



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2022 – 04:06 PM EDT

PDB ID : 7TU2  
Title : Structure of the *L. blandensis* dGTPase R37A mutant bound to Mn  
Authors : Sikkema, A.P.; Klemm, B.P.; Horng, J.C.; Hall, T.M.T.  
Deposited on : 2022-02-02  
Resolution : 2.13 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  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
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) : 2.28.1

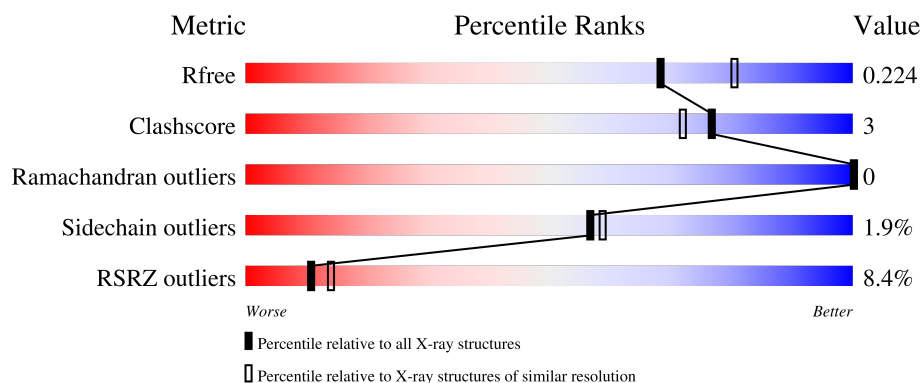
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\leq 5\%$ . 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	464	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	464	<div> <div>7%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>8%</div> </div> </div>
1	C	464	<div> <div>9%</div> <div> <div></div> <div>82%</div> <div>11%</div> <div>7%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10410 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 dGTP triphosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	0	0
			3445	2193	583	661	8			
1	B	426	Total	C	N	O	S	0	0	0
			3383	2158	571	646	8			
1	C	430	Total	C	N	O	S	0	0	0
			3391	2162	570	651	8			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP A3XHN1
A	-20	HIS	-	expression tag	UNP A3XHN1
A	-19	HIS	-	expression tag	UNP A3XHN1
A	-18	HIS	-	expression tag	UNP A3XHN1
A	-17	HIS	-	expression tag	UNP A3XHN1
A	-16	HIS	-	expression tag	UNP A3XHN1
A	-15	HIS	-	expression tag	UNP A3XHN1
A	-14	SER	-	expression tag	UNP A3XHN1
A	-13	SER	-	expression tag	UNP A3XHN1
A	-12	GLY	-	expression tag	UNP A3XHN1
A	-11	VAL	-	expression tag	UNP A3XHN1
A	-10	ASP	-	expression tag	UNP A3XHN1
A	-9	LEU	-	expression tag	UNP A3XHN1
A	-8	GLY	-	expression tag	UNP A3XHN1
A	-7	THR	-	expression tag	UNP A3XHN1
A	-6	GLU	-	expression tag	UNP A3XHN1
A	-5	ASN	-	expression tag	UNP A3XHN1
A	-4	LEU	-	expression tag	UNP A3XHN1
A	-3	TYR	-	expression tag	UNP A3XHN1
A	-2	PHE	-	expression tag	UNP A3XHN1
A	-1	GLN	-	expression tag	UNP A3XHN1
A	0	SER	-	expression tag	UNP A3XHN1
A	1	ASN	-	expression tag	UNP A3XHN1

