



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 21, 2023 – 08:06 PM JST

PDB ID : 7WHG
Title : Lokiarchaeota gelsolin (2DGel) bound to two molecules of rabbit actin
Authors : Robinson, R.C.; Akil, C.
Deposited on : 2021-12-30
Resolution : 3.25 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 ⓘ 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 ⓘ](#)) 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 : 2.36
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

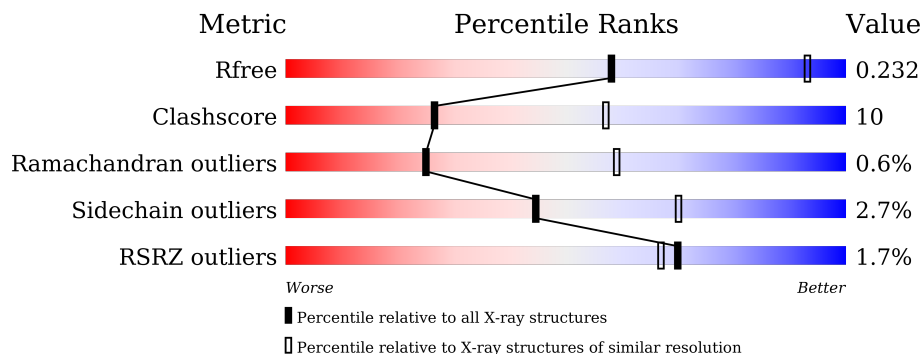
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 $\leq 5\%$. 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	377	 2% 76% 21% ..
1	B	377	 % 80% 18% ..
2	G	335	 2% 40% 24% . 34%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7607 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.

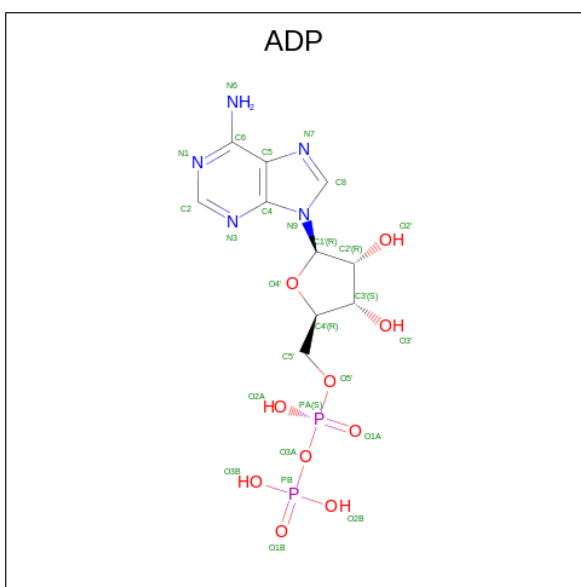
- Molecule 1 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	371	Total	C	N	O	S	0	0	0
			2899	1833	488	558	20			
1	B	371	Total	C	N	O	S	0	0	0
			2900	1837	489	553	21			

- Molecule 2 is a protein called Lokiarchaeota gelsolin (2DGel).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	221	Total	C	N	O	S	0	0	0
			1745	1107	289	344	5			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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		

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

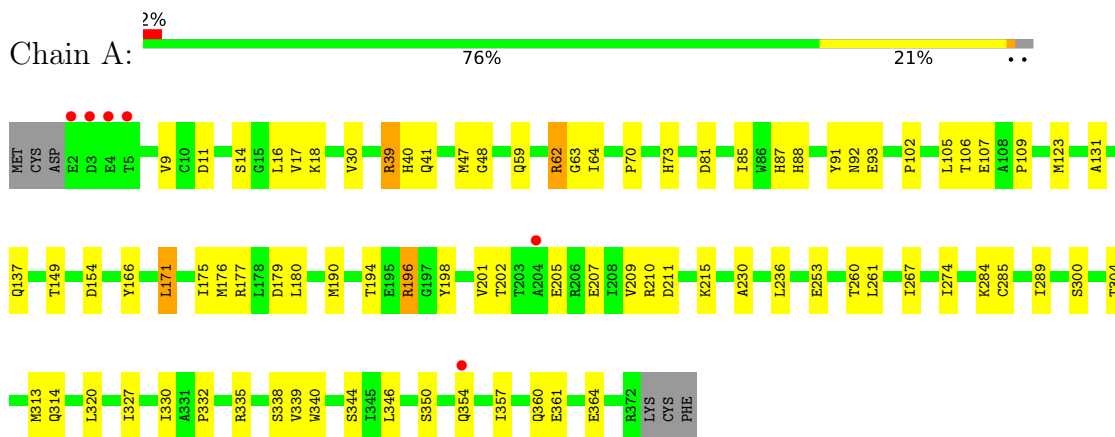
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Ca 2	0	0
4	B	1	Total 1	Ca 1	0	0
4	G	6	Total 6	Ca 6	0	0

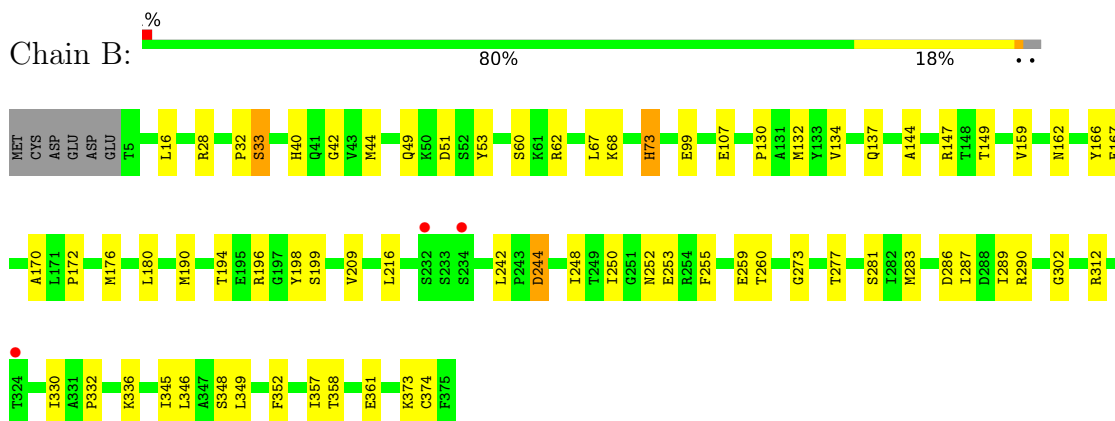
3 Residue-property plots [i](#)

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.

