wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 12:10 AM EDT

PDB ID	:	7R6V
Title	:	Human EXOG complexed with dRP-containing DNA
Authors	:	Szymanski, M.R.; Yin, Y.W.
Deposited on	:	2021-06-23
Resolution	:	2.16 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

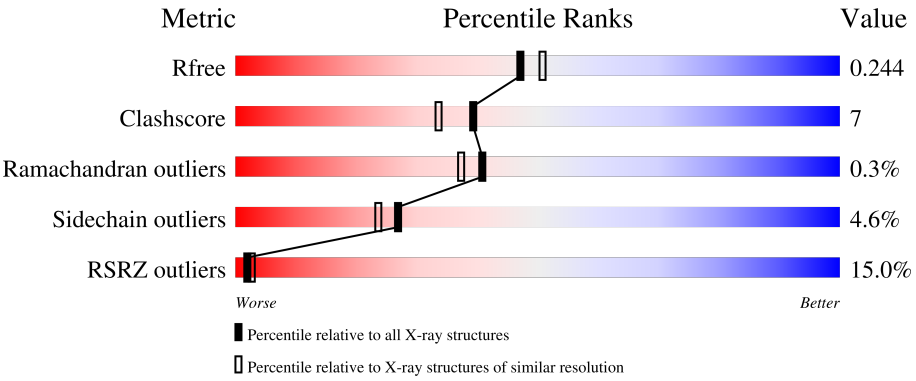
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 <=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	D	311	13% 80% 12% • 6%
1	E	311	11% 82% 10% • 7%
1	G	311	12% 77% 14% • 7%
1	I	311	14% 77% 14% • 6%
2	F	10	20% 30% 40% 30%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	10	30% 20% 70% 10%
2	J	10	30% 40% 40% 20%
2	K	10	40% 60% 30% 10%
3	A	12	42% 42% 33% 25%
3	B	12	17% 58% 25% 17%
3	L	12	42% 83% 8% 8%
3	M	12	50% 33% 50% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	D	401	-	-	-	X
4	MG	I	402	-	-	-	X
5	SO4	D	402	-	-	X	-
5	SO4	I	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11230 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 Nuclease EXOG, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	293	Total	C	N	O	S	0	0	0
			2346	1493	399	443	11			
1	E	289	Total	C	N	O	S	0	0	0
			2311	1470	393	437	11			
1	G	289	Total	C	N	O	S	0	0	0
			2315	1473	394	437	11			
1	I	293	Total	C	N	O	S	0	0	0
			2350	1496	400	443	11			

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*GP*AP*CP*GP*TP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	P	0	0	0
			140	68	25	41	6			
2	H	9	Total	C	N	O	P	0	0	0
			184	87	33	55	9			
2	J	8	Total	C	N	O	P	0	0	0
			165	78	30	49	8			
2	K	9	Total	C	N	O	P	0	0	0
			184	87	33	55	9			

- Molecule 3 is a DNA chain called DNA (5'-D(*CP*GP*CP*AP*CP*GP*TP*CP*AP*GP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	10	Total	C	N	O	P	0	0	0
			206	97	41	58	10			
3	A	9	Total	C	N	O	P	0	0	0
			186	88	38	51	9			
3	L	11	Total	C	N	O	P	0	0	0
			227	107	46	63	11			

Continued on next page...

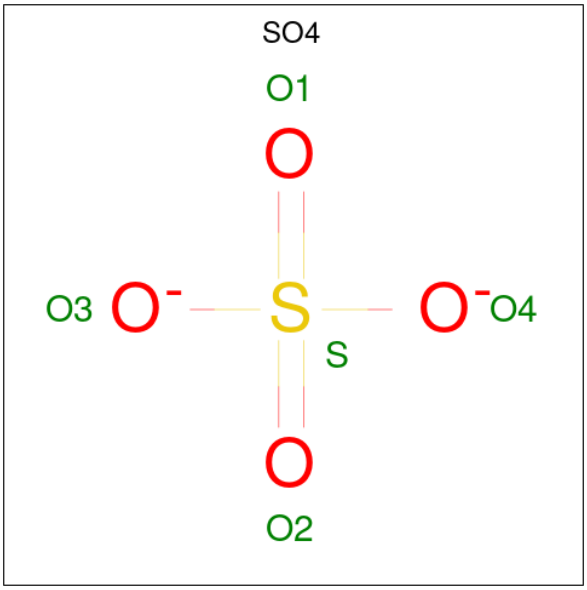
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	10	Total	C	N	O	P	0	0	0
			205	97	41	57	10			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	I	2	Total	Mg	0	0
			2	2		
4	J	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

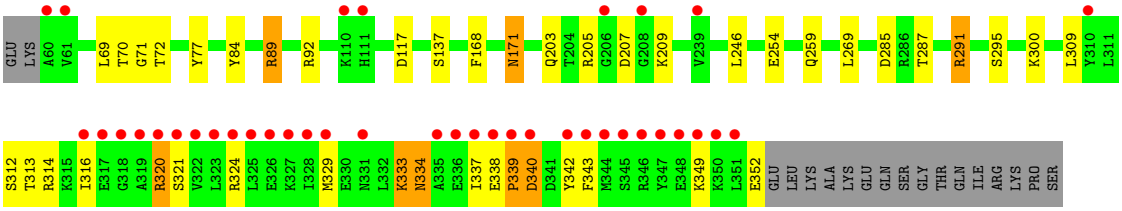
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	93	Total O 93 93	0	0
6	E	95	Total O 95 95	0	0
6	F	7	Total O 7 7	0	0
6	H	6	Total O 6 6	0	0
6	B	2	Total O 2 2	0	0
6	A	8	Total O 8 8	0	0
6	G	81	Total O 81 81	0	0
6	I	87	Total O 87 87	0	0
6	J	6	Total O 6 6	0	0
6	K	4	Total O 4 4	0	0
6	M	1	Total O 1 1	0	0

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.

