



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 08:54 am BST

PDB ID : 5XSI  
Title : The catalytic domain of GdpP  
Authors : Wang, F.; Gu, L.  
Deposited on : 2017-06-14  
Resolution : 2.20 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 : 2.11  
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) : 2.11

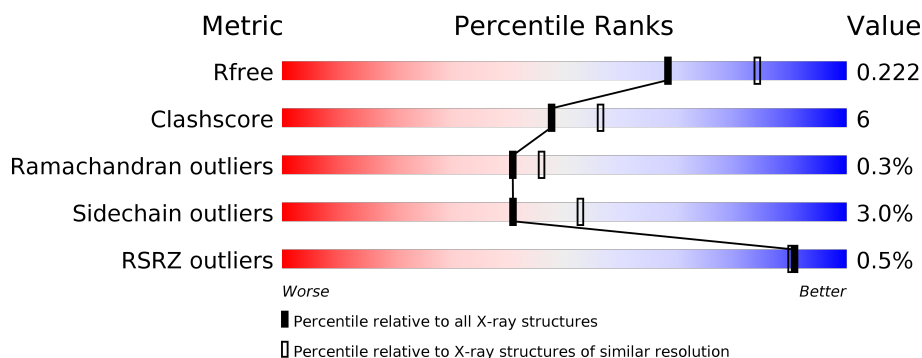
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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  $\leq 5\%$ . 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	343	 84% 11% . .
1	B	343	 82% 14% . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5538 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 Phosphodiesterase acting on cyclic dinucleotides.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	0	0
			2597	1619	460	509	9			
1	B	333	Total	C	N	O	S	0	0	0
			2597	1619	460	509	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	GLY	-	expression tag	UNP A0A0U1MUE2
A	314	SER	-	expression tag	UNP A0A0U1MUE2
A	315	MET	-	expression tag	UNP A0A0U1MUE2
B	313	GLY	-	expression tag	UNP A0A0U1MUE2
B	314	SER	-	expression tag	UNP A0A0U1MUE2
B	315	MET	-	expression tag	UNP A0A0U1MUE2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

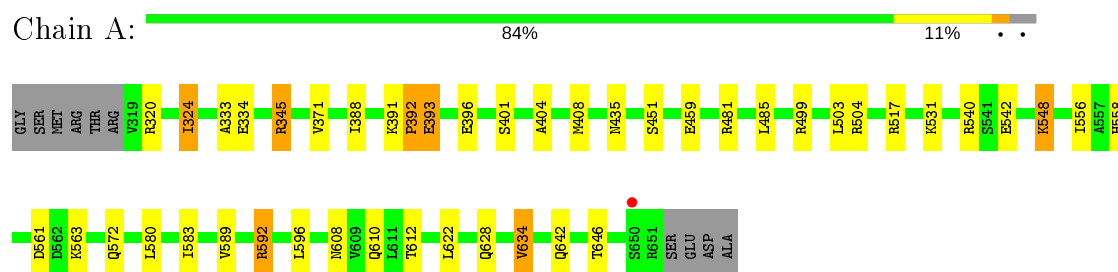
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	187	Total	O	0	0
			187	187		
3	B	153	Total	O	0	0
			153	153		

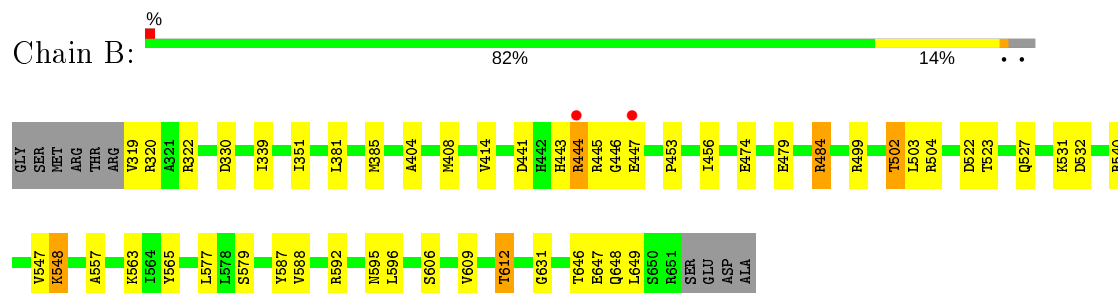
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Phosphodiesterase acting on cyclic dinucleotides



