



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 08:22 PM JST

PDB ID : 7DRP  
Title : Structure of ATP-grasp ligase PsnB complexed with phosphomimetic variant of minimal precursor, Mg, and ADP  
Authors : Song, I.; Yu, J.; Song, W.; Kim, S.  
Deposited on : 2020-12-29  
Resolution : 2.98 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

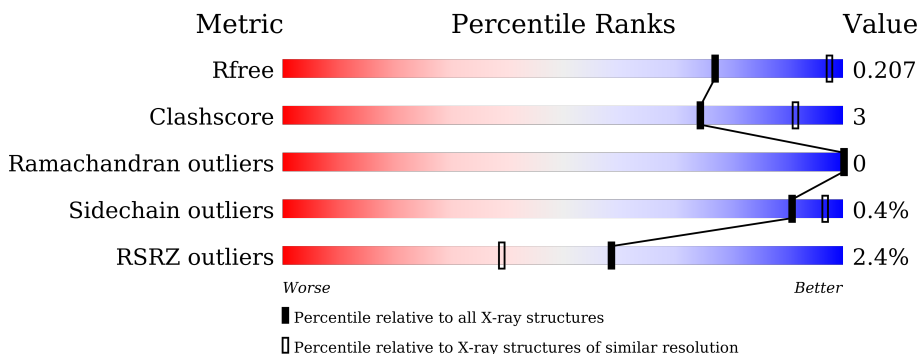
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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	334	
1	B	334	
1	C	334	
1	D	334	
2	E	25	
2	F	25	

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	DV9	E	24	-	-	-	X
4	MG	A	403	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9483 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 ATP-grasp domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	2338	1470	417	440	11	0	0	0
1	B	295	2203	1382	395	415	11	0	0	0
1	C	311	2368	1486	431	440	11	0	0	0
1	D	296	2210	1383	401	414	12	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A6G4D7
A	-18	GLY	-	expression tag	UNP A6G4D7
A	-17	SER	-	expression tag	UNP A6G4D7
A	-16	SER	-	expression tag	UNP A6G4D7
A	-15	HIS	-	expression tag	UNP A6G4D7
A	-14	HIS	-	expression tag	UNP A6G4D7
A	-13	HIS	-	expression tag	UNP A6G4D7
A	-12	HIS	-	expression tag	UNP A6G4D7
A	-11	HIS	-	expression tag	UNP A6G4D7
A	-10	HIS	-	expression tag	UNP A6G4D7
A	-9	SER	-	expression tag	UNP A6G4D7
A	-8	SER	-	expression tag	UNP A6G4D7
A	-7	GLY	-	expression tag	UNP A6G4D7
A	-6	LEU	-	expression tag	UNP A6G4D7
A	-5	VAL	-	expression tag	UNP A6G4D7
A	-4	PRO	-	expression tag	UNP A6G4D7
A	-3	ARG	-	expression tag	UNP A6G4D7
A	-2	GLY	-	expression tag	UNP A6G4D7
A	-1	SER	-	expression tag	UNP A6G4D7
A	0	HIS	-	expression tag	UNP A6G4D7
B	-19	MET	-	expression tag	UNP A6G4D7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A6G4D7
B	-17	SER	-	expression tag	UNP A6G4D7
B	-16	SER	-	expression tag	UNP A6G4D7
B	-15	HIS	-	expression tag	UNP A6G4D7
B	-14	HIS	-	expression tag	UNP A6G4D7
B	-13	HIS	-	expression tag	UNP A6G4D7
B	-12	HIS	-	expression tag	UNP A6G4D7
B	-11	HIS	-	expression tag	UNP A6G4D7
B	-10	HIS	-	expression tag	UNP A6G4D7
B	-9	SER	-	expression tag	UNP A6G4D7
B	-8	SER	-	expression tag	UNP A6G4D7
B	-7	GLY	-	expression tag	UNP A6G4D7
B	-6	LEU	-	expression tag	UNP A6G4D7
B	-5	VAL	-	expression tag	UNP A6G4D7
B	-4	PRO	-	expression tag	UNP A6G4D7
B	-3	ARG	-	expression tag	UNP A6G4D7
B	-2	GLY	-	expression tag	UNP A6G4D7
B	-1	SER	-	expression tag	UNP A6G4D7
B	0	HIS	-	expression tag	UNP A6G4D7
C	-19	MET	-	expression tag	UNP A6G4D7
C	-18	GLY	-	expression tag	UNP A6G4D7
C	-17	SER	-	expression tag	UNP A6G4D7
C	-16	SER	-	expression tag	UNP A6G4D7
C	-15	HIS	-	expression tag	UNP A6G4D7
C	-14	HIS	-	expression tag	UNP A6G4D7
C	-13	HIS	-	expression tag	UNP A6G4D7
C	-12	HIS	-	expression tag	UNP A6G4D7
C	-11	HIS	-	expression tag	UNP A6G4D7
C	-10	HIS	-	expression tag	UNP A6G4D7
C	-9	SER	-	expression tag	UNP A6G4D7
C	-8	SER	-	expression tag	UNP A6G4D7
C	-7	GLY	-	expression tag	UNP A6G4D7
C	-6	LEU	-	expression tag	UNP A6G4D7
C	-5	VAL	-	expression tag	UNP A6G4D7
C	-4	PRO	-	expression tag	UNP A6G4D7
C	-3	ARG	-	expression tag	UNP A6G4D7
C	-2	GLY	-	expression tag	UNP A6G4D7
C	-1	SER	-	expression tag	UNP A6G4D7
C	0	HIS	-	expression tag	UNP A6G4D7
D	-19	MET	-	expression tag	UNP A6G4D7
D	-18	GLY	-	expression tag	UNP A6G4D7
D	-17	SER	-	expression tag	UNP A6G4D7

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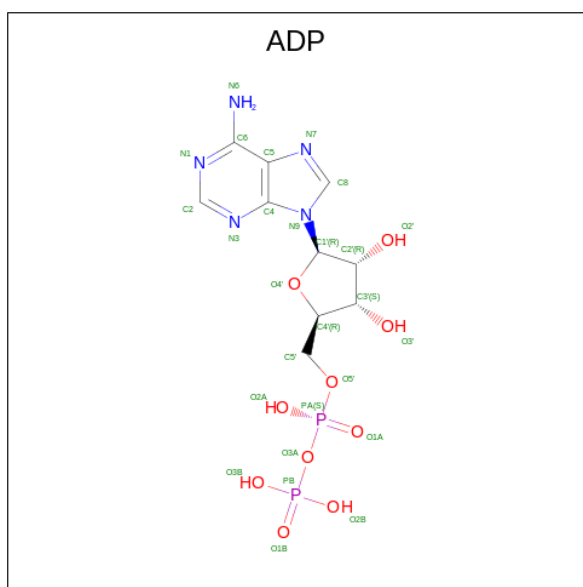
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A6G4D7
D	-15	HIS	-	expression tag	UNP A6G4D7
D	-14	HIS	-	expression tag	UNP A6G4D7
D	-13	HIS	-	expression tag	UNP A6G4D7
D	-12	HIS	-	expression tag	UNP A6G4D7
D	-11	HIS	-	expression tag	UNP A6G4D7
D	-10	HIS	-	expression tag	UNP A6G4D7
D	-9	SER	-	expression tag	UNP A6G4D7
D	-8	SER	-	expression tag	UNP A6G4D7
D	-7	GLY	-	expression tag	UNP A6G4D7
D	-6	LEU	-	expression tag	UNP A6G4D7
D	-5	VAL	-	expression tag	UNP A6G4D7
D	-4	PRO	-	expression tag	UNP A6G4D7
D	-3	ARG	-	expression tag	UNP A6G4D7
D	-2	GLY	-	expression tag	UNP A6G4D7
D	-1	SER	-	expression tag	UNP A6G4D7
D	0	HIS	-	expression tag	UNP A6G4D7

- Molecule 2 is a protein called PsnA214-38, Precursor peptide, phospho-mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	F	18	Total	C	N	O	0	0	0		
			127	83	18	26					
2	E	15	Total	C	F	N	O	P	0	0	0
			109	67	2	15	24	1			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		
4	D	2	Total	Mg	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	6	Total	O	0	0
			6	6		

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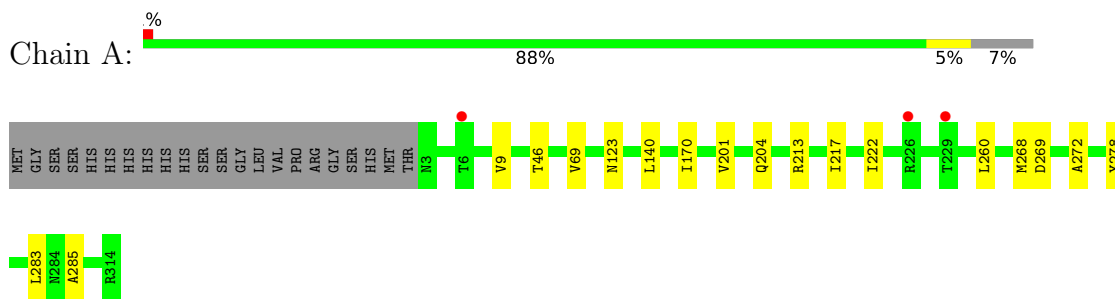
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
5	B	1	Total O 1 1	0	0
5	C	2	Total O 2 2	0	0
5	D	3	Total O 3 3	0	0