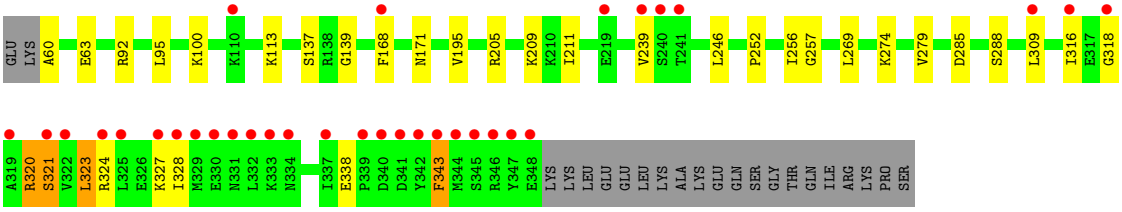
• Molecule 1: Nuclease EXOG, mitochondrial

Chain D:



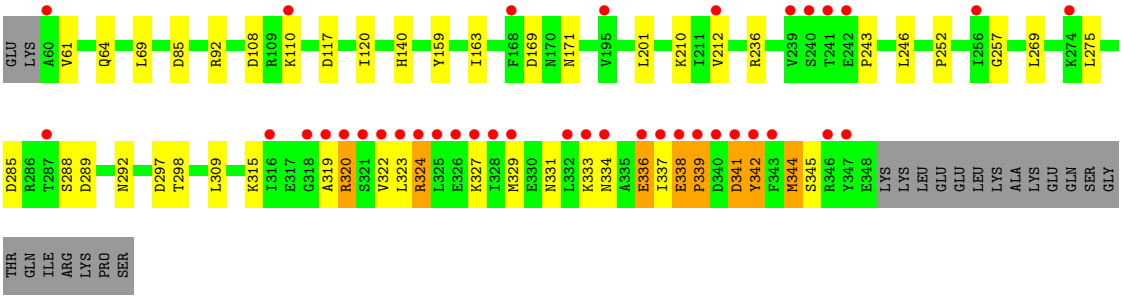
• Molecule 1: Nuclease EXOG, mitochondrial

Chain E:



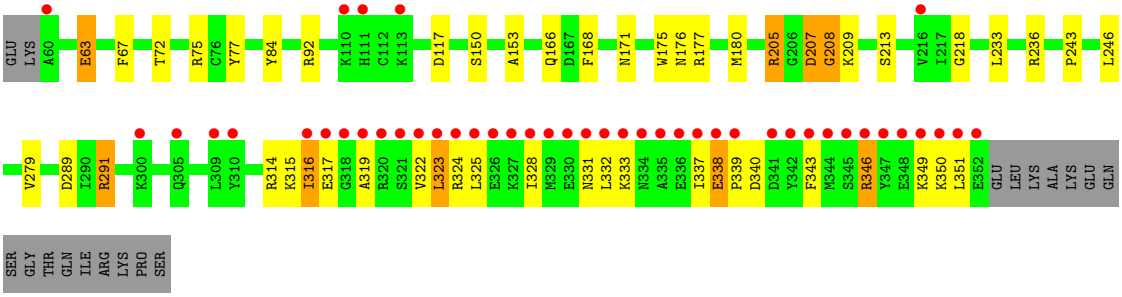
• Molecule 1: Nuclease EXOG, mitochondrial

Chain G:



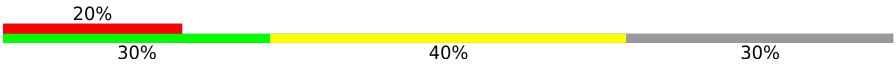
• Molecule 1: Nuclease EXOG, mitochondrial

Chain I:



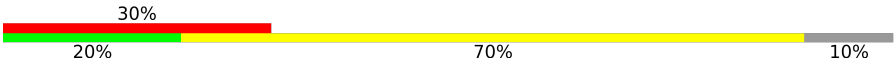
• Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*GP*TP*GP*CP*G)-3')

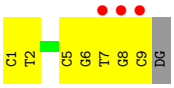
Chain F:



• Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*GP*TP*GP*CP*G)-3')

Chain H:



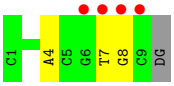


• Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*GP*TP*GP*CP*G)-3')

Chain J:

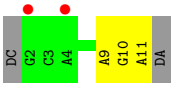
• Molecule 2: DNA (5'-D(*CP*TP*GP*AP*CP*GP*TP*GP*CP*G)-3')