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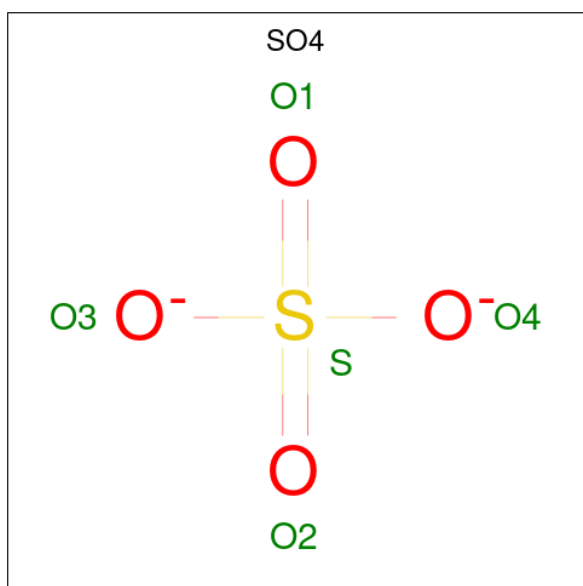
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP A3XHN1
A	37	ALA	ARG	engineered mutation	UNP A3XHN1
B	-21	MET	-	expression tag	UNP A3XHN1
B	-20	HIS	-	expression tag	UNP A3XHN1
B	-19	HIS	-	expression tag	UNP A3XHN1
B	-18	HIS	-	expression tag	UNP A3XHN1
B	-17	HIS	-	expression tag	UNP A3XHN1
B	-16	HIS	-	expression tag	UNP A3XHN1
B	-15	HIS	-	expression tag	UNP A3XHN1
B	-14	SER	-	expression tag	UNP A3XHN1
B	-13	SER	-	expression tag	UNP A3XHN1
B	-12	GLY	-	expression tag	UNP A3XHN1
B	-11	VAL	-	expression tag	UNP A3XHN1
B	-10	ASP	-	expression tag	UNP A3XHN1
B	-9	LEU	-	expression tag	UNP A3XHN1
B	-8	GLY	-	expression tag	UNP A3XHN1
B	-7	THR	-	expression tag	UNP A3XHN1
B	-6	GLU	-	expression tag	UNP A3XHN1
B	-5	ASN	-	expression tag	UNP A3XHN1
B	-4	LEU	-	expression tag	UNP A3XHN1
B	-3	TYR	-	expression tag	UNP A3XHN1
B	-2	PHE	-	expression tag	UNP A3XHN1
B	-1	GLN	-	expression tag	UNP A3XHN1
B	0	SER	-	expression tag	UNP A3XHN1
B	1	ASN	-	expression tag	UNP A3XHN1
B	2	ALA	-	expression tag	UNP A3XHN1
B	37	ALA	ARG	engineered mutation	UNP A3XHN1
C	-21	MET	-	expression tag	UNP A3XHN1
C	-20	HIS	-	expression tag	UNP A3XHN1
C	-19	HIS	-	expression tag	UNP A3XHN1
C	-18	HIS	-	expression tag	UNP A3XHN1
C	-17	HIS	-	expression tag	UNP A3XHN1
C	-16	HIS	-	expression tag	UNP A3XHN1
C	-15	HIS	-	expression tag	UNP A3XHN1
C	-14	SER	-	expression tag	UNP A3XHN1
C	-13	SER	-	expression tag	UNP A3XHN1
C	-12	GLY	-	expression tag	UNP A3XHN1
C	-11	VAL	-	expression tag	UNP A3XHN1
C	-10	ASP	-	expression tag	UNP A3XHN1
C	-9	LEU	-	expression tag	UNP A3XHN1
C	-8	GLY	-	expression tag	UNP A3XHN1
C	-7	THR	-	expression tag	UNP A3XHN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	GLU	-	expression tag	UNP A3XHN1
C	-5	ASN	-	expression tag	UNP A3XHN1
C	-4	LEU	-	expression tag	UNP A3XHN1
C	-3	TYR	-	expression tag	UNP A3XHN1
C	-2	PHE	-	expression tag	UNP A3XHN1
C	-1	GLN	-	expression tag	UNP A3XHN1
C	0	SER	-	expression tag	UNP A3XHN1
C	1	ASN	-	expression tag	UNP A3XHN1
C	2	ALA	-	expression tag	UNP A3XHN1
C	37	ALA	ARG	engineered mutation	UNP A3XHN1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mn 1	0	0
3	B	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0

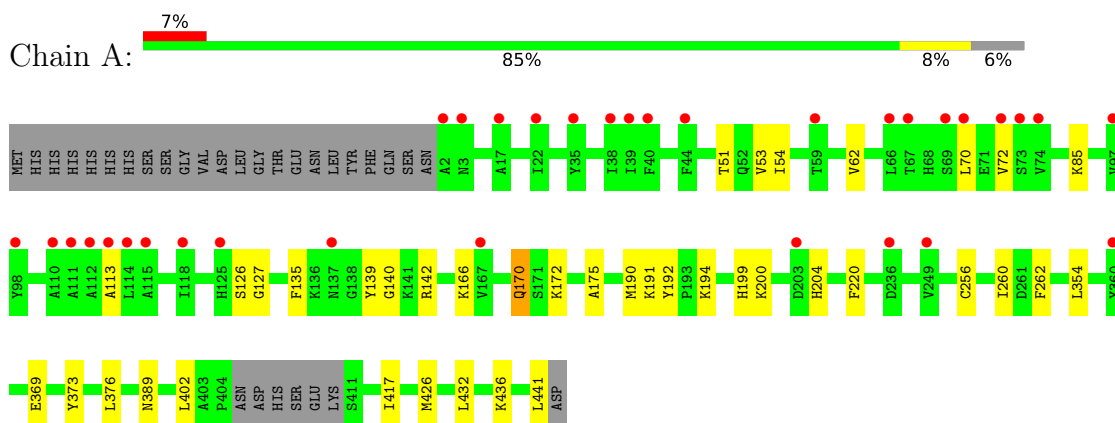
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	74	Total 74	O 74	0	0
4	C	30	Total 30	O 30	0	0

