



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2026 – 10:34 AM EDT

PDB ID : 9ZXA / pdb_00009zxa
Title : Crystal structure of the N42L2 polynucleotide kinase domain complexed with ADP and Mg.
Authors : Wang, H.; Stanley, R.E.
Deposited on : 2026-01-03
Resolution : 1.89 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

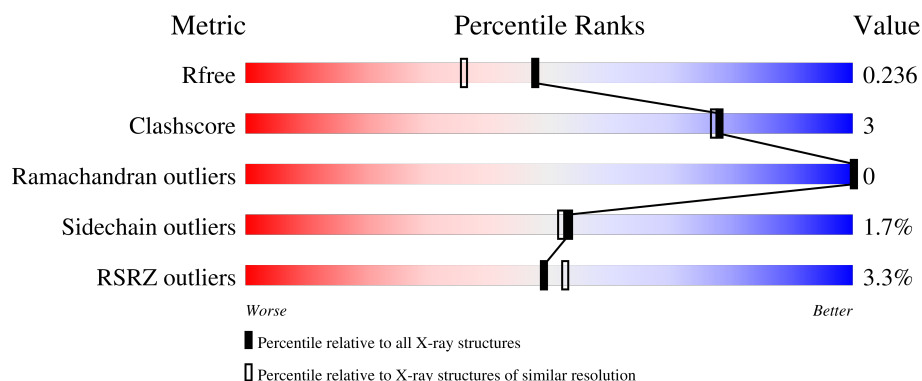
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	161	5% 80% 11% 10%
1	B	161	3% 80% 7% 13%
1	C	161	% 82% • 14%
1	D	161	2% 80% 8% 12%
1	E	161	2% 81% 8% 11%

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Mol	Chain	Length	Quality of chain
1	F	161	4% 81% 6% 12%
1	G	161	2% 82% • 14%
1	H	161	3% 83% 5% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19670 atoms, of which 9256 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 NEDD4-binding protein 2-like 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	145	Total	C	H	N	O	S	0	0	0
			2367	757	1170	216	220	4			
1	B	140	Total	C	H	N	O	S	0	0	0
			2284	727	1134	208	211	4			
1	C	139	Total	C	H	N	O	S	0	2	0
			2271	723	1124	207	213	4			
1	D	141	Total	C	H	N	O	S	0	2	0
			2309	734	1145	211	215	4			
1	E	143	Total	C	H	N	O	S	0	0	0
			2326	740	1153	213	216	4			
1	F	142	Total	C	H	N	O	S	0	0	0
			2324	741	1152	213	214	4			
1	G	139	Total	C	H	N	O	S	0	2	0
			2290	728	1138	210	210	4			
1	H	141	Total	C	H	N	O	S	0	2	0
			2308	734	1144	211	215	4			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	GLY	-	expression tag	UNP Q92802
A	390	SER	-	expression tag	UNP Q92802
A	391	HIS	-	expression tag	UNP Q92802
A	392	MET	-	expression tag	UNP Q92802
A	393	ASP	-	expression tag	UNP Q92802
A	394	TYR	-	expression tag	UNP Q92802
A	395	LYS	-	expression tag	UNP Q92802
A	396	ASP	-	expression tag	UNP Q92802
A	397	ASP	-	expression tag	UNP Q92802
A	398	ASP	-	expression tag	UNP Q92802
A	399	ASP	-	expression tag	UNP Q92802
A	400	LYS	-	expression tag	UNP Q92802
B	389	GLY	-	expression tag	UNP Q92802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	390	SER	-	expression tag	UNP Q92802
B	391	HIS	-	expression tag	UNP Q92802
B	392	MET	-	expression tag	UNP Q92802
B	393	ASP	-	expression tag	UNP Q92802
B	394	TYR	-	expression tag	UNP Q92802
B	395	LYS	-	expression tag	UNP Q92802
B	396	ASP	-	expression tag	UNP Q92802
B	397	ASP	-	expression tag	UNP Q92802
B	398	ASP	-	expression tag	UNP Q92802
B	399	ASP	-	expression tag	UNP Q92802
B	400	LYS	-	expression tag	UNP Q92802
C	389	GLY	-	expression tag	UNP Q92802
C	390	SER	-	expression tag	UNP Q92802
C	391	HIS	-	expression tag	UNP Q92802
C	392	MET	-	expression tag	UNP Q92802
C	393	ASP	-	expression tag	UNP Q92802
C	394	TYR	-	expression tag	UNP Q92802
C	395	LYS	-	expression tag	UNP Q92802
C	396	ASP	-	expression tag	UNP Q92802
C	397	ASP	-	expression tag	UNP Q92802
C	398	ASP	-	expression tag	UNP Q92802
C	399	ASP	-	expression tag	UNP Q92802
C	400	LYS	-	expression tag	UNP Q92802
D	389	GLY	-	expression tag	UNP Q92802
D	390	SER	-	expression tag	UNP Q92802
D	391	HIS	-	expression tag	UNP Q92802
D	392	MET	-	expression tag	UNP Q92802
D	393	ASP	-	expression tag	UNP Q92802
D	394	TYR	-	expression tag	UNP Q92802
D	395	LYS	-	expression tag	UNP Q92802
D	396	ASP	-	expression tag	UNP Q92802
D	397	ASP	-	expression tag	UNP Q92802
D	398	ASP	-	expression tag	UNP Q92802
D	399	ASP	-	expression tag	UNP Q92802
D	400	LYS	-	expression tag	UNP Q92802
E	389	GLY	-	expression tag	UNP Q92802
E	390	SER	-	expression tag	UNP Q92802
E	391	HIS	-	expression tag	UNP Q92802
E	392	MET	-	expression tag	UNP Q92802
E	393	ASP	-	expression tag	UNP Q92802
E	394	TYR	-	expression tag	UNP Q92802
E	395	LYS	-	expression tag	UNP Q92802

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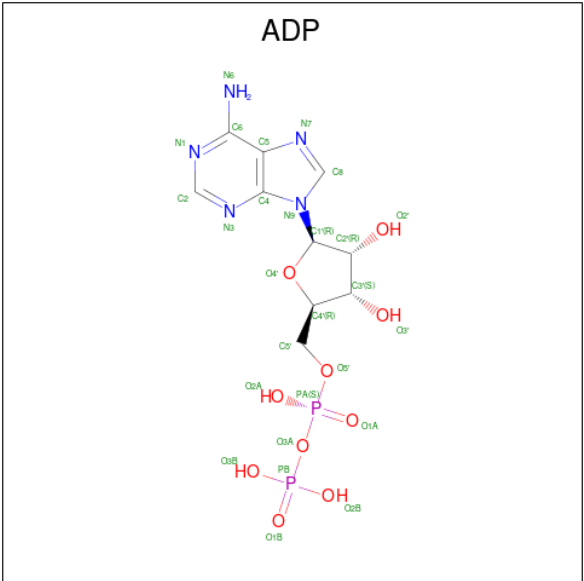
Chain	Residue	Modelled	Actual	Comment	Reference
E	396	ASP	-	expression tag	UNP Q92802
E	397	ASP	-	expression tag	UNP Q92802
E	398	ASP	-	expression tag	UNP Q92802
E	399	ASP	-	expression tag	UNP Q92802
E	400	LYS	-	expression tag	UNP Q92802
F	389	GLY	-	expression tag	UNP Q92802
F	390	SER	-	expression tag	UNP Q92802
F	391	HIS	-	expression tag	UNP Q92802
F	392	MET	-	expression tag	UNP Q92802
F	393	ASP	-	expression tag	UNP Q92802
F	394	TYR	-	expression tag	UNP Q92802
F	395	LYS	-	expression tag	UNP Q92802
F	396	ASP	-	expression tag	UNP Q92802
F	397	ASP	-	expression tag	UNP Q92802
F	398	ASP	-	expression tag	UNP Q92802
F	399	ASP	-	expression tag	UNP Q92802
F	400	LYS	-	expression tag	UNP Q92802
G	389	GLY	-	expression tag	UNP Q92802
G	390	SER	-	expression tag	UNP Q92802
G	391	HIS	-	expression tag	UNP Q92802
G	392	MET	-	expression tag	UNP Q92802
G	393	ASP	-	expression tag	UNP Q92802
G	394	TYR	-	expression tag	UNP Q92802
G	395	LYS	-	expression tag	UNP Q92802
G	396	ASP	-	expression tag	UNP Q92802
G	397	ASP	-	expression tag	UNP Q92802
G	398	ASP	-	expression tag	UNP Q92802
G	399	ASP	-	expression tag	UNP Q92802
G	400	LYS	-	expression tag	UNP Q92802
H	389	GLY	-	expression tag	UNP Q92802
H	390	SER	-	expression tag	UNP Q92802
H	391	HIS	-	expression tag	UNP Q92802
H	392	MET	-	expression tag	UNP Q92802
H	393	ASP	-	expression tag	UNP Q92802
H	394	TYR	-	expression tag	UNP Q92802
H	395	LYS	-	expression tag	UNP Q92802
H	396	ASP	-	expression tag	UNP Q92802
H	397	ASP	-	expression tag	UNP Q92802
H	398	ASP	-	expression tag	UNP Q92802
H	399	ASP	-	expression tag	UNP Q92802
H	400	LYS	-	expression tag	UNP Q92802

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		
2	G	1	Total	Mg	0	0
			1	1		
2	H	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	B	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	C	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	D	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	E	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	F	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	G	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0
3	H	1	Total 39	C 10	H 12	N 5	O 10	P 2	0	0

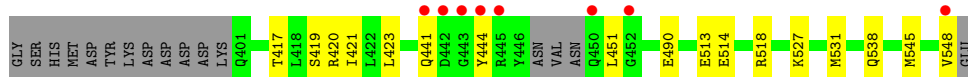
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total 107	O 107	0	0
4	B	111	Total 111	O 111	0	0
4	C	135	Total 135	O 135	0	0
4	D	102	Total 102	O 102	0	0
4	E	110	Total 110	O 110	0	0
4	F	93	Total 93	O 93	0	0
4	G	108	Total 108	O 108	0	0
4	H	105	Total 105	O 105	0	0

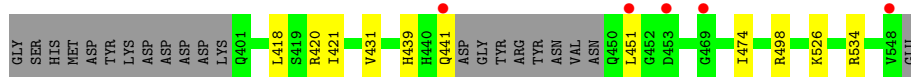
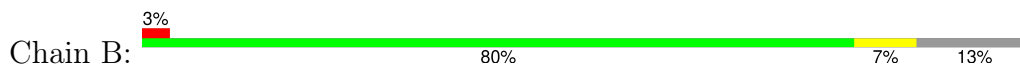
3 Residue-property plots [i](#)

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.