Chain K:



• Molecule 3: DNA (5'-D(*CP*GP*CP*AP*CP*GP*TP*CP*AP*GP*AP*A)-3')

Chain B:

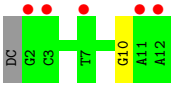


• Molecule 3: DNA (5'-D(*CP*GP*CP*AP*CP*GP*TP*CP*AP*GP*AP*A)-3')

Chain A:

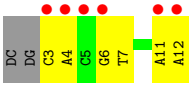
• Molecule 3: DNA (5'-D(*CP*GP*CP*AP*CP*GP*TP*CP*AP*GP*AP*A)-3')

Chain L:



• Molecule 3: DNA (5'-D(*CP*GP*CP*AP*CP*GP*TP*CP*AP*GP*AP*A)-3')

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.75Å 79.08Å 79.64Å 69.05° 65.02° 89.72°	Depositor
Resolution (Å)	50.00 – 2.16 45.10 – 2.16	Depositor EDS
% Data completeness (in resolution range)	97.0 (50.00-2.16) 90.0 (45.10-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.17	Depositor
R, R_{free}	0.200 , 0.240 0.212 , 0.244	Depositor DCC
R_{free} test set	1988 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.689	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, 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	D	0.29	0/2402	0.52	0/3253
1	E	0.29	0/2367	0.51	0/3208
1	G	0.29	0/2371	0.52	0/3212
1	I	0.30	0/2406	0.51	0/3257
2	F	0.59	0/156	0.88	0/239
2	H	0.56	0/205	0.86	0/314
2	J	0.75	1/184 (0.5%)	0.99	1/282 (0.4%)
2	K	0.52	0/205	0.83	0/314
3	A	0.65	0/209	0.81	0/320
3	B	0.46	0/231	0.81	0/354
3	L	0.45	0/255	0.79	0/391
3	M	0.63	0/230	0.87	0/352
All	All	0.35	1/11221 (0.0%)	0.59	1/15496 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	7	DT	O3'-P	6.19	1.68	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	7	DT	P-O3'-C3'	-6.32	112.12	119.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	319	ALA	Peptide

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	D	2346	0	2289	39	0
1	E	2311	0	2250	25	0
1	G	2315	0	2259	33	0
1	I	2350	0	2300	40	0
2	F	140	0	81	4	0
2	H	184	0	102	6	0
2	J	165	0	91	3	0
2	K	184	0	102	2	0
3	A	186	0	101	10	0
3	B	206	0	112	3	0
3	L	227	0	123	1	0
3	M	205	0	112	5	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	I	2	0	0	0	0
4	J	1	0	0	0	0
5	D	5	0	0	2	0
5	G	5	0	0	0	0
5	I	5	0	0	2	0
6	A	8	0	0	0	0
6	B	2	0	0	0	0
6	D	93	0	0	2	0
6	E	95	0	0	3	0
6	F	7	0	0	1	0
6	G	81	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	6	0	0	1	0
6	I	87	0	0	5	0
6	J	6	0	0	1	0
6	K	4	0	0	0	0
6	M	1	0	0	0	0
All	All	11230	0	9922	151	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 7.

The worst 5 of 151 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:E:320:ARG:HD3	1:E:321:SER:H	1.27	0.99
1:G:315:LYS:HD3	1:G:327:LYS:HE2	1.54	0.90
1:E:60:ALA:N	6:E:401:HOH:O	2.07	0.86
1:D:309:LEU:HD11	1:D:339:PRO:HG3	1.59	0.84
1:D:339:PRO:HG2	1:D:342:TYR:HB3	1.57	0.83

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	D	291/311 (94%)	287 (99%)	3 (1%)	1 (0%)	41	37
1	E	287/311 (92%)	281 (98%)	6 (2%)	0	100	100
1	G	287/311 (92%)	281 (98%)	5 (2%)	1 (0%)	41	37
1	I	291/311 (94%)	285 (98%)	5 (2%)	1 (0%)	41	37
All	All	1156/1244 (93%)	1134 (98%)	19 (2%)	3 (0%)	41	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	208	GLY
1	D	339	PRO
1	G	339	PRO

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	D	258/276 (94%)	245 (95%)	13 (5%)	24	21
1	E	254/276 (92%)	249 (98%)	5 (2%)	55	59
1	G	255/276 (92%)	243 (95%)	12 (5%)	26	23
1	I	259/276 (94%)	242 (93%)	17 (7%)	16	11
All	All	1026/1104 (93%)	979 (95%)	47 (5%)	27	23

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	342	TYR
1	I	316	ILE
1	G	344	MET
1	I	207	ASP
1	I	324	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	334	ASN

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 9 ligands modelled in this entry, 6 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	$\#\|Z\| > 2$
5	SO4	D	402	-	4,4,4	0.18	0	6,6,6	0.28	0
5	SO4	G	401	-	4,4,4	0.32	0	6,6,6	0.28	0
5	SO4	I	403	-	4,4,4	0.34	0	6,6,6	0.19	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.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	402	SO4	2	0
5	I	403	SO4	2	0