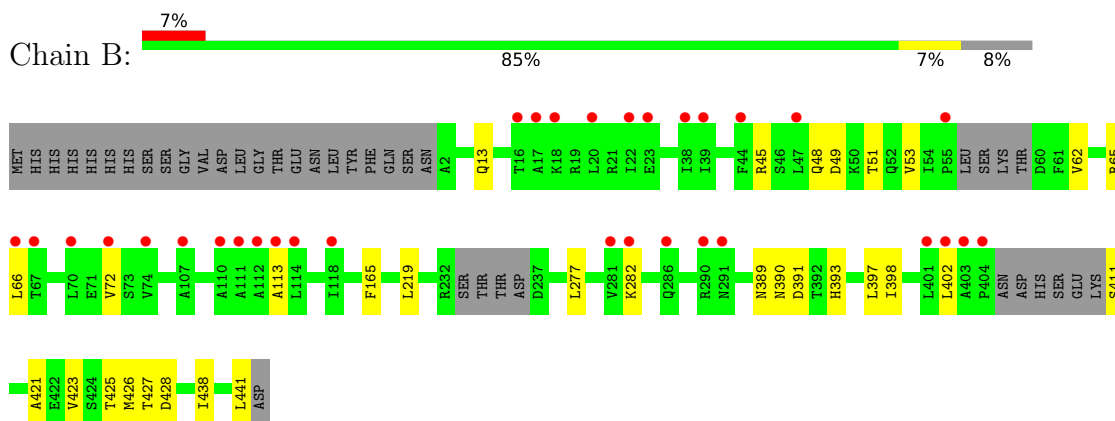
### 3 Residue-property plots [i](#)

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.

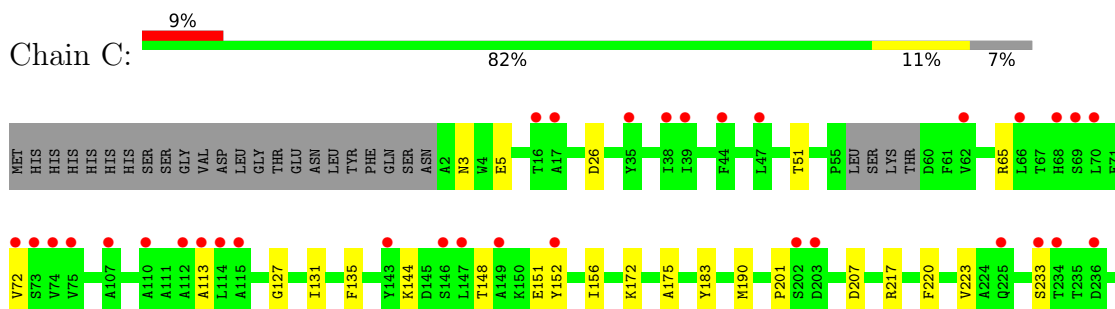
- Molecule 1: dGTP triphosphohydrolase

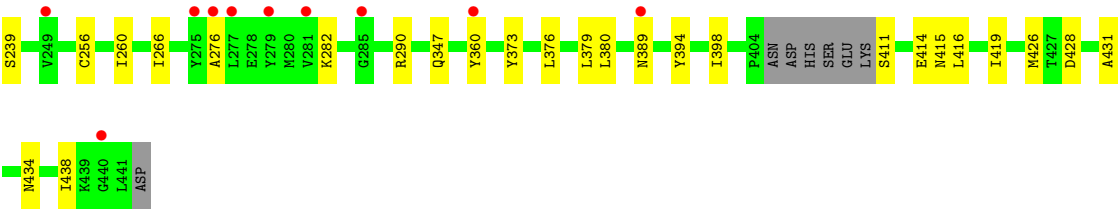


- Molecule 1: dGTP triphosphohydrolase



- Molecule 1: dGTP triphosphohydrolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.93Å 179.93Å 110.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.22 – 2.13 39.72 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.2 (36.22-2.13) 91.1 (39.72-2.13)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.204 , 0.226 0.204 , 0.224	Depositor DCC
$R_{free}$ test set	1662 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: MN, SO4

