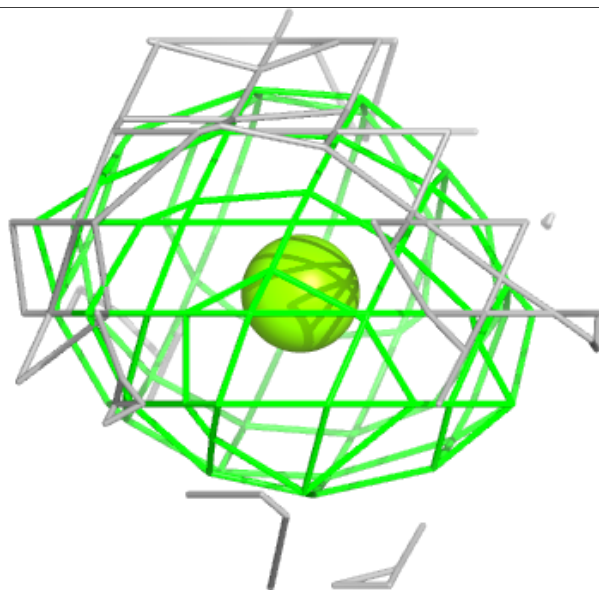
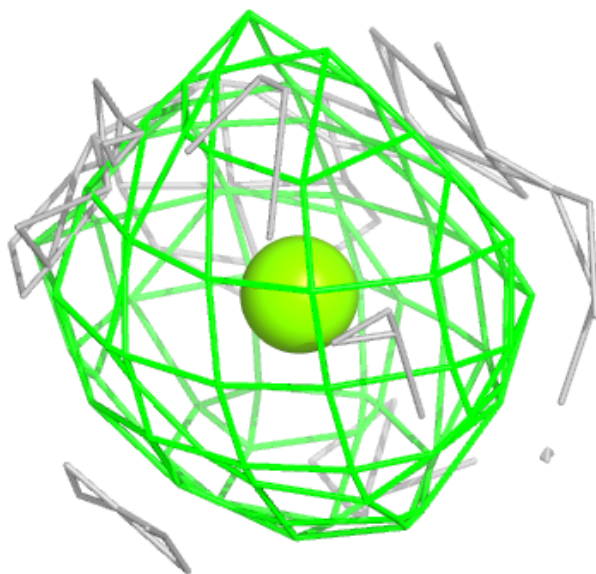
### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

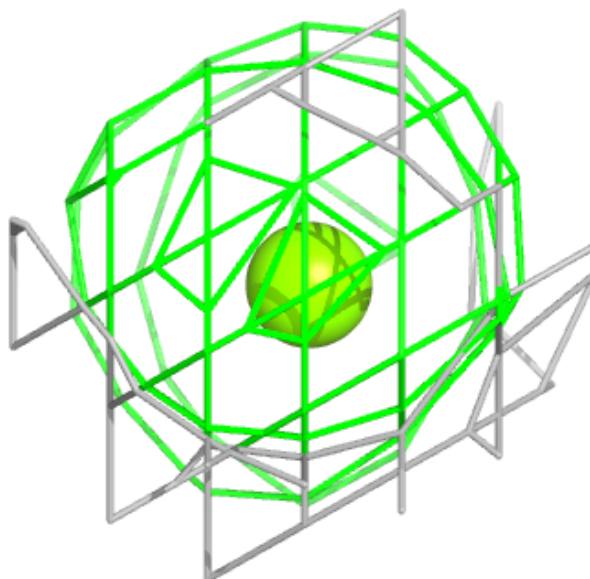
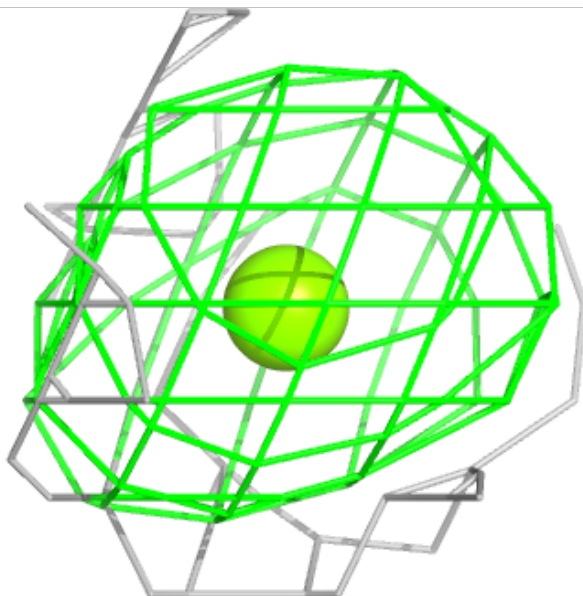
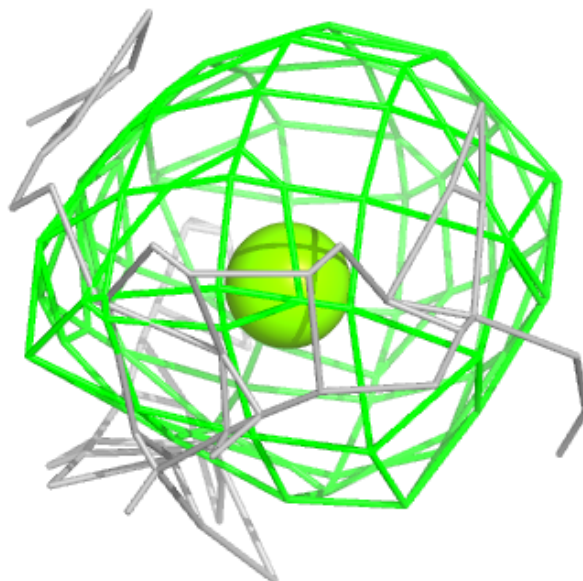
**Electron density around MG A 701:**

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



**Electron density around MG B 701:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.