



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:23 AM UTC

PDB ID : 6XU1 / pdb_00006xu1
Title : Crystal structure of tetrameric human H215A-SAMHD1 (residues 109-626) with GTP, dAMPNPP and Mg
Authors : Morris, E.R.; Kunzelmann, S.; Caswell, S.J.; Arnold, L.H.; Purkiss, A.G.; Kelly, G.; Taylor, I.A.
Deposited on : 2020-01-17
Resolution : 2.20 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

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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

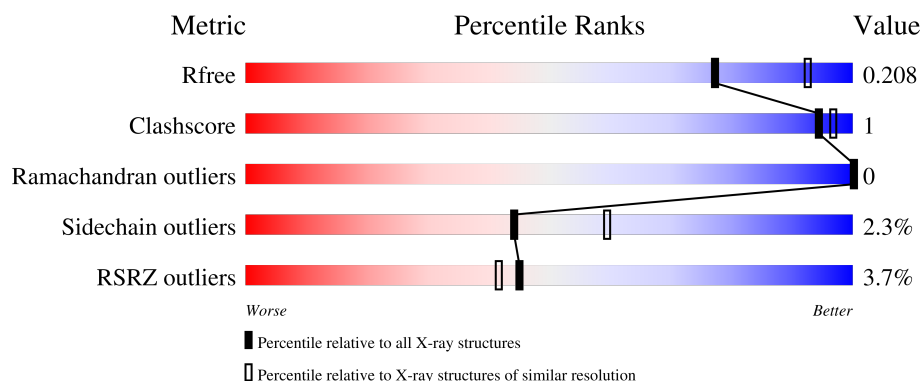
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	520	4% 87% 5% • 8%
1	B	520	2% 85% 6% • 8%
1	C	520	2% 86% 5% • 8%
1	D	520	2% 85% 6% • 8%

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Mol	Chain	Length	Quality of chain
1	E	520	7% 82% 6% 11%
1	F	520	2% 83% 8% 8%
1	G	520	2% 85% 6% 8%
1	H	520	7% 87% 5% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 32438 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 Deoxynucleoside triphosphate triphosphohydrolase SAMHD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3882	2485	672	705	20			
1	B	479	Total	C	N	O	S	0	0	0
			3882	2487	673	702	20			
1	C	478	Total	C	N	O	S	0	0	0
			3864	2475	668	701	20			
1	D	478	Total	C	N	O	S	0	0	0
			3868	2479	668	701	20			
1	E	464	Total	C	N	O	S	0	0	0
			3757	2404	651	682	20			
1	F	480	Total	C	N	O	S	0	0	0
			3894	2494	676	704	20			
1	G	479	Total	C	N	O	S	0	0	0
			3882	2486	674	702	20			
1	H	478	Total	C	N	O	S	0	0	0
			3844	2467	667	690	20			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	expression tag	UNP Q9Y3Z3
A	108	SER	-	expression tag	UNP Q9Y3Z3
A	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
B	107	GLY	-	expression tag	UNP Q9Y3Z3
B	108	SER	-	expression tag	UNP Q9Y3Z3
B	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
C	107	GLY	-	expression tag	UNP Q9Y3Z3
C	108	SER	-	expression tag	UNP Q9Y3Z3
C	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
D	107	GLY	-	expression tag	UNP Q9Y3Z3
D	108	SER	-	expression tag	UNP Q9Y3Z3
D	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
E	107	GLY	-	expression tag	UNP Q9Y3Z3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	108	SER	-	expression tag	UNP Q9Y3Z3
E	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
F	107	GLY	-	expression tag	UNP Q9Y3Z3
F	108	SER	-	expression tag	UNP Q9Y3Z3
F	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
G	107	GLY	-	expression tag	UNP Q9Y3Z3
G	108	SER	-	expression tag	UNP Q9Y3Z3
G	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3
H	107	GLY	-	expression tag	UNP Q9Y3Z3
H	108	SER	-	expression tag	UNP Q9Y3Z3
H	215	ALA	HIS	engineered mutation	UNP Q9Y3Z3

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

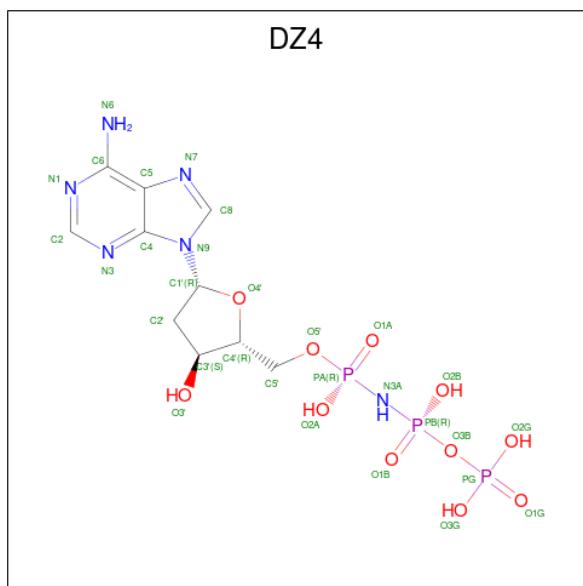
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total	Mg	0	0
			3	3		
3	D	4	Total	Mg	0	0
			4	4		
3	E	3	Total	Mg	0	0
			3	3		
3	F	3	Total	Mg	0	0
			3	3		
3	G	3	Total	Mg	0	0
			3	3		
3	H	3	Total	Mg	0	0
			3	3		

- Molecule 4 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amin o}phosphoryl]adenosine (CCD ID: DZ4) (formula: C₁₀H₁₇N₆O₁₁P₃) (labeled as "Ligand of Interest" by depositor).



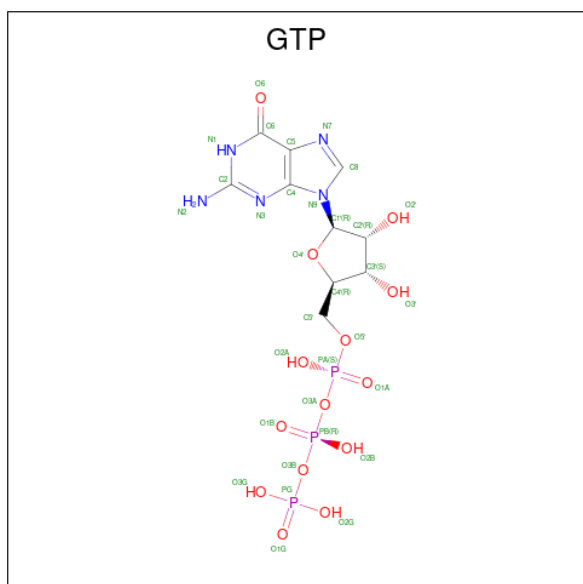
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	6	11	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	C	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	D	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	E	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	E	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	F	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	F	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	G	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	G	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	H	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
4	H	1	Total	C	N	O	P	0	0
			30	10	6	11	3		

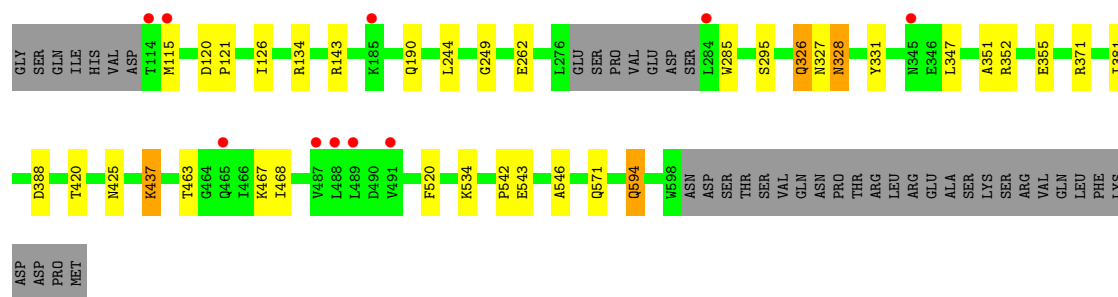
- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



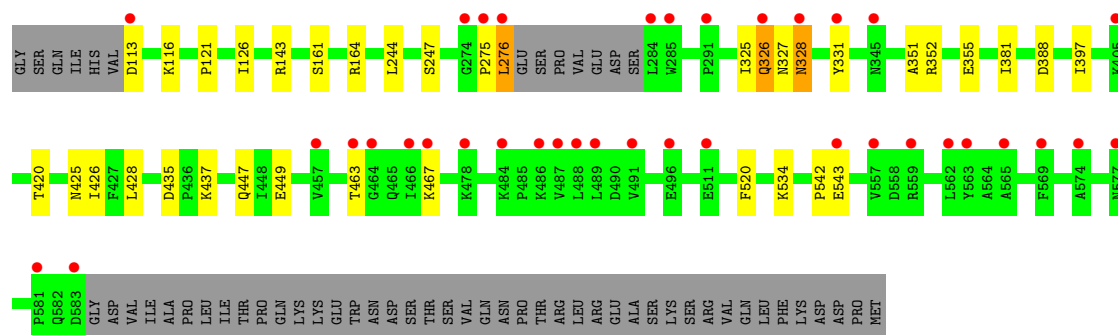
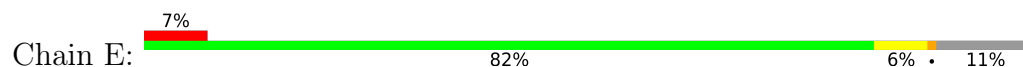
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	G	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	H	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is water.

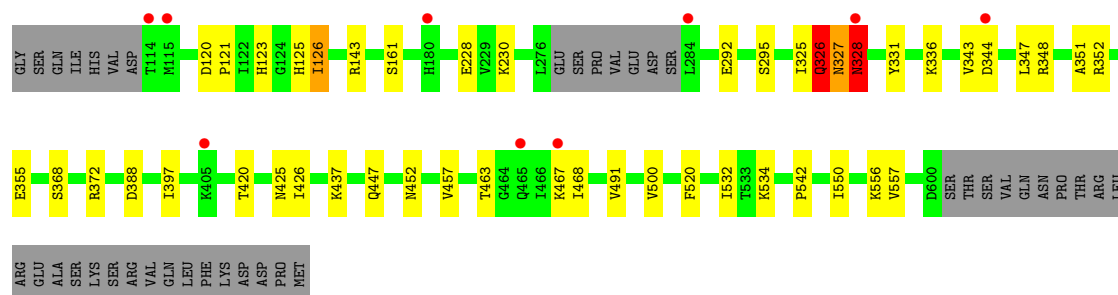
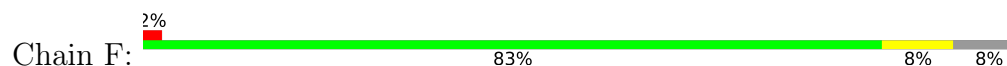
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	113	Total	O	0	0
			113	113		
6	C	116	Total	O	0	0
			116	116		
6	D	99	Total	O	0	0
			99	99		
6	E	71	Total	O	0	0
			71	71		
6	F	124	Total	O	0	0
			124	124		
6	G	115	Total	O	0	0
			115	115		
6	H	59	Total	O	0	0
			59	59		



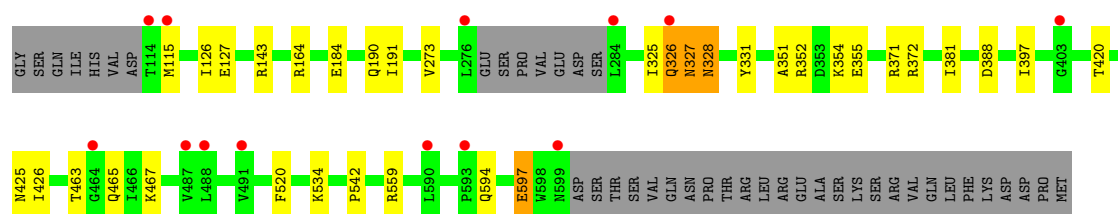
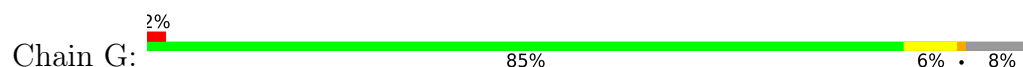
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



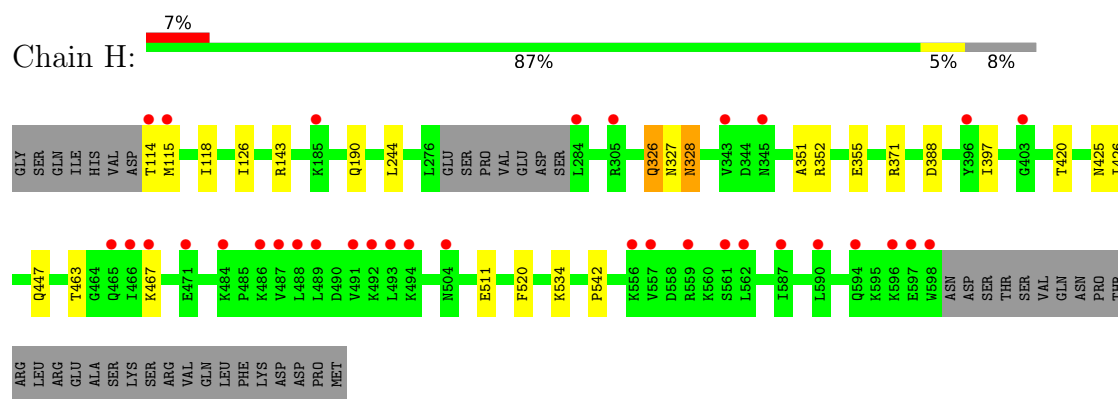
- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



- Molecule 1: Deoxynucleoside triphosphate triphosphohydrolase SAMHD1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.37Å 171.86Å 179.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	107.30 – 2.20 107.30 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (107.30-2.20) 98.7 (107.30-2.20)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.176 , 0.202 0.183 , 0.208	Depositor DCC
R_{free} test set	10526 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	32438	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: FE, GTP, MG, DZ4

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	1.34	9/3974 (0.2%)	1.17	5/5375 (0.1%)
1	B	1.33	12/3974 (0.3%)	1.17	6/5372 (0.1%)
1	C	1.33	11/3956 (0.3%)	1.16	6/5350 (0.1%)
1	D	1.31	11/3960 (0.3%)	1.15	4/5355 (0.1%)
1	E	1.22	8/3845 (0.2%)	1.13	6/5197 (0.1%)
1	F	1.38	22/3986 (0.6%)	1.19	11/5387 (0.2%)
1	G	1.29	9/3974 (0.2%)	1.12	8/5373 (0.1%)
1	H	1.20	4/3936 (0.1%)	1.11	2/5325 (0.0%)
All	All	1.30	86/31605 (0.3%)	1.15	48/42734 (0.1%)

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	491	VAL	C-O	-9.85	1.13	1.24
1	A	161	SER	CB-OG	8.69	1.59	1.42
1	F	327	ASN	C-O	-8.01	1.14	1.24
1	A	489	LEU	C-O	-7.75	1.14	1.24
1	F	347	LEU	C-O	-7.44	1.15	1.24
1	G	355	GLU	CD-OE1	7.16	1.39	1.25
1	B	355	GLU	CD-OE1	7.12	1.38	1.25
1	B	425	ASN	CG-ND2	6.97	1.47	1.33
1	C	355	GLU	CD-OE1	6.95	1.38	1.25
1	D	425	ASN	CG-ND2	6.83	1.47	1.33
1	D	262	GLU	C-O	6.80	1.31	1.24
1	B	371	ARG	C-O	-6.79	1.16	1.24
1	C	347	LEU	C-O	-6.70	1.15	1.24
1	A	328	ASN	CG-ND2	6.54	1.47	1.33
1	A	114	THR	C-O	6.51	1.32	1.23
1	F	343	VAL	CA-CB	6.43	1.63	1.54
1	F	355	GLU	CD-OE1	6.40	1.37	1.25
1	A	115	MET	C-O	-6.39	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	457	VAL	C-O	-6.38	1.16	1.23
1	G	371	ARG	C-O	-6.36	1.16	1.24
1	D	468	ILE	C-O	-6.32	1.17	1.24
1	E	275	PRO	C-O	-6.25	1.15	1.24
1	D	327	ASN	C-O	-6.24	1.16	1.24
1	D	371	ARG	C-O	-6.19	1.16	1.24
1	A	327	ASN	C-O	-6.19	1.16	1.24
1	C	184	GLU	C-O	-6.10	1.17	1.24
1	D	355	GLU	CD-OE1	6.08	1.36	1.25
1	E	449	GLU	CD-OE2	5.99	1.36	1.25
1	F	372	ARG	CZ-NH2	5.95	1.41	1.33
1	F	500	VAL	C-O	-5.91	1.17	1.24
1	F	228	GLU	CD-OE2	5.83	1.36	1.25
1	B	447	GLN	CD-NE2	5.77	1.45	1.33
1	C	327	ASN	C-O	-5.71	1.17	1.24
1	B	447	GLN	CG-CD	5.69	1.66	1.52
1	B	468	ILE	C-O	-5.66	1.17	1.24
1	A	355	GLU	CD-OE1	5.65	1.36	1.25
1	C	468	ILE	C-O	-5.62	1.18	1.24
1	G	328	ASN	CG-ND2	5.61	1.45	1.33
1	F	372	ARG	CZ-NH1	5.61	1.40	1.32
1	E	247	SER	CB-OG	-5.61	1.30	1.42
1	C	126	ILE	CB-CG1	-5.58	1.42	1.53
1	B	191	ILE	C-O	-5.58	1.18	1.24
1	B	184	GLU	C-O	-5.57	1.17	1.24
1	F	344	ASP	C-O	5.55	1.30	1.24
1	F	447	GLN	CD-NE2	5.54	1.44	1.33
1	D	347	LEU	C-O	-5.54	1.17	1.24
1	B	449	GLU	CD-OE2	5.52	1.35	1.25
1	B	327	ASN	CG-ND2	5.52	1.44	1.33
1	G	184	GLU	C-O	-5.50	1.17	1.24
1	B	328	ASN	CG-ND2	5.49	1.44	1.33
1	F	368	SER	CB-OG	-5.47	1.31	1.42
1	A	543	GLU	N-CA	5.46	1.53	1.46
1	G	191	ILE	C-O	-5.37	1.18	1.24
1	F	550	ILE	C-O	-5.37	1.18	1.24
1	F	125	HIS	C-O	-5.36	1.17	1.24
1	C	125	HIS	C-O	-5.35	1.17	1.24
1	F	161	SER	CB-OG	5.30	1.52	1.42
1	H	371	ARG	C-O	-5.30	1.17	1.24
1	D	546	ALA	C-O	-5.26	1.17	1.23
1	E	355	GLU	CD-OE1	5.26	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	115	MET	CA-C	5.25	1.59	1.52
1	H	355	GLU	CD-OE1	5.25	1.35	1.25
1	C	262	GLU	C-O	5.23	1.30	1.24
1	F	326	GLN	CD-OE1	-5.20	1.13	1.23
1	G	327	ASN	C-O	-5.19	1.17	1.24
1	D	115	MET	CA-C	5.18	1.59	1.52
1	G	273	VAL	C-O	-5.17	1.18	1.24
1	A	354	LYS	C-O	-5.15	1.17	1.24
1	F	532	ILE	C-O	-5.15	1.18	1.24
1	D	328	ASN	CG-ND2	5.15	1.44	1.33
1	B	327	ASN	C-O	-5.13	1.17	1.24
1	E	121	PRO	C-O	-5.13	1.17	1.24
1	F	468	ILE	C-O	-5.13	1.18	1.24
1	E	435	ASP	CG-OD2	5.11	1.35	1.25
1	E	326	GLN	C-O	5.10	1.29	1.23
1	F	327	ASN	CG-ND2	5.08	1.44	1.33
1	F	126	ILE	CB-CG1	-5.08	1.43	1.53
1	E	161	SER	CB-OG	5.08	1.52	1.42
1	H	328	ASN	CG-ND2	5.07	1.44	1.33
1	G	372	ARG	CD-NE	-5.07	1.39	1.46
1	C	447	GLN	CG-CD	5.06	1.64	1.52
1	F	123	HIS	C-O	-5.04	1.17	1.24
1	D	249	GLY	C-O	-5.04	1.18	1.24
1	C	331	TYR	CZ-OH	5.04	1.48	1.38
1	C	371	ARG	C-O	-5.02	1.18	1.24
1	G	326	GLN	CG-CD	5.01	1.64	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	328	ASN	N-CA-C	7.63	122.62	113.16
1	C	328	ASN	N-CA-C	7.54	122.19	112.92
1	B	328	ASN	N-CA-C	7.39	122.01	112.92
1	G	328	ASN	N-CA-C	7.22	121.80	112.92
1	H	328	ASN	N-CA-C	7.18	121.75	112.92
1	E	328	ASN	N-CA-C	7.17	121.74	112.92
1	A	328	ASN	N-CA-C	7.14	121.70	112.92
1	C	437	LYS	CB-CG-CD	6.93	127.24	111.30
1	D	328	ASN	N-CA-C	6.61	121.04	112.92
1	C	354	LYS	CD-CE-NZ	6.36	132.26	111.90
1	E	164	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	D	437	LYS	CB-CG-CD	6.32	125.83	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	275	PRO	CB-CA-C	-6.26	101.22	111.56
1	E	437	LYS	CA-CB-CG	6.25	126.60	114.10
1	F	348	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	B	437	LYS	CB-CG-CD	6.03	125.17	111.30
1	F	328	ASN	N-CA-CB	-5.91	101.40	110.44
1	C	325	ILE	CB-CG1-CD1	-5.82	101.57	113.80
1	A	164	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	D	262	GLU	CB-CG-CD	5.67	122.25	112.60
1	F	292	GLU	CG-CD-OE2	-5.65	105.39	118.40
1	F	325	ILE	CB-CG1-CD1	-5.64	101.95	113.80
1	F	295	SER	CA-CB-OG	5.55	122.20	111.10
1	G	559	ARG	CB-CG-CD	5.47	123.87	111.30
1	C	164	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	597	GLU	CA-CB-CG	5.41	124.93	114.10
1	G	597	GLU	CA-CB-CG	5.41	124.93	114.10
1	B	325	ILE	CB-CG1-CD1	-5.38	102.50	113.80
1	E	116	LYS	CD-CE-NZ	5.32	128.92	111.90
1	A	489	LEU	N-CA-C	5.27	117.49	108.90
1	G	325	ILE	CB-CA-C	-5.24	102.43	110.50
1	F	292	GLU	CG-CD-OE1	5.24	130.44	118.40
1	B	495	ALA	CA-C-N	5.22	128.96	120.60
1	B	495	ALA	C-N-CA	5.22	128.96	120.60
1	H	118	ILE	CB-CG1-CD1	-5.22	102.85	113.80
1	E	325	ILE	CB-CG1-CD1	-5.21	102.85	113.80
1	F	326	GLN	CB-CG-CD	5.21	121.45	112.60
1	A	489	LEU	CD1-CG-CD2	-5.17	99.43	110.80
1	F	230	LYS	N-CA-C	-5.15	97.33	107.69
1	G	164	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	G	354	LYS	CG-CD-CE	-5.08	99.61	111.30
1	D	134	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	G	465	GLN	N-CA-C	-5.06	106.70	112.92
1	G	327	ASN	CA-C-O	-5.04	114.65	120.49
1	F	437	LYS	CB-CG-CD	5.03	122.86	111.30
1	C	354	LYS	CG-CD-CE	-5.02	99.75	111.30
1	F	336	LYS	CB-CA-C	-5.02	102.46	110.79
1	B	326	GLN	CB-CG-CD	5.00	121.11	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3882	0	3823	9	0
1	B	3882	0	3841	17	0
1	C	3864	0	3808	10	0
1	D	3868	0	3819	12	0
1	E	3757	0	3700	14	0
1	F	3894	0	3858	13	0
1	G	3882	0	3838	10	0
1	H	3844	0	3793	11	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	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
4	A	60	0	26	0	0
4	B	30	0	13	0	0
4	C	90	0	39	1	0
4	D	60	0	26	0	0
4	E	60	0	26	0	0
4	F	60	0	26	0	0
4	G	60	0	26	0	0
4	H	60	0	26	0	0
5	A	32	0	12	0	0
5	B	32	0	12	0	0
5	C	32	0	12	0	0
5	D	32	0	12	1	0
5	E	64	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	32	0	11	0	0
5	H	32	0	12	0	0
6	A	99	0	0	0	0
6	B	113	0	0	3	0
6	C	116	0	0	3	0
6	D	99	0	0	1	0
6	E	71	0	0	0	0
6	F	124	0	0	1	1
6	G	115	0	0	0	1
6	H	59	0	0	0	0
All	All	32438	0	30783	81	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 1.

All (81) 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:F:328:ASN:N	1:F:328:ASN:OD1	2.05	0.85
1:B:437:LYS:NZ	6:B:802:HOH:O	2.26	0.68
1:E:425:ASN:OD1	1:F:425:ASN:ND2	2.28	0.66
1:B:331:TYR:OH	6:B:801:HOH:O	2.14	0.62
1:A:425:ASN:OD1	1:B:425:ASN:ND2	2.26	0.61
1:E:326:GLN:CD	1:H:326:GLN:NE2	2.60	0.60
1:F:331:TYR:OH	6:F:801:HOH:O	2.03	0.59
1:D:534:LYS:HE3	1:D:542:PRO:O	2.04	0.58
1:C:534:LYS:HE3	1:C:542:PRO:O	2.04	0.56
1:B:466:ILE:HD12	6:B:854:HOH:O	2.05	0.55
1:B:326:GLN:HG3	1:B:327:ASN:N	2.22	0.54
1:B:534:LYS:HE3	1:B:542:PRO:O	2.08	0.54
1:F:326:GLN:HG2	1:G:327:ASN:O	2.07	0.54
1:F:326:GLN:HG3	1:F:327:ASN:N	2.23	0.53
1:G:397:ILE:HG21	1:G:426:ILE:HD11	1.92	0.52
1:F:534:LYS:HE3	1:F:542:PRO:O	2.09	0.51
1:A:326:GLN:HB3	1:D:326:GLN:NE2	2.26	0.51
1:E:534:LYS:HE3	1:E:542:PRO:O	2.11	0.50
1:E:327:ASN:O	1:H:326:GLN:HG2	2.12	0.49
1:E:397:ILE:HG21	1:E:426:ILE:HD11	1.94	0.49
1:G:534:LYS:HE3	1:G:542:PRO:O	2.13	0.49
4:C:706:DZ4:PA	6:C:825:HOH:O	2.69	0.49
1:H:326:GLN:HG3	1:H:327:ASN:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:GLN:NE2	1:C:326:GLN:HB3	2.28	0.48
1:A:534:LYS:HE3	1:A:542:PRO:O	2.14	0.48
1:B:397:ILE:HG21	1:B:426:ILE:HD11	1.95	0.47
1:A:326:GLN:CG	1:D:326:GLN:HE22	2.27	0.47
1:B:326:GLN:HG2	1:C:327:ASN:O	2.14	0.47
1:H:397:ILE:HG21	1:H:426:ILE:HD11	1.97	0.47
1:E:428:LEU:HD13	1:F:425:ASN:HB2	1.96	0.47
1:D:331:TYR:OH	6:D:801:HOH:O	2.06	0.46
1:E:276:LEU:HD23	1:E:276:LEU:N	2.31	0.46
1:F:143:ARG:HD2	1:F:420:THR:HA	1.98	0.45
1:C:285:TRP:CH2	1:C:295:SER:HB3	2.51	0.45
1:B:452:ASN:OD1	1:B:557:VAL:HG21	2.17	0.45
1:C:143:ARG:HD2	1:C:420:THR:HA	1.99	0.45
1:G:143:ARG:HD2	1:G:420:THR:HA	1.99	0.45
1:G:425:ASN:OD1	1:H:425:ASN:ND2	2.47	0.45
1:B:364:HIS:HE1	6:C:912:HOH:O	2.01	0.44
1:H:143:ARG:HD2	1:H:420:THR:HA	1.99	0.44
1:A:351:ALA:O	1:A:520:PHE:HA	2.18	0.44
1:F:351:ALA:O	1:F:520:PHE:HA	2.19	0.43
1:B:351:ALA:O	1:B:520:PHE:HA	2.18	0.43
1:D:285:TRP:CH2	1:D:295:SER:HB3	2.53	0.43
1:E:143:ARG:HD2	1:E:420:THR:HA	2.00	0.43
1:G:115:MET:HE3	1:G:127:GLU:HB3	2.01	0.43
1:B:381:ILE:HD12	1:B:381:ILE:HA	1.92	0.43
1:A:143:ARG:HD2	1:A:420:THR:HA	2.00	0.42
1:B:143:ARG:HD2	1:B:420:THR:HA	2.01	0.42
1:D:351:ALA:O	1:D:520:PHE:HA	2.19	0.42
1:H:534:LYS:HE3	1:H:542:PRO:O	2.18	0.42
1:B:326:GLN:NE2	1:C:326:GLN:CD	2.78	0.42
1:D:143:ARG:HD2	1:D:420:THR:HA	2.02	0.42
1:D:381:ILE:HD12	1:D:381:ILE:HA	1.94	0.42
1:E:326:GLN:HB3	1:H:326:GLN:NE2	2.34	0.42
1:F:452:ASN:OD1	1:F:557:VAL:HG21	2.20	0.42
1:E:351:ALA:O	1:E:520:PHE:HA	2.20	0.41
1:A:120:ASP:OD1	1:A:121:PRO:HD2	2.20	0.41
1:C:331:TYR:CD1	1:C:331:TYR:C	2.99	0.41
1:C:351:ALA:O	1:C:520:PHE:HA	2.20	0.41
1:F:397:ILE:HG21	1:F:426:ILE:HD11	2.02	0.41
1:G:381:ILE:HD12	1:G:381:ILE:HA	1.94	0.41
1:A:331:TYR:CD1	1:A:331:TYR:C	2.98	0.41
1:E:381:ILE:HD12	1:E:381:ILE:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:ASP:OD1	1:F:121:PRO:HD2	2.20	0.41
1:F:326:GLN:NE2	1:G:326:GLN:HB3	2.36	0.41
1:D:120:ASP:OD1	1:D:121:PRO:HD2	2.21	0.41
1:E:326:GLN:CD	1:H:326:GLN:HE22	2.27	0.41
1:E:331:TYR:CD1	1:E:331:TYR:C	2.99	0.41
1:G:351:ALA:O	1:G:520:PHE:HA	2.20	0.41
1:C:455:LYS:NZ	5:D:707:GTP:O2G	2.54	0.41
1:D:571:GLN:NE2	1:D:594:GLN:OE1	2.48	0.41
1:E:244:LEU:HD23	1:E:244:LEU:C	2.46	0.41
1:H:244:LEU:HD23	1:H:244:LEU:C	2.46	0.41
1:H:351:ALA:O	1:H:520:PHE:HA	2.20	0.41
1:B:331:TYR:CD1	1:B:331:TYR:C	2.99	0.40
1:B:580:LYS:HD2	1:B:598:TRP:HB3	2.03	0.40
1:G:331:TYR:CD1	1:G:331:TYR:C	2.99	0.40
1:D:244:LEU:HD23	1:D:244:LEU:C	2.46	0.40
1:A:326:GLN:HB3	1:D:326:GLN:HE22	1.87	0.40
1:C:354:LYS:NZ	6:C:807:HOH:O	2.54	0.40

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)
6:F:923:HOH:O	6:G:912:HOH:O[3_655]	2.08	0.12

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	476/520 (92%)	466 (98%)	10 (2%)	0	100	100
1	B	475/520 (91%)	468 (98%)	7 (2%)	0	100	100
1	C	474/520 (91%)	464 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	474/520 (91%)	466 (98%)	8 (2%)	0	100	100
1	E	460/520 (88%)	452 (98%)	8 (2%)	0	100	100
1	F	476/520 (92%)	470 (99%)	6 (1%)	0	100	100
1	G	475/520 (91%)	466 (98%)	9 (2%)	0	100	100
1	H	474/520 (91%)	466 (98%)	8 (2%)	0	100	100
All	All	3784/4160 (91%)	3718 (98%)	66 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	416/463 (90%)	408 (98%)	8 (2%)	50	66
1	B	417/463 (90%)	409 (98%)	8 (2%)	50	66
1	C	414/463 (89%)	404 (98%)	10 (2%)	43	58
1	D	415/463 (90%)	404 (97%)	11 (3%)	39	53
1	E	403/463 (87%)	393 (98%)	10 (2%)	42	56
1	F	419/463 (90%)	411 (98%)	8 (2%)	50	66
1	G	417/463 (90%)	408 (98%)	9 (2%)	45	61
1	H	409/463 (88%)	398 (97%)	11 (3%)	39	53
All	All	3310/3704 (89%)	3235 (98%)	75 (2%)	44	59

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	126	ILE
1	A	190	GLN
1	A	284	LEU
1	A	328	ASN

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Mol	Chain	Res	Type
1	A	388	ASP
1	A	463	THR
1	A	597	GLU
1	B	126	ILE
1	B	263	GLU
1	B	326	GLN
1	B	328	ASN
1	B	352	ARG
1	B	388	ASP
1	B	463	THR
1	B	467	LYS
1	C	126	ILE
1	C	190	GLN
1	C	328	ASN
1	C	352	ARG
1	C	388	ASP
1	C	437	LYS
1	C	463	THR
1	C	467	LYS
1	C	469	LYS
1	C	594	GLN
1	D	126	ILE
1	D	190	GLN
1	D	326	GLN
1	D	328	ASN
1	D	352	ARG
1	D	388	ASP
1	D	437	LYS
1	D	463	THR
1	D	467	LYS
1	D	543	GLU
1	D	594	GLN
1	E	113	ASP
1	E	126	ILE
1	E	276	LEU
1	E	328	ASN
1	E	352	ARG
1	E	388	ASP
1	E	447	GLN
1	E	463	THR
1	E	467	LYS
1	E	543	GLU

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Mol	Chain	Res	Type
1	F	126	ILE
1	F	326	GLN
1	F	328	ASN
1	F	352	ARG
1	F	388	ASP
1	F	463	THR
1	F	467	LYS
1	F	556	LYS
1	G	126	ILE
1	G	190	GLN
1	G	328	ASN
1	G	352	ARG
1	G	388	ASP
1	G	463	THR
1	G	467	LYS
1	G	594	GLN
1	G	597	GLU
1	H	114	THR
1	H	126	ILE
1	H	190	GLN
1	H	326	GLN
1	H	328	ASN
1	H	352	ARG
1	H	388	ASP
1	H	447	GLN
1	H	463	THR
1	H	467	LYS
1	H	511	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	200	GLN
1	A	248	ASN
1	A	328	ASN
1	A	364	HIS
1	A	375	GLN
1	A	380	ASN
1	A	447	GLN
1	A	571	GLN
1	B	149	GLN

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Mol	Chain	Res	Type
1	B	200	GLN
1	B	326	GLN
1	B	328	ASN
1	B	364	HIS
1	B	517	HIS
1	B	567	GLN
1	B	571	GLN
1	C	149	GLN
1	C	190	GLN
1	C	200	GLN
1	C	248	ASN
1	C	328	ASN
1	C	367	ASN
1	C	375	GLN
1	C	380	ASN
1	C	517	HIS
1	C	571	GLN
1	C	594	GLN
1	D	149	GLN
1	D	200	GLN
1	D	243	HIS
1	D	248	ASN
1	D	326	GLN
1	D	328	ASN
1	D	367	ASN
1	D	517	HIS
1	D	567	GLN
1	E	149	GLN
1	E	163	ASN
1	E	200	GLN
1	E	248	ASN
1	E	328	ASN
1	E	364	HIS
1	E	367	ASN
1	E	425	ASN
1	F	149	GLN
1	F	200	GLN
1	F	248	ASN
1	F	364	HIS
1	F	425	ASN
1	F	461	GLN
1	F	571	GLN

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Mol	Chain	Res	Type
1	G	149	GLN
1	G	190	GLN
1	G	200	GLN
1	G	248	ASN
1	G	328	ASN
1	G	367	ASN
1	G	571	GLN
1	G	594	GLN
1	H	200	GLN
1	H	248	ASN
1	H	326	GLN
1	H	328	ASN
1	H	367	ASN
1	H	517	HIS
1	H	567	GLN
1	H	571	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 33 are monoatomic - leaving 24 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
4	DZ4	D	706	2,3	31,32,32	1.41	4 (12%)	44,50,50	1.49	5 (11%)
5	GTP	A	706	3	33,34,34	1.52	5 (15%)	50,54,54	2.43	15 (30%)
4	DZ4	B	705	2,3	31,32,32	1.10	3 (9%)	44,50,50	1.13	3 (6%)
4	DZ4	C	708	3	31,32,32	1.47	5 (16%)	44,50,50	1.69	6 (13%)
5	GTP	H	707	3	33,34,34	1.57	7 (21%)	50,54,54	1.66	12 (24%)
4	DZ4	G	706	2,3	31,32,32	1.54	4 (12%)	44,50,50	1.34	4 (9%)
4	DZ4	F	706	3	31,32,32	1.32	5 (16%)	44,50,50	1.89	6 (13%)
4	DZ4	A	705	2,3	31,32,32	1.90	4 (12%)	44,50,50	1.25	4 (9%)
4	DZ4	E	705	2,3	31,32,32	1.39	5 (16%)	44,50,50	1.48	5 (11%)
4	DZ4	H	706	2,3	31,32,32	2.88	6 (19%)	44,50,50	1.55	5 (11%)
4	DZ4	C	706	2,3	31,32,32	1.42	6 (19%)	44,50,50	1.44	5 (11%)
4	DZ4	E	708	3	31,32,32	1.53	6 (19%)	44,50,50	1.72	7 (15%)
4	DZ4	G	701	3	31,32,32	1.46	5 (16%)	44,50,50	1.85	5 (11%)
4	DZ4	A	707	3	31,32,32	1.31	3 (9%)	44,50,50	1.59	4 (9%)
4	DZ4	C	701	3	31,32,32	1.21	5 (16%)	44,50,50	1.74	5 (11%)
4	DZ4	D	701	3	31,32,32	1.39	5 (16%)	44,50,50	1.63	5 (11%)
5	GTP	E	706	3	33,34,34	2.01	8 (24%)	50,54,54	2.39	22 (44%)
4	DZ4	F	705	2,3	31,32,32	1.90	5 (16%)	44,50,50	1.50	4 (9%)
5	GTP	E	707	3	33,34,34	1.54	6 (18%)	50,54,54	1.73	13 (26%)
5	GTP	C	707	3	33,34,34	2.15	10 (30%)	50,54,54	1.87	14 (28%)
5	GTP	B	706	3	33,34,34	2.18	7 (21%)	50,54,54	1.88	15 (30%)
4	DZ4	H	701	3	31,32,32	1.31	4 (12%)	44,50,50	1.68	8 (18%)
5	GTP	D	707	3	33,34,34	1.50	6 (18%)	50,54,54	2.12	17 (34%)
5	GTP	G	707	3	33,34,34	1.86	9 (27%)	50,54,54	1.81	12 (24%)