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	0.45	0/3510	0.63	0/4740
1	B	0.42	0/3446	0.59	0/4650
1	C	0.40	0/3455	0.58	0/4669
All	All	0.42	0/10411	0.60	0/14059

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	3445	0	3410	20	0
1	B	3383	0	3342	12	0
1	C	3391	0	3329	29	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	69	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	74	0	0	0	0
4	C	30	0	0	0	0
All	All	10410	0	10081	60	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 (60) 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:53:VAL:HG23	1:A:54:ILE:HD12	1.78	0.66
1:C:72:VAL:HG12	1:C:113:ALA:HB1	1.77	0.65
1:B:72:VAL:HG12	1:B:113:ALA:HB1	1.82	0.62
1:C:415:ASN:O	1:C:419:ILE:HG13	2.03	0.59
1:A:72:VAL:HG12	1:A:113:ALA:HB1	1.85	0.59
1:C:233:SER:HB2	1:C:239:SER:HB3	1.85	0.58
1:C:434:ASN:O	1:C:438:ILE:HG12	2.04	0.58
1:C:201:PRO:HD2	1:C:207:ASP:HB3	1.85	0.57
1:C:127:GLY:O	1:C:131:ILE:HD12	2.06	0.56
1:C:3:ASN:HB3	1:C:5:GLU:OE1	2.06	0.56
1:A:51:THR:HG23	1:A:54:ILE:O	2.06	0.55
1:C:51:THR:HG23	1:C:428:ASP:OD2	2.07	0.55
1:B:49:ASP:HB2	1:B:427:THR:HB	1.89	0.54
1:B:165:PHE:CZ	1:B:219:LEU:HD12	2.44	0.53
1:A:402:LEU:HD22	1:A:426:MET:HE1	1.92	0.51
1:C:376:LEU:O	1:C:380:LEU:HD12	2.10	0.51
1:B:421:ALA:O	1:B:425:THR:HG23	2.11	0.50
1:A:432:LEU:HG	1:A:436:LYS:HD2	1.94	0.50
1:C:144:LYS:HE2	1:C:152:TYR:CE2	2.47	0.49
1:B:51:THR:HG23	1:B:428:ASP:OD2	2.12	0.49
1:A:127:GLY:HA2	1:A:376:LEU:HD12	1.94	0.49
1:B:402:LEU:HD11	1:B:438:ILE:HD11	1.95	0.48
1:C:172:LYS:HG2	1:C:175:ALA:HB3	1.95	0.48
1:C:411:SER:HB2	1:C:414:GLU:HB2	1.95	0.47
1:C:183:TYR:CD2	1:C:223:VAL:HA	2.50	0.47
1:A:139:TYR:O	1:A:142:ARG:NH1	2.48	0.47
1:B:393:HIS:O	1:B:397:LEU:HD12	2.14	0.47
1:C:144:LYS:HE2	1:C:152:TYR:CZ	2.50	0.47
1:C:282:LYS:HD3	1:C:347:GLN:NE2	2.29	0.46
1:A:199:HIS:CE1	1:A:200:LYS:HD2	2.50	0.46
1:B:45:ARG:O	1:B:48:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:152:TYR:CD2	1:C:156:ILE:HD13	2.52	0.45
1:C:190:MET:HG2	1:C:220:PHE:CZ	2.52	0.45
1:A:262:PHE:HE1	1:A:354:LEU:HD23	1.82	0.44
1:A:166:LYS:HG2	1:A:170:GLN:HG3	1.98	0.44
1:C:135:PHE:CE1	1:C:416:LEU:HD12	2.51	0.44
1:A:441:LEU:HD21	1:B:441:LEU:HD13	1.99	0.44
1:C:426:MET:CE	1:C:431:ALA:HA	2.48	0.44
1:A:126:SER:OG	1:A:369:GLU:HB3	2.17	0.43
1:A:191:LYS:HD2	1:A:192:TYR:CZ	2.53	0.43
1:A:190:MET:HG2	1:A:220:PHE:CZ	2.53	0.43
1:A:417:ILE:HD12	1:A:417:ILE:HA	1.89	0.43
1:C:379:LEU:HD13	1:C:426:MET:HE1	2.00	0.42
1:C:360:TYR:H	1:C:360:TYR:HD1	1.68	0.42
1:C:394:TYR:O	1:C:398:ILE:HG12	2.20	0.42
1:C:148:THR:HG23	1:C:151:GLU:OE1	2.20	0.42
1:B:389:ASN:C	1:B:391:ASP:H	2.23	0.42
1:C:360:TYR:CD1	1:C:360:TYR:N	2.88	0.41
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.91	0.41
1:B:398:ILE:HD13	1:B:398:ILE:HA	1.94	0.41
1:C:65:ARG:HG2	1:C:65:ARG:NH1	2.34	0.41
1:A:142:ARG:NH1	1:A:142:ARG:HB2	2.35	0.41
1:A:256:CYS:O	1:A:260:ILE:HB	2.21	0.41
1:C:65:ARG:HG2	1:C:65:ARG:HH11	1.86	0.41
1:C:266:ILE:HD13	1:C:276:ALA:HB2	2.02	0.41
1:C:135:PHE:HE1	1:C:416:LEU:HD12	1.85	0.40
1:C:256:CYS:O	1:C:260:ILE:HB	2.21	0.40
1:B:423:VAL:HA	1:B:426:MET:HE2	2.02	0.40
1:A:135:PHE:HA	1:A:140:GLY:HA3	2.03	0.40
1:A:172:LYS:HG2	1:A:175:ALA:HB3	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	430/464 (93%)	421 (98%)	9 (2%)	0	100	100
1	B	418/464 (90%)	411 (98%)	7 (2%)	0	100	100
1	C	424/464 (91%)	415 (98%)	9 (2%)	0	100	100
All	All	1272/1392 (91%)	1247 (98%)	25 (2%)	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	367/399 (92%)	360 (98%)	7 (2%)	57	59
1	B	358/399 (90%)	349 (98%)	9 (2%)	47	47
1	C	357/399 (90%)	352 (99%)	5 (1%)	67	70
All	All	1082/1197 (90%)	1061 (98%)	21 (2%)	57	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	85	LYS
1	A	170	GLN
1	A	194	LYS
1	A	204	HIS
1	A	373	TYR
1	A	389	ASN
1	B	13	GLN
1	B	53	VAL
1	B	62	VAL
1	B	65	ARG
1	B	66	LEU
1	B	277	LEU
1	B	282	LYS
1	B	390	ASN