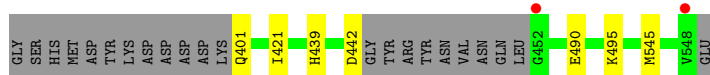
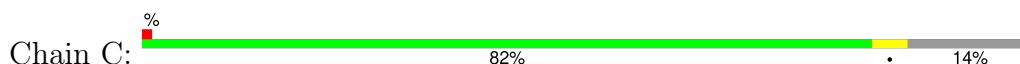
- Molecule 1: NEDD4-binding protein 2-like 2



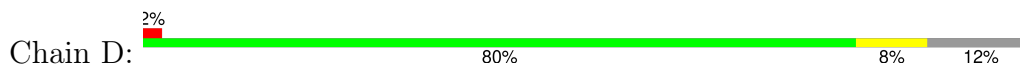
- Molecule 1: NEDD4-binding protein 2-like 2



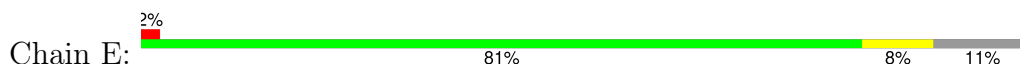
- Molecule 1: NEDD4-binding protein 2-like 2



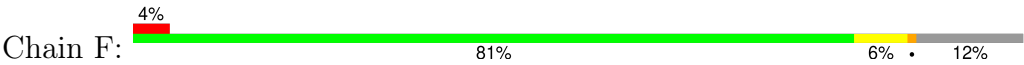
- Molecule 1: NEDD4-binding protein 2-like 2



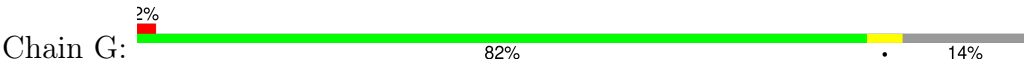
- Molecule 1: NEDD4-binding protein 2-like 2



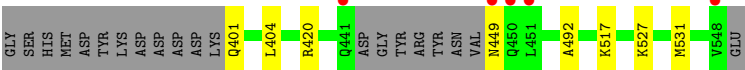
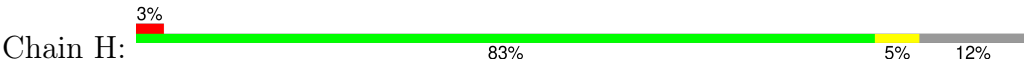
- Molecule 1: NEDD4-binding protein 2-like 2



• Molecule 1: NEDD4-binding protein 2-like 2



• Molecule 1: NEDD4-binding protein 2-like 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.58Å 115.02Å 90.03Å 90.00° 109.64° 90.00°	Depositor
Resolution (Å)	34.12 – 1.89 34.12 – 1.89	Depositor EDS
% Data completeness (in resolution range)	88.6 (34.12-1.89) 88.6 (34.12-1.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 1.89Å)	Xtriage
Refinement program	PHENIX ("2.0_5936": ???)	Depositor
R, R_{free}	0.197 , 0.237 0.197 , 0.236	Depositor DCC
R_{free} test set	4323 reflections (4.40%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19670	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7123e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, 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	0.30	0/1224	0.35	0/1649
1	B	0.30	0/1175	0.36	0/1583
1	C	0.35	0/1179	0.39	0/1589
1	D	0.32	0/1196	0.35	0/1612
1	E	0.31	0/1198	0.35	0/1615
1	F	0.27	0/1197	0.34	0/1611
1	G	0.30	0/1185	0.36	0/1596
1	H	0.29	0/1196	0.35	0/1612
All	All	0.31	0/9550	0.36	0/12867

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	1197	1170	1170	11	0
1	B	1150	1134	1132	7	0
1	C	1147	1124	1115	6	0
1	D	1164	1145	1136	8	0
1	E	1173	1153	1153	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1172	1152	1151	10	0
1	G	1152	1138	1133	5	0
1	H	1164	1144	1136	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	12	12	0	0
3	B	27	12	12	0	0
3	C	27	12	12	0	0
3	D	27	12	12	0	0
3	E	27	12	12	0	0
3	F	27	12	12	0	0
3	G	27	12	12	0	0
3	H	27	12	12	0	0
4	A	107	0	0	2	0
4	B	111	0	0	1	0
4	C	135	0	0	1	0
4	D	102	0	0	0	0
4	E	110	0	0	0	0
4	F	93	0	0	0	0
4	G	108	0	0	0	0
4	H	105	0	0	5	0
All	All	10414	9256	9222	52	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.

The worst 5 of 52 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:GLN:HE21	1:A:451:LEU:HD12	1.52	0.72
1:C:401:GLN:N	4:C:2101:HOH:O	2.22	0.71
1:H:449:ASN:N	4:H:2101:HOH:O	2.25	0.68
1:B:421:ILE:HD11	1:C:421:ILE:CD1	2.24	0.68
1:H:401:GLN:N	4:H:2102:HOH:O	2.26	0.67

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	141/161 (88%)	140 (99%)	1 (1%)	0	100	100
1	B	136/161 (84%)	134 (98%)	2 (2%)	0	100	100
1	C	137/161 (85%)	136 (99%)	1 (1%)	0	100	100
1	D	139/161 (86%)	138 (99%)	1 (1%)	0	100	100
1	E	139/161 (86%)	138 (99%)	1 (1%)	0	100	100
1	F	136/161 (84%)	132 (97%)	4 (3%)	0	100	100
1	G	137/161 (85%)	135 (98%)	2 (2%)	0	100	100
1	H	139/161 (86%)	138 (99%)	1 (1%)	0	100	100
All	All	1104/1288 (86%)	1091 (99%)	13 (1%)	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	128/143 (90%)	125 (98%)	3 (2%)	44	40
1	B	124/143 (87%)	120 (97%)	4 (3%)	34	27
1	C	125/143 (87%)	124 (99%)	1 (1%)	73	75
1	D	127/143 (89%)	125 (98%)	2 (2%)	55	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	127/143 (89%)	125 (98%)	2 (2%)	55	54
1	F	126/143 (88%)	122 (97%)	4 (3%)	34	27
1	G	125/143 (87%)	124 (99%)	1 (1%)	73	75
1	H	127/143 (89%)	127 (100%)	0	100	100
All	All	1009/1144 (88%)	992 (98%)	17 (2%)	53	52

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	446	TYR
1	G	468	GLN
1	C	495	LYS
1	D	423	LEU
1	D	426	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	401	GLN
1	G	468	GLN
1	H	459	GLN
1	H	401	GLN
1	E	441	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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	C	2002	2	28,29,29	1.50	5 (17%)	43,45,45	1.81	9 (20%)
3	ADP	E	2002	2	28,29,29	1.48	6 (21%)	43,45,45	1.80	10 (23%)
3	ADP	G	2002	2	28,29,29	1.44	5 (17%)	43,45,45	1.87	10 (23%)
3	ADP	A	2002	2	28,29,29	1.49	5 (17%)	43,45,45	1.78	10 (23%)
3	ADP	H	2002	2	28,29,29	1.59	5 (17%)	43,45,45	1.82	11 (25%)
3	ADP	D	2002	2	28,29,29	1.56	4 (14%)	43,45,45	1.77	10 (23%)
3	ADP	F	2002	2	28,29,29	1.36	4 (14%)	43,45,45	1.80	10 (23%)
3	ADP	B	2002	2	28,29,29	1.33	4 (14%)	43,45,45	1.82	9 (20%)

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	C	2002	2	-	1/16/32/32	0/3/3/3
3	ADP	E	2002	2	-	2/16/32/32	0/3/3/3
3	ADP	G	2002	2	-	2/16/32/32	0/3/3/3
3	ADP	A	2002	2	-	2/16/32/32	0/3/3/3
3	ADP	H	2002	2	-	2/16/32/32	0/3/3/3
3	ADP	D	2002	2	-	2/16/32/32	0/3/3/3
3	ADP	F	2002	2	-	1/16/32/32	0/3/3/3
3	ADP	B	2002	2	-	1/16/32/32	0/3/3/3

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2002	ADP	C5-C4	5.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2002	ADP	C5-C4	4.79	1.47	1.39
3	H	2002	ADP	C5-C4	4.40	1.46	1.39
3	F	2002	ADP	C5-C4	4.16	1.46	1.39
3	E	2002	ADP	C5-C4	4.15	1.46	1.39

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2002	ADP	C5-C4-N3	-5.53	119.10	126.72
3	C	2002	ADP	C5-C4-N3	-5.36	119.34	126.72
3	H	2002	ADP	C5-C4-N3	-5.15	119.62	126.72
3	E	2002	ADP	C5-C4-N3	-5.13	119.66	126.72
3	D	2002	ADP	C5-C4-N3	-5.07	119.73	126.72

There are no chirality outliers.