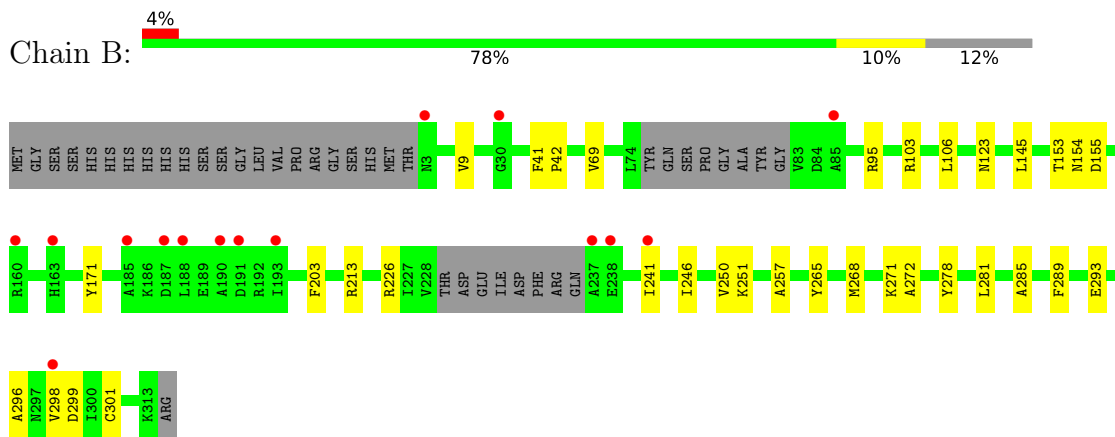
### 3 Residue-property plots [i](#)

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.

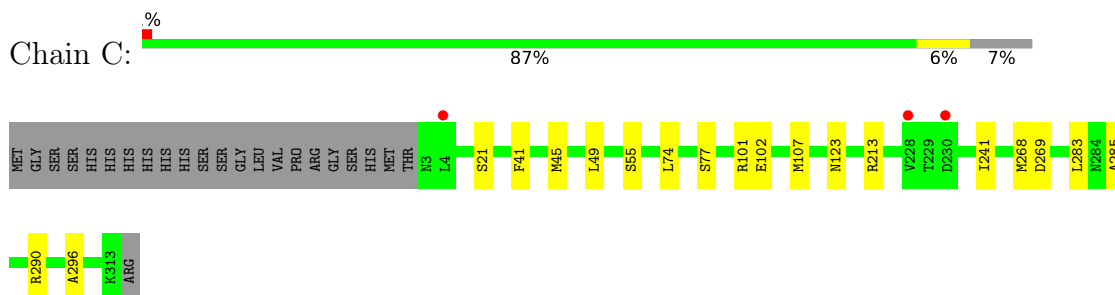
- Molecule 1: ATP-grasp domain-containing protein



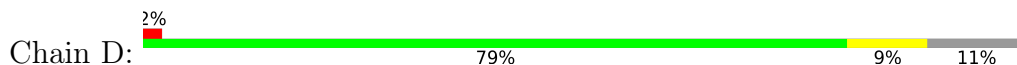
- Molecule 1: ATP-grasp domain-containing protein

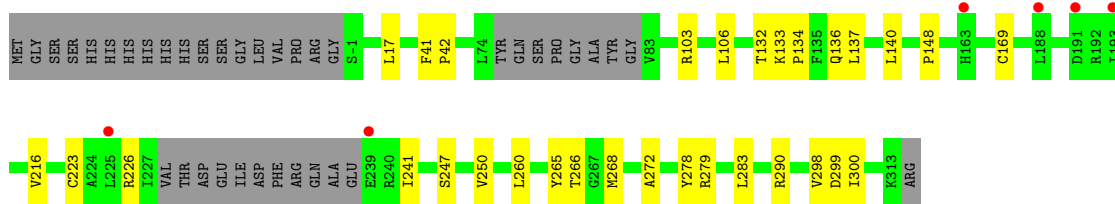


- Molecule 1: ATP-grasp domain-containing protein

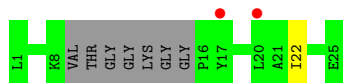


- Molecule 1: ATP-grasp domain-containing protein

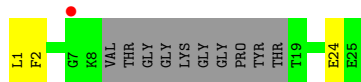




- Molecule 2: PsnA214-38, Precursor peptide, phospho-mimic



- Molecule 2: PsnA214-38, Precursor peptide, phospho-mimic



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.59Å 91.66Å 98.20Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	33.19 – 2.98 33.19 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (33.19-2.98) 99.0 (33.19-2.98)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 3.00Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.206 , 0.210 0.204 , 0.207	Depositor DCC
$R_{free}$ test set	1558 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.4	Xtrriage
Anisotropy	0.472	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9483	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% 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: DV9, ADP, 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	0.34	0/2378	0.50	0/3236
1	B	0.34	0/2237	0.51	0/3043
1	C	0.32	0/2408	0.50	0/3268
1	D	0.32	0/2245	0.50	0/3052
2	E	0.51	0/92	0.73	0/119
2	F	0.53	0/122	0.67	0/160
All	All	0.34	0/9482	0.51	0/12878

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	2338	0	2276	11	0
1	B	2203	0	2140	22	0
1	C	2368	0	2340	10	0
1	D	2210	0	2135	17	0
2	E	109	0	83	3	0
2	F	127	0	106	1	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	6	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	1	0
5	D	3	0	0	0	0
All	All	9483	0	9128	59	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 (59) 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:D:268:MET:HG2	1:D:283:LEU:HG	1.81	0.63
1:C:123:ASN:ND2	1:C:285:ALA:O	2.35	0.60
1:A:213:ARG:NH1	1:A:269:ASP:OD1	2.37	0.57
1:B:42:PRO:HG2	1:B:103:ARG:CZ	2.36	0.54
1:B:123:ASN:ND2	1:B:285:ALA:O	2.41	0.54
1:A:268:MET:HG2	1:A:283:LEU:HG	1.90	0.53
1:A:170:ILE:HD11	1:A:204:GLN:HB2	1.91	0.53
1:C:77:SER:OG	2:F:22:ILE:HD12	2.09	0.53
1:B:9:VAL:HB	1:B:69:VAL:HG22	1.90	0.52
1:C:213:ARG:NE	1:C:269:ASP:OD1	2.41	0.52
1:D:140:LEU:HD23	1:D:260:LEU:HD23	1.93	0.50
1:B:226:ARG:O	1:B:241:ILE:HA	2.11	0.50
1:B:241:ILE:HG22	1:B:296:ALA:HB2	1.93	0.50
1:A:201:VAL:HG21	2:E:2:PHE:CD2	2.47	0.49
1:B:271:LYS:HB2	1:B:281:LEU:HD11	1.94	0.49
1:D:272:ALA:HA	1:D:278:TYR:HA	1.94	0.49
1:C:268:MET:HB3	1:C:283:LEU:HG	1.95	0.49
1:D:216:VAL:HB	1:D:266:THR:HG22	1.94	0.48
1:D:132:THR:O	1:D:136:GLN:N	2.39	0.48
1:C:41:PHE:HA	1:C:45:MET:HB3	1.95	0.47
1:D:148:PRO:HD3	1:D:279:ARG:HB3	1.95	0.47
1:C:21:SER:OG	1:C:290:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:SER:HB2	1:D:250:VAL:HG23	1.97	0.47
1:A:123:ASN:ND2	1:A:285:ALA:O	2.48	0.47
1:D:223:CYS:SG	1:D:300:ILE:HD11	2.56	0.46
1:A:201:VAL:HG21	2:E:2:PHE:HD2	1.81	0.46
1:D:226:ARG:O	1:D:241:ILE:HA	2.16	0.46
1:B:289:PHE:CE1	1:B:301:CYS:HB2	2.51	0.46
1:C:241:ILE:HG22	1:C:296:ALA:HB2	1.97	0.46
1:D:17:LEU:HD23	1:D:290:ARG:NH2	2.31	0.45
1:A:272:ALA:HA	1:A:278:TYR:HA	1.99	0.45
1:B:41:PHE:CZ	1:B:106:LEU:HD23	2.52	0.45
1:D:42:PRO:HG2	1:D:103:ARG:CZ	2.46	0.45
1:A:9:VAL:HB	1:A:69:VAL:HG22	1.98	0.45
1:D:133:LYS:HB2	1:D:134:PRO:HD3	1.99	0.45
1:A:217:ILE:HB	1:A:222:ILE:HD11	1.98	0.44
1:A:46:THR:HG23	1:B:155:ASP:HB2	1.99	0.44
1:B:246:ILE:HD12	1:B:250:VAL:HG12	1.98	0.44
1:B:272:ALA:HA	1:B:278:TYR:HA	1.99	0.44
1:B:41:PHE:HB3	1:B:42:PRO:HD3	1.99	0.44
1:B:298:VAL:HG22	1:B:299:ASP:H	1.83	0.43
1:B:246:ILE:HG13	1:B:251:LYS:HG3	1.99	0.43
1:D:298:VAL:HG22	1:D:299:ASP:H	1.82	0.43
1:A:140:LEU:HD23	1:A:260:LEU:HD23	2.01	0.43
1:D:106:LEU:HA	1:D:106:LEU:HD12	1.75	0.43
1:B:41:PHE:HZ	1:B:106:LEU:HD23	1.83	0.43
1:B:95:ARG:NE	2:E:1:LEU:HD12	2.33	0.42
1:B:293:GLU:HA	1:B:298:VAL:HG12	2.00	0.42
1:D:41:PHE:CZ	1:D:106:LEU:HD23	2.54	0.42
1:B:145:LEU:HD22	1:B:257:ALA:HB2	2.01	0.42
1:B:268:MET:HE2	1:B:268:MET:HB2	1.62	0.41
1:B:213:ARG:HA	1:B:268:MET:O	2.20	0.41
1:D:137:LEU:HD12	1:D:137:LEU:HA	1.82	0.41
1:C:102:GLU:OE2	5:C:501:HOH:O	2.22	0.41
1:C:49:LEU:HA	1:C:55:SER:O	2.21	0.41
1:B:171:TYR:HB3	1:B:203:PHE:CD1	2.56	0.41
1:D:41:PHE:HB3	1:D:42:PRO:HD3	2.03	0.40
1:C:74:LEU:HD22	1:C:107:MET:HB3	2.03	0.40
1:B:153:THR:OG1	1:B:154:ASN:N	2.54	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	310/334 (93%)	294 (95%)	16 (5%)	0	100	100
1	B	289/334 (86%)	277 (96%)	12 (4%)	0	100	100
1	C	309/334 (92%)	299 (97%)	10 (3%)	0	100	100
1	D	290/334 (87%)	276 (95%)	14 (5%)	0	100	100
2	E	10/25 (40%)	8 (80%)	2 (20%)	0	100	100
2	F	13/25 (52%)	12 (92%)	1 (8%)	0	100	100
All	All	1221/1386 (88%)	1166 (96%)	55 (4%)	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	234/274 (85%)	234 (100%)	0	100	100
1	B	220/274 (80%)	219 (100%)	1 (0%)	88	95
1	C	240/274 (88%)	239 (100%)	1 (0%)	91	97
1	D	219/274 (80%)	217 (99%)	2 (1%)	78	91
2	E	7/17 (41%)	7 (100%)	0	100	100
2	F	10/17 (59%)	10 (100%)	0	100	100
All	All	930/1130 (82%)	926 (100%)	4 (0%)	91	97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	265	TYR
1	C	101	ARG
1	D	169	CYS
1	D	265	TYR

