



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:58 AM UTC

PDB ID : 9NM5 / pdb_00009nm5
Title : Crystal structure of human glutamine synthetase in complex with ADP and phosphinothricin phosphate
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Deposited on : 2025-03-04
Resolution : 1.85 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

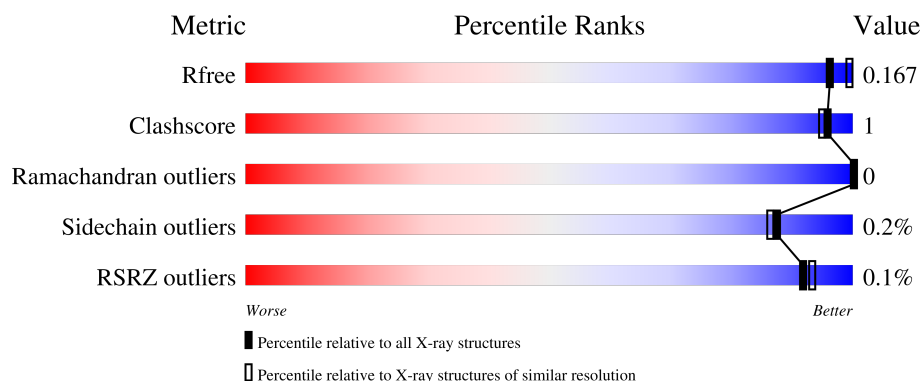
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	373	97% ..
1	B	373	96% ..
1	C	373	97% ..
1	H	373	98% ..
1	I	373	98% ..

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Mol	Chain	Length	Quality of chain
2	D	373	<div><div></div><div>97%</div><div></div></div> <div>..</div>
2	E	373	<div><div></div><div>98%</div><div></div></div> <div>..</div>
2	F	373	<div><div></div><div>96%</div><div></div></div> <div>..</div>
2	G	373	<div><div></div><div>97%</div><div></div></div> <div>..</div>
2	J	373	<div><div>%</div><div></div><div></div></div> <div>96%</div> <div>..</div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 33375 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	4	0
			2947	1851	520	554	22			
1	B	371	Total	C	N	O	S	0	3	0
			2918	1836	510	550	22			
1	C	370	Total	C	N	O	S	0	4	0
			2940	1846	517	555	22			
1	H	370	Total	C	N	O	S	0	3	0
			2906	1831	510	543	22			
1	I	371	Total	C	N	O	S	0	3	0
			2910	1832	508	548	22			

- Molecule 2 is a protein called Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	371	Total	C	N	O	S	0	4	0
			2929	1842	512	552	23			
2	E	371	Total	C	N	O	S	0	4	0
			2925	1840	513	550	22			
2	F	370	Total	C	N	O	S	0	3	0
			2898	1826	505	545	22			
2	G	370	Total	C	N	O	S	0	4	0
			2910	1831	508	549	22			
2	J	370	Total	C	N	O	S	0	3	0
			2904	1828	507	547	22			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

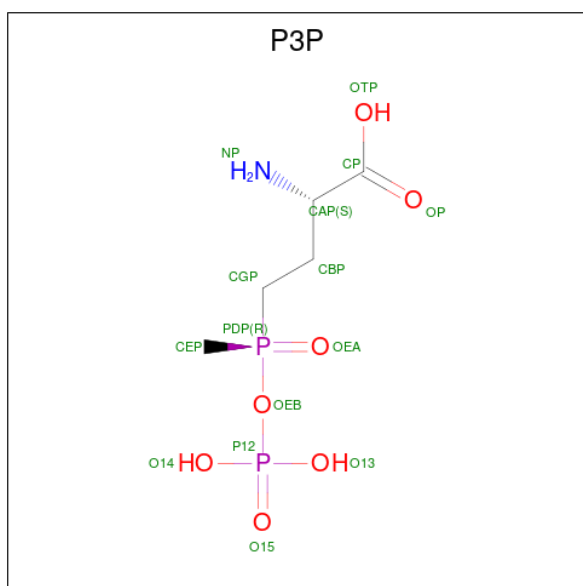
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total 3	Mn 3	0	0
4	C	3	Total 3	Mn 3	0	0
4	D	3	Total 3	Mn 3	0	0
4	E	3	Total 3	Mn 3	0	0
4	F	3	Total 3	Mn 3	0	0
4	G	3	Total 3	Mn 3	0	0
4	H	3	Total 3	Mn 3	0	0
4	I	3	Total 3	Mn 3	0	0
4	J	3	Total 3	Mn 3	0	0

- Molecule 5 is (2S)-2-AMINO-4-[METHYL(PHOSPHONOOXY)PHOSPHORYL]BUTANOIC ACID (CCD ID: P3P) (formula: $C_5H_{13}NO_7P_2$) (labeled as "Ligand of Interest" by depositor).



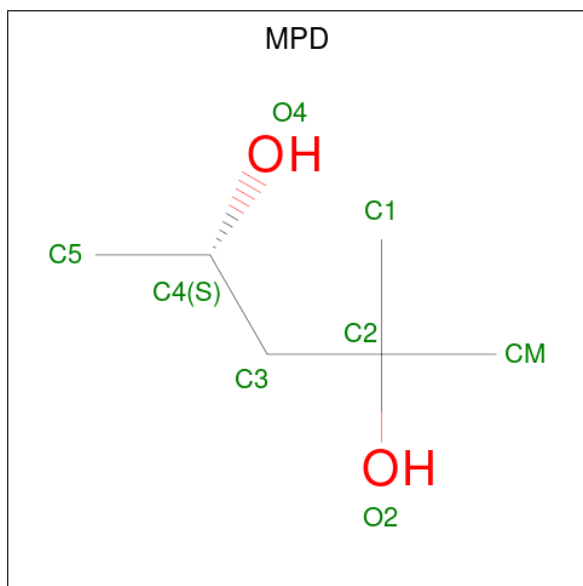
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	C	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	D	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	E	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	F	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	G	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	H	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	I	1	Total	C	N	O	P	0	0
			15	5	1	7	2		
5	J	1	Total	C	N	O	P	0	0
			15	5	1	7	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	E	1	Total	C	O	0	0
			8	6	2		
6	E	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	F	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	G	1	Total	C	O	0	0
			8	6	2		
6	H	1	Total	C	O	0	0
			8	6	2		
6	H	1	Total	C	O	0	0
			8	6	2		
6	H	1	Total	C	O	0	0
			8	6	2		
6	I	1	Total	C	O	0	0
			8	6	2		
6	I	1	Total	C	O	0	0
			8	6	2		
6	J	1	Total	C	O	0	0
			8	6	2		
6	J	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Cl 2	0	0
7	B	1	Total 1	Cl 1	0	0
7	C	1	Total 1	Cl 1	0	0
7	D	1	Total 1	Cl 1	0	0
7	F	2	Total 2	Cl 2	0	0
7	G	1	Total 1	Cl 1	0	0
7	I	2	Total 2	Cl 2	0	0

- Molecule 8 is water.

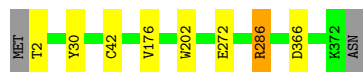
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	392	Total 392	O 392	0	0
8	B	370	Total 370	O 370	0	0
8	C	407	Total 407	O 407	0	0
8	D	397	Total 397	O 397	0	0
8	E	376	Total 376	O 376	0	0
8	F	323	Total 323	O 323	0	0
8	G	300	Total 300	O 300	0	0
8	H	357	Total 357	O 357	0	0
8	I	331	Total 331	O 331	0	0
8	J	307	Total 307	O 307	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamine synthetase

Chain A:  97% ..



- Molecule 1: Glutamine synthetase

Chain B:  96% ..



- Molecule 1: Glutamine synthetase

Chain C:  97% ..



- Molecule 1: Glutamine synthetase

Chain H:  98% ..



- Molecule 1: Glutamine synthetase

Chain I:  98% ..



- Molecule 2: Glutamine synthetase

Chain D:  97% ..



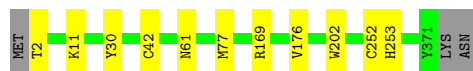
- Molecule 2: Glutamine synthetase

Chain E: 98% ..



- Molecule 2: Glutamine synthetase

Chain F: 96% ..



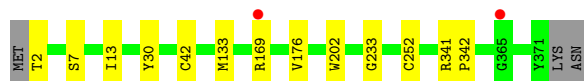
- Molecule 2: Glutamine synthetase

Chain G: 97% ..



- Molecule 2: Glutamine synthetase

Chain J: 96% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.40Å 130.98Å 191.62Å 90.00° 101.41° 90.00°	Depositor
Resolution (Å)	37.54 – 1.85 37.54 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.54-1.85) 99.2 (37.54-1.85)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.86Å)	Xtriage
Refinement program	PHENIX (dev_5484: ???)	Depositor
R, R_{free}	0.131 , 0.159 0.141 , 0.167	Depositor DCC
R_{free} test set	18649 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	33375	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, CSO, MN, P3P, CL, MPD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.22	0/3030	0.43	0/4099
1	B	0.22	0/2998	0.43	0/4061
1	C	0.24	0/3023	0.45	0/4091
1	H	0.21	0/2986	0.41	0/4044
1	I	0.20	0/2990	0.41	0/4052
2	D	0.23	0/3020	0.44	0/4091
2	E	0.22	0/3016	0.44	0/4086
2	F	0.19	0/2986	0.39	0/4048
2	G	0.20	0/3001	0.39	0/4069
2	J	0.20	0/2992	0.39	0/4056
All	All	0.22	0/30042	0.42	0/40697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2947	0	2818	6	0
1	B	2918	0	2756	8	0
1	C	2940	0	2802	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2906	0	2755	4	0
1	I	2910	0	2738	5	0
2	D	2929	0	2777	6	0
2	E	2925	0	2775	6	0
2	F	2898	0	2734	7	0
2	G	2910	0	2741	7	0
2	J	2904	0	2738	8	0
3	A	27	0	11	0	0
3	B	27	0	11	0	0
3	C	27	0	12	0	0
3	D	27	0	11	0	0
3	E	27	0	11	0	0
3	F	27	0	11	0	0
3	G	27	0	11	0	0
3	H	27	0	11	0	0
3	I	27	0	12	0	0
3	J	27	0	11	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
4	G	3	0	0	0	0
4	H	3	0	0	0	0
4	I	3	0	0	0	0
4	J	3	0	0	0	0
5	A	15	0	10	0	0
5	B	15	0	10	0	0
5	C	15	0	10	0	0
5	D	15	0	10	0	0
5	E	15	0	10	0	0
5	F	15	0	10	0	0
5	G	15	0	10	0	0
5	H	15	0	10	0	0
5	I	15	0	10	0	0
5	J	15	0	10	0	0
6	A	16	0	28	1	0
6	B	16	0	28	0	0
6	C	16	0	28	0	0
6	D	16	0	28	0	0
6	E	16	0	28	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	16	0	28	0	0
6	G	16	0	28	0	0
6	H	24	0	42	0	0
6	I	16	0	28	0	0
6	J	16	0	28	1	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	2	0	0	0	0
7	G	1	0	0	0	0
7	I	2	0	0	0	0
8	A	392	0	0	3	0
8	B	370	0	0	1	0
8	C	407	0	0	1	0
8	D	397	0	0	0	0
8	E	376	0	0	3	0
8	F	323	0	0	1	0
8	G	300	0	0	3	0
8	H	357	0	0	1	0
8	I	331	0	0	1	0
8	J	307	0	0	2	0
All	All	33375	0	28140	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (64) 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)
6:A:406:MPD:HM1	8:A:854:HOH:O	1.86	0.74
1:B:2:THR:N	8:B:501:HOH:O	2.22	0.72
1:C:246[B]:ASN:ND2	8:C:501:HOH:O	2.24	0.70
2:J:2:THR:N	8:J:501:HOH:O	2.27	0.67
2:E:286:ARG:NH2	2:E:366:ASP:O	2.30	0.64
2:G:91:LYS:NZ	8:G:504:HOH:O	2.33	0.61
1:A:176:VAL:HG21	1:A:202:TRP:CE3	2.39	0.58
2:G:246[A]:ASN:ND2	8:G:506:HOH:O	2.36	0.58
2:E:176:VAL:HG21	2:E:202:TRP:CE3	2.38	0.57
2:F:2:THR:N	8:F:502:HOH:O	2.37	0.57
2:F:176:VAL:HG21	2:F:202:TRP:CE3	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2:THR:N	8:H:505:HOH:O	2.37	0.57
2:D:2:THR:HG21	8:J:736:HOH:O	2.05	0.56
1:H:176:VAL:HG21	1:H:202:TRP:CE3	2.41	0.56
2:J:133:MET:HE2	2:J:252:CYS:SG	2.49	0.53
2:D:176:VAL:HG21	2:D:202:TRP:CE3	2.43	0.53
2:F:176:VAL:HG21	2:F:202:TRP:CD2	2.43	0.53
2:G:176:VAL:HG21	2:G:202:TRP:CE3	2.44	0.53
1:B:176:VAL:HG21	1:B:202:TRP:CE3	2.43	0.53
1:C:176:VAL:HG21	1:C:202:TRP:CE3	2.45	0.52
2:E:176:VAL:HG21	2:E:202:TRP:CD2	2.45	0.51
2:J:176:VAL:HG21	2:J:202:TRP:CE3	2.45	0.51
2:G:2:THR:N	8:G:508:HOH:O	2.44	0.50
1:H:176:VAL:HG21	1:H:202:TRP:CD2	2.46	0.50
1:A:176:VAL:HG21	1:A:202:TRP:CD2	2.46	0.50
2:E:246[A]:ASN:ND2	8:E:507:HOH:O	2.44	0.50
1:I:176:VAL:HG21	1:I:202:TRP:CE3	2.47	0.49
2:G:176:VAL:HG21	2:G:202:TRP:CD2	2.47	0.49
1:I:176:VAL:HG21	1:I:202:TRP:CD2	2.48	0.48
2:D:371:TYR:O	2:D:372:LYS:CB	2.63	0.47
2:J:176:VAL:HG21	2:J:202:TRP:CD2	2.50	0.46
1:B:13:ILE:HD11	1:C:11:LYS:HE3	1.96	0.46
2:D:176:VAL:HG21	2:D:202:TRP:CD2	2.50	0.46
1:C:176:VAL:HG21	1:C:202:TRP:CD2	2.51	0.45
2:E:2:THR:N	8:E:512:HOH:O	2.49	0.45
6:E:406:MPD:H11	6:E:406:MPD:O4	2.18	0.44
1:B:176:VAL:HG21	1:B:202:TRP:CD2	2.51	0.44
1:H:133:MET:HE2	1:H:252:CYS:SG	2.58	0.43
1:I:2:THR:N	8:I:508:HOH:O	2.50	0.43
1:B:30:TYR:O	1:B:42:CYS:HA	2.19	0.43
1:A:30:TYR:O	1:A:42:CYS:HA	2.19	0.43
1:C:16:VAL:O	1:C:19[B]:SER:OG	2.32	0.43
2:J:7:SER:HB3	2:J:233:GLY:HA3	2.00	0.42
6:J:406:MPD:O4	6:J:406:MPD:H11	2.19	0.42
1:B:264:GLU:OE2	1:B:334:LYS:NZ	2.40	0.42
1:A:286:ARG:NH2	1:A:366:ASP:O	2.41	0.42
1:I:7:SER:HB3	1:I:233:GLY:HA3	2.02	0.42
1:A:2:THR:N	8:A:512:HOH:O	2.51	0.42
2:G:341:ARG:N	2:G:342:PRO:CD	2.83	0.42
1:B:61:ASN:HA	1:B:77:MET:O	2.20	0.42
2:F:11:LYS:HE3	2:J:13:ILE:HD11	2.02	0.42
2:E:286:ARG:NE	8:E:514:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:TYR:O	1:I:42:CYS:HA	2.20	0.42
1:A:272:GLU:OE2	8:A:501:HOH:O	2.22	0.41
2:F:30:TYR:O	2:F:42:CYS:HA	2.20	0.41
1:C:341:ARG:N	1:C:342:PRO:CD	2.83	0.41
2:J:341:ARG:N	2:J:342:PRO:CD	2.83	0.41
1:B:133:MET:HE2	1:B:252:CYS:SG	2.61	0.41
2:D:7:SER:HB3	2:D:233:GLY:HA3	2.03	0.41
2:F:252:CYS:O	2:F:253:HIS:C	2.64	0.41
2:F:61:ASN:HA	2:F:77:MET:O	2.20	0.41
2:G:16:VAL:O	2:G:19[B]:SER:OG	2.32	0.41
2:J:30:TYR:O	2:J:42:CYS:HA	2.22	0.40
2:D:57:LEU:HD13	2:D:97:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	372/373 (100%)	366 (98%)	6 (2%)	0	100	100
1	B	371/373 (100%)	363 (98%)	8 (2%)	0	100	100
1	C	371/373 (100%)	364 (98%)	7 (2%)	0	100	100
1	H	370/373 (99%)	361 (98%)	9 (2%)	0	100	100
1	I	371/373 (100%)	364 (98%)	7 (2%)	0	100	100
2	D	373/373 (100%)	366 (98%)	7 (2%)	0	100	100
2	E	373/373 (100%)	366 (98%)	7 (2%)	0	100	100
2	F	371/373 (100%)	362 (98%)	9 (2%)	0	100	100
2	G	372/373 (100%)	366 (98%)	6 (2%)	0	100	100
2	J	371/373 (100%)	362 (98%)	9 (2%)	0	100	100
All	All	3715/3730 (100%)	3640 (98%)	75 (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	313/313 (100%)	312 (100%)	1 (0%)	86	85
1	B	304/313 (97%)	304 (100%)	0	100	100
1	C	312/313 (100%)	312 (100%)	0	100	100
1	H	302/313 (96%)	301 (100%)	1 (0%)	86	85
1	I	301/313 (96%)	301 (100%)	0	100	100
2	D	309/314 (98%)	307 (99%)	2 (1%)	78	73
2	E	308/314 (98%)	308 (100%)	0	100	100
2	F	302/314 (96%)	301 (100%)	1 (0%)	86	85
2	G	304/314 (97%)	304 (100%)	0	100	100
2	J	303/314 (96%)	302 (100%)	1 (0%)	86	85
All	All	3058/3135 (98%)	3052 (100%)	6 (0%)	87	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	ARG
2	D	38	GLU
2	D	169	ARG
2	F	169	ARG
1	H	286	ARG
2	J	169	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	69	GLN
1	A	127	GLN

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Mol	Chain	Res	Type
1	B	69	GLN
1	C	69	GLN
1	C	127	GLN
2	D	265	ASN
2	E	8	HIS
2	E	61	ASN
2	F	69	GLN
2	F	127	GLN
2	F	265	ASN
2	G	69	GLN
1	H	8	HIS
1	H	69	GLN
1	H	152	ASN
1	H	265	ASN
1	I	246	ASN
1	I	265	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	I	53	1	3,6,7	0.65	0	1,6,8	0.15	0
1	CSO	C	53	1	3,6,7	0.67	0	1,6,8	0.37	0
1	CSO	A	53	1	3,6,7	0.60	0	1,6,8	0.14	0
1	CSO	B	53	1	3,6,7	0.65	0	1,6,8	0.02	0
1	CSO	H	53	1	3,6,7	0.67	0	1,6,8	0.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	I	53	1	-	0/1/5/7	-
1	CSO	C	53	1	-	0/1/5/7	-
1	CSO	A	53	1	-	0/1/5/7	-
1	CSO	B	53	1	-	0/1/5/7	-
1	CSO	H	53	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 81 ligands modelled in this entry, 40 are monoatomic - leaving 41 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	$\# Z > 2$
6	MPD	I	406	-	7,7,7	0.40	0	9,10,10	0.52	0
5	P3P	G	405	4	9,14,14	2.50	1 (11%)	11,21,21	0.82	0
5	P3P	D	405	4	9,14,14	2.58	1 (11%)	11,21,21	0.86	0
6	MPD	A	407	-	7,7,7	0.37	0	9,10,10	0.63	0
6	MPD	H	406	-	7,7,7	0.29	0	9,10,10	0.64	0
6	MPD	G	406	-	7,7,7	0.40	0	9,10,10	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	P3P	A	405	4	9,14,14	2.30	1 (11%)	11,21,21	0.76	0
5	P3P	E	405	4	9,14,14	2.49	1 (11%)	11,21,21	0.80	0
6	MPD	E	406	-	7,7,7	0.42	0	9,10,10	0.51	0
3	ADP	C	401	4	28,29,29	2.73	10 (35%)	43,45,45	2.40	12 (27%)
3	ADP	B	401	4	28,29,29	2.82	10 (35%)	43,45,45	2.32	12 (27%)
6	MPD	C	407	-	7,7,7	0.40	0	9,10,10	0.56	0
3	ADP	G	401	4	28,29,29	2.90	9 (32%)	43,45,45	2.42	12 (27%)
3	ADP	F	401	4	28,29,29	2.94	10 (35%)	43,45,45	2.40	12 (27%)
3	ADP	H	401	4	28,29,29	2.84	10 (35%)	43,45,45	2.43	13 (30%)
6	MPD	B	407	-	7,7,7	0.40	0	9,10,10	0.57	0
5	P3P	I	405	4	9,14,14	2.58	1 (11%)	11,21,21	0.92	0
3	ADP	D	401	4	28,29,29	2.74	10 (35%)	43,45,45	2.37	13 (30%)
6	MPD	B	406	-	7,7,7	0.41	0	9,10,10	0.49	0
6	MPD	H	408	-	7,7,7	0.41	0	9,10,10	0.51	0
3	ADP	I	401	4	28,29,29	2.82	10 (35%)	43,45,45	2.38	12 (27%)
5	P3P	F	405	4	9,14,14	2.40	1 (11%)	11,21,21	0.80	0
3	ADP	E	401	4	28,29,29	2.85	10 (35%)	43,45,45	2.41	11 (25%)
5	P3P	C	405	4	9,14,14	2.68	1 (11%)	11,21,21	0.84	0
6	MPD	D	406	-	7,7,7	0.43	0	9,10,10	0.45	0
6	MPD	F	406	-	7,7,7	0.43	0	9,10,10	0.57	0
6	MPD	E	407	-	7,7,7	0.42	0	9,10,10	0.53	0
6	MPD	J	407	-	7,7,7	0.36	0	9,10,10	0.69	0
5	P3P	J	405	4	9,14,14	2.41	1 (11%)	11,21,21	0.80	0
6	MPD	J	406	-	7,7,7	0.43	0	9,10,10	0.55	0
6	MPD	A	406	-	7,7,7	0.32	0	9,10,10	0.52	0
6	MPD	I	407	-	7,7,7	0.38	0	9,10,10	0.56	0
5	P3P	H	405	4	9,14,14	2.76	1 (11%)	11,21,21	0.91	0
6	MPD	H	407	-	7,7,7	0.36	0	9,10,10	0.58	0
3	ADP	A	401	4	28,29,29	2.85	10 (35%)	43,45,45	2.42	11 (25%)
5	P3P	B	405	4	9,14,14	2.47	1 (11%)	11,21,21	0.89	0
6	MPD	C	406	-	7,7,7	0.42	0	9,10,10	0.70	0
6	MPD	F	407	-	7,7,7	0.42	0	9,10,10	0.56	0
3	ADP	J	401	4	28,29,29	2.93	10 (35%)	43,45,45	2.40	13 (30%)
6	MPD	G	407	-	7,7,7	0.39	0	9,10,10	0.54	0
6	MPD	D	407	-	7,7,7	0.38	0	9,10,10	0.63	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	I	406	-	-	1/5/5/5	-
5	P3P	G	405	4	-	4/12/16/16	-
5	P3P	D	405	4	-	5/12/16/16	-
6	MPD	A	407	-	-	2/5/5/5	-
6	MPD	H	406	-	-	0/5/5/5	-
6	MPD	G	406	-	-	0/5/5/5	-
5	P3P	A	405	4	-	4/12/16/16	-
5	P3P	E	405	4	-	4/12/16/16	-
6	MPD	E	406	-	-	1/5/5/5	-
3	ADP	C	401	4	-	7/16/32/32	0/3/3/3
3	ADP	B	401	4	-	5/16/32/32	0/3/3/3
6	MPD	C	407	-	-	0/5/5/5	-
3	ADP	G	401	4	-	8/16/32/32	0/3/3/3
3	ADP	F	401	4	-	8/16/32/32	0/3/3/3
3	ADP	H	401	4	-	8/16/32/32	0/3/3/3
6	MPD	B	407	-	-	2/5/5/5	-
5	P3P	I	405	4	-	4/12/16/16	-
3	ADP	D	401	4	-	6/16/32/32	0/3/3/3
6	MPD	B	406	-	-	1/5/5/5	-
6	MPD	H	408	-	-	3/5/5/5	-
3	ADP	I	401	4	-	8/16/32/32	0/3/3/3
5	P3P	F	405	4	-	4/12/16/16	-
3	ADP	E	401	4	-	7/16/32/32	0/3/3/3
5	P3P	C	405	4	-	4/12/16/16	-
6	MPD	D	406	-	-	1/5/5/5	-
6	MPD	F	406	-	-	1/5/5/5	-
6	MPD	E	407	-	-	0/5/5/5	-
6	MPD	J	407	-	-	2/5/5/5	-
5	P3P	J	405	4	-	4/12/16/16	-
6	MPD	J	406	-	-	1/5/5/5	-
6	MPD	A	406	-	-	0/5/5/5	-
6	MPD	I	407	-	-	3/5/5/5	-
5	P3P	H	405	4	-	4/12/16/16	-
6	MPD	H	407	-	-	0/5/5/5	-
3	ADP	A	401	4	-	8/16/32/32	0/3/3/3
5	P3P	B	405	4	-	4/12/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	C	406	-	-	0/5/5/5	-
6	MPD	F	407	-	-	2/5/5/5	-
3	ADP	J	401	4	-	7/16/32/32	0/3/3/3
6	MPD	G	407	-	-	4/5/5/5	-
6	MPD	D	407	-	-	0/5/5/5	-