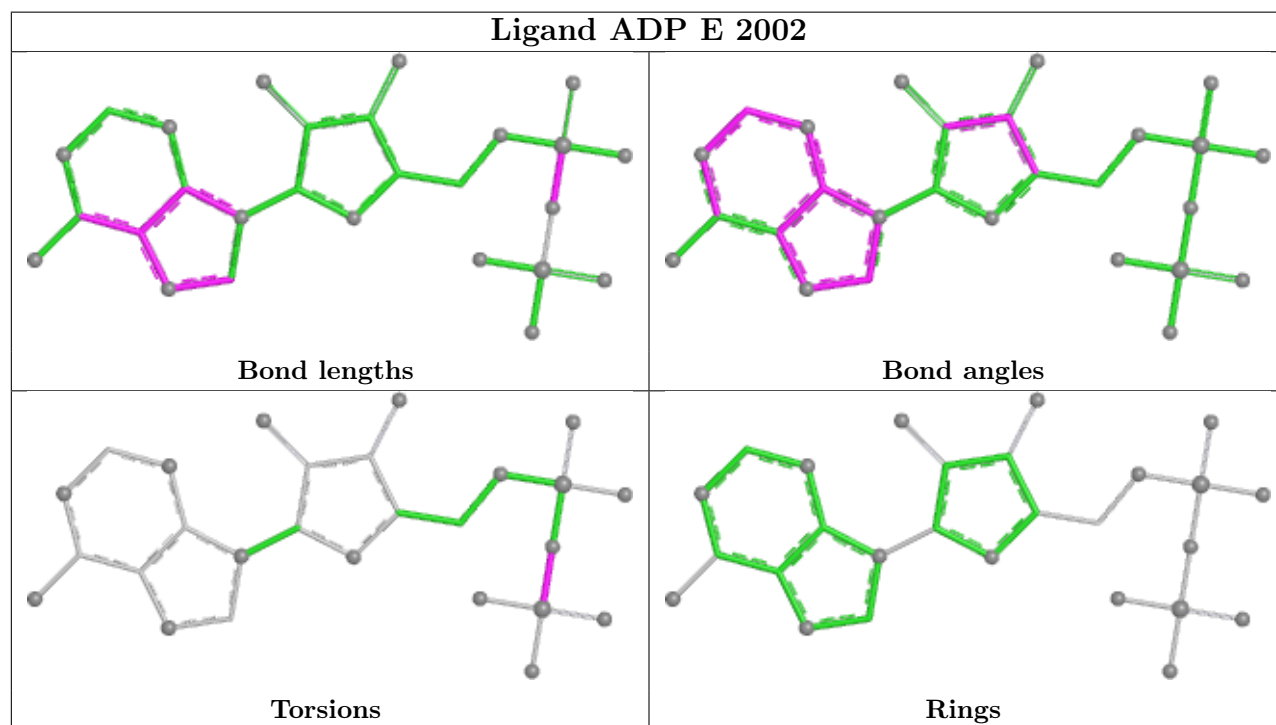
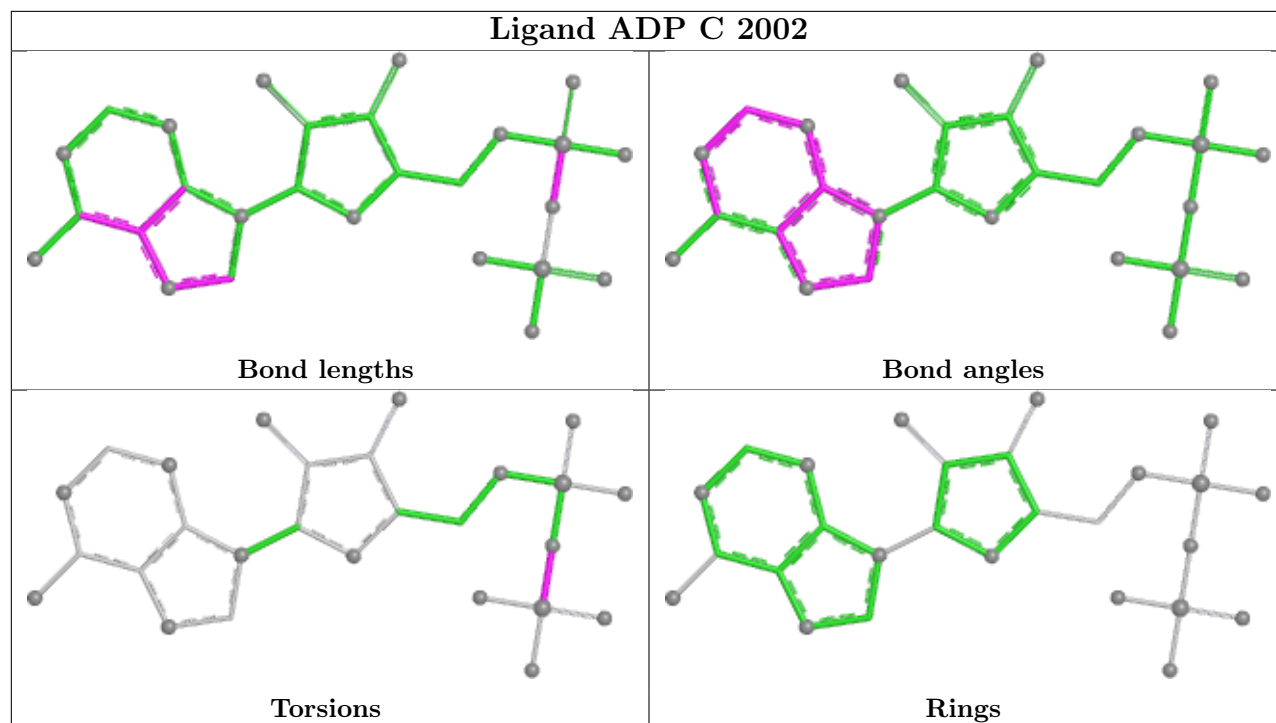
5 of 13 torsion outliers are listed below:

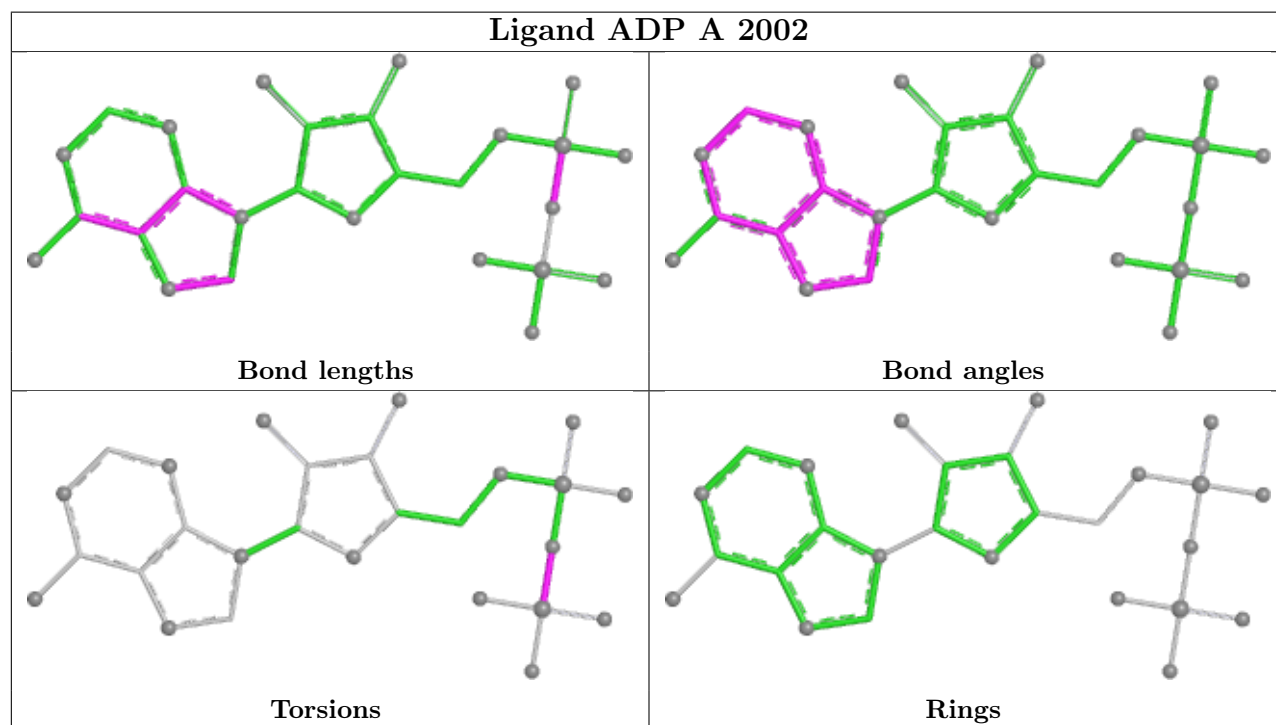
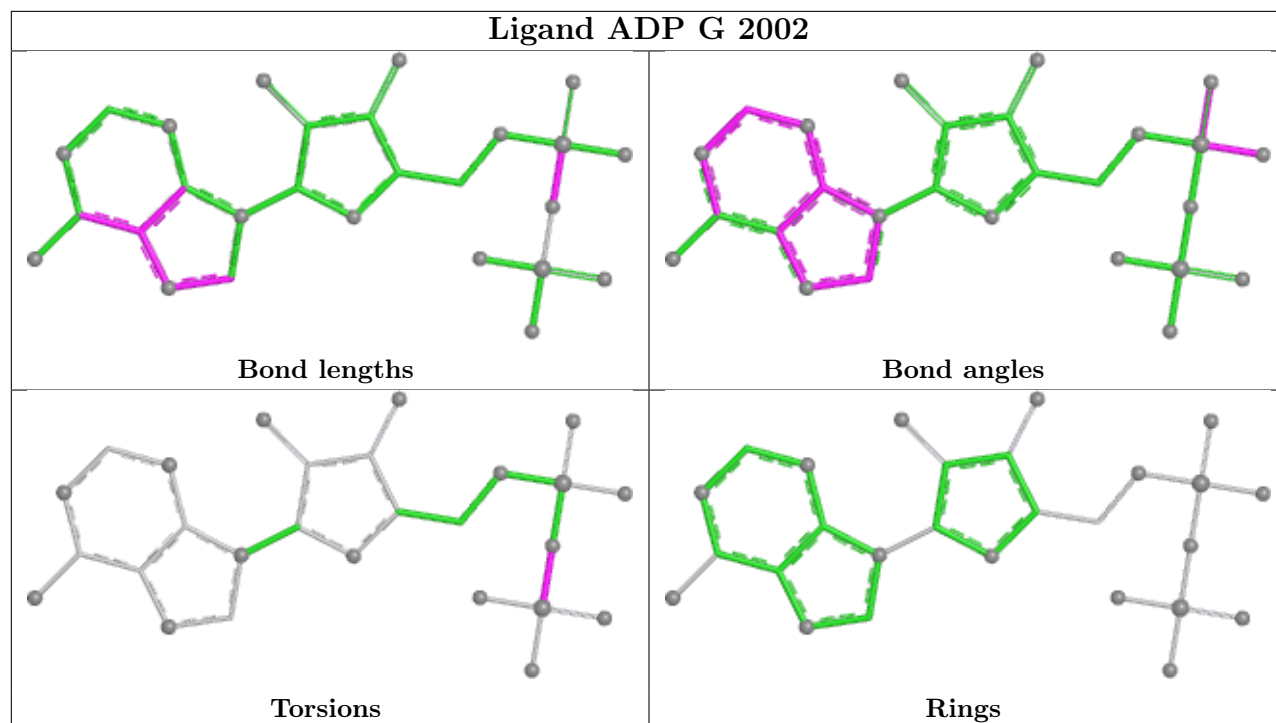
Mol	Chain	Res	Type	Atoms
3	A	2002	ADP	PA-O3A-PB-O2B
3	D	2002	ADP	PA-O3A-PB-O2B
3	B	2002	ADP	PA-O3A-PB-O1B
3	C	2002	ADP	PA-O3A-PB-O1B
3	E	2002	ADP	PA-O3A-PB-O1B