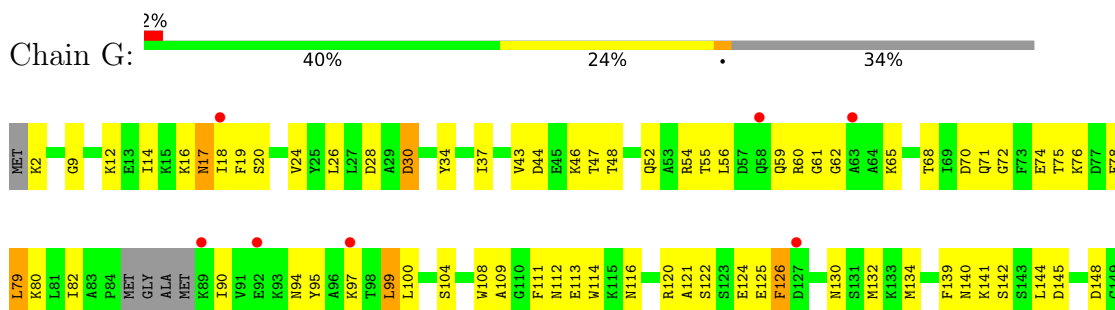
- Molecule 1: Actin, alpha skeletal muscle



- Molecule 1: Actin, alpha skeletal muscle



- Molecule 2: Lokiarchaeota gelsolin (2DGel)



F150	L2286	GLU	GLU
D153	L206	GLY	GLY
L154	A204	GLU	GLU
G155	L206	ASP	ARG
W177	D207	ASP	ARG
S180	R208	ASP	ASP
I181	K213	ASP	ASP
R185	A217	ILE	ILE
L188	L2286	ALA	ALA
E191	GLU	ALA	ILE
D199	GLY	PRO	GLN
I200	ARG	PRO	LYS
E201	ILE	THR	THR
A204	THR	GLY	GLY
L206	ALA	ARG	ARG
D207	ILE	ARG	ARG
R208	LEU	ARG	CYS
K213	THR	PRO	PRO
A217	ILE	GLU	GLU
L2286	LYS	CYS	CYS
GLU	THR	ASN	ASN
GLY	GLU	ILE	ILE
GLU	GLY	ASP	LYS
ASP	ARG	PRO	PRO
ASP	ARG	GLN	GLN
ASP	ASP	MET	PRO
ASP	ASP	ILE	GLU
ASP	ASP	ILE	LEU
ASP	ASP	HIS	LEU
ASP	ASP	GLU	LYS
ASP	ASP	THR	THR
ASP	ASP	VAL	VAL
ASP	ASP	VAL	VAL
ASP	ASP	LYS	LYS
ASP	ASP	SER	SER
ASP	ASP	VAL	VAL
ASP	ASP	THR	THR
ASP	ASP	ILE	ILE
ASP	ASP	ILE	ILE
ASP	ASP	LEU	LEU
ASP	ASP	ASP	ASP
TYR	PRO	ARG	ARG
PRO	ARG	VAL	VAL
ARG	VAL	GLY	GLY
VAL	TYR	GLY	GLY
TYR	GLY	LYS	LYS
GLY	LYS	PHE	PHE
LYS	LYS	LYS	LYS
LYS	CYS	CYS	CYS
PHE	GLY	GLY	GLY
VAL	SER	SER	SER
GLY	ALA	ALA	ALA
LYS	ALA	ALA	ALA
PHE	PRO	PRO	PRO
LYS	GLY	GLY	GLY
VAL	VAL	VAL	VAL
GLU	GLU	GLU	GLU
TRP	TRP	TRP	TRP
ARG	ARG	ARG	ARG
GLU	GLU	GLU	GLU
ARG	ARG	ARG	ARG

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.66Å 72.06Å 100.39Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	20.00 – 3.25 19.91 – 3.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.25) 87.9 (19.91-3.25)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 3.29Å)	Xtrriage
Refinement program	PHENIX 1.17.1	Depositor
R, R_{free}	0.175 , 0.232 0.172 , 0.232	Depositor DCC
R_{free} test set	845 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtrriage
Anisotropy	0.152	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP, HIC, CA

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	0.60	0/2948	0.76	2/3994 (0.1%)
1	B	0.49	0/2950	0.66	0/3994
2	G	0.57	1/1771 (0.1%)	0.68	1/2380 (0.0%)
All	All	0.55	1/7669 (0.0%)	0.70	3/10368 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	191	GLU	CB-CG	5.06	1.61	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	226	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	171	LEU	CA-CB-CG	-5.31	103.09	115.30
1	A	320	LEU	CB-CG-CD2	-5.14	102.27	111.00

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	2899	0	2861	51	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2900	0	2872	47	1
2	G	1745	0	1731	68	0
3	A	27	0	12	1	0
3	B	27	0	12	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	G	6	0	0	0	0
All	All	7607	0	7488	155	1

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 10.

The worst 5 of 155 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:147:ARG:NH2	2:G:70:ASP:OD1	2.10	0.85
2:G:17:ASN:HD22	2:G:82:ILE:HG23	1.47	0.79
2:G:95:TYR:HE2	2:G:226:LEU:HB3	1.48	0.79
1:A:314:GLN:NE2	1:A:327:ILE:O	2.20	0.75
2:G:44:ASP:HB2	2:G:99:LEU:HD21	1.70	0.74

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:GLN:NE2	1:B:99:GLU:OE1[2_555]	2.16	0.04

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	368/377 (98%)	351 (95%)	14 (4%)	3 (1%)	19	52
1	B	368/377 (98%)	356 (97%)	11 (3%)	1 (0%)	41	72
2	G	217/335 (65%)	203 (94%)	12 (6%)	2 (1%)	17	50
All	All	953/1089 (88%)	910 (96%)	37 (4%)	6 (1%)	25	59

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	61	GLY
2	G	217	ALA
1	B	244	ASP
1	A	62	ARG
1	A	201	VAL

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	313/319 (98%)	307 (98%)	6 (2%)	57	76
1	B	313/319 (98%)	308 (98%)	5 (2%)	62	79
2	G	186/283 (66%)	175 (94%)	11 (6%)	19	50
All	All	812/921 (88%)	790 (97%)	22 (3%)	44	70

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	54	ARG
2	G	99	LEU
2	G	97	LYS
2	G	126	PHE
1	B	33	SER

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

Mol	Chain	Res	Type
1	A	88	HIS
2	G	140	ASN
2	G	162	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](#)

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
1	HIC	B	73	1	8,11,12	1.83	2 (25%)	6,14,16	1.67	1 (16%)
1	HIC	A	73	1	8,11,12	2.07	2 (25%)	6,14,16	0.91	0

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HIC	B	73	1	-	2/5/6/8	0/1/1/1
1	HIC	A	73	1	-	3/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	73	HIC	CD2-CG	4.78	1.43	1.36
1	B	73	HIC	CD2-CG	4.23	1.42	1.36
1	A	73	HIC	CD2-NE2	2.49	1.41	1.38
1	B	73	HIC	CD2-NE2	2.11	1.41	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	HIC	CB-CA-C	-3.51	104.89	111.47

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	73	HIC	O-C-CA-CB
1	A	73	HIC	CA-CB-CG-ND1
1	A	73	HIC	C-CA-CB-CG
1	B	73	HIC	CA-CB-CG-ND1
1	B	73	HIC	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	73	HIC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 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	A	401	4	24,29,29	0.93	1 (4%)	29,45,45	1.61	5 (17%)
3	ADP	B	401	4	24,29,29	1.09	1 (4%)	29,45,45	1.66	8 (27%)

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	A	401	4	-	0/12/32/32	0/3/3/3
3	ADP	B	401	4	-	3/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	ADP	C5-C4	2.90	1.48	1.40
3	A	401	ADP	C2'-C1'	-2.25	1.50	1.53

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ADP	C4-C5-N7	-4.13	105.10	109.40
3	A	401	ADP	N3-C2-N1	-3.59	123.07	128.68
3	B	401	ADP	C1'-N9-C4	-2.92	121.52	126.64
3	A	401	ADP	N6-C6-N1	2.87	124.53	118.57
3	B	401	ADP	C5-C6-N6	2.75	124.53	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	ADP	C5'-O5'-PA-O1A
3	B	401	ADP	C5'-O5'-PA-O3A
3	B	401	ADP	C5'-O5'-PA-O2A