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	ADP	C3'-C4'	-8.24	1.32	1.53
3	G	401	ADP	C3'-C4'	-8.18	1.32	1.53
3	J	401	ADP	C3'-C4'	-8.16	1.32	1.53
3	I	401	ADP	C3'-C4'	-8.14	1.32	1.53
3	E	401	ADP	C3'-C4'	-8.06	1.32	1.53
3	A	401	ADP	C3'-C4'	-8.04	1.32	1.53
3	H	401	ADP	C3'-C4'	-7.98	1.32	1.53
3	B	401	ADP	C3'-C4'	-7.90	1.32	1.53
3	J	401	ADP	O4'-C4'	7.89	1.62	1.45
3	F	401	ADP	O4'-C4'	7.89	1.62	1.45
5	H	405	P3P	PDP-CGP	7.88	1.87	1.79
3	G	401	ADP	O4'-C4'	7.86	1.62	1.45
5	C	405	P3P	PDP-CGP	7.73	1.86	1.79
3	D	401	ADP	C3'-C4'	-7.70	1.33	1.53
3	E	401	ADP	O4'-C4'	7.65	1.62	1.45
3	C	401	ADP	C3'-C4'	-7.60	1.33	1.53
3	H	401	ADP	O4'-C4'	7.55	1.61	1.45
3	I	401	ADP	O4'-C4'	7.54	1.61	1.45
3	B	401	ADP	O4'-C4'	7.45	1.61	1.45
3	A	401	ADP	O4'-C4'	7.38	1.61	1.45
5	I	405	P3P	PDP-CGP	7.38	1.86	1.79
5	D	405	P3P	PDP-CGP	7.30	1.86	1.79
3	D	401	ADP	O4'-C4'	7.28	1.61	1.45
5	G	405	P3P	PDP-CGP	7.11	1.86	1.79
3	C	401	ADP	O4'-C4'	7.08	1.60	1.45
5	E	405	P3P	PDP-CGP	7.02	1.86	1.79
5	B	405	P3P	PDP-CGP	7.00	1.86	1.79
5	F	405	P3P	PDP-CGP	6.68	1.85	1.79
5	J	405	P3P	PDP-CGP	6.68	1.85	1.79
5	A	405	P3P	PDP-CGP	6.38	1.85	1.79
3	F	401	ADP	O4'-C1'	-4.95	1.30	1.42
3	H	401	ADP	O4'-C1'	-4.87	1.30	1.42
3	A	401	ADP	O4'-C1'	-4.87	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ADP	O4'-C1'	-4.86	1.30	1.42
3	I	401	ADP	O4'-C1'	-4.78	1.31	1.42
3	G	401	ADP	O4'-C1'	-4.77	1.31	1.42
3	J	401	ADP	O4'-C1'	-4.62	1.31	1.42
3	C	401	ADP	O4'-C1'	-4.61	1.31	1.42
3	D	401	ADP	O4'-C1'	-4.59	1.31	1.42
3	B	401	ADP	O4'-C1'	-4.51	1.31	1.42
3	E	401	ADP	C6-N6	4.40	1.45	1.34
3	B	401	ADP	C6-N6	4.37	1.45	1.34
3	J	401	ADP	PA-O3A	4.36	1.64	1.59
3	A	401	ADP	C6-N6	4.35	1.45	1.34
3	D	401	ADP	C6-N6	4.33	1.45	1.34
3	J	401	ADP	C6-N6	4.32	1.45	1.34
3	G	401	ADP	C6-N6	4.30	1.45	1.34
3	F	401	ADP	PA-O3A	4.23	1.64	1.59
3	F	401	ADP	C6-N6	4.22	1.45	1.34
3	I	401	ADP	C6-N6	4.20	1.44	1.34
3	H	401	ADP	C6-N6	4.18	1.44	1.34
3	A	401	ADP	PA-O3A	4.17	1.64	1.59
3	C	401	ADP	C6-N6	3.94	1.44	1.34
3	B	401	ADP	PA-O3A	3.84	1.63	1.59
3	G	401	ADP	PA-O3A	3.72	1.63	1.59
3	C	401	ADP	C5-C4	-3.24	1.33	1.39
3	H	401	ADP	PA-O3A	3.23	1.63	1.59
3	E	401	ADP	PA-O3A	3.18	1.62	1.59
3	I	401	ADP	PA-O3A	3.09	1.62	1.59
3	C	401	ADP	PA-O3A	3.01	1.62	1.59
3	G	401	ADP	O3'-C3'	3.00	1.50	1.43
3	B	401	ADP	O3'-C3'	2.98	1.50	1.43
3	E	401	ADP	O3'-C3'	2.97	1.50	1.43
3	H	401	ADP	C5-C4	-2.95	1.33	1.39
3	A	401	ADP	C5-C4	-2.87	1.34	1.39
3	G	401	ADP	O2'-C2'	-2.83	1.35	1.43
3	F	401	ADP	O3'-C3'	2.82	1.49	1.43
3	E	401	ADP	O2'-C2'	-2.81	1.36	1.43
3	J	401	ADP	O2'-C2'	-2.81	1.36	1.43
3	G	401	ADP	C5-C4	-2.81	1.34	1.39
3	E	401	ADP	C5-C4	-2.80	1.34	1.39
3	H	401	ADP	O3'-C3'	2.79	1.49	1.43
3	I	401	ADP	C5-C4	-2.75	1.34	1.39
3	D	401	ADP	C5-C4	-2.74	1.34	1.39
3	B	401	ADP	O2'-C2'	-2.73	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	401	ADP	O2'-C2'	-2.71	1.36	1.43
3	A	401	ADP	O2'-C2'	-2.68	1.36	1.43
3	F	401	ADP	C5-C4	-2.68	1.34	1.39
3	C	401	ADP	O3'-C3'	2.67	1.49	1.43
3	J	401	ADP	O3'-C3'	2.66	1.49	1.43
3	H	401	ADP	C8-N9	-2.63	1.33	1.37
3	A	401	ADP	O3'-C3'	2.62	1.49	1.43
3	D	401	ADP	PA-O3A	2.58	1.62	1.59
3	D	401	ADP	C8-N9	-2.57	1.33	1.37
3	J	401	ADP	C5-C4	-2.56	1.34	1.39
3	D	401	ADP	O3'-C3'	2.53	1.49	1.43
3	C	401	ADP	C5-N7	-2.53	1.34	1.39
3	D	401	ADP	O2'-C2'	-2.51	1.36	1.43
3	H	401	ADP	O2'-C2'	-2.51	1.36	1.43
3	C	401	ADP	C8-N9	-2.48	1.33	1.37
3	F	401	ADP	C8-N9	-2.46	1.33	1.37
3	I	401	ADP	O3'-C3'	2.45	1.49	1.43
3	A	401	ADP	C8-N9	-2.43	1.33	1.37
3	C	401	ADP	O2'-C2'	-2.42	1.37	1.43
3	I	401	ADP	O2'-C2'	-2.41	1.37	1.43
3	F	401	ADP	C5-N7	-2.41	1.34	1.39
3	H	401	ADP	C5-N7	-2.40	1.34	1.39
3	J	401	ADP	C8-N9	-2.38	1.33	1.37
3	I	401	ADP	C8-N9	-2.36	1.33	1.37
3	I	401	ADP	C5-N7	-2.36	1.34	1.39
3	B	401	ADP	C5-C4	-2.35	1.34	1.39
3	E	401	ADP	C8-N9	-2.35	1.33	1.37
3	G	401	ADP	C8-N9	-2.35	1.33	1.37
3	J	401	ADP	C5-N7	-2.34	1.34	1.39
3	D	401	ADP	C5-N7	-2.28	1.34	1.39
3	B	401	ADP	C8-N9	-2.09	1.34	1.37
3	E	401	ADP	C5-N7	-2.07	1.35	1.39
3	B	401	ADP	C5-N7	-2.06	1.35	1.39
3	A	401	ADP	C4-N9	-2.02	1.33	1.37

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	401	ADP	N6-C6-N1	-6.34	104.25	118.38
3	J	401	ADP	N6-C6-N1	-6.25	104.45	118.38
3	F	401	ADP	N6-C6-N1	-6.21	104.53	118.38
3	A	401	ADP	N6-C6-N1	-6.21	104.55	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	401	ADP	N6-C6-N1	-6.19	104.59	118.38
3	E	401	ADP	N6-C6-N1	-6.16	104.66	118.38
3	I	401	ADP	N6-C6-N1	-6.05	104.90	118.38
3	C	401	ADP	N3-C2-N1	-6.04	119.43	128.58
3	D	401	ADP	N6-C6-N1	-5.95	105.12	118.38
3	B	401	ADP	N6-C6-N1	-5.87	105.30	118.38
3	E	401	ADP	N3-C2-N1	-5.85	119.73	128.58
3	I	401	ADP	N3-C2-N1	-5.84	119.74	128.58
3	A	401	ADP	N3-C2-N1	-5.80	119.80	128.58
3	C	401	ADP	N6-C6-N1	-5.75	105.56	118.38
3	H	401	ADP	N3-C2-N1	-5.75	119.88	128.58
3	G	401	ADP	N3-C2-N1	-5.70	119.96	128.58
3	J	401	ADP	N3-C2-N1	-5.66	120.01	128.58
3	B	401	ADP	N3-C2-N1	-5.65	120.02	128.58
3	D	401	ADP	N3-C2-N1	-5.65	120.03	128.58
3	F	401	ADP	N3-C2-N1	-5.61	120.09	128.58
3	C	401	ADP	N9-C8-N7	-5.34	106.36	113.94
3	H	401	ADP	N9-C8-N7	-5.24	106.50	113.94
3	G	401	ADP	N9-C8-N7	-5.15	106.63	113.94
3	A	401	ADP	N9-C8-N7	-5.14	106.64	113.94
3	F	401	ADP	N9-C8-N7	-5.14	106.65	113.94
3	E	401	ADP	N9-C8-N7	-5.09	106.71	113.94
3	D	401	ADP	N9-C8-N7	-5.05	106.77	113.94
3	I	401	ADP	N9-C8-N7	-5.05	106.78	113.94
3	J	401	ADP	N9-C8-N7	-5.00	106.84	113.94
3	J	401	ADP	C5-C6-N6	4.95	135.54	123.29
3	G	401	ADP	C5-C6-N6	4.93	135.48	123.29
3	E	401	ADP	C5-C6-N6	4.88	135.36	123.29
3	F	401	ADP	C5-C6-N6	4.87	135.35	123.29
3	H	401	ADP	C5-C6-N6	4.86	135.32	123.29
3	B	401	ADP	N9-C8-N7	-4.84	107.06	113.94
3	A	401	ADP	C5-C6-N6	4.84	135.26	123.29
3	E	401	ADP	C5-C4-N3	-4.72	120.21	126.72
3	C	401	ADP	C5-C4-N3	-4.72	120.22	126.72
3	I	401	ADP	C5-C4-N3	-4.67	120.28	126.72
3	D	401	ADP	C5-C6-N6	4.67	134.85	123.29
3	B	401	ADP	C5-C4-N3	-4.67	120.29	126.72
3	H	401	ADP	C5-C4-N3	-4.67	120.29	126.72
3	I	401	ADP	C5-C6-N6	4.66	134.83	123.29
3	J	401	ADP	C5-C4-N3	-4.61	120.37	126.72
3	G	401	ADP	C5-C4-N3	-4.60	120.38	126.72
3	F	401	ADP	C5-C4-N3	-4.60	120.39	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	ADP	C5-C4-N3	-4.59	120.39	126.72
3	A	401	ADP	C5-C4-N3	-4.56	120.43	126.72
3	B	401	ADP	C5-C6-N6	4.56	134.57	123.29
3	A	401	ADP	C4-N9-C1'	-4.52	116.07	126.63
3	A	401	ADP	C4-N9-C8	4.45	110.41	105.74
3	G	401	ADP	C4-N9-C1'	-4.44	116.26	126.63
3	H	401	ADP	C4-N9-C1'	-4.43	116.27	126.63
3	C	401	ADP	C4-N9-C8	4.43	110.39	105.74
3	D	401	ADP	C4-N9-C8	4.36	110.32	105.74
3	H	401	ADP	C4-N9-C8	4.34	110.30	105.74
3	G	401	ADP	C4-N9-C8	4.34	110.29	105.74
3	E	401	ADP	C4-N9-C1'	-4.34	116.49	126.63
3	I	401	ADP	C4-N9-C1'	-4.33	116.50	126.63
3	C	401	ADP	C5-C6-N6	4.33	134.00	123.29
3	F	401	ADP	C4-N9-C1'	-4.32	116.54	126.63
3	F	401	ADP	C4-N9-C8	4.29	110.24	105.74
3	D	401	ADP	C4-N9-C1'	-4.29	116.61	126.63
3	J	401	ADP	C4-N9-C1'	-4.25	116.68	126.63
3	C	401	ADP	C4-N9-C1'	-4.20	116.81	126.63
3	E	401	ADP	C4-N9-C8	4.16	110.11	105.74
3	I	401	ADP	C4-N9-C8	4.11	110.06	105.74
3	B	401	ADP	C4-N9-C8	4.10	110.04	105.74
3	J	401	ADP	C4-N9-C8	4.07	110.01	105.74
3	B	401	ADP	C4-N9-C1'	-4.06	117.14	126.63
3	C	401	ADP	N3-C4-N9	3.79	133.61	127.17
3	B	401	ADP	N3-C4-N9	3.67	133.41	127.17
3	D	401	ADP	N3-C4-N9	3.63	133.33	127.17
3	I	401	ADP	N3-C4-N9	3.55	133.21	127.17
3	F	401	ADP	N3-C4-N9	3.52	133.15	127.17
3	H	401	ADP	N3-C4-N9	3.50	133.12	127.17
3	E	401	ADP	N3-C4-N9	3.49	133.10	127.17
3	G	401	ADP	N3-C4-N9	3.46	133.06	127.17
3	A	401	ADP	N3-C4-N9	3.40	132.94	127.17
3	J	401	ADP	N3-C4-N9	3.38	132.91	127.17
3	E	401	ADP	C2-N3-C4	3.34	120.00	111.83
3	C	401	ADP	C2-N3-C4	3.28	119.83	111.83
3	A	401	ADP	C2-N3-C4	3.26	119.79	111.83
3	I	401	ADP	C2-N3-C4	3.25	119.76	111.83
3	H	401	ADP	C2-N3-C4	3.24	119.75	111.83
3	G	401	ADP	C2-N3-C4	3.19	119.63	111.83
3	J	401	ADP	C2-N3-C4	3.15	119.53	111.83
3	F	401	ADP	C2-N3-C4	3.15	119.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ADP	C2-N3-C4	3.09	119.38	111.83
3	F	401	ADP	C5-N7-C8	3.06	108.25	103.45
3	G	401	ADP	C5-N7-C8	3.05	108.25	103.45
3	C	401	ADP	C5-N7-C8	3.03	108.21	103.45
3	J	401	ADP	C5-N7-C8	3.01	108.18	103.45
3	H	401	ADP	C5-N7-C8	3.00	108.16	103.45
3	D	401	ADP	C2-N3-C4	3.00	119.15	111.83
3	E	401	ADP	C5-N7-C8	2.99	108.16	103.45
3	D	401	ADP	C5-N7-C8	2.96	108.10	103.45
3	I	401	ADP	C5-N7-C8	2.93	108.06	103.45
3	A	401	ADP	C1'-N9-C8	2.89	133.52	127.09
3	G	401	ADP	C1'-N9-C8	2.86	133.45	127.09
3	I	401	ADP	C1'-N9-C8	2.86	133.45	127.09
3	H	401	ADP	C1'-N9-C8	2.85	133.43	127.09
3	A	401	ADP	C5-N7-C8	2.85	107.93	103.45
3	E	401	ADP	C1'-N9-C8	2.83	133.38	127.09
3	B	401	ADP	C5-N7-C8	2.81	107.86	103.45
3	J	401	ADP	C1'-N9-C8	2.80	133.30	127.09
3	F	401	ADP	C1'-N9-C8	2.76	133.22	127.09
3	D	401	ADP	C1'-N9-C8	2.69	133.07	127.09
3	B	401	ADP	C1'-N9-C8	2.58	132.82	127.09
3	C	401	ADP	C1'-N9-C8	2.57	132.80	127.09
3	D	401	ADP	C6-C5-C4	2.36	120.40	117.18
3	C	401	ADP	C6-C5-C4	2.29	120.30	117.18
3	H	401	ADP	O2A-PA-O3A	2.28	113.45	107.27
3	B	401	ADP	C6-C5-C4	2.27	120.28	117.18
3	J	401	ADP	C6-C5-C4	2.15	120.11	117.18
3	F	401	ADP	C6-C5-C4	2.09	120.04	117.18
3	I	401	ADP	C6-C5-C4	2.09	120.03	117.18
3	H	401	ADP	C6-C5-C4	2.06	119.99	117.18
3	D	401	ADP	O2A-PA-O3A	2.06	112.83	107.27
3	J	401	ADP	C4-C5-N7	-2.04	108.25	110.58
3	G	401	ADP	C4-C5-N7	-2.03	108.26	110.58

There are no chirality outliers.

All (137) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	PA-O3A-PB-O2B
3	C	401	ADP	PA-O3A-PB-O2B
3	F	401	ADP	PA-O3A-PB-O2B
5	A	405	P3P	CBP-CAP-CP-OTP

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Mol	Chain	Res	Type	Atoms
5	C	405	P3P	CBP-CAP-CP-OTP
5	D	405	P3P	CBP-CAP-CP-OTP
5	E	405	P3P	CBP-CAP-CP-OTP
5	F	405	P3P	CBP-CAP-CP-OTP
5	G	405	P3P	CBP-CAP-CP-OTP
5	I	405	P3P	CBP-CAP-CP-OTP
5	J	405	P3P	CBP-CAP-CP-OTP
5	I	405	P3P	NP-CAP-CP-OTP
5	H	405	P3P	CBP-CAP-CP-OTP
5	B	405	P3P	NP-CAP-CP-OTP
5	F	405	P3P	NP-CAP-CP-OTP
5	B	405	P3P	CBP-CAP-CP-OTP
5	A	405	P3P	NP-CAP-CP-OTP
5	C	405	P3P	NP-CAP-CP-OTP
5	D	405	P3P	NP-CAP-CP-OTP
5	E	405	P3P	NP-CAP-CP-OTP
5	G	405	P3P	NP-CAP-CP-OTP
5	H	405	P3P	NP-CAP-CP-OTP
5	J	405	P3P	NP-CAP-CP-OTP
5	C	405	P3P	CBP-CAP-CP-OP
5	D	405	P3P	CBP-CAP-CP-OP
5	E	405	P3P	CBP-CAP-CP-OP
5	F	405	P3P	CBP-CAP-CP-OP
5	G	405	P3P	CBP-CAP-CP-OP
5	J	405	P3P	CBP-CAP-CP-OP
5	A	405	P3P	CBP-CAP-CP-OP
5	B	405	P3P	CBP-CAP-CP-OP
5	I	405	P3P	CBP-CAP-CP-OP
5	H	405	P3P	CBP-CAP-CP-OP
3	E	401	ADP	O4'-C4'-C5'-O5'
3	F	401	ADP	O4'-C4'-C5'-O5'
5	A	405	P3P	NP-CAP-CP-OP
5	B	405	P3P	NP-CAP-CP-OP
5	C	405	P3P	NP-CAP-CP-OP
5	D	405	P3P	NP-CAP-CP-OP
5	E	405	P3P	NP-CAP-CP-OP
5	F	405	P3P	NP-CAP-CP-OP
5	G	405	P3P	NP-CAP-CP-OP
5	H	405	P3P	NP-CAP-CP-OP
5	I	405	P3P	NP-CAP-CP-OP
5	J	405	P3P	NP-CAP-CP-OP
3	F	401	ADP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	B	401	ADP	PA-O3A-PB-O2B
3	D	401	ADP	PA-O3A-PB-O2B
3	E	401	ADP	PA-O3A-PB-O2B
3	G	401	ADP	PA-O3A-PB-O2B
3	H	401	ADP	PA-O3A-PB-O2B
3	J	401	ADP	PA-O3A-PB-O2B
3	A	401	ADP	C2'-C1'-N9-C8
3	B	401	ADP	C2'-C1'-N9-C8
3	C	401	ADP	C2'-C1'-N9-C8
3	D	401	ADP	C2'-C1'-N9-C8
3	E	401	ADP	C2'-C1'-N9-C8
3	F	401	ADP	C2'-C1'-N9-C8
3	G	401	ADP	C2'-C1'-N9-C8
3	H	401	ADP	C2'-C1'-N9-C8
3	I	401	ADP	C2'-C1'-N9-C8
3	J	401	ADP	C2'-C1'-N9-C8
6	E	406	MPD	O2-C2-C3-C4
6	I	406	MPD	O2-C2-C3-C4
6	B	407	MPD	C1-C2-C3-C4
6	F	407	MPD	C1-C2-C3-C4
6	G	407	MPD	C1-C2-C3-C4
6	H	408	MPD	C1-C2-C3-C4
3	B	401	ADP	O4'-C4'-C5'-O5'
3	E	401	ADP	C3'-C4'-C5'-O5'
3	I	401	ADP	O4'-C4'-C5'-O5'
3	J	401	ADP	C5'-O5'-PA-O1A
6	H	408	MPD	C2-C3-C4-C5
3	F	401	ADP	PB-O3A-PA-O2A
3	A	401	ADP	O4'-C4'-C5'-O5'
3	G	401	ADP	O4'-C4'-C5'-O5'
3	H	401	ADP	O4'-C4'-C5'-O5'
3	B	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	O4'-C4'-C5'-O5'
3	I	401	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	PB-O3A-PA-O2A
3	H	401	ADP	PB-O3A-PA-O2A
3	D	401	ADP	O4'-C4'-C5'-O5'
3	I	401	ADP	PA-O3A-PB-O2B
5	D	405	P3P	PDP-OEB-P12-O14
3	D	401	ADP	O4'-C1'-N9-C8
3	E	401	ADP	O4'-C1'-N9-C8
3	G	401	ADP	O4'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
3	I	401	ADP	O4'-C1'-N9-C8
3	A	401	ADP	PB-O3A-PA-O1A
3	A	401	ADP	PB-O3A-PA-O2A
3	B	401	ADP	PB-O3A-PA-O2A
3	C	401	ADP	PB-O3A-PA-O1A
3	D	401	ADP	PB-O3A-PA-O2A
3	E	401	ADP	PB-O3A-PA-O2A
3	F	401	ADP	PB-O3A-PA-O1A
3	G	401	ADP	PB-O3A-PA-O1A
3	G	401	ADP	PB-O3A-PA-O2A
3	H	401	ADP	PB-O3A-PA-O1A
3	I	401	ADP	PB-O3A-PA-O1A
3	I	401	ADP	PB-O3A-PA-O2A
3	J	401	ADP	PB-O3A-PA-O2A
6	A	407	MPD	O2-C2-C3-C4
6	B	406	MPD	O2-C2-C3-C4
6	D	406	MPD	O2-C2-C3-C4
6	F	406	MPD	O2-C2-C3-C4
6	G	407	MPD	O2-C2-C3-C4
6	J	406	MPD	O2-C2-C3-C4
3	C	401	ADP	O4'-C1'-N9-C8
3	J	401	ADP	O4'-C1'-N9-C8
3	A	401	ADP	C3'-C4'-C5'-O5'
3	H	401	ADP	C3'-C4'-C5'-O5'
6	G	407	MPD	C2-C3-C4-O4
6	I	407	MPD	C2-C3-C4-O4
3	A	401	ADP	C2'-C1'-N9-C4
3	C	401	ADP	C2'-C1'-N9-C4
3	D	401	ADP	C2'-C1'-N9-C4
3	F	401	ADP	C2'-C1'-N9-C4
3	G	401	ADP	C2'-C1'-N9-C4
3	H	401	ADP	C2'-C1'-N9-C4
3	I	401	ADP	C2'-C1'-N9-C4
3	J	401	ADP	C2'-C1'-N9-C4
6	A	407	MPD	CM-C2-C3-C4
6	B	407	MPD	CM-C2-C3-C4
6	F	407	MPD	CM-C2-C3-C4
6	G	407	MPD	CM-C2-C3-C4
6	H	408	MPD	CM-C2-C3-C4
6	I	407	MPD	C1-C2-C3-C4
6	I	407	MPD	CM-C2-C3-C4
6	J	407	MPD	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
6	J	407	MPD	CM-C2-C3-C4
3	G	401	ADP	C3'-C4'-C5'-O5'
3	A	401	ADP	O4'-C1'-N9-C8
3	F	401	ADP	O4'-C1'-N9-C8
3	H	401	ADP	O4'-C1'-N9-C8
3	E	401	ADP	PB-O3A-PA-O1A
3	J	401	ADP	PB-O3A-PA-O1A

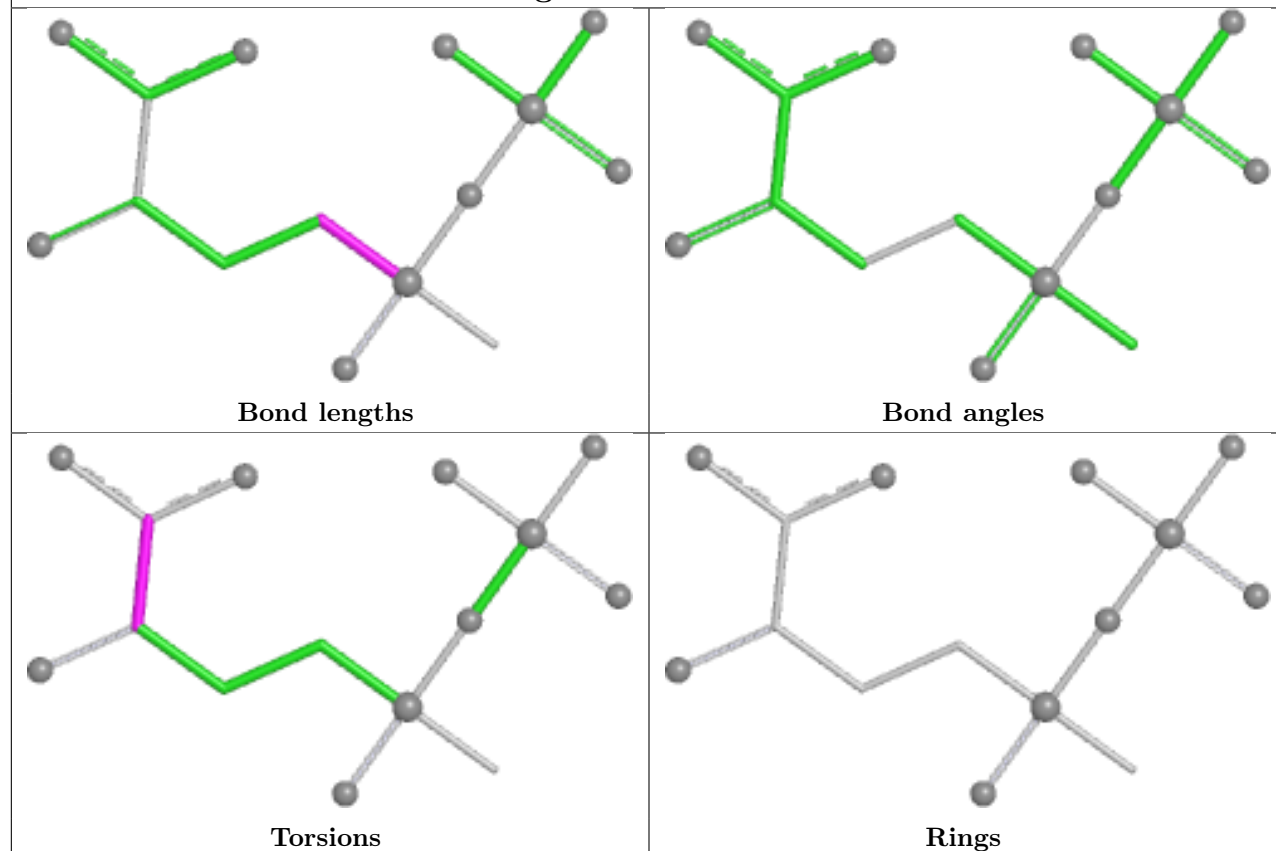
There are no ring outliers.

3 monomers are involved in 3 short contacts:

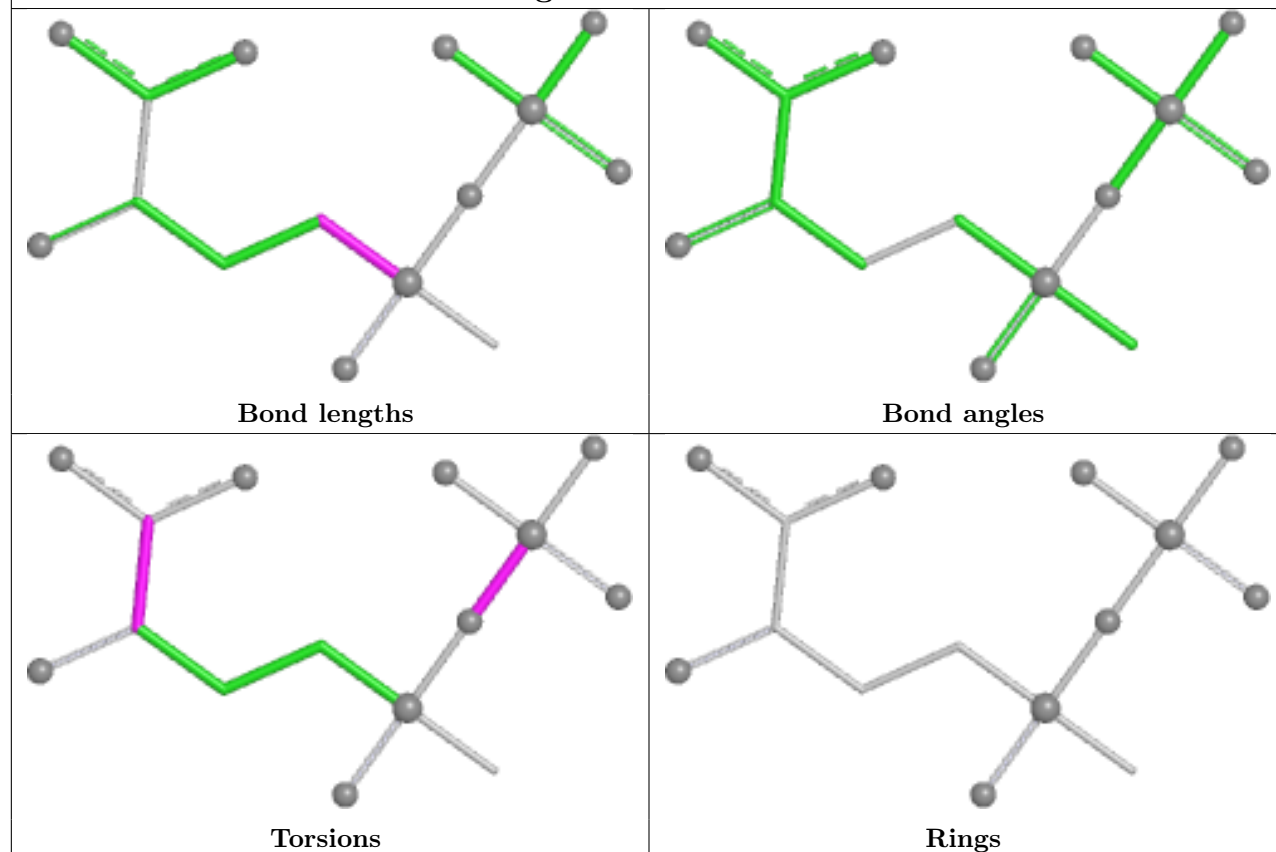
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	406	MPD	1	0
6	J	406	MPD	1	0
6	A	406	MPD	1	0

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.