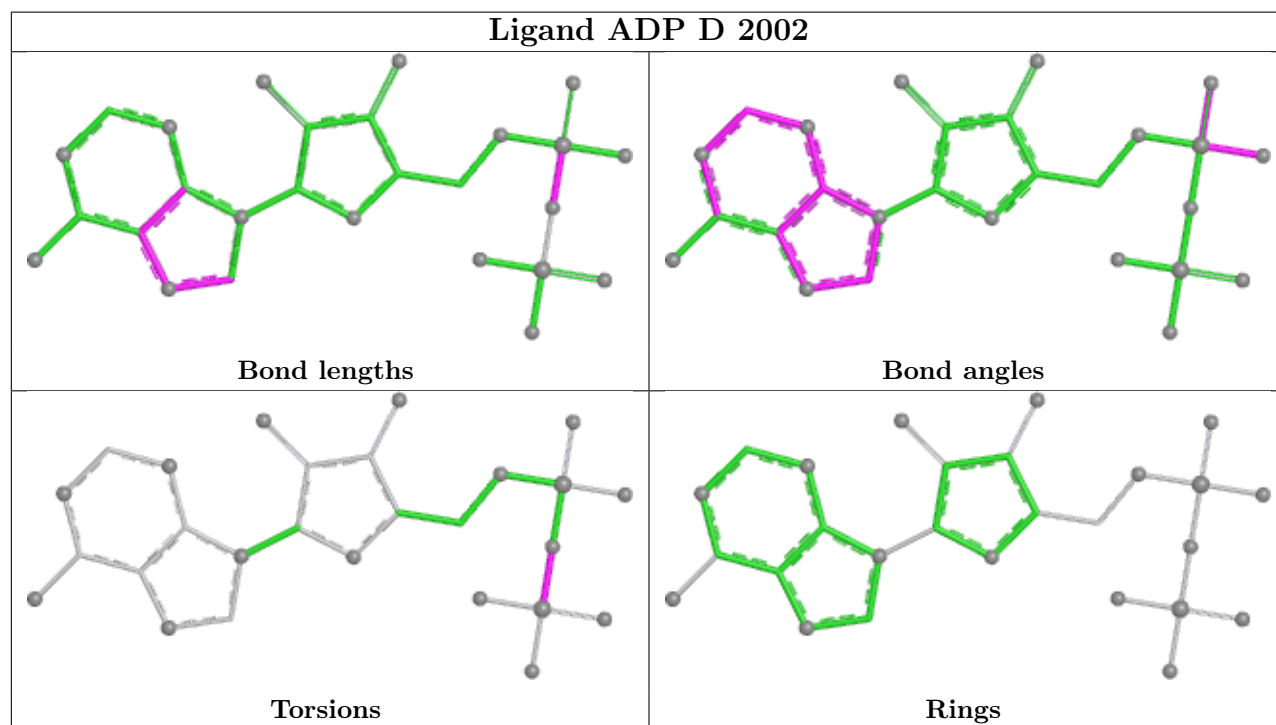
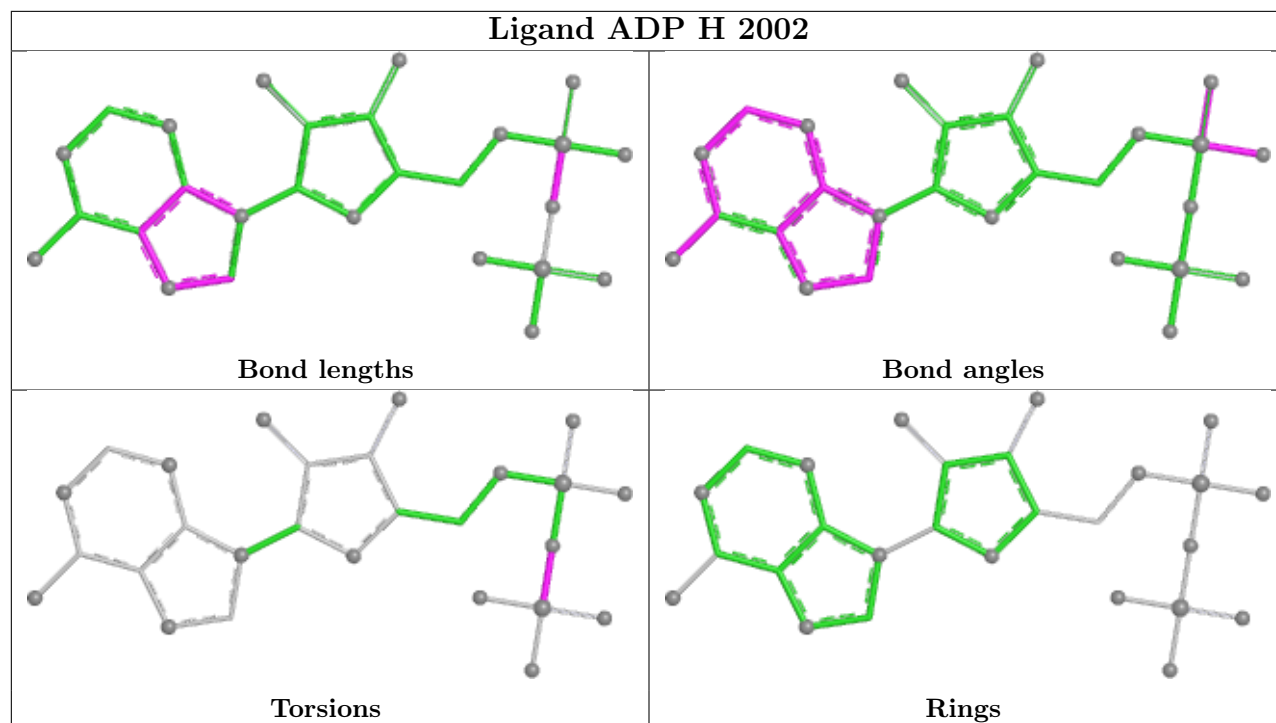
There are no ring outliers.

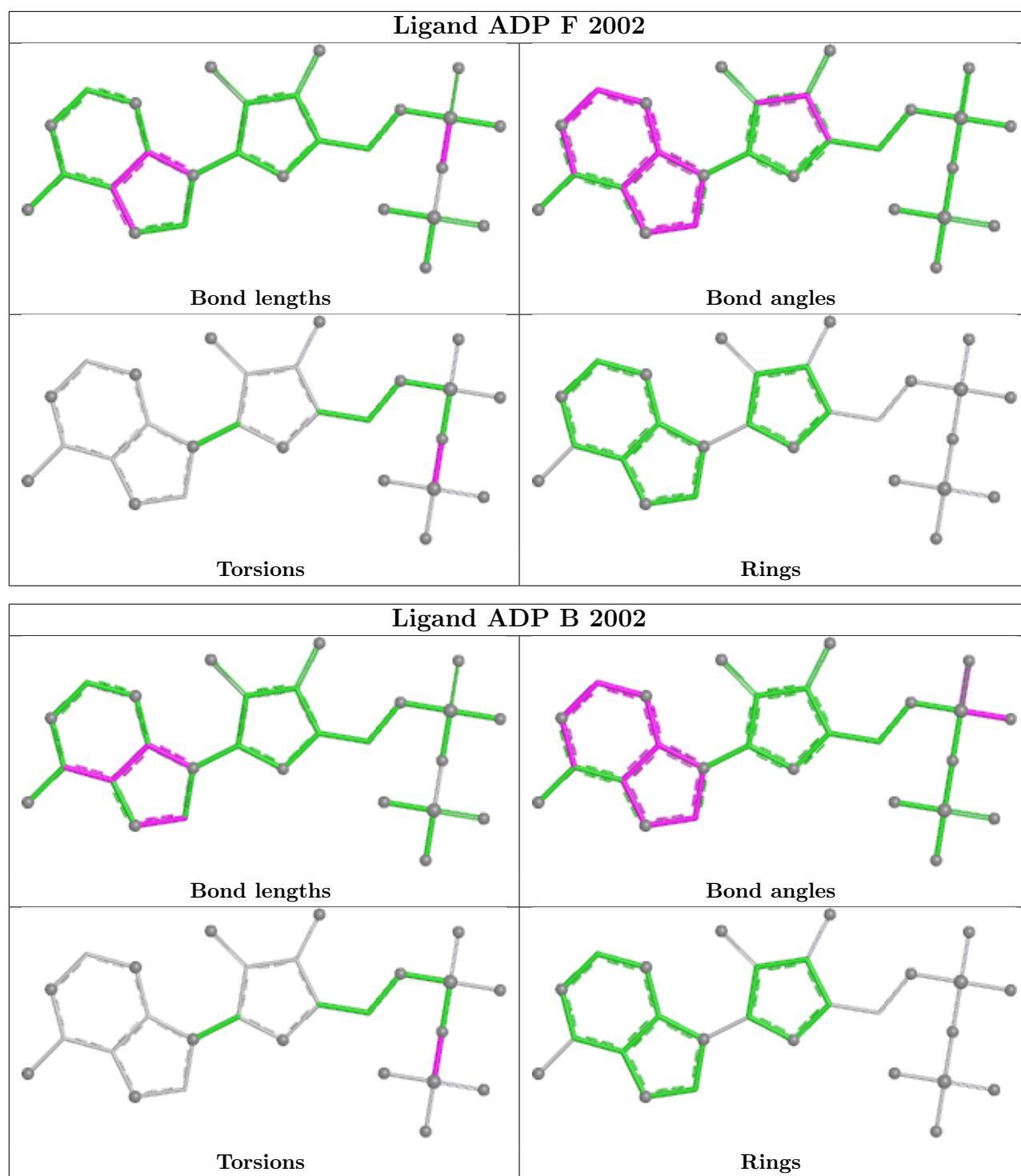
No monomer is involved in short contacts.