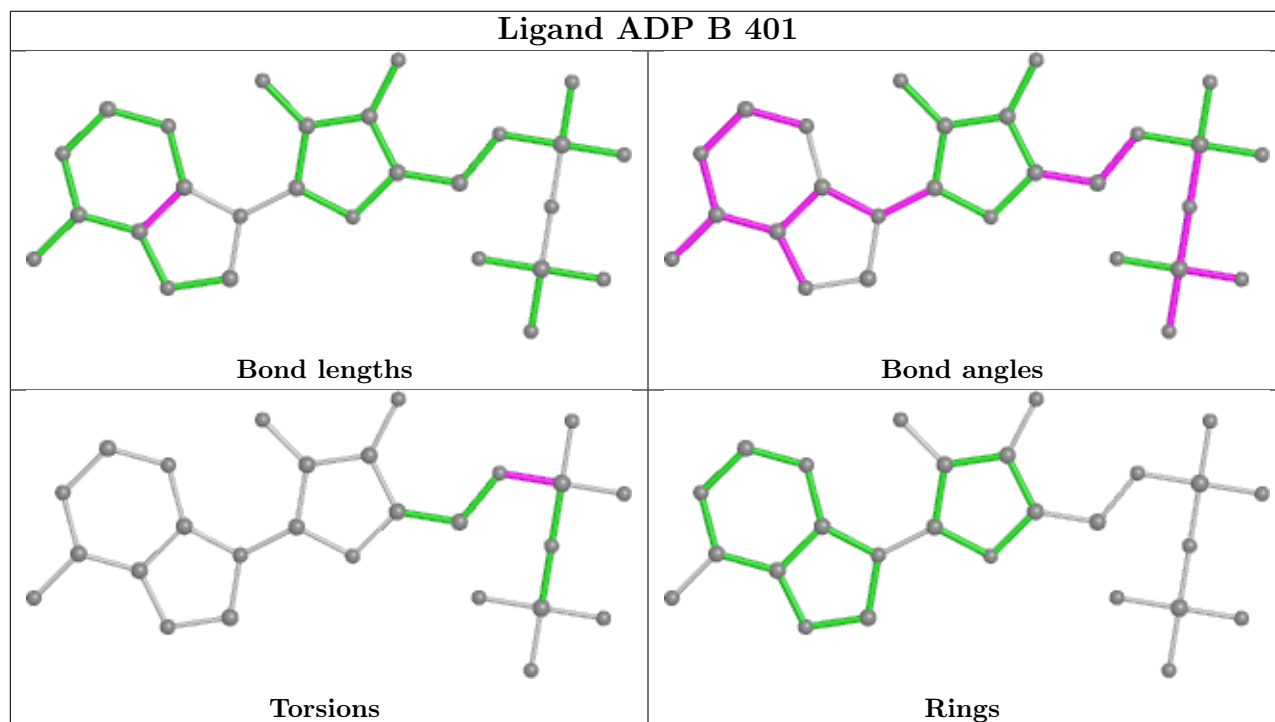
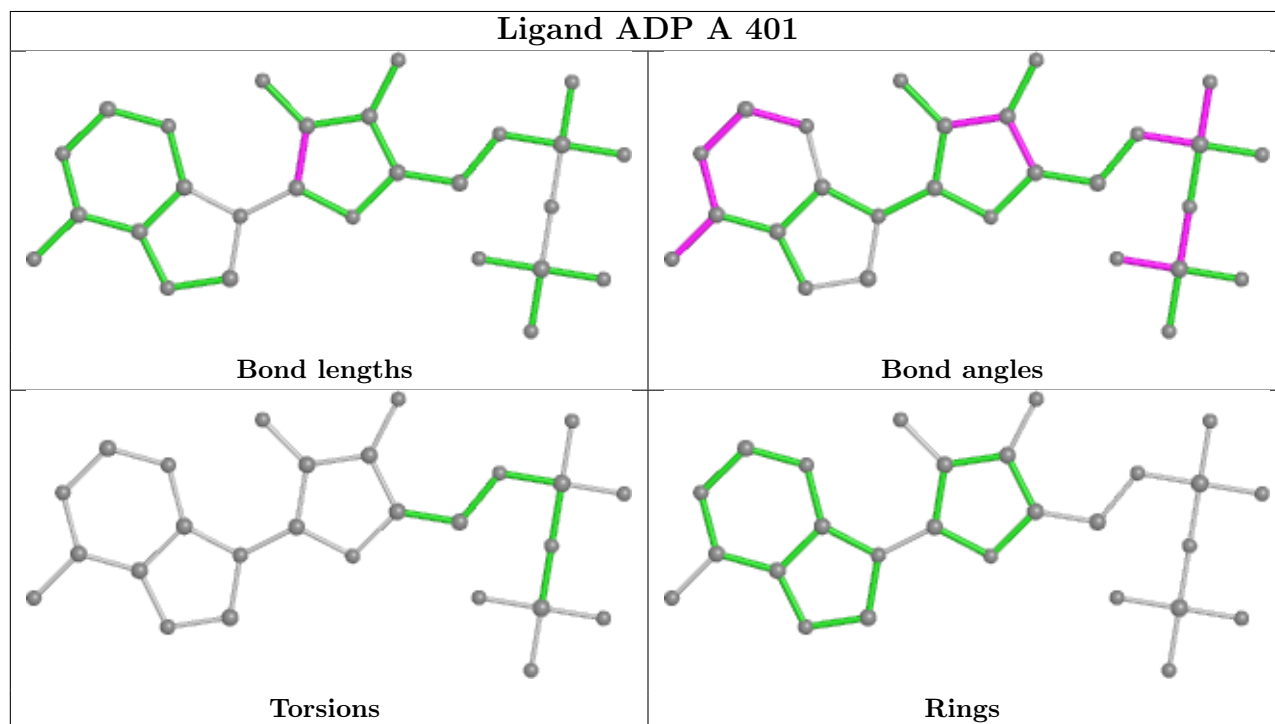
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ADP	1	0

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 [i](#)

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, 95th 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	A	370/377 (98%)	-0.50	6 (1%) 72 69	15, 45, 91, 154	0
1	B	370/377 (98%)	-0.32	3 (0%) 86 86	40, 74, 115, 144	0
2	G	221/335 (65%)	-0.02	7 (3%) 47 45	35, 77, 133, 152	0
All	All	961/1089 (88%)	-0.32	16 (1%) 70 67	15, 64, 118, 154	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASP	4.1
1	B	324	THR	3.5
1	A	4	GLU	3.4
2	G	18	ILE	3.2
1	A	204	ALA	2.9

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, 95th 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
1	HIC	B	73	11/12	0.86	0.32	79,84,86,87	0
1	HIC	A	73	11/12	0.93	0.22	40,54,64,65	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