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
4	DZ4	D	706	2,3	-	1/19/34/34	0/3/3/3
5	GTP	A	706	3	-	6/22/38/38	0/3/3/3
4	DZ4	B	705	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	C	708	3	-	5/19/34/34	0/3/3/3
5	GTP	H	707	3	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DZ4	G	706	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	F	706	3	-	3/19/34/34	0/3/3/3
4	DZ4	A	705	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	E	705	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	H	706	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	C	706	2,3	-	1/19/34/34	0/3/3/3
4	DZ4	E	708	3	-	5/19/34/34	0/3/3/3
4	DZ4	G	701	3	-	4/19/34/34	0/3/3/3
4	DZ4	A	707	3	-	2/19/34/34	0/3/3/3
4	DZ4	C	701	3	-	3/19/34/34	0/3/3/3
4	DZ4	D	701	3	-	5/19/34/34	0/3/3/3
5	GTP	E	706	3	-	9/22/38/38	0/3/3/3
4	DZ4	F	705	2,3	-	3/19/34/34	0/3/3/3
5	GTP	E	707	3	-	6/22/38/38	0/3/3/3
5	GTP	C	707	3	-	7/22/38/38	0/3/3/3
5	GTP	B	706	3	-	6/22/38/38	0/3/3/3
4	DZ4	H	701	3	-	4/19/34/34	0/3/3/3
5	GTP	D	707	3	-	7/22/38/38	0/3/3/3
5	GTP	G	707	3	-	7/22/38/38	0/3/3/3

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	706	DZ4	PA-O1A	7.97	1.58	1.46
5	E	706	GTP	PB-O3B	7.34	1.67	1.59
4	A	705	DZ4	PB-O1B	7.32	1.57	1.46
5	B	706	GTP	PB-O3A	7.27	1.67	1.59
4	H	706	DZ4	PB-O1B	7.15	1.57	1.46
4	H	706	DZ4	PB-O3B	-6.43	1.51	1.59
5	C	707	GTP	PB-O3A	6.27	1.66	1.59
5	B	706	GTP	PA-O3A	6.18	1.66	1.59
4	H	706	DZ4	PB-N3A	6.17	1.79	1.63
4	F	705	DZ4	PA-O1A	6.16	1.55	1.46
5	C	707	GTP	PA-O3A	6.12	1.66	1.59
4	H	706	DZ4	PG-O2G	-6.08	1.32	1.54
4	A	705	DZ4	PA-O1A	5.99	1.55	1.46
4	F	705	DZ4	PB-O1B	5.88	1.55	1.46
4	G	706	DZ4	PA-O1A	4.90	1.53	1.46
4	C	708	DZ4	PB-O3B	4.75	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	708	DZ4	PB-O3B	4.60	1.64	1.59
5	G	707	GTP	C6-N1	-4.59	1.30	1.38
4	G	706	DZ4	PB-O1B	4.51	1.53	1.46
4	C	706	DZ4	PB-O1B	4.51	1.53	1.46
4	G	701	DZ4	PB-O1B	4.44	1.52	1.46
5	A	706	GTP	PB-O3A	4.38	1.64	1.59
4	D	701	DZ4	PB-O3B	4.30	1.64	1.59
5	G	707	GTP	C5-N7	-4.27	1.30	1.39
5	D	707	GTP	PB-O3A	4.11	1.63	1.59
4	A	707	DZ4	PB-O1B	4.10	1.52	1.46
4	E	705	DZ4	PA-O1A	4.09	1.52	1.46
4	H	701	DZ4	PB-O1B	3.95	1.52	1.46
4	D	706	DZ4	PA-O1A	3.87	1.52	1.46
4	F	706	DZ4	PA-O1A	3.85	1.52	1.46
4	D	706	DZ4	PB-O1B	3.80	1.51	1.46
4	D	701	DZ4	PB-O1B	3.80	1.51	1.46
4	E	705	DZ4	PB-O1B	3.78	1.51	1.46
4	A	707	DZ4	PB-O2B	-3.73	1.46	1.56
5	A	706	GTP	PB-O3B	3.68	1.63	1.59
5	C	707	GTP	C5-N7	-3.65	1.31	1.39
4	H	706	DZ4	PG-O1G	3.62	1.61	1.50
4	C	706	DZ4	PA-O1A	3.51	1.51	1.46
4	E	708	DZ4	PB-O1B	3.44	1.51	1.46
5	B	706	GTP	O4'-C1'	3.43	1.49	1.42
5	G	707	GTP	C5-C4	3.42	1.48	1.38
4	C	708	DZ4	PB-O1B	3.41	1.51	1.46
5	G	707	GTP	C4-N9	-3.40	1.29	1.38
4	C	701	DZ4	PB-O1B	3.34	1.51	1.46
5	E	706	GTP	C5-N7	-3.33	1.32	1.39
5	H	707	GTP	PB-O3B	3.30	1.63	1.59
4	B	705	DZ4	PB-O1B	3.27	1.51	1.46
5	E	707	GTP	C5-C4	3.25	1.47	1.38
4	G	701	DZ4	PA-O2A	-3.24	1.48	1.56
5	E	707	GTP	C5-N7	-3.18	1.32	1.39
4	F	705	DZ4	PB-O2B	-3.17	1.48	1.56
4	A	707	DZ4	PA-O2A	-3.13	1.48	1.56
4	F	705	DZ4	PA-O2A	-3.13	1.48	1.56
5	H	707	GTP	PB-O3A	-3.12	1.56	1.59
4	G	701	DZ4	PA-O1A	3.10	1.50	1.46
4	H	701	DZ4	PB-O3B	3.06	1.62	1.59
4	D	706	DZ4	PB-O2B	-3.05	1.48	1.56
4	E	708	DZ4	PB-O2B	-3.05	1.48	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	701	DZ4	PA-O2A	-3.04	1.48	1.56
4	G	706	DZ4	PB-O2B	-3.00	1.48	1.56
5	E	707	GTP	C4-N9	-2.99	1.30	1.38
5	E	707	GTP	O2'-C2'	2.96	1.50	1.43
5	E	707	GTP	PA-O3A	2.96	1.62	1.59
4	F	706	DZ4	PG-O2G	-2.96	1.43	1.54
5	E	706	GTP	PB-O2B	-2.96	1.41	1.55
5	B	706	GTP	C3'-C4'	2.95	1.60	1.53
5	A	706	GTP	C6-N1	-2.95	1.33	1.38
5	C	707	GTP	C2-N1	-2.95	1.30	1.37
4	F	706	DZ4	PB-O2B	-2.94	1.49	1.56
5	H	707	GTP	O4'-C1'	-2.92	1.35	1.42
4	C	708	DZ4	PB-O2B	-2.87	1.49	1.56
5	H	707	GTP	PA-O3A	-2.85	1.56	1.59
5	G	707	GTP	O6-C6	2.83	1.28	1.23
4	D	706	DZ4	PB-O3B	2.83	1.62	1.59
4	E	708	DZ4	PA-O1A	2.82	1.50	1.46
5	C	707	GTP	C4-N9	-2.81	1.30	1.38
4	D	701	DZ4	PA-O2A	-2.81	1.49	1.56
5	D	707	GTP	C5-N7	-2.80	1.33	1.39
5	E	706	GTP	PG-O1G	-2.77	1.41	1.50
5	B	706	GTP	O6-C6	2.76	1.28	1.23
4	E	708	DZ4	PA-O2A	-2.76	1.49	1.56
5	G	707	GTP	O4'-C1'	2.75	1.48	1.42
4	F	706	DZ4	PA-O2A	-2.72	1.49	1.56
4	E	705	DZ4	PA-O2A	-2.70	1.49	1.56
5	G	707	GTP	O3'-C3'	-2.67	1.36	1.43
5	C	707	GTP	C6-N1	-2.66	1.33	1.38
4	C	701	DZ4	PA-O2A	-2.66	1.49	1.56
4	G	706	DZ4	PG-O3G	-2.66	1.44	1.54
4	H	701	DZ4	PA-O1A	2.64	1.50	1.46
4	F	706	DZ4	PB-O1B	2.63	1.50	1.46
5	D	707	GTP	C4-N9	-2.62	1.31	1.38
5	H	707	GTP	C5-C4	2.59	1.45	1.38
4	E	705	DZ4	PG-O3G	-2.57	1.45	1.54
4	C	708	DZ4	PG-O3G	-2.44	1.45	1.54
5	E	706	GTP	PA-O2A	-2.44	1.44	1.55
5	E	706	GTP	C8-N9	-2.39	1.32	1.37
4	E	705	DZ4	PB-N3A	2.37	1.69	1.63
5	A	706	GTP	C2-N2	-2.37	1.28	1.34
5	C	707	GTP	PG-O1G	-2.36	1.43	1.50
4	C	708	DZ4	PA-O2A	-2.36	1.50	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	701	DZ4	PG-O2G	-2.35	1.46	1.54
4	D	701	DZ4	PG-O3G	-2.35	1.46	1.54
4	A	705	DZ4	PG-O2G	-2.33	1.46	1.54
5	G	707	GTP	PB-O2B	-2.33	1.44	1.55
5	D	707	GTP	PA-O5'	2.32	1.68	1.59
4	C	701	DZ4	PG-O2G	-2.30	1.46	1.54
5	C	707	GTP	O4'-C4'	-2.29	1.39	1.45
5	E	706	GTP	PG-O2G	-2.27	1.46	1.54
4	E	708	DZ4	PG-O2G	-2.26	1.46	1.54
5	D	707	GTP	C8-N9	-2.23	1.32	1.37
5	H	707	GTP	PG-O1G	-2.22	1.43	1.50
4	C	706	DZ4	PA-O2A	-2.22	1.50	1.56
4	B	705	DZ4	PA-O2A	-2.21	1.50	1.56
4	F	705	DZ4	PG-O3G	-2.19	1.46	1.54
5	E	706	GTP	C4-N9	-2.18	1.32	1.38
5	A	706	GTP	PB-O2B	-2.18	1.45	1.55
5	E	707	GTP	C4-N3	2.17	1.39	1.34
4	C	706	DZ4	PB-O2B	-2.16	1.51	1.56
4	D	701	DZ4	PB-O2B	-2.16	1.51	1.56
5	C	707	GTP	O3'-C3'	-2.16	1.37	1.43
5	H	707	GTP	PG-O3G	-2.14	1.46	1.54
5	D	707	GTP	PB-O2B	-2.14	1.45	1.55
4	C	701	DZ4	PB-O2B	-2.09	1.51	1.56
4	C	701	DZ4	PA-N3A	2.09	1.68	1.63
5	B	706	GTP	PG-O2G	-2.07	1.47	1.54
5	C	707	GTP	C2'-C3'	-2.05	1.47	1.53
5	G	707	GTP	PB-O3B	2.05	1.61	1.59
4	C	706	DZ4	PG-O2G	-2.04	1.47	1.54
5	B	706	GTP	C5-C4	2.03	1.44	1.38
4	B	705	DZ4	PA-O1A	2.02	1.49	1.46
4	G	701	DZ4	PB-O2B	-2.01	1.51	1.56
4	A	705	DZ4	PB-O2B	-2.01	1.51	1.56
4	C	706	DZ4	PB-O3B	2.00	1.61	1.59

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	DZ4	O1A-PA-N3A	-7.77	100.33	111.77
5	A	706	GTP	C5-C4-N3	-7.66	116.21	128.39
5	E	706	GTP	O5'-C5'-C4'	7.49	134.50	108.99
5	A	706	GTP	C2-N3-C4	7.07	124.48	112.30
5	A	706	GTP	N9-C4-N3	6.87	139.70	125.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	705	DZ4	O2B-PB-O1B	6.37	123.52	109.87
4	G	701	DZ4	O1B-PB-N3A	-6.28	102.52	111.77
4	A	707	DZ4	O1A-PA-N3A	-6.22	102.61	111.77
4	F	706	DZ4	O1A-PA-N3A	-6.02	102.91	111.77
4	E	708	DZ4	O1B-PB-N3A	-5.95	103.01	111.77
5	B	706	GTP	O2B-PB-O3A	-5.87	91.40	107.27
4	F	706	DZ4	O2B-PB-O1B	5.81	122.33	109.87
5	C	707	GTP	O2B-PB-O3A	-5.65	91.99	107.27
4	H	706	DZ4	O5'-PA-O1A	-5.65	97.49	114.27
4	H	701	DZ4	O1A-PA-N3A	-5.42	103.79	111.77
4	C	701	DZ4	O5'-PA-O1A	-5.41	98.23	114.27
5	D	707	GTP	C5-C4-N3	-5.40	119.79	128.39
4	H	706	DZ4	O2B-PB-O1B	5.27	121.18	109.87
4	F	706	DZ4	O1B-PB-N3A	-5.19	104.13	111.77
5	G	707	GTP	C5-C4-N3	-5.19	120.13	128.39
4	F	705	DZ4	O2B-PB-O1B	5.18	120.97	109.87
4	D	701	DZ4	O2A-PA-O1A	5.15	120.92	109.87
4	C	708	DZ4	O1B-PB-N3A	-5.00	104.40	111.77
4	G	701	DZ4	O2B-PB-O1B	4.94	120.46	109.87
5	A	706	GTP	O2B-PB-O3A	-4.86	94.13	107.27
4	G	701	DZ4	O1A-PA-N3A	-4.86	104.61	111.77
4	D	701	DZ4	O1B-PB-N3A	-4.86	104.61	111.77
4	G	701	DZ4	O2A-PA-O1A	4.85	120.26	109.87
4	B	705	DZ4	O2B-PB-O1B	4.82	120.20	109.87
4	F	705	DZ4	O2A-PA-O1A	4.81	120.19	109.87
4	C	706	DZ4	O1B-PB-N3A	-4.79	104.71	111.77
4	F	706	DZ4	O5'-PA-O1A	-4.79	100.06	114.27
5	D	707	GTP	C2-N3-C4	4.78	120.53	112.30
4	A	707	DZ4	O2B-PB-O1B	4.76	120.07	109.87
4	D	701	DZ4	O1A-PA-N3A	-4.72	104.82	111.77
4	H	701	DZ4	O2B-PB-O1B	4.71	119.97	109.87
4	C	708	DZ4	O2A-PA-O1A	4.67	119.89	109.87
4	G	706	DZ4	O2B-PB-O1B	4.65	119.85	109.87
5	E	706	GTP	O3B-PG-O1G	-4.64	86.64	111.04
5	E	706	GTP	O2G-PG-O3B	-4.61	89.16	104.64
4	E	708	DZ4	O2B-PB-O1B	4.55	119.62	109.87
4	E	708	DZ4	O5'-PA-O1A	-4.54	100.80	114.27
4	D	701	DZ4	O2B-PB-O1B	4.50	119.52	109.87
4	H	706	DZ4	O2A-PA-O1A	4.42	119.34	109.87
4	A	705	DZ4	O2A-PA-O1A	4.32	119.14	109.87
4	C	708	DZ4	O2B-PB-O1B	4.26	119.00	109.87
4	D	706	DZ4	O1A-PA-N3A	-4.24	105.52	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	705	DZ4	O5'-PA-O1A	-4.21	101.79	114.27
4	A	705	DZ4	O2B-PB-O1B	4.21	118.89	109.87
4	D	706	DZ4	O2B-PB-O1B	4.18	118.83	109.87
5	E	706	GTP	C5-C4-N3	-4.16	121.77	128.39
4	H	701	DZ4	O2A-PA-O1A	4.14	118.75	109.87
4	C	706	DZ4	O2A-PA-O1A	4.14	118.74	109.87
5	E	707	GTP	O2B-PB-O3A	-4.09	96.23	107.27
5	G	707	GTP	O2B-PB-O3A	-4.07	96.27	107.27
4	F	706	DZ4	O2A-PA-O1A	4.07	118.59	109.87
5	B	706	GTP	O2B-PB-O1B	4.05	131.28	112.44
4	A	707	DZ4	O2A-PA-O1A	4.04	118.53	109.87
4	D	706	DZ4	O2A-PA-O1A	3.99	118.43	109.87
4	H	701	DZ4	O5'-PA-O1A	-3.98	102.47	114.27
5	G	707	GTP	N9-C4-N3	3.96	133.88	125.95
5	D	707	GTP	O5'-C5'-C4'	3.93	122.36	108.99
5	E	706	GTP	PA-O5'-C5'	3.91	143.77	121.35
4	C	708	DZ4	O2A-PA-O5'	-3.81	96.55	106.69
5	E	706	GTP	O4'-C4'-C5'	-3.80	97.18	109.33
5	B	706	GTP	C2-N3-C4	3.78	118.80	112.30
5	H	707	GTP	C5-C4-N3	-3.76	122.40	128.39
5	H	707	GTP	N9-C4-N3	3.74	133.44	125.95
5	E	706	GTP	O2G-PG-O1G	3.74	125.40	110.83
4	G	701	DZ4	O5'-PA-O1A	-3.71	103.26	114.27
5	E	706	GTP	O2B-PB-O3A	-3.71	97.24	107.27
5	C	707	GTP	C5-C4-N3	-3.71	122.49	128.39
4	E	708	DZ4	O2A-PA-O1A	3.71	117.82	109.87
4	C	706	DZ4	O2B-PB-O1B	3.65	117.70	109.87
5	E	707	GTP	N9-C4-N3	3.64	133.23	125.95
5	D	707	GTP	O2B-PB-O3A	-3.60	97.55	107.27
5	C	707	GTP	N9-C4-N3	3.42	132.80	125.95
5	D	707	GTP	N9-C4-N3	3.41	132.76	125.95
5	E	707	GTP	C2-N3-C4	3.40	118.15	112.30
5	E	707	GTP	O6-C6-C5	-3.38	117.60	126.53
4	G	706	DZ4	O1A-PA-N3A	-3.38	106.80	111.77
5	A	706	GTP	O2A-PA-O1A	3.36	128.07	112.44
5	B	706	GTP	C5-C4-N3	-3.35	123.06	128.39
5	A	706	GTP	O3B-PG-O1G	-3.31	93.65	111.04
4	C	701	DZ4	O2B-PB-O1B	3.21	116.76	109.87
5	E	706	GTP	C2-N3-C4	3.21	117.83	112.30
5	E	707	GTP	C5-C4-N3	-3.20	123.30	128.39
4	C	701	DZ4	O2A-PA-O1A	3.19	116.70	109.87
5	C	707	GTP	O2A-PA-O3A	3.18	115.86	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	705	DZ4	O2A-PA-O1A	3.17	116.67	109.87
5	A	706	GTP	O6-C6-C5	-3.17	118.17	126.53
5	E	706	GTP	N9-C4-N3	3.12	132.19	125.95
4	E	705	DZ4	O3B-PB-N3A	-3.11	97.95	106.59
5	C	707	GTP	O3G-PG-O2G	3.10	119.43	107.80
5	D	707	GTP	O3G-PG-O2G	3.09	119.39	107.80
5	C	707	GTP	O2B-PB-O1B	3.07	126.72	112.44
5	D	707	GTP	C2-N1-C6	-3.06	119.56	125.11
5	H	707	GTP	O3G-PG-O2G	3.05	119.25	107.80
5	C	707	GTP	O3'-C3'-C4'	-3.02	102.41	111.08
5	B	706	GTP	C3'-C2'-C1'	2.99	107.13	101.46
5	D	707	GTP	O3G-PG-O3B	2.97	114.60	104.64
4	A	707	DZ4	O5'-PA-O1A	-2.95	105.52	114.27
5	D	707	GTP	N2-C2-N1	2.94	122.98	116.76
5	E	707	GTP	C6-C5-C4	-2.94	114.40	118.83
4	D	706	DZ4	O5'-PA-O1A	-2.90	105.67	114.27
5	B	706	GTP	O2G-PG-O3B	-2.89	94.95	104.64
5	G	707	GTP	C4-C5-N7	-2.89	106.09	110.67
5	D	707	GTP	N2-C2-N3	-2.87	114.08	119.67
4	G	706	DZ4	O2A-PA-O1A	2.85	115.97	109.87
4	H	701	DZ4	O3B-PB-N3A	-2.82	98.76	106.59
5	G	707	GTP	O2B-PB-O3B	2.78	114.79	107.27
5	B	706	GTP	O5'-PA-O1A	-2.78	97.93	108.94
5	C	707	GTP	O5'-PA-O1A	-2.78	97.93	108.94
4	H	701	DZ4	O3G-PG-O2G	2.77	118.20	107.80
4	G	706	DZ4	O1B-PB-N3A	-2.77	107.69	111.77
4	E	705	DZ4	O2A-PA-O5'	-2.76	99.34	106.69
4	C	706	DZ4	O5'-PA-O1A	-2.71	106.23	114.27
4	E	708	DZ4	O3B-PB-N3A	-2.71	99.08	106.59
4	H	701	DZ4	O3G-PG-O3B	-2.70	95.59	104.64
5	D	707	GTP	O5'-PA-O1A	-2.69	98.26	108.94
4	D	701	DZ4	O5'-PA-O1A	-2.69	106.30	114.27
4	H	706	DZ4	O2A-PA-O5'	-2.65	99.63	106.69
5	E	706	GTP	O2A-PA-O1A	2.64	124.74	112.44
5	D	707	GTP	O3B-PB-O1B	2.64	118.64	110.70
4	A	705	DZ4	O1A-PA-N3A	-2.63	107.89	111.77
4	C	708	DZ4	O5'-PA-O1A	-2.63	106.45	114.27
4	F	705	DZ4	O2A-PA-O5'	-2.63	99.69	106.69
5	G	707	GTP	O3'-C3'-C4'	-2.63	103.53	111.08
5	G	707	GTP	N2-C2-N3	-2.62	114.56	119.67
5	C	707	GTP	O5'-C5'-C4'	2.62	117.90	108.99
5	A	706	GTP	O4'-C1'-N9	-2.61	102.45	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	707	GTP	C4-C5-N7	-2.60	106.55	110.67
5	E	706	GTP	C2'-C1'-N9	2.60	120.48	113.25
4	H	701	DZ4	O2A-PA-O5'	-2.60	99.78	106.69
5	G	707	GTP	O5'-C5'-C4'	2.57	117.76	108.99
5	A	706	GTP	O3G-PG-O2G	2.57	117.42	107.80
5	H	707	GTP	C6-C5-N7	2.56	134.95	130.29
5	E	707	GTP	O3B-PB-O1B	2.56	118.39	110.70
4	E	708	DZ4	O2A-PA-O5'	-2.55	99.91	106.69
5	D	707	GTP	O2A-PA-O1A	2.54	124.28	112.44
5	E	706	GTP	O2B-PB-O1B	2.54	124.27	112.44
5	A	706	GTP	C2-N1-C6	-2.53	120.52	125.11
4	D	706	DZ4	O1B-PB-N3A	-2.53	108.05	111.77
5	E	707	GTP	O2G-PG-O3B	-2.51	96.22	104.64
5	G	707	GTP	C8-N7-C5	2.51	108.73	104.26
5	E	707	GTP	O6-C6-N1	2.50	124.82	120.11
5	E	706	GTP	O3G-PG-O3B	2.49	112.97	104.64
5	G	707	GTP	C6-C5-C4	2.48	122.55	118.83
5	A	706	GTP	C5-C6-N1	2.46	119.52	113.25
5	A	706	GTP	O3G-PG-O3B	2.44	112.83	104.64
5	B	706	GTP	N9-C4-N3	2.44	130.84	125.95
4	B	705	DZ4	O2A-PA-O1A	2.43	115.09	109.87
5	H	707	GTP	O3G-PG-O1G	-2.43	101.38	110.83
5	D	707	GTP	C6-C5-N7	2.42	134.70	130.29
5	E	707	GTP	C6-C5-N7	2.42	134.70	130.29
5	E	706	GTP	C6-C5-N7	2.42	134.69	130.29
5	B	706	GTP	O6-C6-C5	-2.39	120.22	126.53
5	E	707	GTP	N2-C2-N1	2.37	121.75	116.76
5	H	707	GTP	C2-N1-C6	-2.35	120.85	125.11
5	C	707	GTP	O6-C6-C5	-2.35	120.34	126.53
5	H	707	GTP	O2'-C2'-C1'	-2.34	102.06	110.10
4	A	705	DZ4	O3G-PG-O1G	2.32	119.89	110.83
5	E	706	GTP	O3G-PG-O2G	2.32	116.50	107.80
5	G	707	GTP	C2'-C3'-C4'	2.32	107.09	102.61
5	D	707	GTP	O2'-C2'-C1'	-2.31	102.14	110.10
5	H	707	GTP	O6-C6-C5	-2.31	120.43	126.53
5	E	706	GTP	N2-C2-N1	2.29	121.59	116.76
5	E	707	GTP	O2G-PG-O1G	2.28	119.73	110.83
4	B	705	DZ4	O1A-PA-N3A	-2.27	108.42	111.77
5	B	706	GTP	O2A-PA-O1A	2.27	123.00	112.44
4	C	701	DZ4	O1B-PB-N3A	-2.26	108.44	111.77
5	B	706	GTP	O3B-PB-O1B	2.26	117.49	110.70
5	D	707	GTP	O6-C6-C5	-2.25	120.59	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	706	GTP	C4-C5-N7	-2.25	107.11	110.67
5	H	707	GTP	C2-N3-C4	2.24	116.15	112.30
5	H	707	GTP	O5'-PA-O1A	-2.23	100.08	108.94
5	A	706	GTP	C1'-N9-C8	-2.23	120.39	126.73
5	H	707	GTP	C3'-C2'-C1'	2.23	105.68	101.46
5	E	707	GTP	O2B-PB-O3B	2.23	113.30	107.27
5	E	706	GTP	O3A-PA-O1A	-2.21	104.07	110.70
5	B	706	GTP	C6-C5-N7	2.19	134.27	130.29
5	E	706	GTP	N9-C8-N7	-2.18	109.37	113.40
5	C	707	GTP	O2G-PG-O3B	-2.16	97.39	104.64
5	B	706	GTP	O3A-PB-O1B	-2.15	104.22	110.70
5	A	706	GTP	O5'-PA-O1A	-2.14	100.46	108.94
5	B	706	GTP	O3G-PG-O1G	2.13	119.15	110.83
4	E	708	DZ4	O3G-PG-O3B	-2.13	97.48	104.64
5	A	706	GTP	O2B-PB-O1B	2.13	122.35	112.44
4	F	706	DZ4	O2A-PA-O5'	2.13	112.34	106.69
4	H	706	DZ4	O3B-PB-N3A	-2.12	100.72	106.59
5	G	707	GTP	O2A-PA-O3A	2.11	112.98	107.27
5	E	706	GTP	O6-C6-C5	-2.11	120.97	126.53
5	C	707	GTP	N2-C2-N3	-2.08	115.60	119.67
4	C	708	DZ4	O2B-PB-O3B	-2.08	97.71	104.64
4	E	705	DZ4	O1B-PB-N3A	-2.07	108.72	111.77
4	C	706	DZ4	C5-C6-N6	2.07	128.42	123.29
5	C	707	GTP	C2-N3-C4	2.06	115.84	112.30
5	C	707	GTP	C6-C5-N7	2.05	134.02	130.29
5	B	706	GTP	O2'-C2'-C1'	-2.04	103.09	110.10
5	E	706	GTP	C8-N9-C4	2.03	109.83	106.03
5	H	707	GTP	C8-N7-C5	2.03	107.87	104.26

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	DZ4	PA-N3A-PB-O1B
4	A	707	DZ4	PB-N3A-PA-O1A
4	A	707	DZ4	PA-N3A-PB-O1B
4	B	705	DZ4	PA-N3A-PB-O1B
4	C	701	DZ4	PA-N3A-PB-O1B
4	C	706	DZ4	PA-N3A-PB-O1B
4	C	708	DZ4	PB-N3A-PA-O1A
4	C	708	DZ4	PG-O3B-PB-O1B
4	C	708	DZ4	PG-O3B-PB-O2B

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Mol	Chain	Res	Type	Atoms
4	D	701	DZ4	PB-N3A-PA-O1A
4	D	701	DZ4	PA-N3A-PB-O1B
4	D	706	DZ4	PA-N3A-PB-O1B
4	E	705	DZ4	PA-N3A-PB-O1B
4	E	708	DZ4	PB-N3A-PA-O1A
4	E	708	DZ4	PG-O3B-PB-O2B
4	F	705	DZ4	PA-N3A-PB-O1B
4	F	706	DZ4	PB-N3A-PA-O1A
4	G	701	DZ4	PB-N3A-PA-O1A
4	G	701	DZ4	PA-N3A-PB-O1B
4	G	701	DZ4	PG-O3B-PB-O1B
4	G	706	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PG-O3B-PB-O1B
4	H	701	DZ4	PG-O3B-PB-O2B
4	H	706	DZ4	PA-N3A-PB-O1B
5	A	706	GTP	C5'-O5'-PA-O2A
5	D	707	GTP	C5'-O5'-PA-O2A
5	E	706	GTP	PB-O3B-PG-O3G
5	E	706	GTP	C5'-O5'-PA-O3A
5	E	706	GTP	C5'-O5'-PA-O1A
5	E	706	GTP	C4'-C5'-O5'-PA
5	E	707	GTP	PB-O3B-PG-O3G
5	E	707	GTP	C5'-O5'-PA-O2A
5	H	707	GTP	PB-O3B-PG-O3G
5	E	706	GTP	O4'-C4'-C5'-O5'
5	E	706	GTP	C3'-C4'-C5'-O5'
5	C	707	GTP	PB-O3B-PG-O1G
5	E	707	GTP	PB-O3B-PG-O1G
5	G	707	GTP	PB-O3B-PG-O1G
5	A	706	GTP	PB-O3B-PG-O1G
5	B	706	GTP	PB-O3B-PG-O3G
5	C	707	GTP	PB-O3B-PG-O3G
5	G	707	GTP	PB-O3B-PG-O3G
5	C	707	GTP	PG-O3B-PB-O1B
5	C	707	GTP	PB-O3A-PA-O2A
5	D	707	GTP	PG-O3B-PB-O1B
5	E	706	GTP	PB-O3A-PA-O2A
5	G	707	GTP	PG-O3B-PB-O1B
5	D	707	GTP	C4'-C5'-O5'-PA
4	C	708	DZ4	PA-N3A-PB-O3B
5	C	707	GTP	C5'-O5'-PA-O3A

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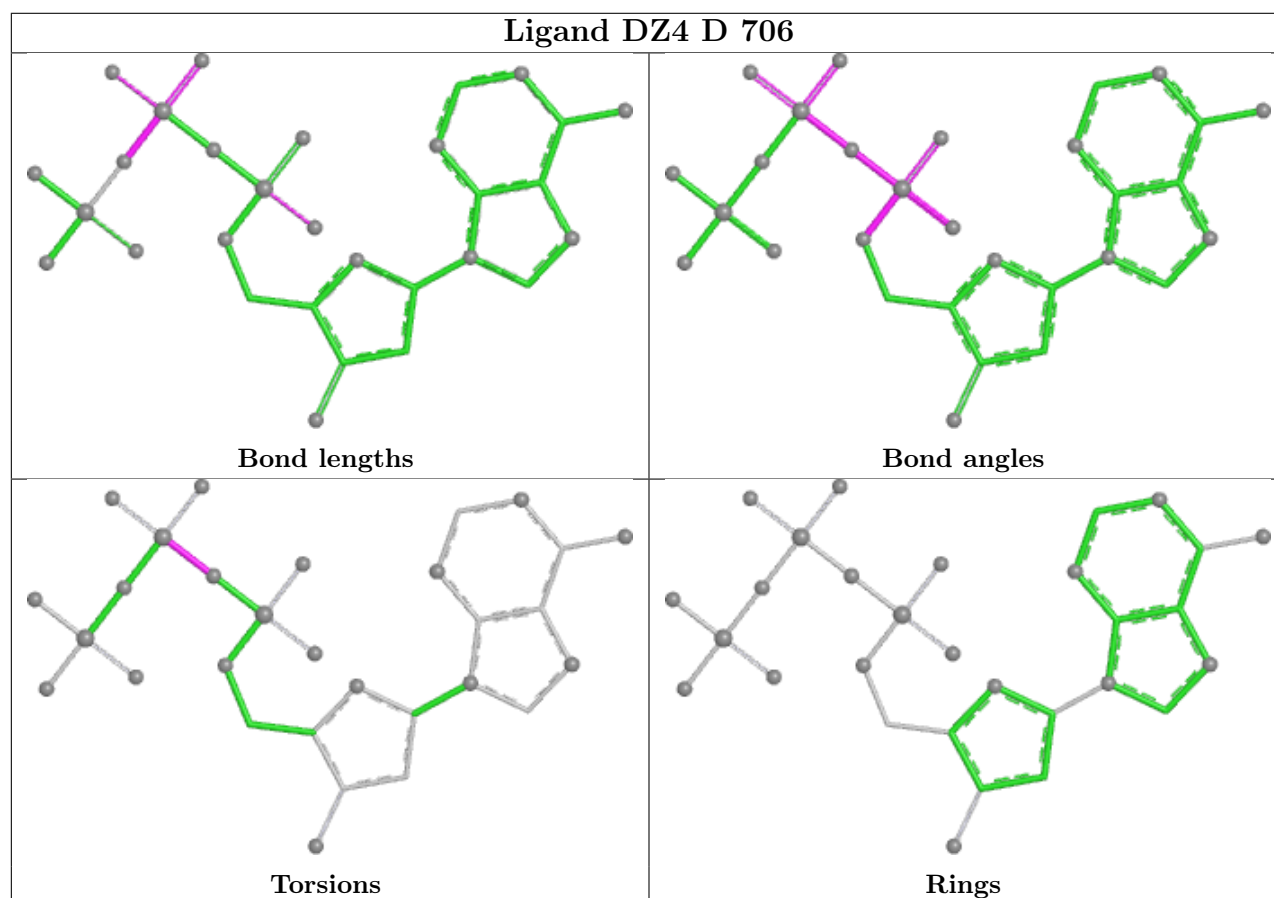
Mol	Chain	Res	Type	Atoms
5	D	707	GTP	C5'-O5'-PA-O3A
5	B	706	GTP	C4'-C5'-O5'-PA
5	C	707	GTP	C4'-C5'-O5'-PA
5	E	707	GTP	C4'-C5'-O5'-PA
5	G	707	GTP	C4'-C5'-O5'-PA
5	B	706	GTP	PB-O3B-PG-O1G
5	D	707	GTP	PB-O3B-PG-O1G
5	A	706	GTP	PB-O3A-PA-O2A
5	B	706	GTP	PB-O3A-PA-O2A
5	D	707	GTP	PB-O3A-PA-O2A
5	E	707	GTP	PB-O3A-PA-O2A
5	G	707	GTP	PB-O3A-PA-O2A
5	H	707	GTP	PB-O3A-PA-O2A
5	A	706	GTP	C4'-C5'-O5'-PA
4	C	701	DZ4	PB-N3A-PA-O1A
4	C	708	DZ4	PA-N3A-PB-O1B
4	E	708	DZ4	PA-N3A-PB-O1B
4	H	701	DZ4	PB-N3A-PA-O1A
5	C	707	GTP	PB-O3A-PA-O1A
5	E	706	GTP	PB-O3A-PA-O1A
4	D	701	DZ4	PG-O3B-PB-O2B
4	G	701	DZ4	PG-O3B-PB-O2B
4	F	705	DZ4	C5'-O5'-PA-N3A
4	F	705	DZ4	C5'-O5'-PA-O2A
5	H	707	GTP	C4'-C5'-O5'-PA
5	E	706	GTP	PB-O3B-PG-O1G
5	A	706	GTP	PG-O3B-PB-O1B
5	A	706	GTP	PB-O3A-PA-O1A
5	B	706	GTP	PG-O3B-PB-O1B
5	B	706	GTP	PB-O3A-PA-O1A
5	E	707	GTP	PB-O3A-PA-O1A
5	G	707	GTP	PG-O3B-PB-O2B
5	G	707	GTP	PB-O3A-PA-O1A
5	H	707	GTP	PG-O3B-PB-O2B
4	C	701	DZ4	PG-O3B-PB-O1B
4	D	701	DZ4	PG-O3B-PB-O1B
4	E	708	DZ4	PG-O3B-PB-O1B
4	F	706	DZ4	PG-O3B-PB-O1B
4	D	701	DZ4	PA-N3A-PB-O3B
4	E	708	DZ4	PA-N3A-PB-O3B
4	F	706	DZ4	PA-N3A-PB-O3B
5	D	707	GTP	PB-O3A-PA-O1A

There are no ring outliers.