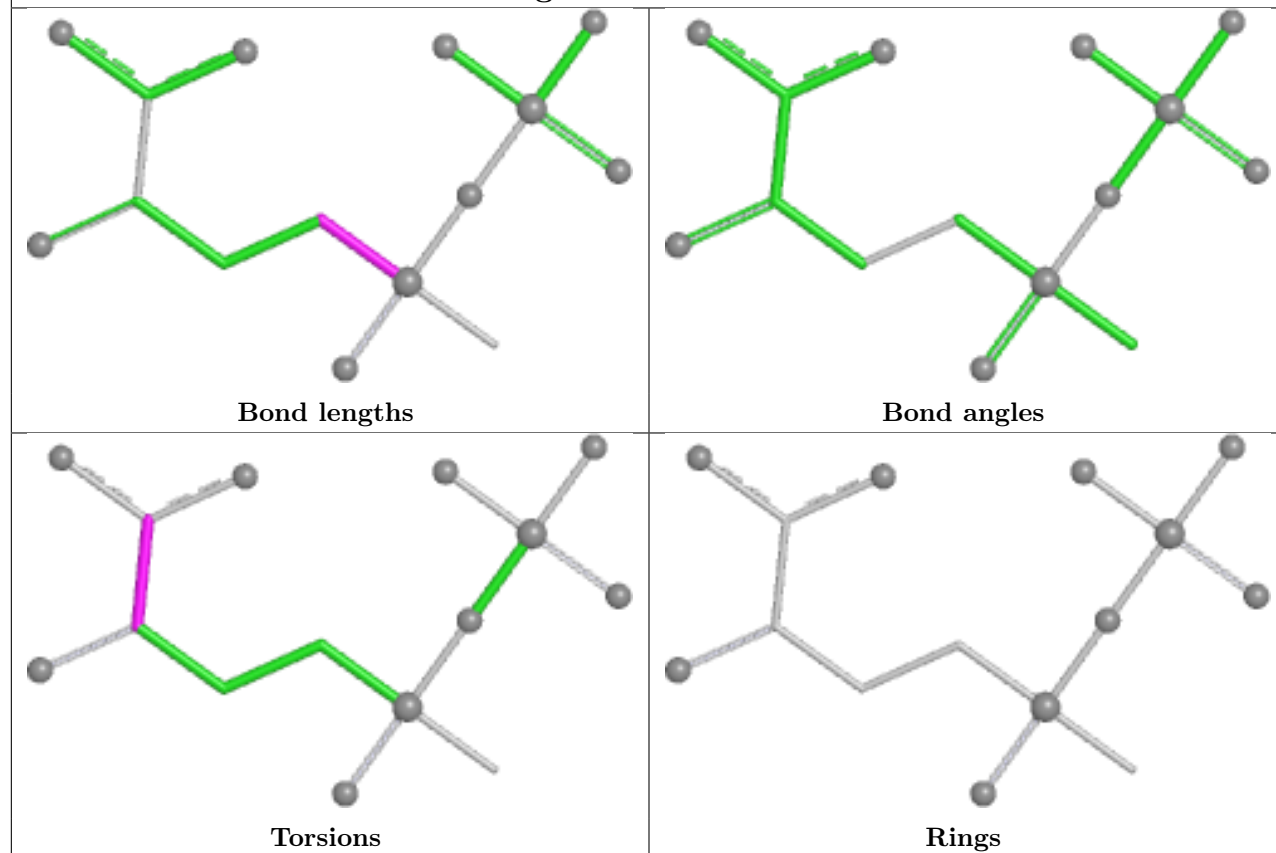
Ligand P3P G 405



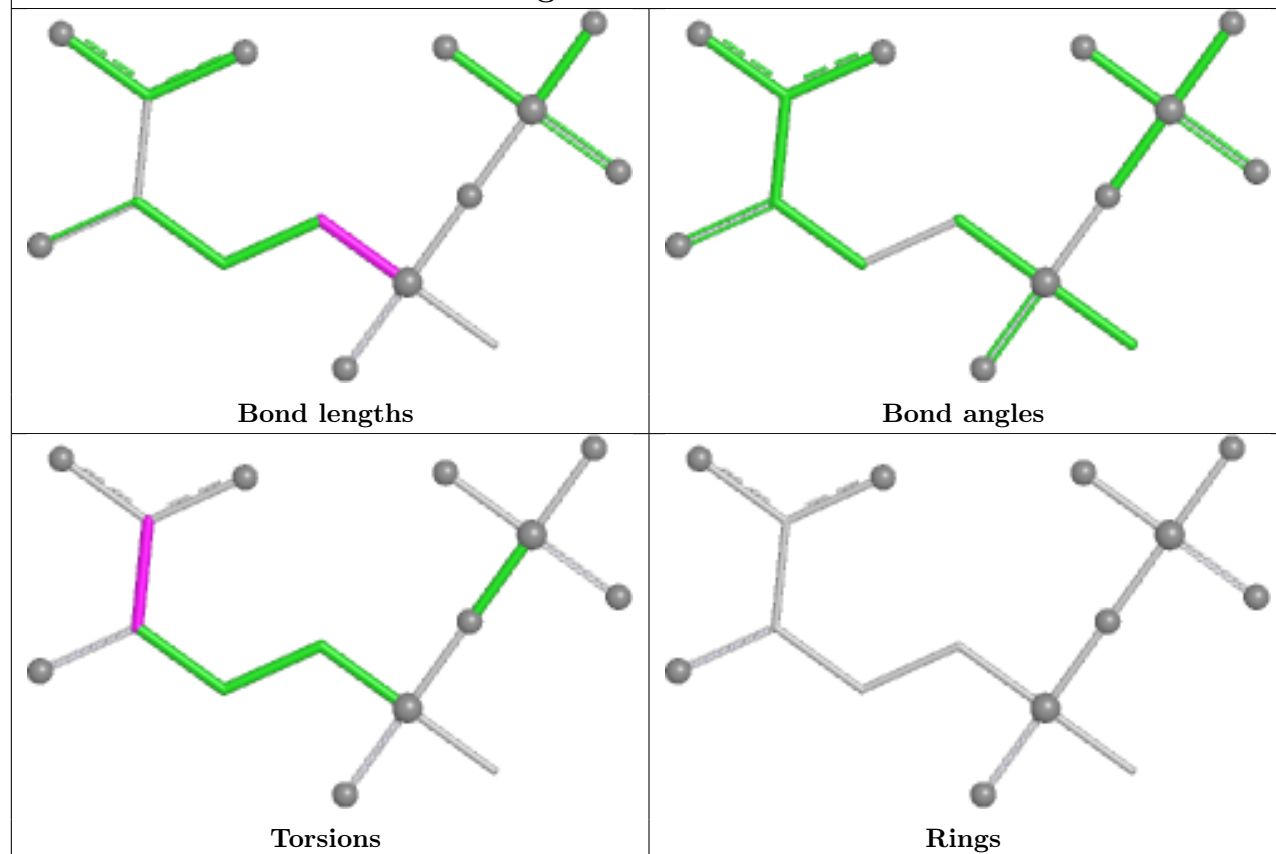
Ligand P3P D 405

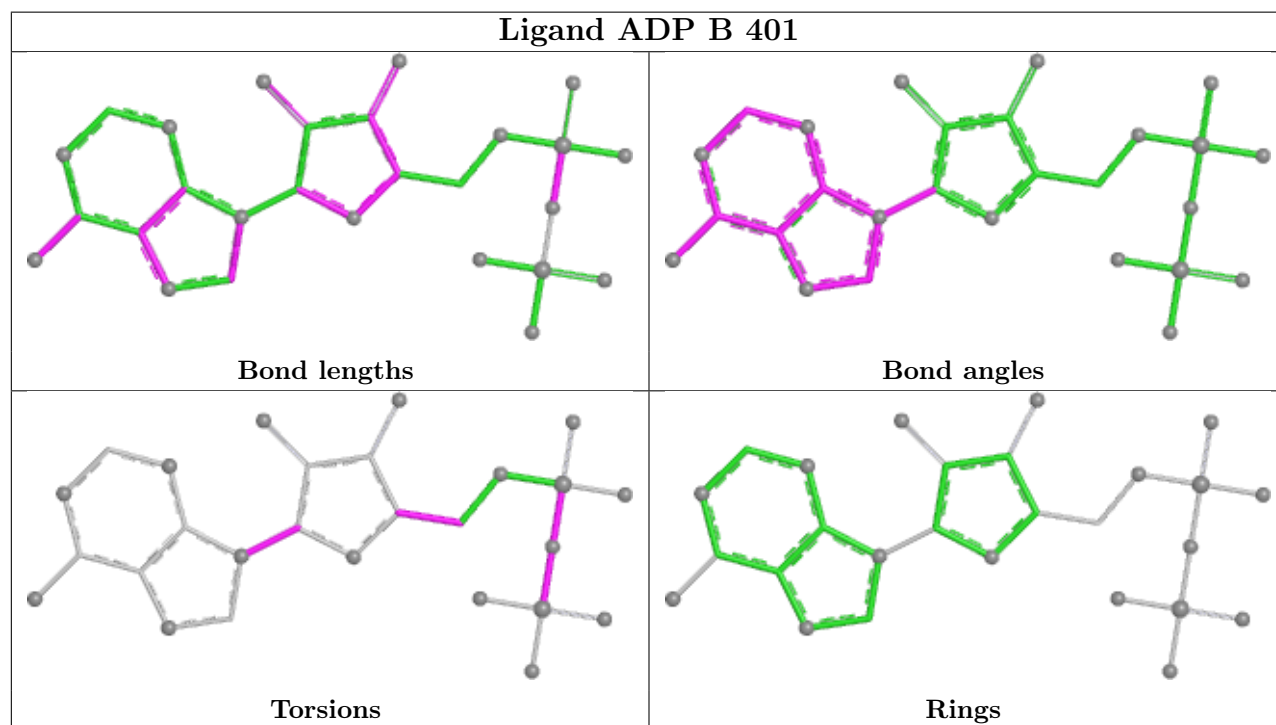
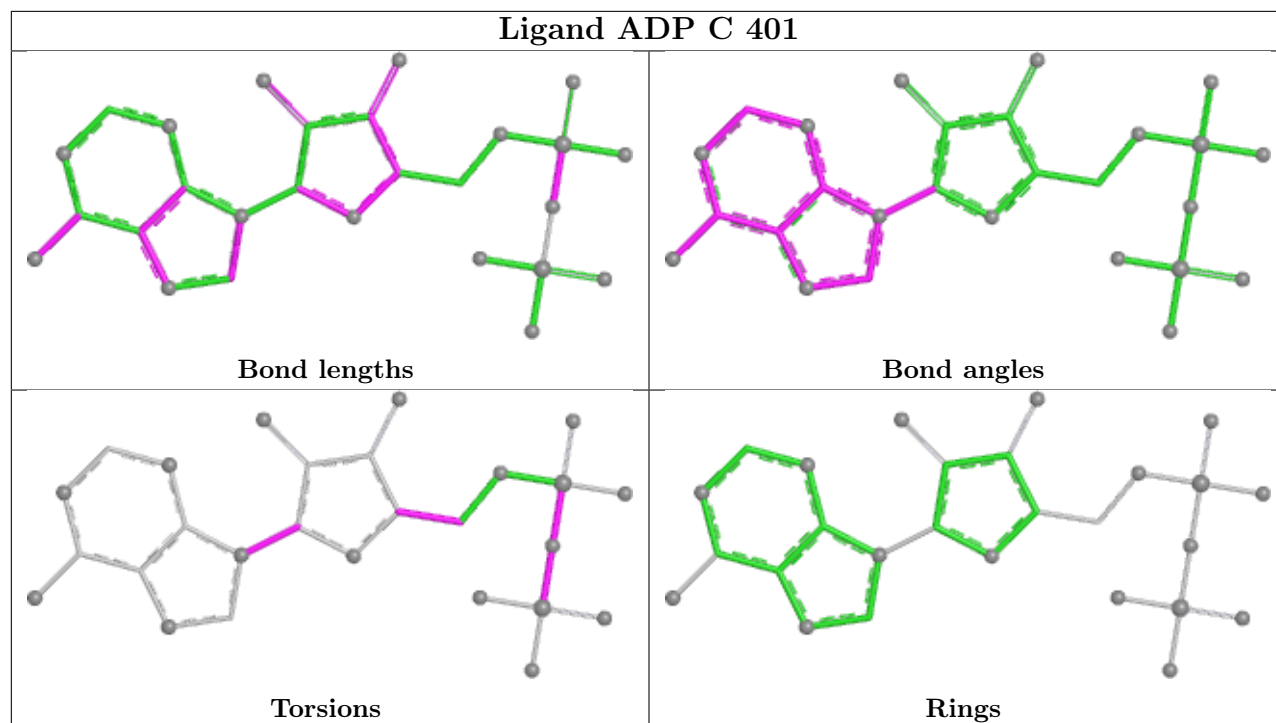


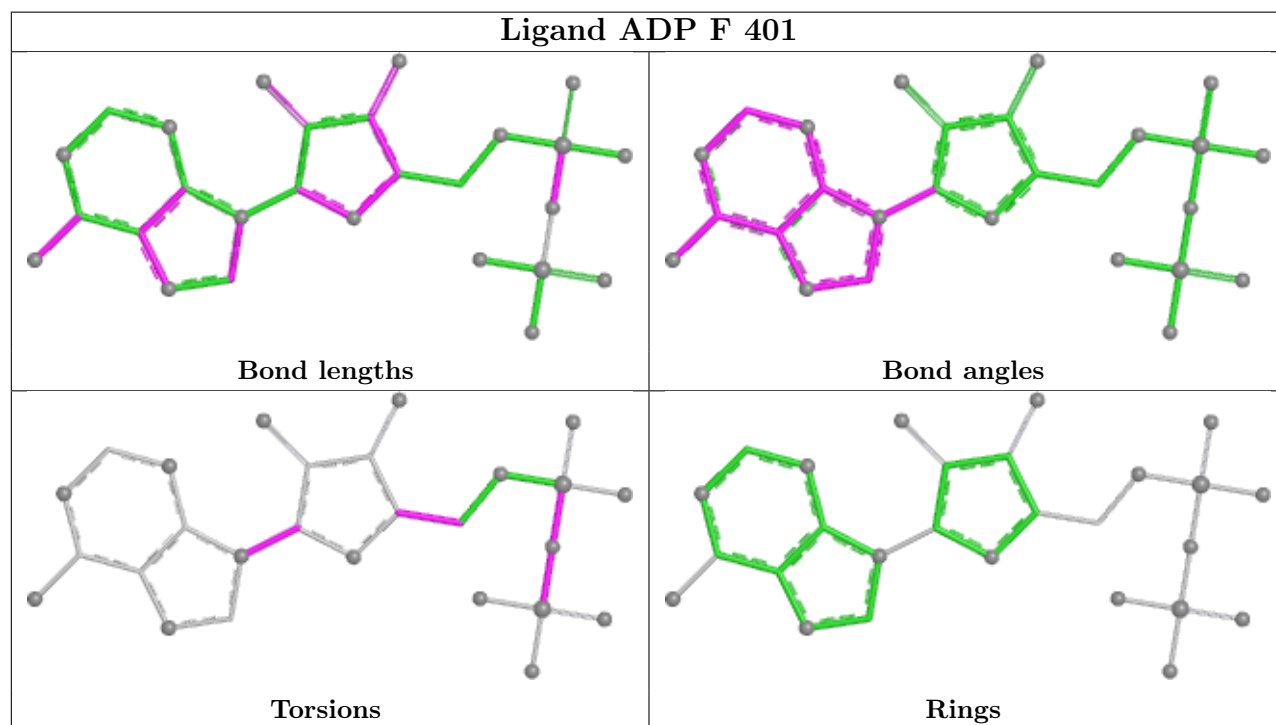
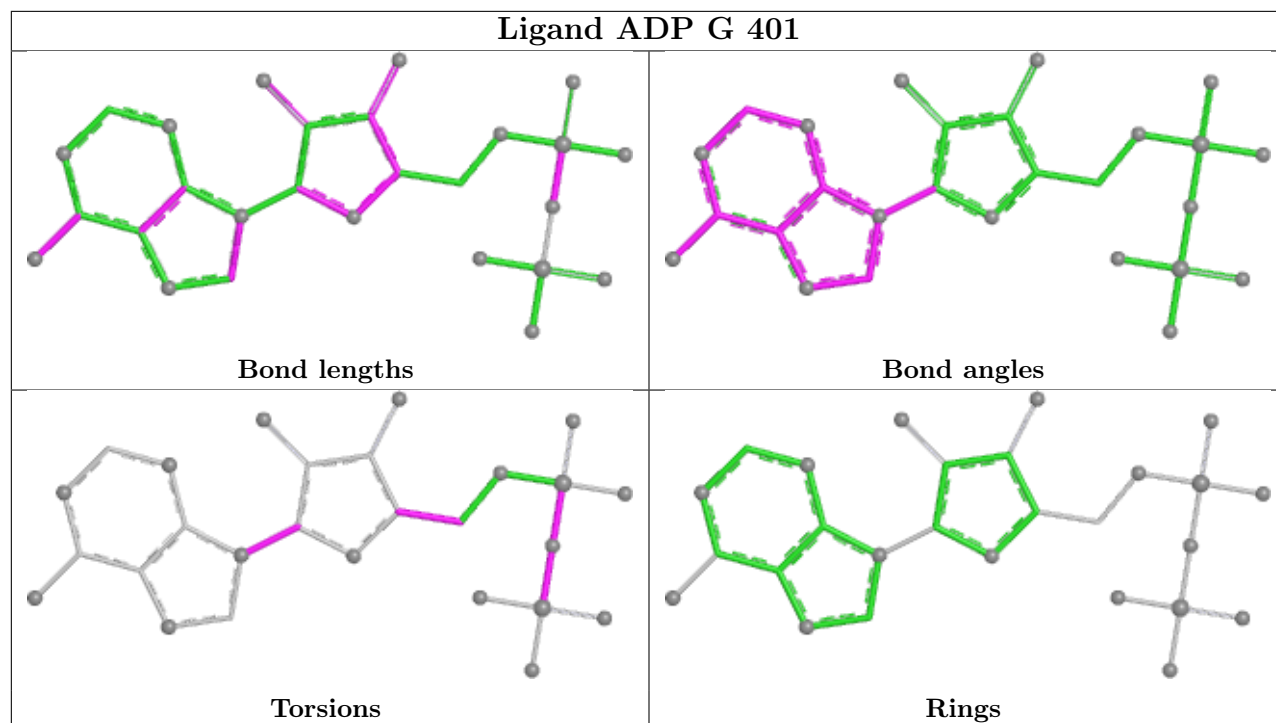
Ligand P3P A 405

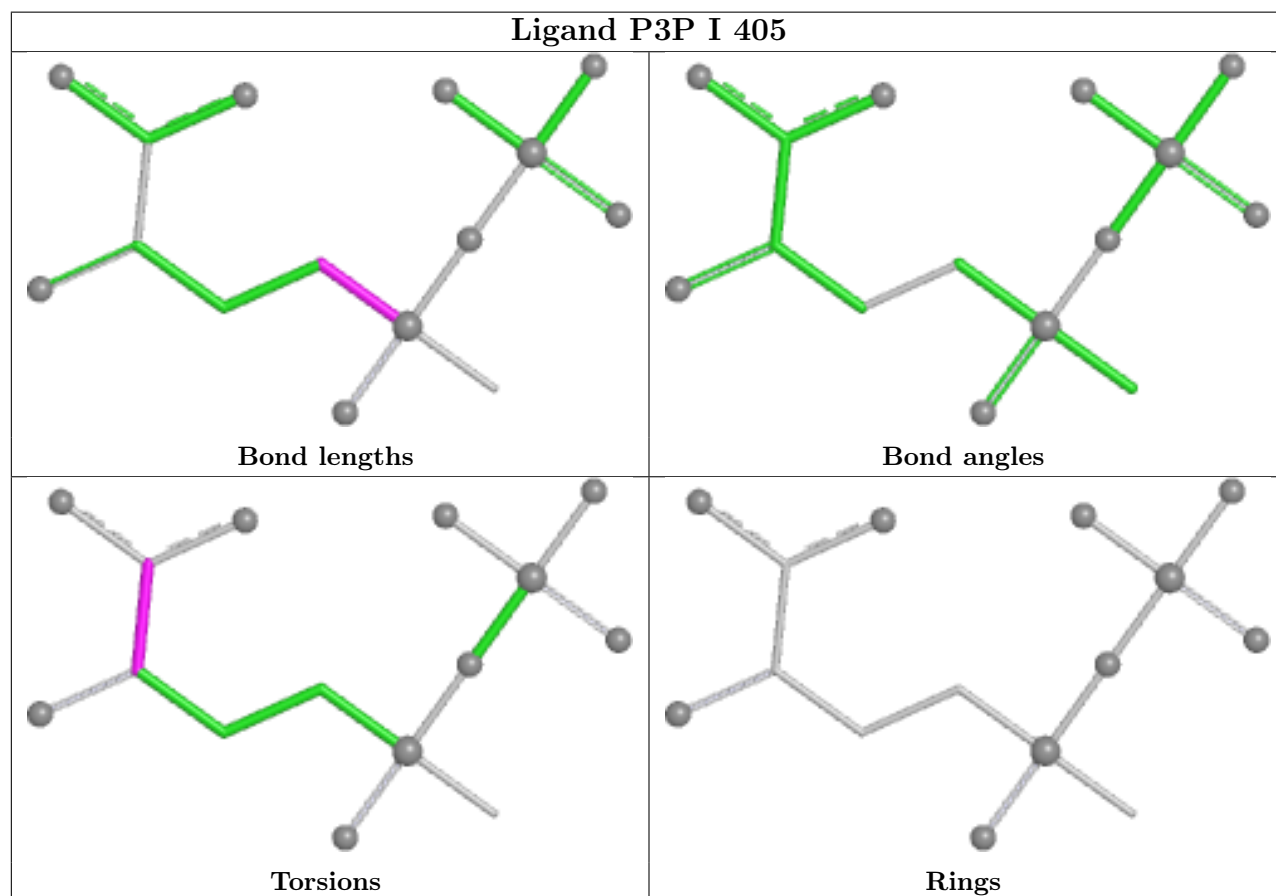
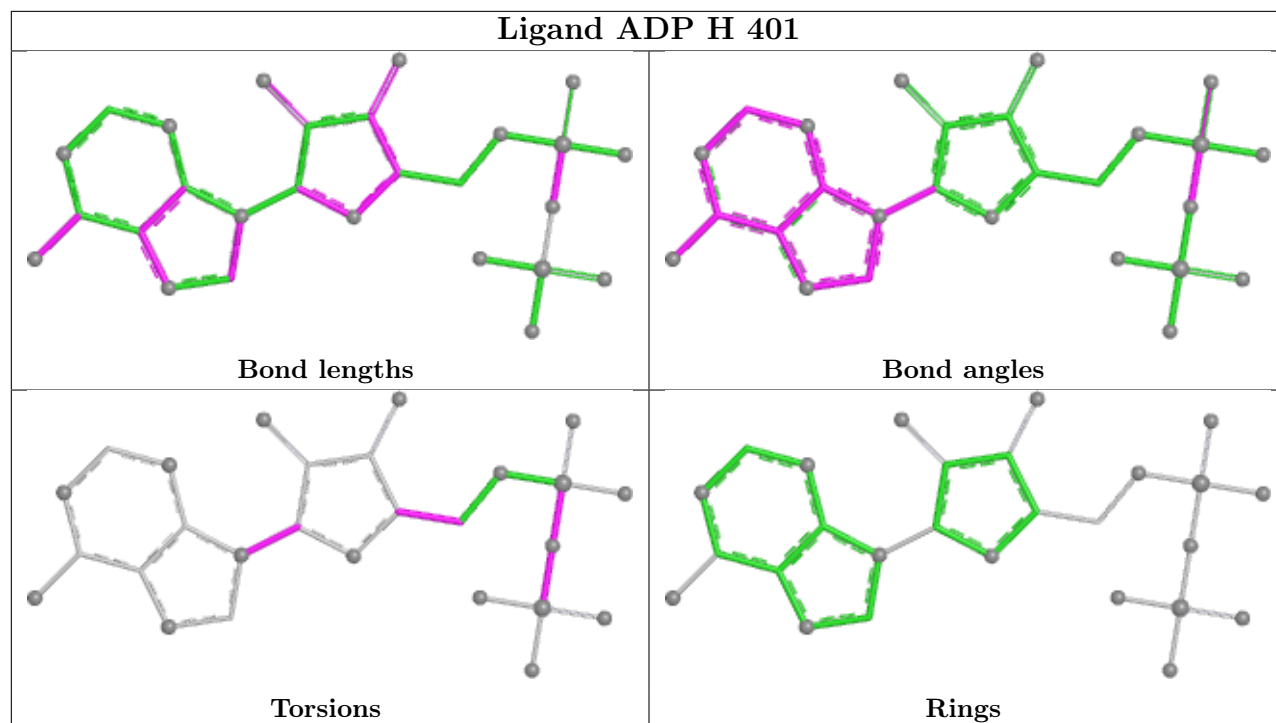