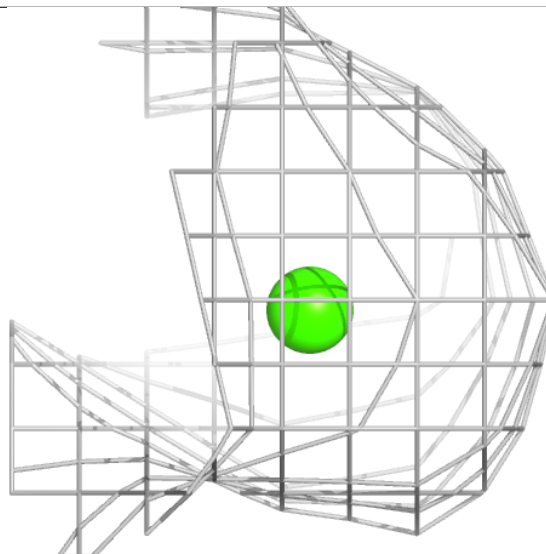
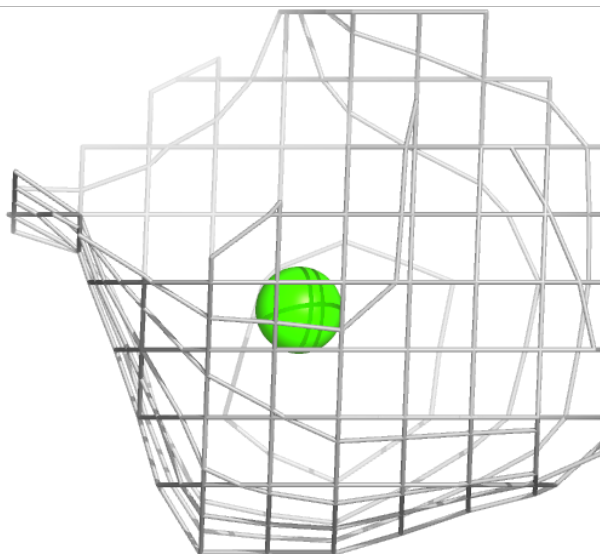
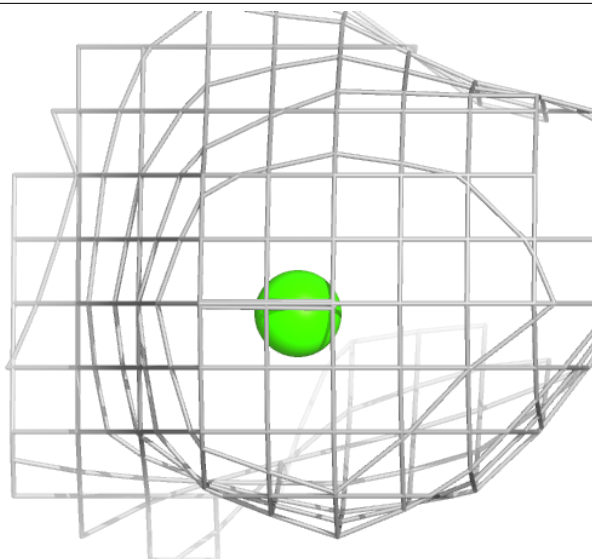
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CA	G	405	1/1	0.68	0.08	116,116,116,116	0
4	CA	B	402	1/1	0.89	0.30	55,55,55,55	0
4	CA	A	403	1/1	0.94	0.21	93,93,93,93	0
4	CA	G	406	1/1	0.94	0.20	78,78,78,78	0
4	CA	G	402	1/1	0.97	0.10	59,59,59,59	0
4	CA	G	403	1/1	0.97	0.06	64,64,64,64	0
3	ADP	B	401	27/27	0.97	0.15	41,48,54,56	0
4	CA	G	401	1/1	0.97	0.18	82,82,82,82	0
4	CA	G	404	1/1	0.98	0.04	35,35,35,35	0
4	CA	A	402	1/1	0.98	0.20	40,40,40,40	0
3	ADP	A	401	27/27	0.98	0.14	28,33,36,37	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.

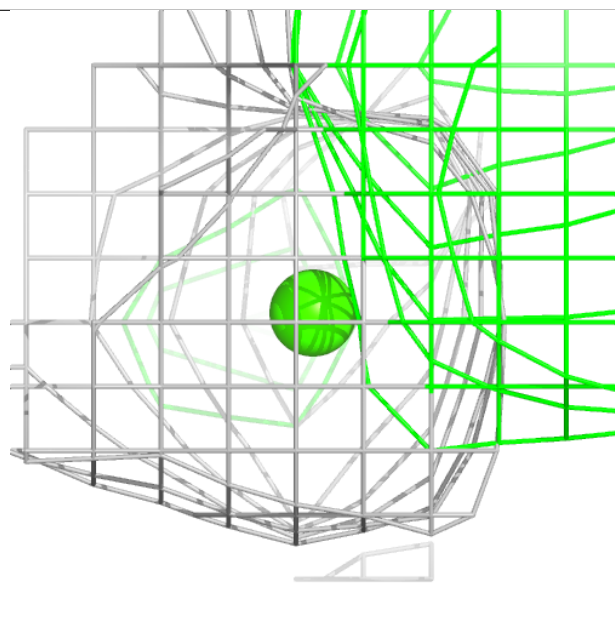
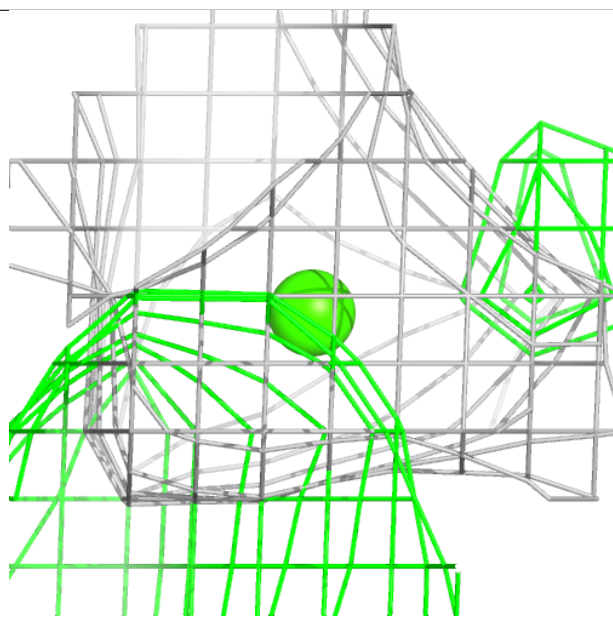
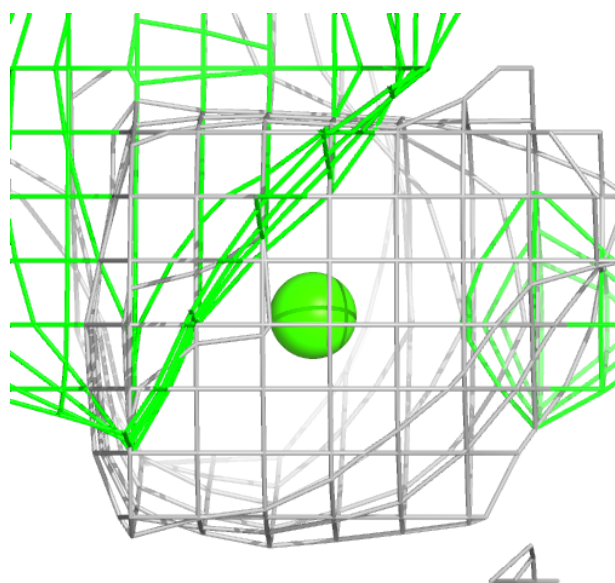
Electron density around CA G 405:

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



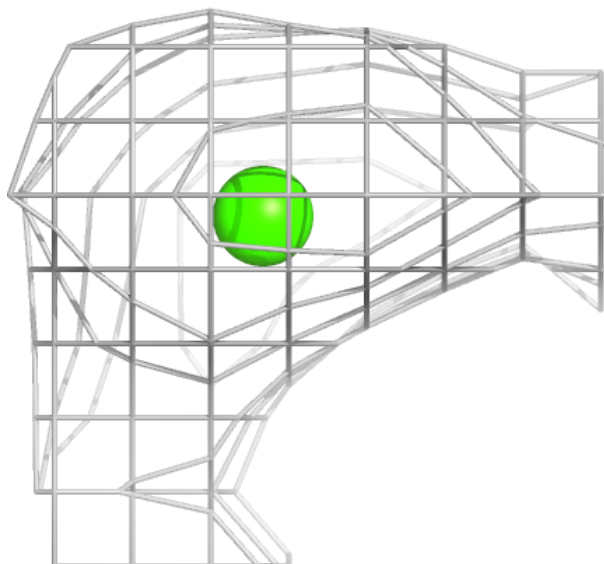
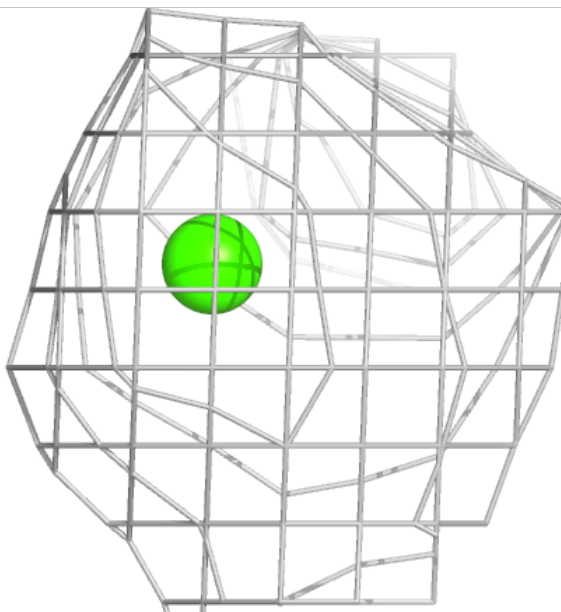
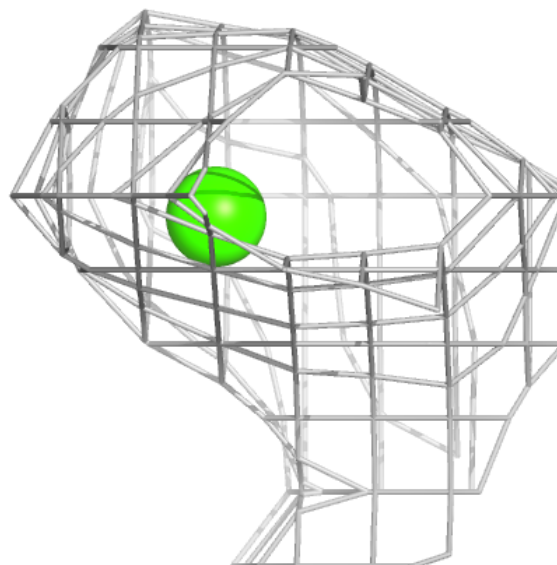
Electron density around CA B 402:

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



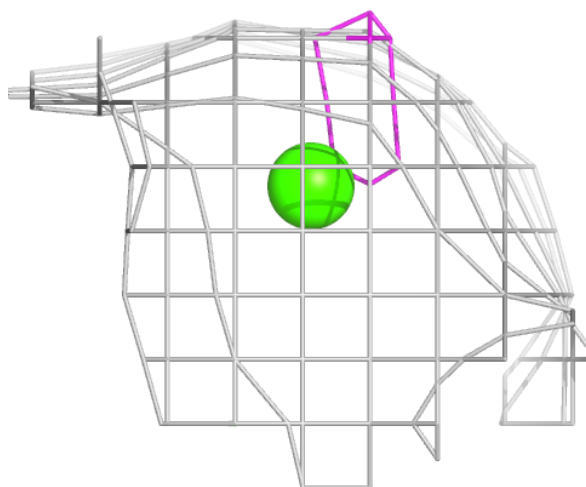
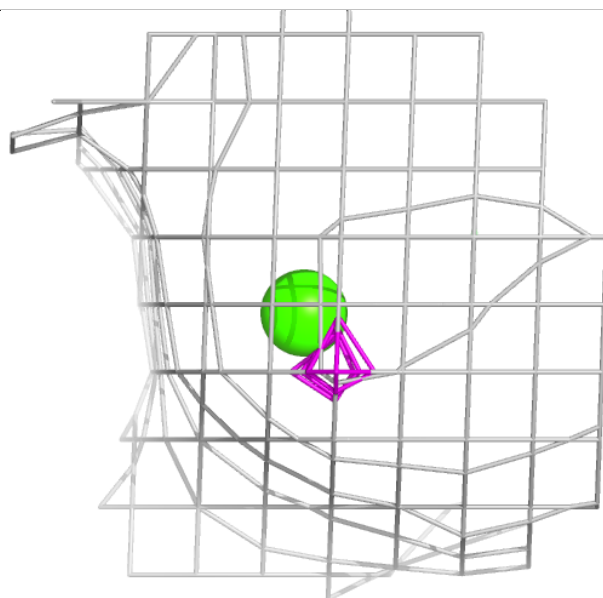
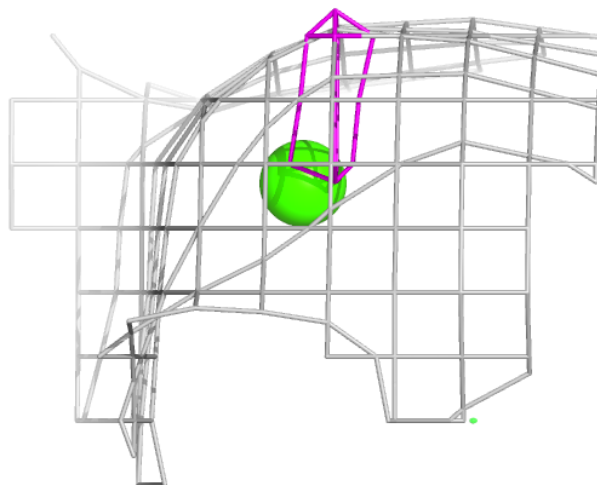
Electron density around CA A 403:

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



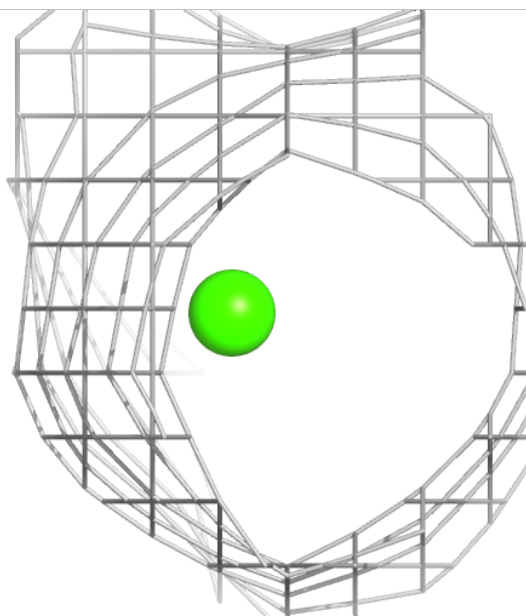
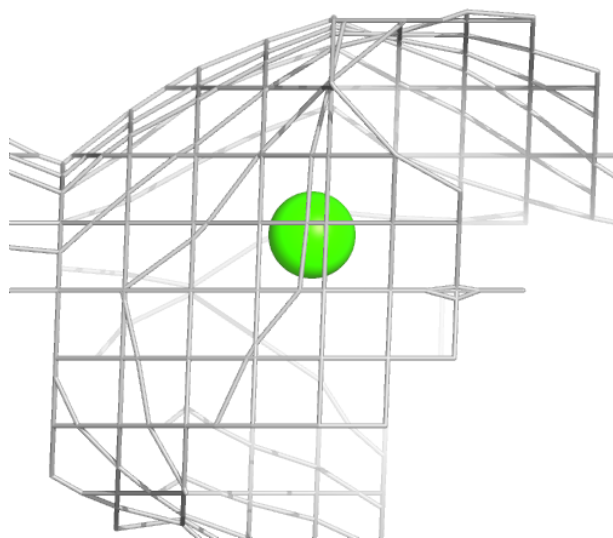
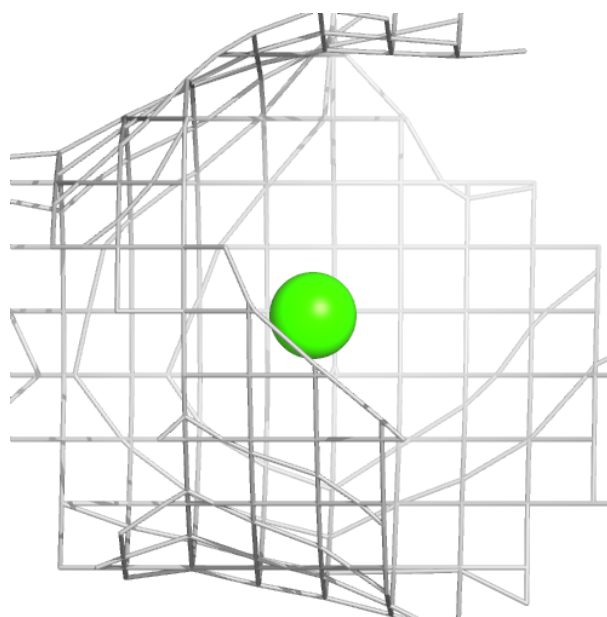
Electron density around CA G 406:

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



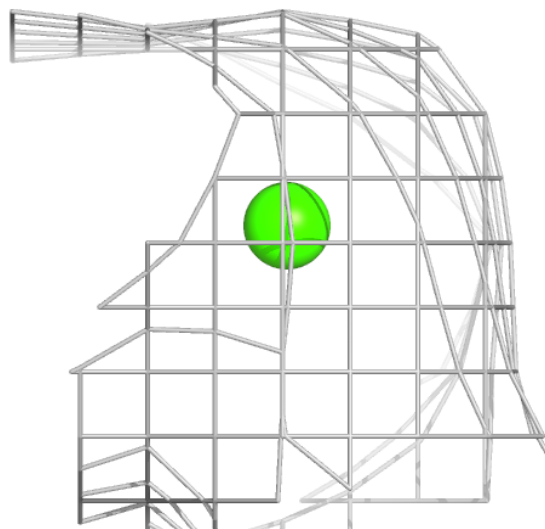
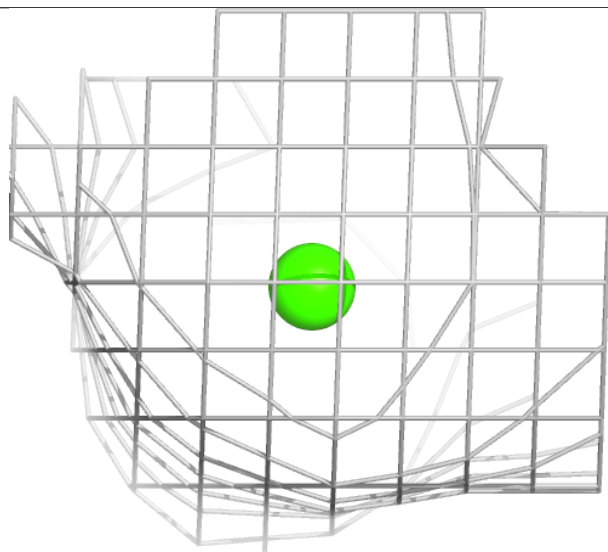
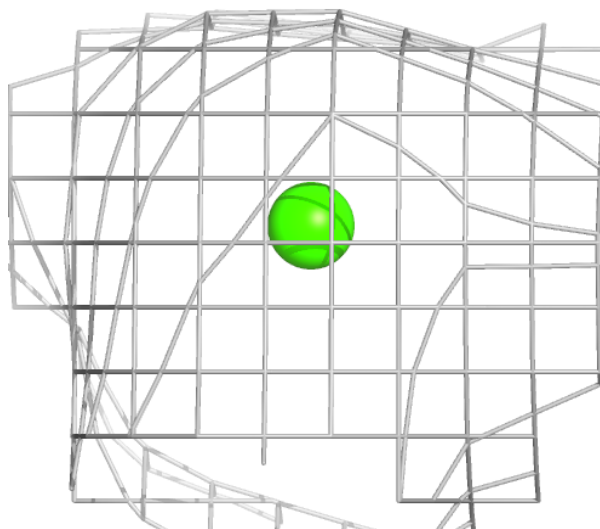
Electron density around CA G 402:

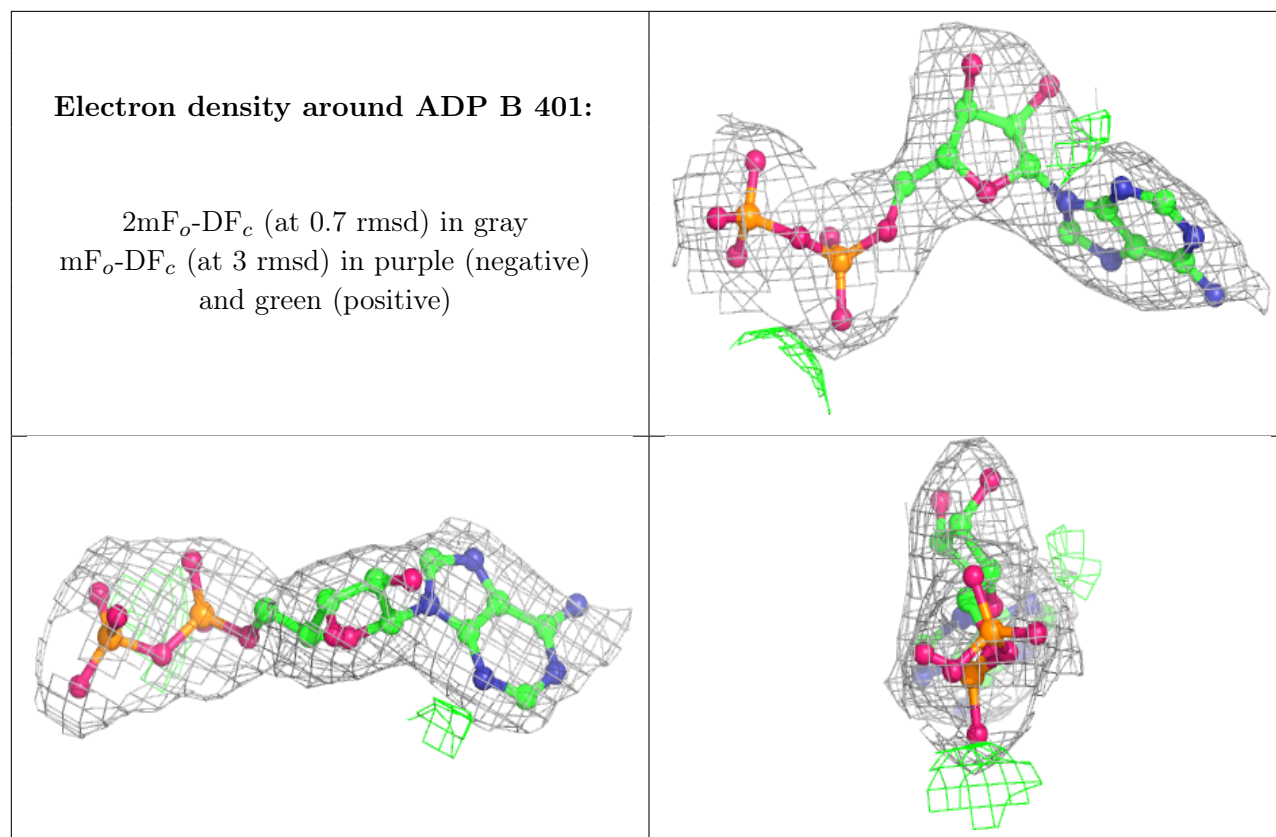
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA G 403:

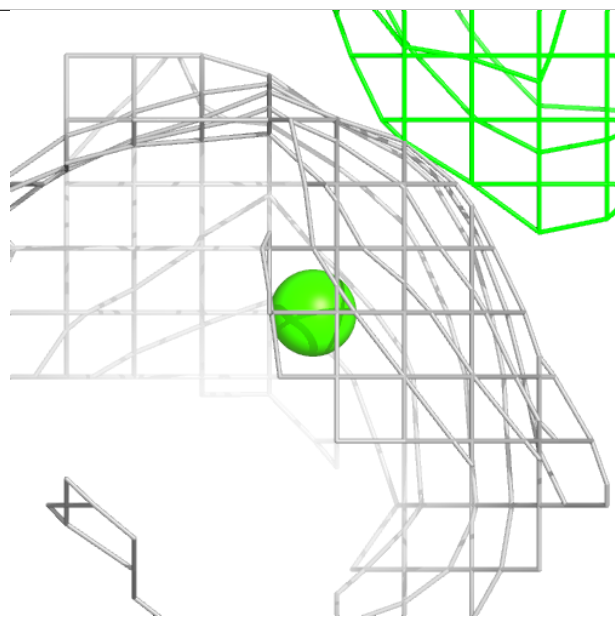
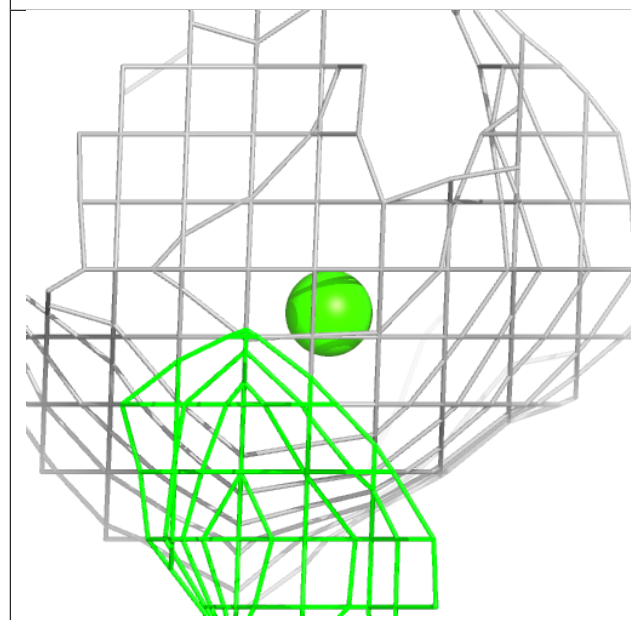
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





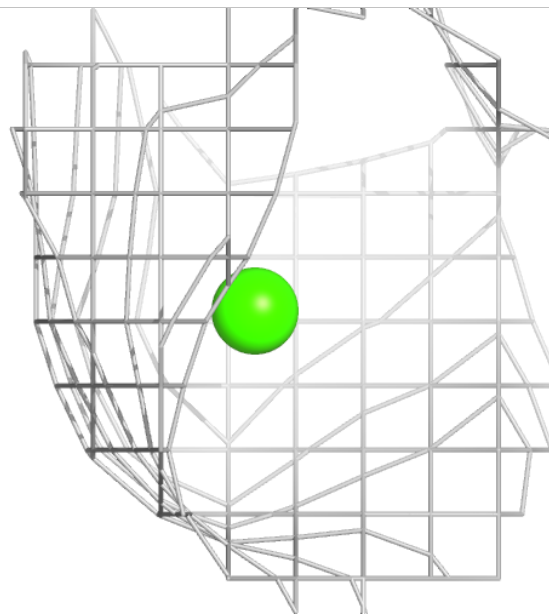
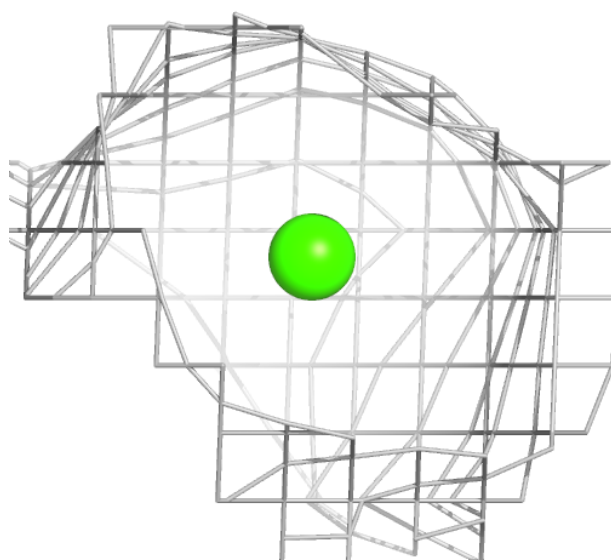
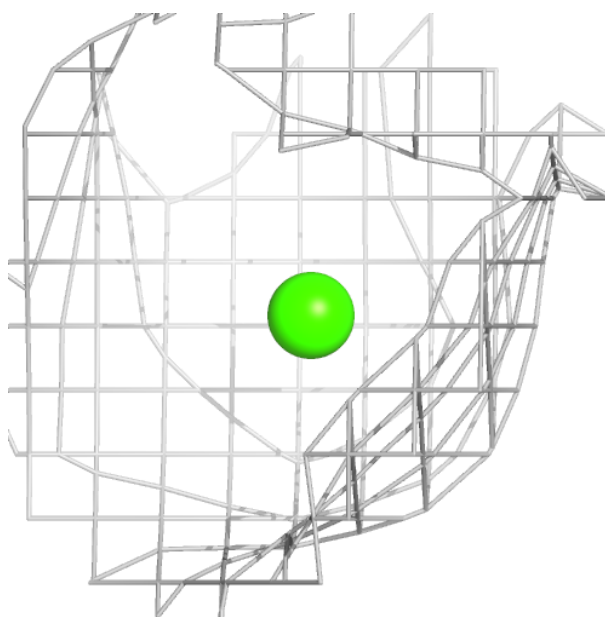
Electron density around CA G 401:

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



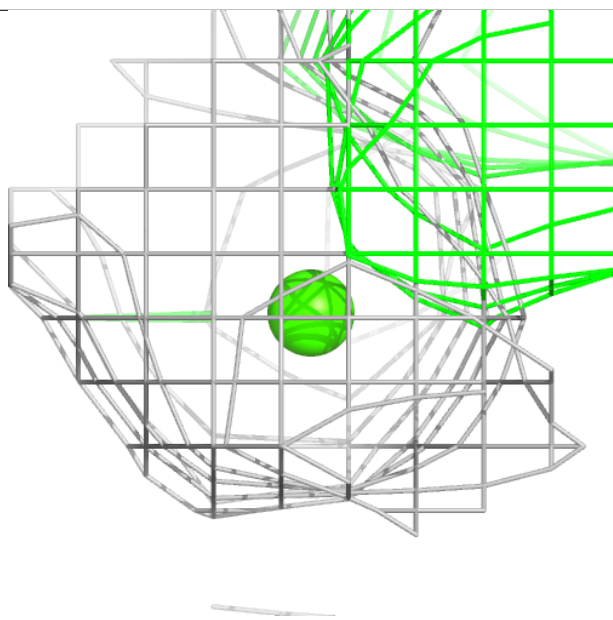
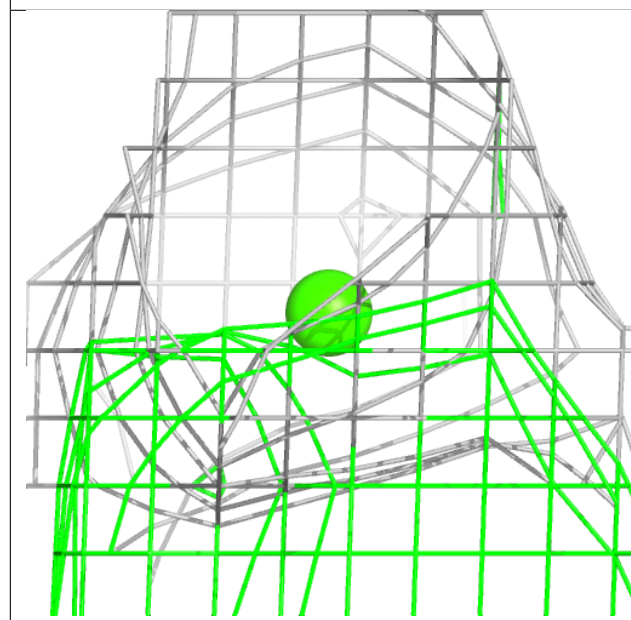
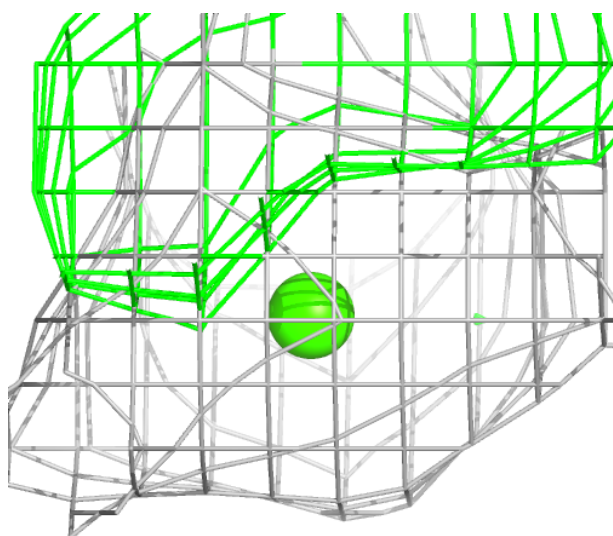
Electron density around CA G 404:

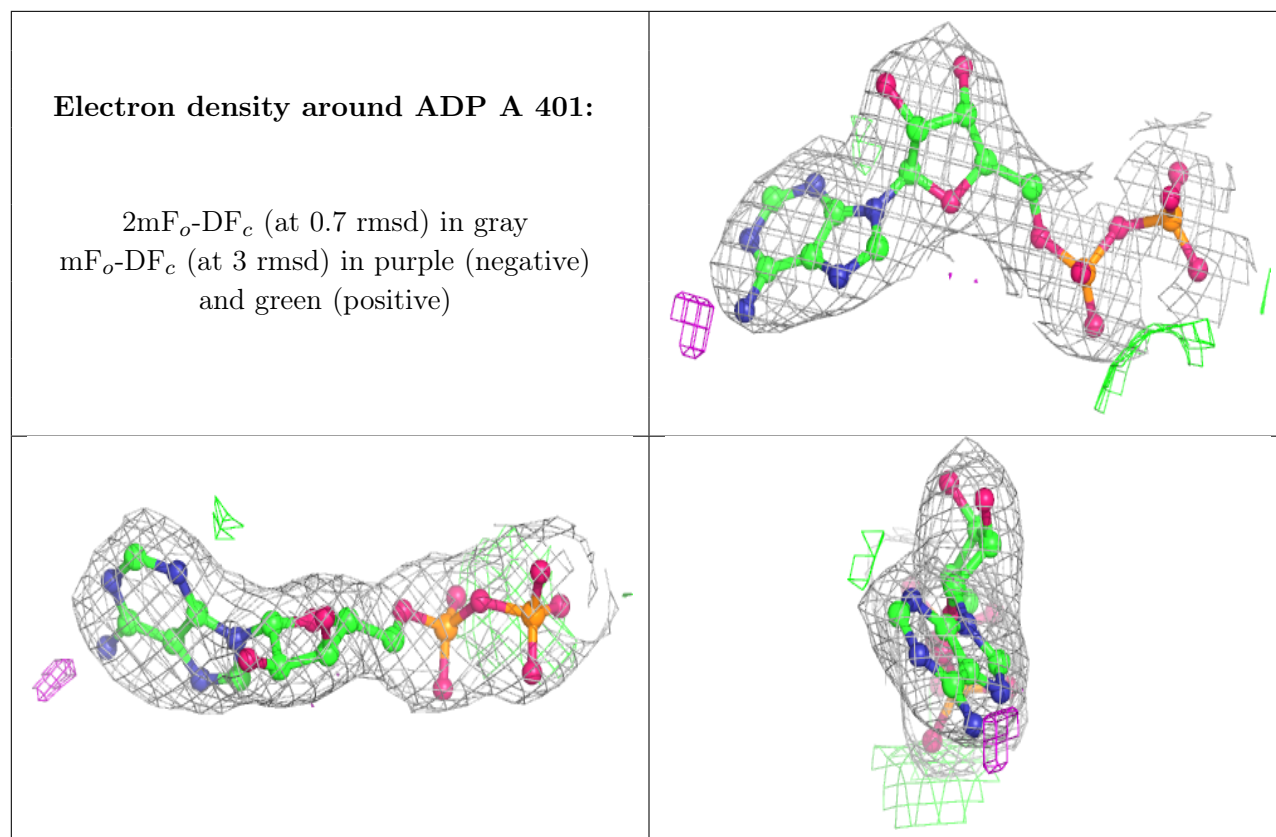
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.