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^{th} 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	D	293/311 (94%)	0.91	39 (13%)	3	4	23, 37, 114, 132	0
1	E	289/311 (92%)	0.77	33 (11%)	5	7	22, 37, 120, 146	0
1	G	289/311 (92%)	0.84	38 (13%)	3	4	22, 37, 117, 142	0
1	I	293/311 (94%)	1.05	45 (15%)	2	2	23, 40, 128, 150	0
2	F	7/10 (70%)	1.03	2 (28%)	0	0	32, 38, 108, 136	0
2	H	9/10 (90%)	1.79	3 (33%)	0	0	36, 54, 160, 179	0
2	J	8/10 (80%)	1.93	3 (37%)	0	0	20, 44, 86, 115	0
2	K	9/10 (90%)	1.91	4 (44%)	0	0	39, 55, 161, 177	0
3	A	9/12 (75%)	2.32	5 (55%)	0	0	60, 92, 129, 131	0
3	B	10/12 (83%)	1.47	2 (20%)	1	1	71, 98, 142, 157	0
3	L	11/12 (91%)	2.77	5 (45%)	0	0	71, 119, 161, 162	0
3	M	10/12 (83%)	2.32	6 (60%)	0	0	81, 104, 147, 155	0
All	All	1237/1332 (92%)	0.96	185 (14%)	2	3	20, 39, 123, 179	0

The worst 5 of 185 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	337	ILE	12.0
1	I	351	LEU	11.5
1	I	342	TYR	11.2
1	D	316	ILE	10.2
1	I	347	TYR	10.1

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

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)

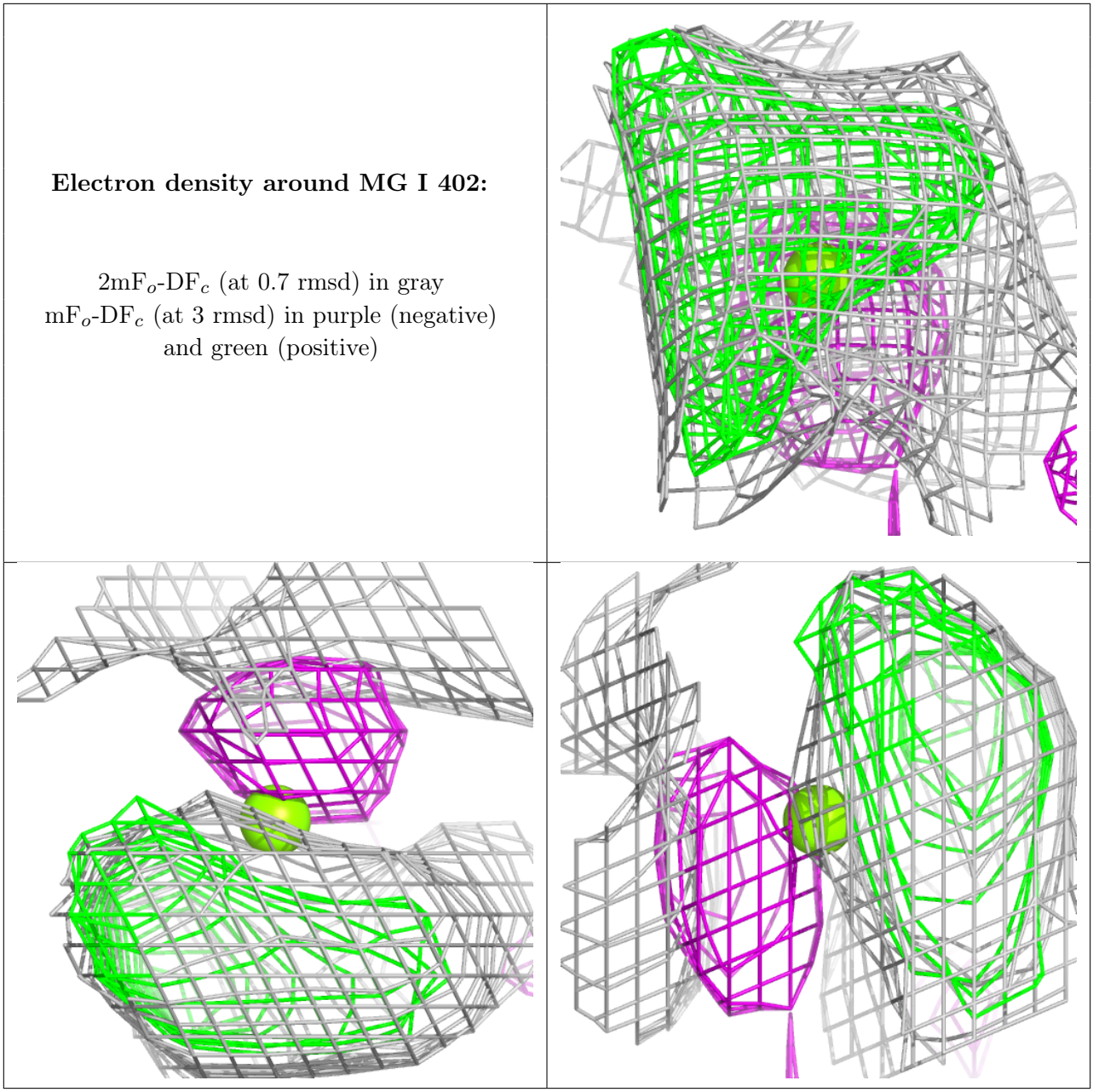
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	I	402	1/1	0.11	0.91	71,71,71,71	0
4	MG	H	101	1/1	0.45	0.13	30,30,30,30	0
4	MG	J	101	1/1	0.47	0.15	33,33,33,33	0
4	MG	D	401	1/1	0.51	1.01	97,97,97,97	0
5	SO4	D	402	5/5	0.66	0.21	65,70,76,132	0
4	MG	F	101	1/1	0.81	0.10	30,30,30,30	0
5	SO4	G	401	5/5	0.82	0.23	46,63,71,106	0
4	MG	I	401	1/1	0.83	0.11	31,31,31,31	0
5	SO4	I	403	5/5	0.90	0.13	54,59,70,97	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.