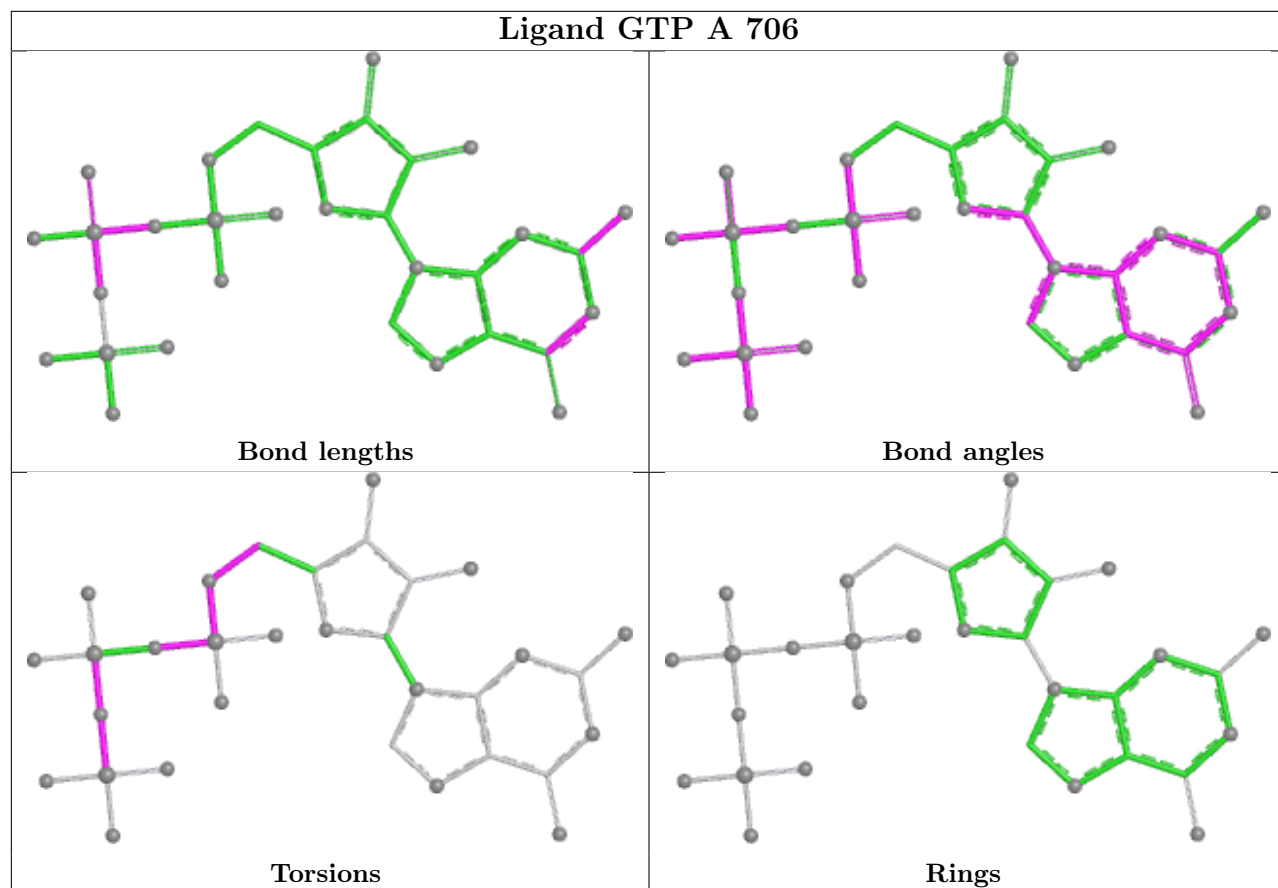
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	706	DZ4	1	0
5	D	707	GTP	1	0

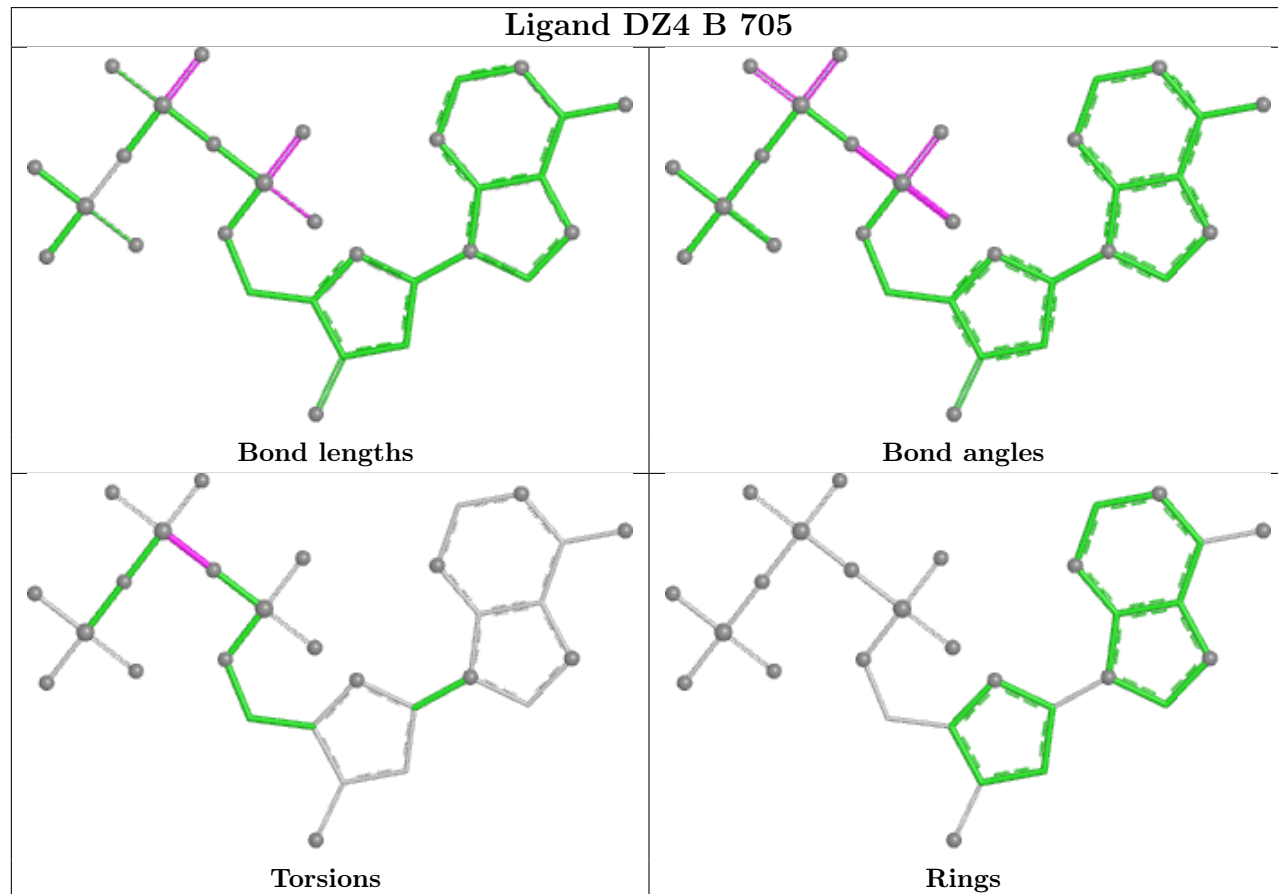
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



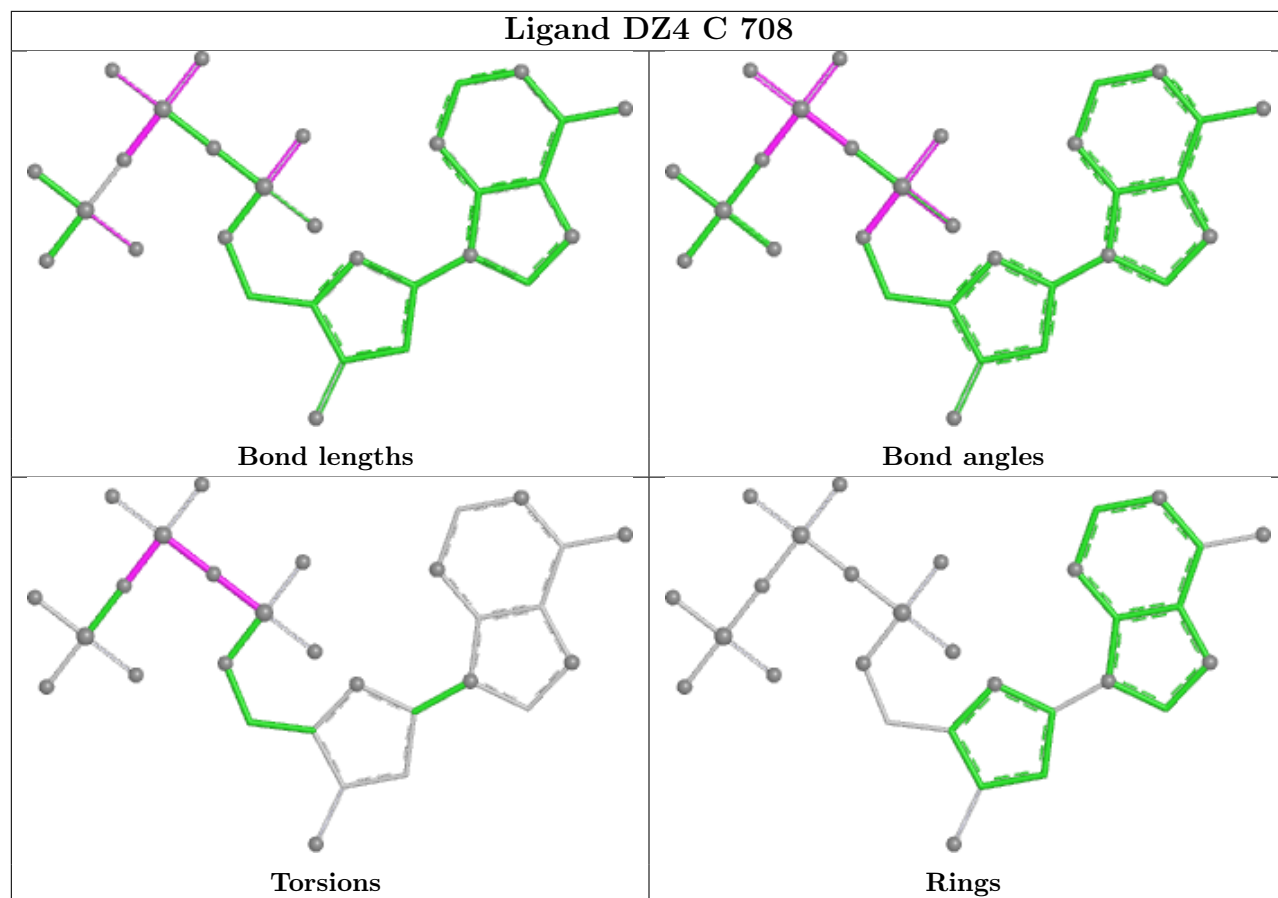
Ligand GTP A 706



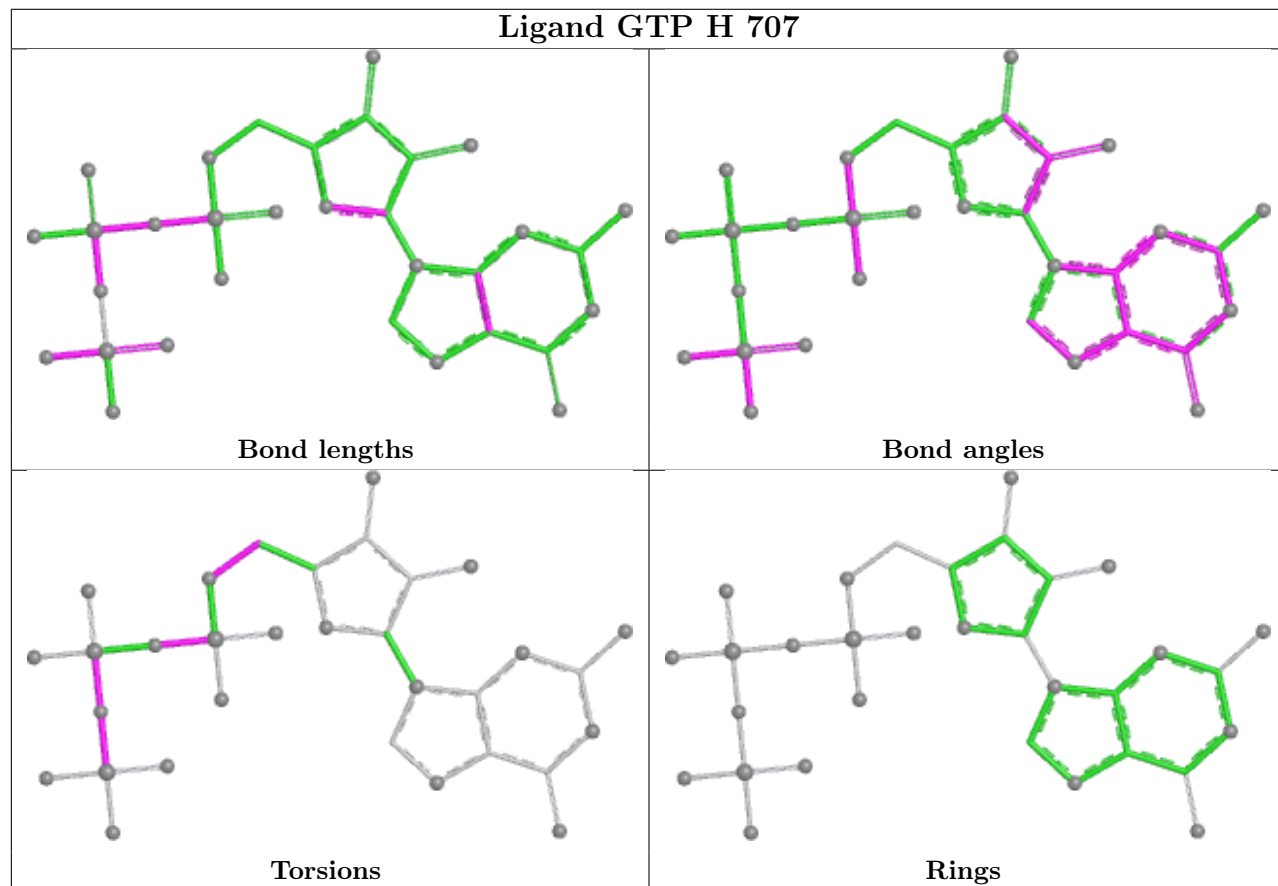
Ligand DZ4 B 705



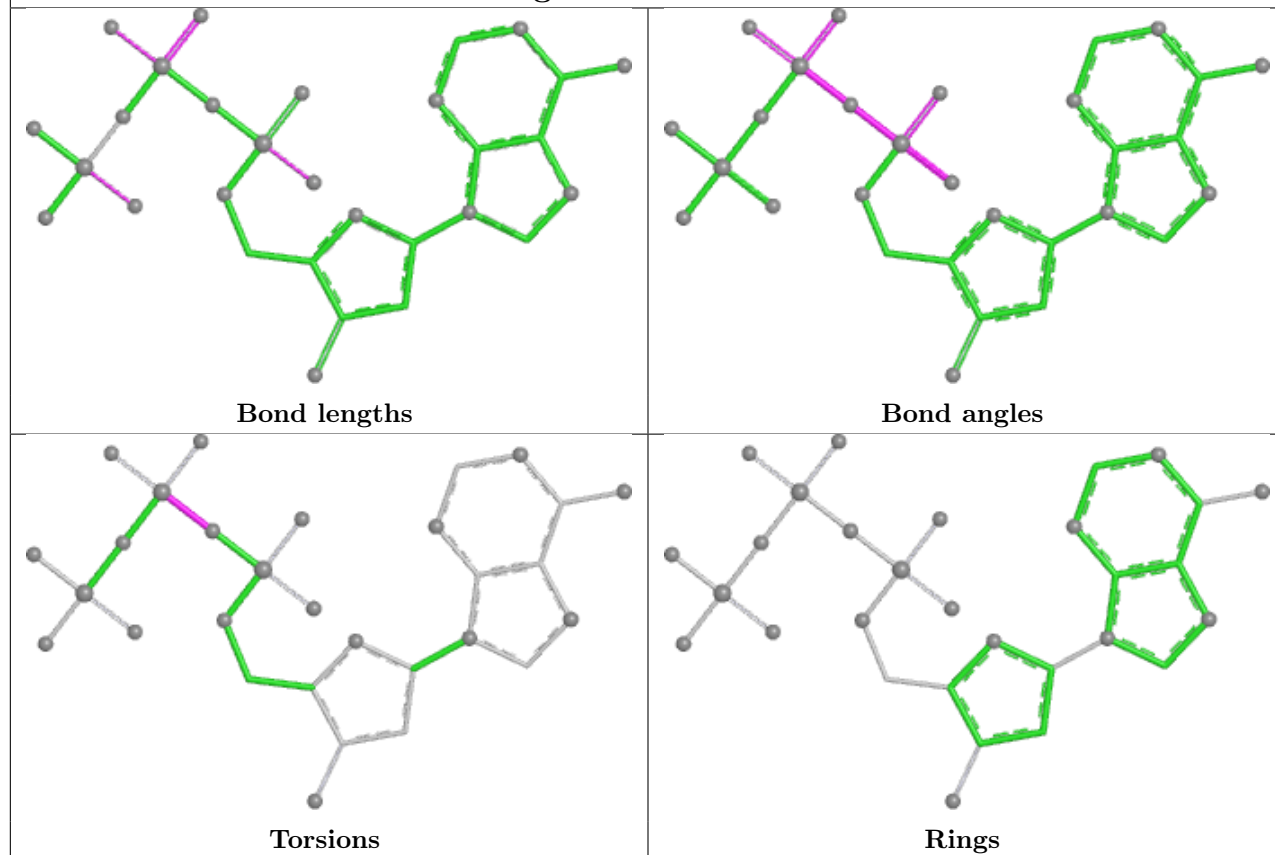
Ligand DZ4 C 708



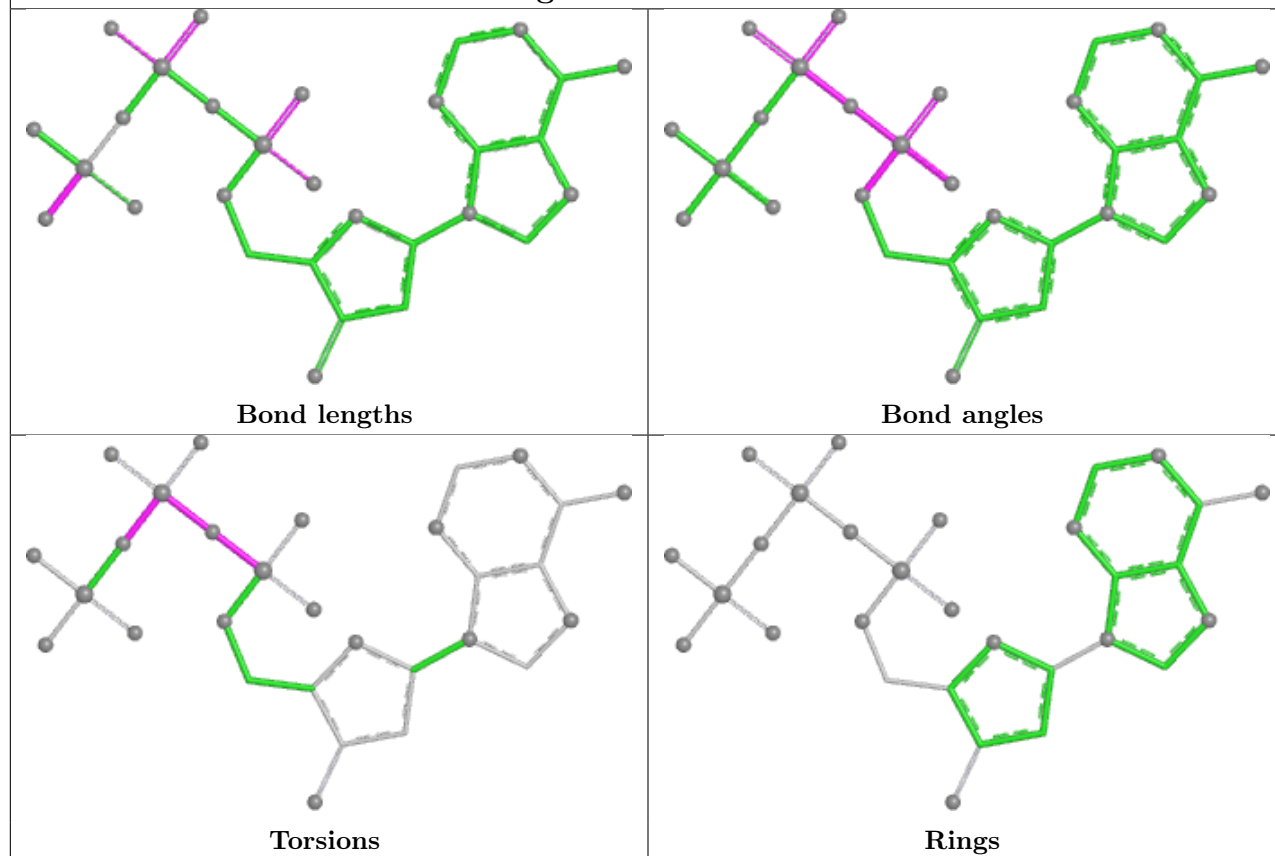
Ligand GTP H 707



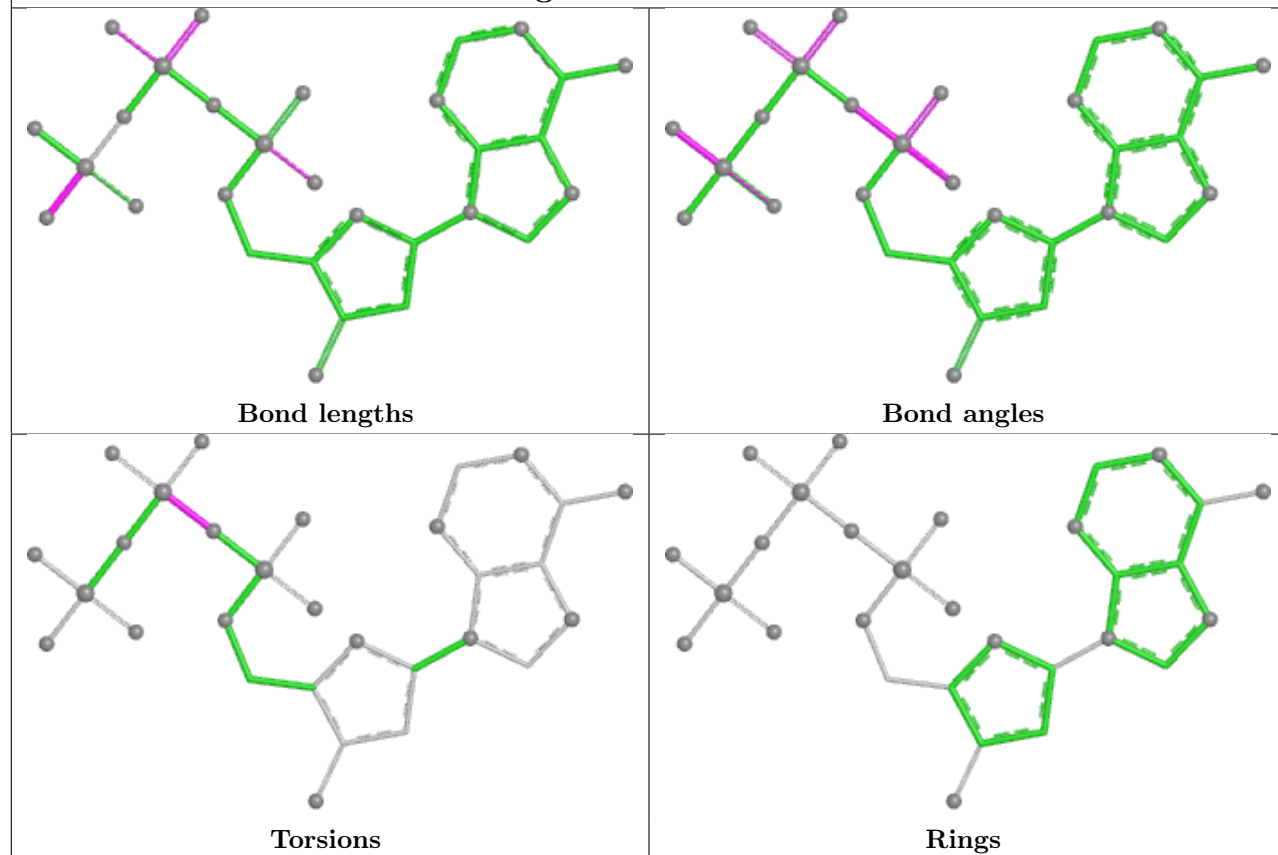
Ligand DZ4 G 706



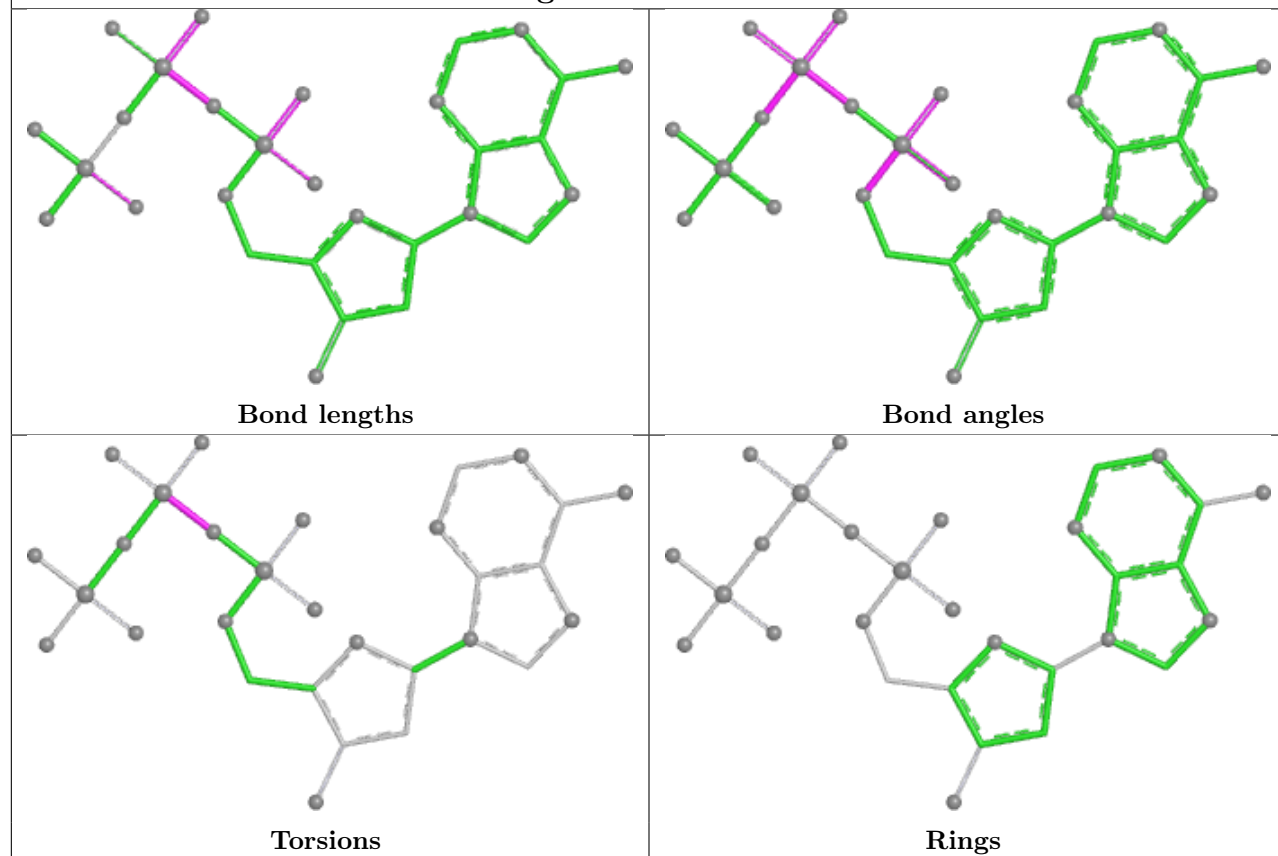
Ligand DZ4 F 706



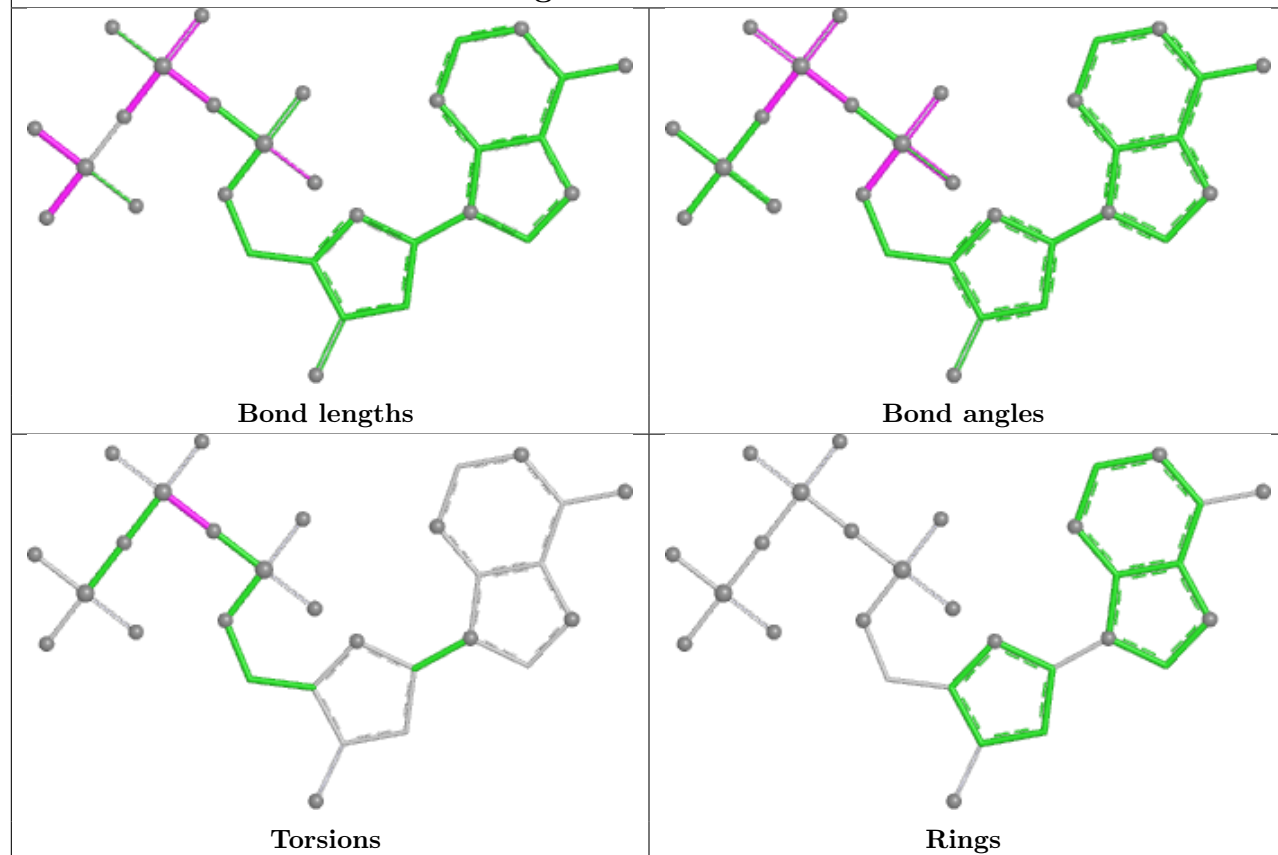
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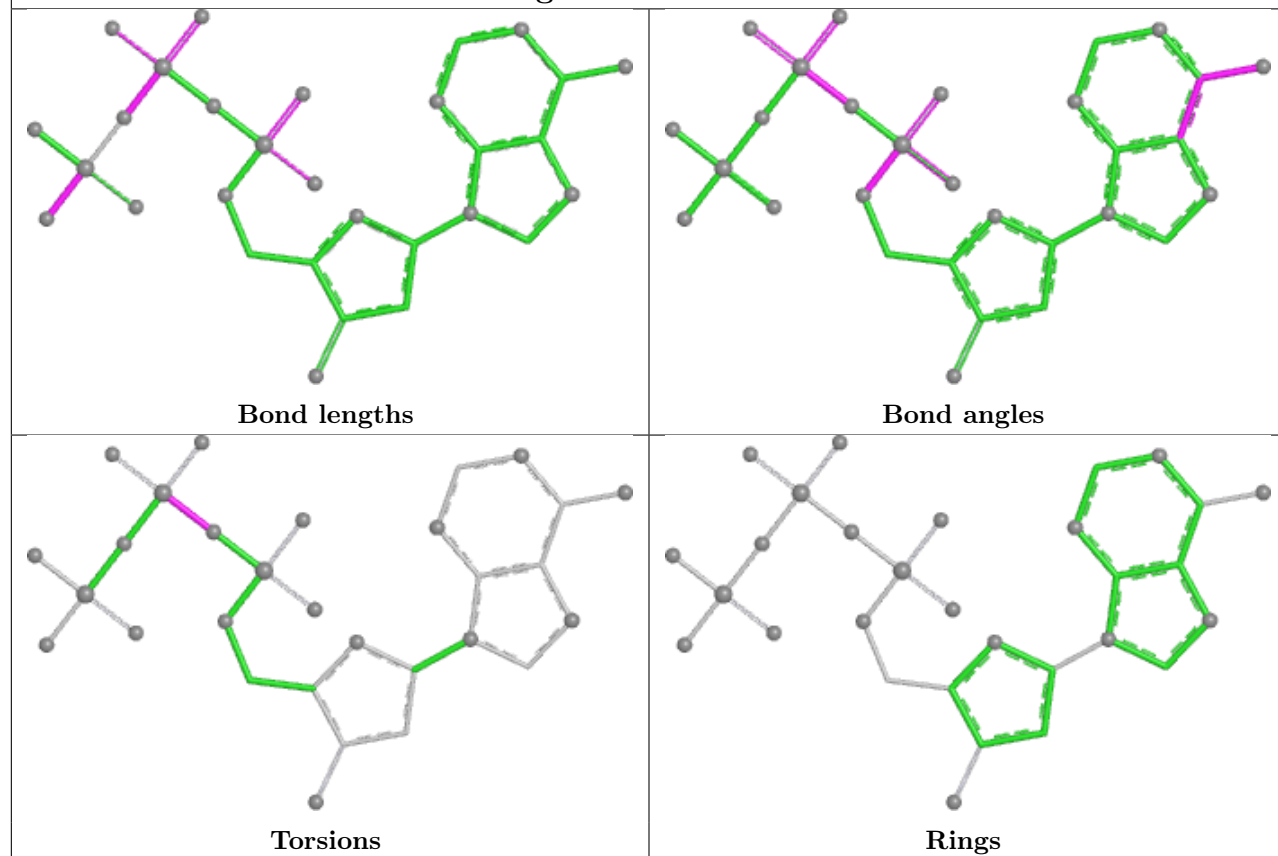
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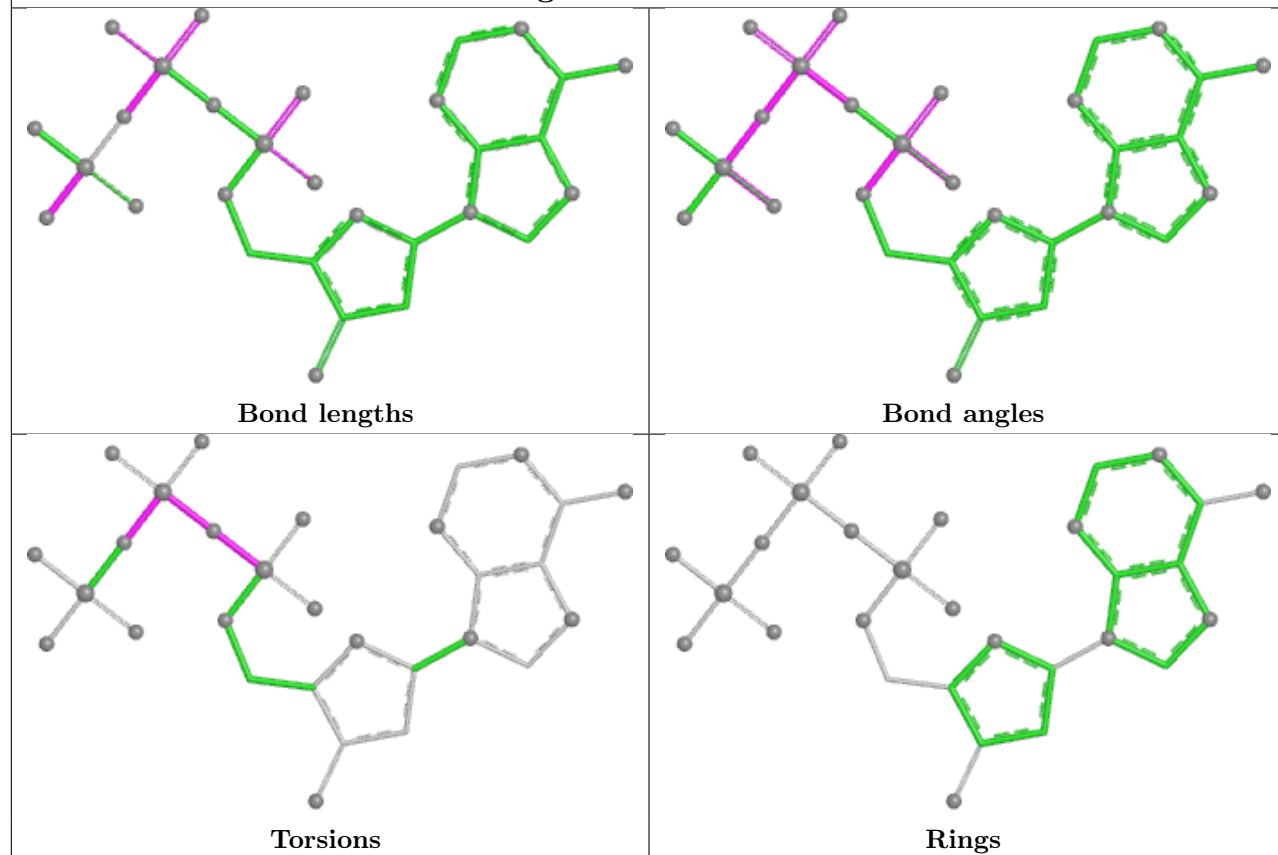
Ligand DZ4 H 706