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Mol	Chain	Res	Type
1	B	411	SER
1	C	26	ASP
1	C	217	ARG
1	C	290	ARG
1	C	373	TYR
1	C	389	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	399	GLN
1	B	96	GLN
1	B	170	GLN
1	C	345	GLN

### 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 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	501	-	4,4,4	0.50	0	6,6,6	0.07	0
2	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	C	501	-	4,4,4	0.15	0	6,6,6	0.25	0

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, 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	434/464 (93%)	0.37	33 (7%) 13 17	40, 59, 85, 116	0
1	B	426/464 (91%)	0.46	32 (7%) 14 18	47, 62, 84, 126	0
1	C	430/464 (92%)	0.63	43 (10%) 7 9	50, 73, 99, 115	0
All	All	1290/1392 (92%)	0.49	108 (8%) 11 14	40, 65, 91, 126	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	THR	6.8
1	C	146	SER	4.8
1	C	16	THR	4.6
1	A	114	LEU	4.2
1	C	143	TYR	4.1
1	B	402	LEU	4.1
1	C	360	TYR	4.0
1	B	404	PRO	4.0
1	C	203	ASP	4.0
1	C	72	VAL	3.9
1	B	401	LEU	3.6
1	B	39	ILE	3.6
1	A	39	ILE	3.5
1	A	72	VAL	3.5
1	C	149	ALA	3.4
1	B	16	THR	3.4
1	C	279	TYR	3.4
1	B	403	ALA	3.4
1	B	20	LEU	3.3
1	A	249	VAL	3.3
1	C	70	LEU	3.3
1	A	74	VAL	3.3
1	B	47	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	17	ALA	3.2
1	A	98	TYR	3.1
1	C	114	LEU	3.1
1	B	70	LEU	3.1
1	C	276	ALA	3.0
1	A	70	LEU	3.0
1	B	22	ILE	3.0
1	A	59	THR	3.0
1	C	73	SER	2.9
1	C	233	SER	2.9
1	C	277	LEU	2.9
1	A	97	VAL	2.9
1	C	47	LEU	2.9
1	A	110	ALA	2.8
1	A	115	ALA	2.8
1	A	35	TYR	2.7
1	B	17	ALA	2.7
1	B	67	THR	2.7
1	C	112	ALA	2.7
1	B	66	LEU	2.7
1	C	38	ILE	2.7
1	C	69	SER	2.7
1	C	440	GLY	2.7