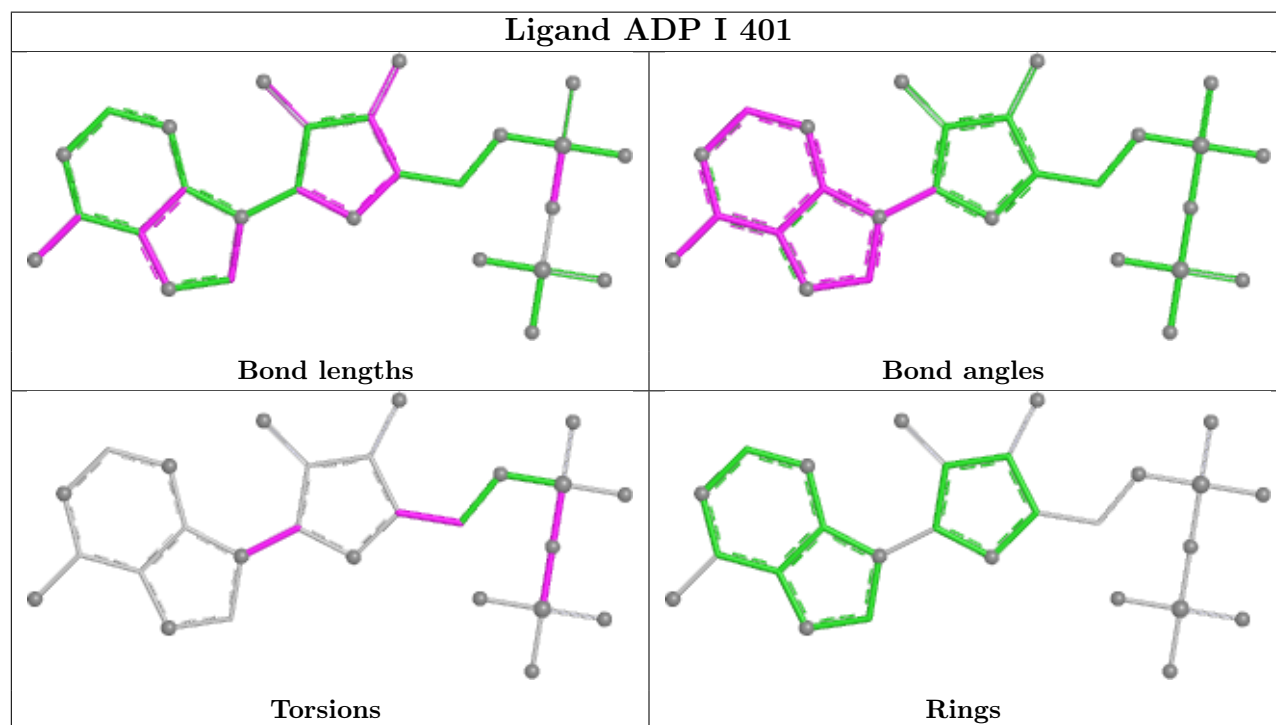
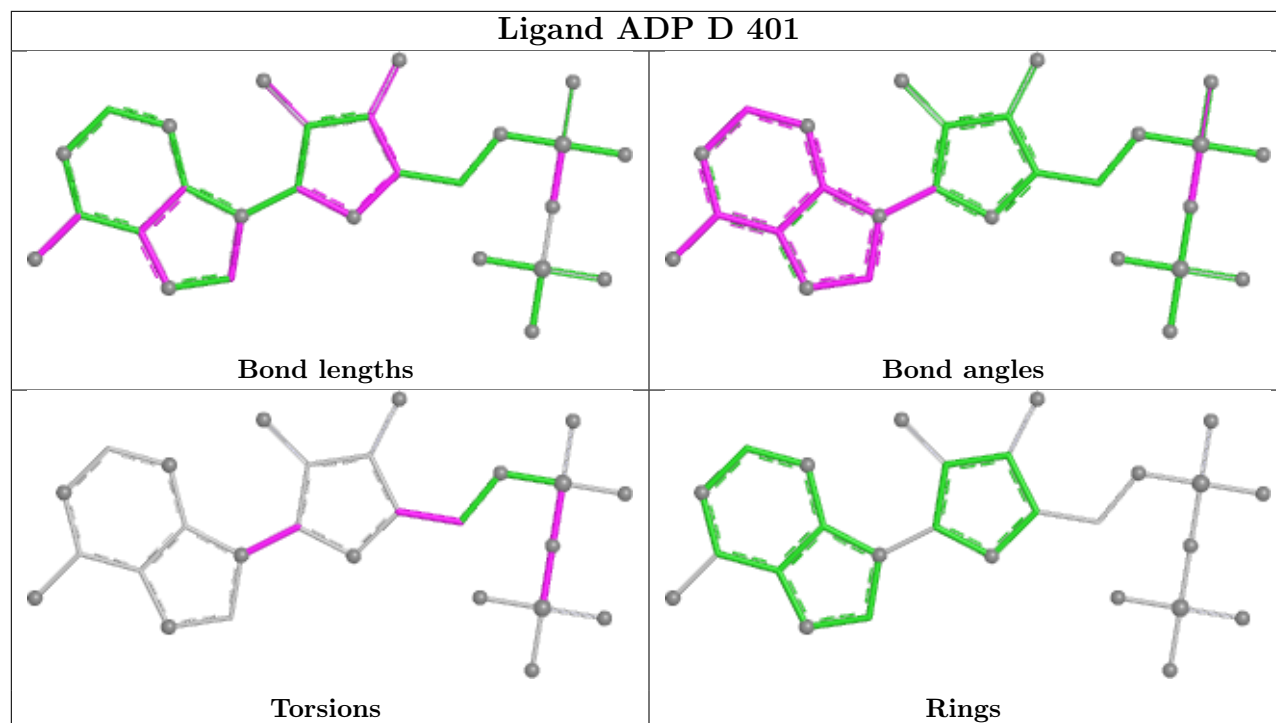
Ligand P3P E 405



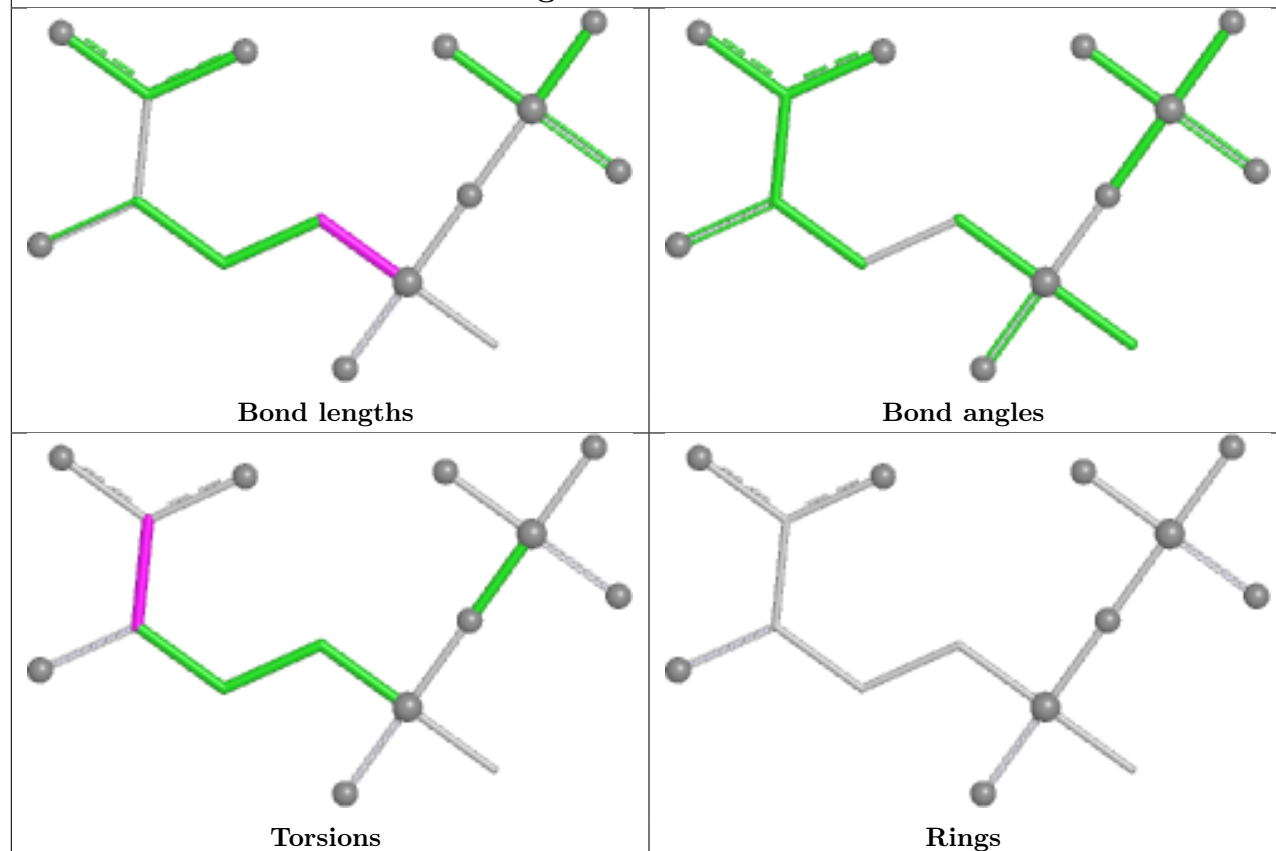




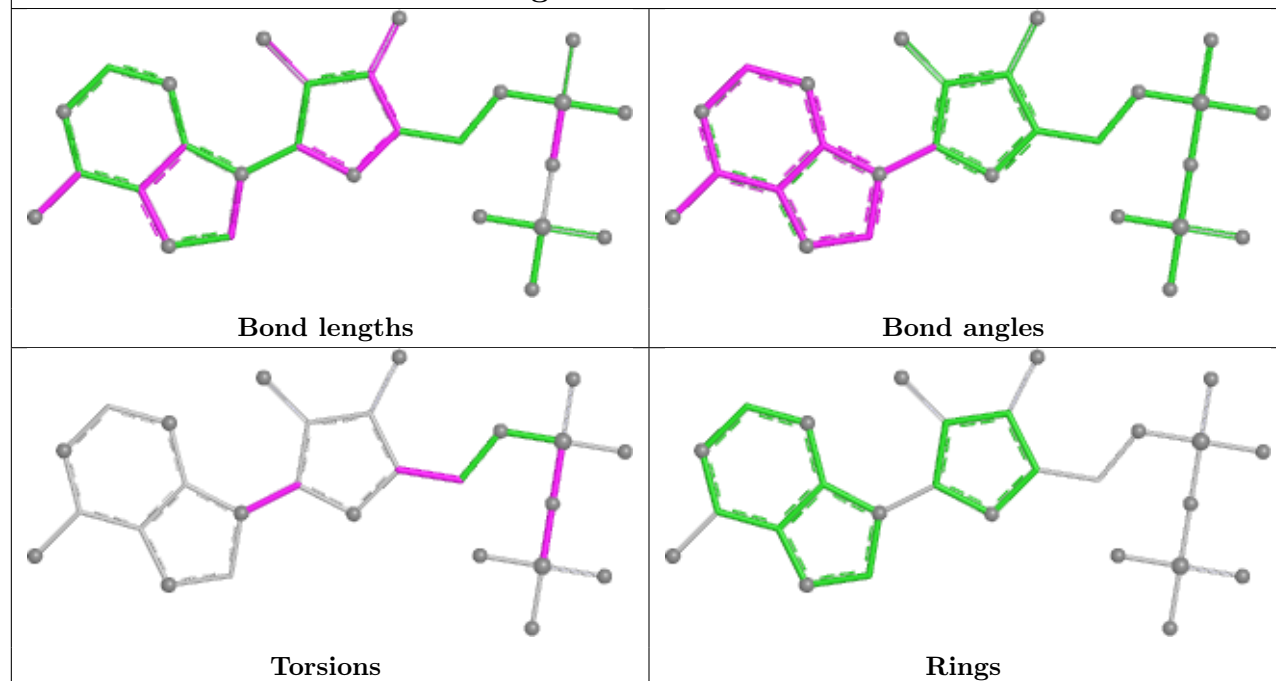




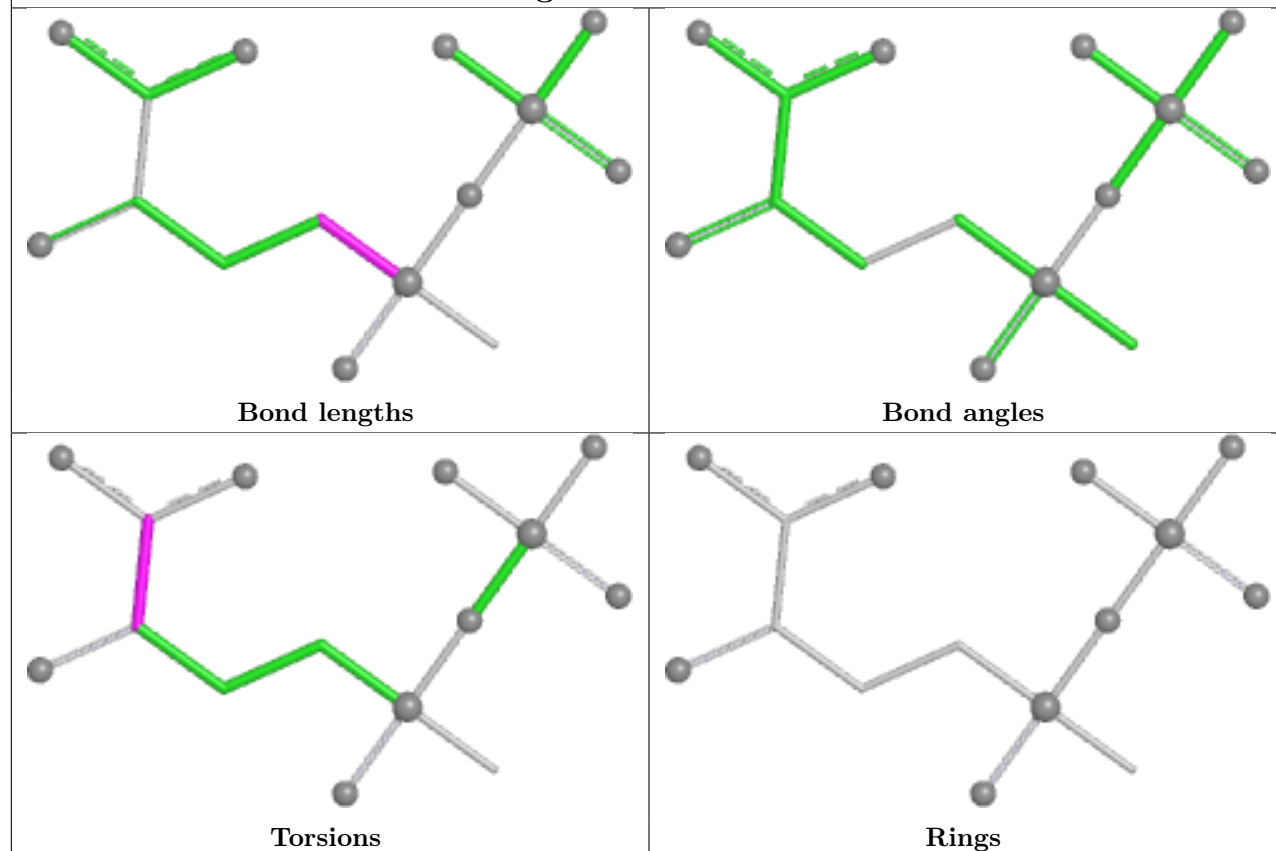
Ligand P3P F 405



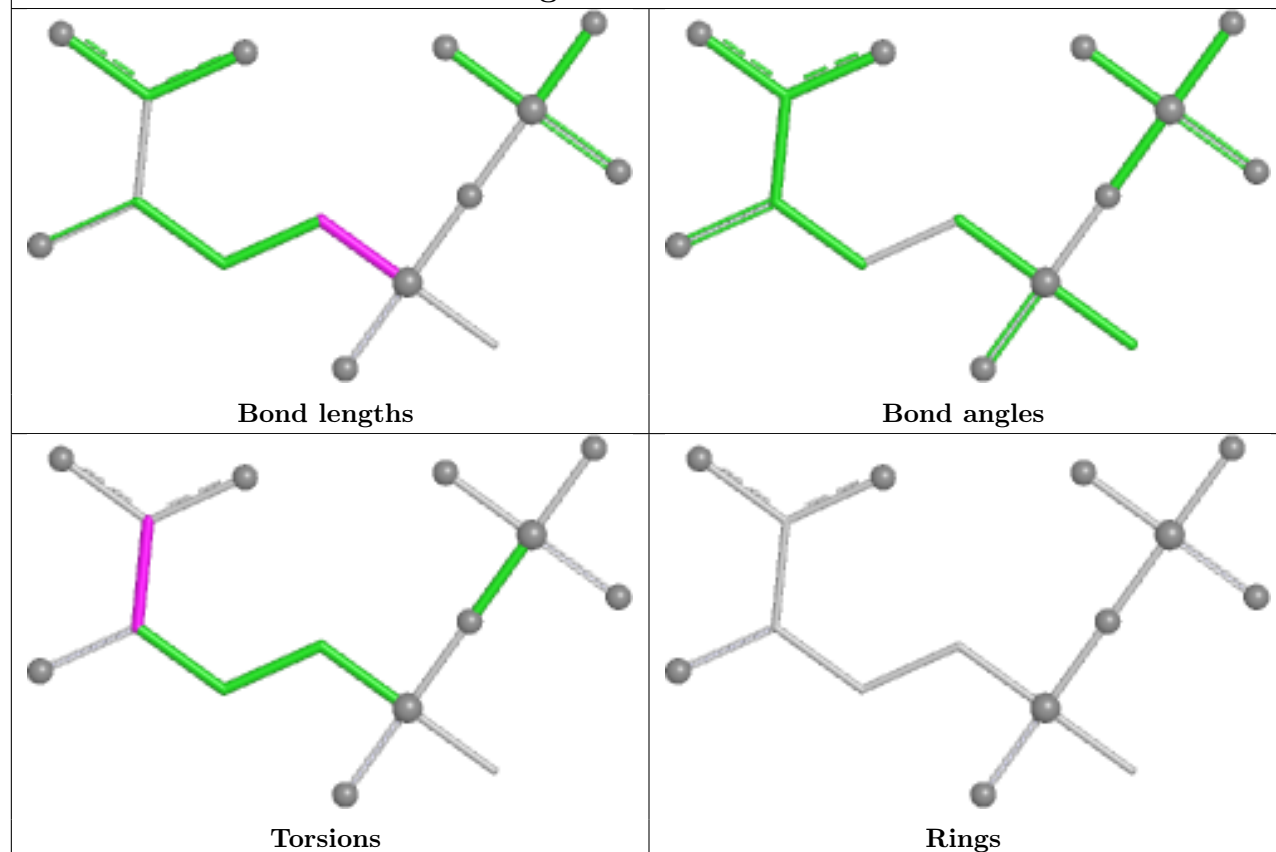
Ligand ADP E 401



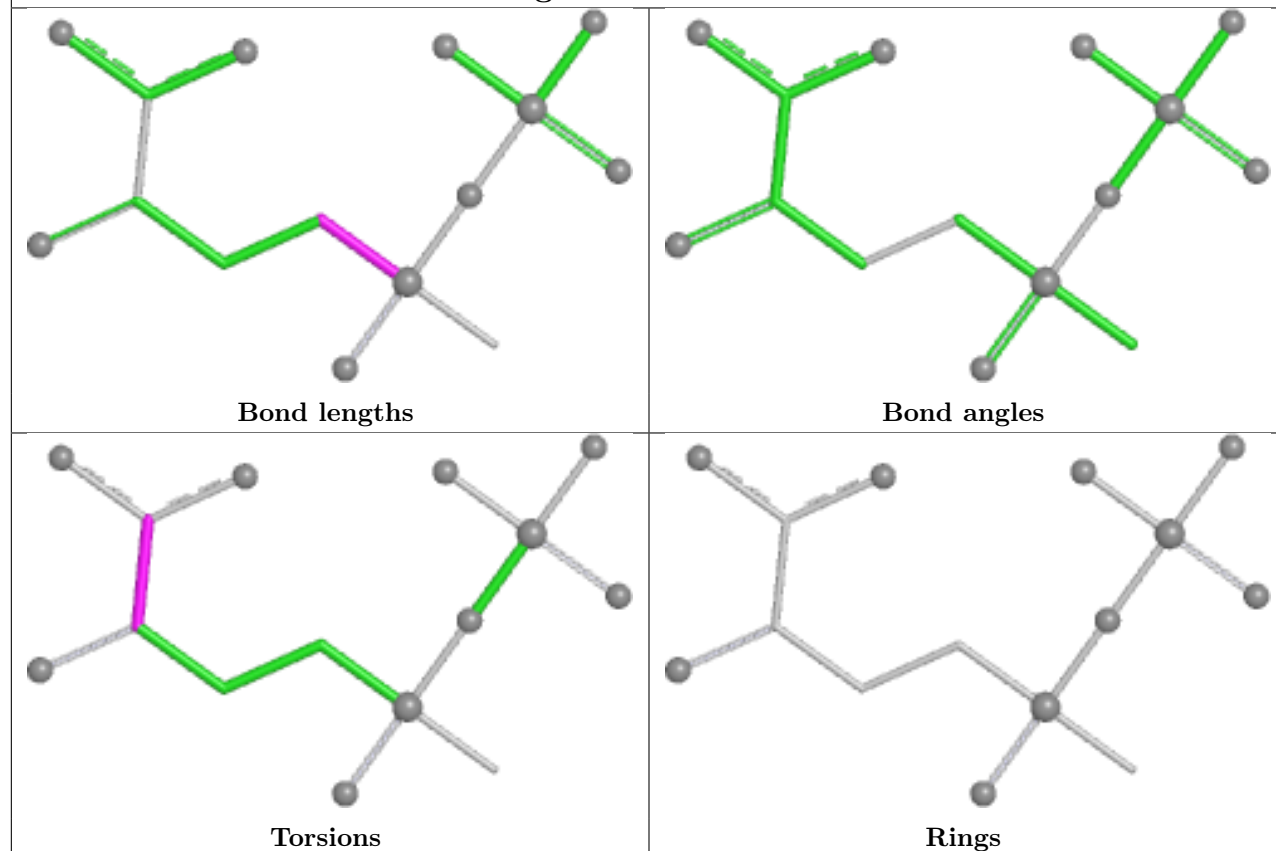
Ligand P3P C 405



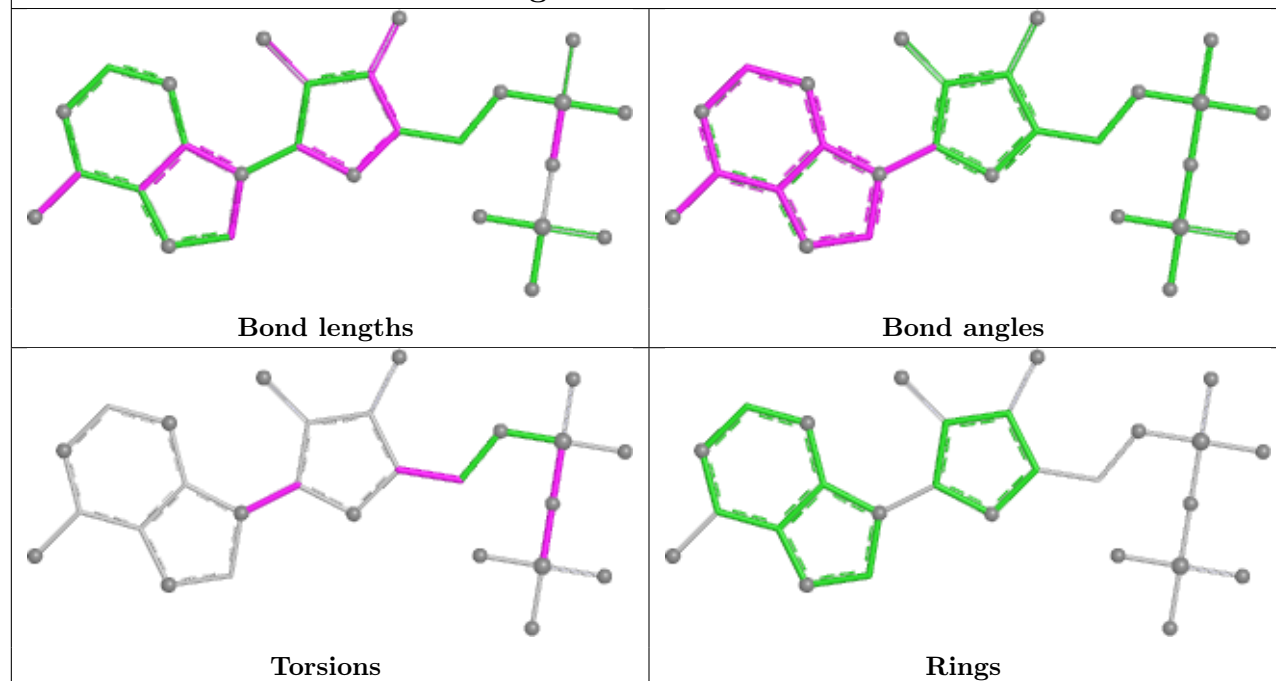
Ligand P3P J 405



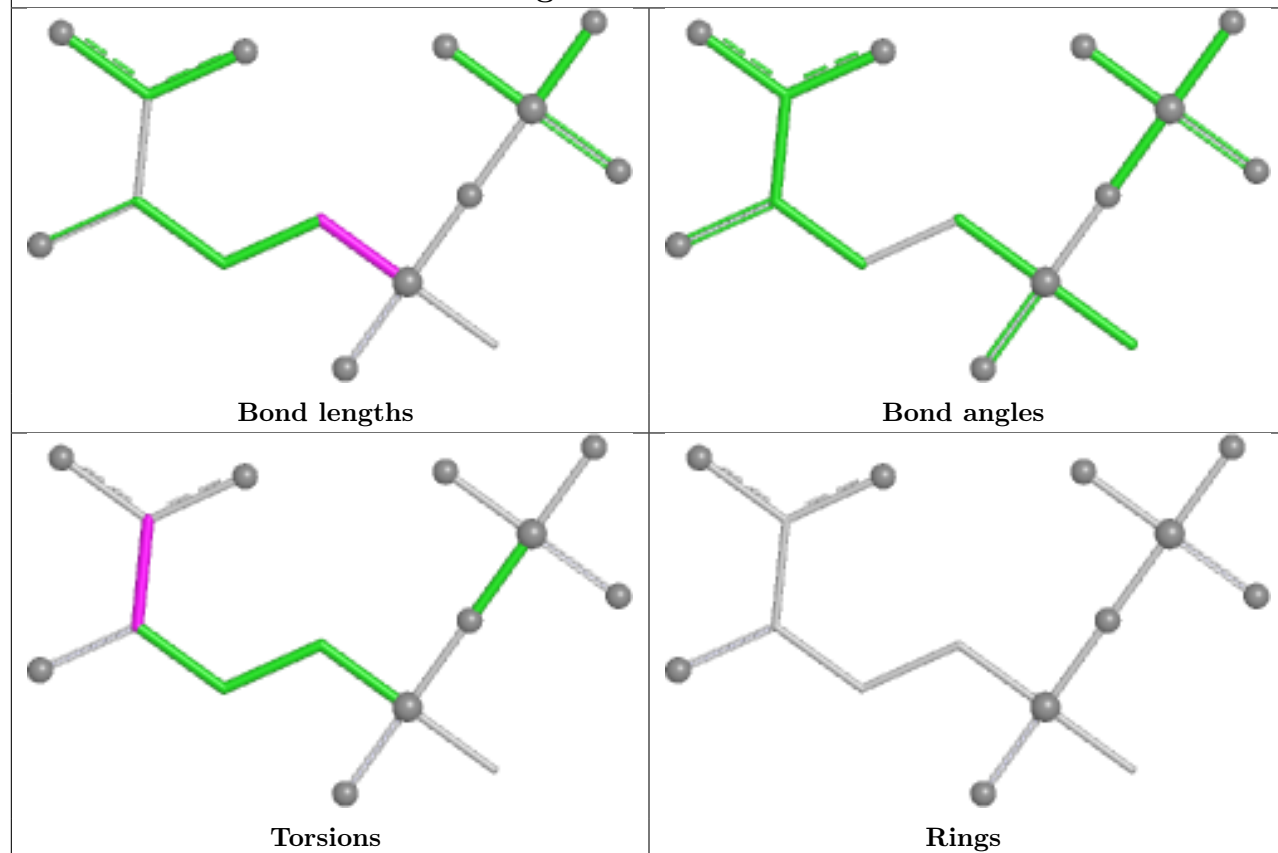
Ligand P3P H 405



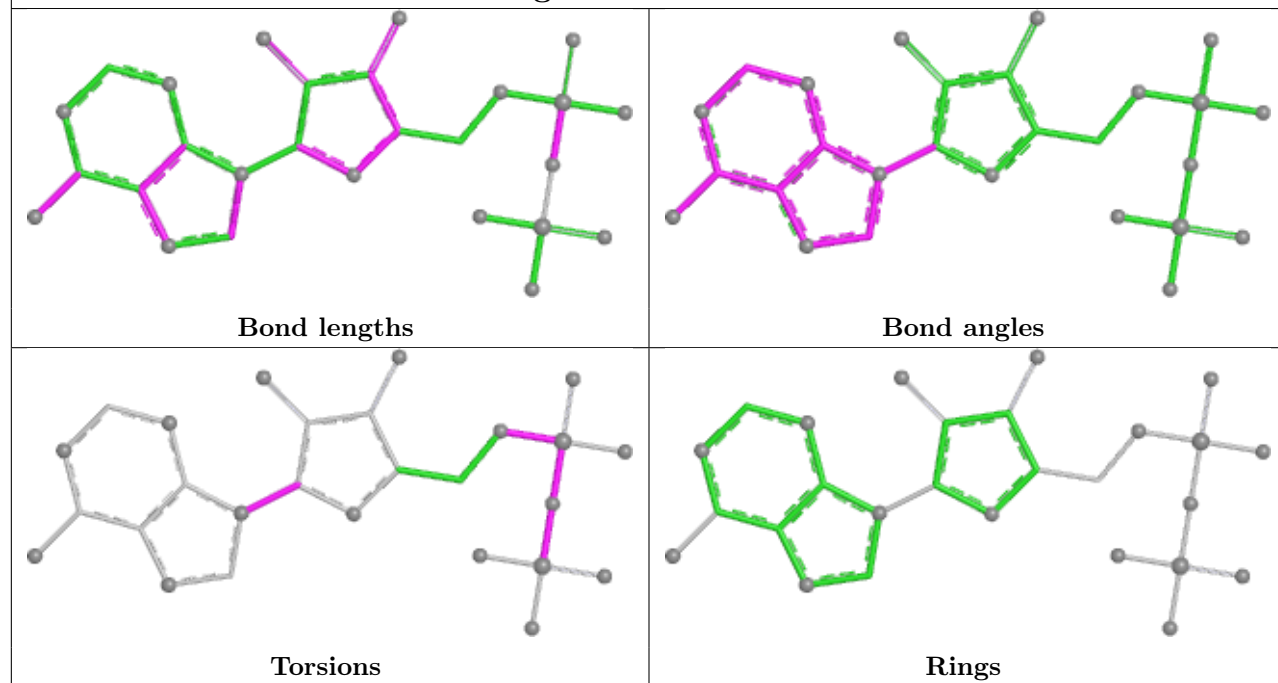
Ligand ADP A 401



Ligand P3P B 405



Ligand ADP J 401



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
1	A	370/373 (99%)	-0.61	0	100	100	10, 16, 31, 61	4 (1%)
1	B	370/373 (99%)	-0.62	0	100	100	10, 16, 30, 51	3 (0%)
1	C	369/373 (98%)	-0.67	0	100	100	9, 14, 27, 45	4 (1%)
1	H	369/373 (98%)	-0.53	0	100	100	11, 19, 33, 49	3 (0%)
1	I	370/373 (99%)	-0.46	1 (0%)	90	92	11, 20, 35, 63	3 (0%)
2	D	371/373 (99%)	-0.65	1 (0%)	90	92	9, 15, 28, 53	4 (1%)
2	E	371/373 (99%)	-0.61	1 (0%)	90	92	10, 17, 30, 50	4 (1%)
2	F	370/373 (99%)	-0.37	0	100	100	12, 22, 38, 55	3 (0%)
2	G	370/373 (99%)	-0.38	0	100	100	13, 21, 39, 54	4 (1%)
2	J	370/373 (99%)	-0.36	2 (0%)	87	90	12, 22, 38, 52	3 (0%)
All	All	3700/3730 (99%)	-0.53	5 (0%)	92	93	9, 18, 34, 63	35 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	365	GLY	2.4
1	I	372	LYS	2.4
2	D	372	LYS	2.2
2	J	169	ARG	2.1
2	E	286	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
1	CSO	A	53	7/8	0.94	0.08	17,20,31,43	0
1	CSO	B	53	7/8	0.95	0.07	18,19,29,37	0
1	CSO	H	53	7/8	0.96	0.07	24,25,36,46	0
1	CSO	I	53	7/8	0.96	0.06	17,18,21,22	0
1	CSO	C	53	7/8	0.97	0.06	16,19,24,36	0