- Molecule 1: Phosphodiesterase acting on cyclic dinucleotides



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.09Å 117.09Å 127.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.42 – 2.20 46.42 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.42-2.20) 99.5 (46.42-2.19)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.98 (at 2.18Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, $R_{free}$	0.174 , 0.226 0.176 , 0.222	Depositor DCC
$R_{free}$ test set	2170 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5538	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

### 5.1 Standard geometry

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

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	0.93	2/2631 (0.1%)	0.85	1/3566 (0.0%)
1	B	0.85	0/2631	0.84	4/3566 (0.1%)
All	All	0.89	2/5262 (0.0%)	0.85	5/7132 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	371	VAL	CB-CG1	5.26	1.64	1.52
1	A	401	SER	CB-OG	-5.11	1.35	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	385	MET	CG-SD-CE	-7.68	87.91	100.20
1	B	540	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	532	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	577	LEU	CA-CB-CG	-5.11	103.55	115.30
1	A	592	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	2597	0	2618	33	0
1	B	2597	0	2618	32	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	187	0	0	6	0
3	B	153	0	0	4	0
All	All	5538	0	5236	64	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 (64) 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:B:474:GLU:OE2	3:B:801:HOH:O	1.65	1.13
1:A:388:ILE:O	1:A:392:PRO:HD2	1.52	1.07
1:A:320:ARG:NH1	1:A:459:GLU:OE2	1.98	0.97
1:B:319:VAL:HG23	1:B:322:ARG:NH2	1.89	0.86
1:B:319:VAL:HG23	1:B:322:ARG:HH22	1.45	0.80
1:A:504:ARG:NH2	3:A:802:HOH:O	2.22	0.72
1:A:504:ARG:HH11	1:A:504:ARG:HG3	1.60	0.66
1:A:333:ALA:O	3:A:801:HOH:O	2.14	0.64
1:B:547:VAL:O	1:B:548:LYS:HE2	1.98	0.64
1:B:612:THR:HB	1:B:648:GLN:OE1	2.01	0.60
1:B:319:VAL:HG23	1:B:322:ARG:CZ	2.32	0.59
1:B:587:TYR:OH	1:B:612:THR:HG21	2.01	0.59
1:A:393:GLU:HG2	1:A:396:GLU:OE2	2.03	0.59
1:A:561:ASP:HA	1:A:634:VAL:HG13	1.85	0.59
1:A:542:GLU:OE1	1:A:563:LYS:NZ	2.33	0.58
1:A:451:SER:HB3	3:A:968:HOH:O	2.04	0.58
1:A:392:PRO:HG3	1:A:485:LEU:HD23	1.88	0.55