1	C	275	TYR	2.6
1	B	38	ILE	2.6
1	A	111	ALA	2.6
1	C	44	PHE	2.6
1	C	66	LEU	2.6
1	B	72	VAL	2.6
1	B	290	ARG	2.5
1	C	35	TYR	2.5
1	B	111	ALA	2.5
1	A	69	SER	2.5
1	C	202	SER	2.5
1	B	44	PHE	2.5
1	C	39	ILE	2.5
1	B	18	LYS	2.4
1	A	22	ILE	2.4
1	A	44	PHE	2.4
1	B	23	GLU	2.4
1	C	285	GLY	2.4
1	B	74	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	110	ALA	2.4
1	B	114	LEU	2.4
1	C	75	VAL	2.4
1	B	107	ALA	2.3
1	C	74	VAL	2.3
1	B	110	ALA	2.3
1	A	125	HIS	2.3
1	A	113	ALA	2.3
1	B	281	VAL	2.3
1	B	113	ALA	2.3
1	C	249	VAL	2.3
1	C	115	ALA	2.2
1	C	147	LEU	2.2
1	A	73	SER	2.2
1	A	38	ILE	2.2
1	A	236	ASP	2.2
1	A	2	ALA	2.2
1	A	360	TYR	2.2
1	C	152	TYR	2.2
1	A	137	ASN	2.2
1	B	291	ASN	2.2
1	C	62	VAL	2.2
1	B	286	GLN	2.2
1	B	112	ALA	2.2
1	C	236	ASP	2.2
1	C	225	GLN	2.1
1	A	66	LEU	2.1
1	A	203	ASP	2.1
1	B	118	ILE	2.1
1	C	389	ASN	2.1
1	A	112	ALA	2.1
1	B	282	LYS	2.1
1	A	67	THR	2.1
1	B	55	PRO	2.1
1	C	68	HIS	2.1
1	A	3	ASN	2.1
1	A	118	ILE	2.1
1	A	17	ALA	2.1
1	A	40	PHE	2.0
1	A	167	VAL	2.0
1	C	107	ALA	2.0
1	C	113	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	281	VAL	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](#)

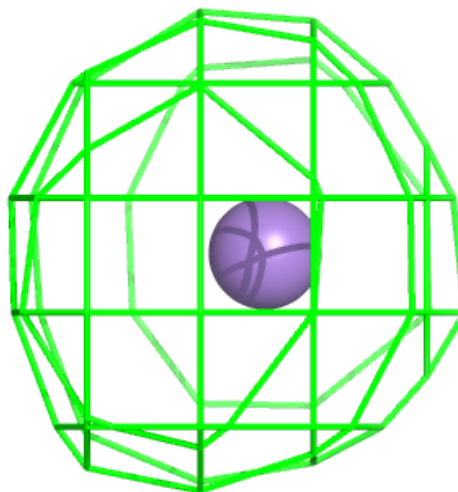
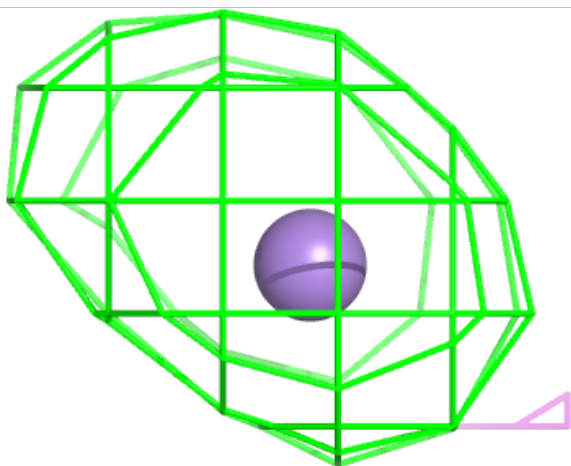
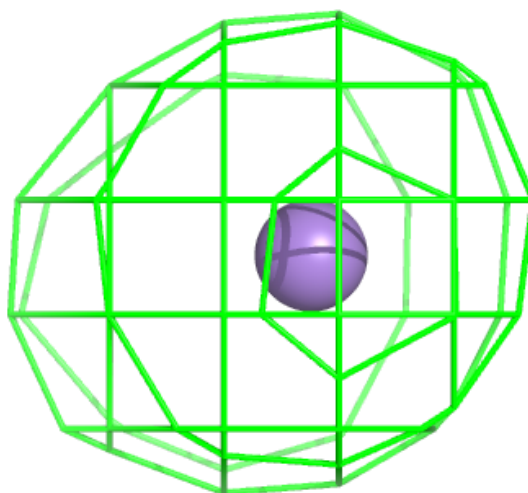
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	SO4	C	501	5/5	0.93	0.12	102,102,105,105	0
3	MN	C	502	1/1	0.95	0.32	75,75,75,75	0
2	SO4	B	501	5/5	0.96	0.12	117,119,120,124	0
2	SO4	A	501	5/5	0.97	0.15	83,84,85,90	0
3	MN	B	502	1/1	0.99	0.18	47,47,47,47	0
3	MN	A	502	1/1	0.99	0.19	45,45,45,45	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 C 502:**