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, 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	145/161 (90%)	0.01	8 (5%) 30 32	16, 27, 70, 87	0
1	B	140/161 (86%)	0.10	5 (3%) 46 49	16, 30, 53, 89	0
1	C	139/161 (86%)	-0.24	2 (1%) 73 76	10, 23, 42, 56	1 (0%)
1	D	141/161 (87%)	0.02	4 (2%) 55 59	12, 29, 51, 89	1 (0%)
1	E	143/161 (88%)	-0.11	3 (2%) 63 67	17, 26, 45, 81	0
1	F	142/161 (88%)	0.12	6 (4%) 40 43	18, 32, 60, 90	0
1	G	139/161 (86%)	0.00	4 (2%) 53 57	17, 27, 49, 89	1 (0%)
1	H	141/161 (87%)	0.18	5 (3%) 47 50	12, 32, 53, 84	1 (0%)
All	All	1130/1288 (87%)	0.01	37 (3%) 49 52	10, 28, 53, 90	4 (0%)

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	452	GLY	6.0
1	E	548	VAL	5.5
1	H	548	VAL	5.1
1	A	442	ASP	4.8
1	D	548	VAL	4.7

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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

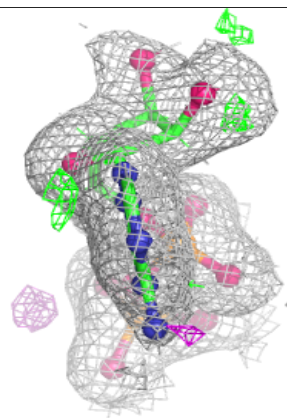
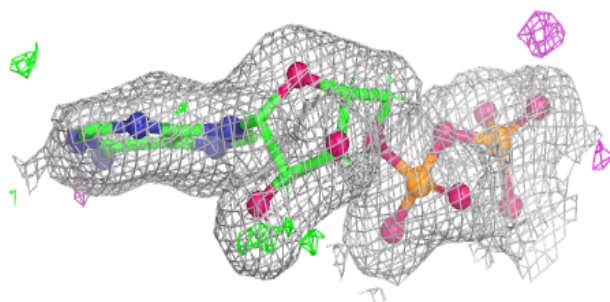
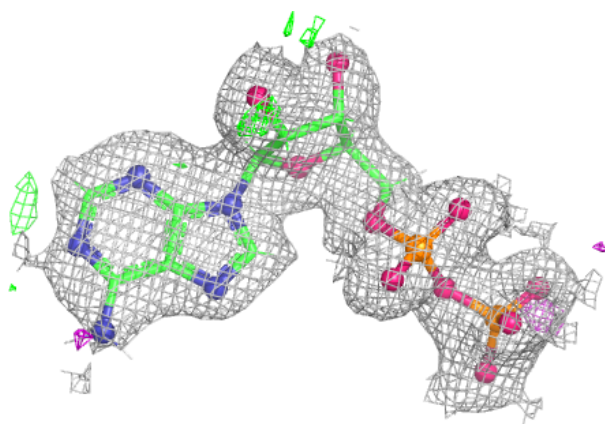
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	C	2002	27/27	0.97	0.07	13,25,38,39	0
3	ADP	D	2002	27/27	0.97	0.06	13,21,36,36	0
3	ADP	E	2002	27/27	0.97	0.08	14,27,42,45	0
3	ADP	G	2002	27/27	0.97	0.06	14,24,40,41	0
3	ADP	A	2002	27/27	0.98	0.06	13,26,41,41	0
3	ADP	B	2002	27/27	0.98	0.05	13,23,32,34	0
2	MG	B	2001	1/1	0.98	0.03	16,16,16,16	0
2	MG	D	2001	1/1	0.98	0.02	17,17,17,17	0
2	MG	F	2001	1/1	0.98	0.03	19,19,19,19	0
3	ADP	F	2002	27/27	0.98	0.06	13,25,34,41	0
2	MG	G	2001	1/1	0.98	0.02	19,19,19,19	0
3	ADP	H	2002	27/27	0.98	0.06	13,24,35,42	0
2	MG	E	2001	1/1	0.99	0.03	20,20,20,20	0
2	MG	C	2001	1/1	0.99	0.02	16,16,16,16	0
2	MG	A	2001	1/1	0.99	0.04	16,16,16,16	0
2	MG	H	2001	1/1	0.99	0.02	20,20,20,20	0

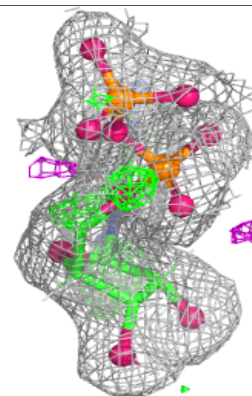
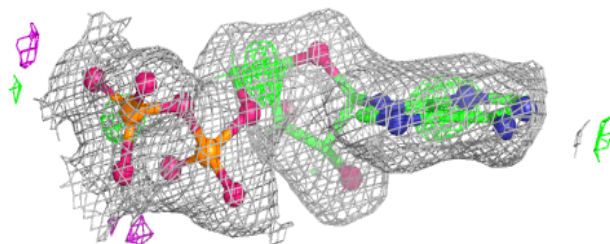
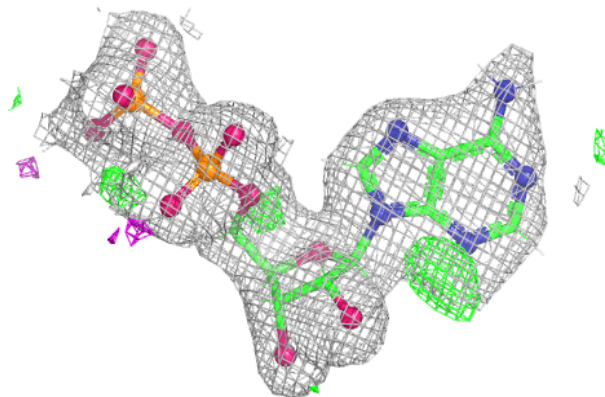
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP C 2002:

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

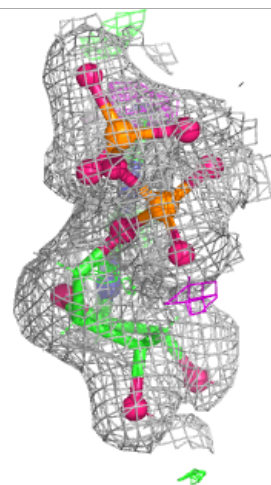
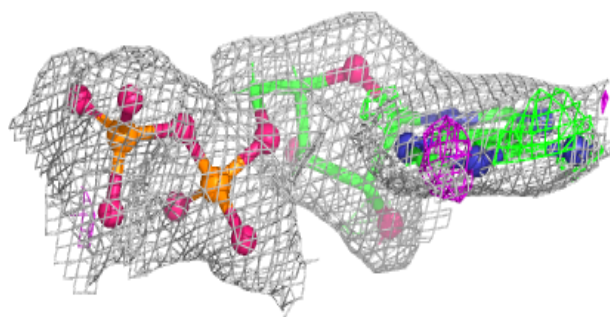
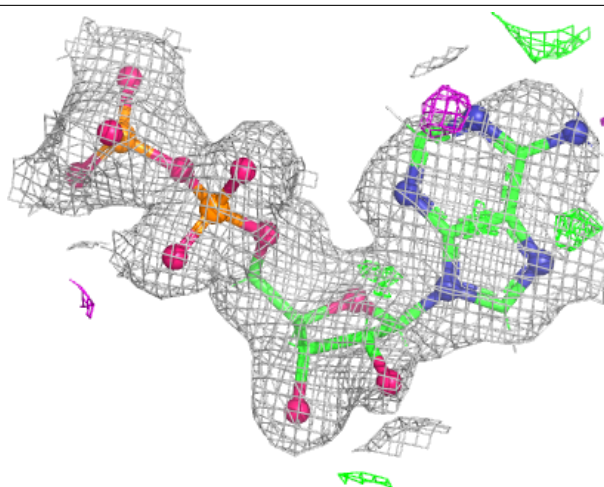
**Electron density around ADP D 2002:**

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



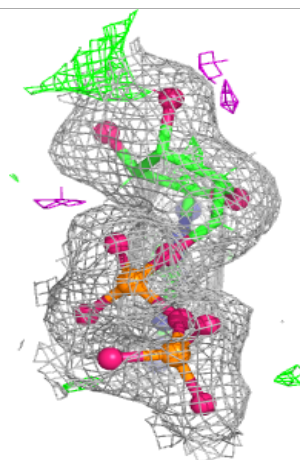
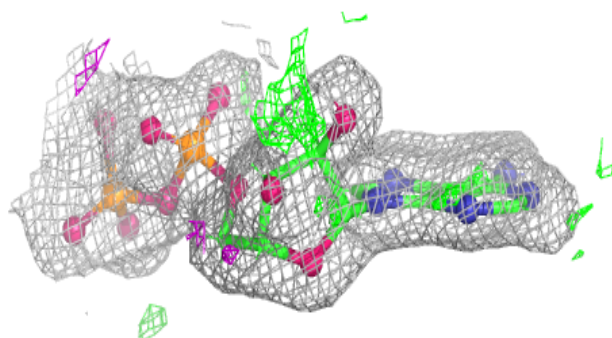
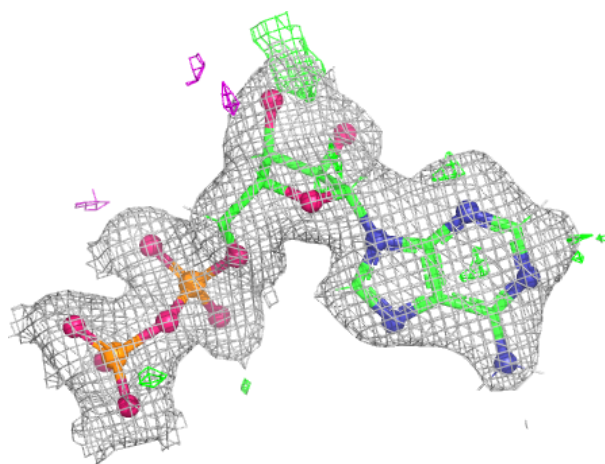
Electron density around ADP E 2002:

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and green (positive)



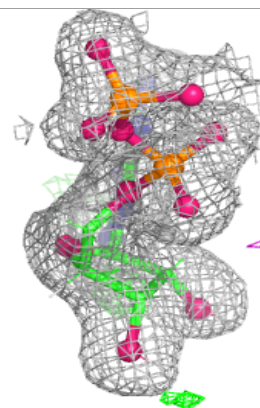
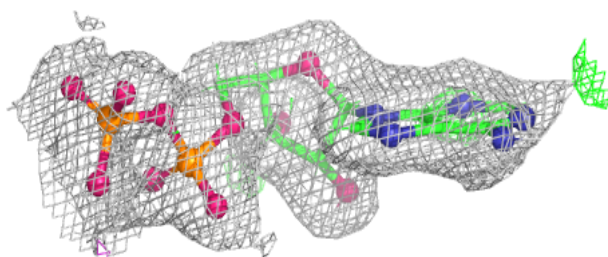
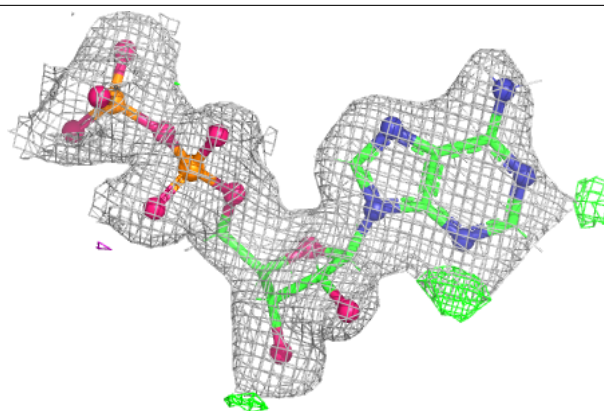
Electron density around ADP G 2002:

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and green (positive)

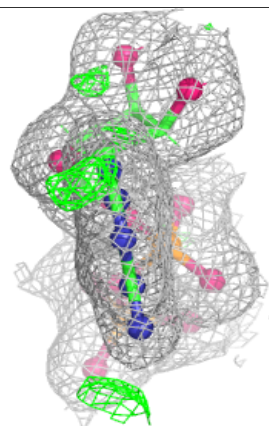
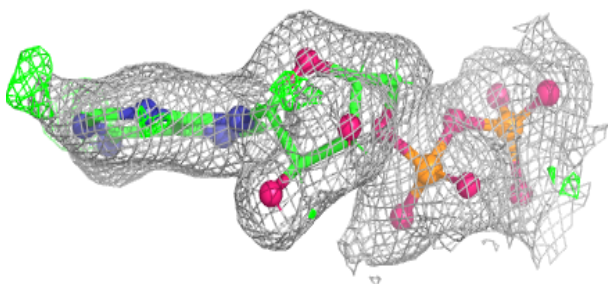
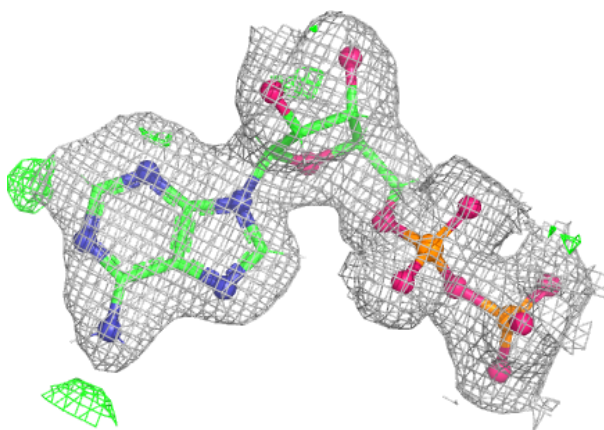


Electron density around ADP A 2002:

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and green (positive)

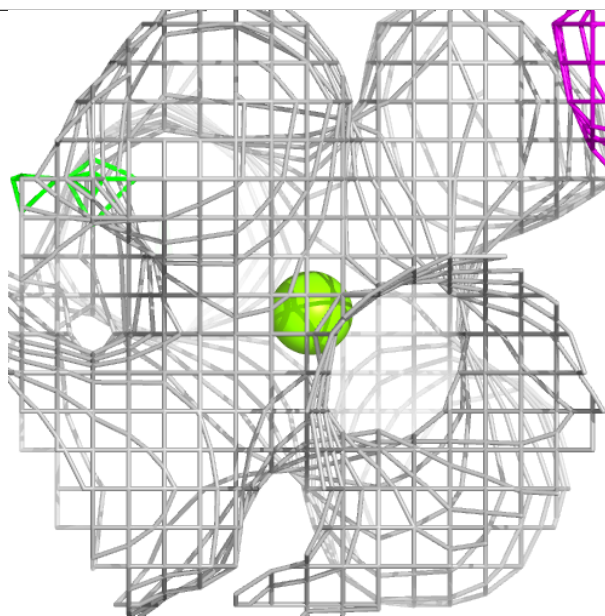
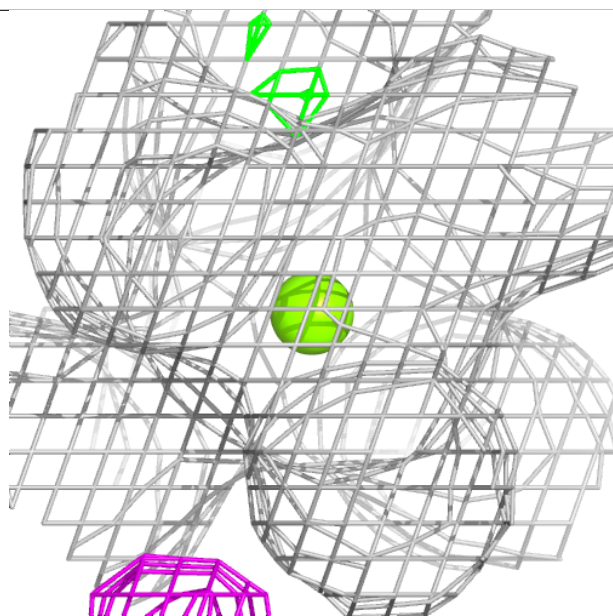
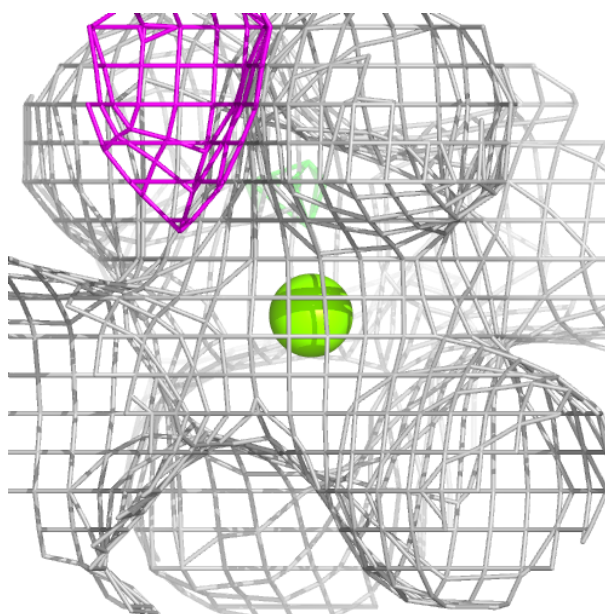
**Electron density around ADP B 2002:**

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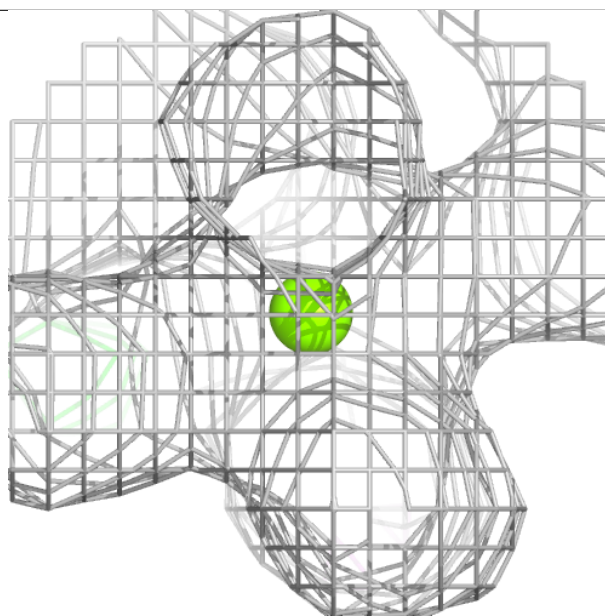
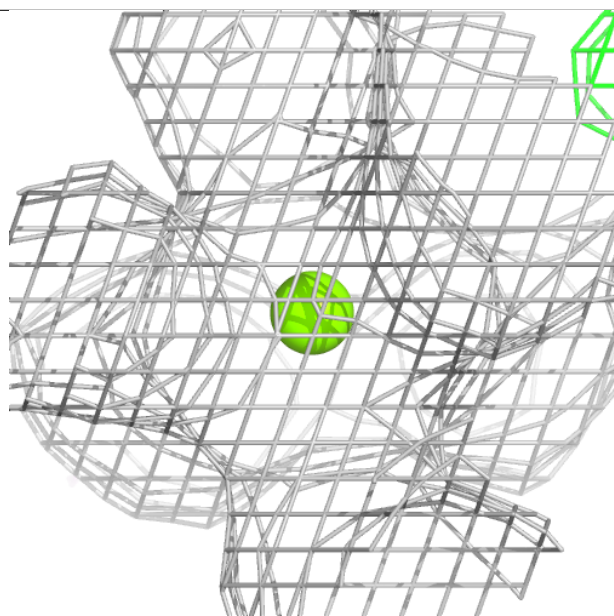
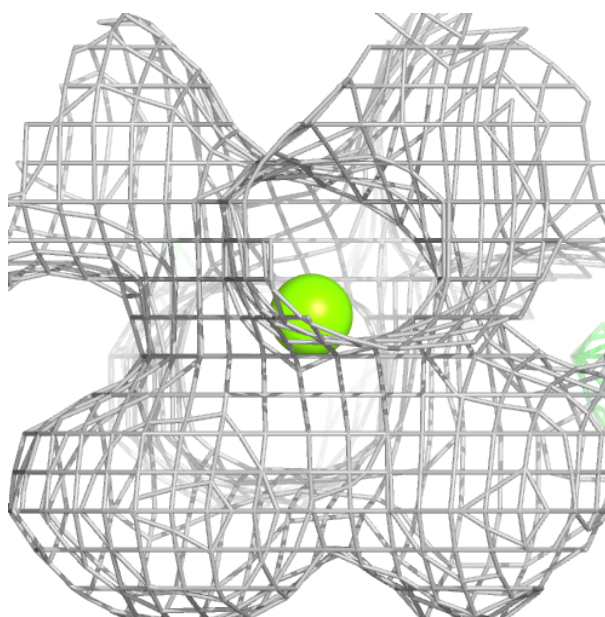
Electron density around MG B 2001:

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and green (positive)