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	DV9	F	24	2	3,4,15	0.75	0	2,4,23	0.70	0
2	DV9	E	24	2	9,14,15	2.81	4 (44%)	8,21,23	2.27	2 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DV9	F	24	2	-	0/0/2/24	-
2	DV9	E	24	2	-	7/14/22/24	-

All (4) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	24	DV9	P01-O14	5.56	1.65	1.54
2	E	24	DV9	P01-O16	-4.63	1.46	1.54
2	E	24	DV9	P01-O15	-2.72	1.46	1.50
2	E	24	DV9	CB-CA	-2.53	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	24	DV9	O16-P01-O15	-5.08	101.64	113.06
2	E	24	DV9	F02-C45-F01	2.42	109.79	106.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	24	DV9	F01-C45-P01-O15
2	E	24	DV9	F01-C45-P01-O16
2	E	24	DV9	F02-C45-P01-O14
2	E	24	DV9	F02-C45-P01-O15
2	E	24	DV9	F02-C45-P01-O16
2	E	24	DV9	F01-C45-P01-O14
2	E	24	DV9	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
3	ADP	B	401	4	24,29,29	0.97	2 (8%)	29,45,45	1.34	4 (13%)
3	ADP	A	401	4	24,29,29	0.94	1 (4%)	29,45,45	1.31	3 (10%)
3	ADP	C	401	4	24,29,29	0.94	1 (4%)	29,45,45	1.22	3 (10%)
3	ADP	D	401	4	24,29,29	1.00	2 (8%)	29,45,45	1.34	3 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	401	4	-	3/12/32/32	0/3/3/3
3	ADP	A	401	4	-	5/12/32/32	0/3/3/3
3	ADP	C	401	4	-	5/12/32/32	0/3/3/3
3	ADP	D	401	4	-	6/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C4	2.17	1.46	1.40
3	D	401	ADP	C2'-C1'	-2.10	1.50	1.53
3	D	401	ADP	C5-C4	2.09	1.46	1.40
3	C	401	ADP	C5-C4	2.07	1.46	1.40
3	A	401	ADP	C5-C4	2.04	1.46	1.40
3	B	401	ADP	C2'-C1'	-2.03	1.50	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C3'-C2'-C1'	3.92	106.88	100.98
3	B	401	ADP	C3'-C2'-C1'	3.41	106.12	100.98
3	B	401	ADP	N3-C2-N1	-3.28	123.54	128.68
3	A	401	ADP	C3'-C2'-C1'	3.22	105.83	100.98
3	C	401	ADP	C3'-C2'-C1'	3.04	105.56	100.98
3	A	401	ADP	N3-C2-N1	-3.03	123.94	128.68
3	C	401	ADP	N3-C2-N1	-2.99	124.00	128.68
3	D	401	ADP	N3-C2-N1	-2.87	124.19	128.68
3	A	401	ADP	C4-C5-N7	-2.76	106.52	109.40
3	B	401	ADP	C4-C5-N7	-2.56	106.73	109.40
3	C	401	ADP	C4-C5-N7	-2.41	106.89	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C4-C5-N7	-2.40	106.90	109.40
3	B	401	ADP	C2-N1-C6	2.02	122.21	118.75

There are no chirality outliers.

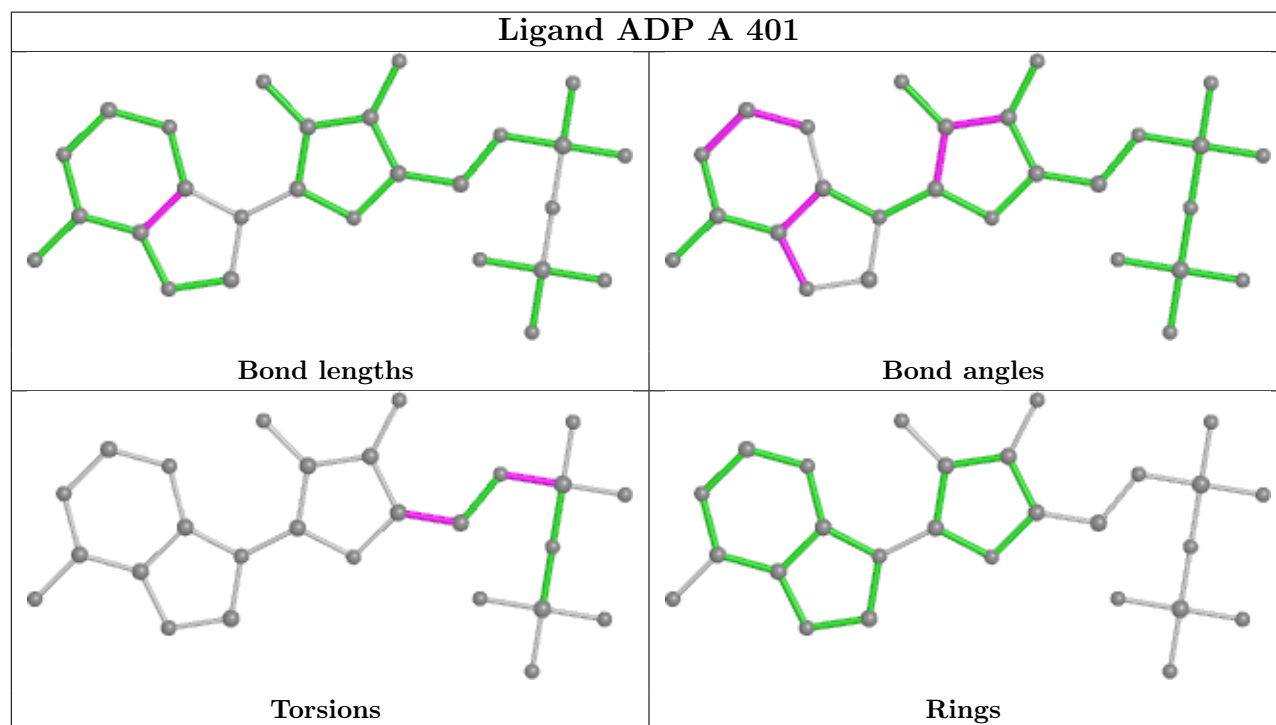
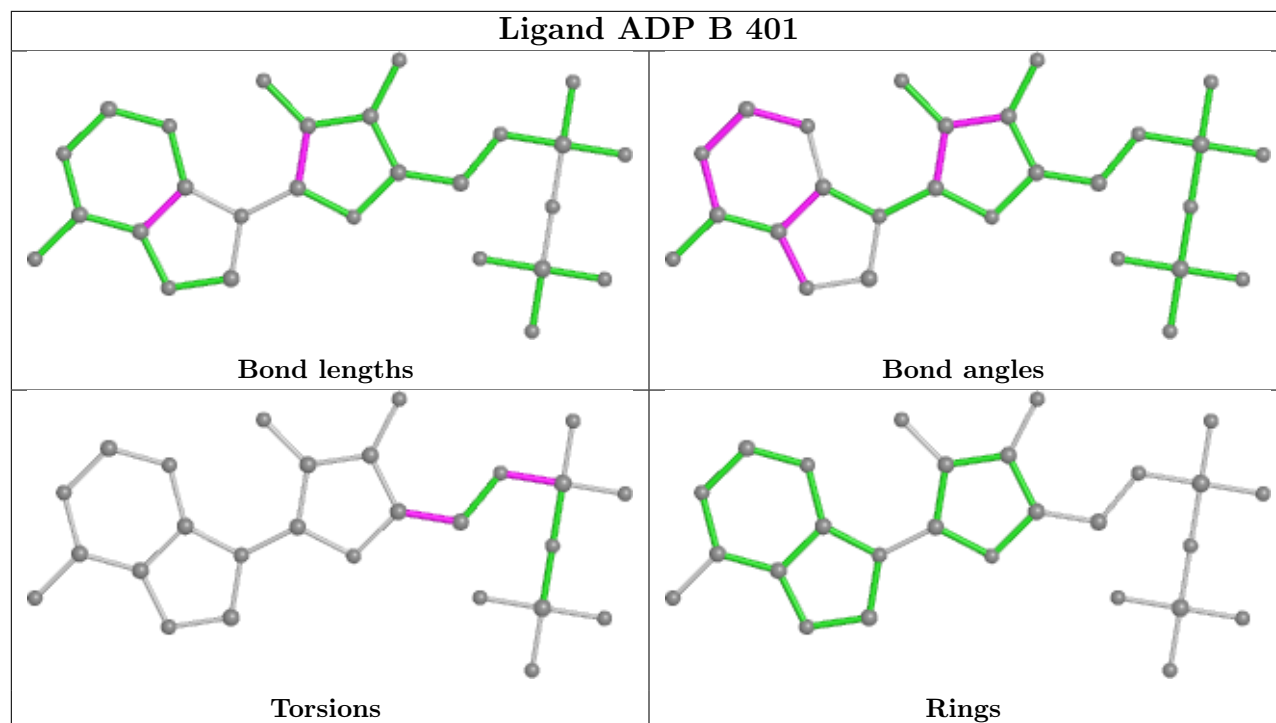
All (19) torsion outliers are listed below:

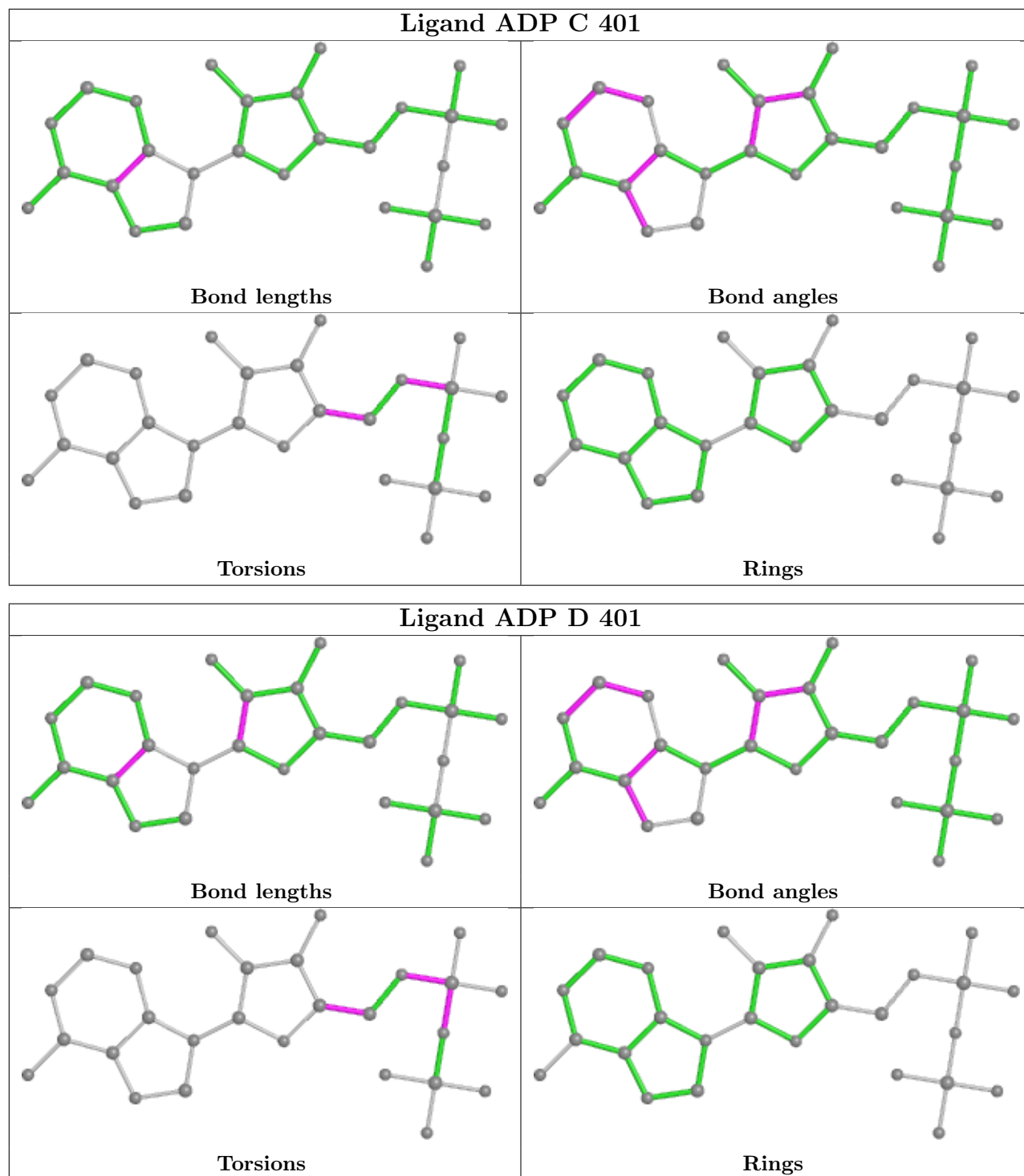
Mol	Chain	Res	Type	Atoms
3	A	401	ADP	C5'-O5'-PA-O1A
3	D	401	ADP	C5'-O5'-PA-O1A
3	D	401	ADP	O4'-C4'-C5'-O5'
3	A	401	ADP	O4'-C4'-C5'-O5'
3	C	401	ADP	O4'-C4'-C5'-O5'
3	D	401	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	C3'-C4'-C5'-O5'
3	B	401	ADP	O4'-C4'-C5'-O5'
3	D	401	ADP	PB-O3A-PA-O5'
3	A	401	ADP	C5'-O5'-PA-O3A
3	C	401	ADP	C5'-O5'-PA-O3A
3	D	401	ADP	C5'-O5'-PA-O3A
3	A	401	ADP	C5'-O5'-PA-O2A
3	D	401	ADP	C5'-O5'-PA-O2A
3	B	401	ADP	C3'-C4'-C5'-O5'
3	B	401	ADP	C5'-O5'-PA-O3A
3	C	401	ADP	C5'-O5'-PA-O1A
3	C	401	ADP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [\(i\)](#)

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

### 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	312/334 (93%)	-0.16	3 (0%) 82 66	48, 64, 82, 100	0
1	B	295/334 (88%)	0.12	15 (5%) 28 16	52, 80, 101, 116	0
1	C	311/334 (93%)	-0.16	3 (0%) 82 66	45, 60, 78, 91	0
1	D	296/334 (88%)	0.03	6 (2%) 65 45	46, 72, 95, 114	0
2	E	14/25 (56%)	0.45	1 (7%) 16 8	55, 73, 99, 103	0
2	F	17/25 (68%)	0.69	2 (11%) 4 2	58, 78, 95, 97	0
All	All	1245/1386 (89%)	-0.03	30 (2%) 59 39	45, 67, 92, 116	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	ILE	4.1
1	B	237	ALA	3.5
1	D	193	ILE	3.4
2	F	20	LEU	3.4
1	D	188	LEU	3.1
1	B	238	GLU	3.1
1	C	228	VAL	2.9
1	B	188	LEU	2.8
1	D	163	HIS	2.8
1	D	191	ASP	2.7
1	B	191	ASP	2.6
1	A	226	ARG	2.6
1	B	30	GLY	2.6
2	F	17	TYR	2.5
1	B	3	ASN	2.4
1	D	225	LEU	2.4
1	B	163	HIS	2.3
2	E	7	GLY	2.3
1	B	160	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	298	VAL	2.2
1	B	241	ILE	2.2
1	C	230	ASP	2.2
1	C	4	LEU	2.1
1	D	239	GLU	2.1
1	B	187	ASP	2.1
1	B	85	ALA	2.0
1	A	229	THR	2.0
1	B	185	ALA	2.0
1	B	190	ALA	2.0
1	A	6	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	DV9	E	24	15/16	0.68	0.52	76,102,115,115	0
2	DV9	F	24	5/16	0.94	0.11	67,67,67,67	0

## 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
4	MG	A	403	1/1	0.78	0.52	67,67,67,67	0
4	MG	B	403	1/1	0.81	0.42	69,69,69,69	0
4	MG	D	403	1/1	0.83	0.46	66,66,66,66	0
4	MG	C	403	1/1	0.84	0.41	62,62,62,62	0
4	MG	D	402	1/1	0.85	0.34	72,72,72,72	0