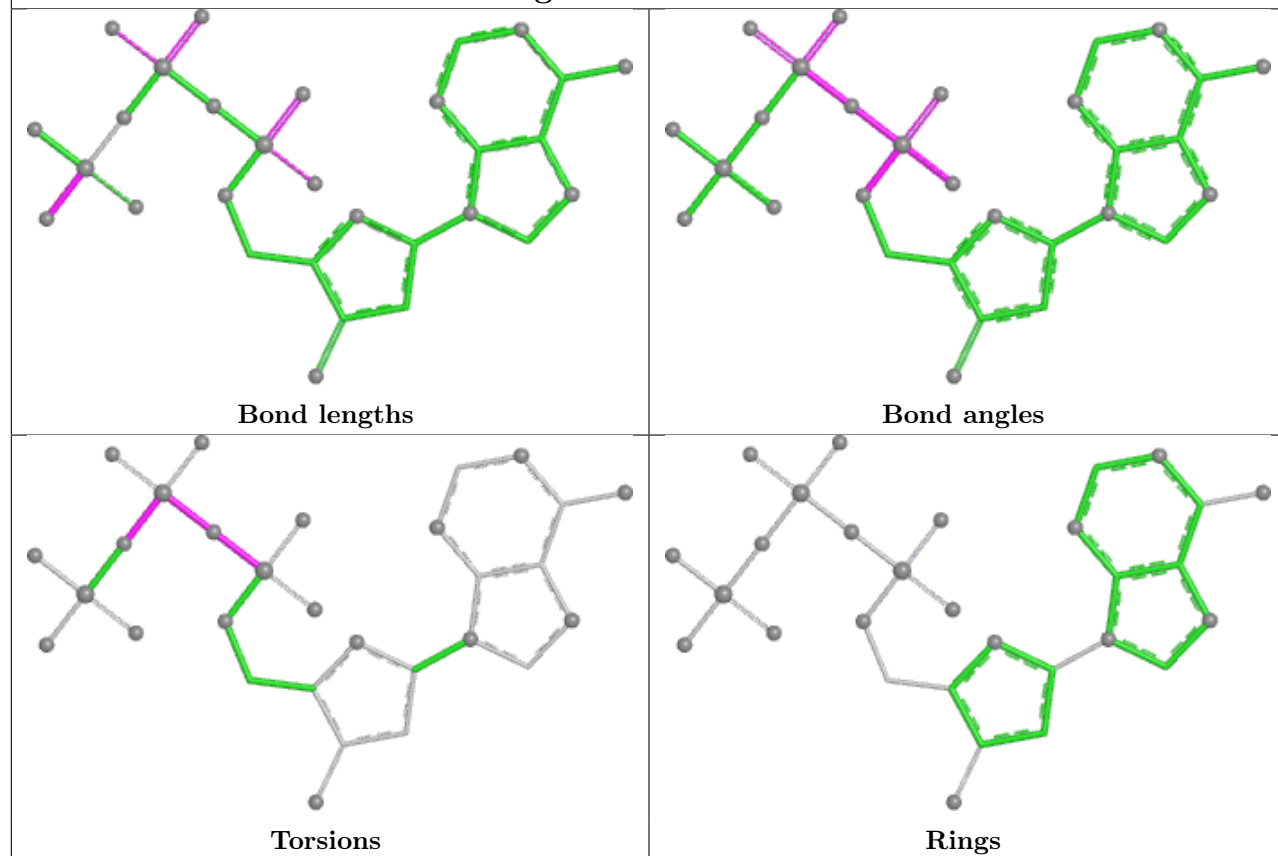
Ligand DZ4 C 706



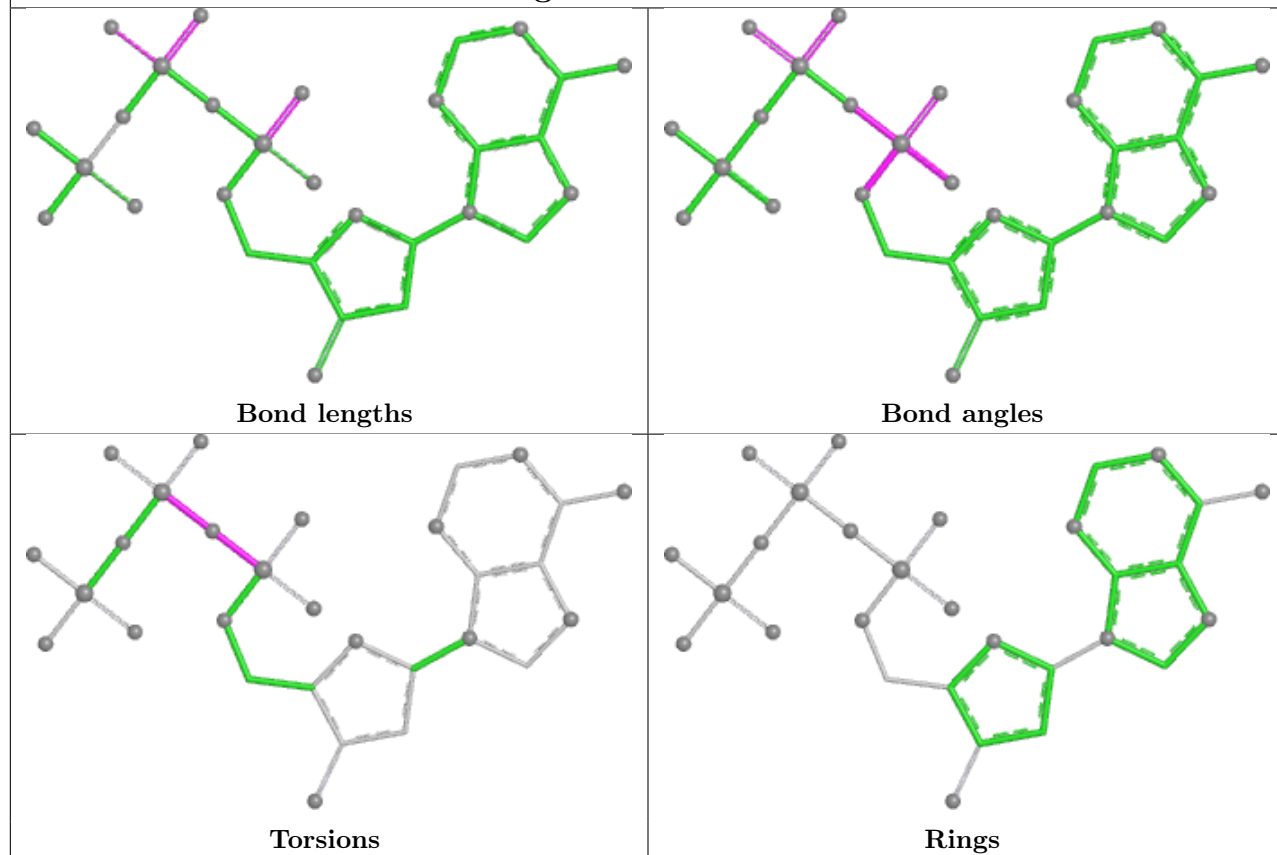
Ligand DZ4 E 708



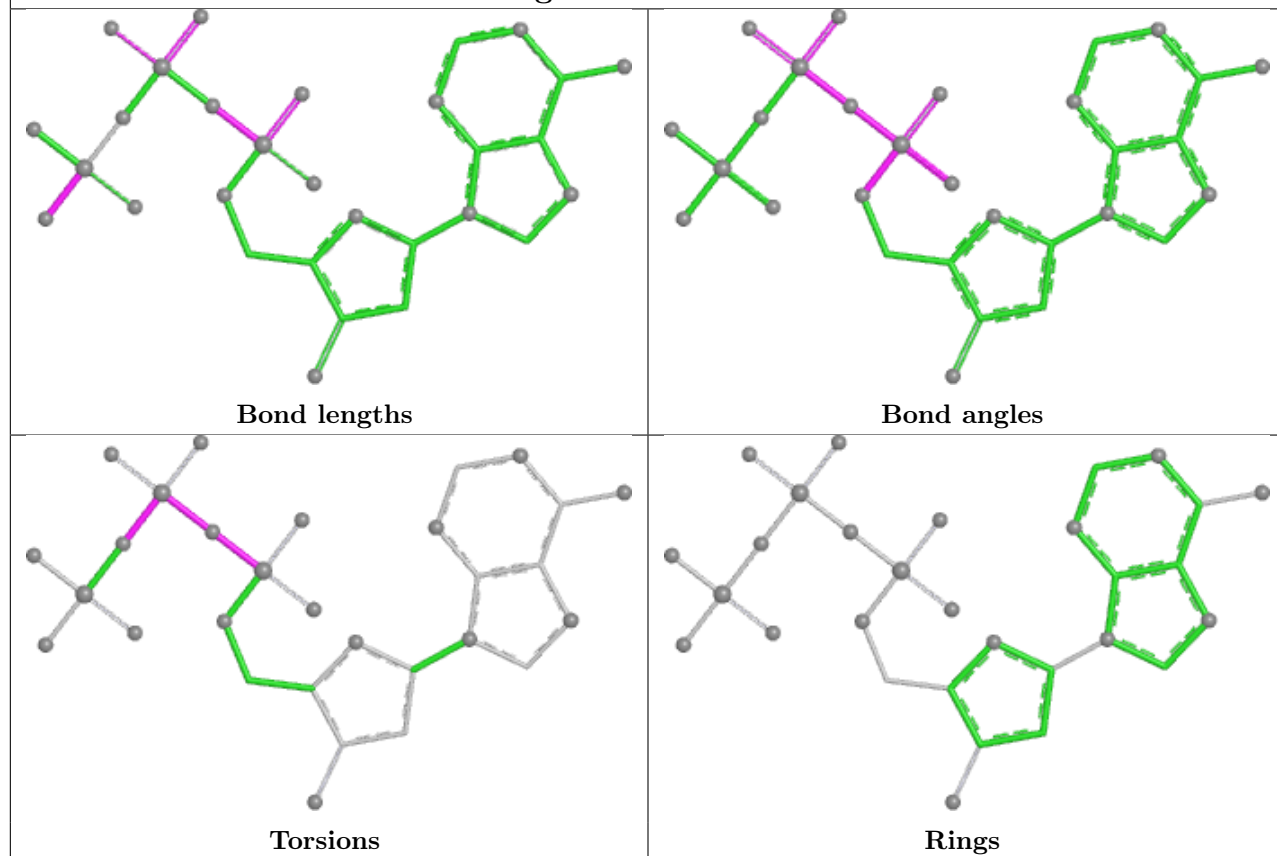
Ligand DZ4 G 701



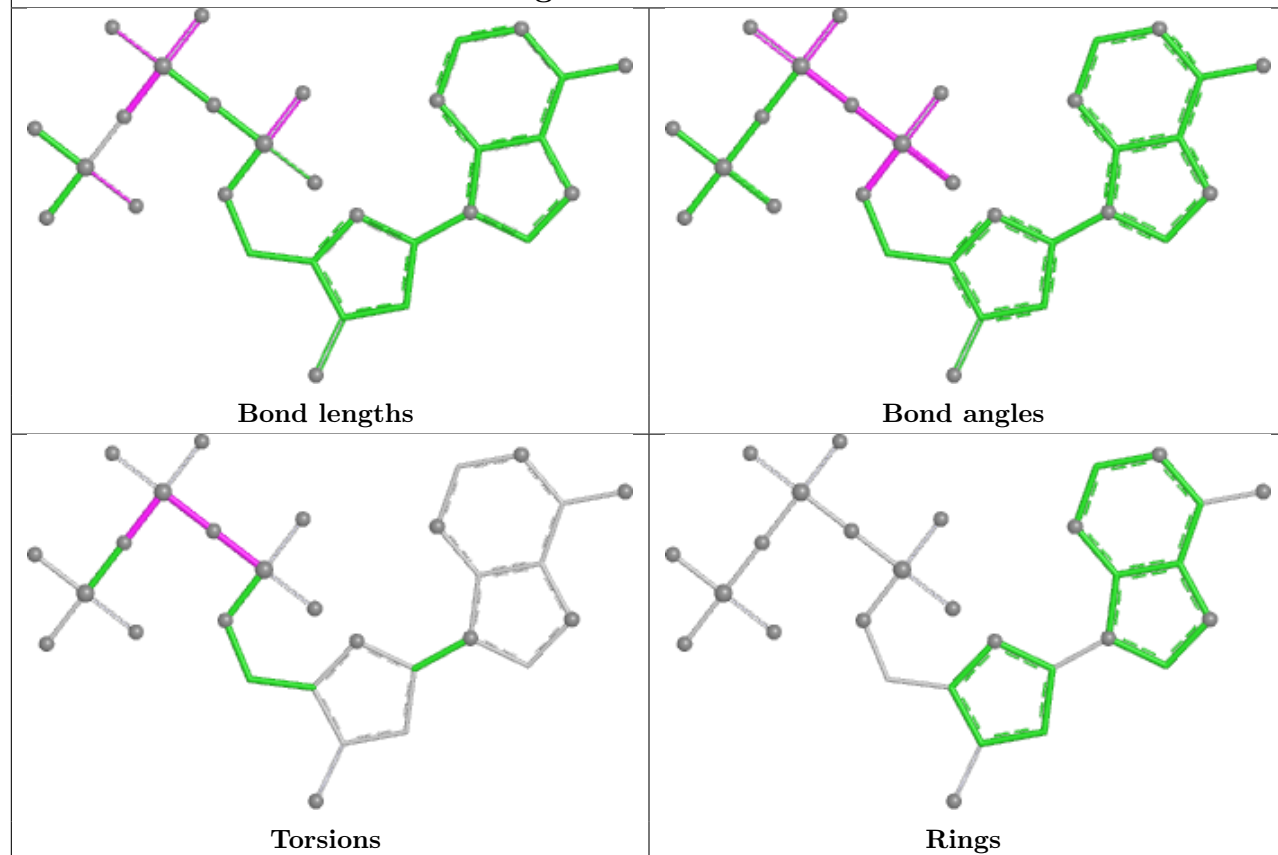
Ligand DZ4 A 707



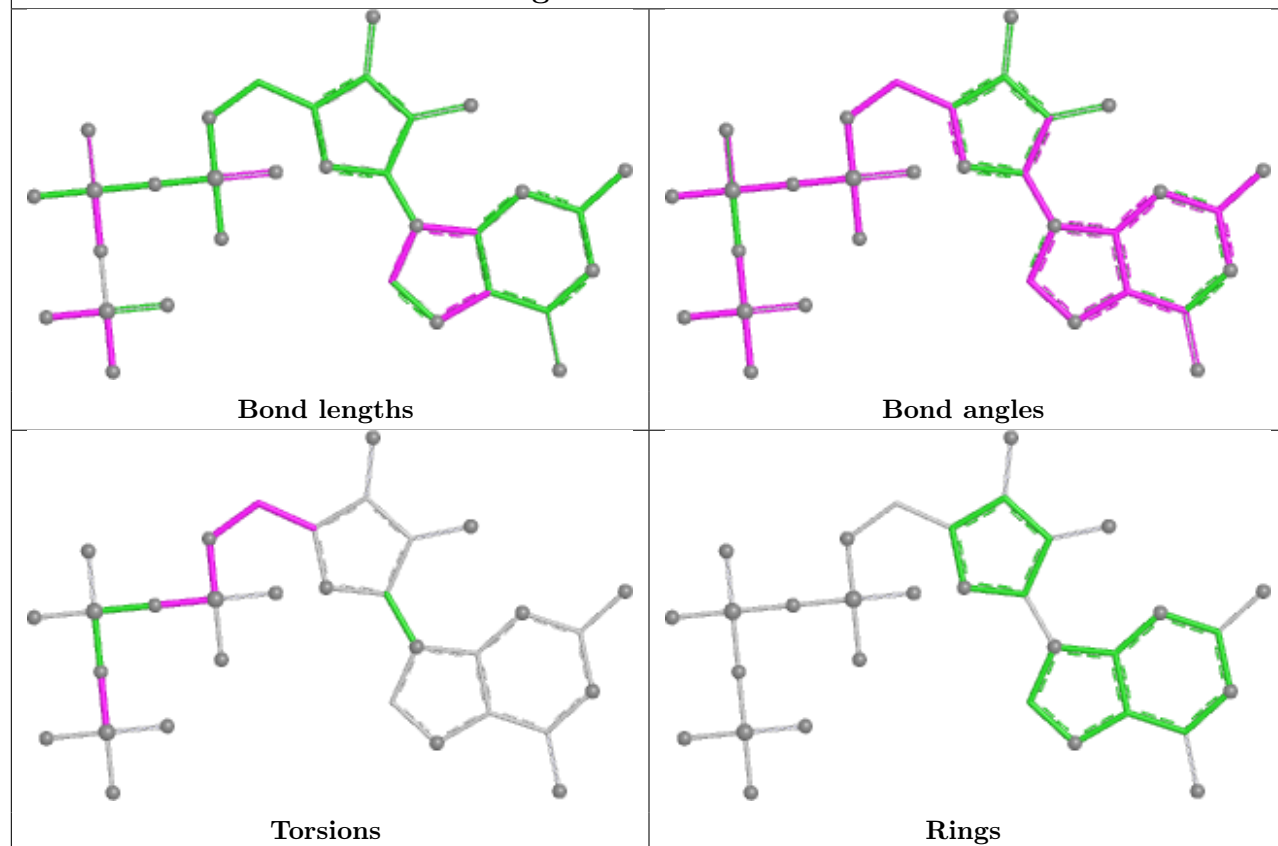
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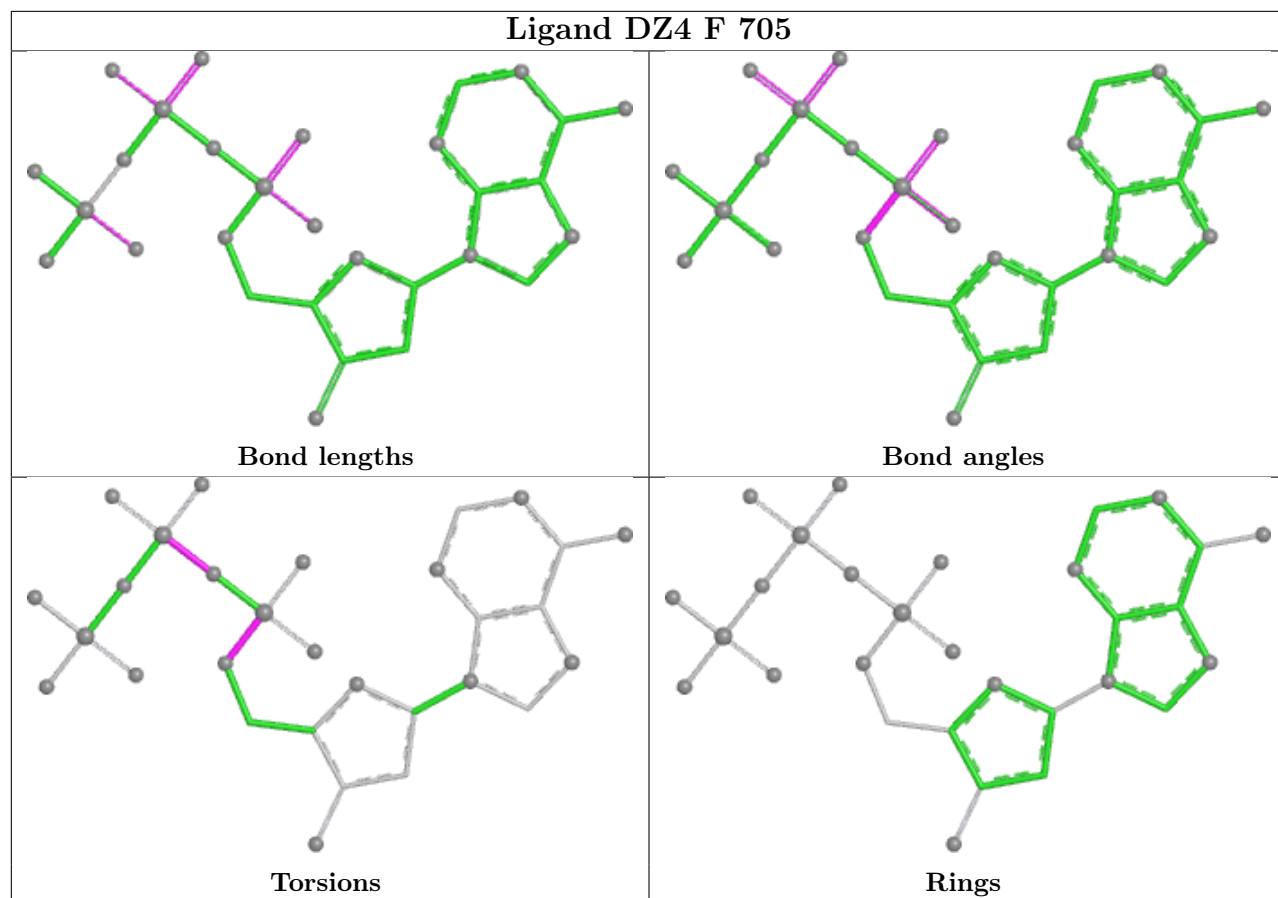
Ligand DZ4 D 701