1:A:517:ARG:NH2	3:A:807:HOH:O	2.40	0.55
1:A:596:LEU:HD21	1:A:628:GLN:OE1	2.08	0.54
1:A:540:ARG:HD2	1:A:572:GLN:HB3	1.89	0.54
1:A:388:ILE:O	1:A:392:PRO:CD	2.42	0.53
1:B:404:ALA:O	1:B:408:MET:HG3	2.09	0.53
1:B:499:ARG:O	1:B:502:THR:HB	2.07	0.53
1:B:444:ARG:NH2	3:B:806:HOH:O	2.42	0.52
1:A:592:ARG:NH2	3:A:809:HOH:O	2.42	0.52
1:B:320:ARG:HG3	1:B:320:ARG:HH11	1.76	0.50
1:B:563:LYS:HG2	1:B:565:TYR:CE1	2.47	0.50
1:B:330:ASP:OD1	3:B:802:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLN:O	1:B:531:LYS:HG2	2.13	0.48
1:A:642:GLN:O	1:A:646:THR:HG23	2.14	0.47
1:A:622:LEU:O	1:A:622:LEU:HD23	2.14	0.47
1:A:531:LYS:HG2	1:B:579:SER:O	2.15	0.47
1:A:608:ASN:OD1	1:A:610:GLN:HB3	2.15	0.47
1:A:435:ASN:ND2	3:A:813:HOH:O	2.48	0.46
1:A:504:ARG:HH11	1:A:504:ARG:CG	2.24	0.46
1:A:388:ILE:C	1:A:392:PRO:HD2	2.30	0.46
1:B:499:ARG:HG3	1:B:503:LEU:HD12	1.97	0.46
1:A:393:GLU:CG	1:A:396:GLU:OE2	2.64	0.45
1:B:339:ILE:O	1:B:414:VAL:HA	2.17	0.45
1:B:523:THR:HG22	1:B:527:GLN:OE1	2.17	0.44
1:A:345:ARG:HG3	1:A:345:ARG:HH11	1.83	0.44
1:B:484:ARG:NH1	1:B:522:ASP:OD2	2.51	0.44
1:B:319:VAL:HG23	1:B:322:ARG:NH1	2.33	0.43
1:B:445:ARG:HG2	1:B:446:GLY:N	2.33	0.43
1:B:484:ARG:HD2	3:B:945:HOH:O	2.18	0.43
1:A:320:ARG:HG2	1:A:324:ILE:CD1	2.49	0.42
1:B:649:LEU:HA	1:B:649:LEU:HD23	1.77	0.42
1:A:345:ARG:HG3	1:A:345:ARG:NH1	2.34	0.42
1:A:499:ARG:HD3	1:A:503:LEU:HD11	2.01	0.42
1:B:609:VAL:HA	1:B:612:THR:CG2	2.49	0.42
1:B:646:THR:O	1:B:647:GLU:C	2.53	0.42
1:A:504:ARG:NH1	1:A:504:ARG:CG	2.79	0.41
1:A:548:LYS:HE3	1:A:556:ILE:HB	2.03	0.41
1:B:557:ALA:HB3	1:B:588:VAL:HG22	2.03	0.41
1:A:404:ALA:O	1:A:408:MET:HG3	2.20	0.41
1:A:558:HIS:HA	1:A:589:VAL:O	2.21	0.41
1:A:320:ARG:HG2	1:A:324:ILE:HD12	2.02	0.41
1:B:447:GLU:CD	1:B:447:GLU:N	2.74	0.41
1:A:580:LEU:HB2	1:A:583:ILE:HD12	2.02	0.40
1:B:351:ILE:HG13	1:B:381:LEU:HD11	2.03	0.40
1:B:441:ASP:OD1	1:B:443:HIS:ND1	2.48	0.40
1:B:596:LEU:HA	1:B:596:LEU:HD12	1.88	0.40
1:B:595:ASN:OD1	1:B:631:GLY:HA2	2.21	0.40
1:B:453:PRO:HG2	1:B:456:ILE:HD11	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	331/343 (96%)	326 (98%)	3 (1%)	2 (1%)	25	26
1	B	331/343 (96%)	322 (97%)	9 (3%)	0	100	100
All	All	662/686 (96%)	648 (98%)	12 (2%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	PRO
1	A	391	LYS