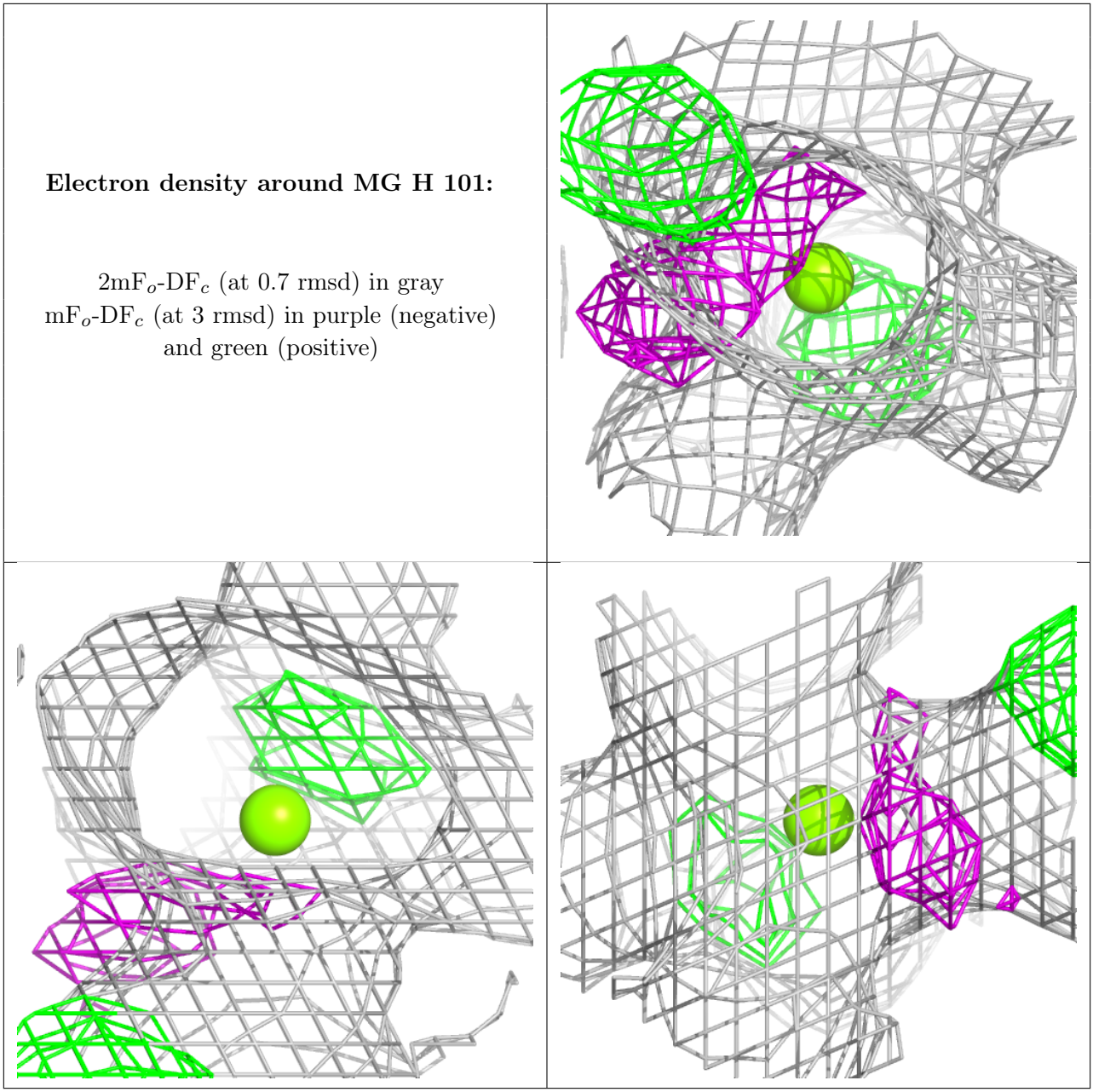
Electron density around MG I 402:

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



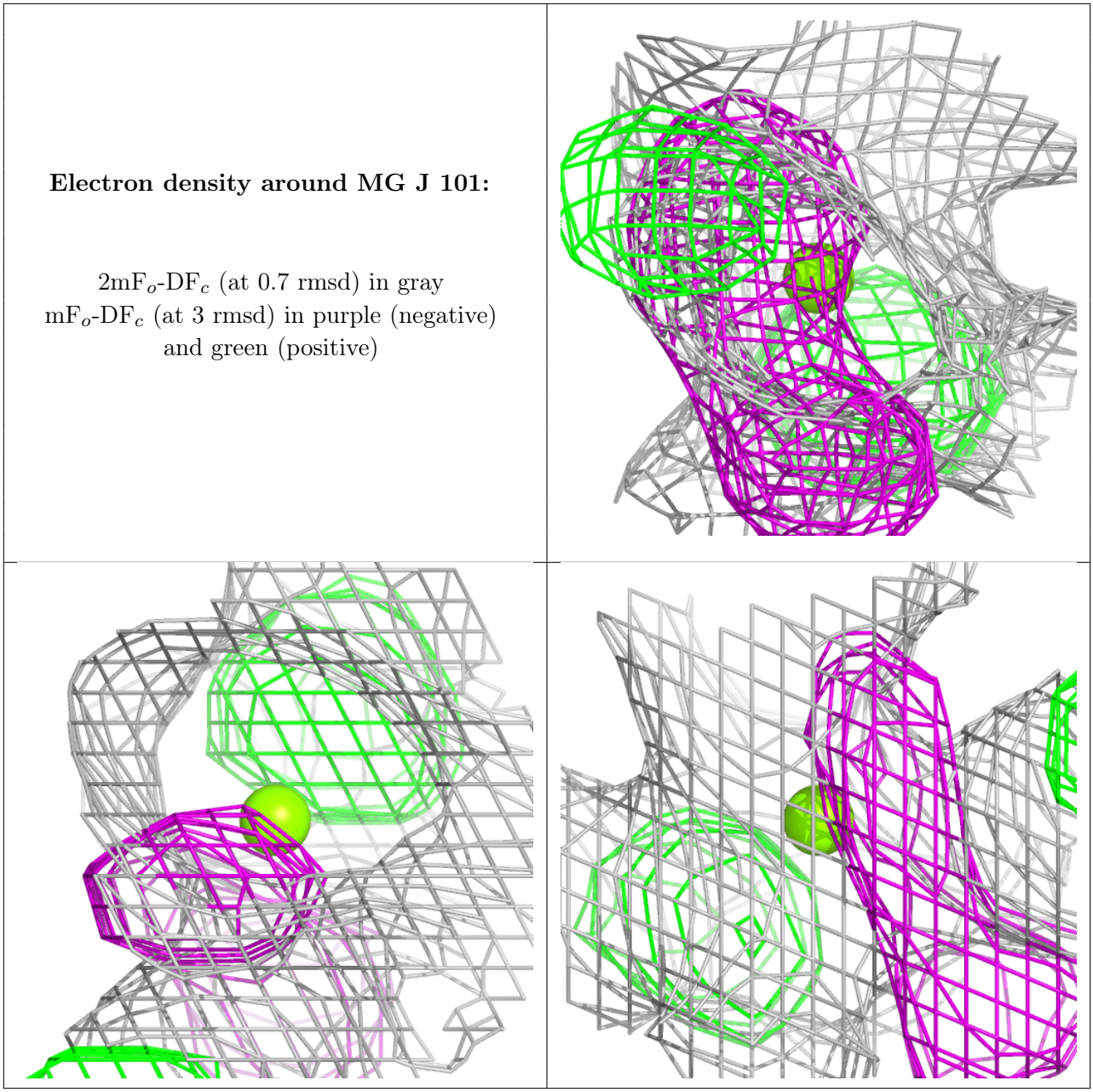
Electron density around MG H 101:

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



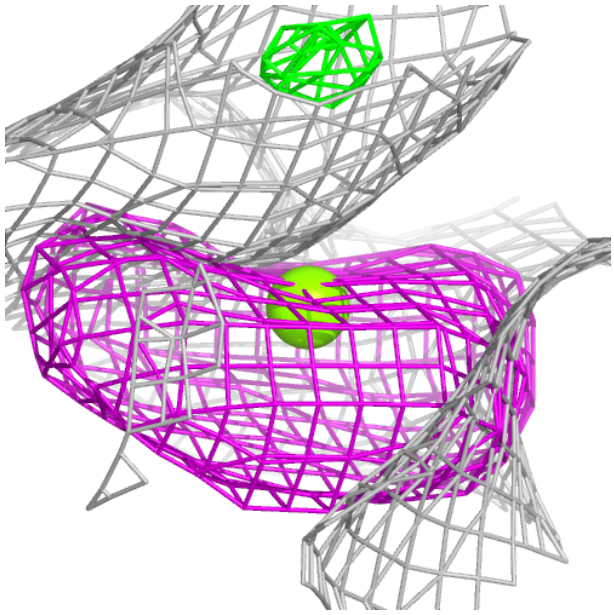
Electron density around MG J 101:

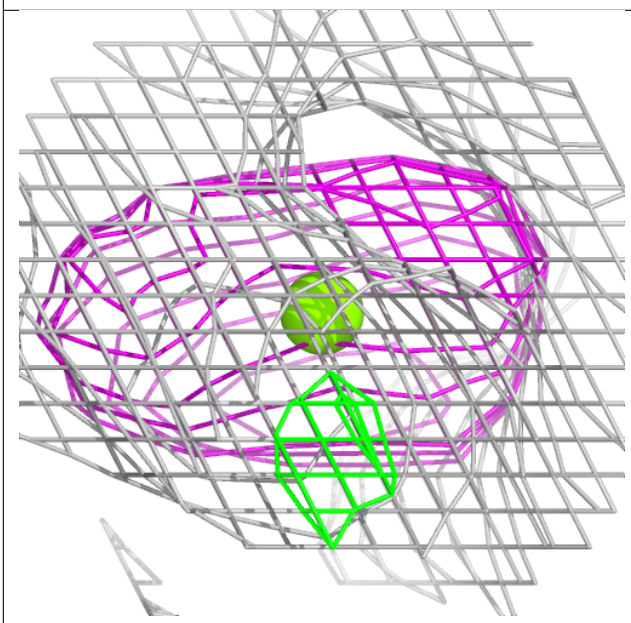
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

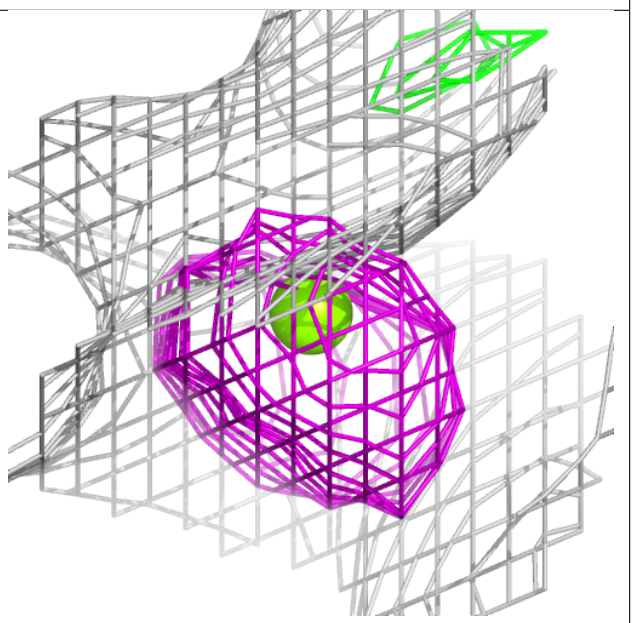


Electron density around MG D 401:

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

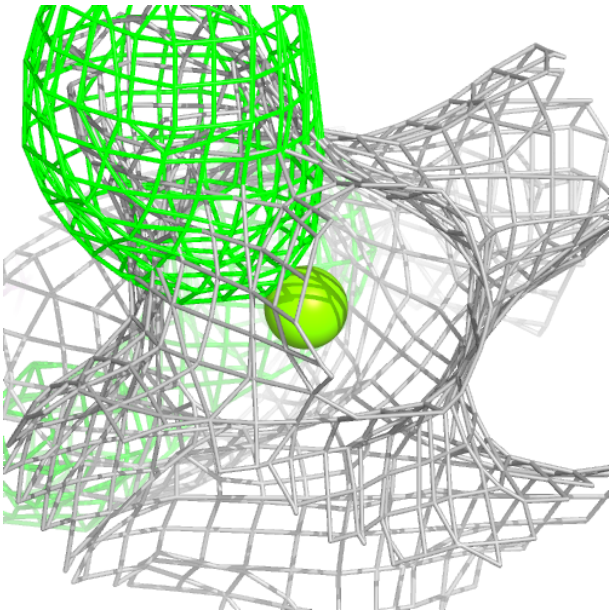


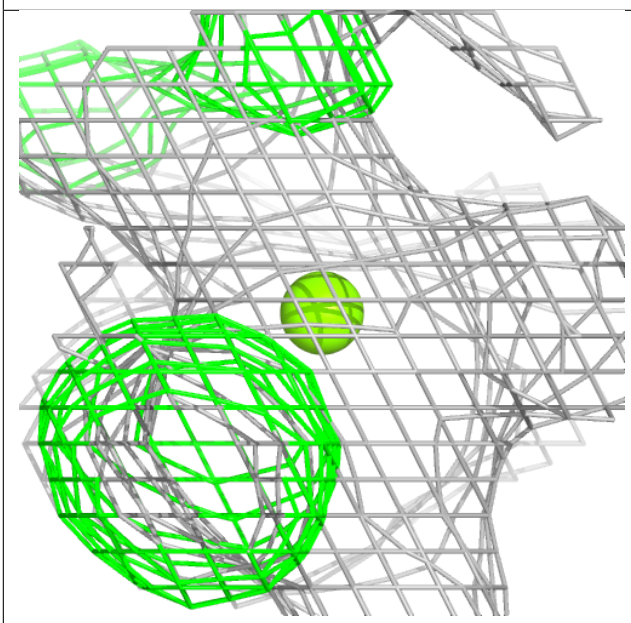


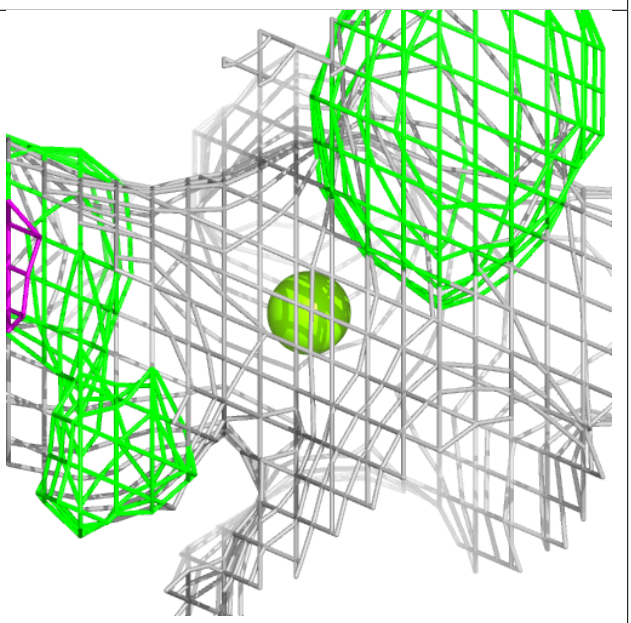


Electron density around MG F 101:

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

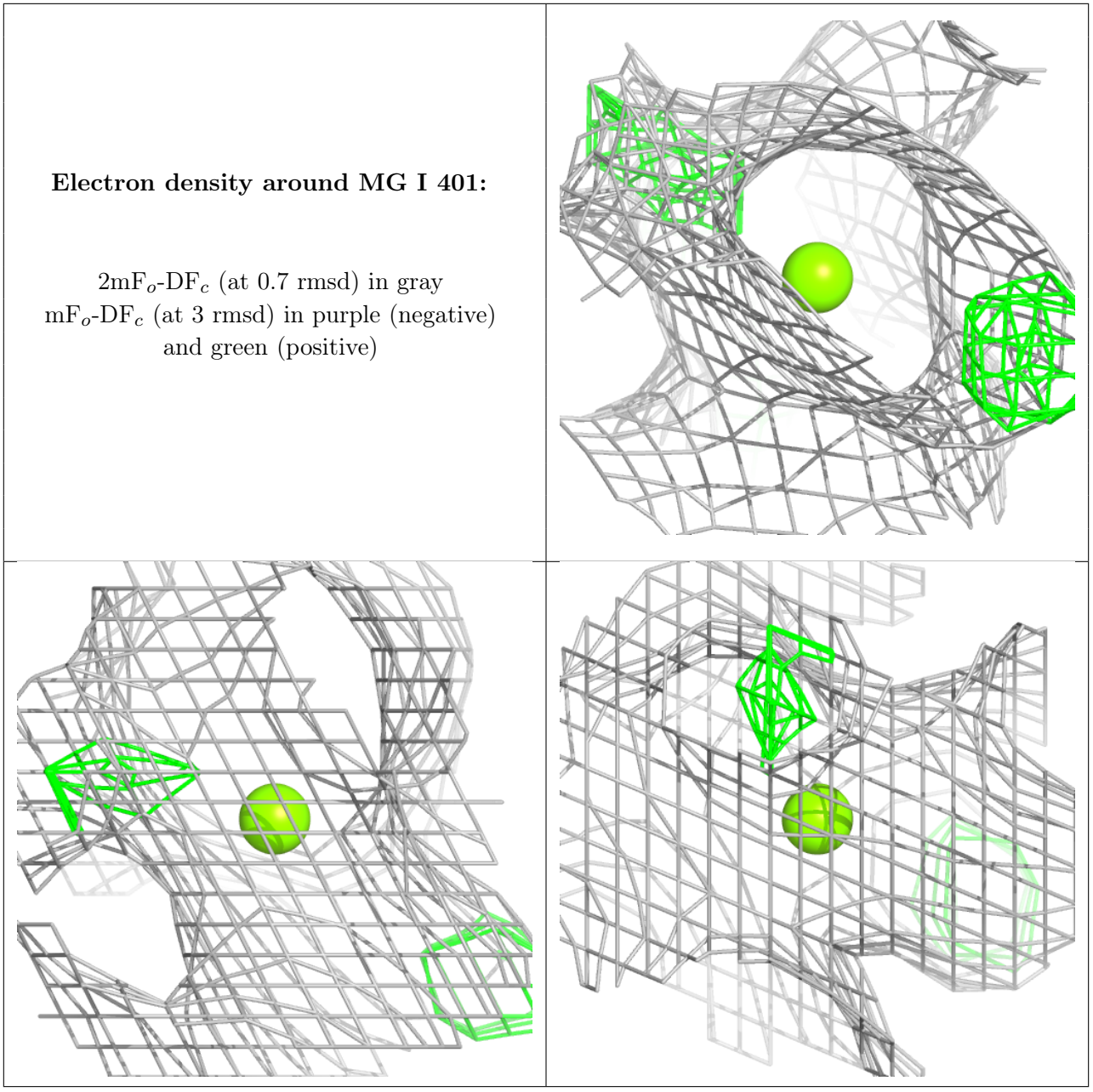






Electron density around MG I 401:

$2mF_o$-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.