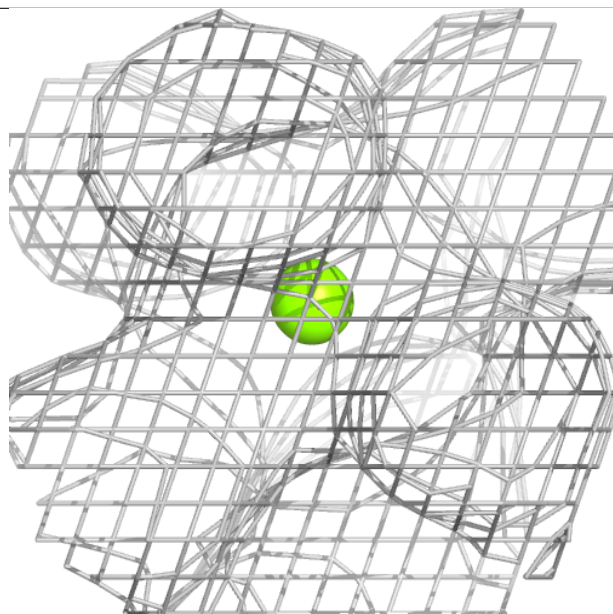
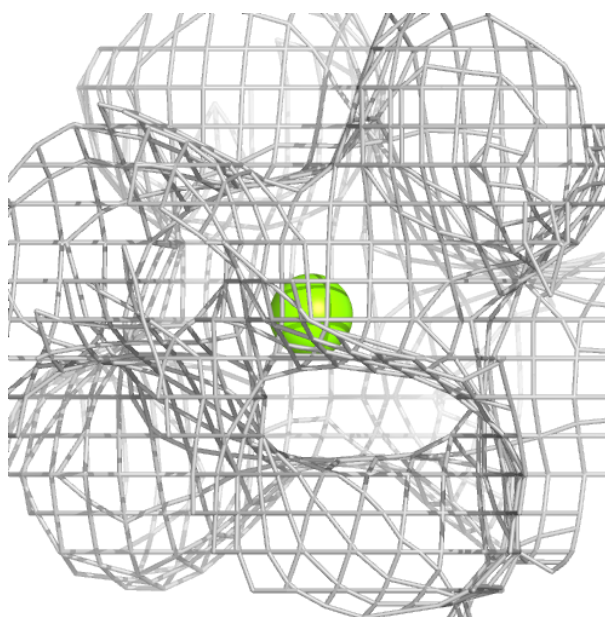
Electron density around MG D 2001:

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and green (positive)



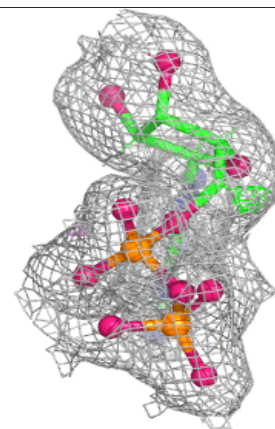
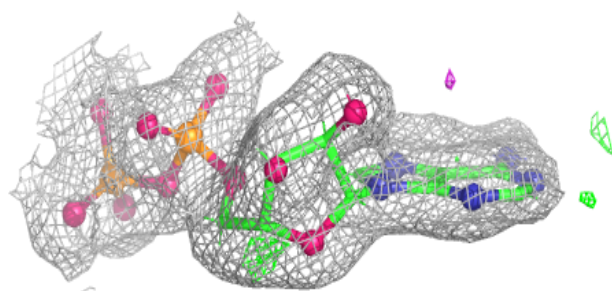
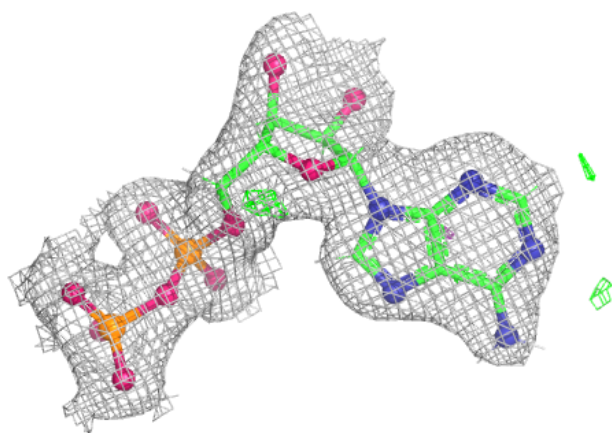
Electron density around MG F 2001:

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and green (positive)



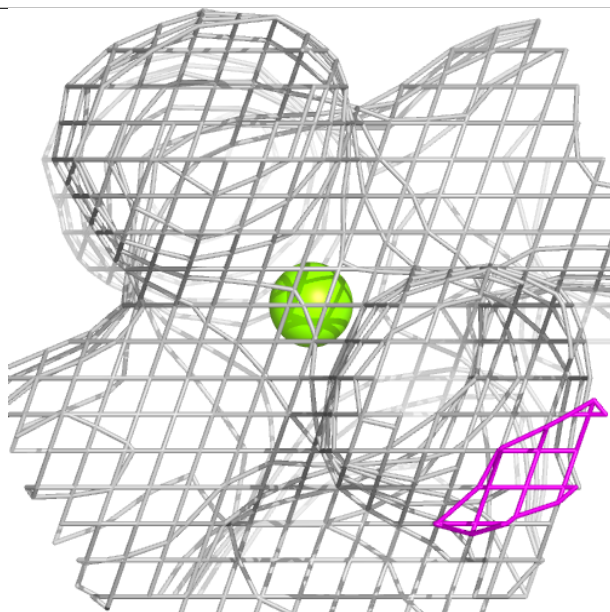
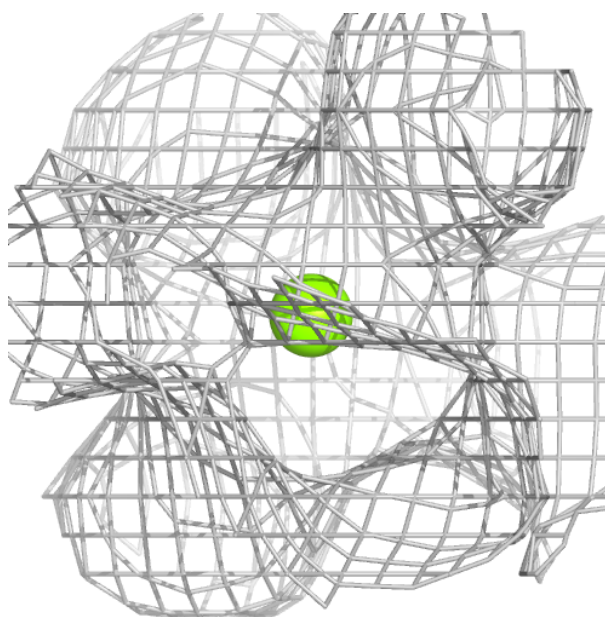
Electron density around ADP F 2002:

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



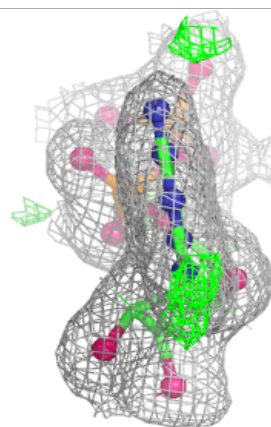
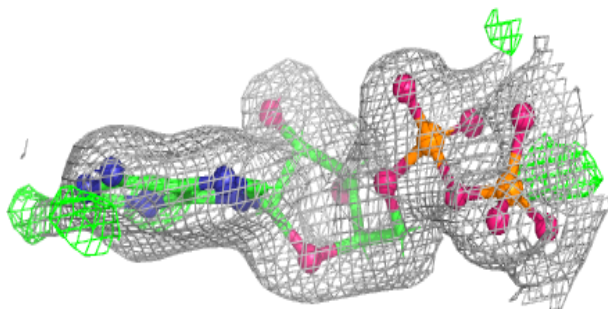
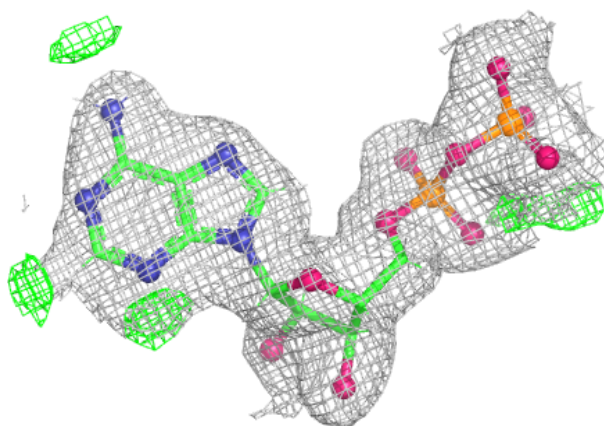
Electron density around MG G 2001:

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and green (positive)



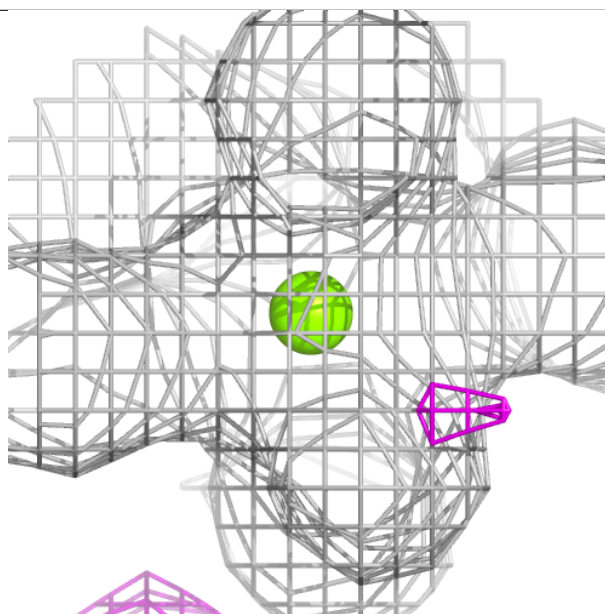
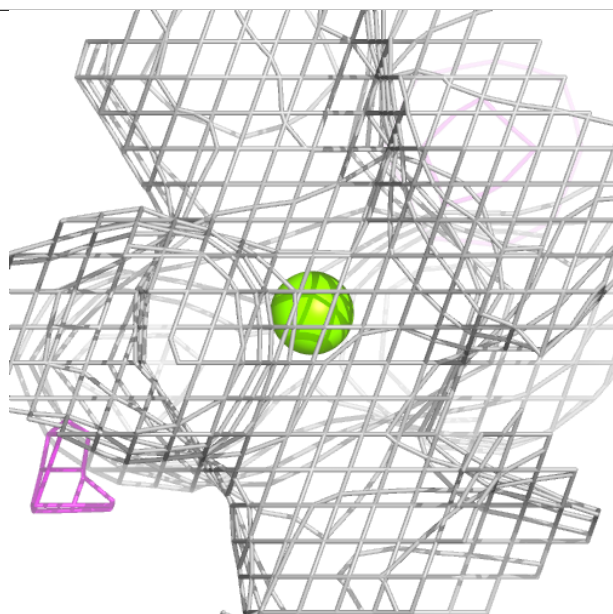
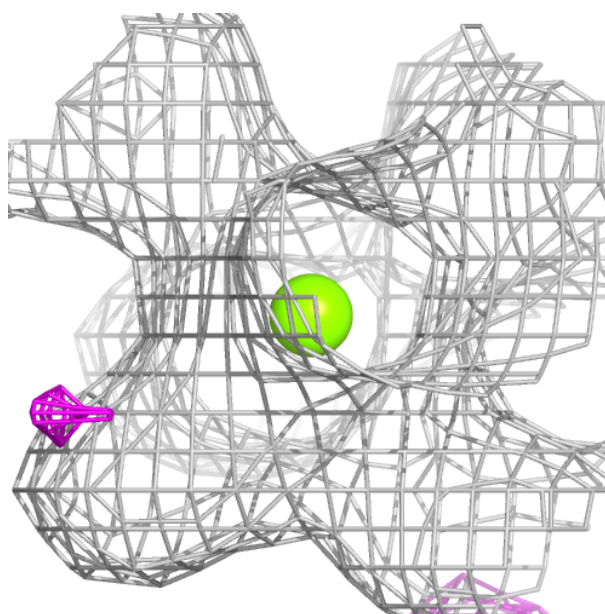
Electron density around ADP H 2002:

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



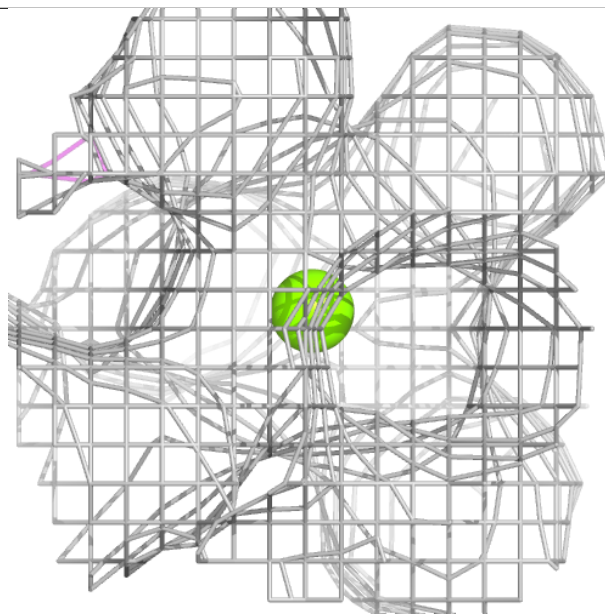
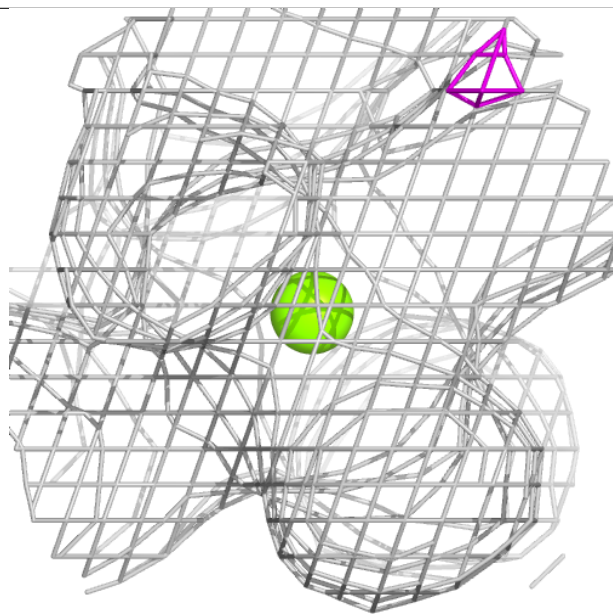
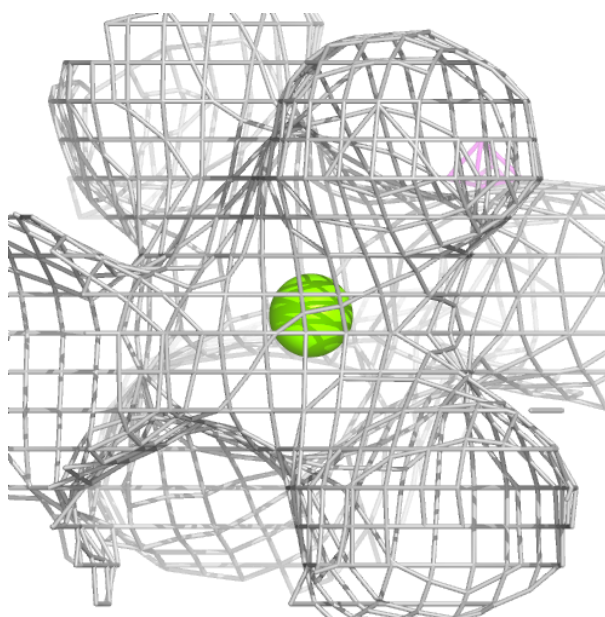
Electron density around MG E 2001:

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



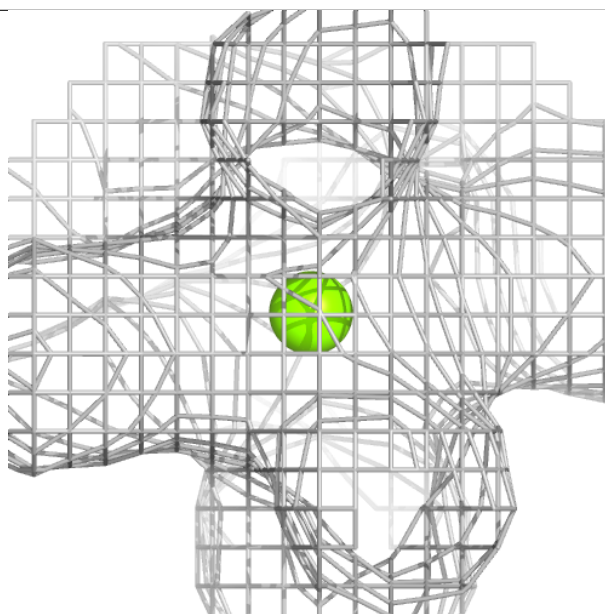
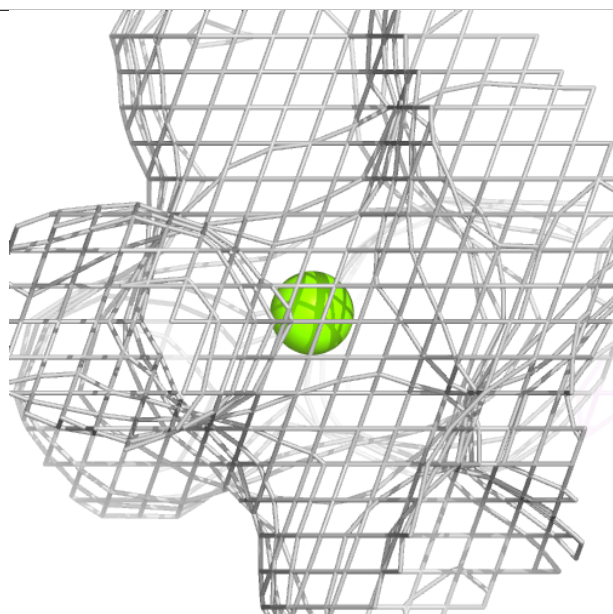
Electron density around MG C 2001:

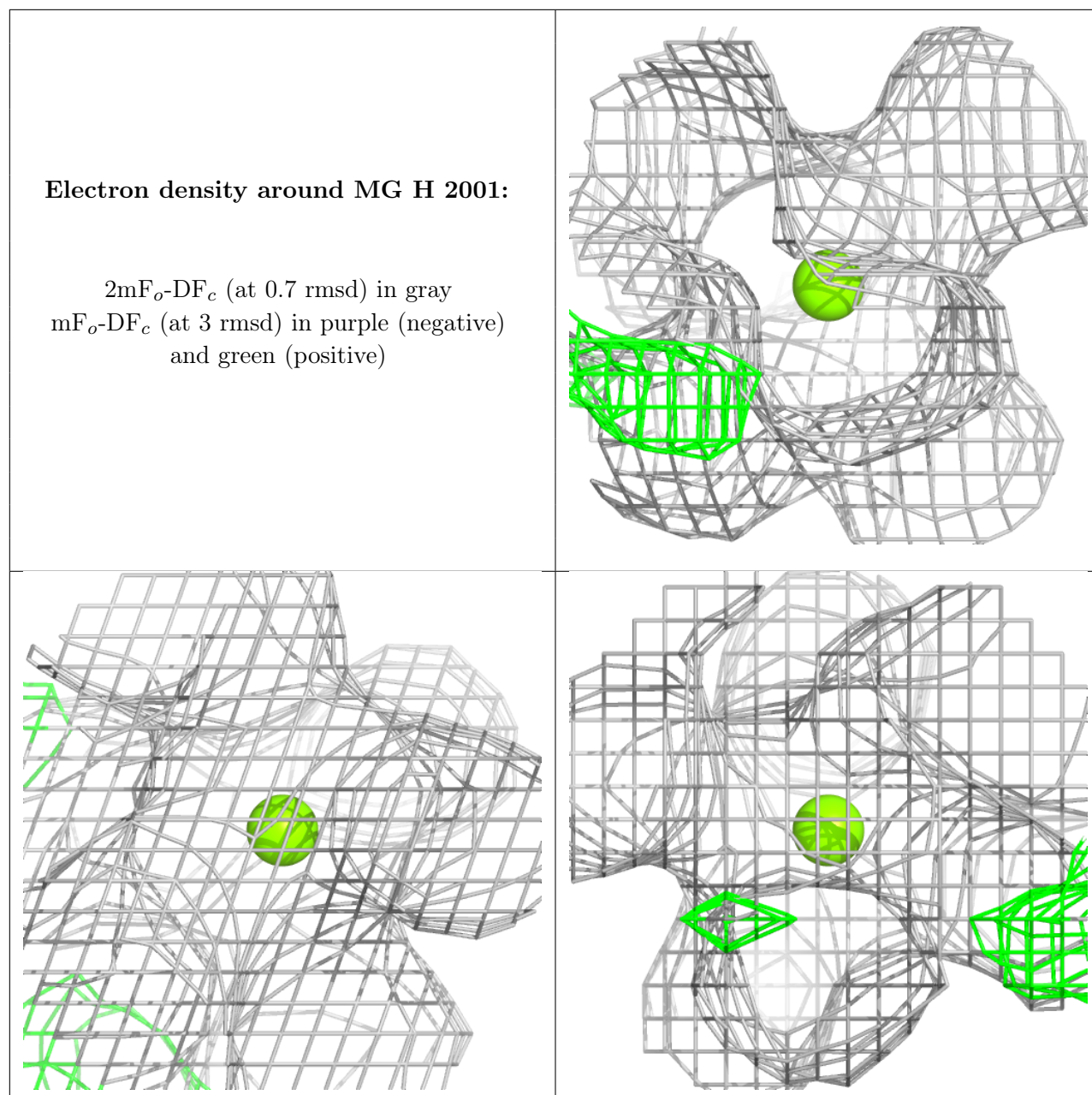
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 2001:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.