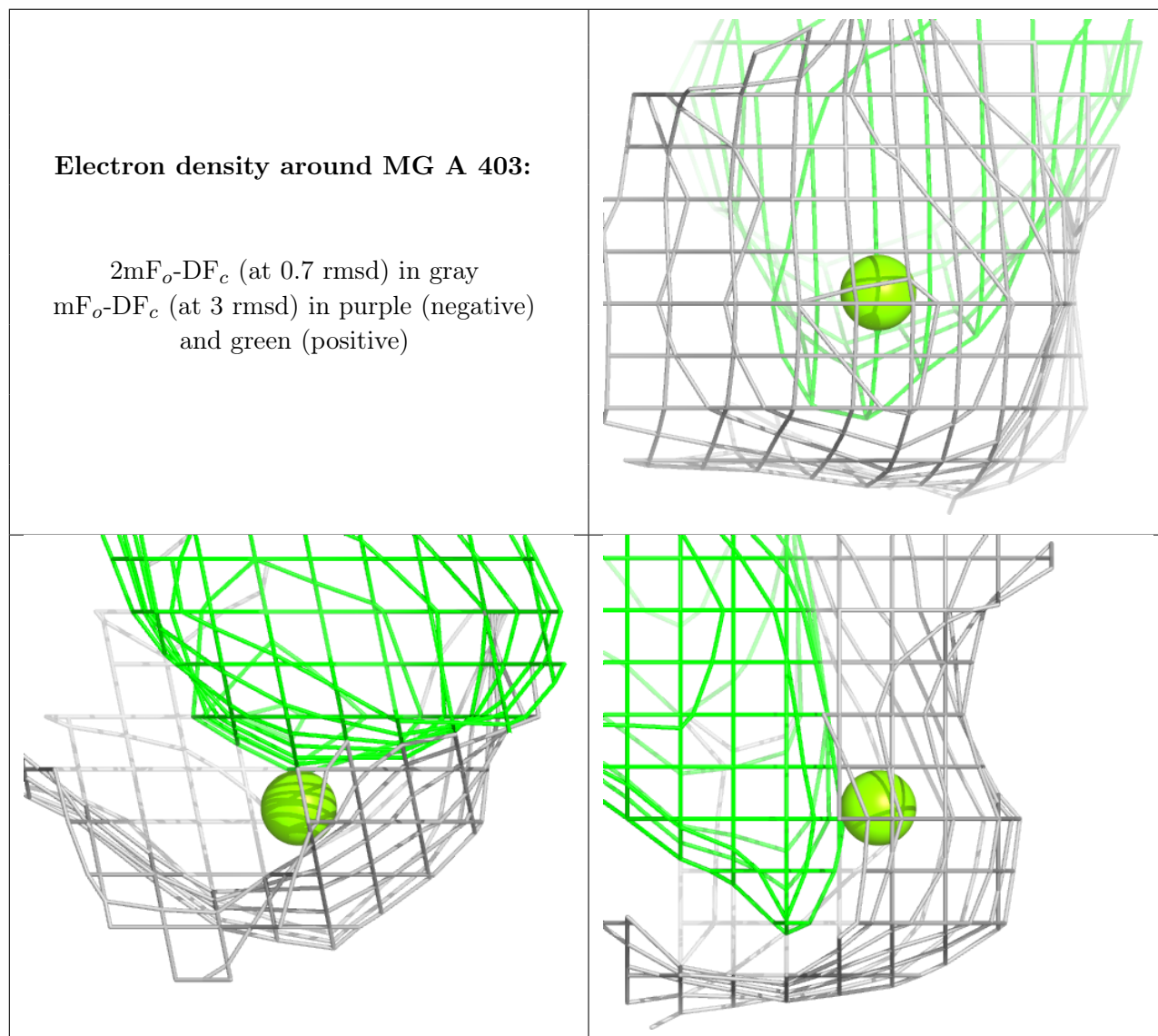
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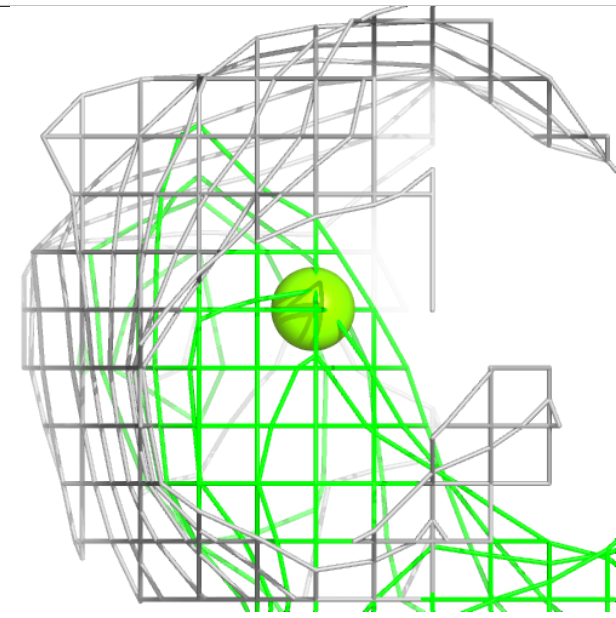
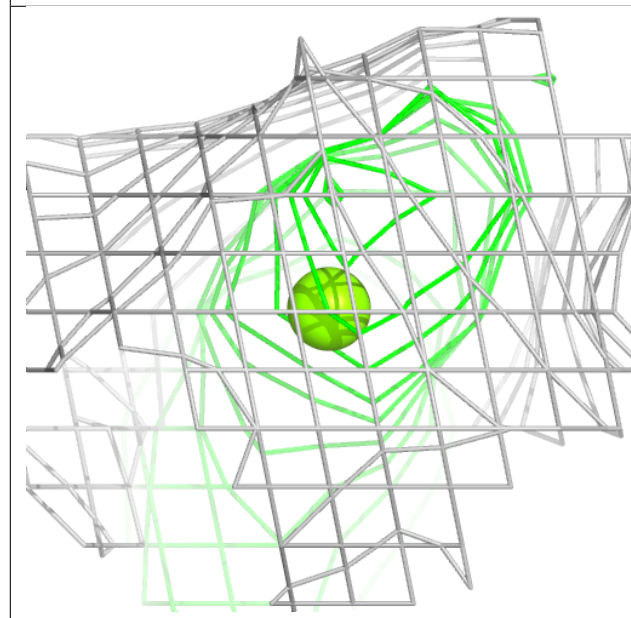
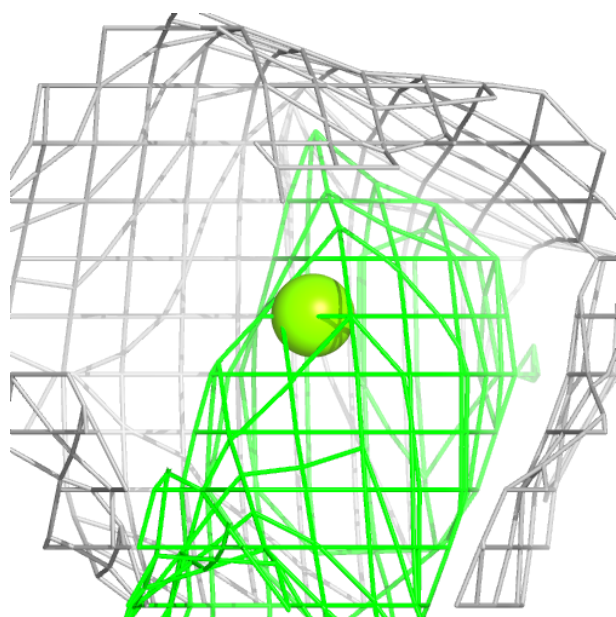
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	C	402	1/1	0.92	0.41	50,50,50,50	0
4	MG	A	402	1/1	0.93	0.43	48,48,48,48	0
3	ADP	D	401	27/27	0.94	0.22	75,78,85,86	0
3	ADP	B	401	27/27	0.94	0.18	69,74,79,81	0
4	MG	B	402	1/1	0.95	0.32	68,68,68,68	0
3	ADP	C	401	27/27	0.95	0.21	50,56,60,65	0
3	ADP	A	401	27/27	0.96	0.18	52,57,63,68	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.