### 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	284/292 (97%)	276 (97%)	8 (3%)	43	56
1	B	284/292 (97%)	275 (97%)	9 (3%)	39	50
All	All	568/584 (97%)	551 (97%)	17 (3%)	41	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	ILE
1	A	334	GLU
1	A	345	ARG
1	A	393	GLU

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Mol	Chain	Res	Type
1	A	481	ARG
1	A	548	LYS
1	A	612	THR
1	A	634	VAL
1	B	444	ARG
1	B	479	GLU
1	B	484	ARG
1	B	502	THR
1	B	504	ARG
1	B	548	LYS
1	B	592	ARG
1	B	606	SER
1	B	612	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/343 (97%)	-0.36	1 (0%) 94 93	20, 33, 50, 75	0
1	B	333/343 (97%)	-0.38	2 (0%) 89 88	21, 37, 53, 83	0
All	All	666/686 (97%)	-0.37	3 (0%) 91 90	20, 35, 52, 83	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	650	SER	2.9
1	B	444	ARG	2.6
1	B	447	GLU	2.5

### 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 carbohydrates 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
2	MN	B	701	1/1	0.97	0.03	50,50,50,50	0
2	MN	B	700	1/1	0.98	0.10	31,31,31,31	0

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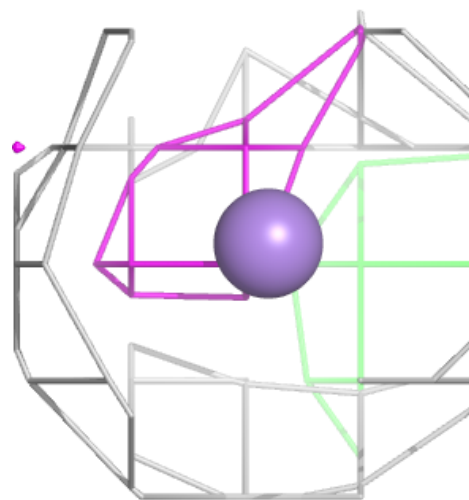
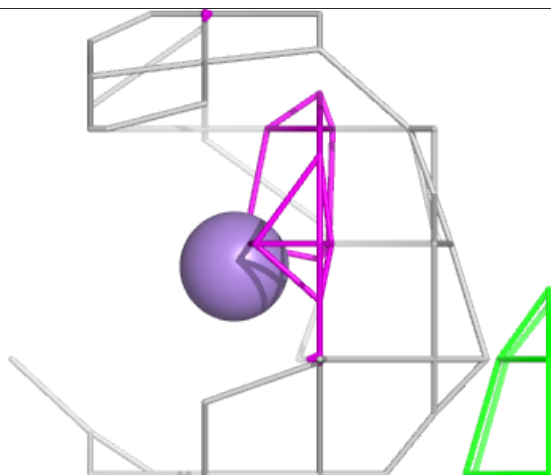
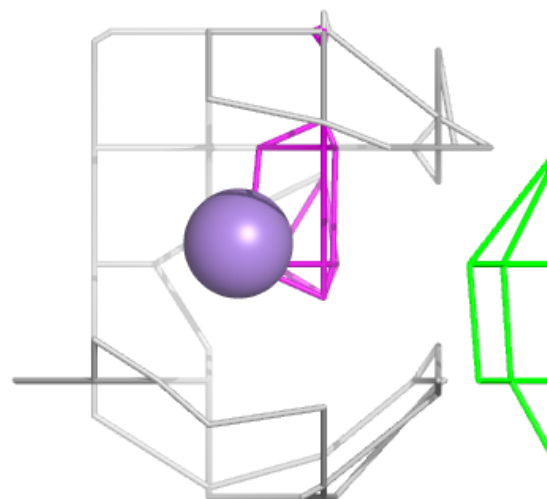
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	A	701	1/1	0.98	0.04	50,50,50,50	0
2	MN	A	700	1/1	1.00	0.12	30,30,30,30	0

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.