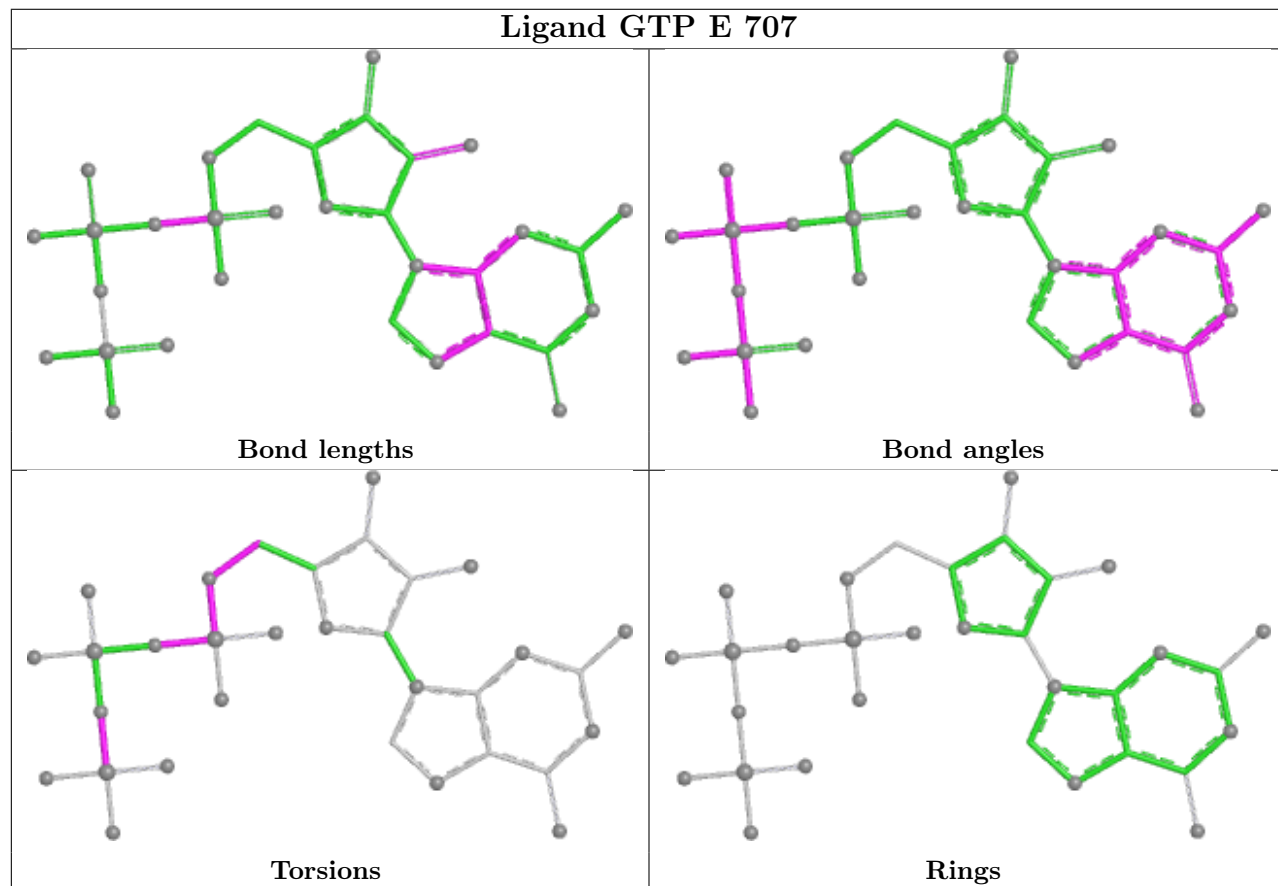
Ligand GTP E 706



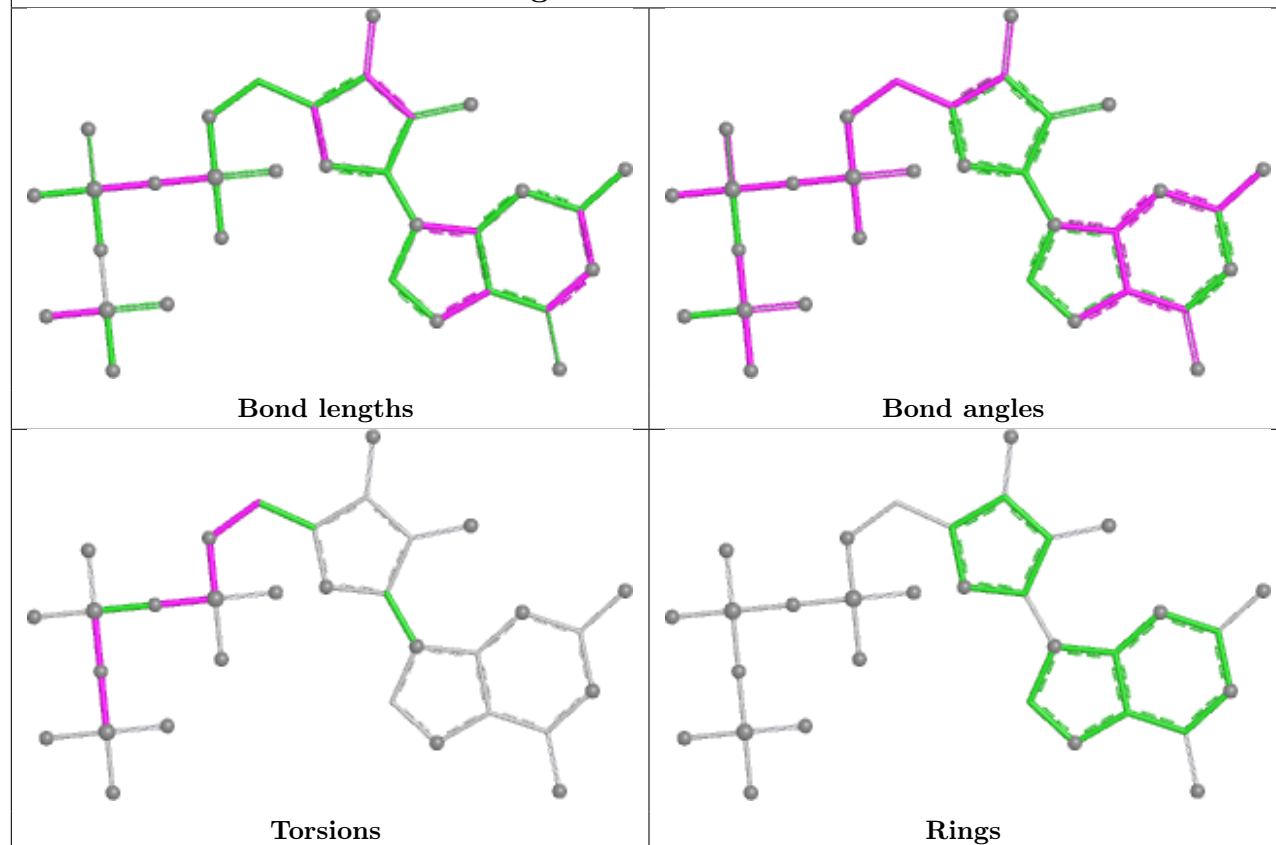
Ligand DZ4 F 705



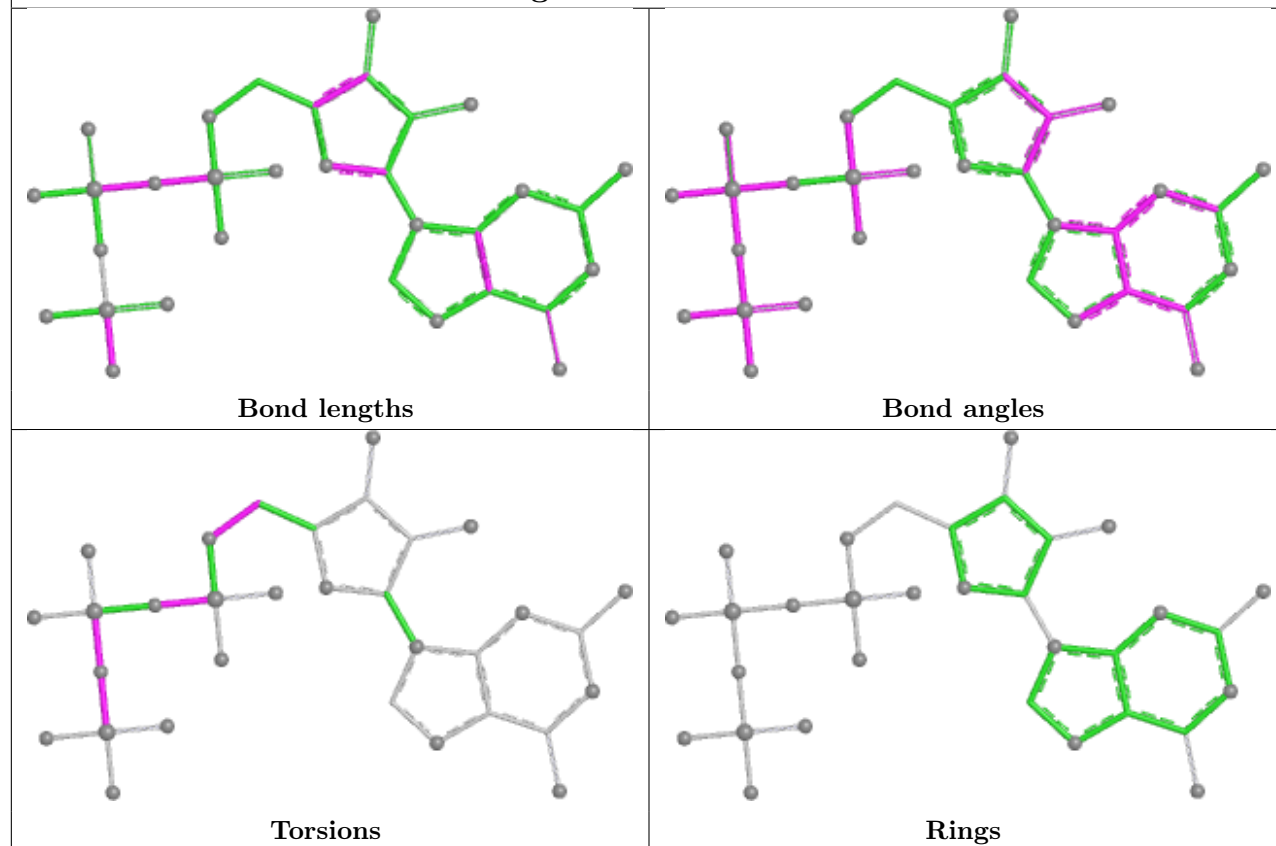
Ligand GTP E 707



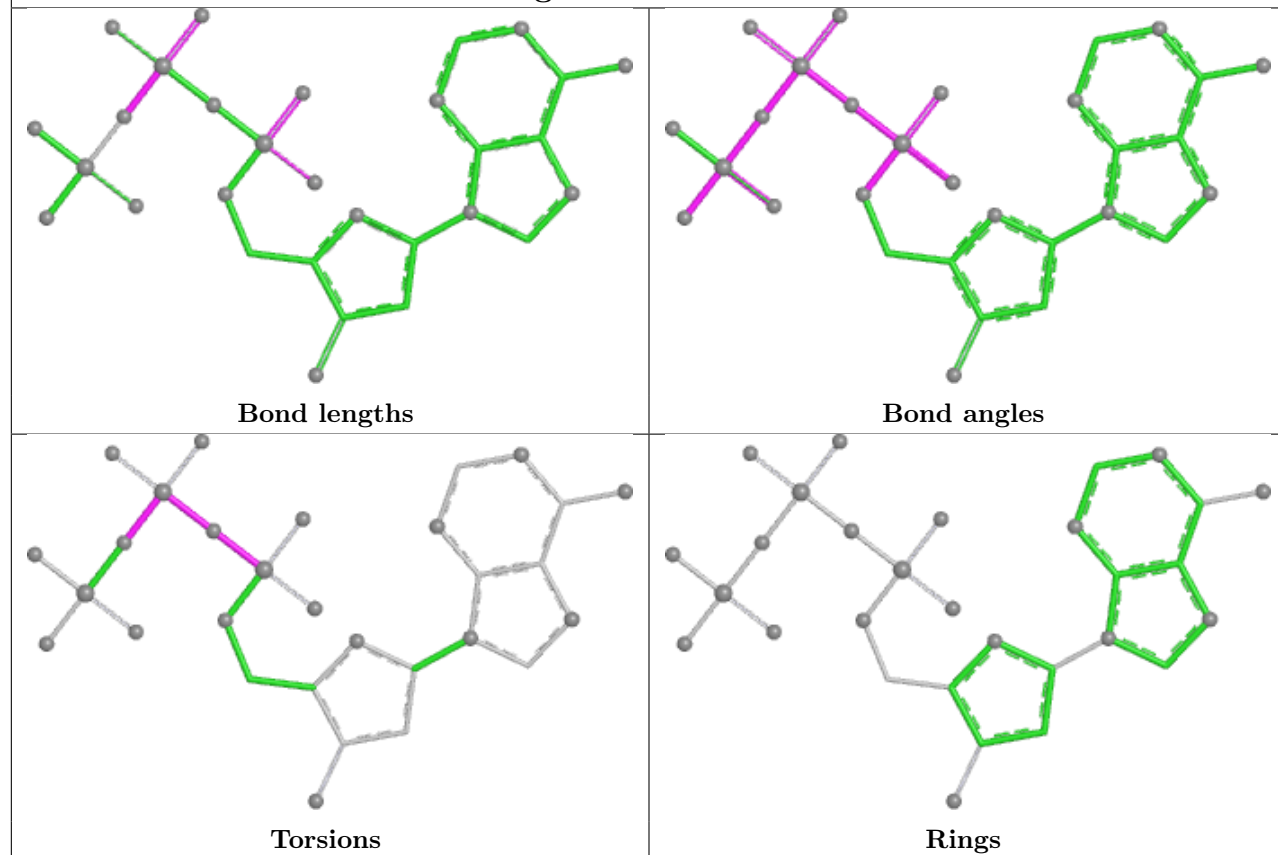
Ligand GTP C 707



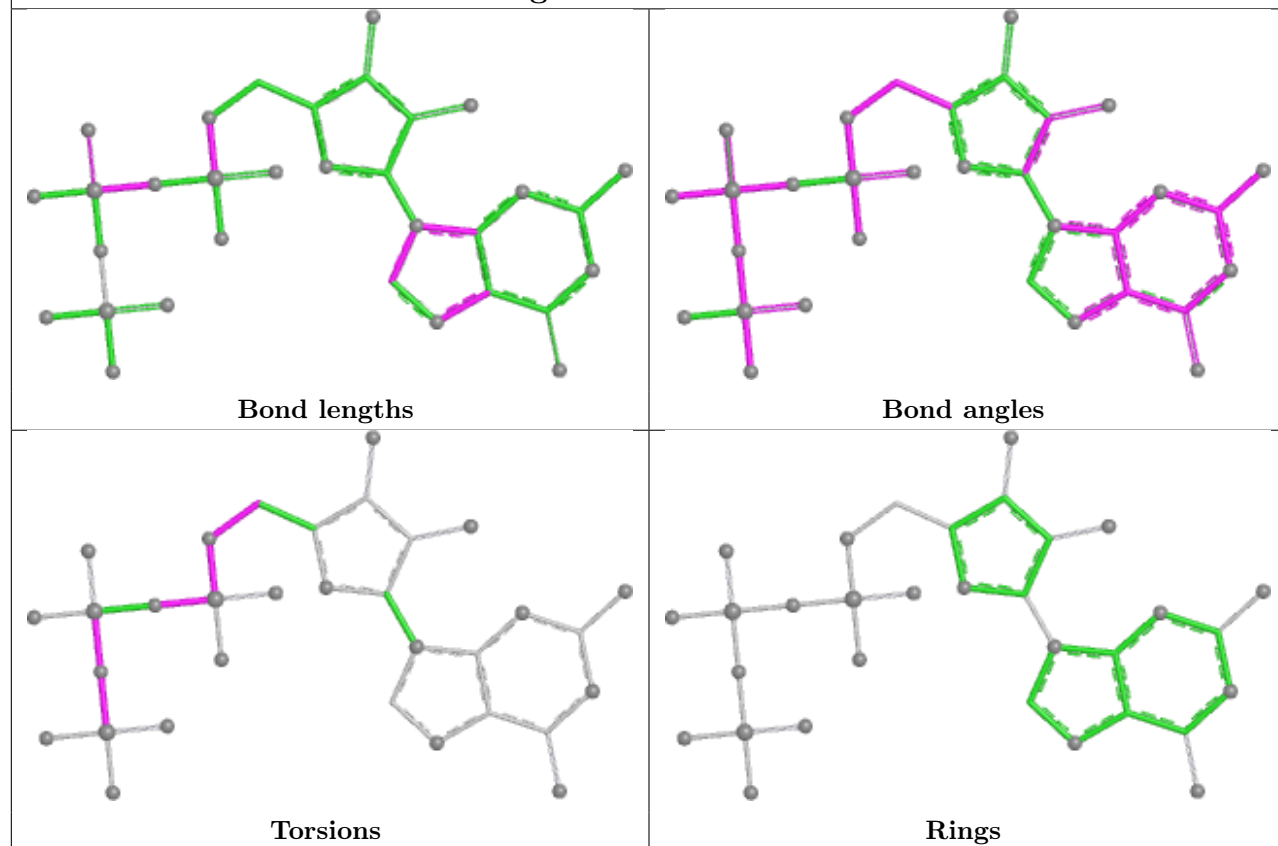
Ligand GTP B 706

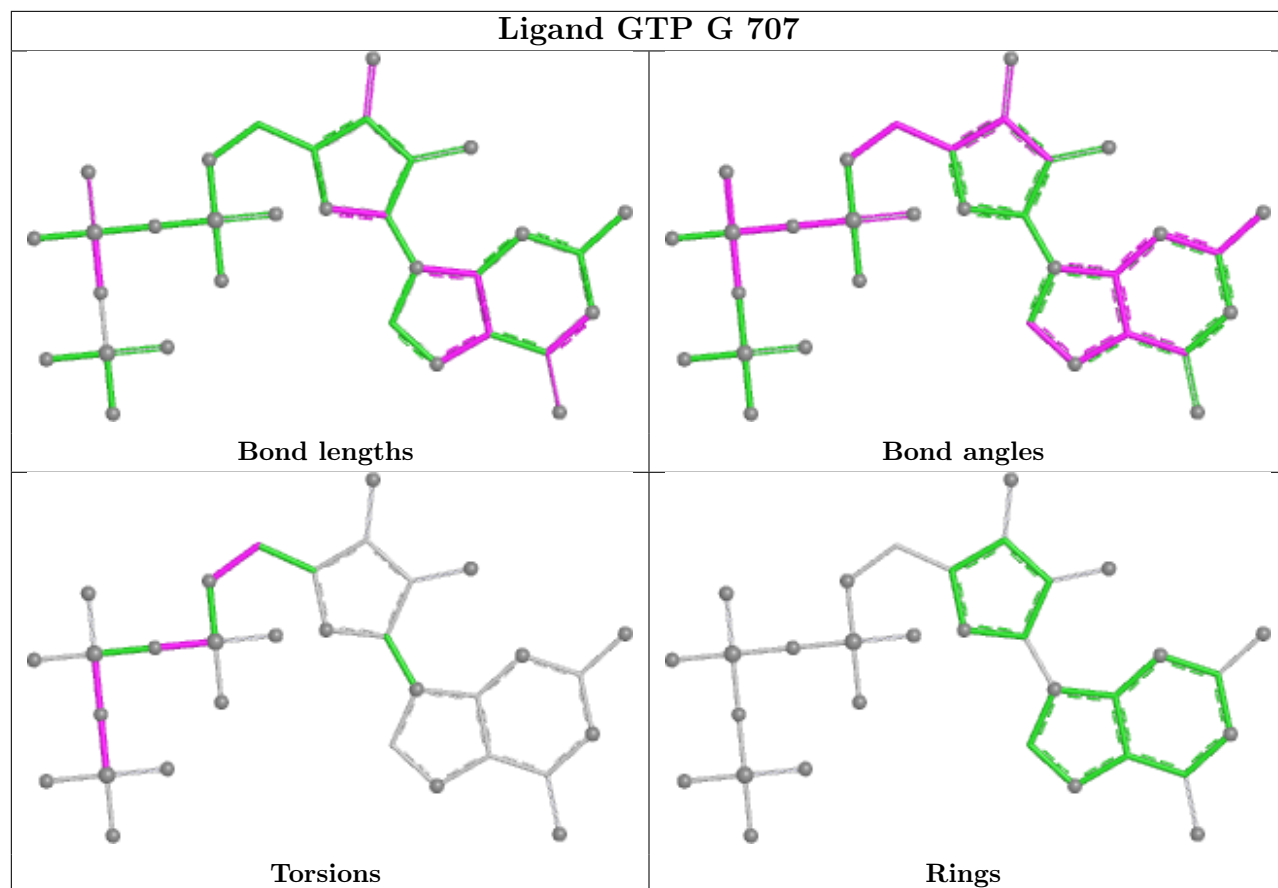


Ligand DZ4 H 701



Ligand GTP D 707





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	480/520 (92%)	-0.10	21 (4%) 39 36	12, 27, 59, 93	0
1	B	479/520 (92%)	-0.20	8 (1%) 69 66	12, 25, 53, 73	0
1	C	478/520 (91%)	-0.15	10 (2%) 63 60	12, 25, 57, 79	0
1	D	478/520 (91%)	-0.15	10 (2%) 63 60	13, 27, 54, 77	0
1	E	464/520 (89%)	0.28	37 (7%) 18 16	14, 34, 70, 96	0
1	F	480/520 (92%)	-0.26	9 (1%) 66 63	11, 24, 47, 65	0
1	G	479/520 (92%)	-0.11	13 (2%) 56 53	13, 27, 56, 87	0
1	H	478/520 (91%)	0.37	34 (7%) 22 19	17, 38, 75, 100	0
All	All	3816/4160 (91%)	-0.04	142 (3%) 45 42	11, 28, 60, 100	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	276	LEU	7.1
1	H	284	LEU	6.4
1	E	284	LEU	5.7
1	B	284	LEU	5.4
1	D	284	LEU	5.1
1	G	284	LEU	4.8
1	H	488	LEU	4.6
1	A	284	LEU	4.4
1	C	284	LEU	4.3
1	E	488	LEU	4.2
1	G	464	GLY	4.2
1	E	113	ASP	4.1
1	G	114	THR	4.1
1	C	488	LEU	4.1
1	H	491	VAL	3.9
1	D	488	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	597	GLU	3.6
1	H	466	ILE	3.6
1	B	597	GLU	3.6
1	A	484	LYS	3.6
1	E	562	LEU	3.5
1	E	491	VAL	3.5
1	F	284	LEU	3.4
1	H	114	THR	3.4
1	E	463	THR	3.3
1	F	114	THR	3.3
1	E	583	ASP	3.3
1	G	599	ASN	3.3
1	G	488	LEU	3.3
1	D	114	THR	3.2
1	H	486	LYS	3.2
1	E	466	ILE	3.2
1	H	345	ASN	3.2
1	A	590	LEU	3.1
1	A	489	LEU	3.1
1	H	596	LYS	3.0
1	D	491	VAL	3.0
1	C	115	MET	3.0
1	E	581	PRO	3.0
1	E	487	VAL	3.0
1	E	489	LEU	2.9
1	E	577	ASN	2.9
1	H	115	MET	2.9
1	G	590	LEU	2.9
1	H	562	LEU	2.9
1	H	493	LEU	2.9
1	H	487	VAL	2.8
1	H	492	LYS	2.8
1	E	574	ALA	2.8
1	A	594	GLN	2.7
1	G	326	GLN	2.7
1	E	484	LYS	2.7
1	H	590	LEU	2.7
1	H	561	SER	2.7
1	F	465	GLN	2.7
1	H	489	LEU	2.6
1	A	596	LYS	2.6
1	A	597	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	113	ASP	2.6
1	A	486	LYS	2.6
1	B	345	ASN	2.6
1	H	587	ILE	2.6
1	E	496	GLU	2.5
1	A	487	VAL	2.5
1	E	457	VAL	2.5
1	D	185	LYS	2.5
1	H	465	GLN	2.5
1	A	483	ALA	2.5
1	A	490	ASP	2.5
1	H	343	VAL	2.5
1	E	563	TYR	2.5
1	E	467	LYS	2.5
1	H	557	VAL	2.4
1	F	405	LYS	2.4
1	C	345	ASN	2.4
1	E	274	GLY	2.4
1	B	466	ILE	2.4
1	F	115	MET	2.4
1	D	345	ASN	2.4
1	F	344	ASP	2.4
1	A	326	GLN	2.4
1	B	405	LYS	2.4
1	A	559	ARG	2.4
1	B	465	GLN	2.4
1	B	327	ASN	2.3
1	C	275	PRO	2.3
1	E	478	LYS	2.3
1	H	403	GLY	2.3
1	G	115	MET	2.3
1	H	559	ARG	2.3
1	E	486	LYS	2.3
1	H	494	LYS	2.3
1	E	326	GLN	2.3
1	E	569	PHE	2.3
1	E	405	LYS	2.3
1	G	593	PRO	2.3
1	E	464	GLY	2.3
1	C	326	GLN	2.3
1	H	471	GLU	2.3
1	F	467	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	115	MET	2.2
1	G	403	GLY	2.2
1	E	557	VAL	2.2
1	H	305	ARG	2.2
1	D	487	VAL	2.2
1	G	491	VAL	2.2
1	E	291	PRO	2.2
1	F	180	HIS	2.2
1	E	331	TYR	2.1
1	H	396	TYR	2.1
1	D	489	LEU	2.1
1	A	557	VAL	2.1
1	E	559	ARG	2.1
1	H	484	LYS	2.1
1	G	487	VAL	2.1
1	H	598	TRP	2.1
1	E	565	ALA	2.1
1	E	511	GLU	2.1
1	E	543	GLU	2.1
1	E	328	ASN	2.1
1	H	504	ASN	2.1
1	A	491	VAL	2.1
1	H	185	LYS	2.1
1	A	466	ILE	2.1
1	A	599	ASN	2.1
1	C	490	ASP	2.1
1	E	275	PRO	2.1
1	E	285	TRP	2.1
1	D	465	GLN	2.0
1	H	594	GLN	2.0
1	A	113	ASP	2.0
1	A	276	LEU	2.0
1	F	328	ASN	2.0
1	C	491	VAL	2.0
1	C	559	ARG	2.0
1	A	437	LYS	2.0
1	H	556	LYS	2.0
1	C	465	GLN	2.0
1	A	488	LEU	2.0
1	E	345	ASN	2.0
1	G	276	LEU	2.0
1	H	467	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	MG	H	704	1/1	0.84	0.09	32,32,32,32	0
3	MG	H	703	1/1	0.94	0.06	15,15,15,15	0
3	MG	D	708	1/1	0.95	0.06	38,38,38,38	0
4	DZ4	H	706	30/30	0.95	0.07	18,22,27,34	0
4	DZ4	A	707	30/30	0.98	0.04	13,15,18,20	0
4	DZ4	C	701	30/30	0.98	0.04	11,13,16,18	0
4	DZ4	E	708	30/30	0.98	0.05	20,23,32,33	0
4	DZ4	G	701	30/30	0.98	0.04	12,15,19,20	0
4	DZ4	H	701	30/30	0.98	0.05	20,23,28,29	0
3	MG	F	702	1/1	0.98	0.02	9,9,9,9	0
5	GTP	D	707	32/32	0.98	0.04	14,16,22,23	0
5	GTP	E	707	32/32	0.98	0.04	18,20,30,33	0
5	GTP	G	707	32/32	0.98	0.04	20,23,32,36	0
3	MG	E	704	1/1	0.99	0.02	16,16,16,16	0
3	MG	A	704	1/1	0.99	0.02	14,14,14,14	0
3	MG	F	704	1/1	0.99	0.02	28,28,28,28	0
3	MG	G	703	1/1	0.99	0.02	11,11,11,11	0
3	MG	G	704	1/1	0.99	0.03	20,20,20,20	0
3	MG	G	705	1/1	0.99	0.04	36,36,36,36	0
3	MG	B	702	1/1	0.99	0.02	9,9,9,9	0
3	MG	B	703	1/1	0.99	0.04	16,16,16,16	0
3	MG	H	705	1/1	0.99	0.03	17,17,17,17	0
4	DZ4	A	705	30/30	0.99	0.04	13,15,19,21	0
3	MG	B	704	1/1	0.99	0.03	17,17,17,17	0
4	DZ4	B	705	30/30	0.99	0.04	12,14,16,16	0
3	MG	C	703	1/1	0.99	0.02	9,9,9,9	0
4	DZ4	C	706	30/30	0.99	0.04	13,14,16,17	0

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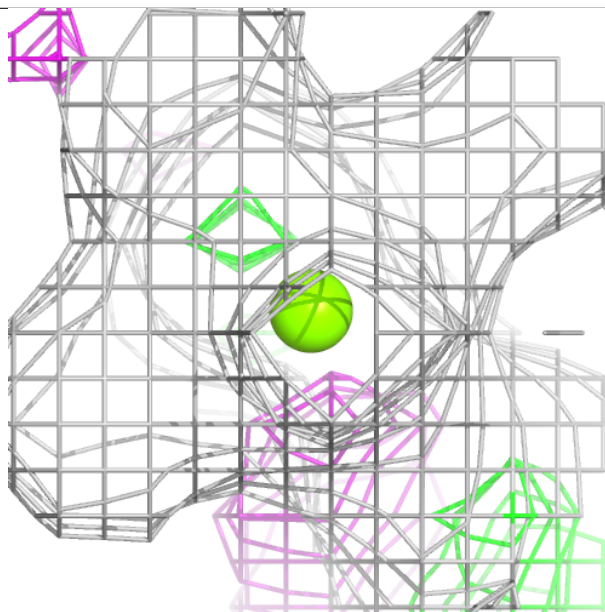
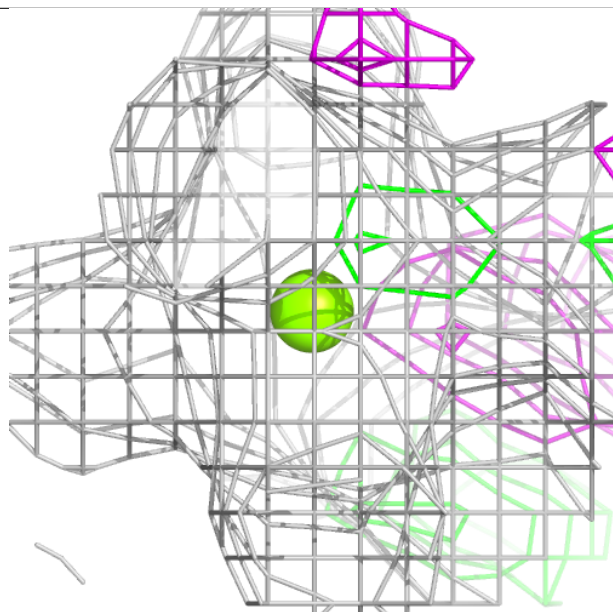
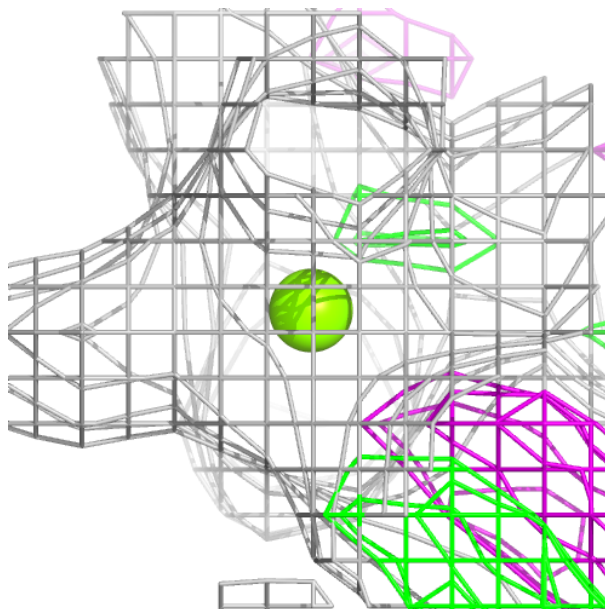
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DZ4	C	708	30/30	0.99	0.04	14,16,20,23	0
4	DZ4	D	701	30/30	0.99	0.04	13,15,19,19	0
4	DZ4	D	706	30/30	0.99	0.04	13,16,19,20	0
4	DZ4	E	705	30/30	0.99	0.04	17,21,23,24	0
3	MG	C	704	1/1	0.99	0.03	13,13,13,13	0
4	DZ4	F	705	30/30	0.99	0.04	12,13,15,16	0
4	DZ4	F	706	30/30	0.99	0.04	11,15,19,20	0
3	MG	C	705	1/1	0.99	0.03	17,17,17,17	0
4	DZ4	G	706	30/30	0.99	0.04	12,13,15,16	0
3	MG	D	704	1/1	0.99	0.02	19,19,19,19	0
3	MG	D	705	1/1	0.99	0.02	18,18,18,18	0
5	GTP	A	706	32/32	0.99	0.03	12,13,18,19	0
5	GTP	B	706	32/32	0.99	0.03	13,17,25,25	0
5	GTP	C	707	32/32	0.99	0.03	14,16,22,23	0
3	MG	A	703	1/1	0.99	0.01	14,14,14,14	0
5	GTP	E	706	32/32	0.99	0.04	13,15,21,23	0
3	MG	E	702	1/1	0.99	0.02	15,15,15,15	0
3	MG	E	703	1/1	0.99	0.02	26,26,26,26	0
5	GTP	H	707	32/32	0.99	0.04	15,17,22,23	0
2	FE	F	701	1/1	1.00	0.01	14,14,14,14	0
3	MG	F	703	1/1	1.00	0.01	15,15,15,15	0
2	FE	G	702	1/1	1.00	0.01	13,13,13,13	0
2	FE	H	702	1/1	1.00	0.01	20,20,20,20	0
3	MG	D	703	1/1	1.00	0.01	8,8,8,8	0
3	MG	A	702	1/1	1.00	0.03	8,8,8,8	0
2	FE	A	701	1/1	1.00	0.01	14,14,14,14	0
2	FE	B	701	1/1	1.00	0.02	13,13,13,13	0
2	FE	C	702	1/1	1.00	0.01	13,13,13,13	0
2	FE	D	702	1/1	1.00	0.01	15,15,15,15	0
2	FE	E	701	1/1	1.00	0.01	17,17,17,17	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.

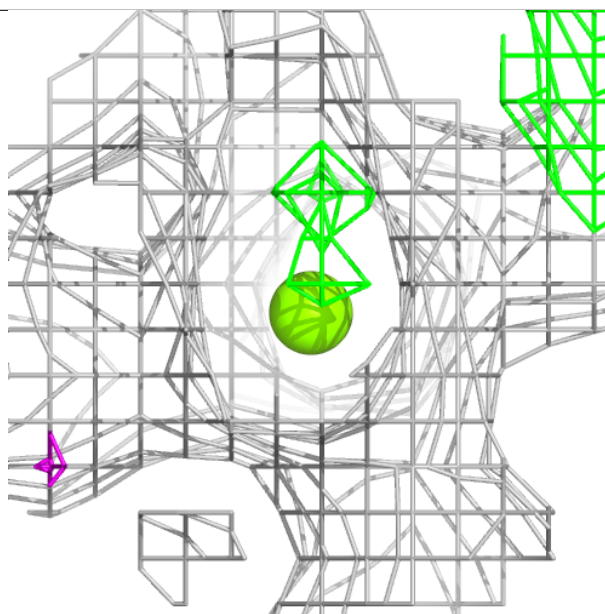
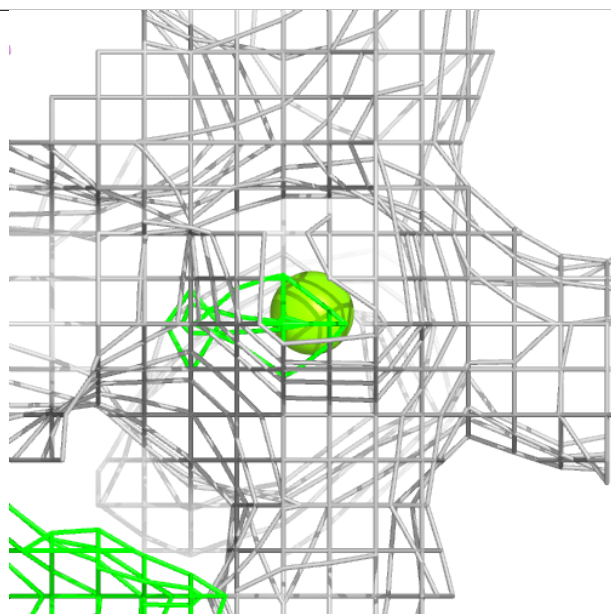
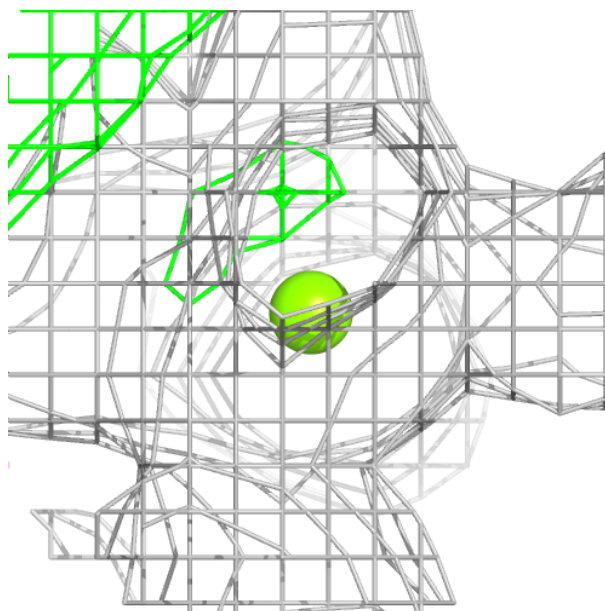
Electron density around MG H 704:

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



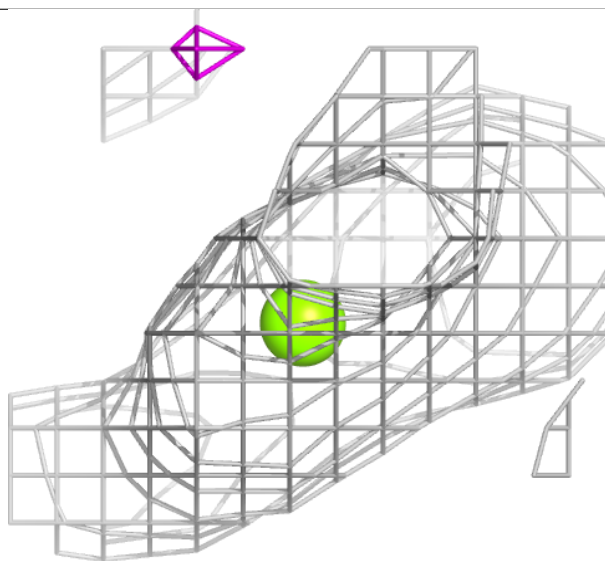
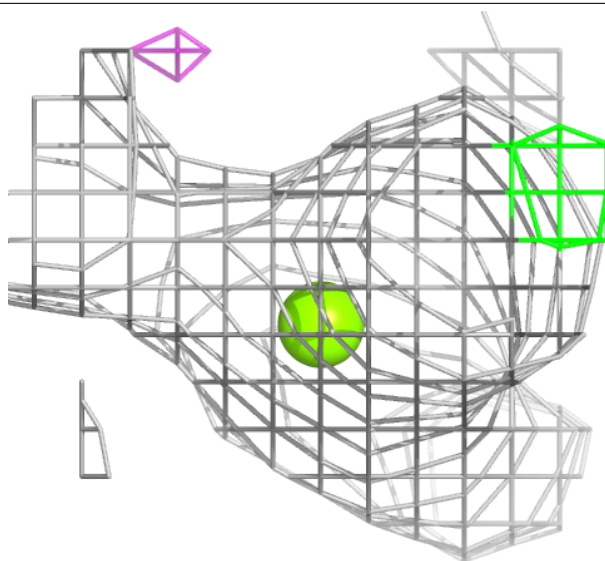
Electron density around MG H 703:

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



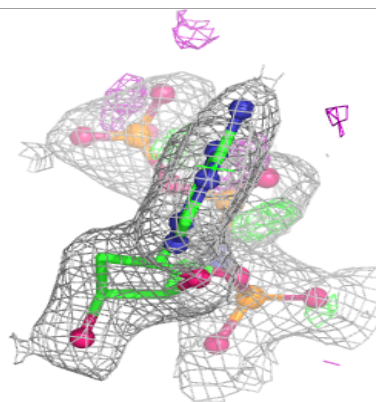
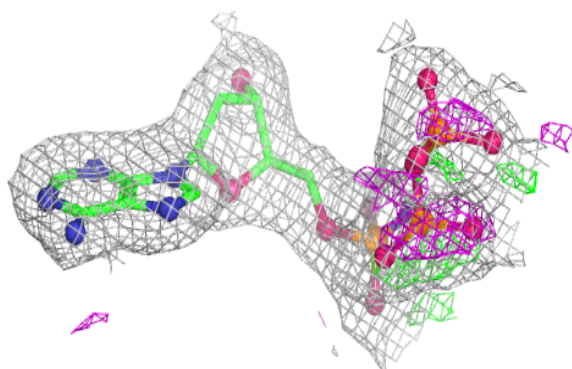
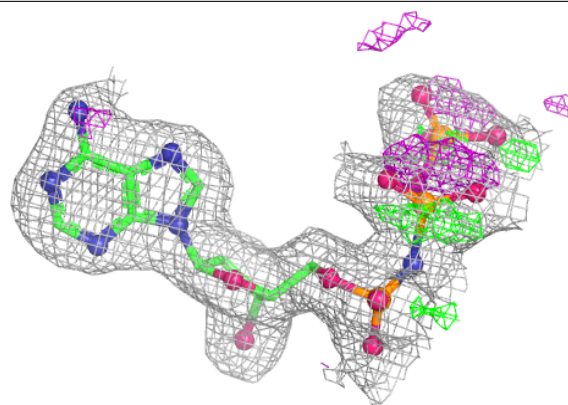
Electron density around MG D 708:

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and green (positive)

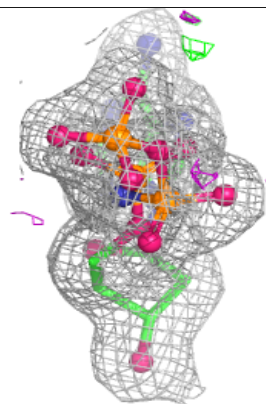
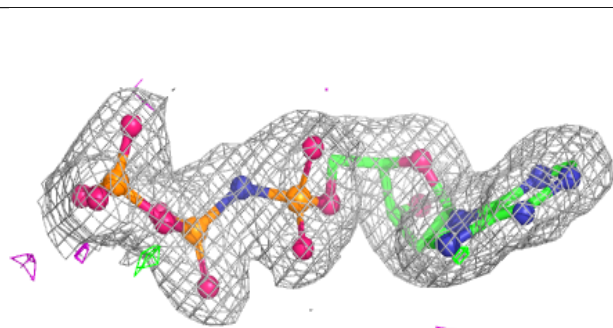
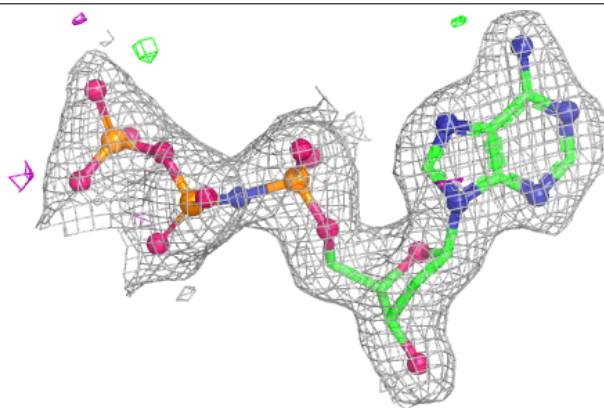


Electron density around DZ4 H 706:

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

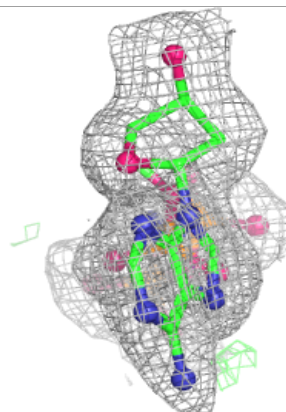
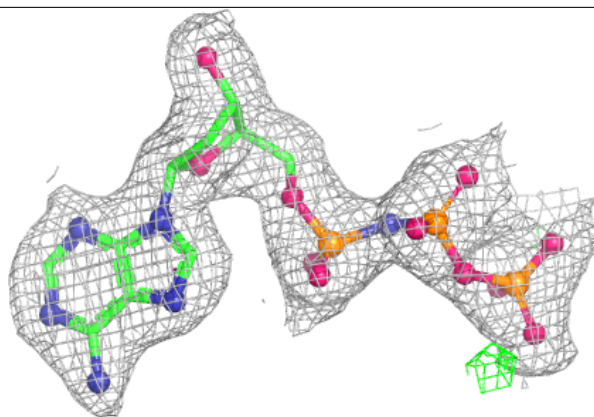
**Electron density around DZ4 A 707:**

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and green (positive)

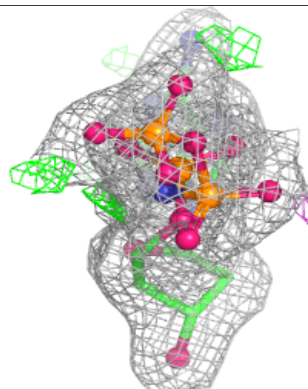
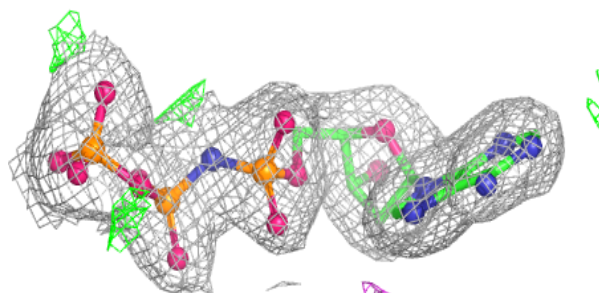
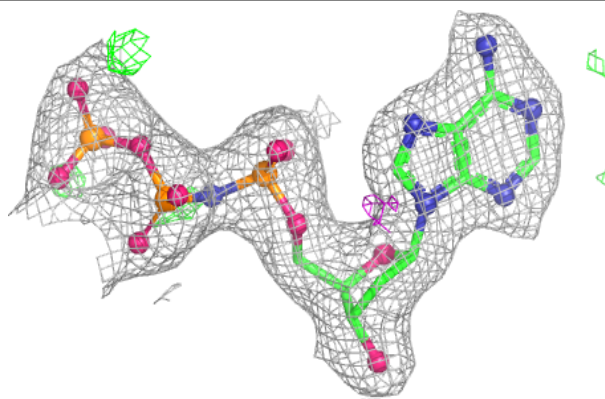


Electron density around DZ4 C 701:

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

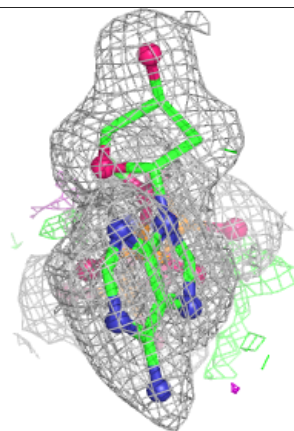
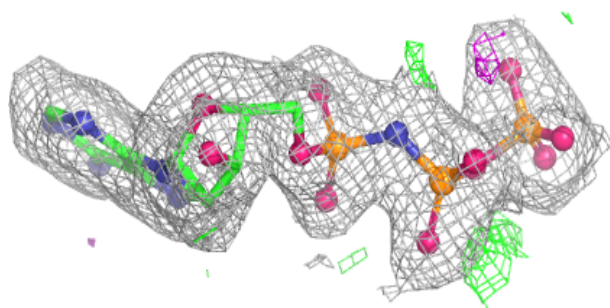
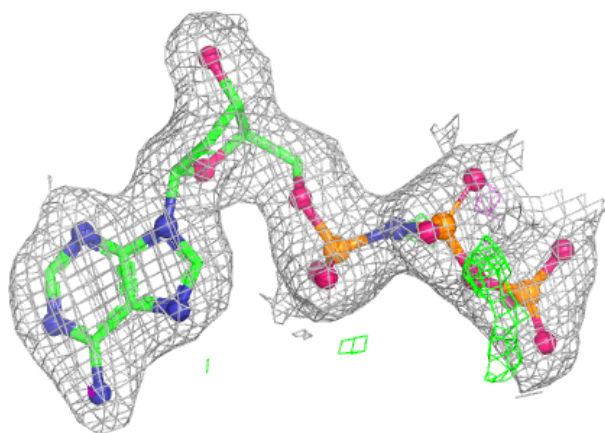
**Electron density around DZ4 E 708:**

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

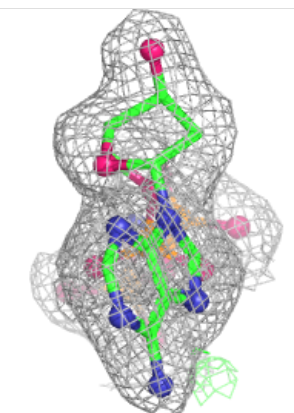
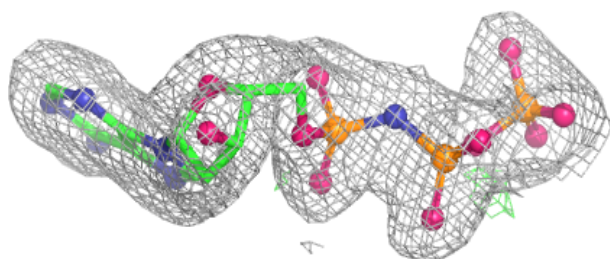
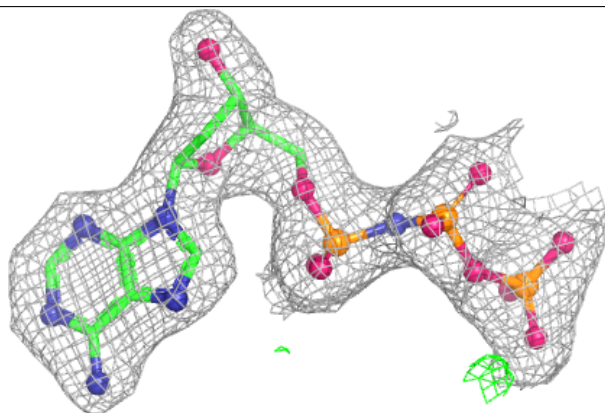


Electron density around DZ4 G 701:

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

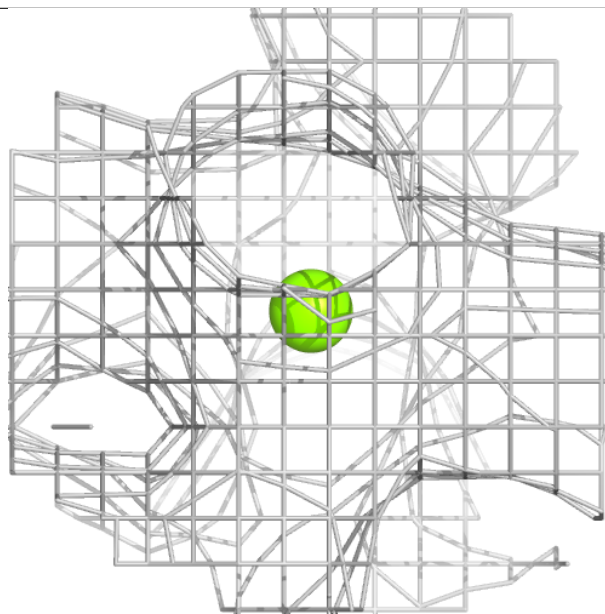
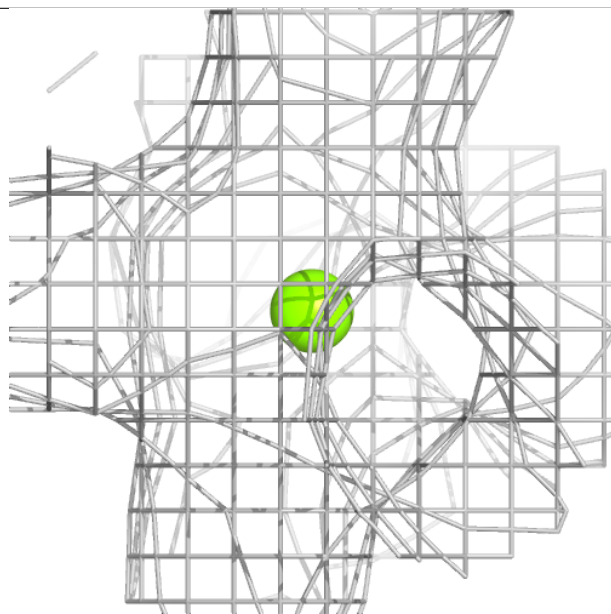
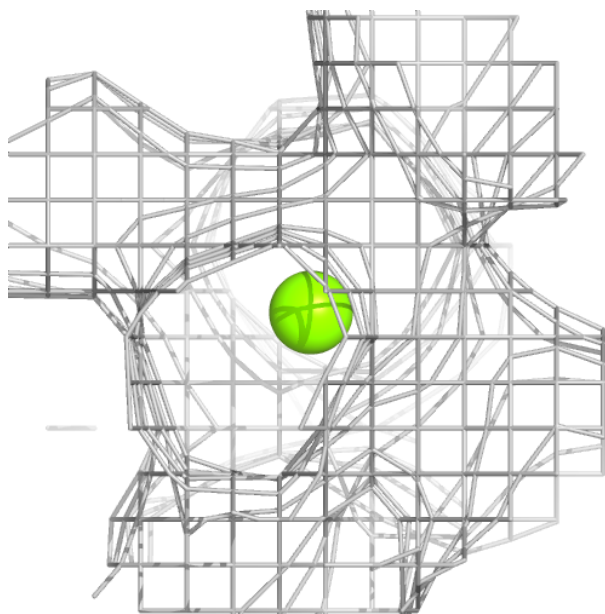
**Electron density around DZ4 H 701:**

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



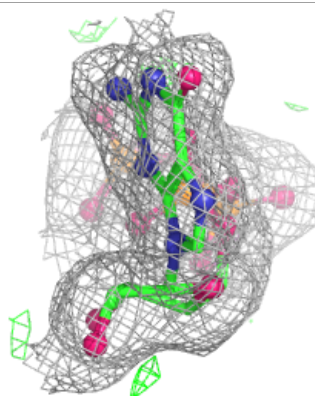
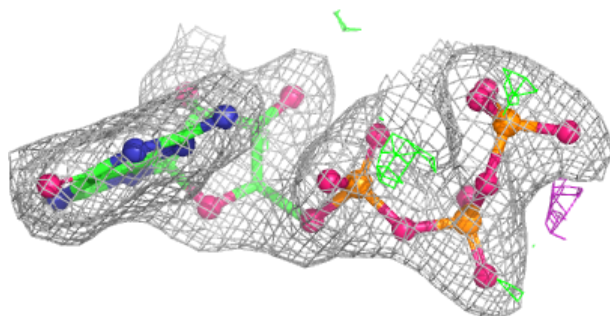
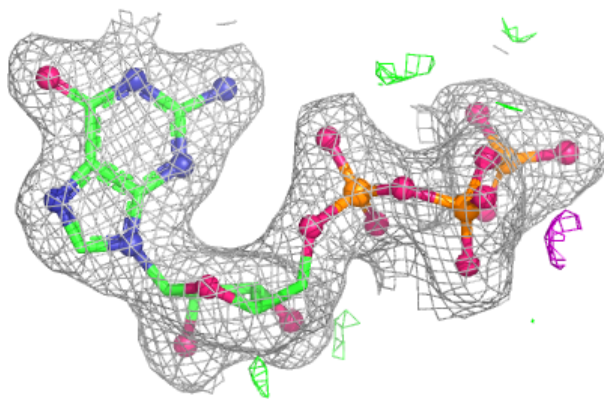
Electron density around MG F 702:

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

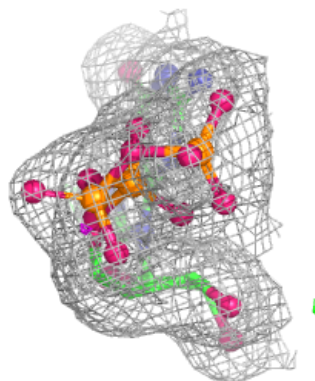
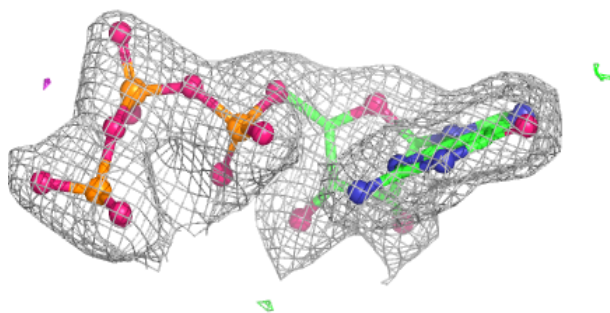
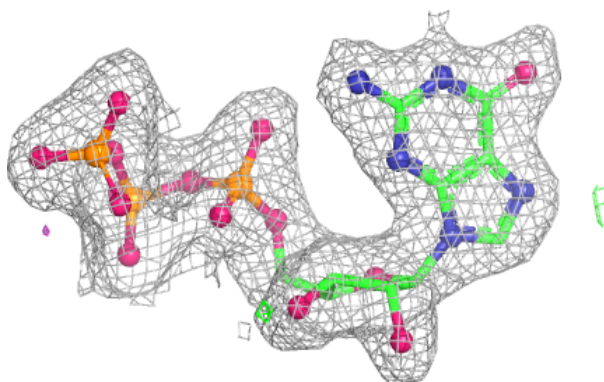


Electron density around GTP D 707:

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

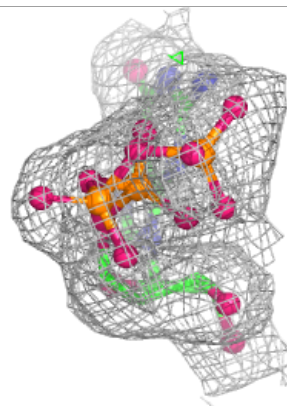
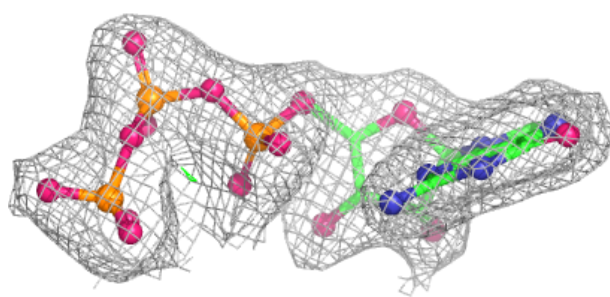
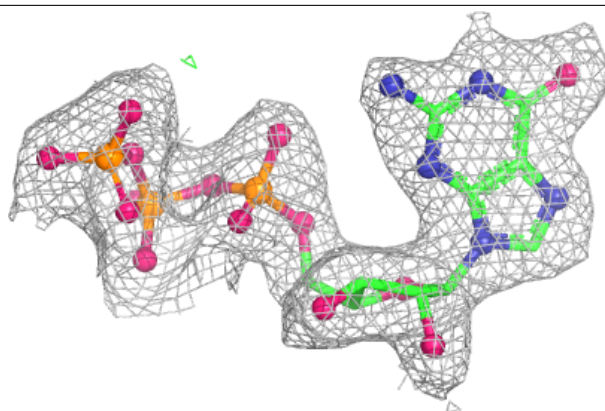
**Electron density around GTP E 707:**

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



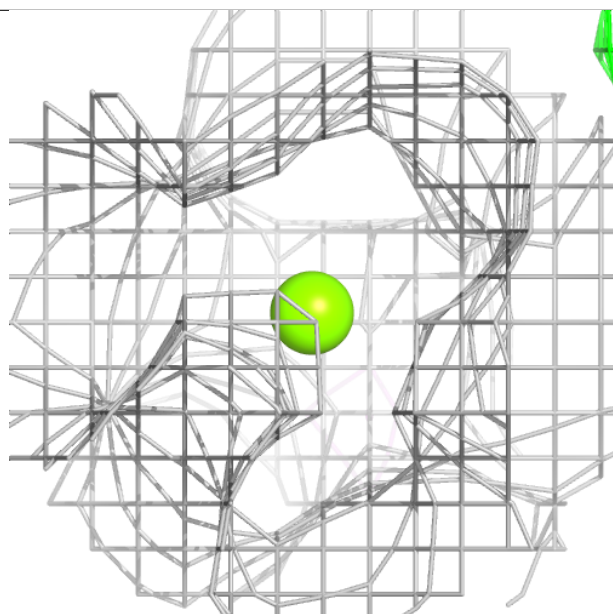
Electron density around GTP G 707:

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



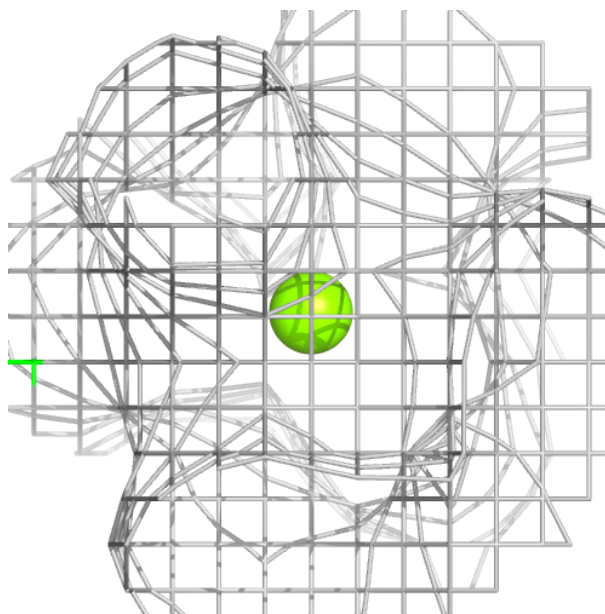
Electron density around MG E 704:

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



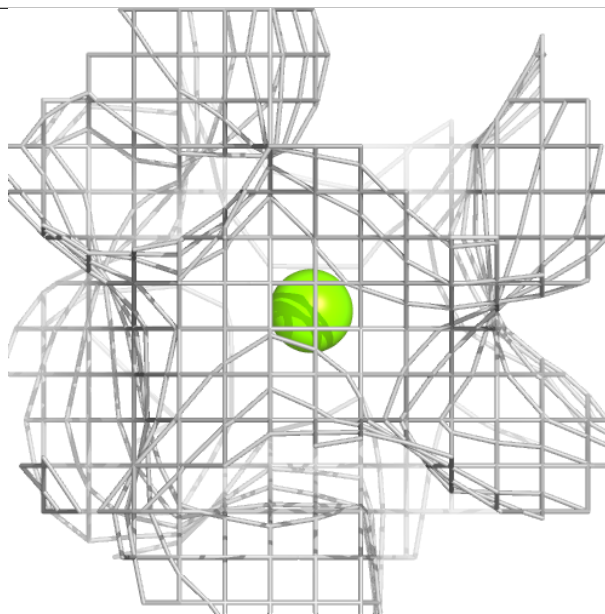
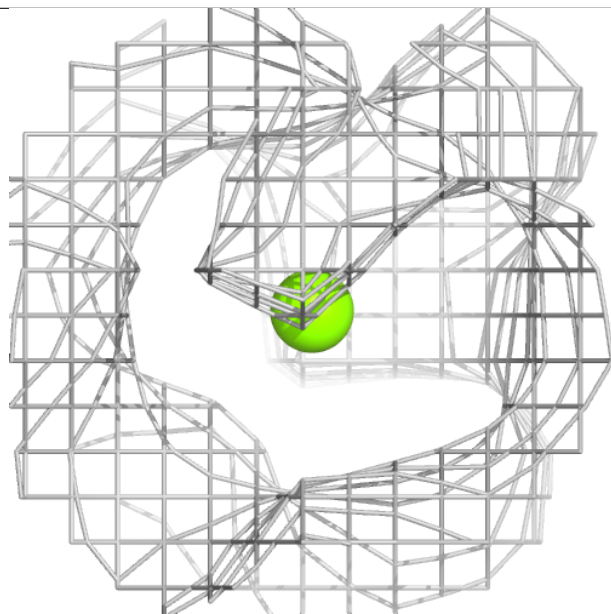
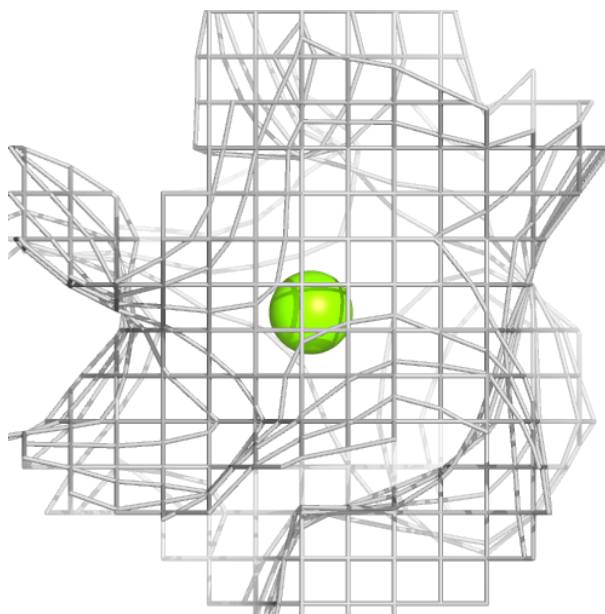
Electron density around MG A 704:

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



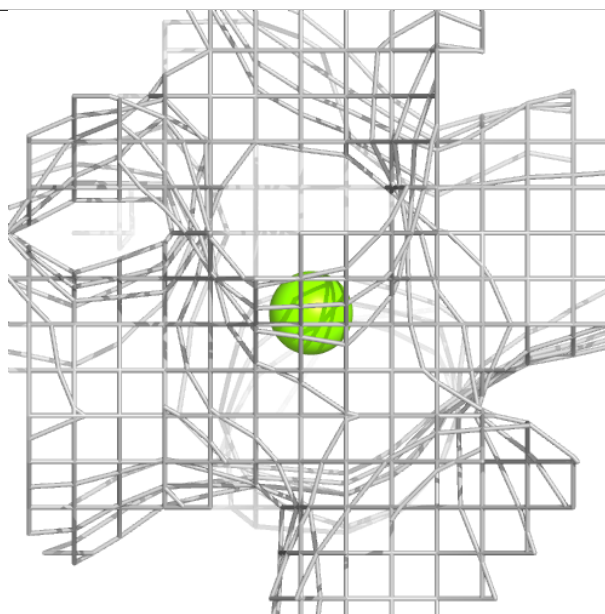
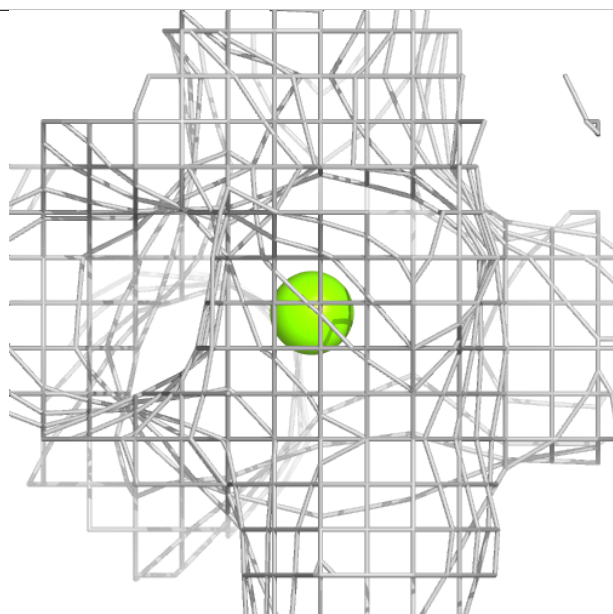
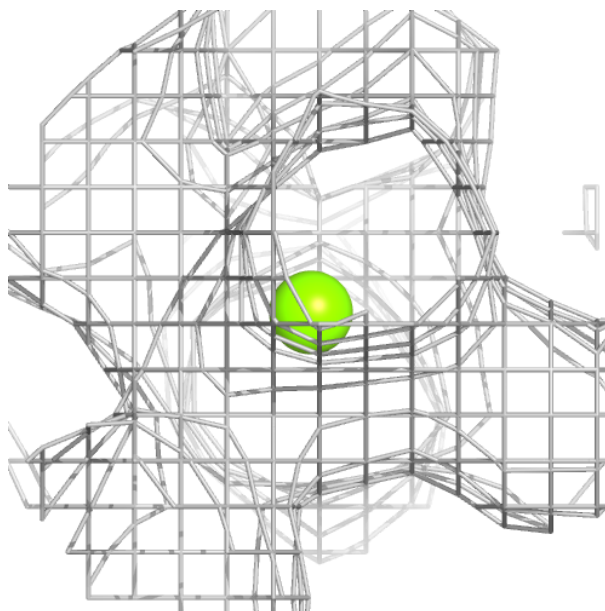
Electron density around MG F 704:

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



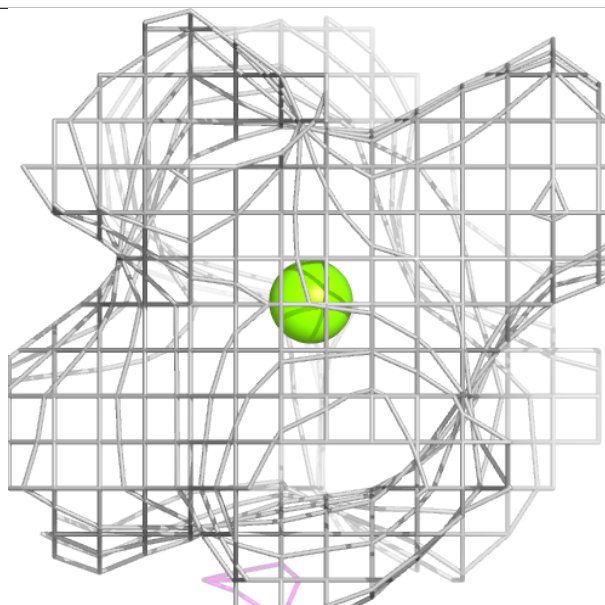
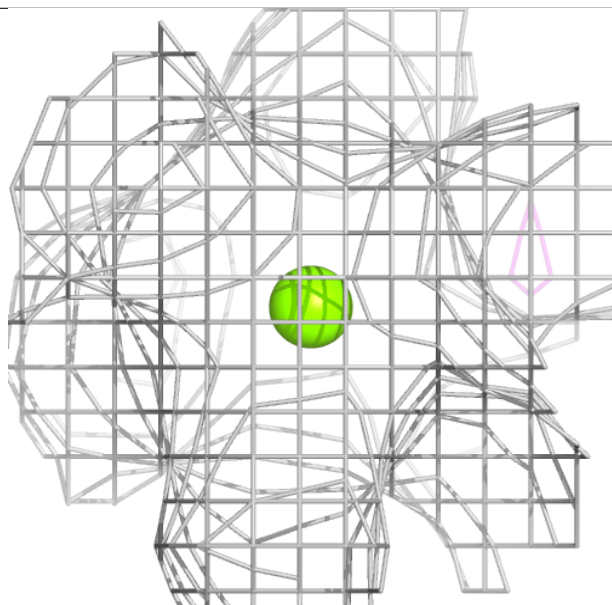
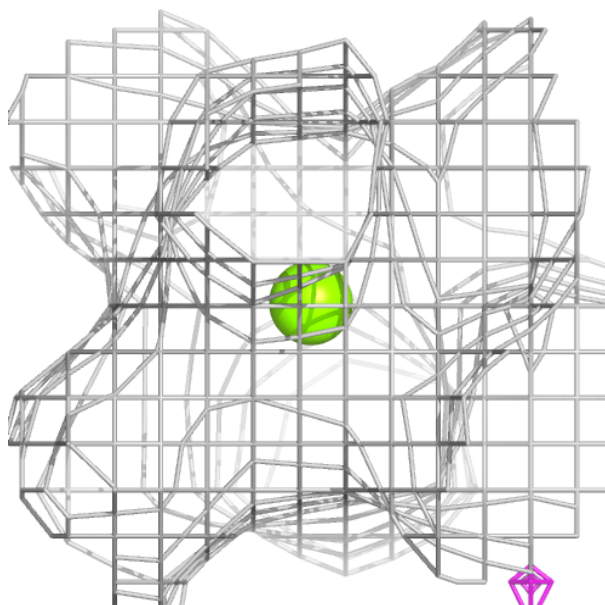
Electron density around MG G 703:

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



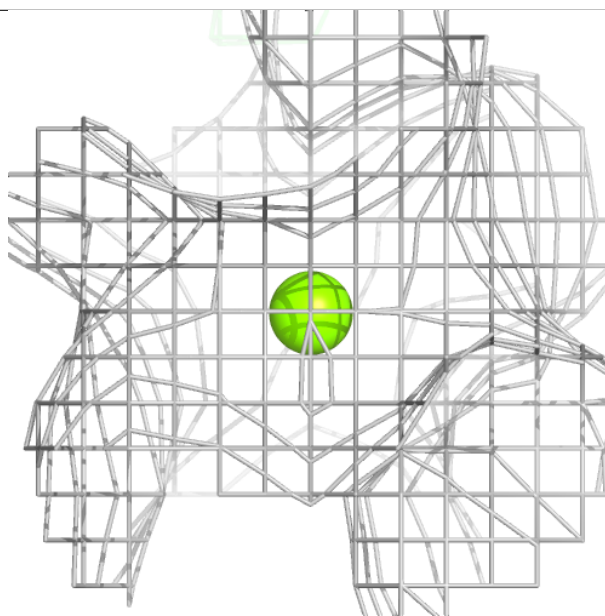
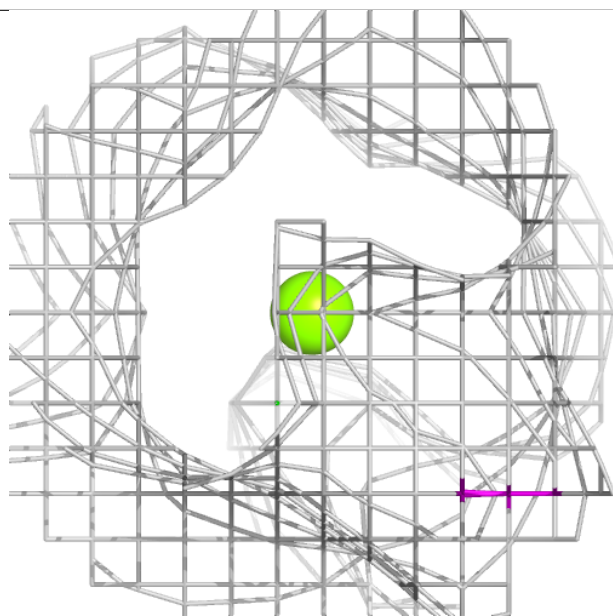
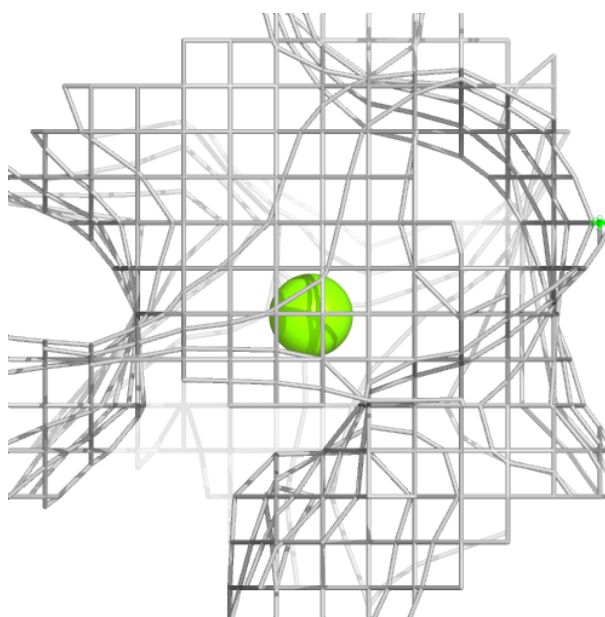
Electron density around MG G 704:

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



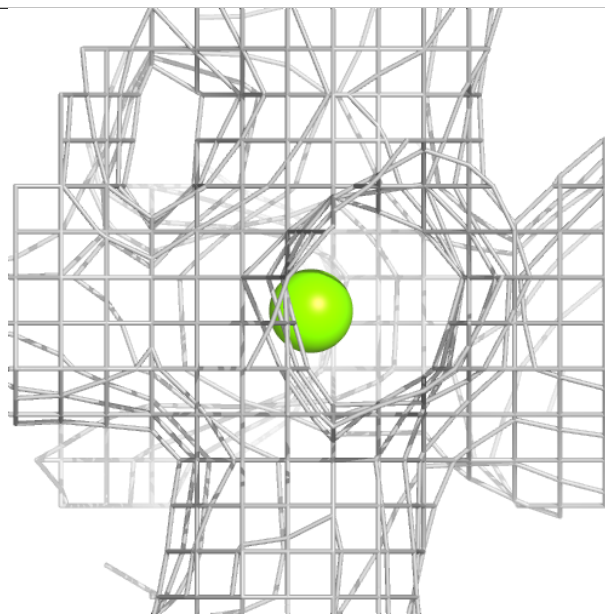
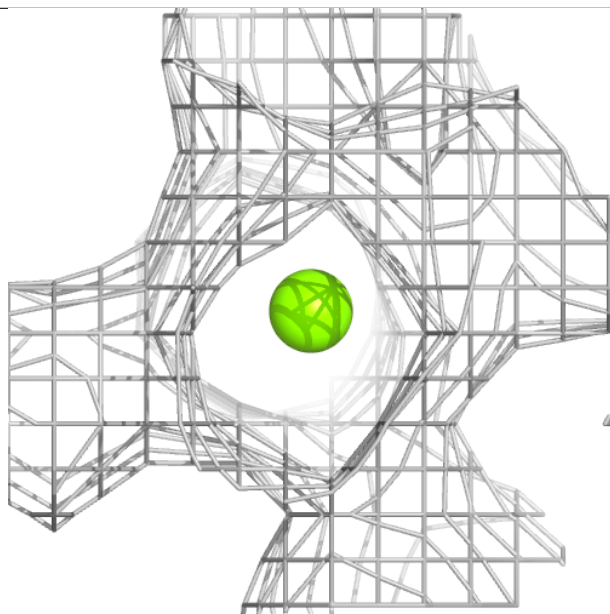
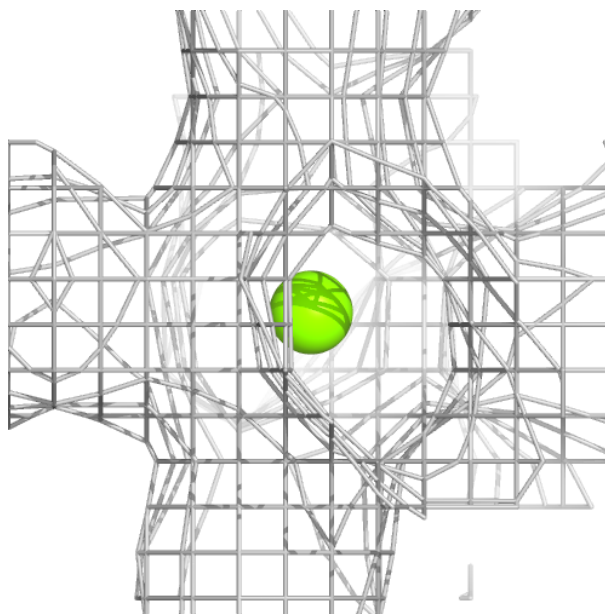
Electron density around MG G 705:

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



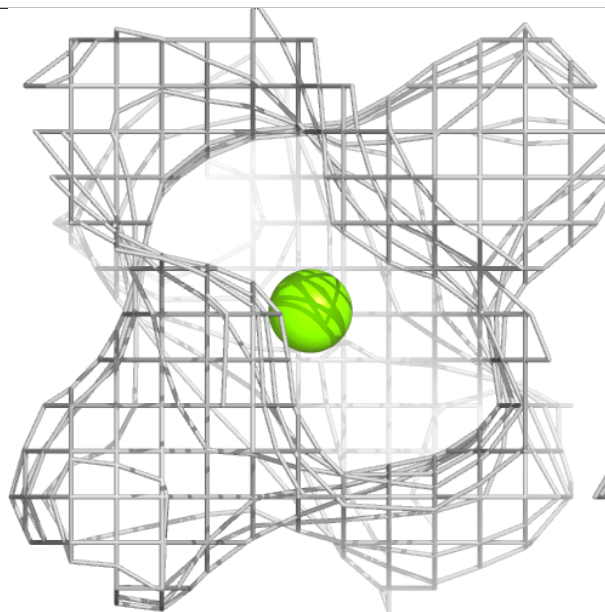
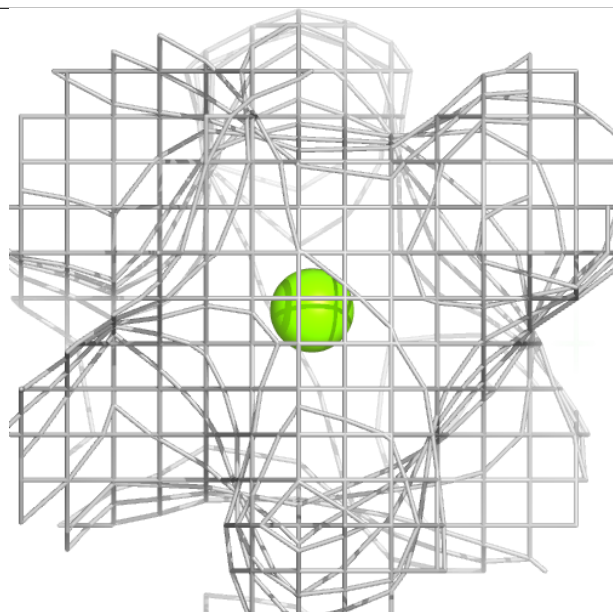
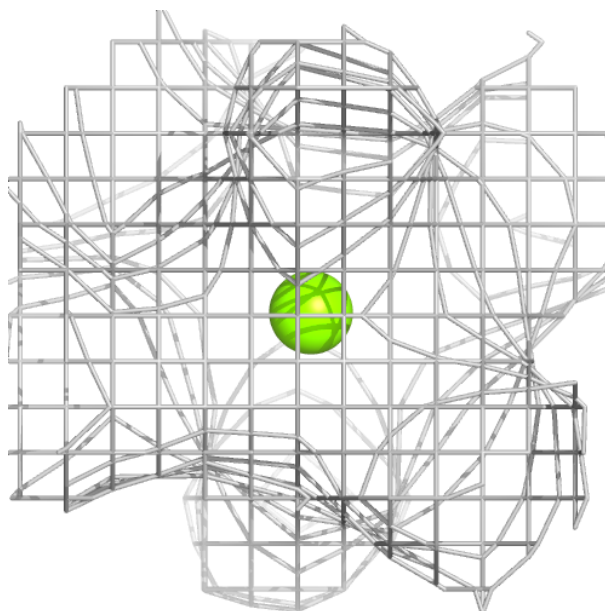
Electron density around MG B 702:

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



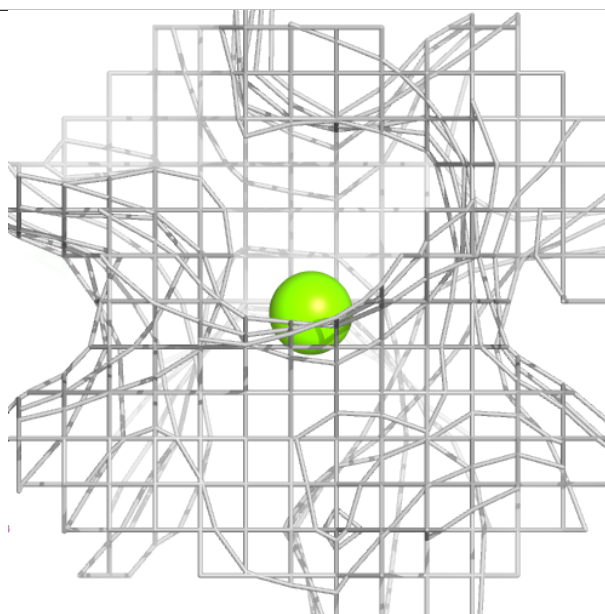
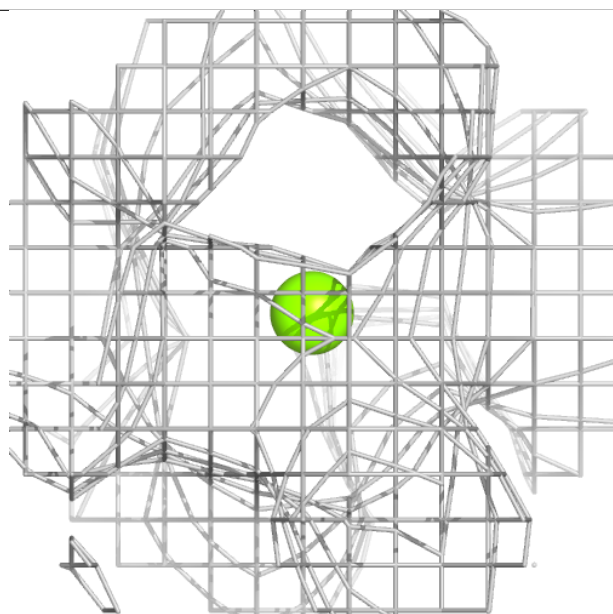
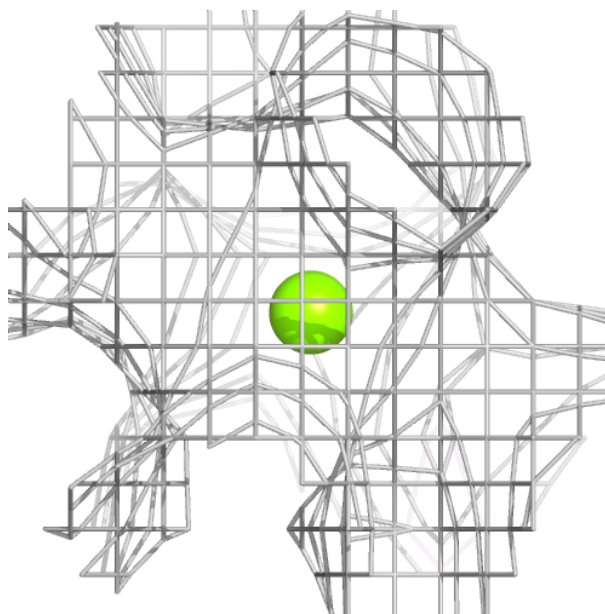
Electron density around MG B 703:

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



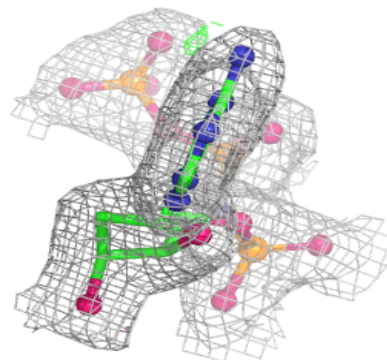
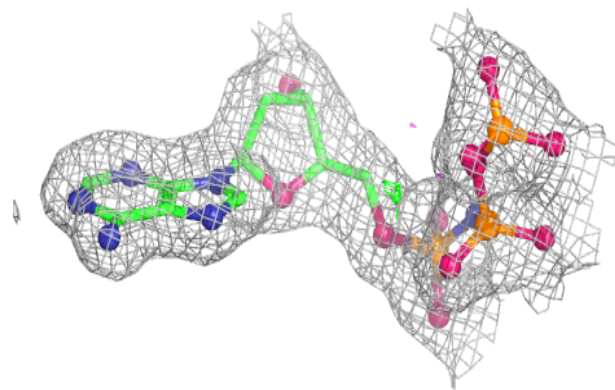
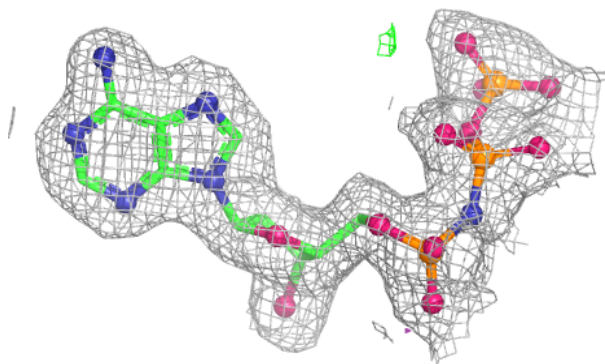
Electron density around MG H 705:

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



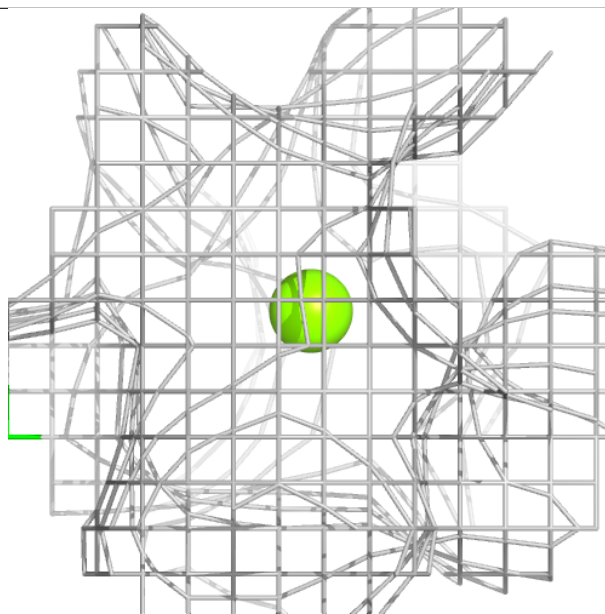
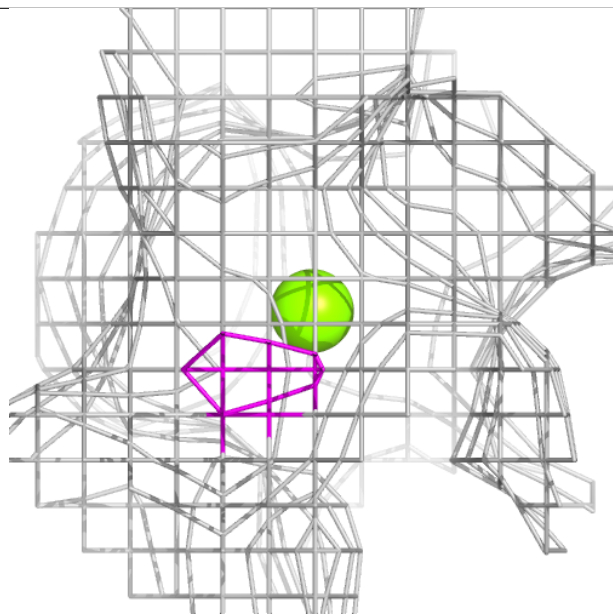
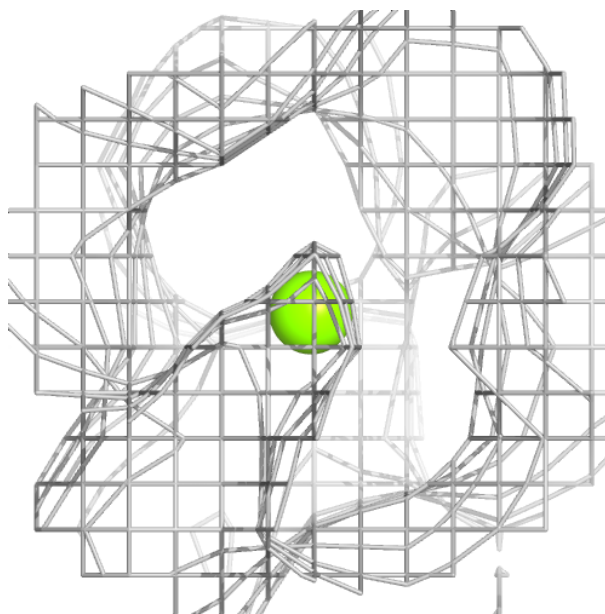
Electron density around DZ4 A 705:

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



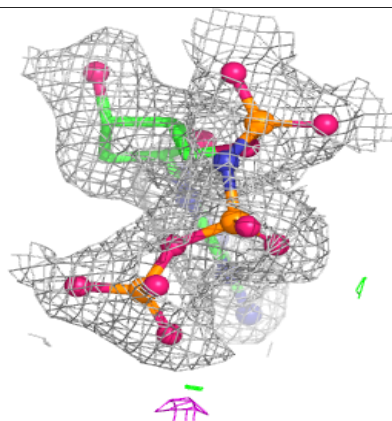
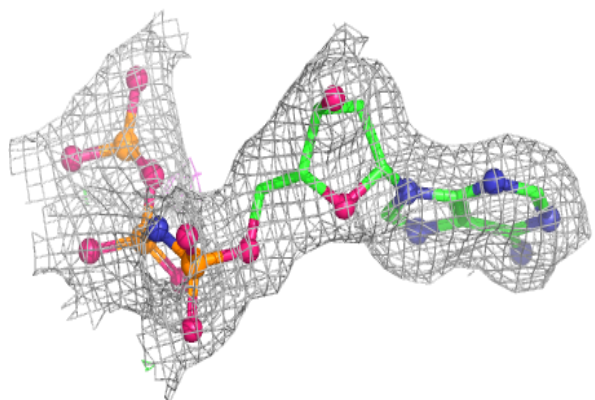
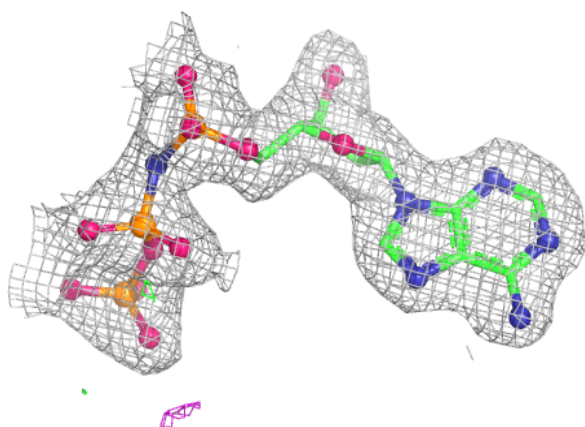
Electron density around MG B 704:

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



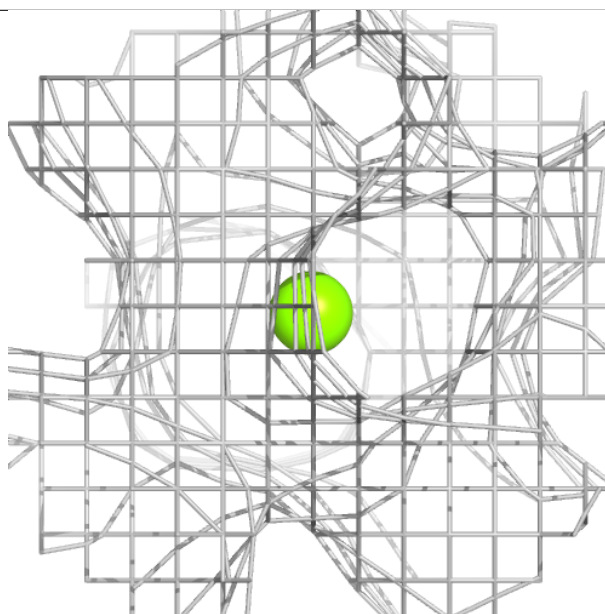
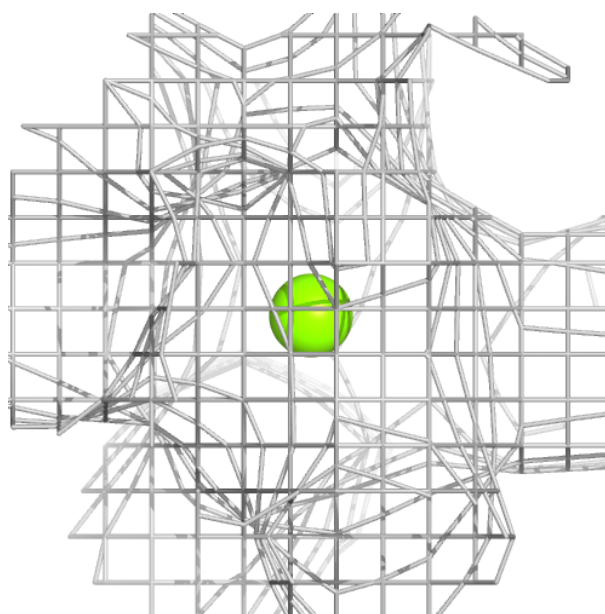
Electron density around DZ4 B 705:

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



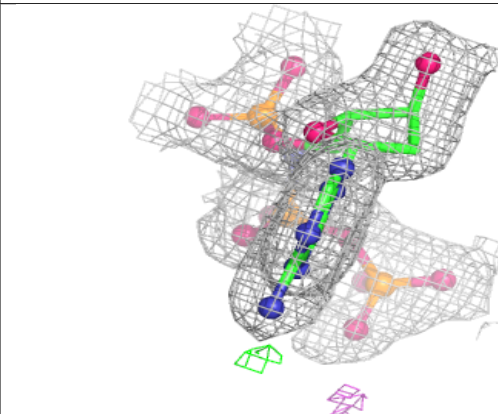
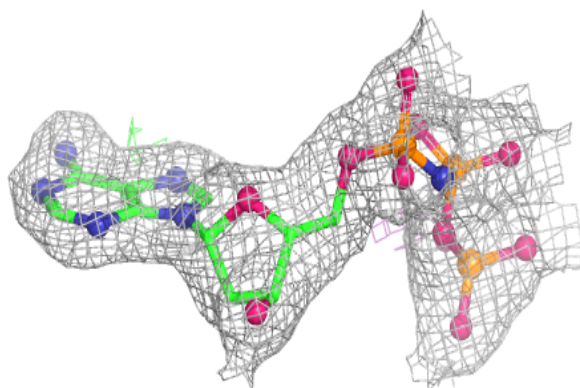
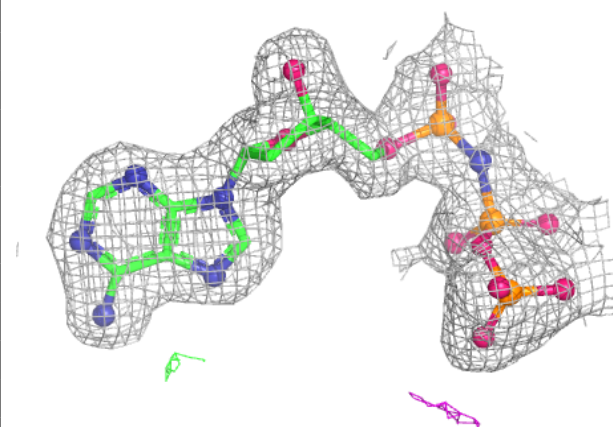
Electron density around MG C 703:

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

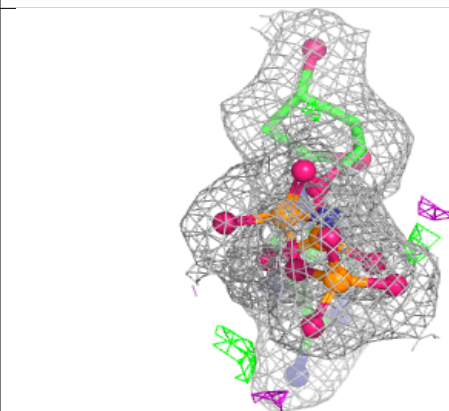
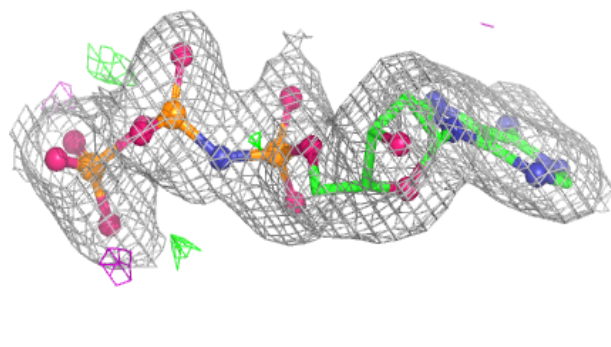
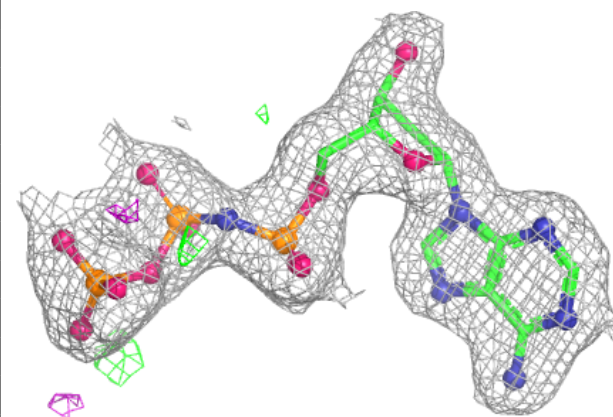