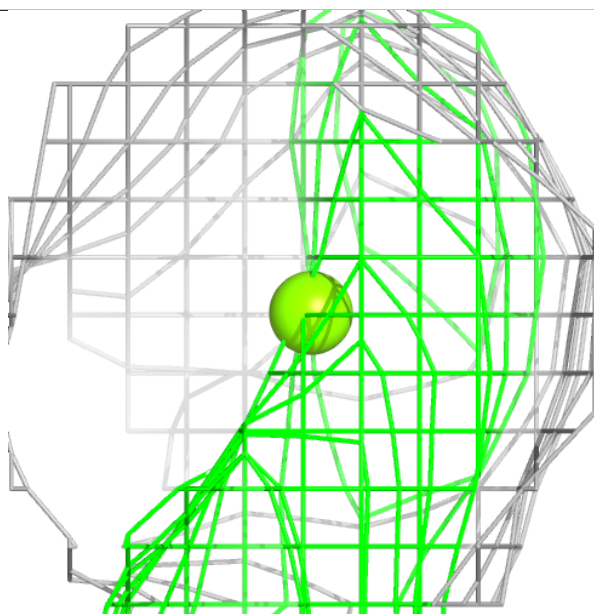
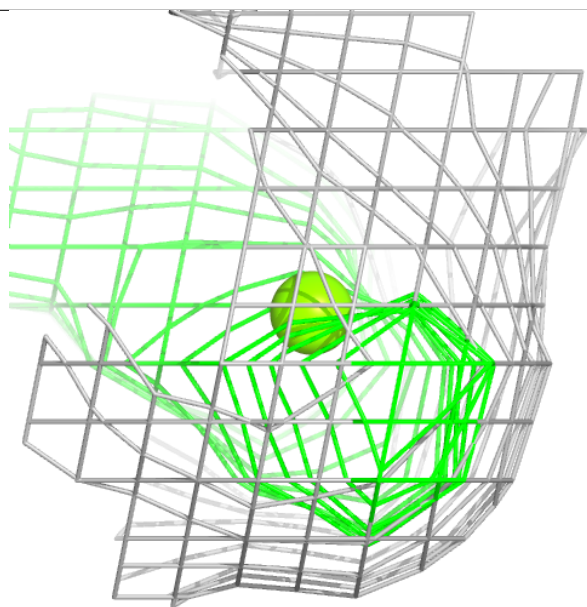
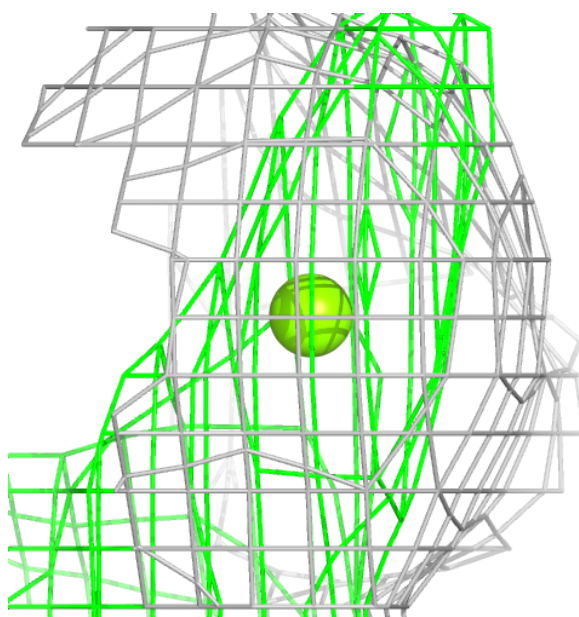
**Electron density around MG B 403:**

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



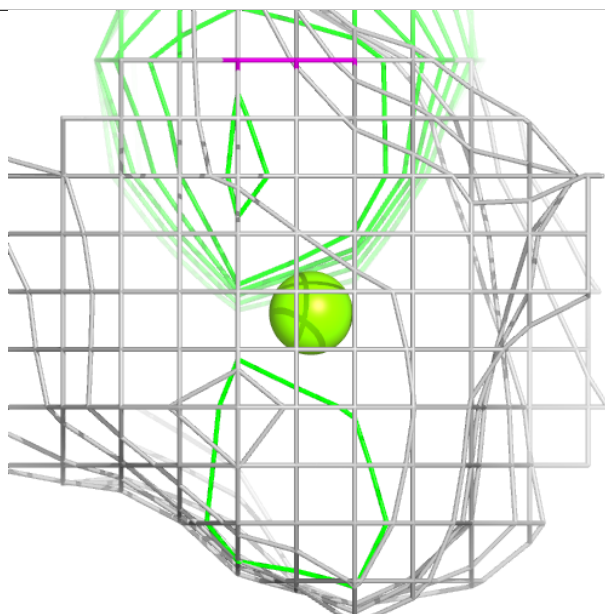
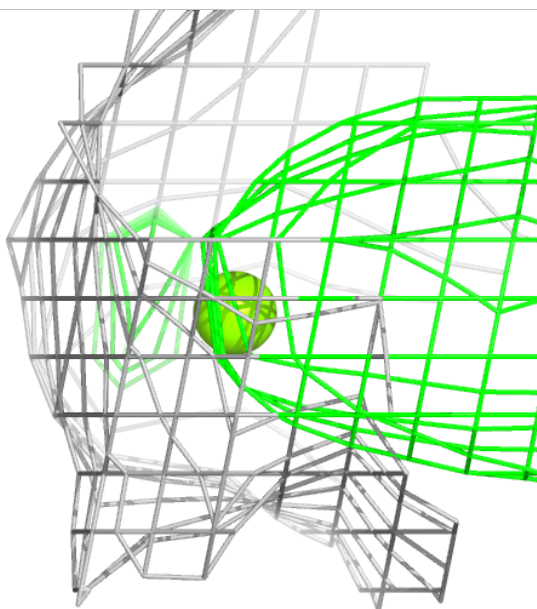
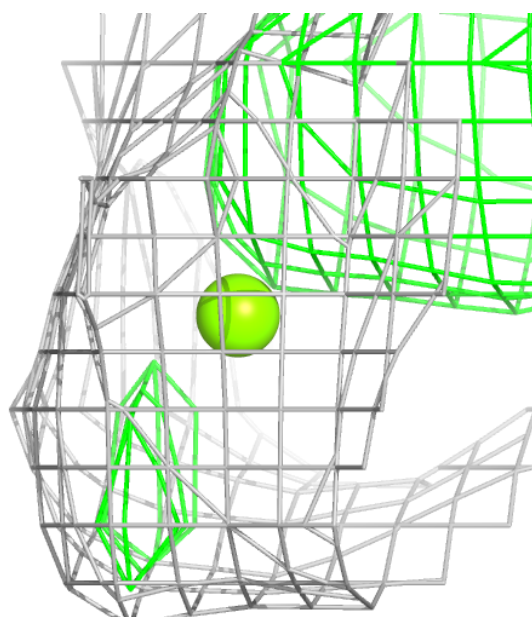
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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



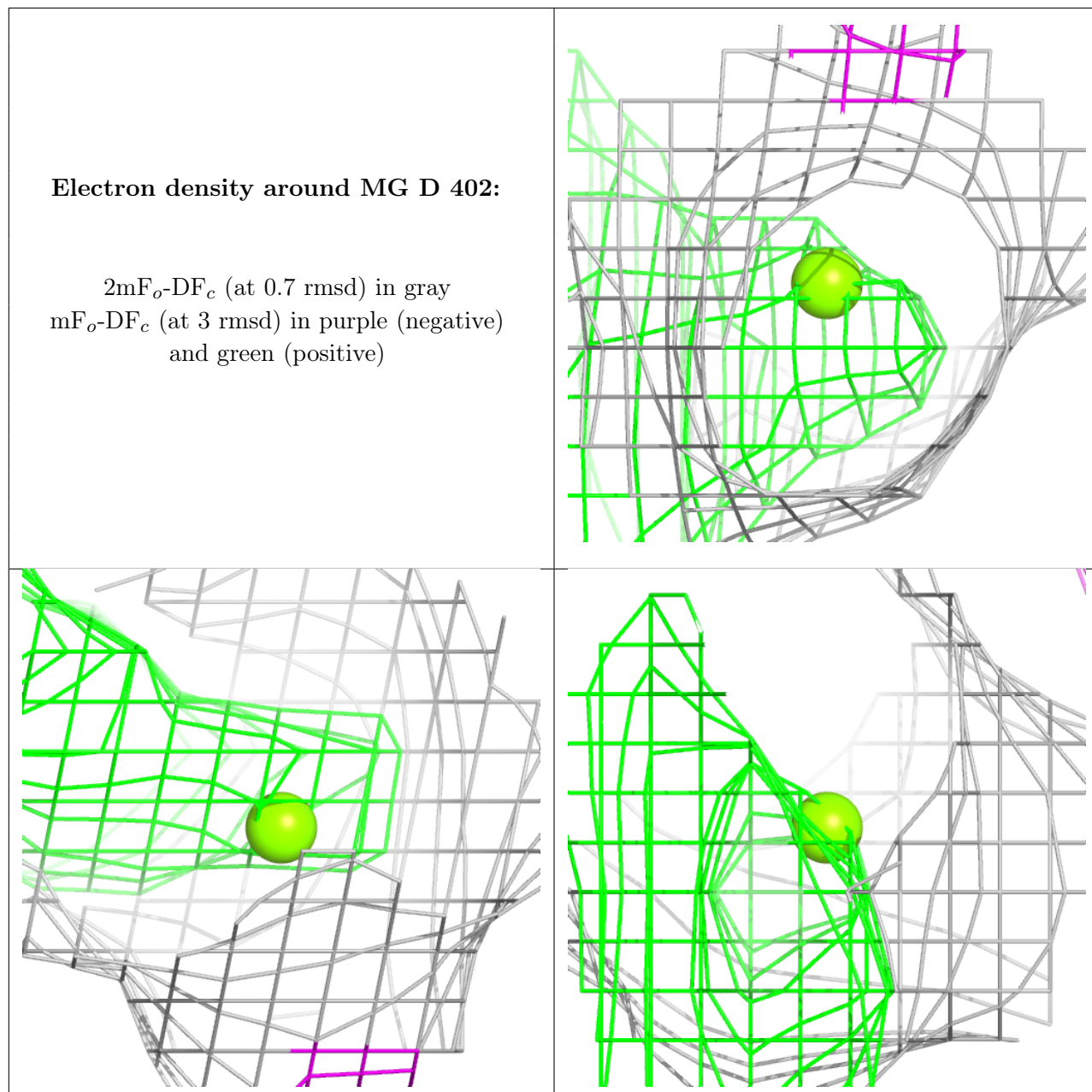
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and green (positive)