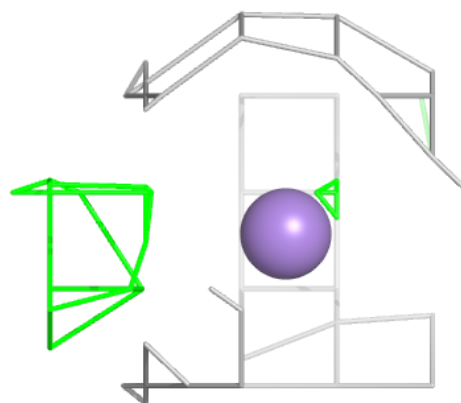
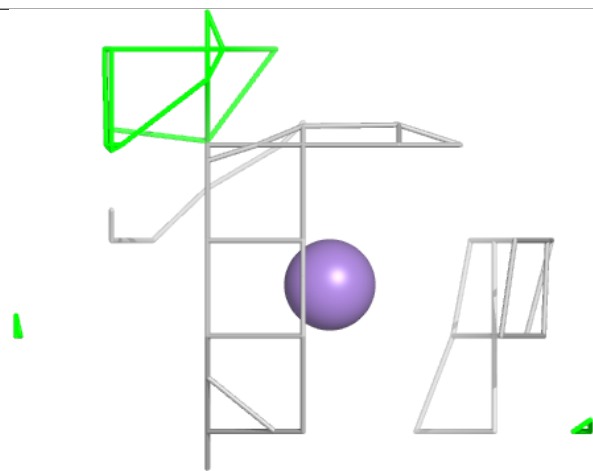
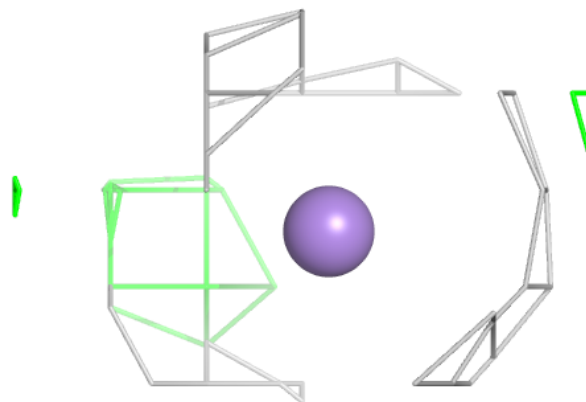
**Electron density around MN B 701:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



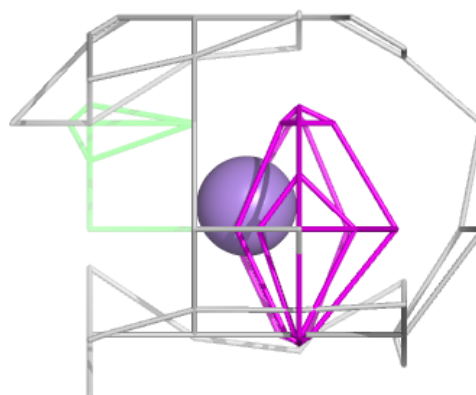
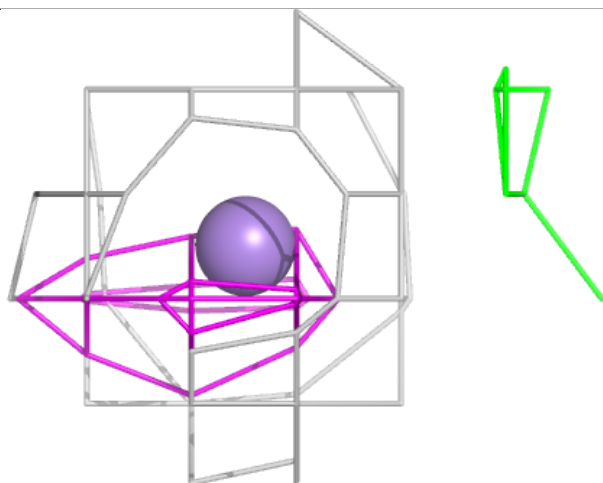
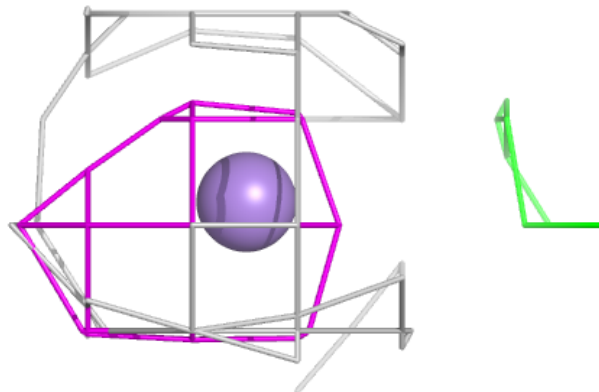
**Electron density around MN B 700:**