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(\AA^2)	Q<0.9
6	MPD	H	408	8/8	0.66	0.20	35,47,51,55	0
6	MPD	H	407	8/8	0.77	0.19	31,42,51,62	0
6	MPD	A	407	8/8	0.81	0.16	27,37,48,54	0
6	MPD	I	407	8/8	0.82	0.15	37,44,49,57	0
6	MPD	J	407	8/8	0.82	0.16	35,38,44,54	0
6	MPD	J	406	8/8	0.83	0.13	29,34,37,38	0
6	MPD	C	406	8/8	0.83	0.13	27,34,38,44	0
6	MPD	C	407	8/8	0.84	0.14	26,29,43,51	0
6	MPD	G	406	8/8	0.84	0.13	26,35,38,47	0
6	MPD	G	407	8/8	0.84	0.13	37,39,43,53	0
6	MPD	B	407	8/8	0.84	0.14	28,34,48,53	0
6	MPD	F	407	8/8	0.85	0.15	35,48,52,58	0
6	MPD	I	406	8/8	0.86	0.12	25,32,36,37	0
6	MPD	F	406	8/8	0.87	0.12	28,33,35,36	0
6	MPD	B	406	8/8	0.87	0.12	29,35,35,36	0
6	MPD	H	406	8/8	0.87	0.12	28,35,40,43	0
6	MPD	E	407	8/8	0.88	0.12	29,36,46,56	0
6	MPD	E	406	8/8	0.88	0.12	25,31,35,39	0
6	MPD	D	406	8/8	0.89	0.11	25,30,35,35	0
6	MPD	D	407	8/8	0.89	0.10	25,32,43,45	0
6	MPD	A	406	8/8	0.89	0.12	25,34,35,36	0
3	ADP	J	401	27/27	0.97	0.06	15,21,26,29	0
3	ADP	H	401	27/27	0.98	0.06	14,18,21,22	0
3	ADP	I	401	27/27	0.98	0.06	14,19,22,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ADP	A	401	27/27	0.98	0.04	10,15,18,22	0
5	P3P	F	405	15/15	0.98	0.05	12,15,19,19	0
5	P3P	G	405	15/15	0.98	0.06	13,16,20,20	0
5	P3P	H	405	15/15	0.98	0.05	11,15,16,16	0
3	ADP	B	401	27/27	0.98	0.05	11,15,19,20	0
3	ADP	F	401	27/27	0.98	0.06	15,21,26,29	0
3	ADP	G	401	27/27	0.98	0.06	16,22,26,27	0
5	P3P	B	405	15/15	0.99	0.04	9,12,16,16	0
5	P3P	C	405	15/15	0.99	0.04	10,11,13,15	0
5	P3P	D	405	15/15	0.99	0.04	8,10,13,13	0
5	P3P	E	405	15/15	0.99	0.04	10,12,14,14	0
3	ADP	E	401	27/27	0.99	0.04	12,15,20,22	0
3	ADP	C	401	27/27	0.99	0.04	10,13,15,18	0
3	ADP	D	401	27/27	0.99	0.04	9,13,17,20	0
5	P3P	I	405	15/15	0.99	0.04	13,14,17,17	0
5	P3P	J	405	15/15	0.99	0.05	14,16,21,22	0
4	MN	A	403	1/1	0.99	0.03	12,12,12,12	0
4	MN	F	404	1/1	0.99	0.03	16,16,16,16	0
4	MN	G	403	1/1	0.99	0.02	17,17,17,17	0
4	MN	H	403	1/1	0.99	0.02	14,14,14,14	0
4	MN	I	403	1/1	0.99	0.02	16,16,16,16	0
5	P3P	A	405	15/15	0.99	0.04	10,12,15,15	0
7	CL	F	408	1/1	0.99	0.04	17,17,17,17	0
7	CL	F	409	1/1	0.99	0.04	18,18,18,18	0
7	CL	G	408	1/1	0.99	0.05	17,17,17,17	0
7	CL	I	408	1/1	0.99	0.03	18,18,18,18	0
7	CL	I	409	1/1	0.99	0.03	18,18,18,18	0
4	MN	F	403	1/1	1.00	0.02	17,17,17,17	0
4	MN	A	402	1/1	1.00	0.01	12,12,12,12	0
4	MN	G	402	1/1	1.00	0.02	16,16,16,16	0
4	MN	A	404	1/1	1.00	0.01	11,11,11,11	0
4	MN	G	404	1/1	1.00	0.03	16,16,16,16	0
4	MN	H	402	1/1	1.00	0.01	13,13,13,13	0
4	MN	B	402	1/1	1.00	0.01	12,12,12,12	0
4	MN	H	404	1/1	1.00	0.02	14,14,14,14	0
4	MN	I	402	1/1	1.00	0.02	14,14,14,14	0
4	MN	B	403	1/1	1.00	0.02	12,12,12,12	0
4	MN	I	404	1/1	1.00	0.02	14,14,14,14	0
4	MN	J	402	1/1	1.00	0.02	15,15,15,15	0
4	MN	J	403	1/1	1.00	0.02	16,16,16,16	0
4	MN	J	404	1/1	1.00	0.02	15,15,15,15	0
4	MN	B	404	1/1	1.00	0.02	11,11,11,11	0

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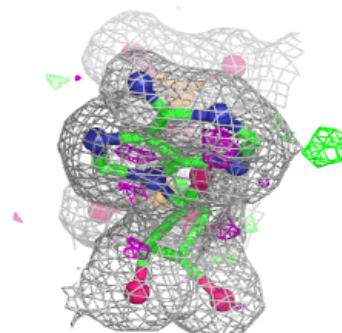
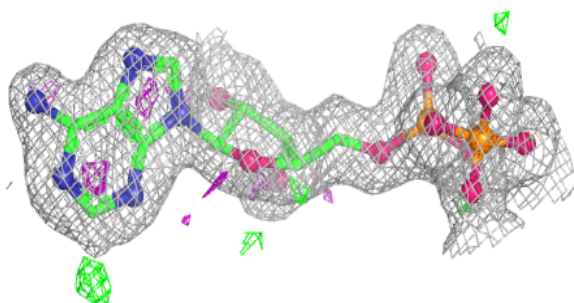
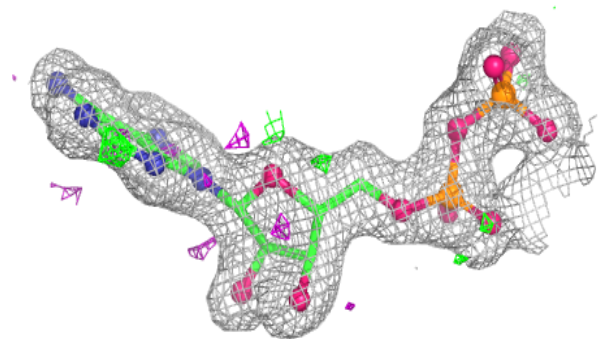
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MN	C	402	1/1	1.00	0.01	11,11,11,11	0
4	MN	C	403	1/1	1.00	0.02	10,10,10,10	0
4	MN	C	404	1/1	1.00	0.01	9,9,9,9	0
4	MN	D	402	1/1	1.00	0.01	11,11,11,11	0
4	MN	D	403	1/1	1.00	0.01	11,11,11,11	0
7	CL	A	408	1/1	1.00	0.05	14,14,14,14	0
7	CL	A	409	1/1	1.00	0.03	14,14,14,14	0
7	CL	B	408	1/1	1.00	0.06	12,12,12,12	0
7	CL	C	408	1/1	1.00	0.03	12,12,12,12	0
7	CL	D	408	1/1	1.00	0.04	14,14,14,14	0
4	MN	D	404	1/1	1.00	0.02	9,9,9,9	0
4	MN	E	402	1/1	1.00	0.01	12,12,12,12	0
4	MN	E	403	1/1	1.00	0.02	13,13,13,13	0
4	MN	E	404	1/1	1.00	0.02	11,11,11,11	0
4	MN	F	402	1/1	1.00	0.02	15,15,15,15	0

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

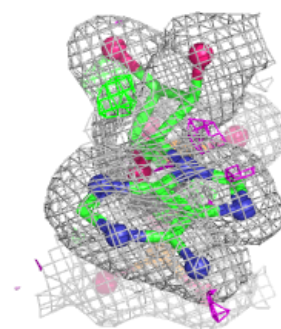
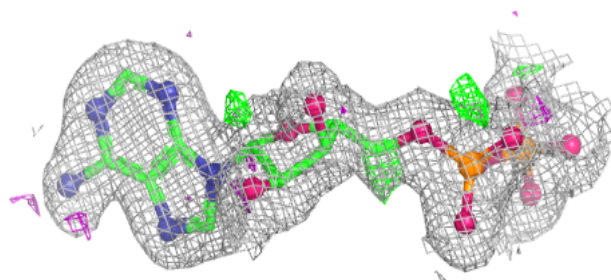
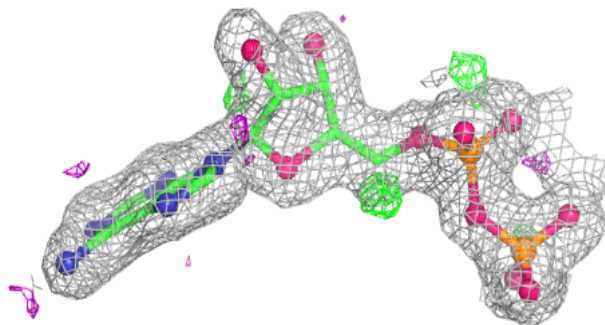
Electron density around ADP J 401:

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

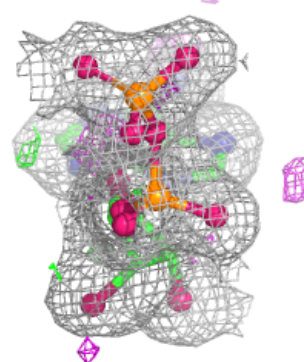
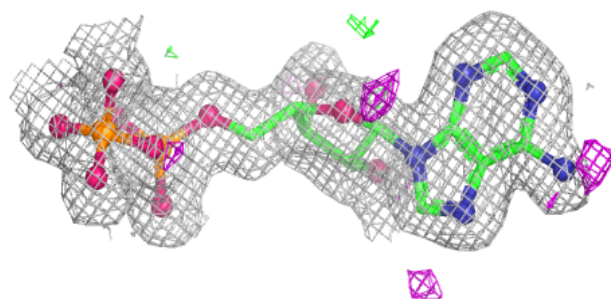
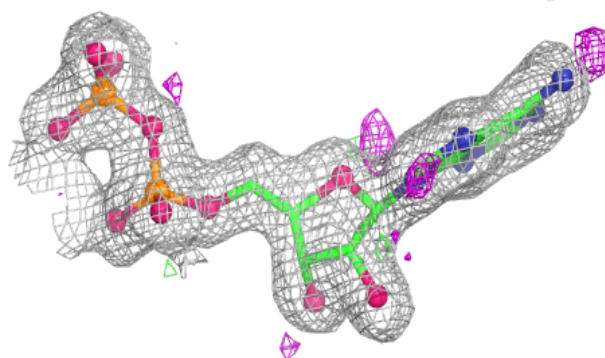


Electron density around ADP H 401:

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and green (positive)

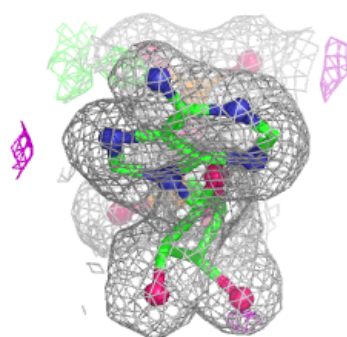
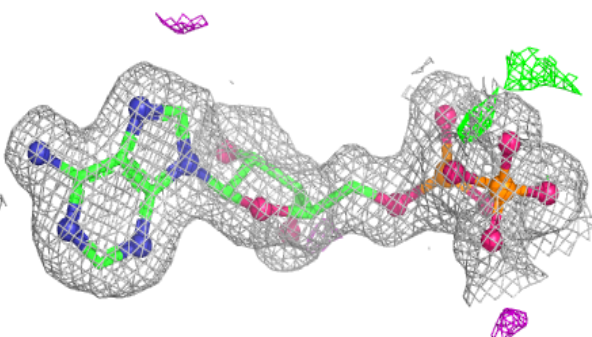
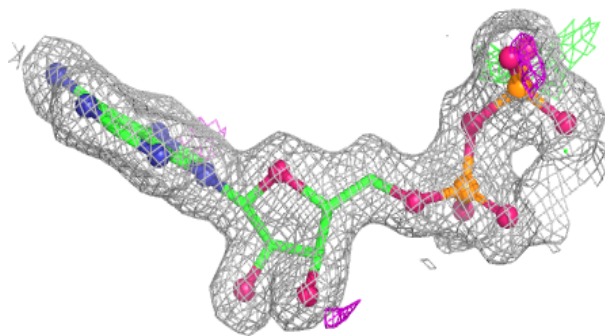
**Electron density around ADP I 401:**

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

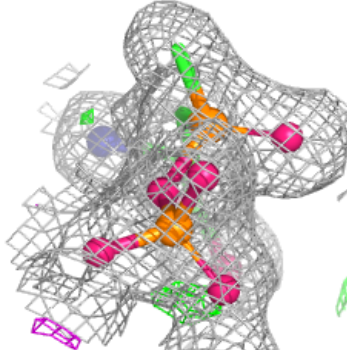
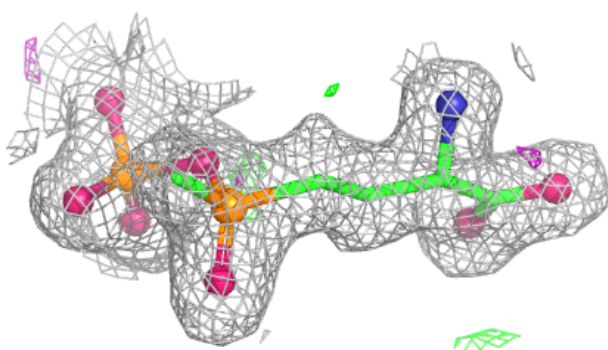
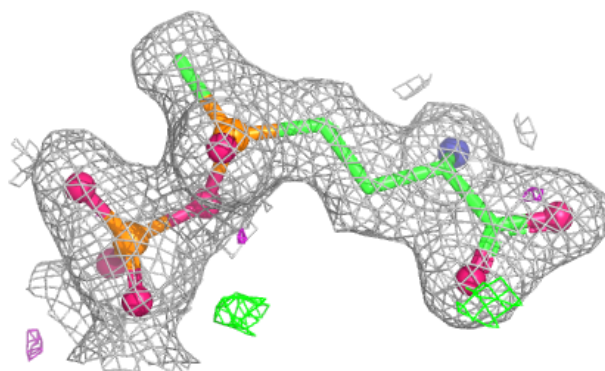


Electron density around ADP A 401:

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and green (positive)

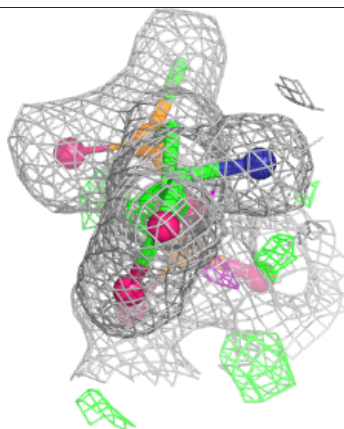
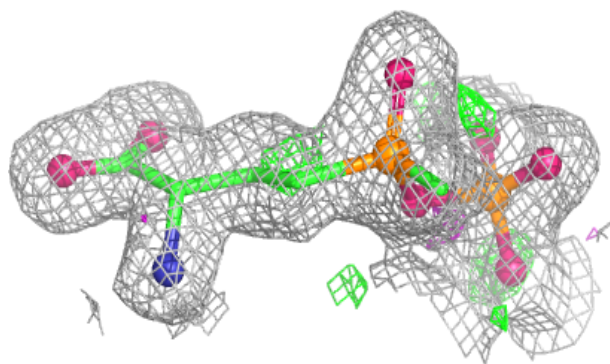
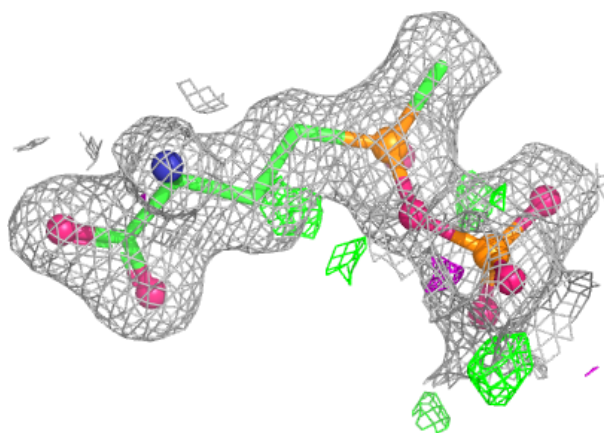
**Electron density around P3P F 405:**

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

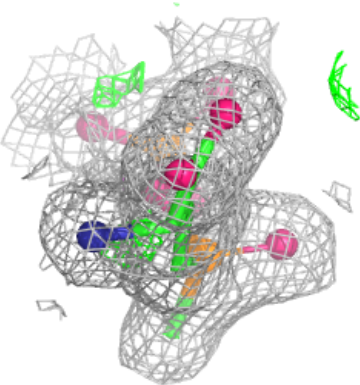
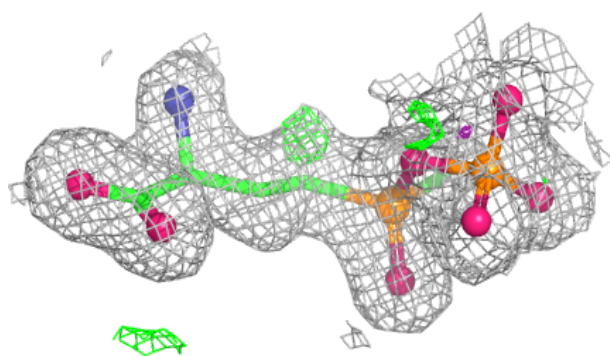
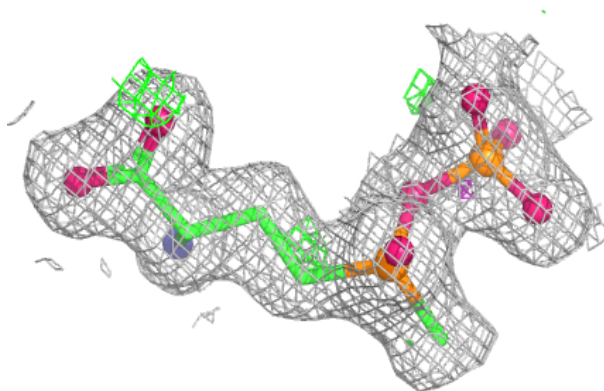


Electron density around P3P G 405:

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

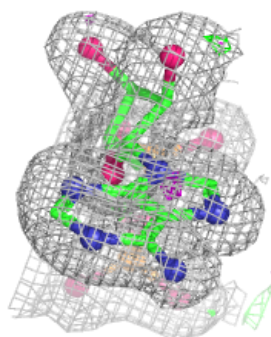
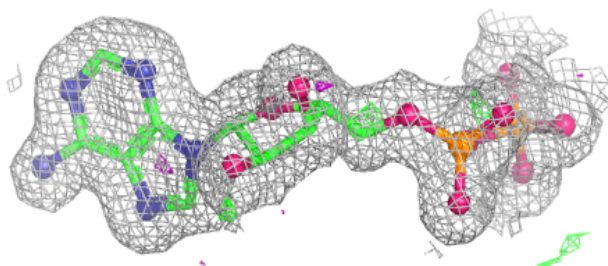
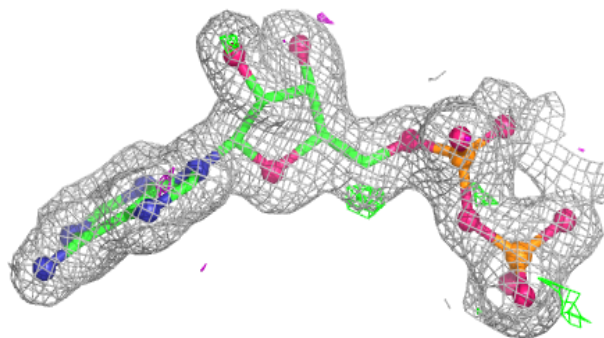
**Electron density around P3P H 405:**

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

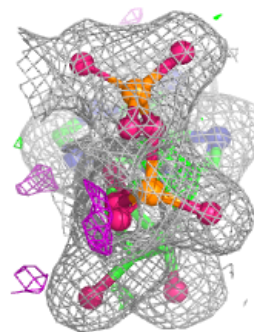
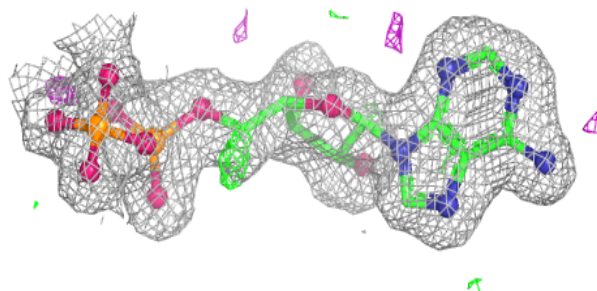
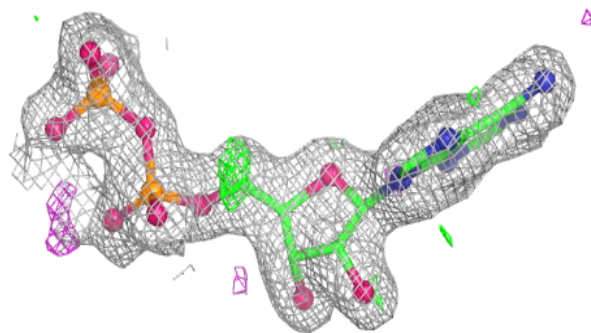


Electron density around ADP B 401:

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

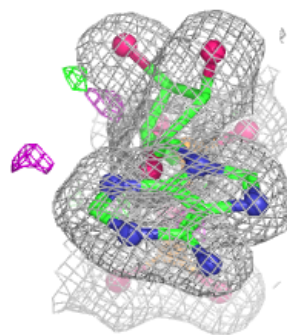
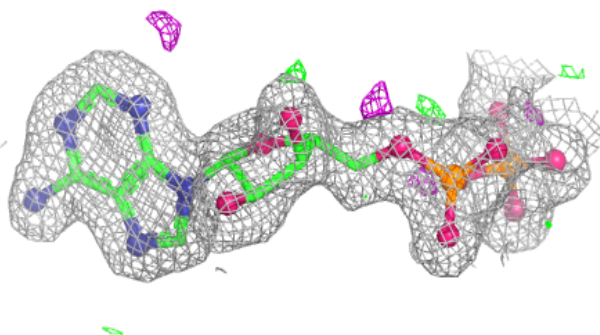
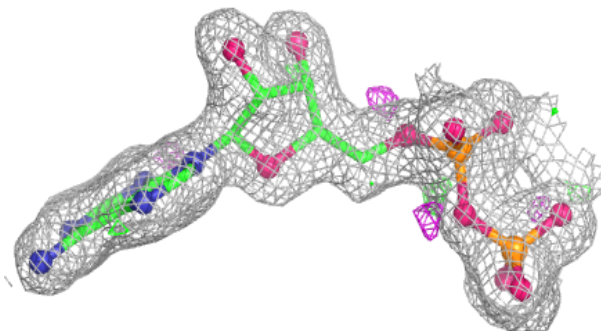
**Electron density around ADP F 401:**