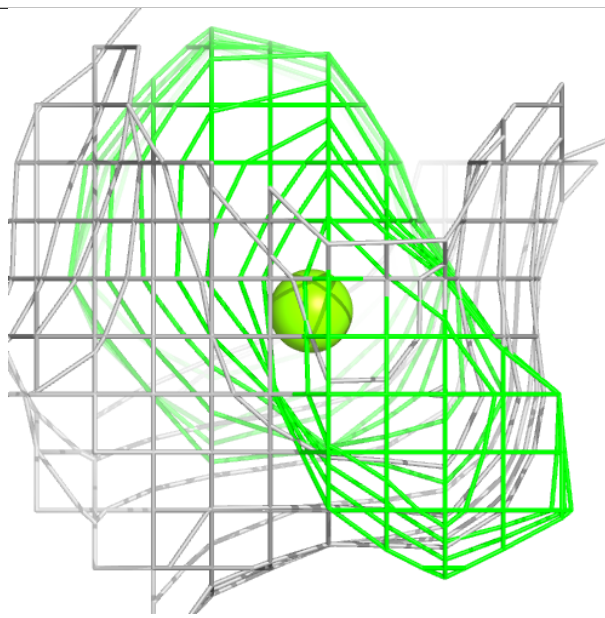
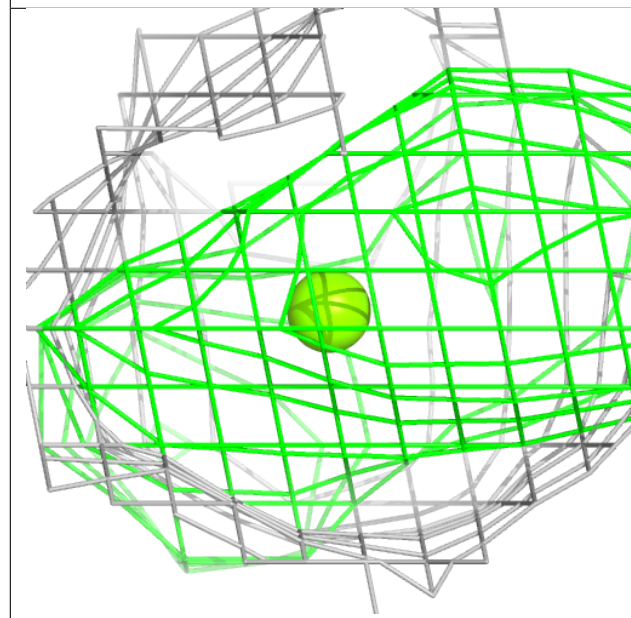
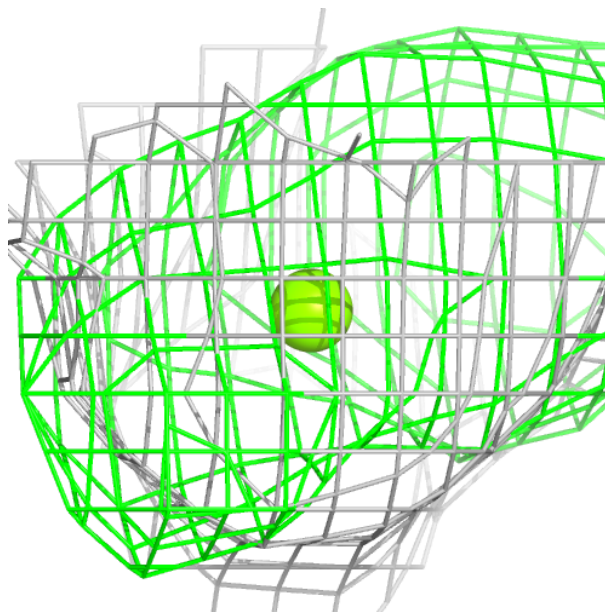
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and green (positive)



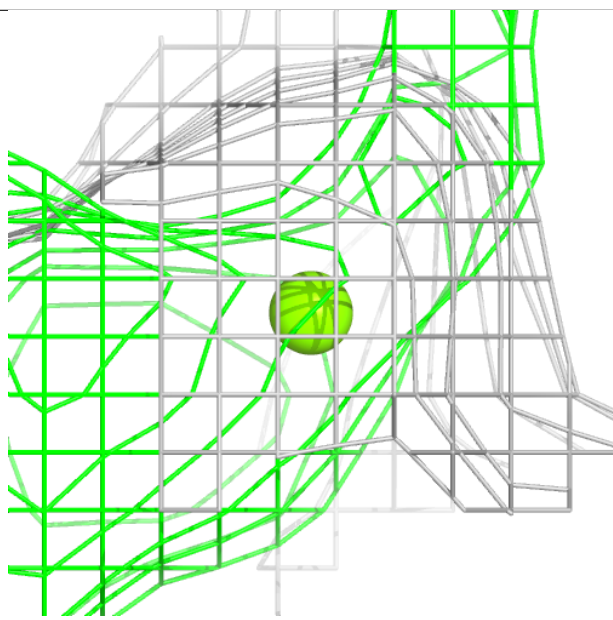
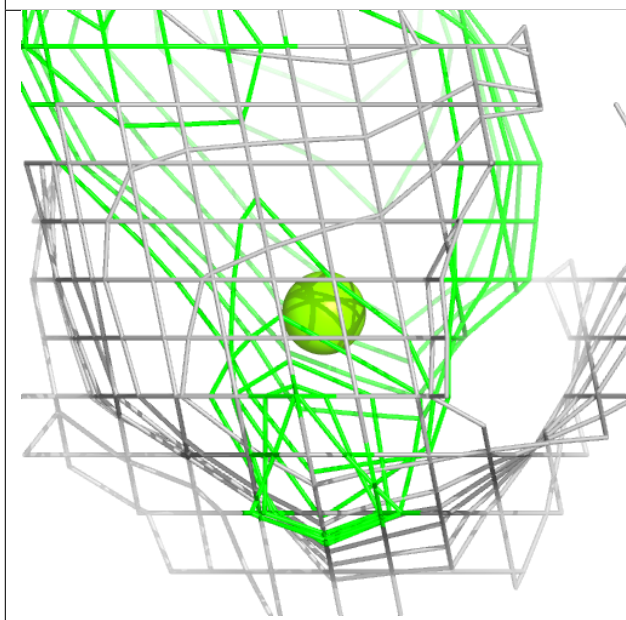
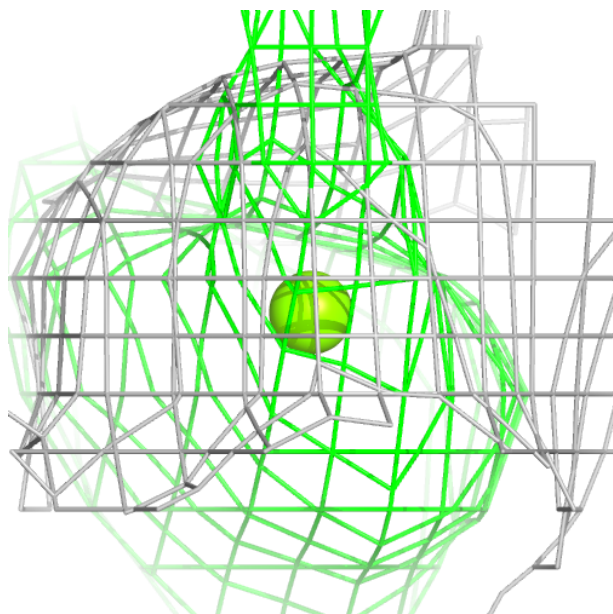
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and green (positive)



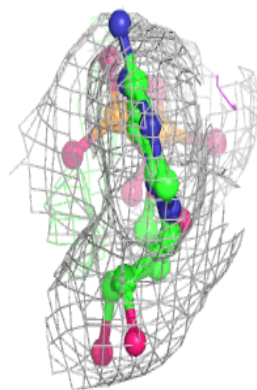
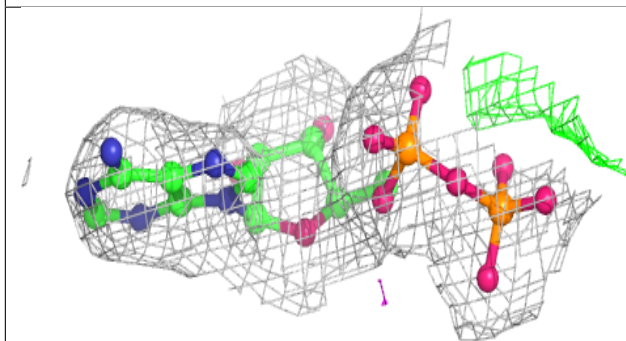
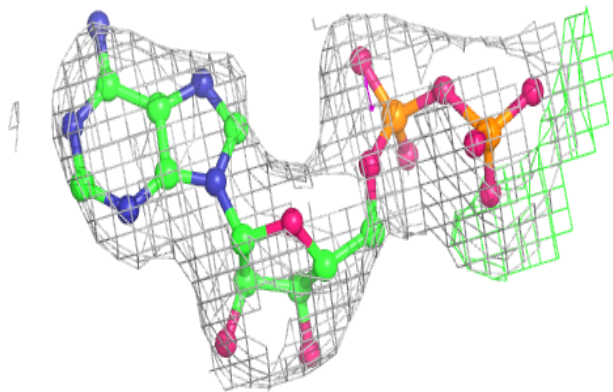
**Electron density around MG A 402:**