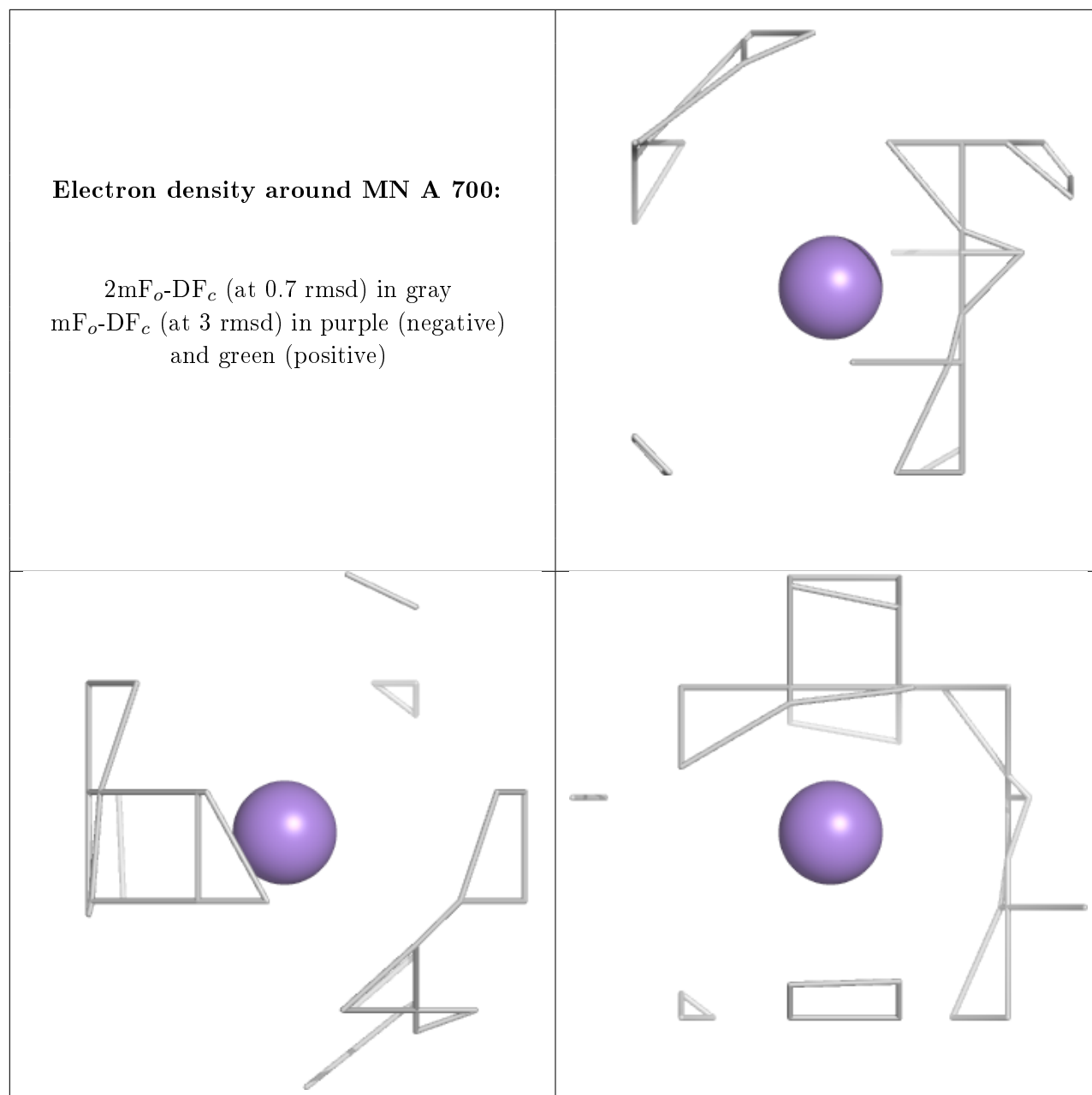
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around MN 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)





## 6.5 Other polymers ⓘ

There are no such residues in this entry.