Electron density around DZ4 C 706:

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

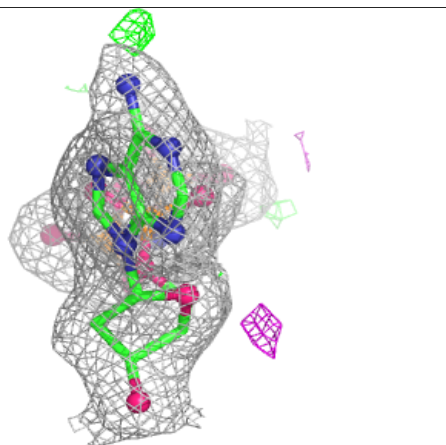
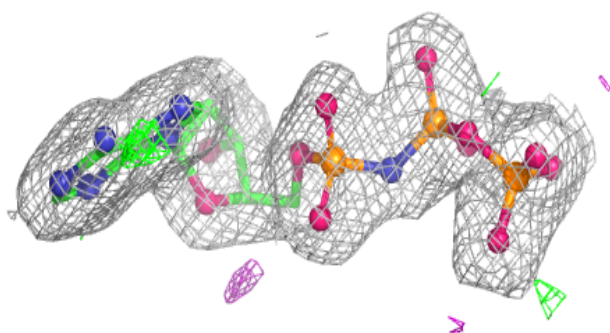
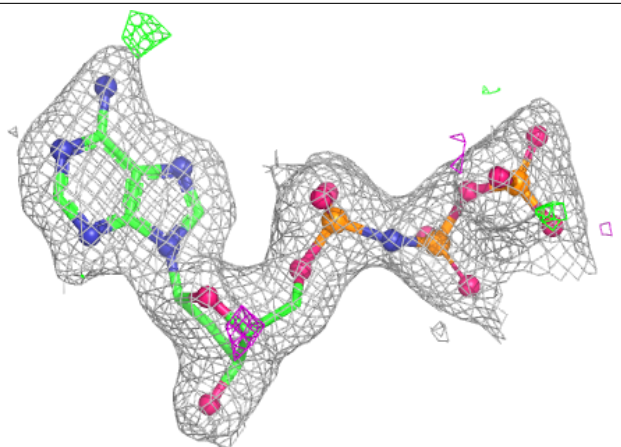
**Electron density around DZ4 C 708:**

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

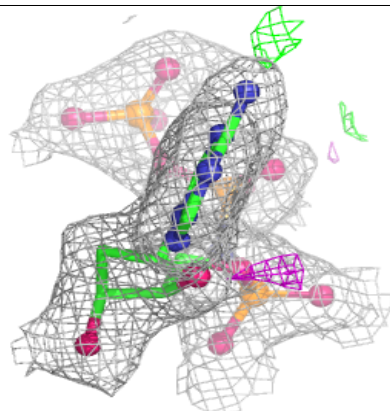
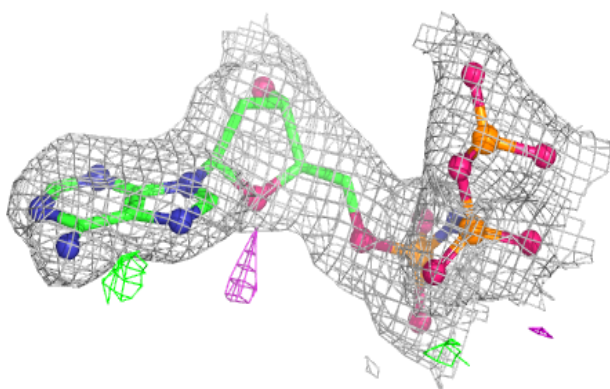
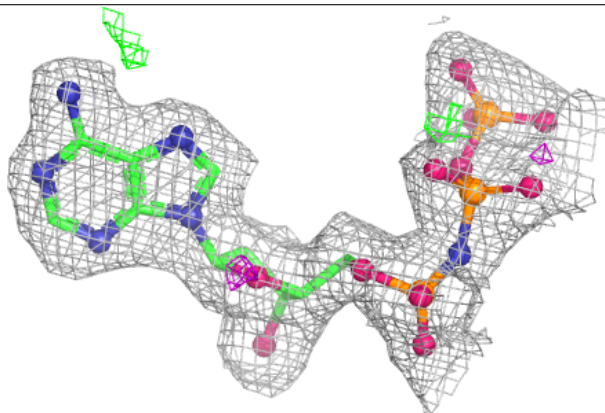


Electron density around DZ4 D 701:

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

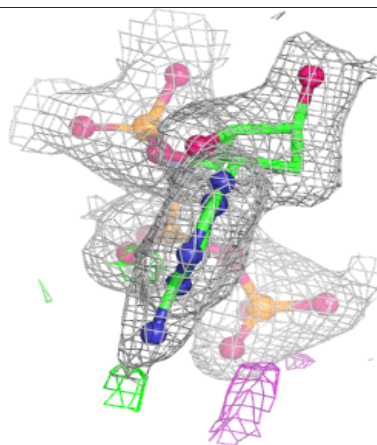
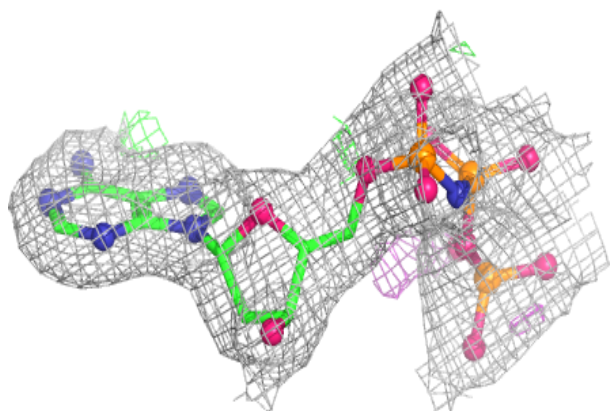
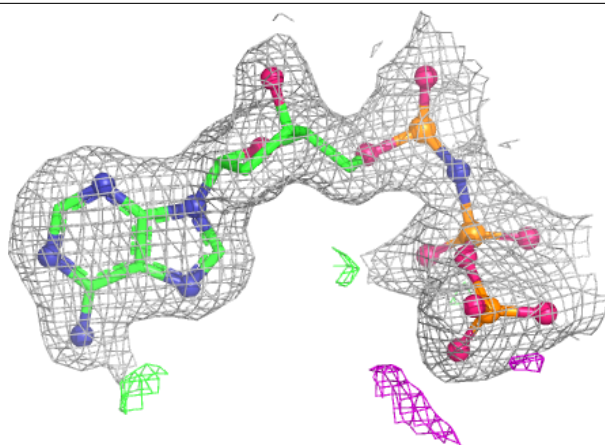
**Electron density around DZ4 D 706:**

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



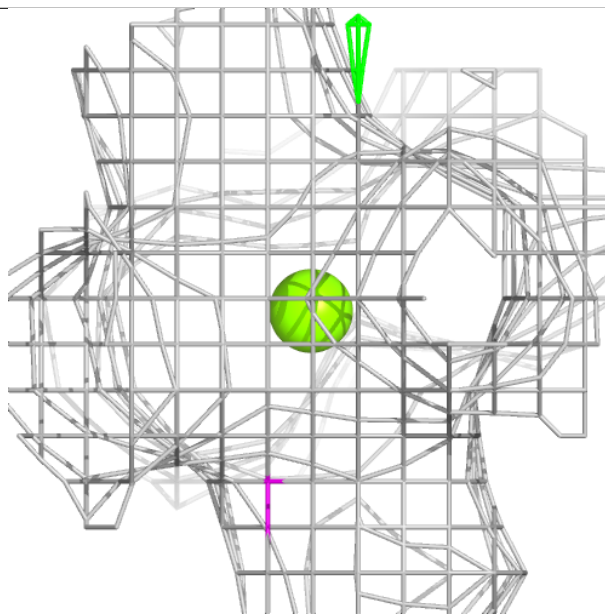
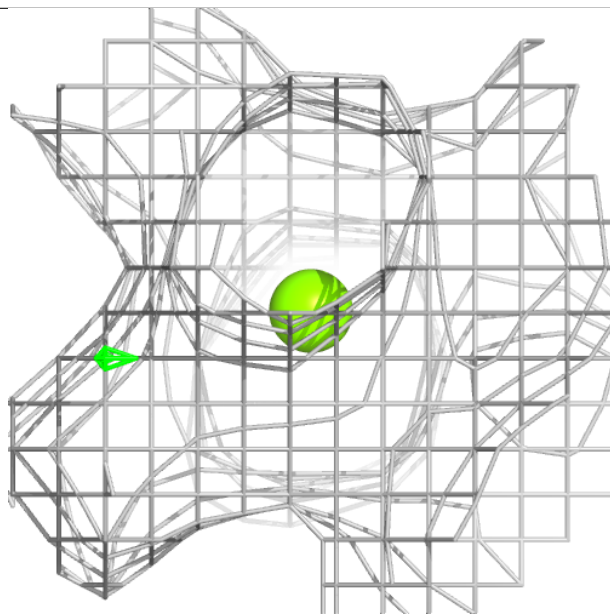
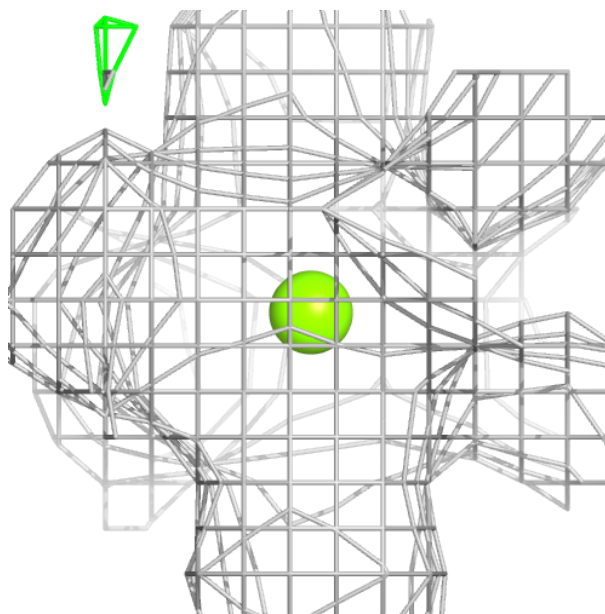
Electron density around DZ4 E 705:

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



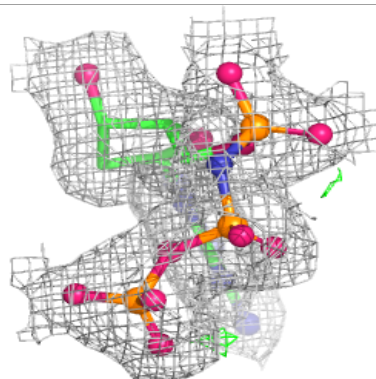
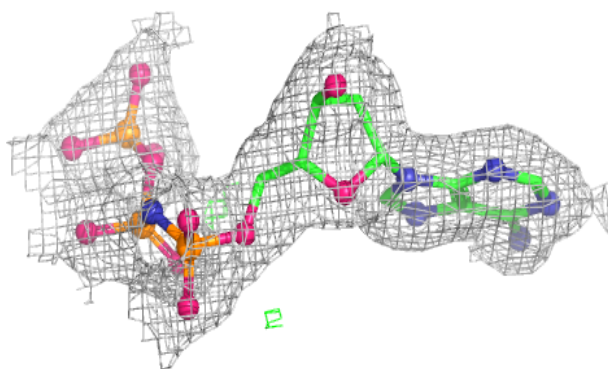
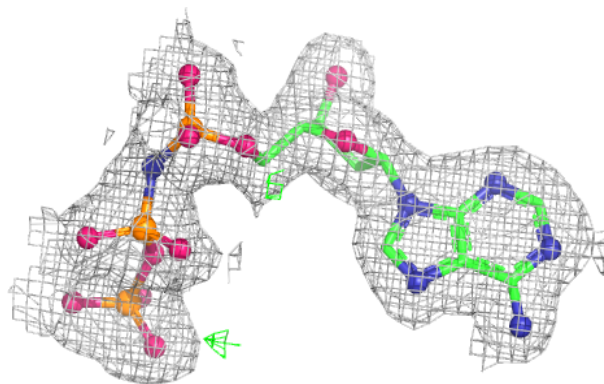
Electron density around MG C 704:

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

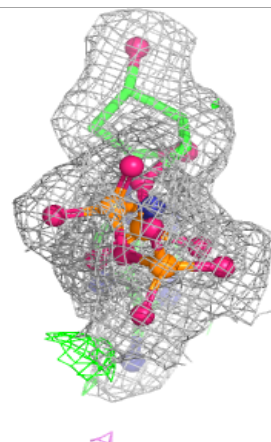
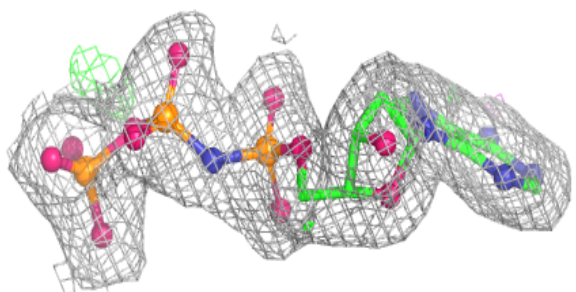
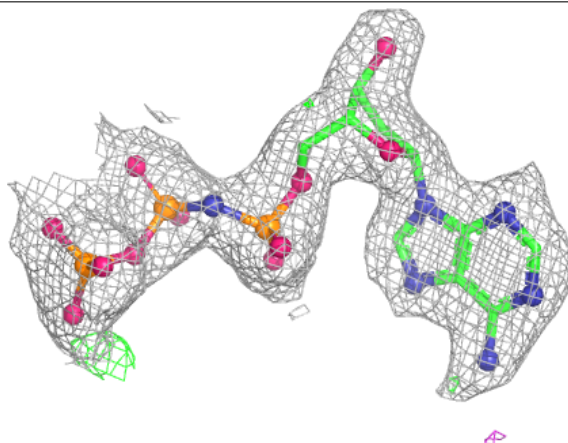


Electron density around DZ4 F 705:

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

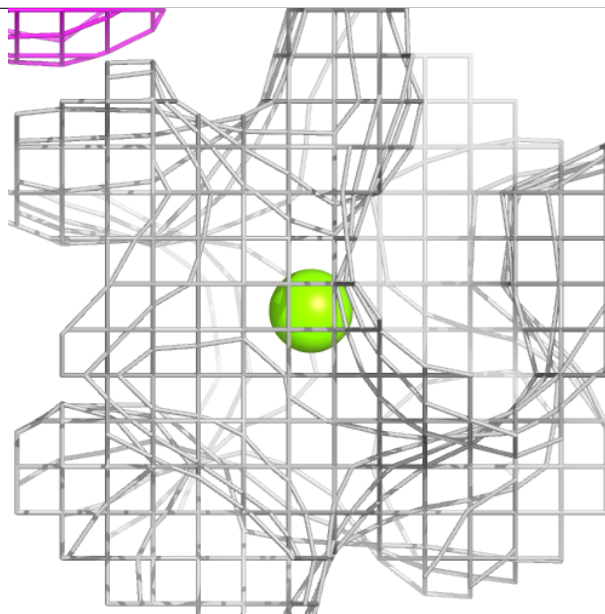
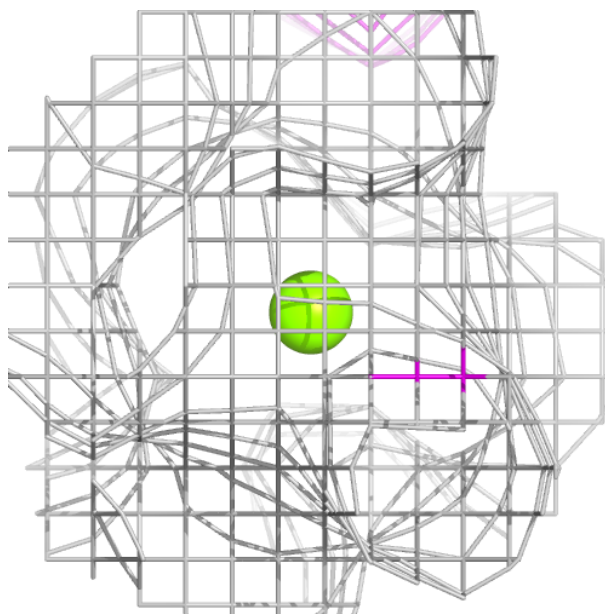
**Electron density around DZ4 F 706:**

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



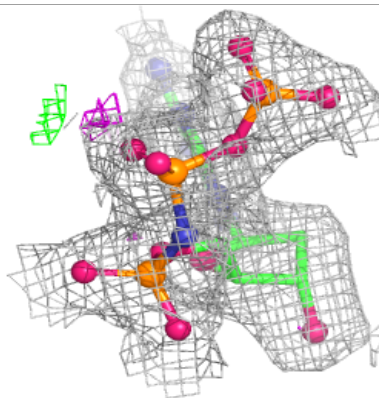
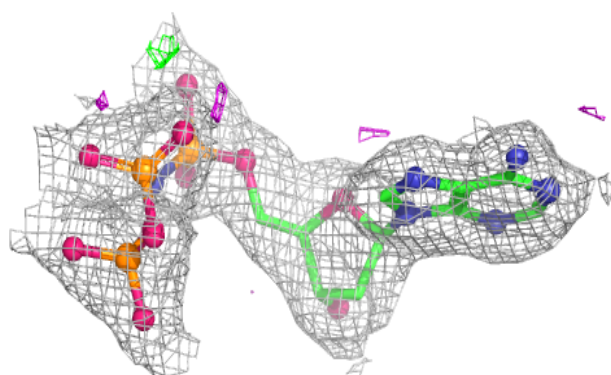
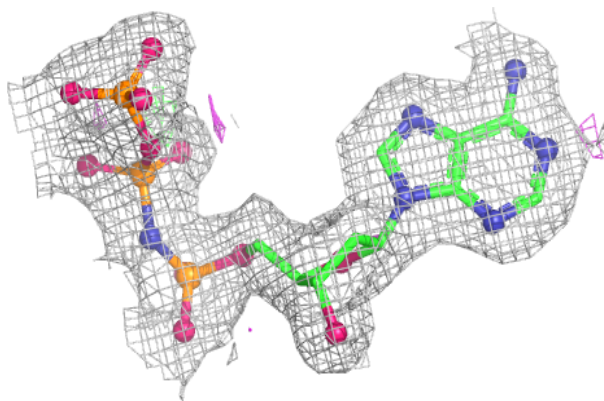
Electron density around MG C 705:

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



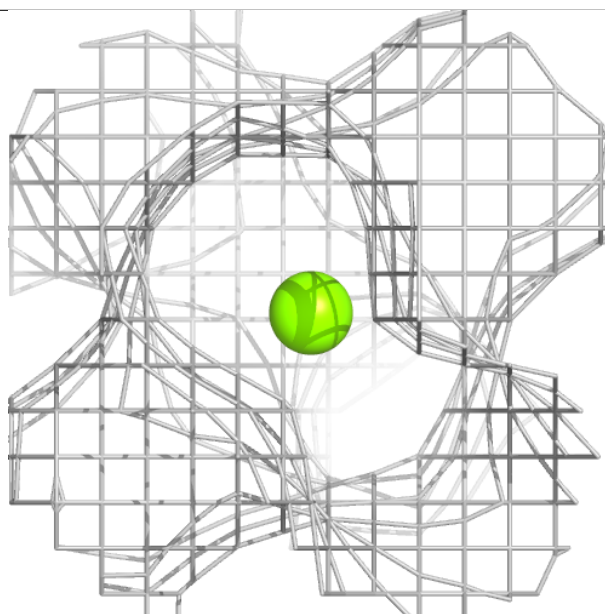
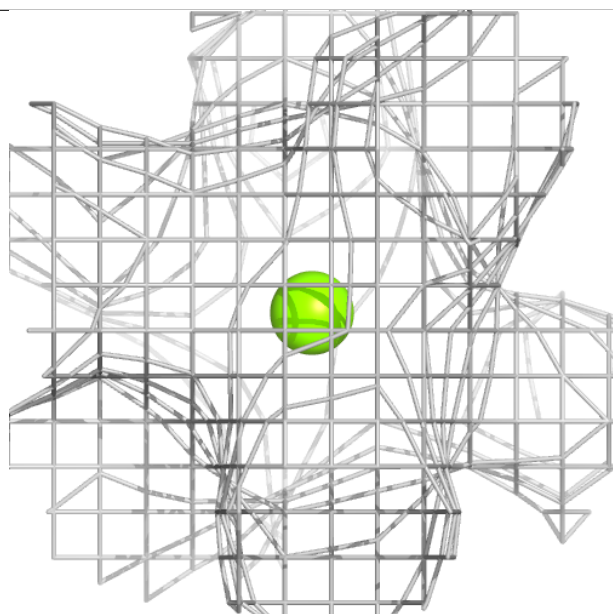
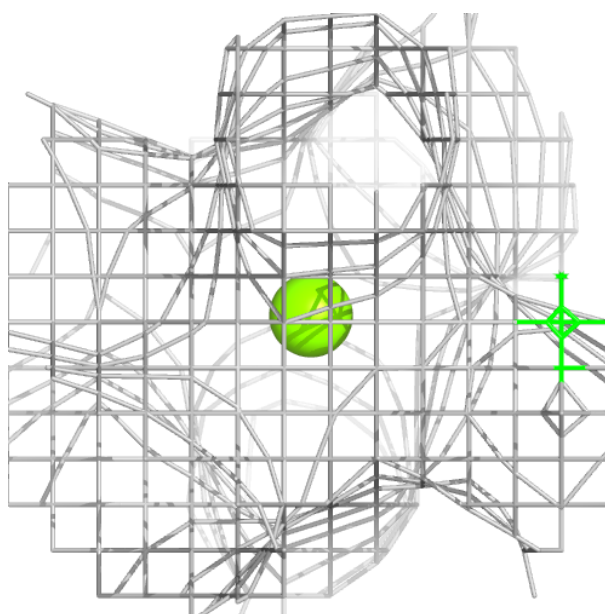
Electron density around DZ4 G 706:

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



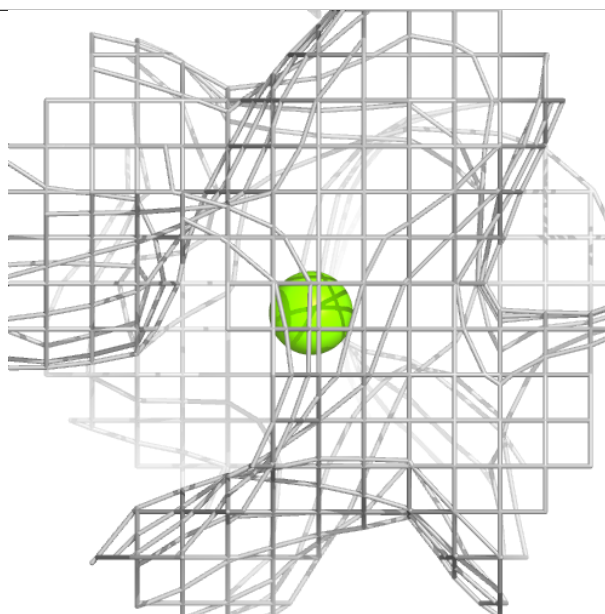
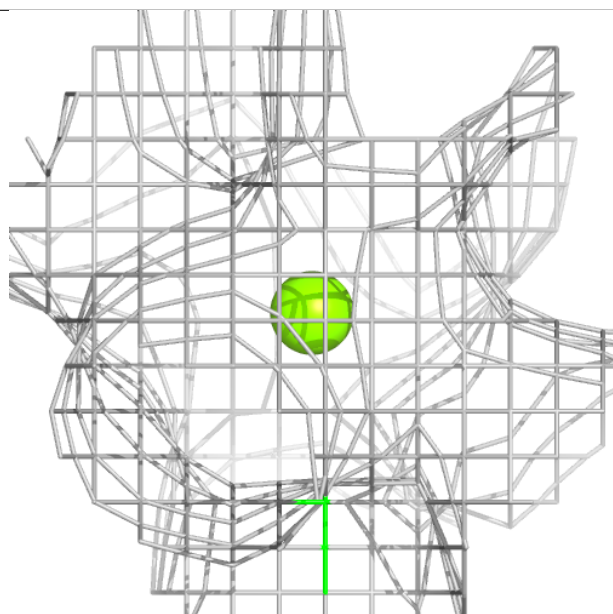
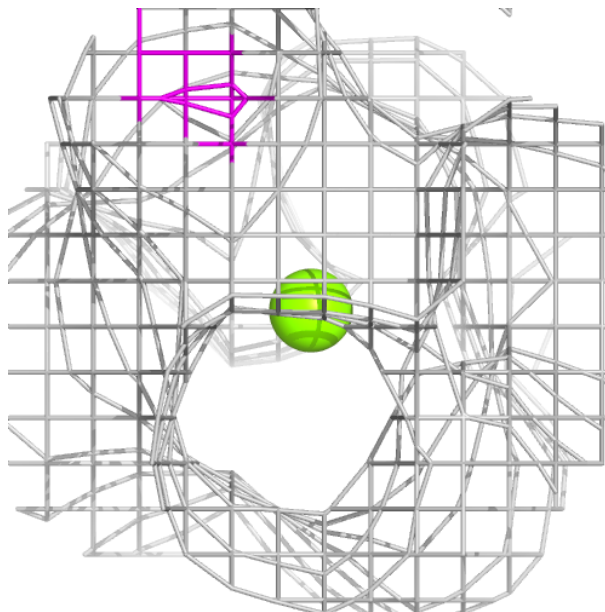
Electron density around MG D 704:

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



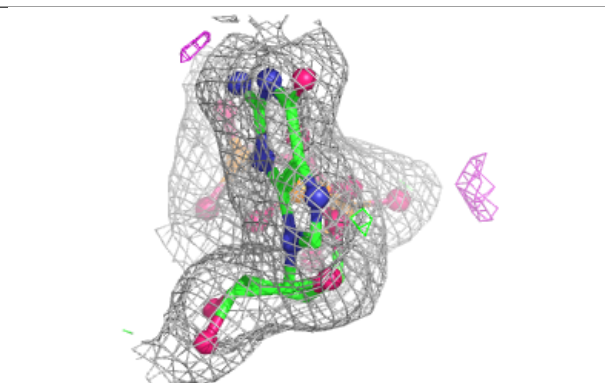
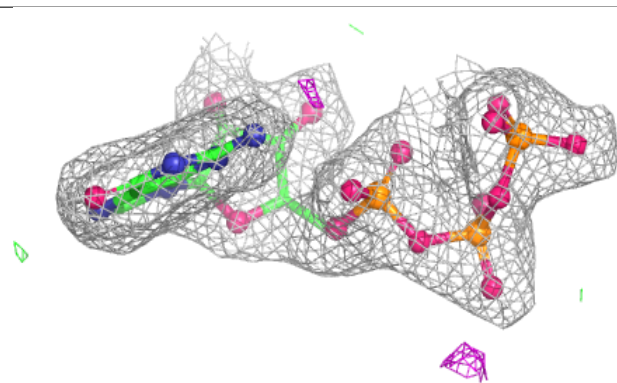
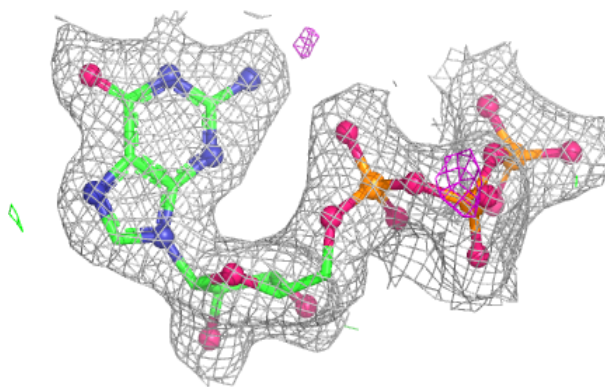
Electron density around MG D 705:

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

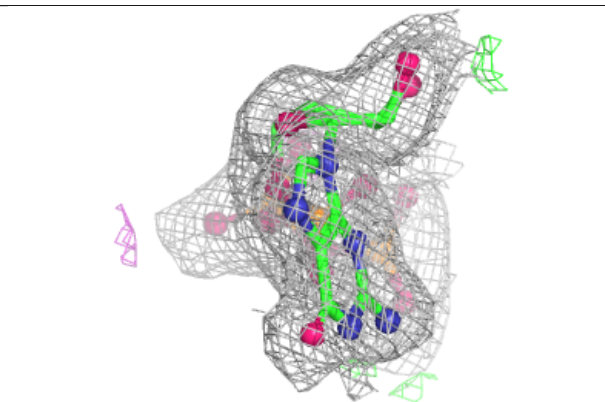
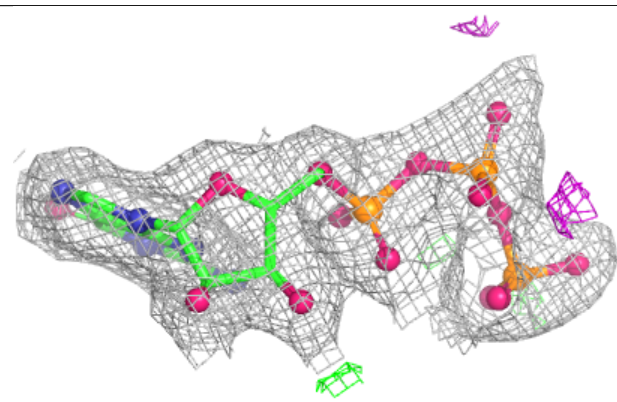
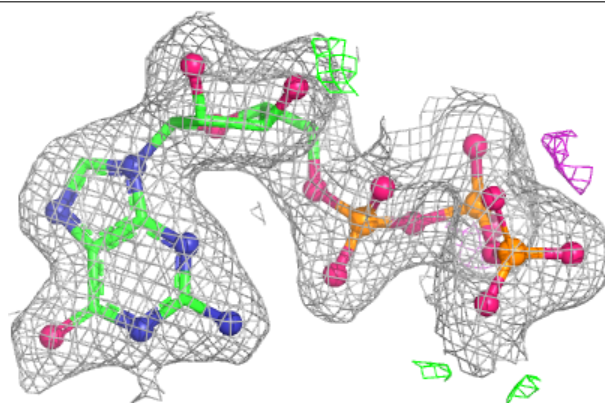


Electron density around GTP A 706:

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

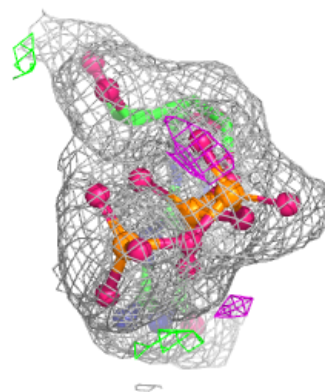
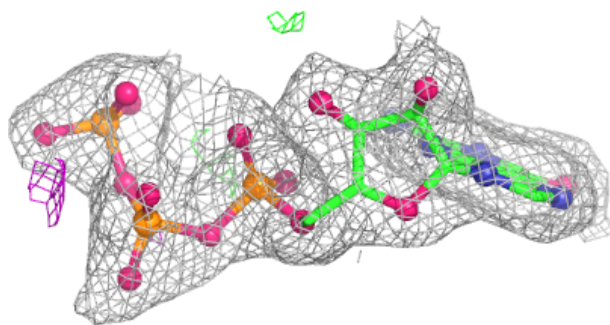
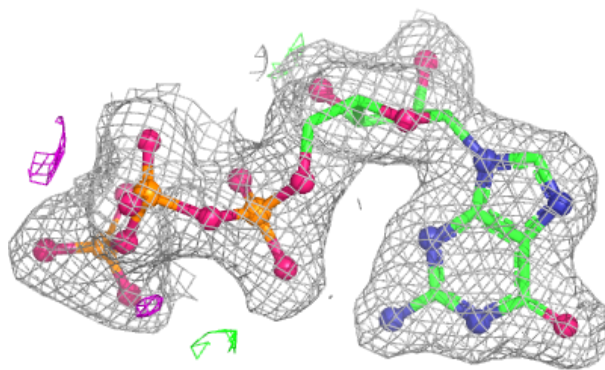
**Electron density around GTP B 706:**

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



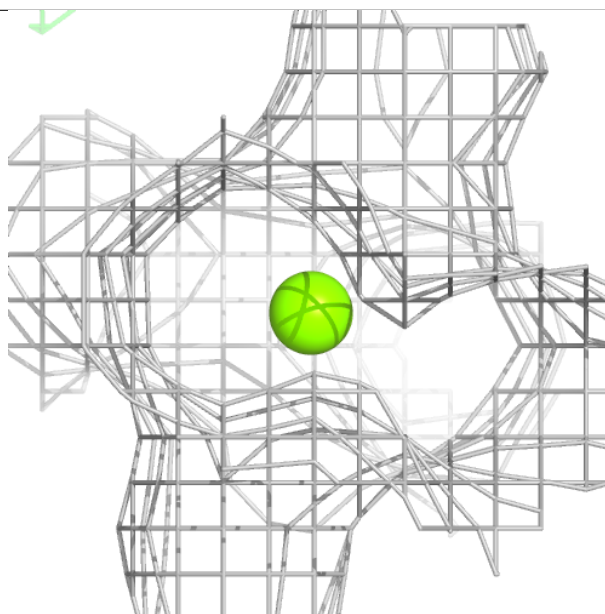
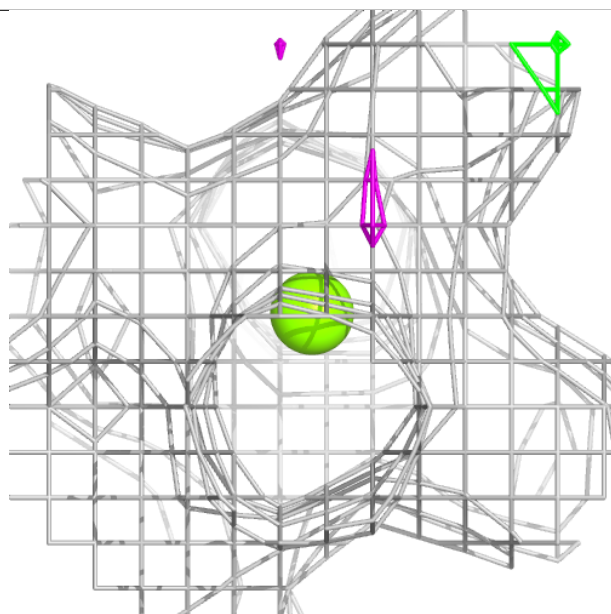
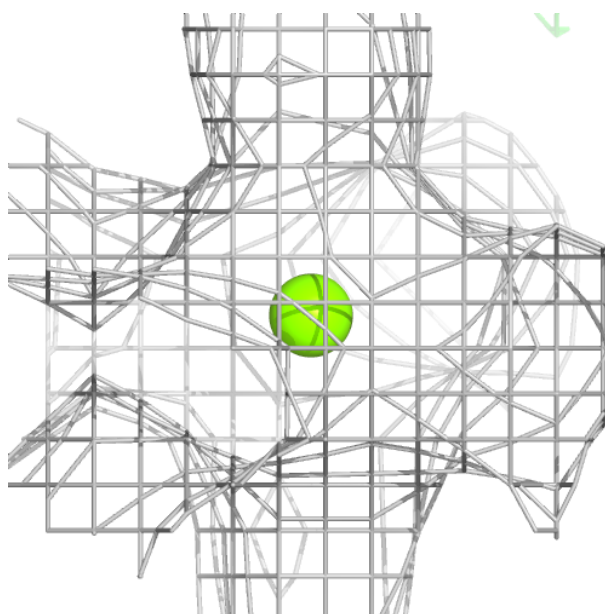
Electron density around GTP C 707:

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



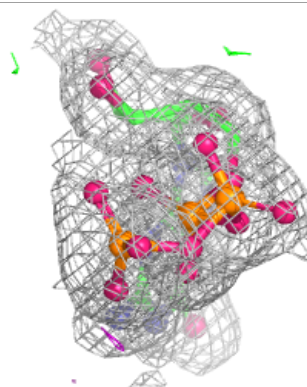
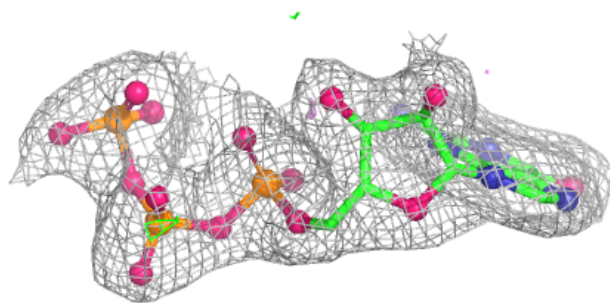
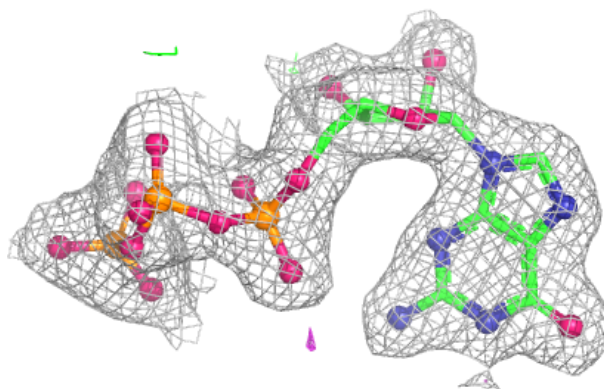
Electron density around MG A 703:

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



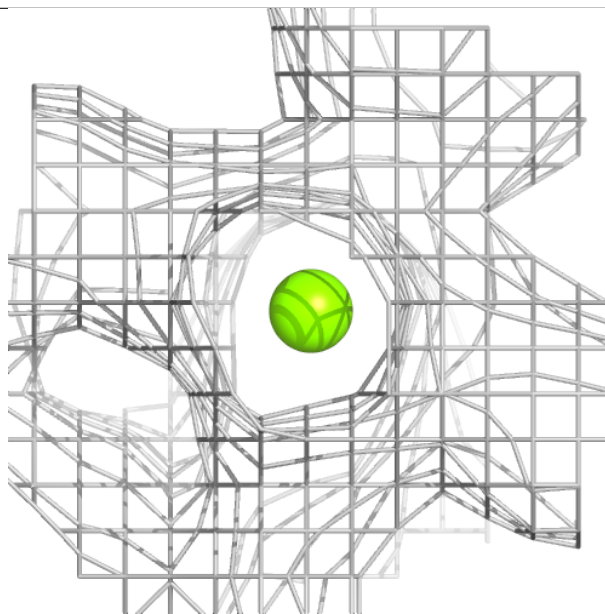
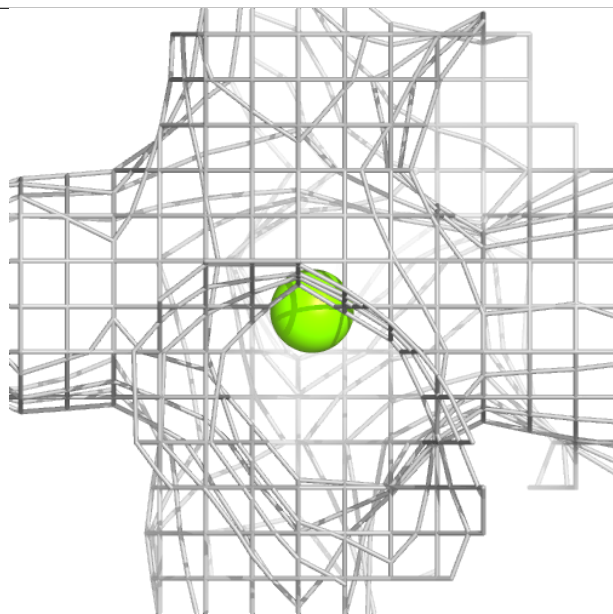
Electron density around GTP E 706:

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



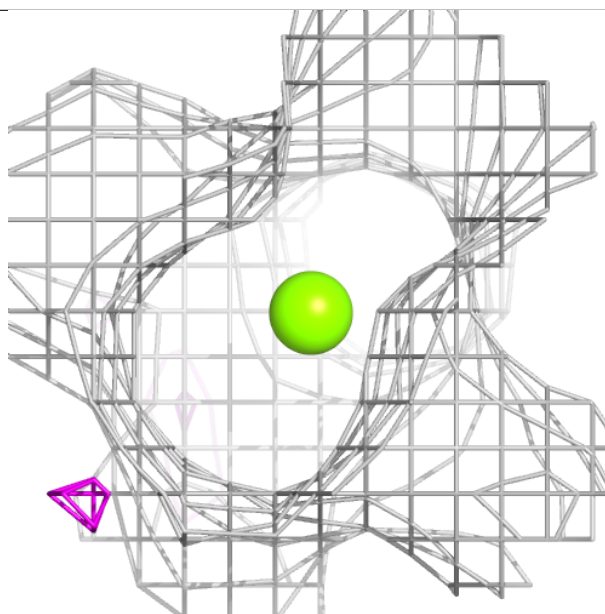
Electron density around MG E 702:

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



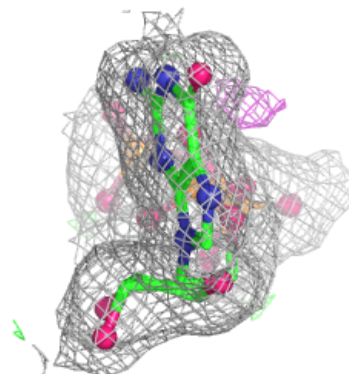
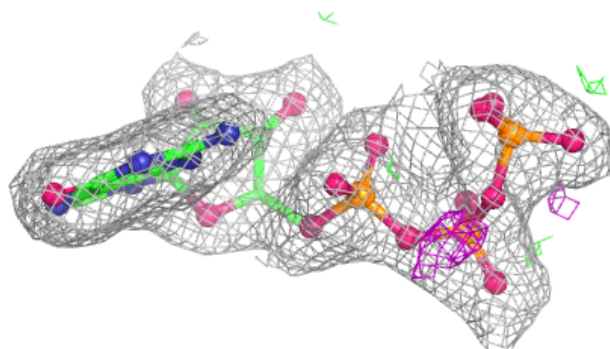
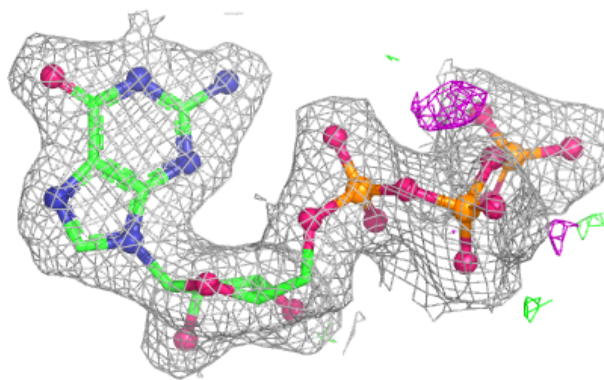
Electron density around MG E 703:

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



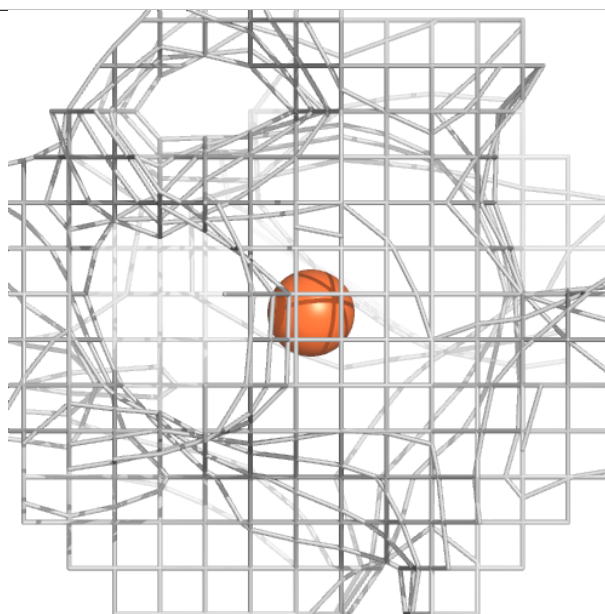
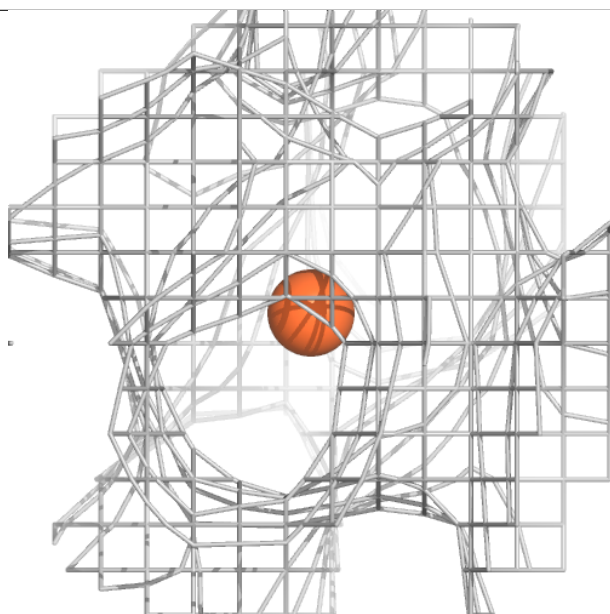
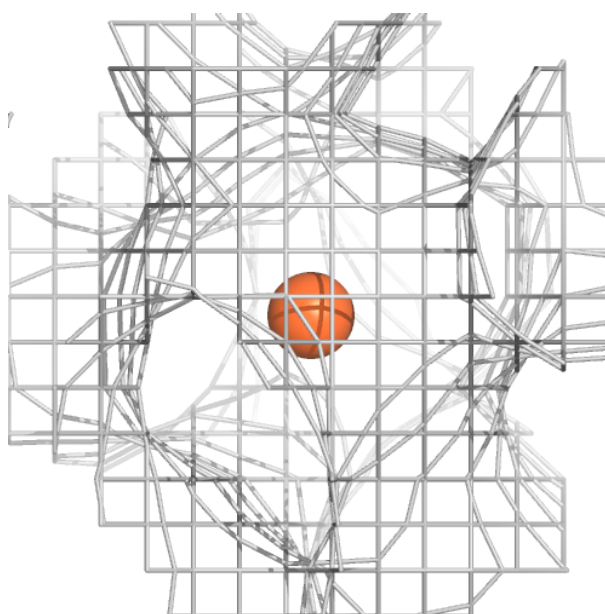
Electron density around GTP H 707:

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



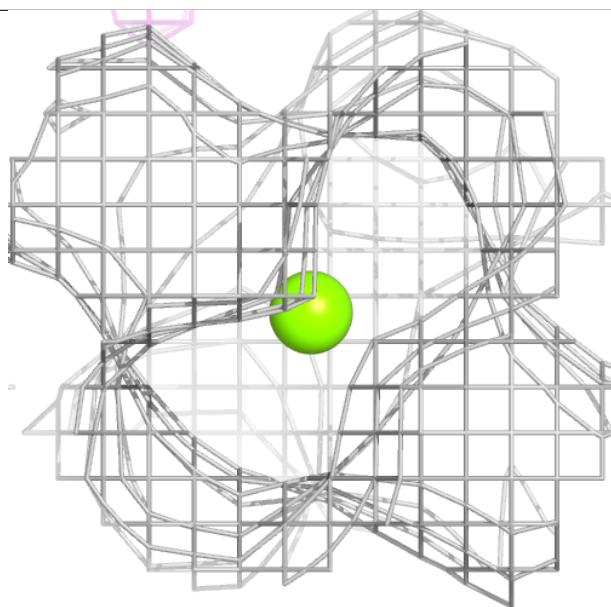
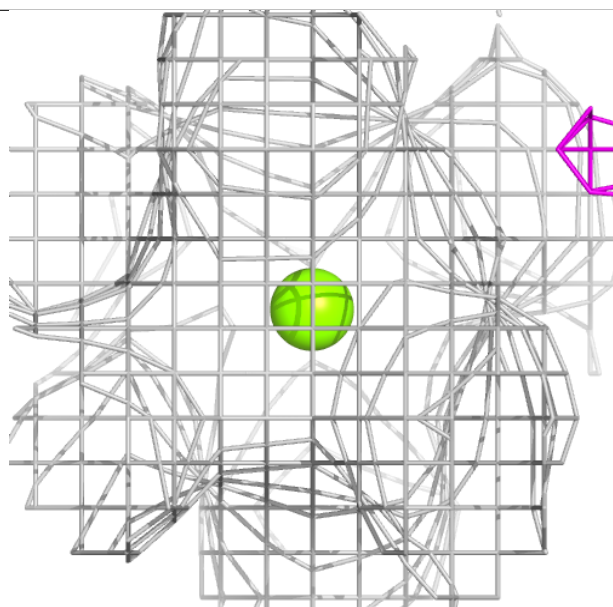
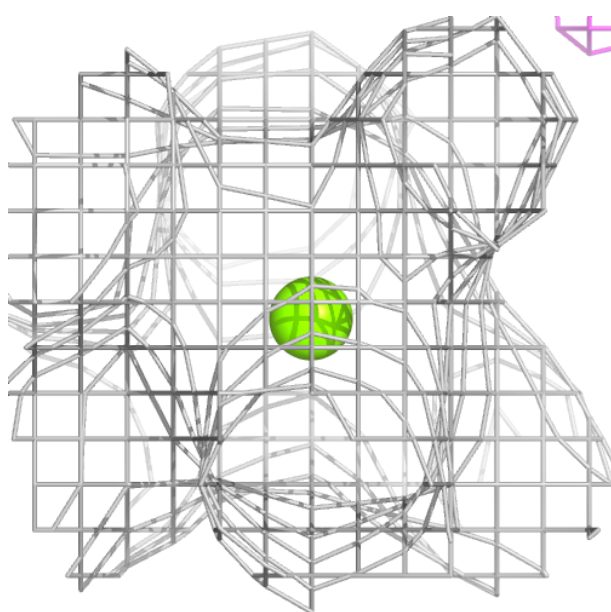
Electron density around FE F 701:

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



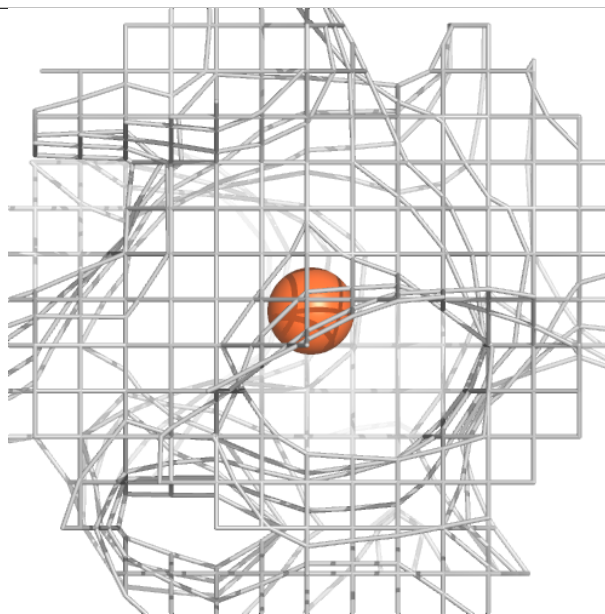
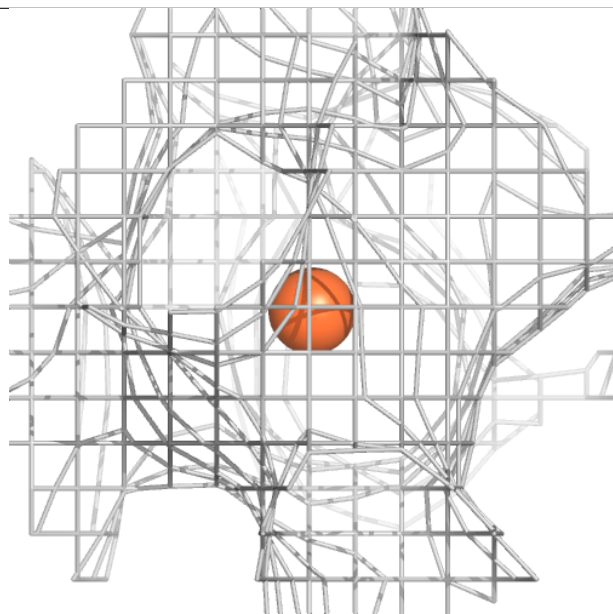
Electron density around MG F 703:

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



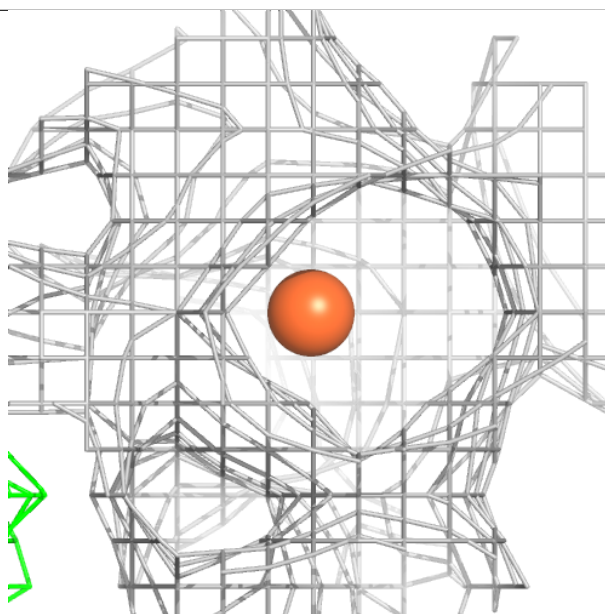
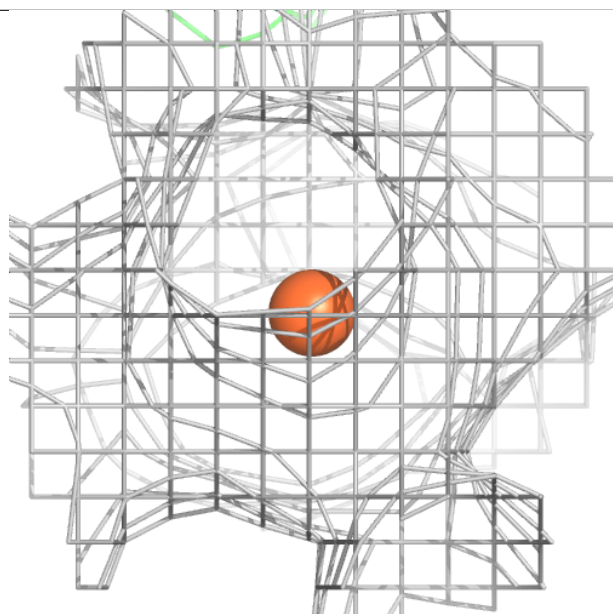
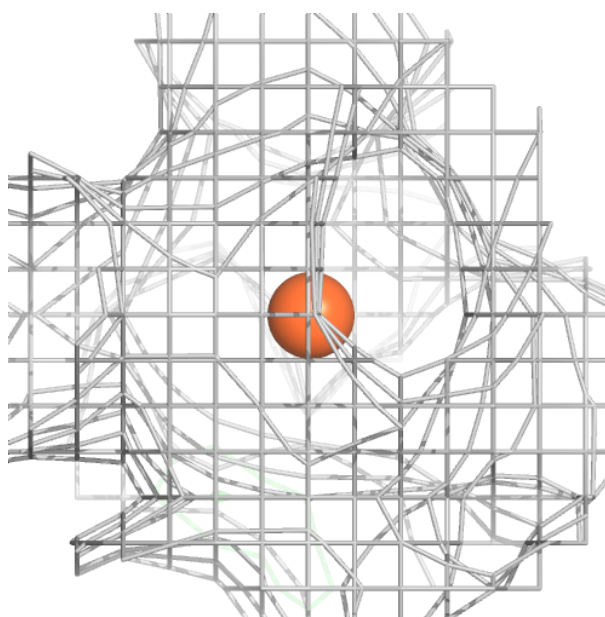
Electron density around FE G 702:

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



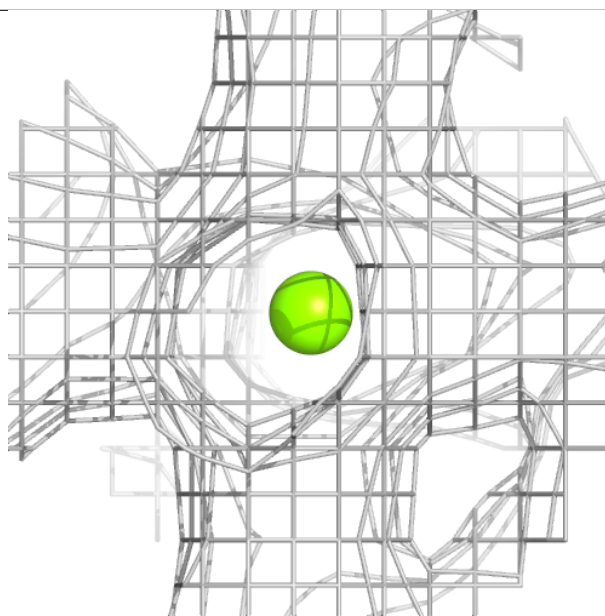
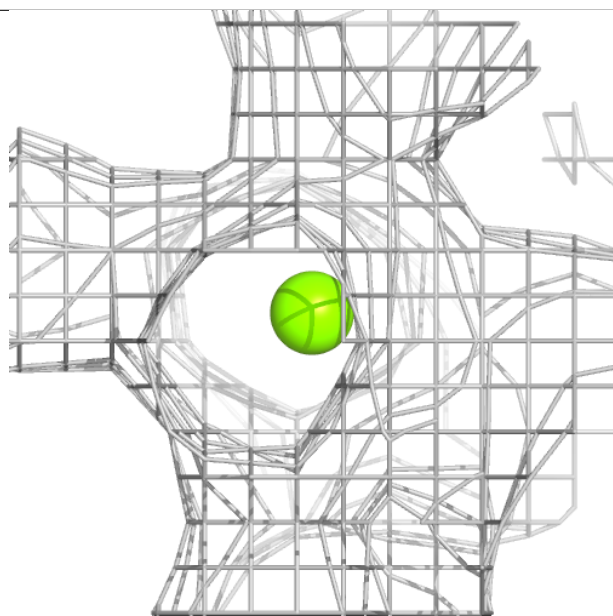
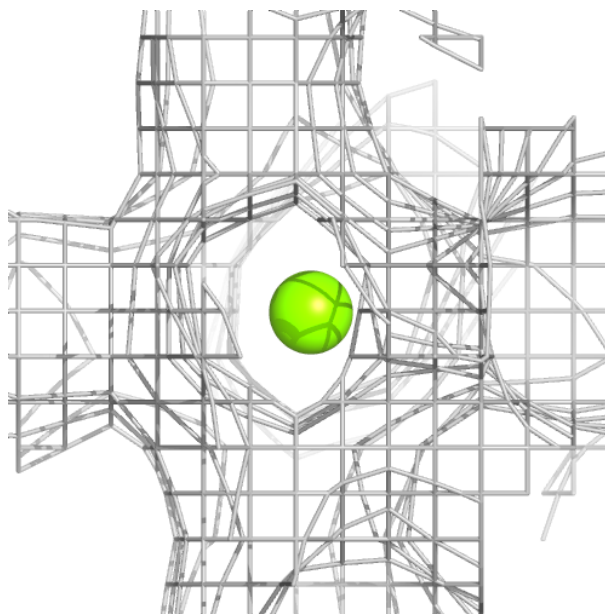
Electron density around FE H 702:

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



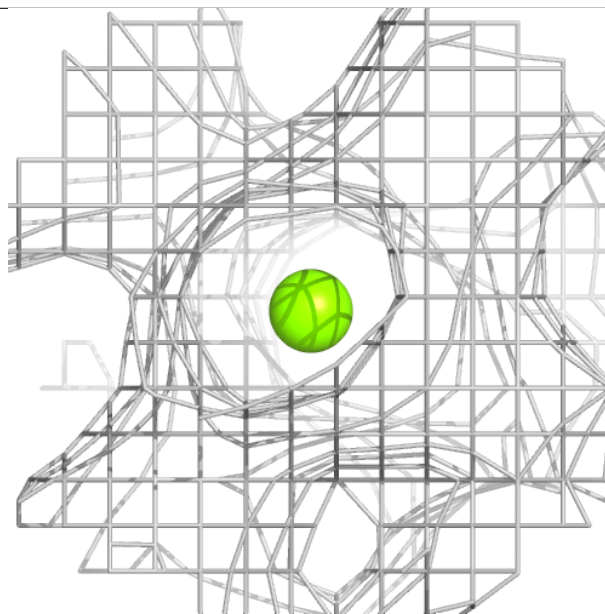
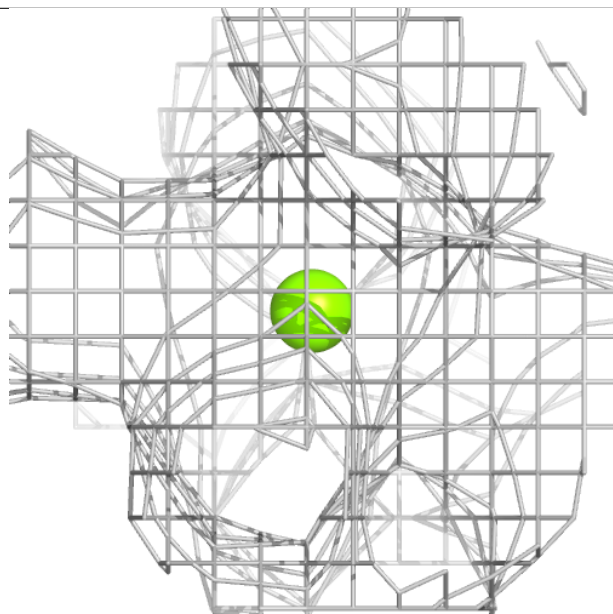
Electron density around MG D 703:

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



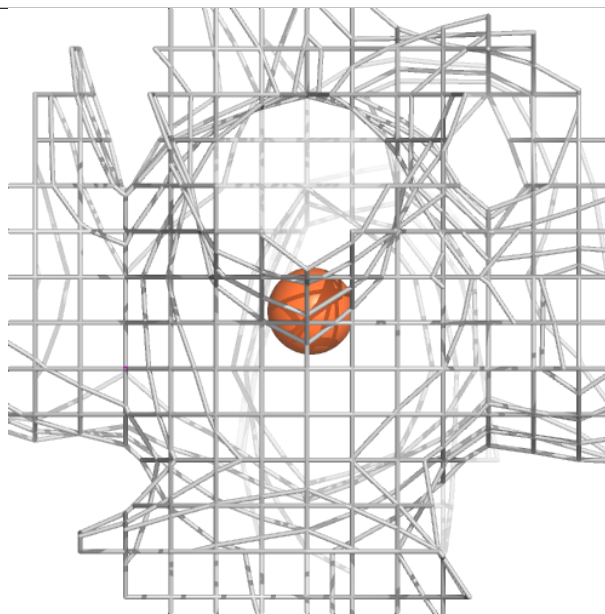
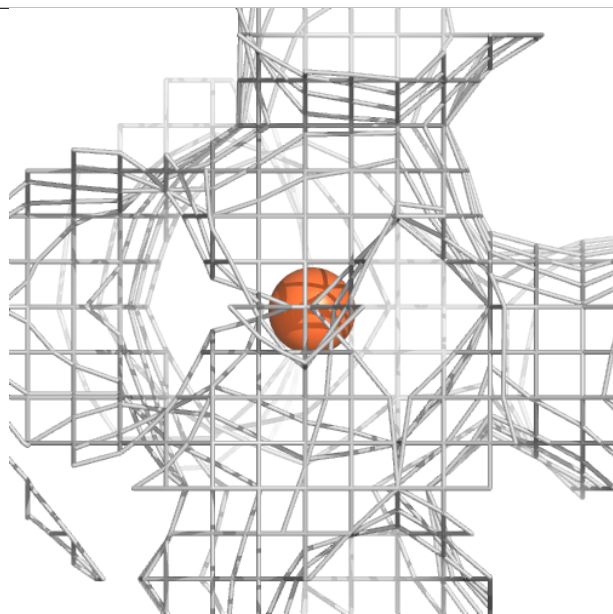
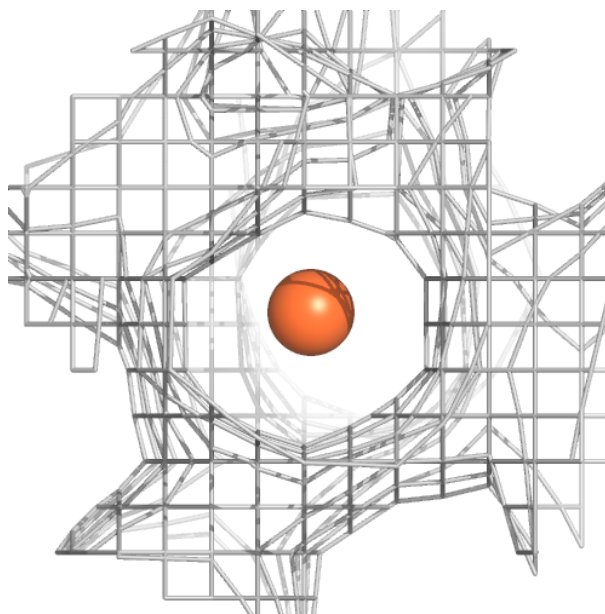
Electron density around MG A 702:

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



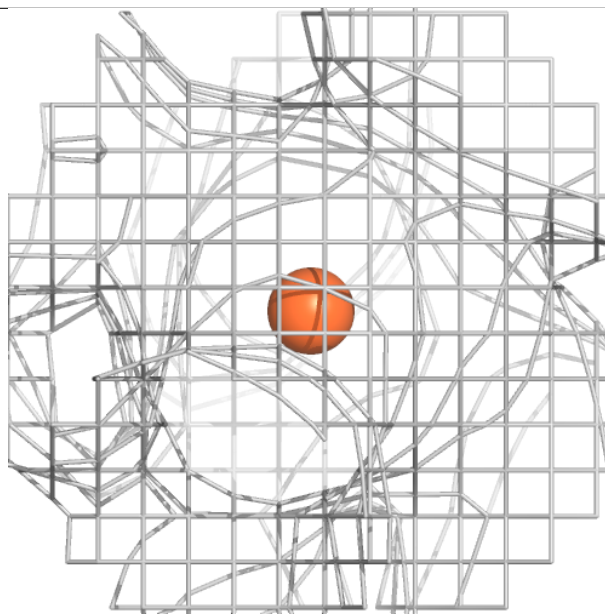
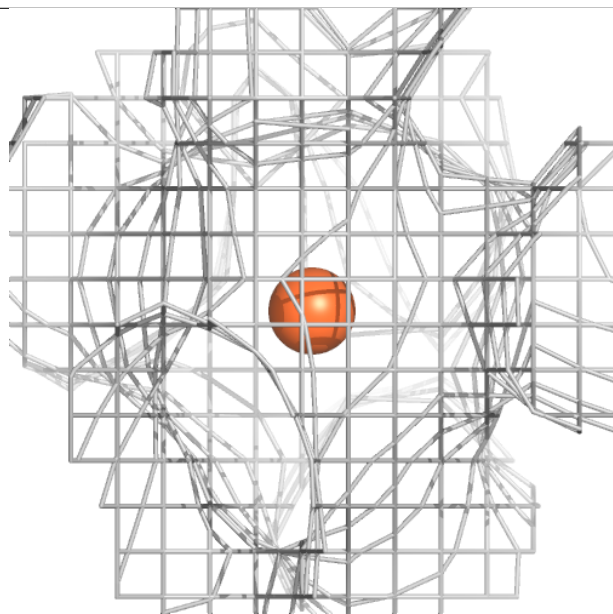
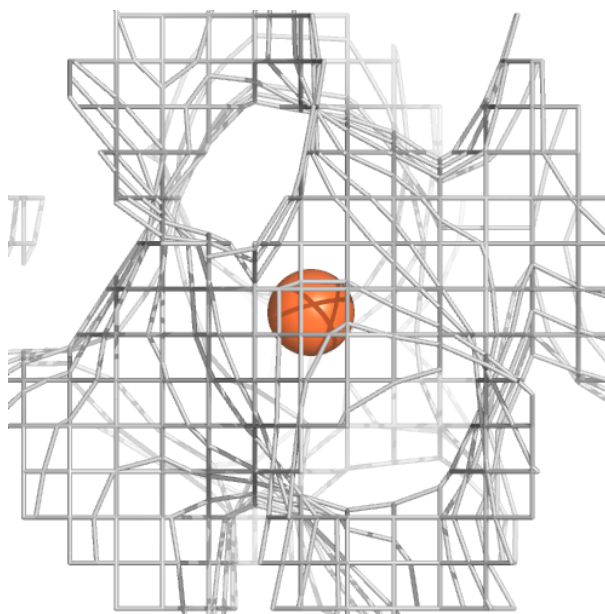
Electron density around FE A 701:

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



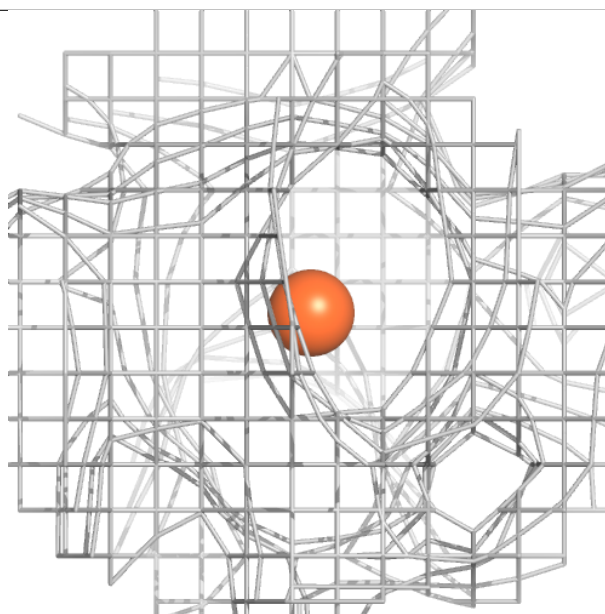
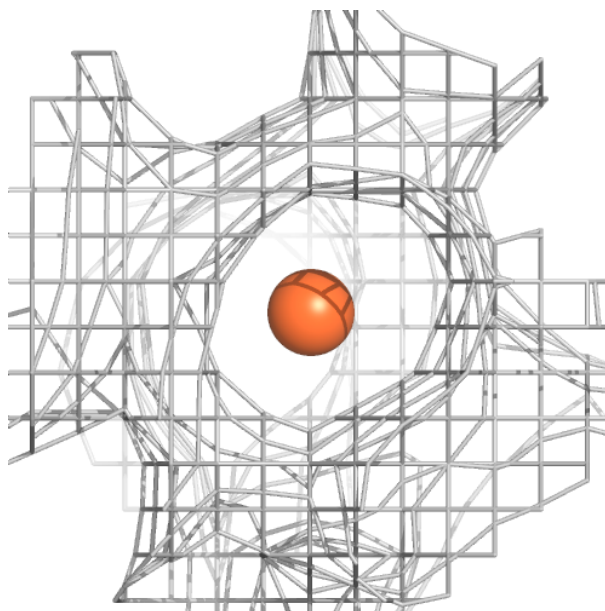
Electron density around FE B 701:

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



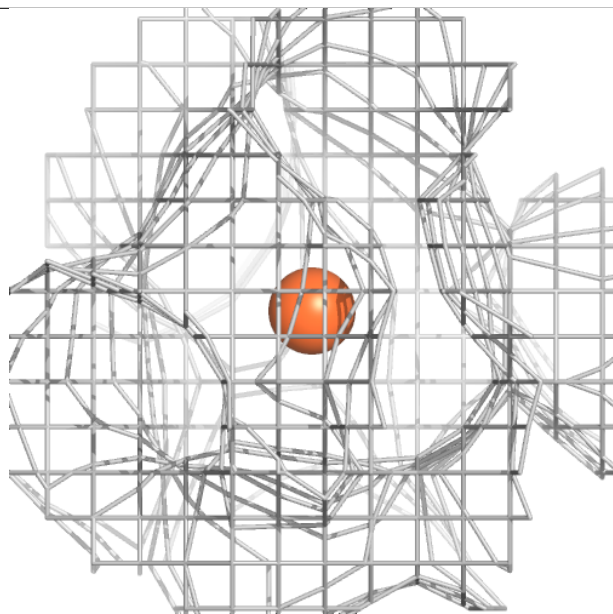
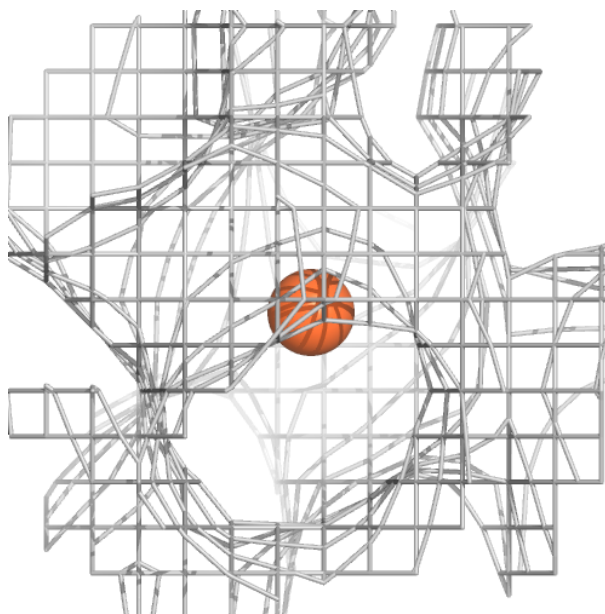
Electron density around FE C 702:

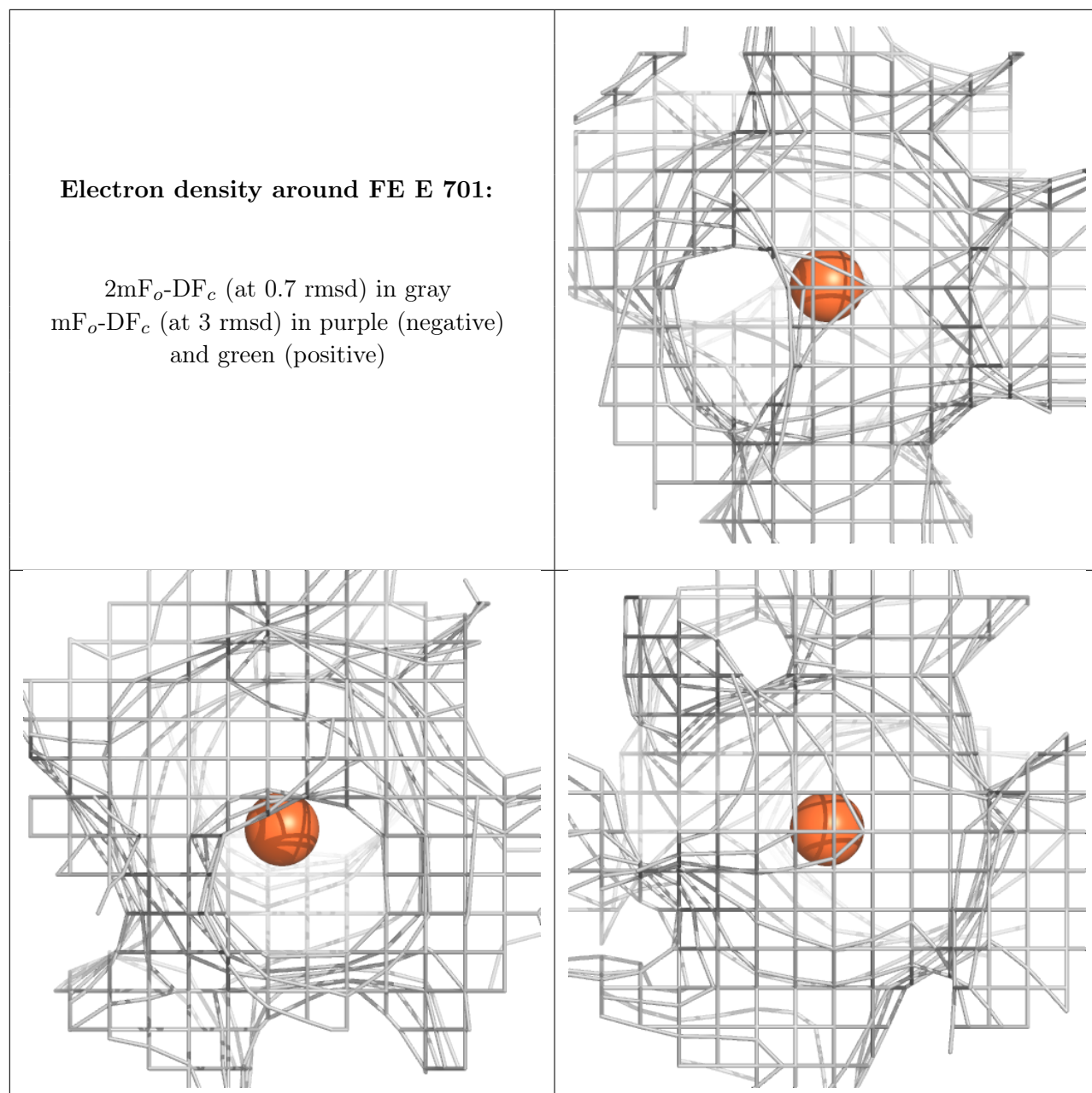
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE D 702:

$2mF_o-DF_c$ (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.