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

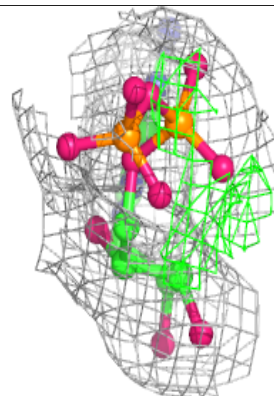
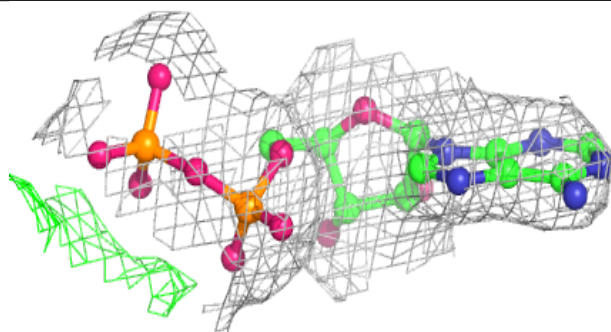
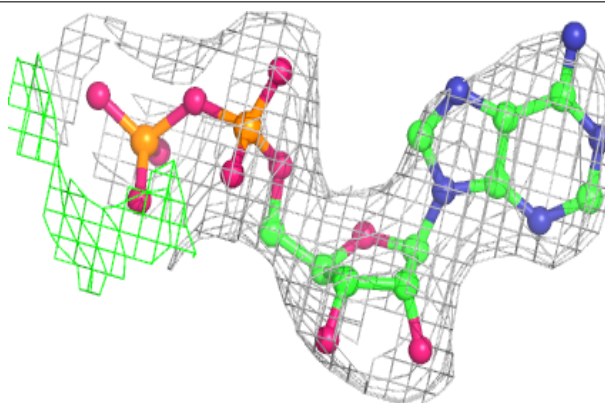


**Electron density around ADP D 401:**

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

**Electron density around ADP B 401:**

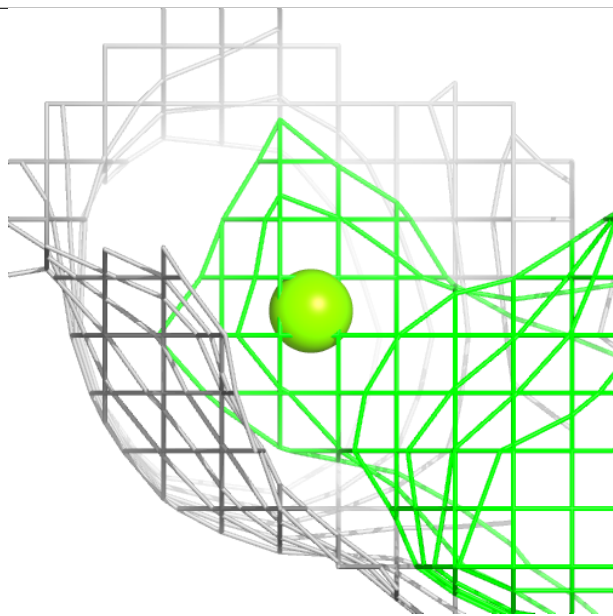
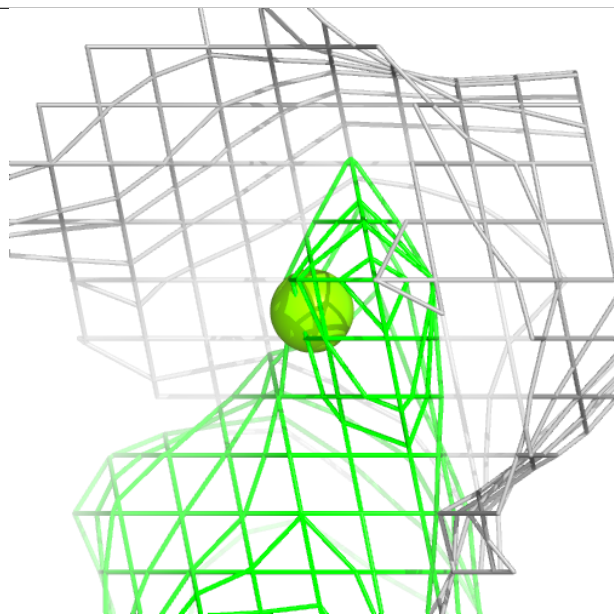
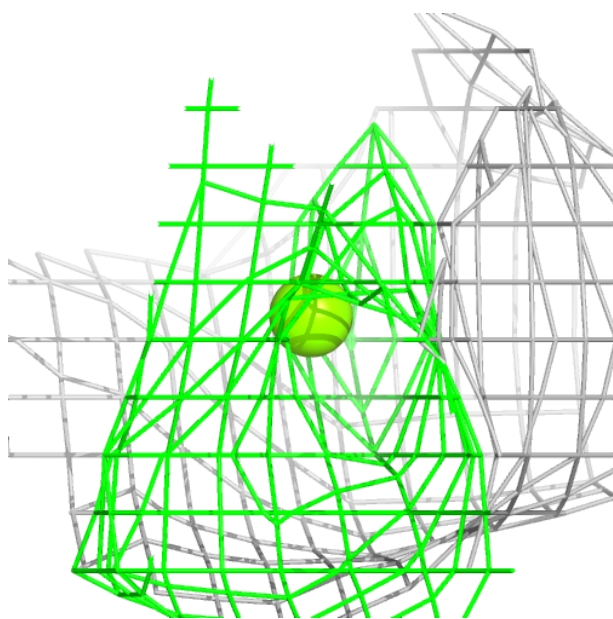
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

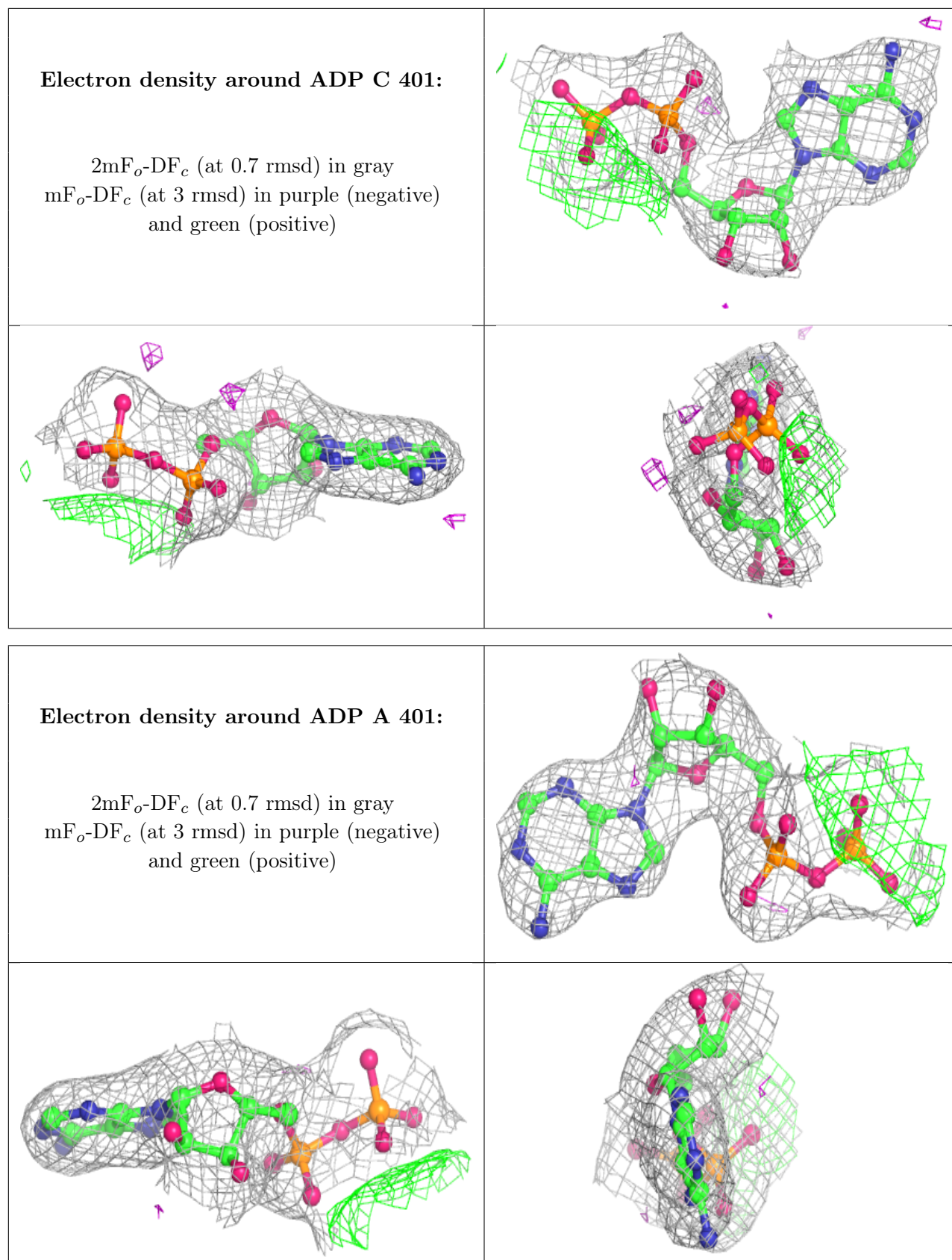




**Electron density around MG B 402:**

$2mF_o-DF_c$  (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.