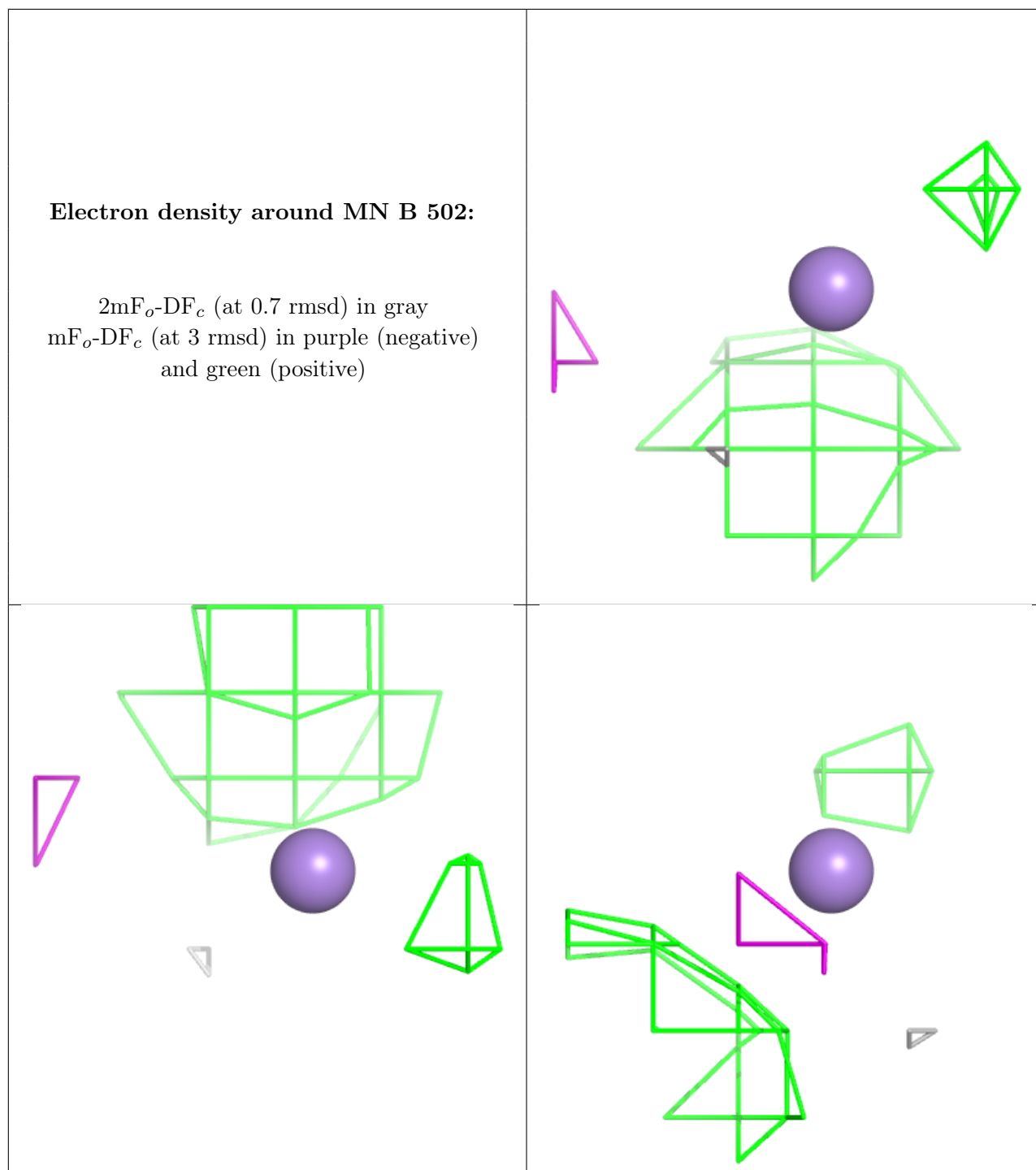
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

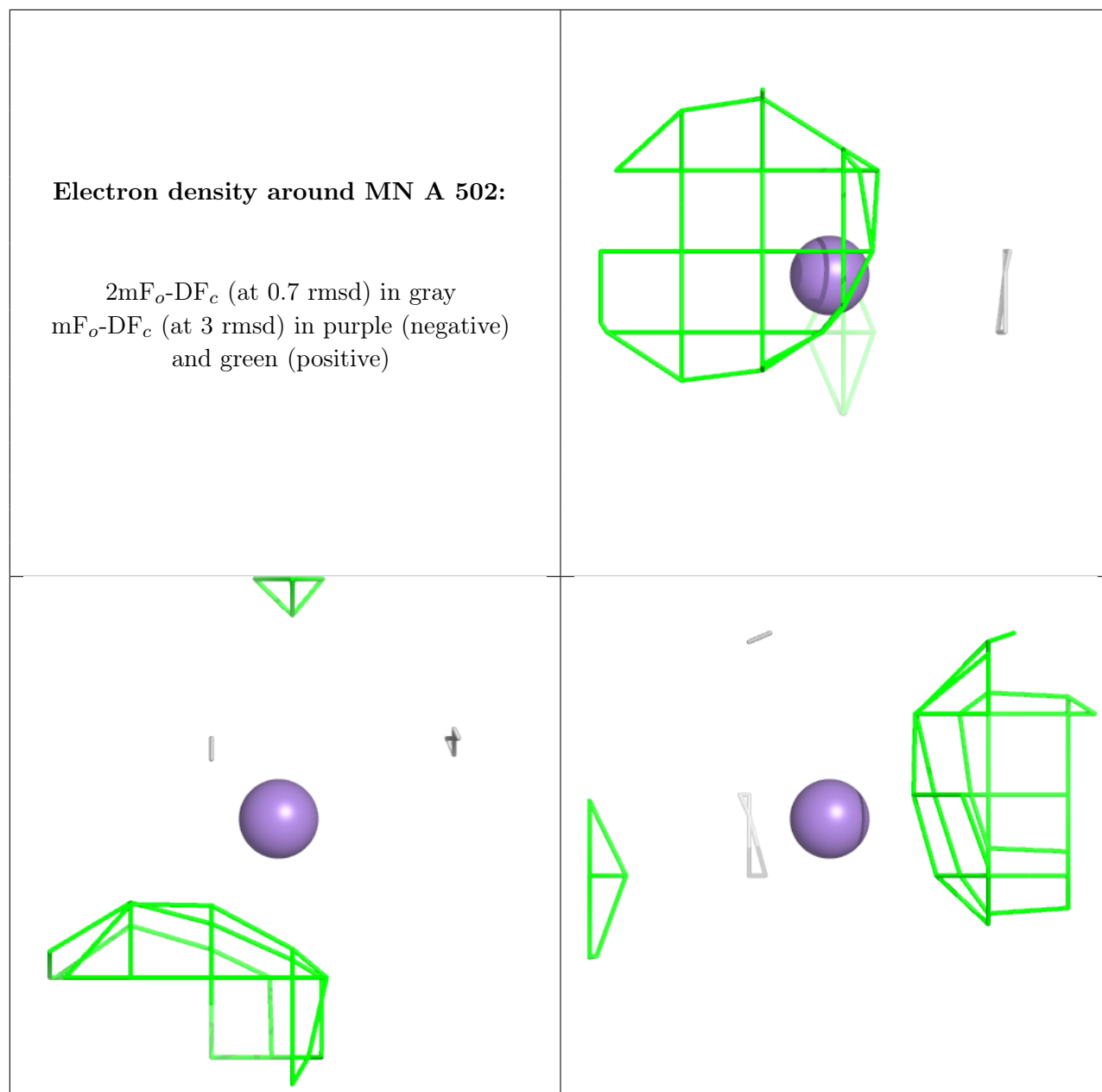


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**Electron density around MN B 502:**

$2mF_o - DF_c$  (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.