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

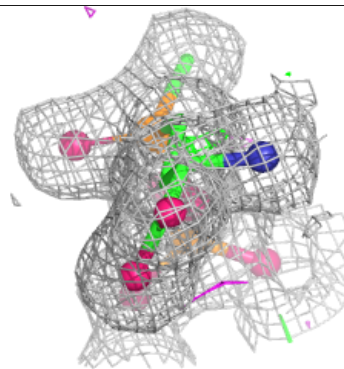
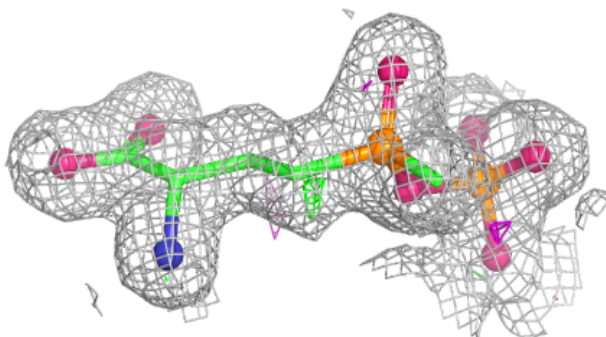
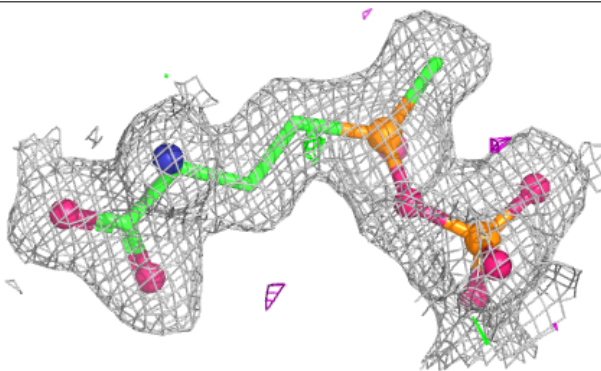


Electron density around ADP G 401:

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

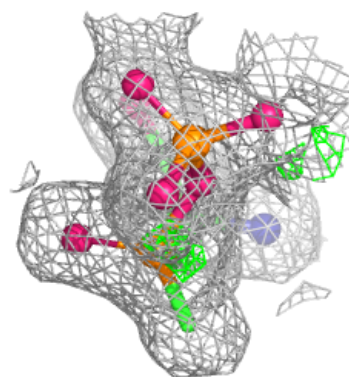
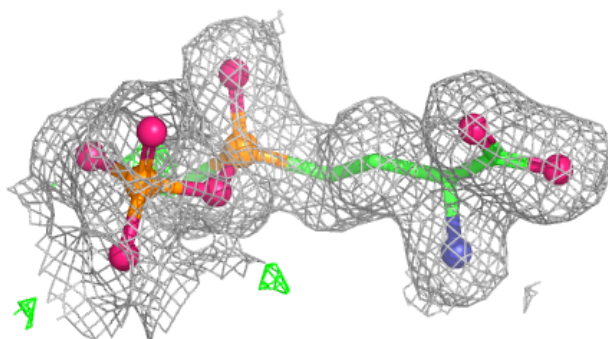
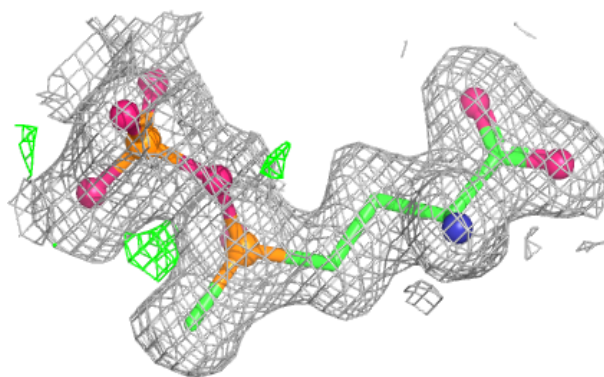
**Electron density around P3P B 405:**

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

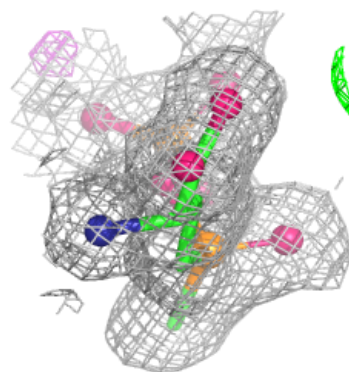
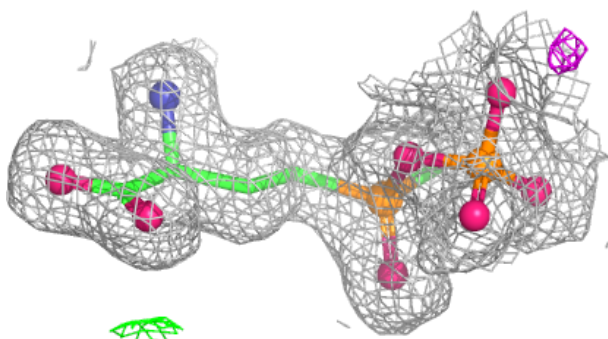
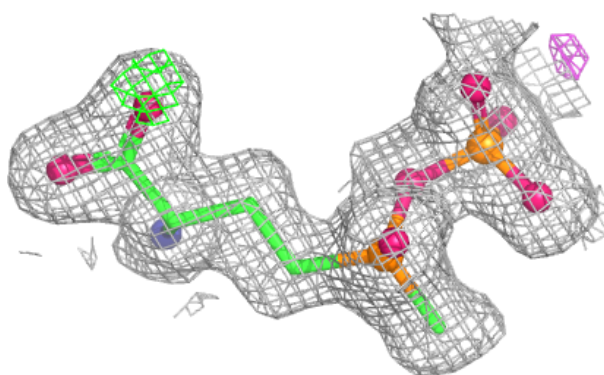


Electron density around P3P C 405:

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

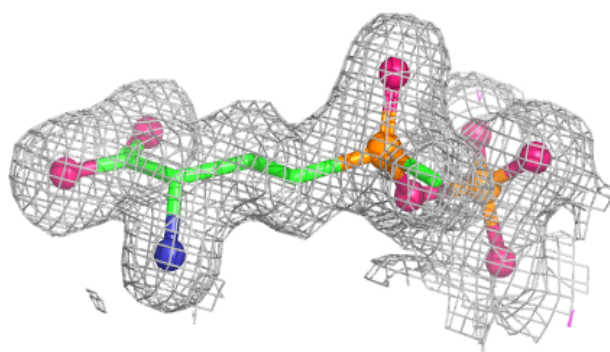
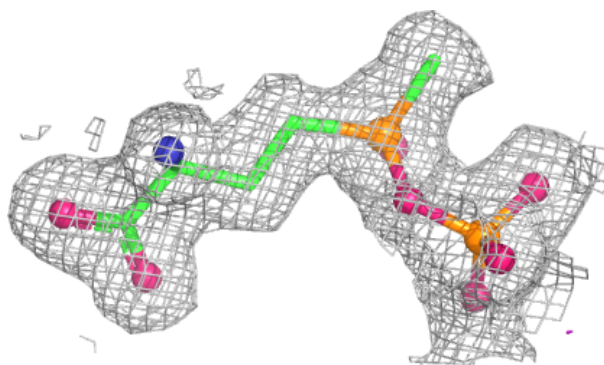
**Electron density around P3P D 405:**

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

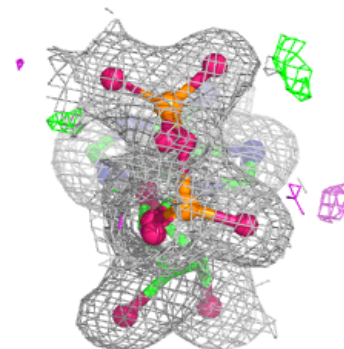
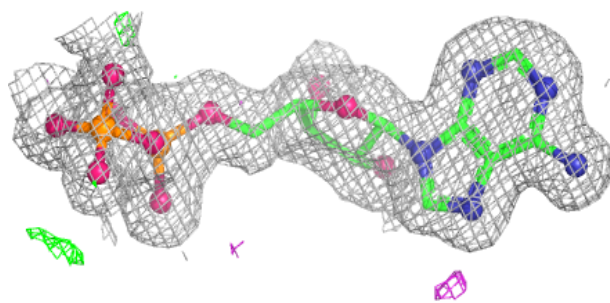
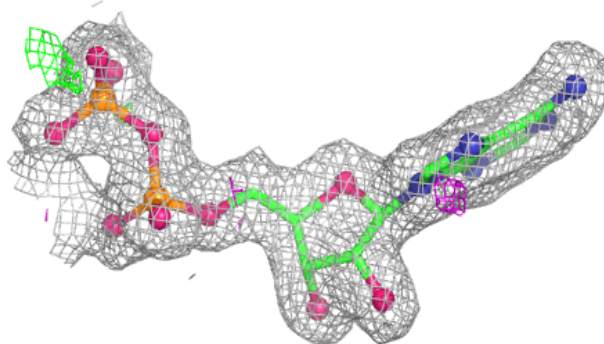


Electron density around P3P E 405:

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

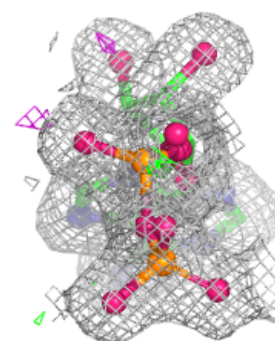
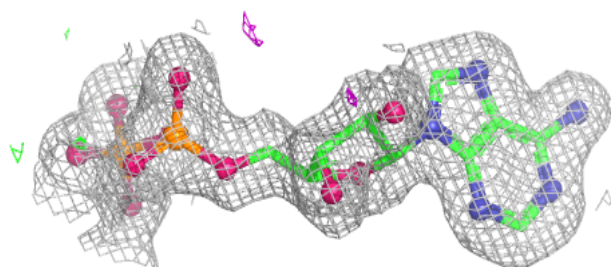
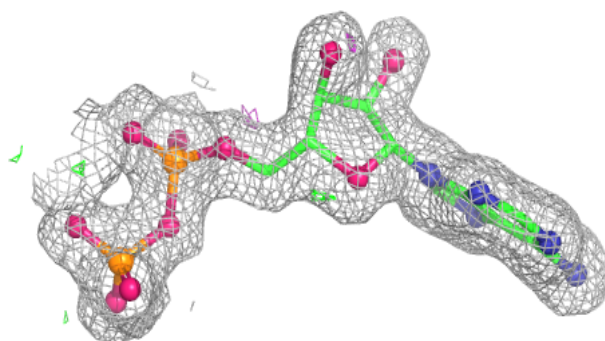
**Electron density around ADP E 401:**

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

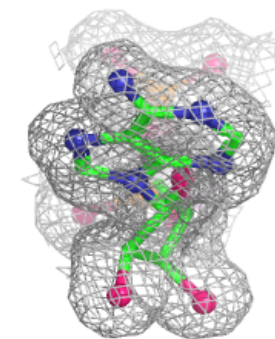
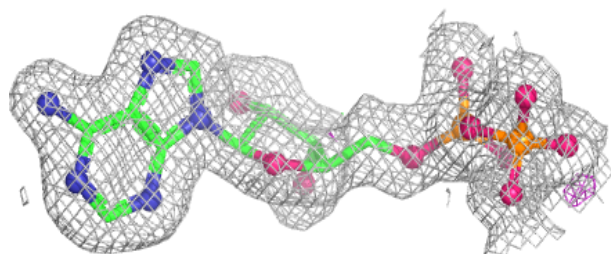
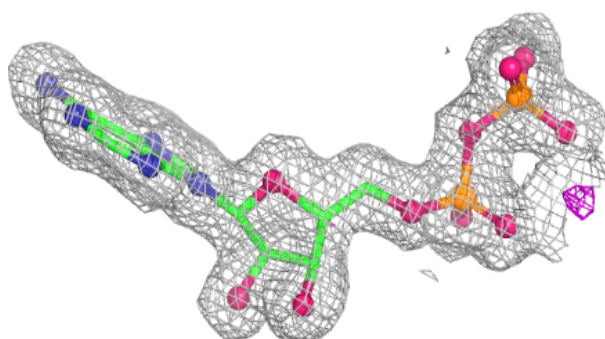


Electron density around ADP C 401:

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

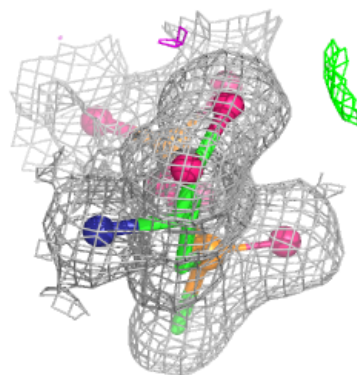
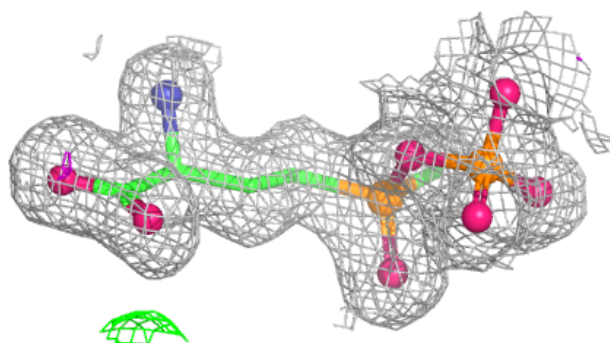
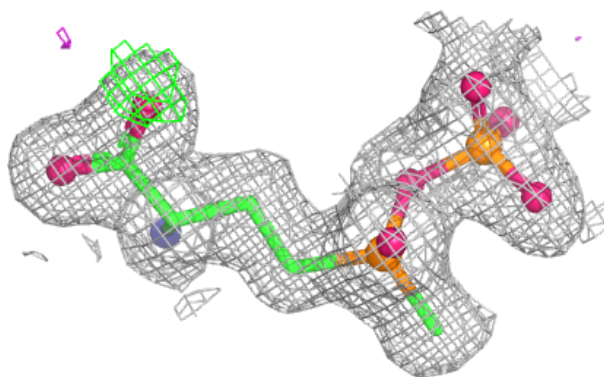
**Electron density around ADP D 401:**

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

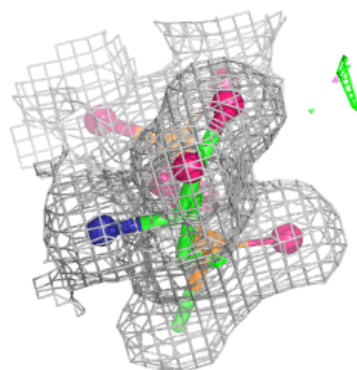
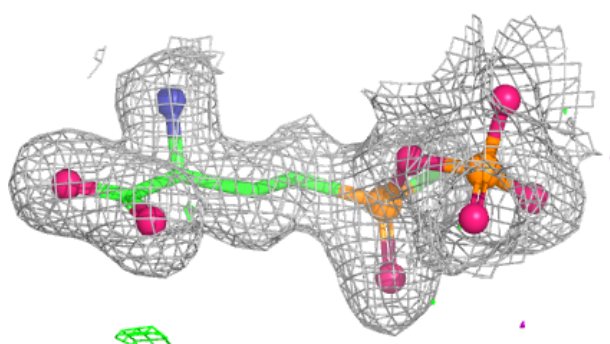
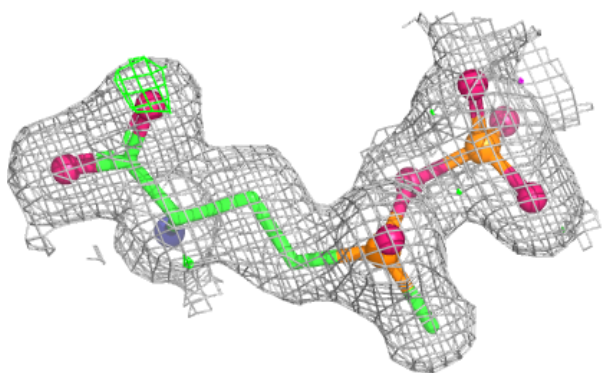


Electron density around P3P I 405:

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

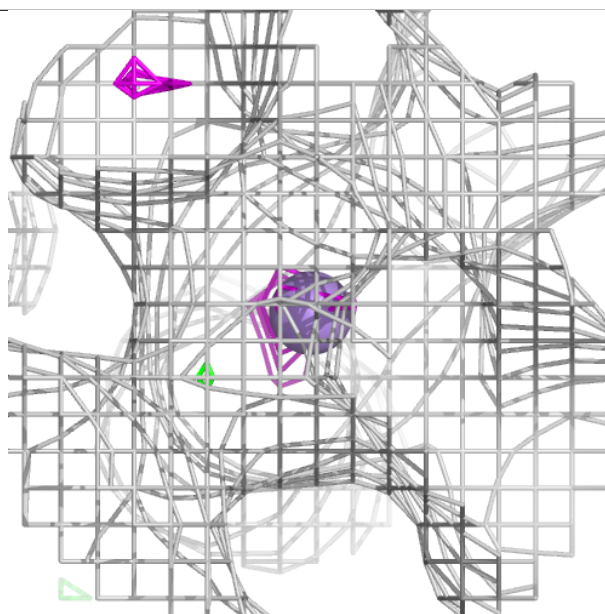
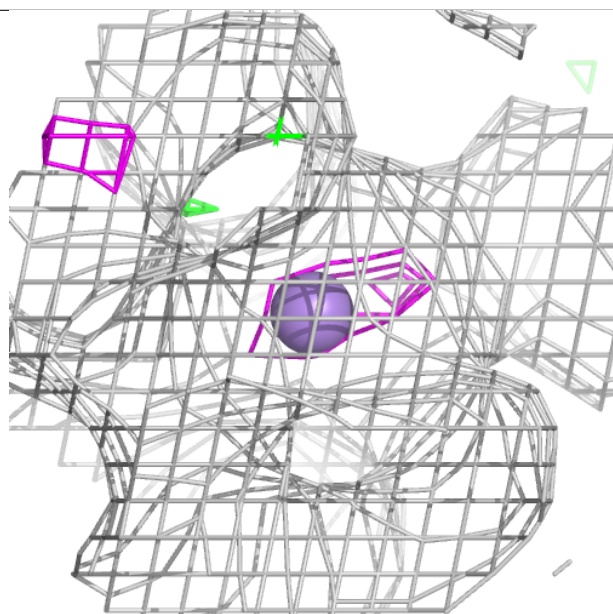
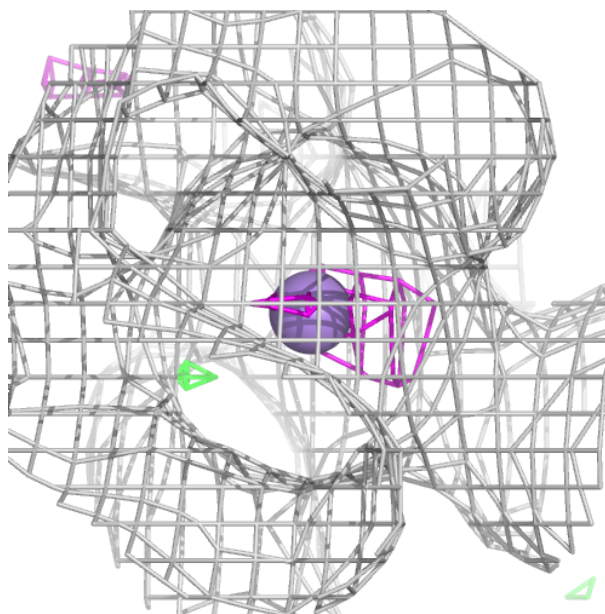
**Electron density around P3P J 405:**

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



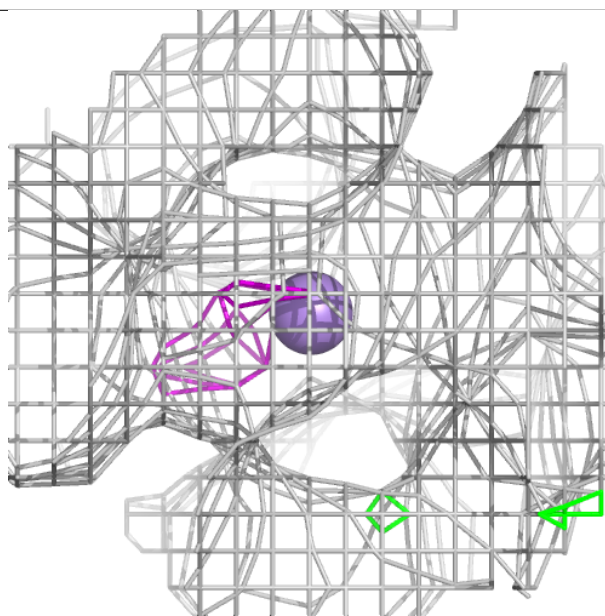
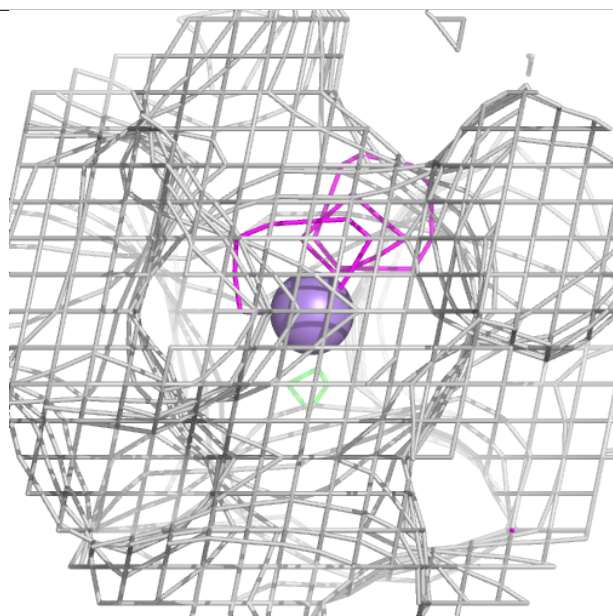
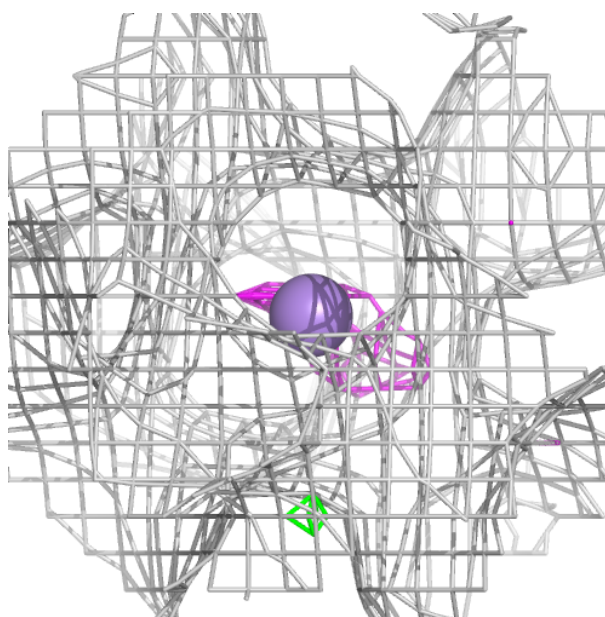
Electron density around MN A 403:

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



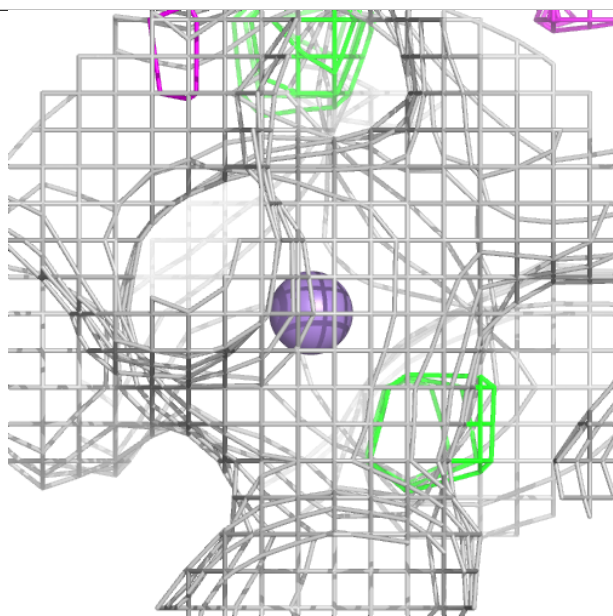
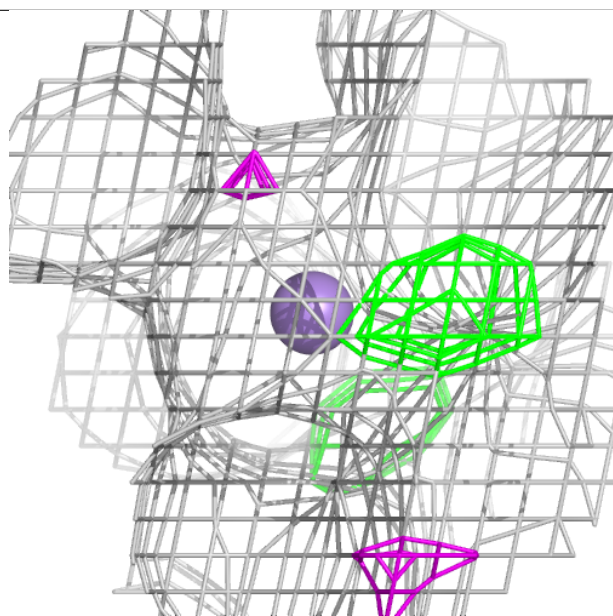
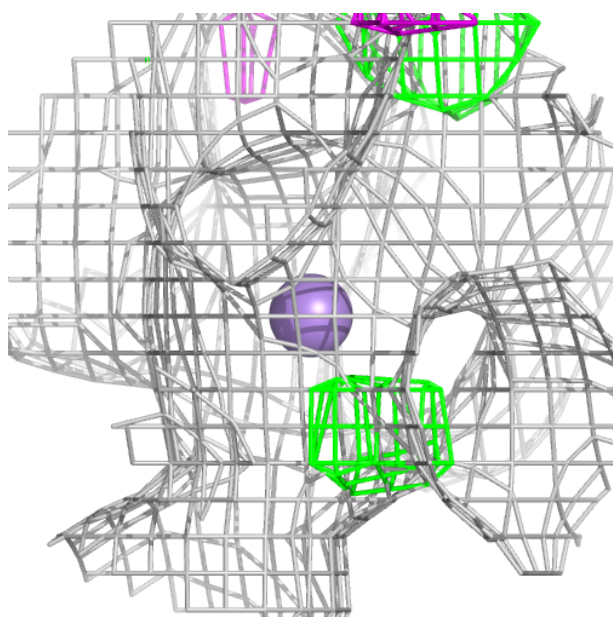
Electron density around MN F 404:

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



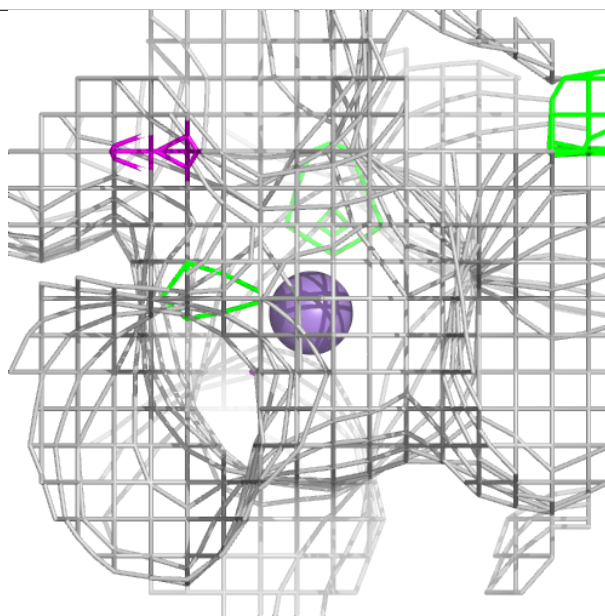
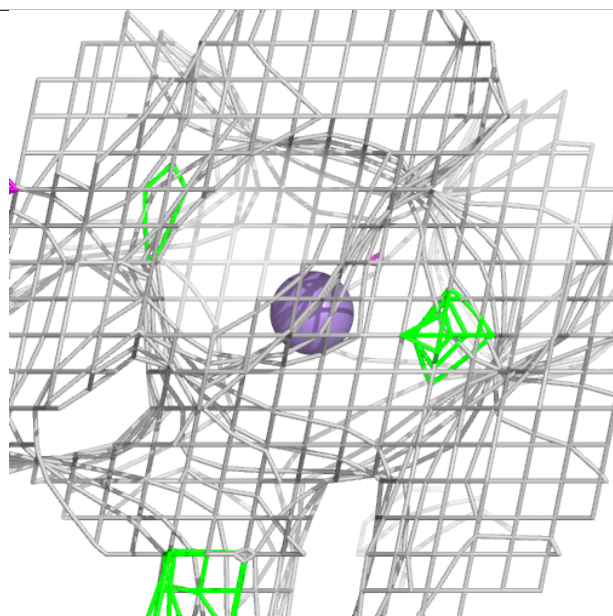
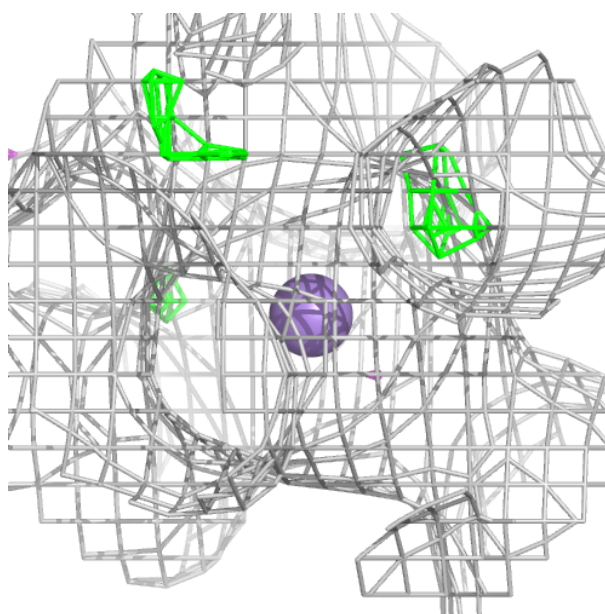
Electron density around MN G 403:

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



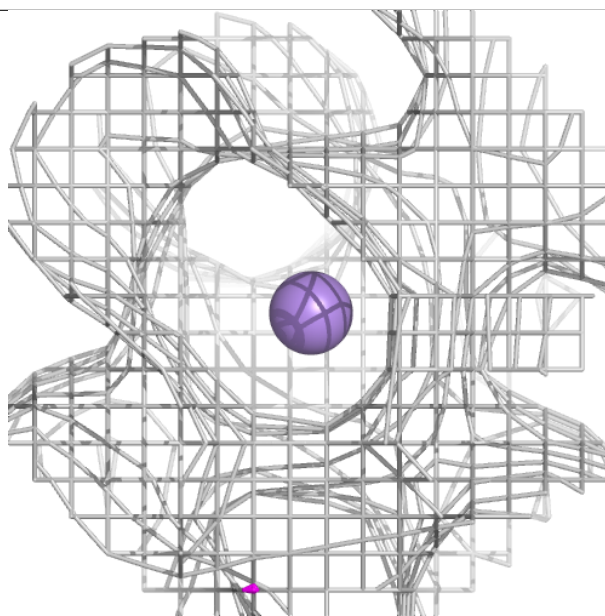
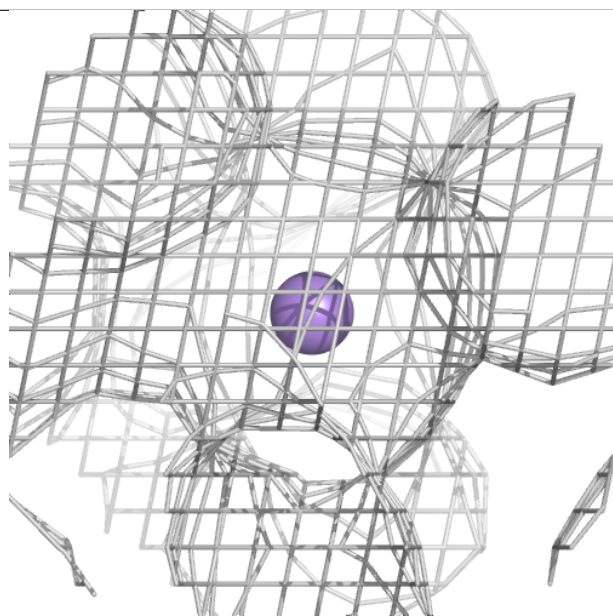
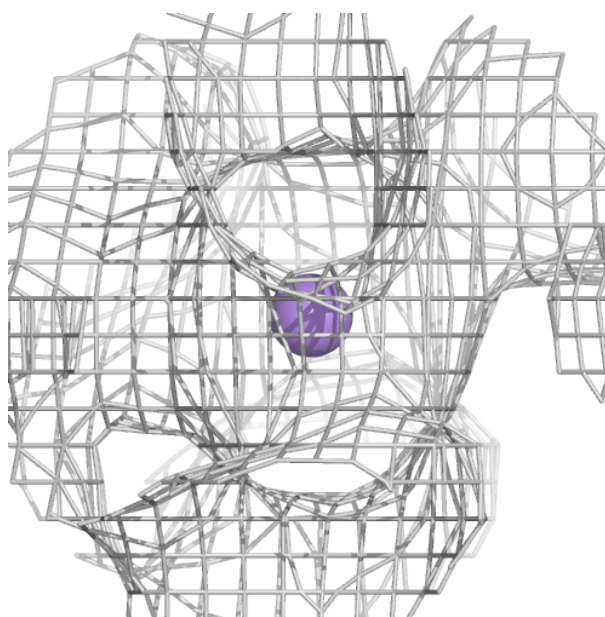
Electron density around MN H 403:

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



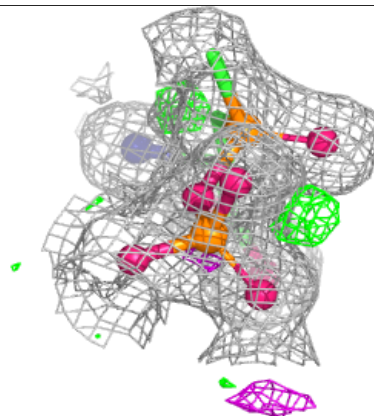
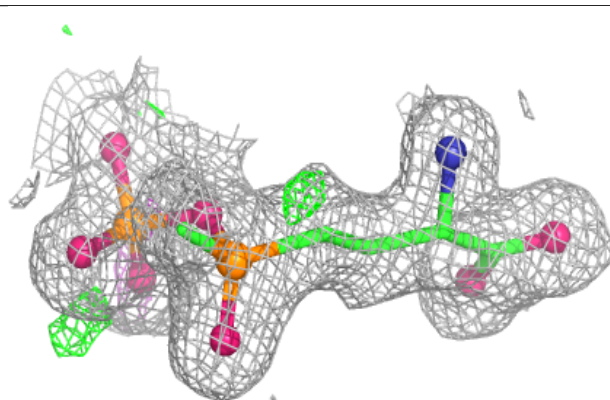
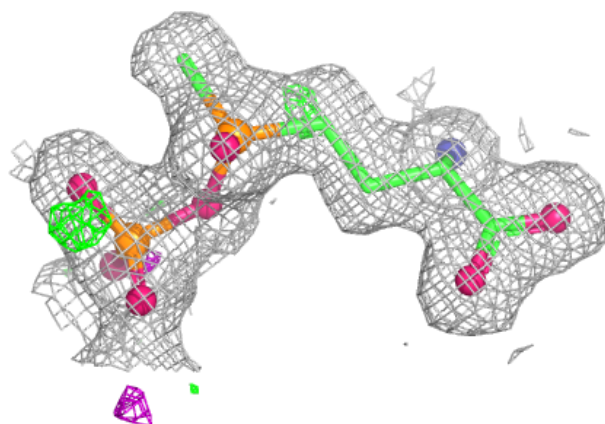
Electron density around MN I 403:

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



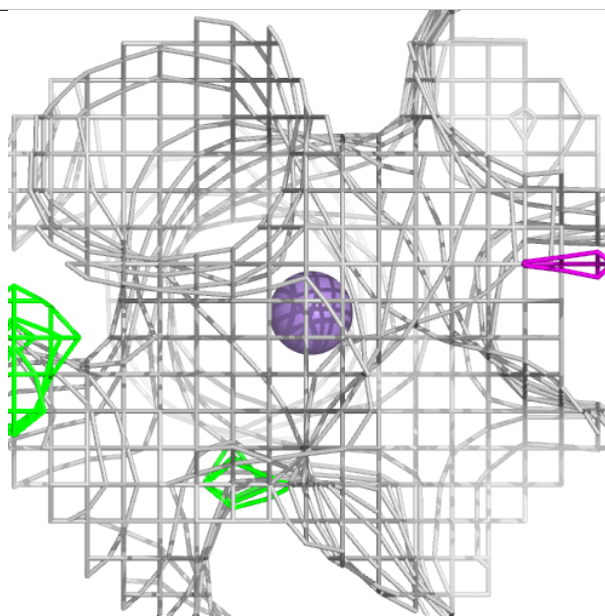
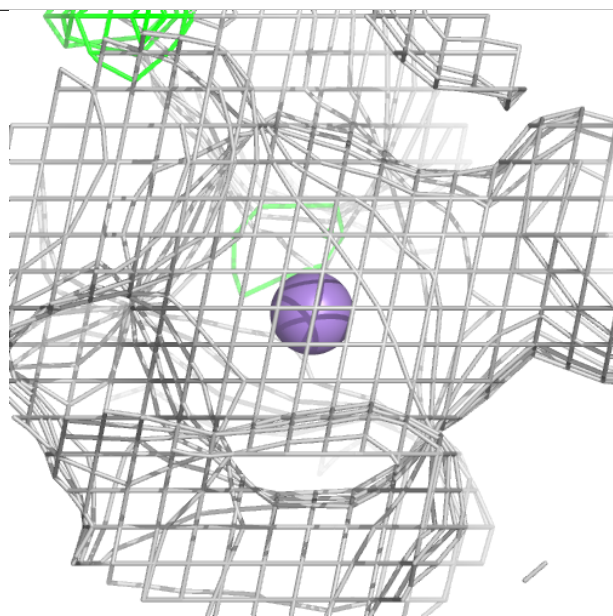
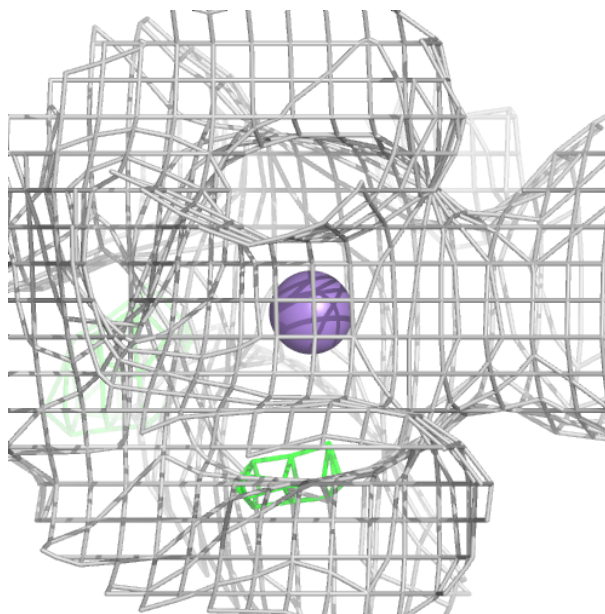
Electron density around P3P A 405:

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



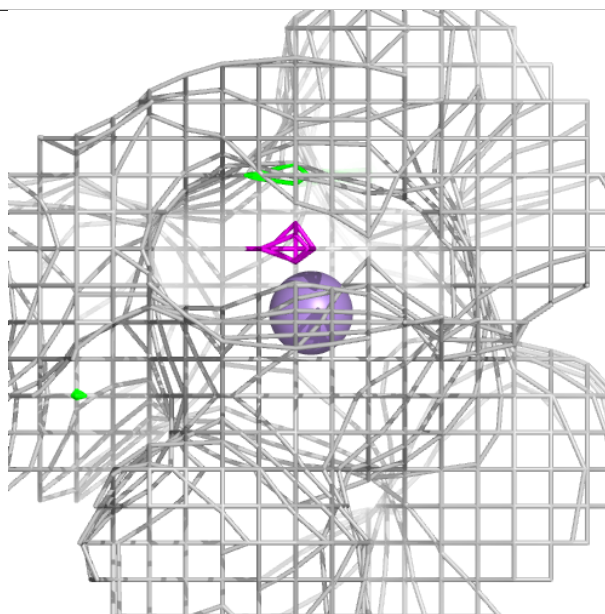
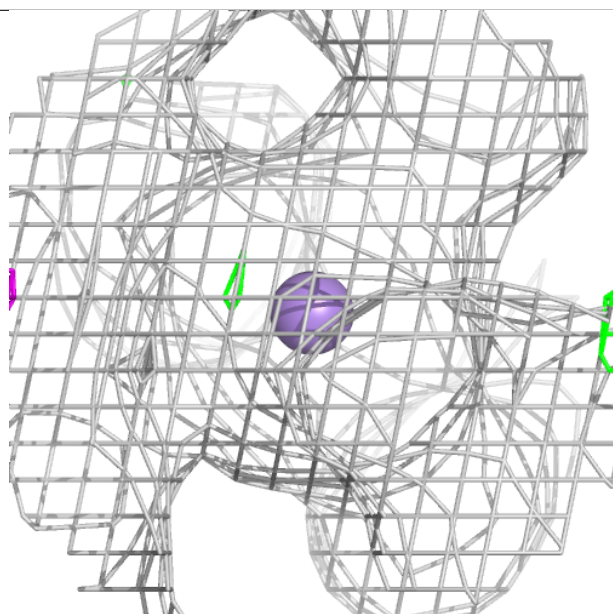
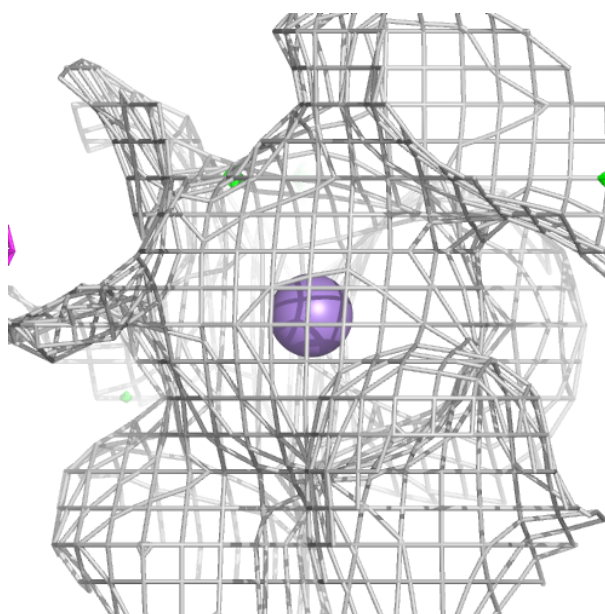
Electron density around MN F 403:

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



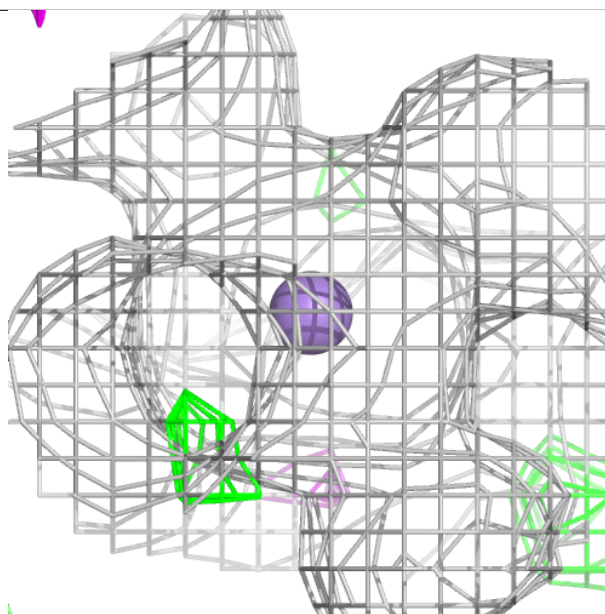
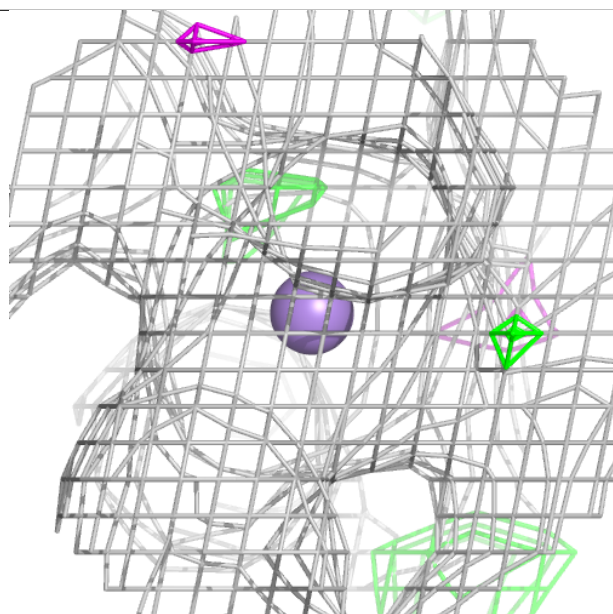
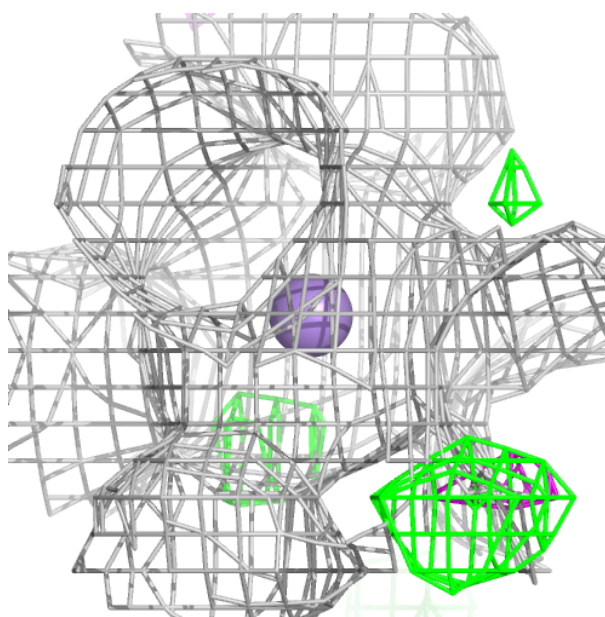
Electron density around MN A 402:

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



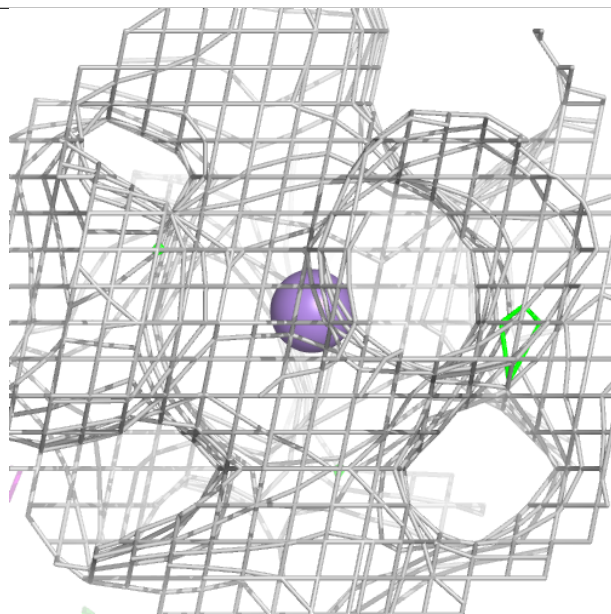
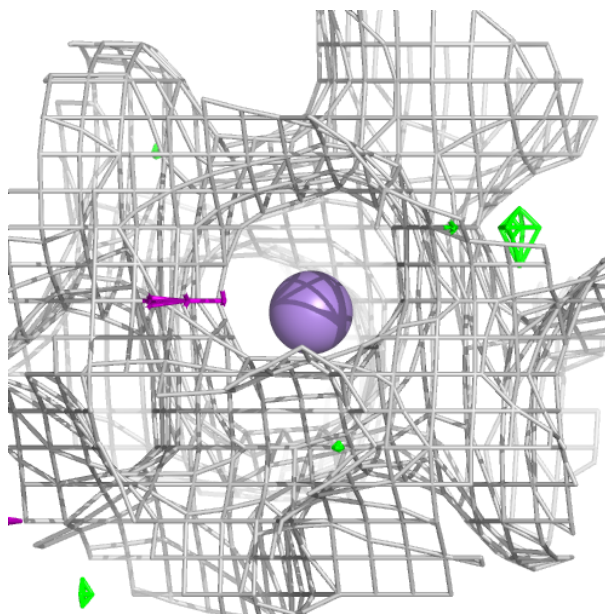
Electron density around MN G 402:

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



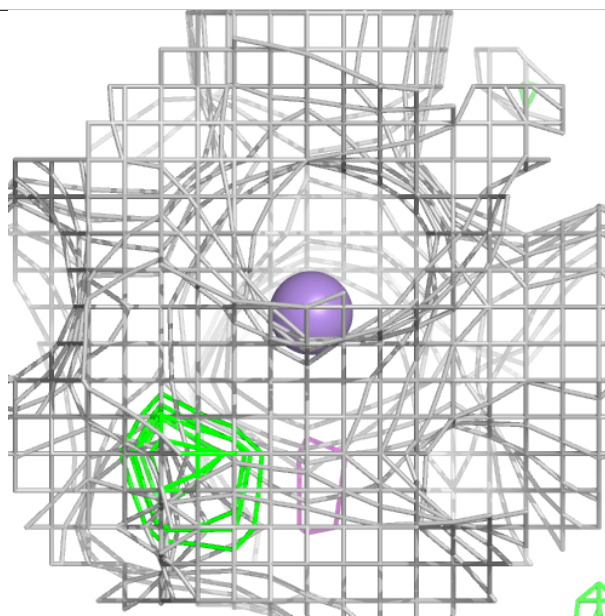
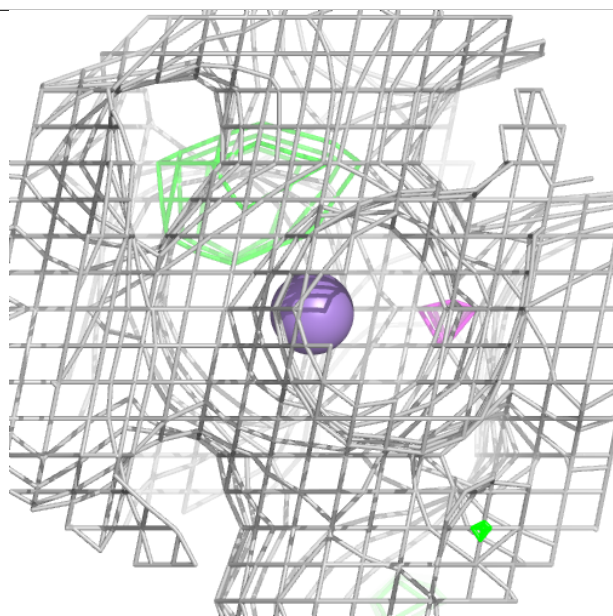
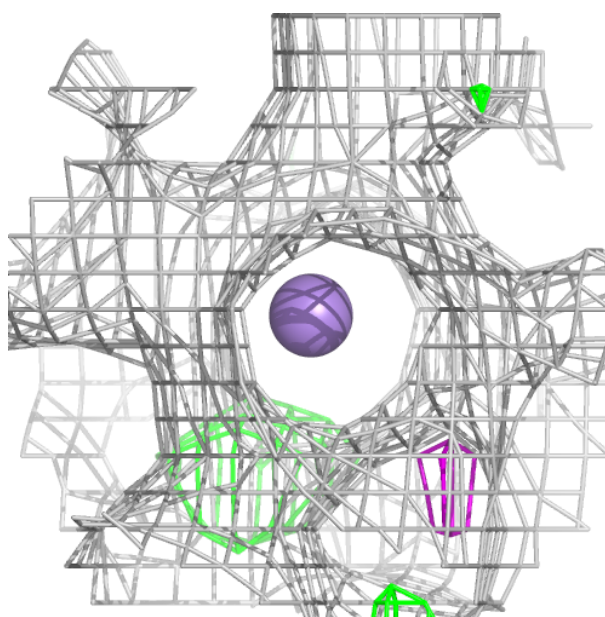
Electron density around MN A 404:

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



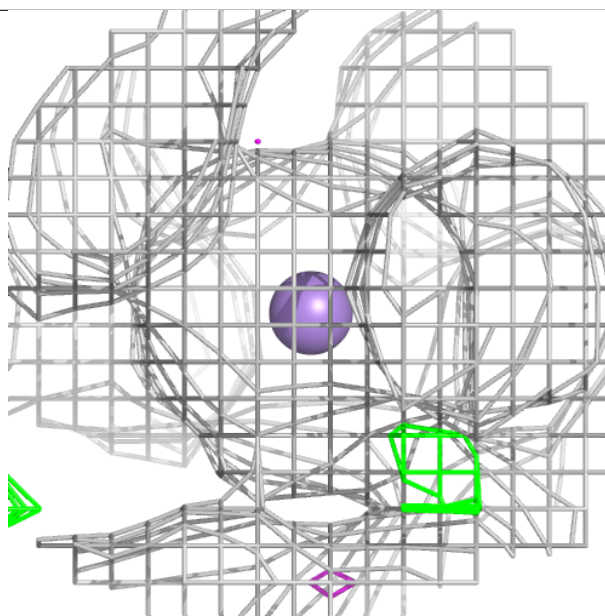
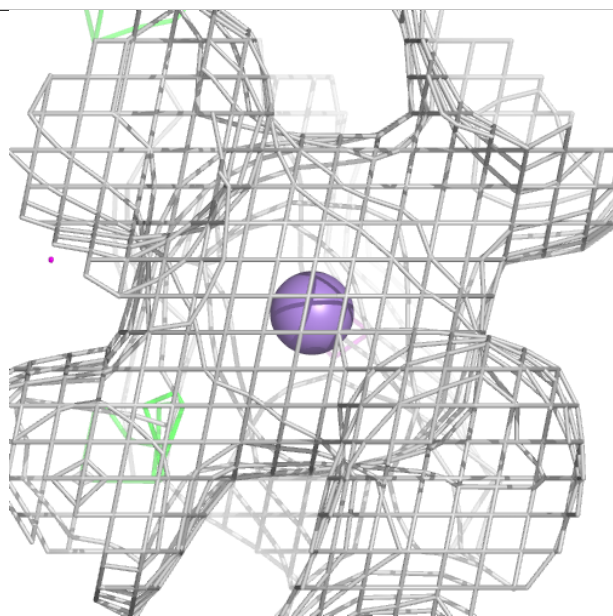
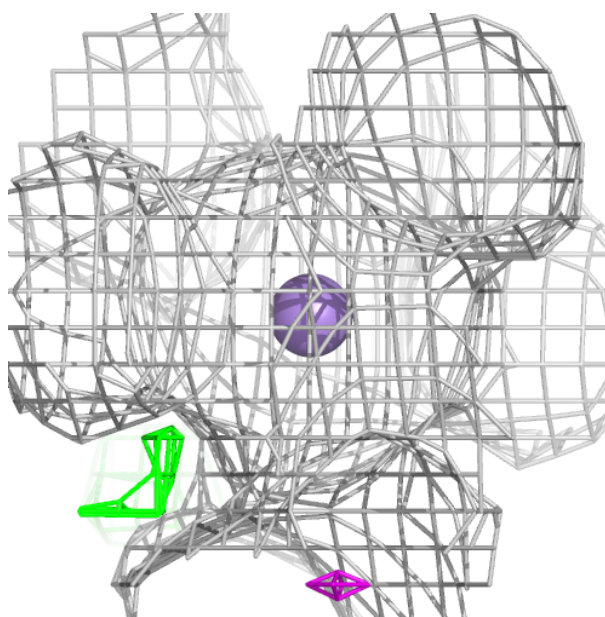
Electron density around MN G 404:

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



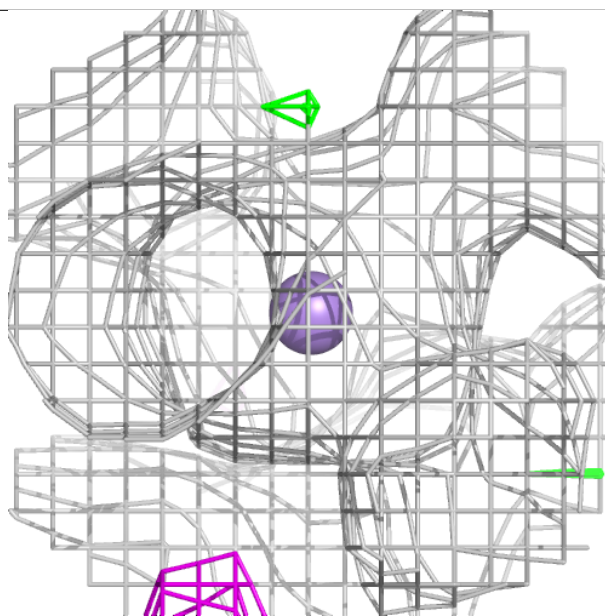
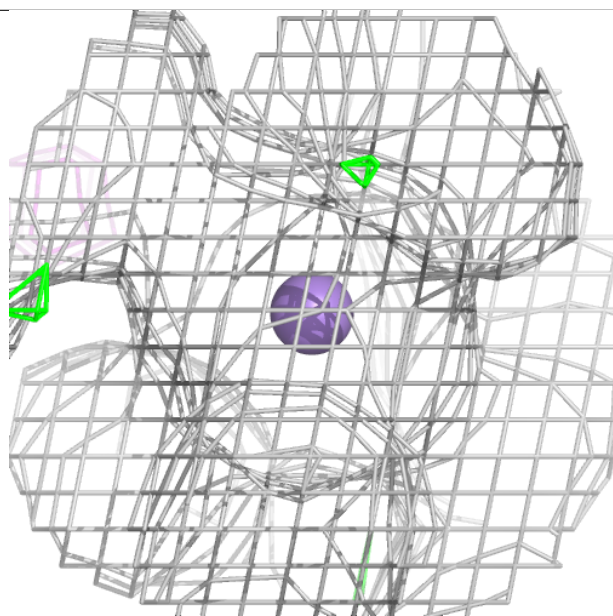
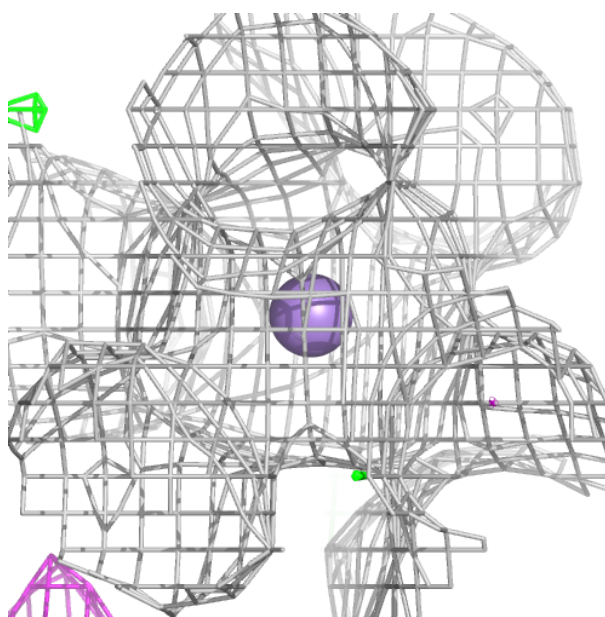
Electron density around MN H 402:

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



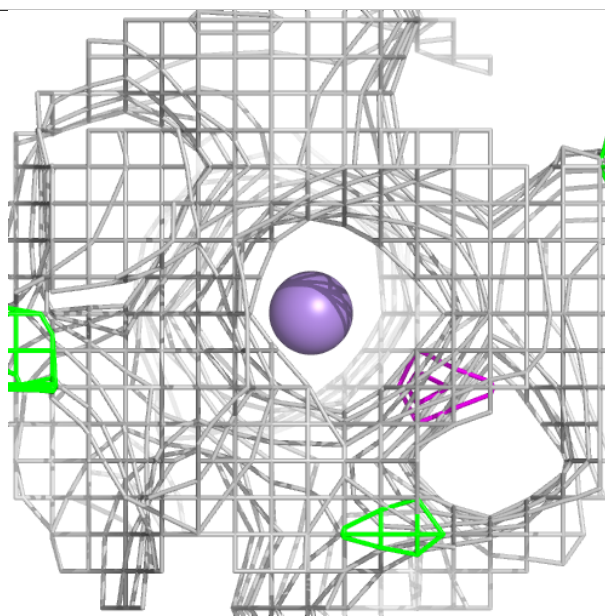
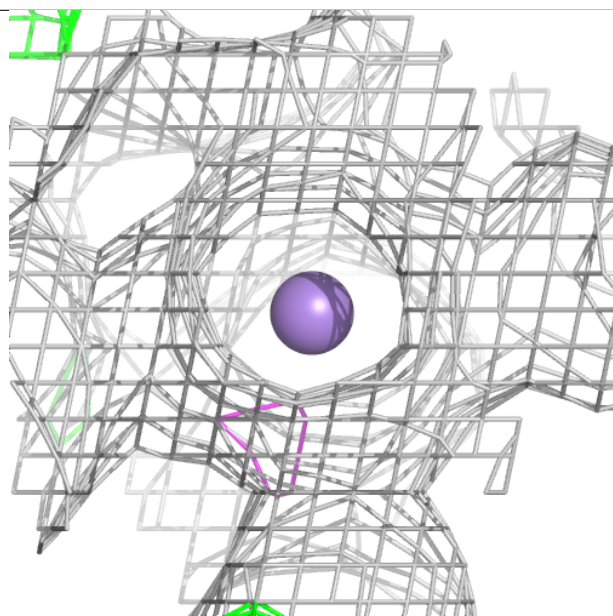
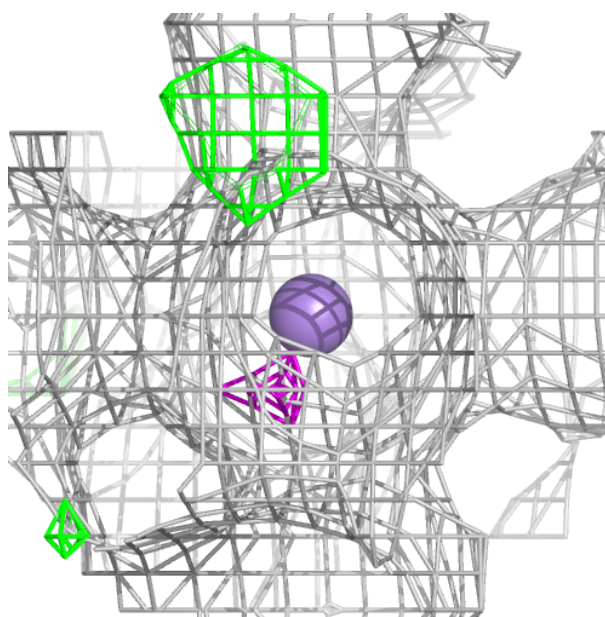
Electron density around MN B 402:

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



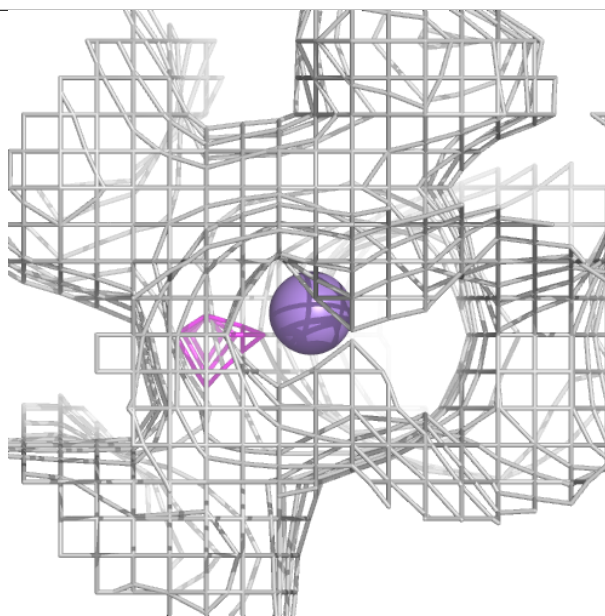
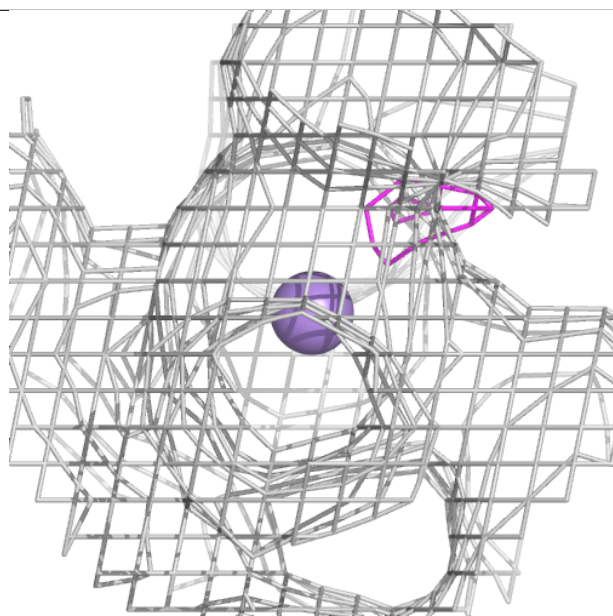
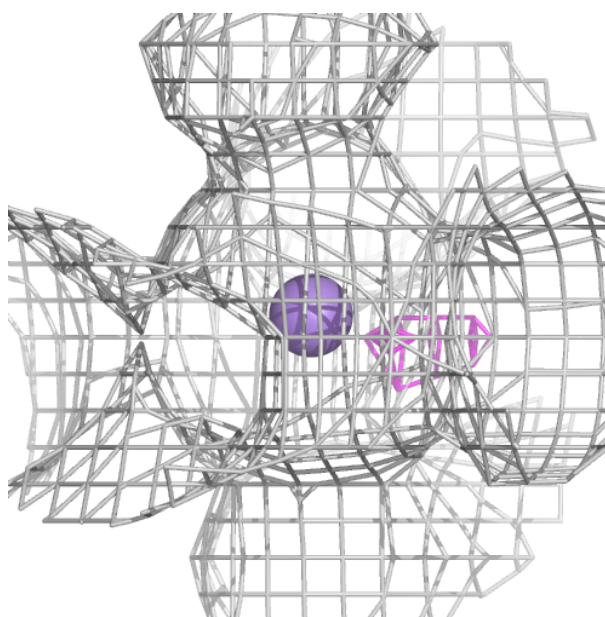
Electron density around MN H 404:

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



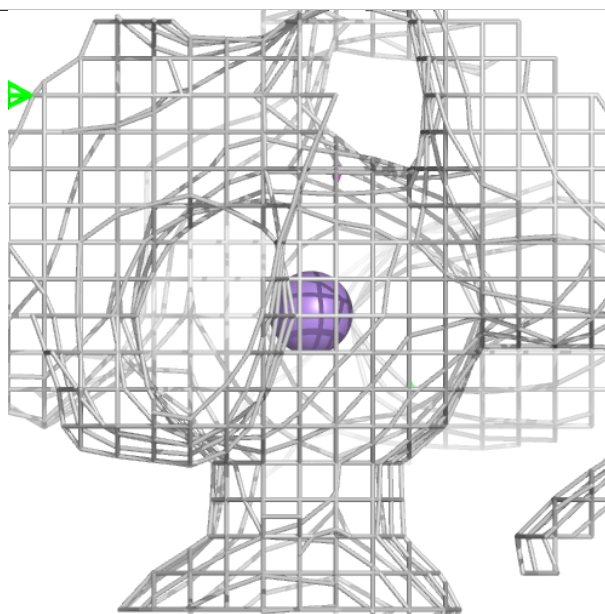
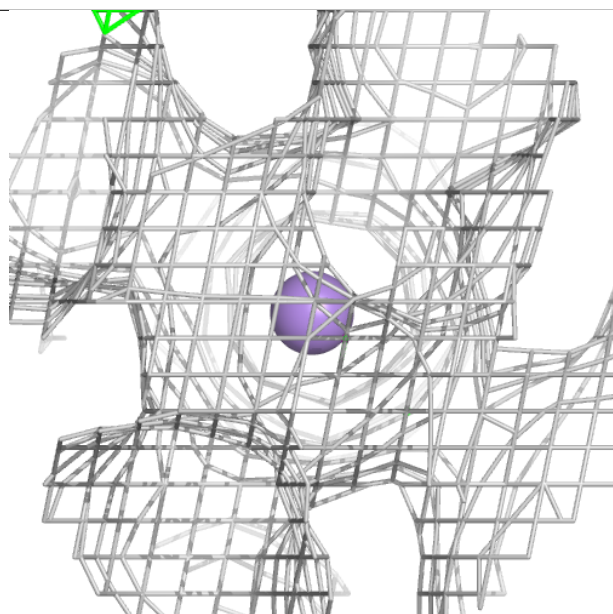
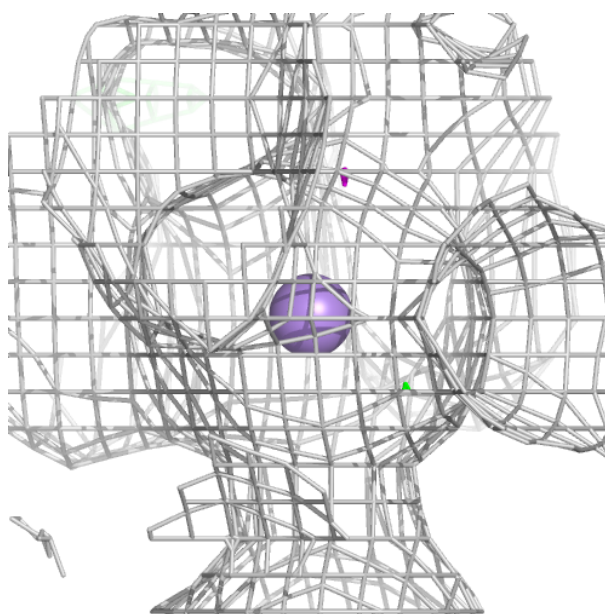
Electron density around MN I 402:

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



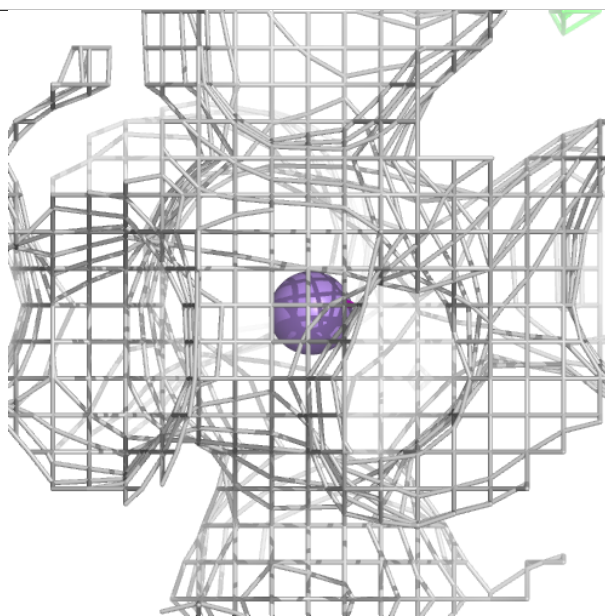
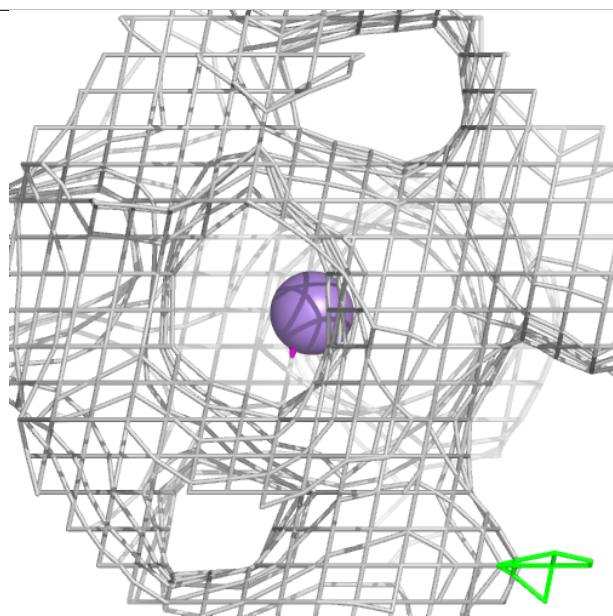
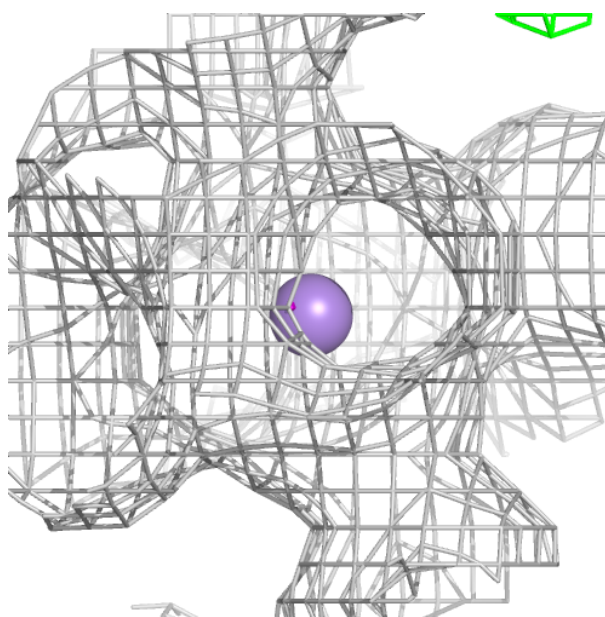
Electron density around MN B 403:

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



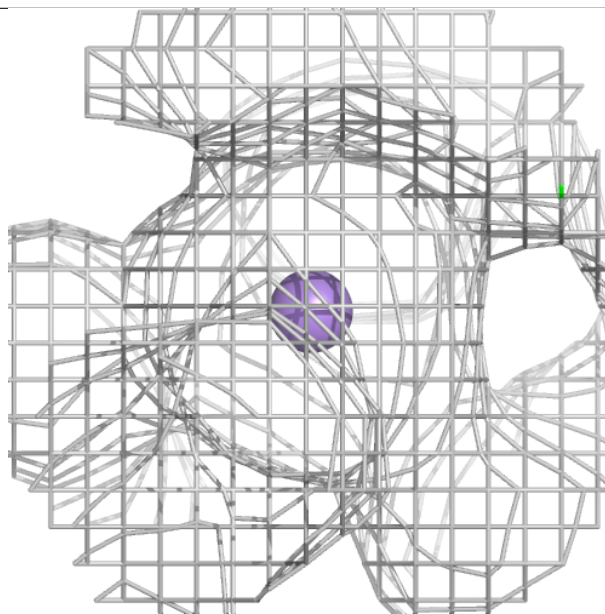
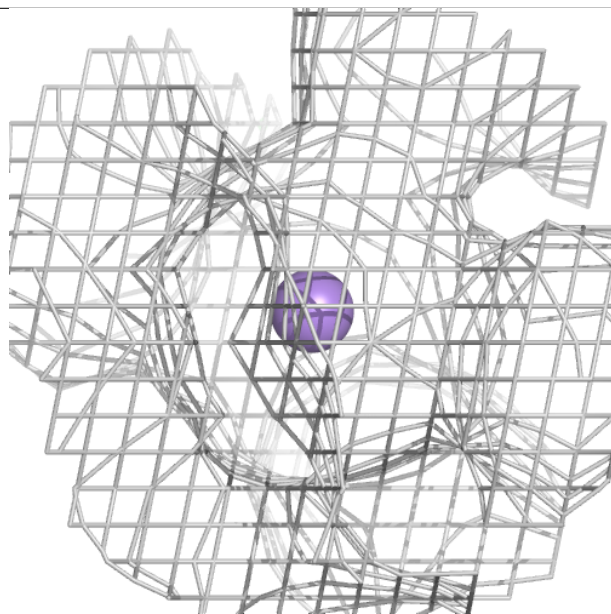
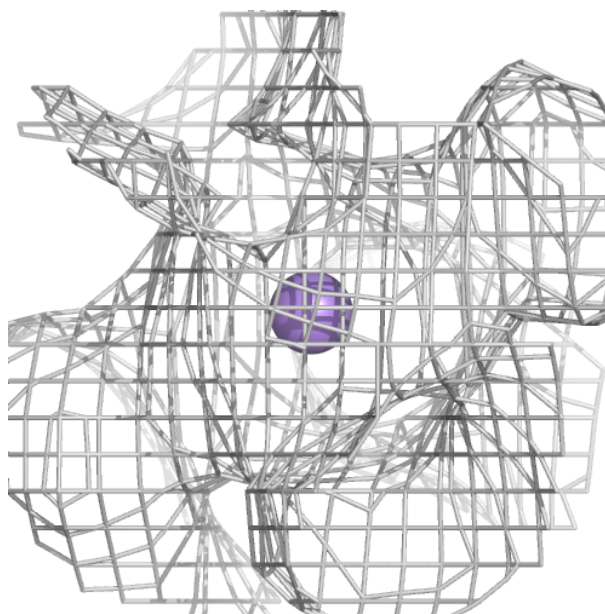
Electron density around MN I 404:

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



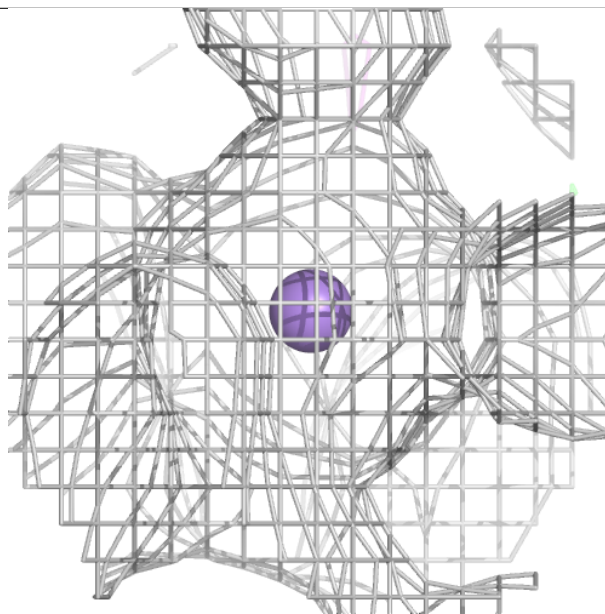
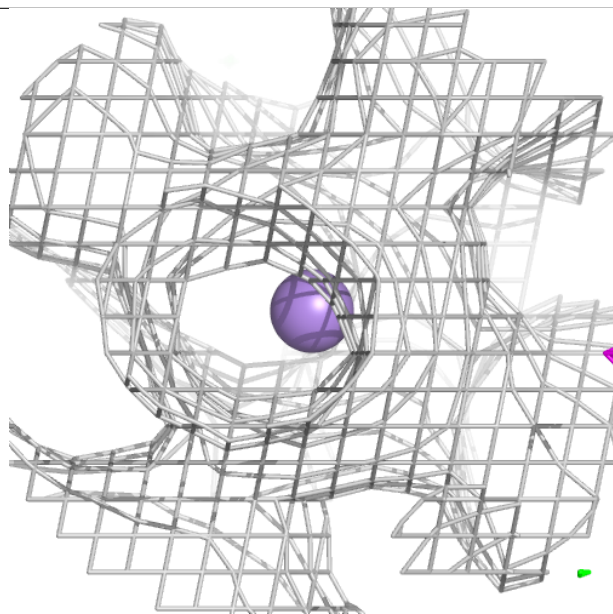
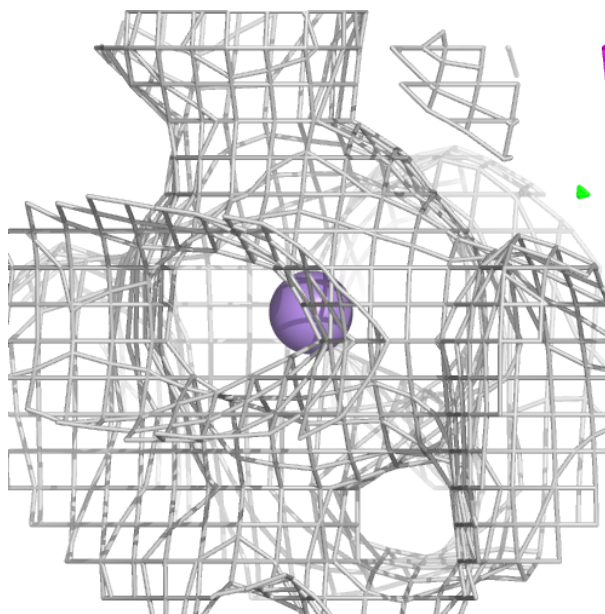
Electron density around MN J 402:

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



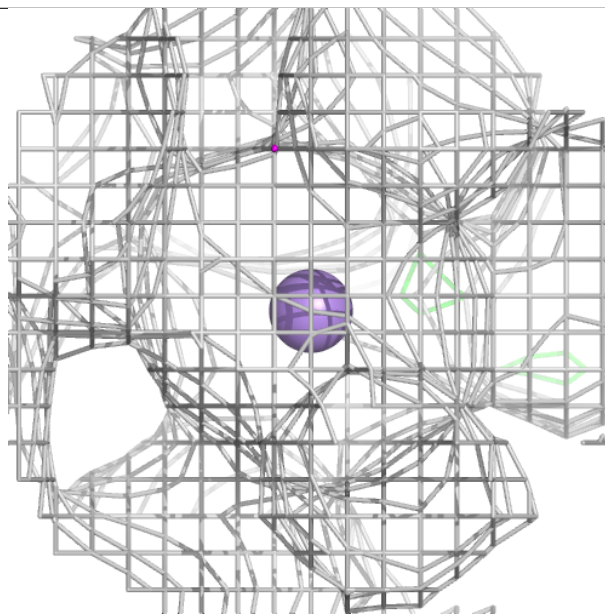
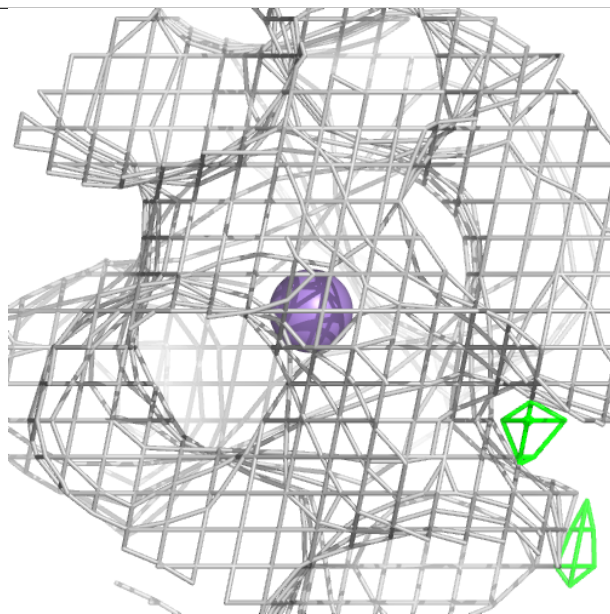
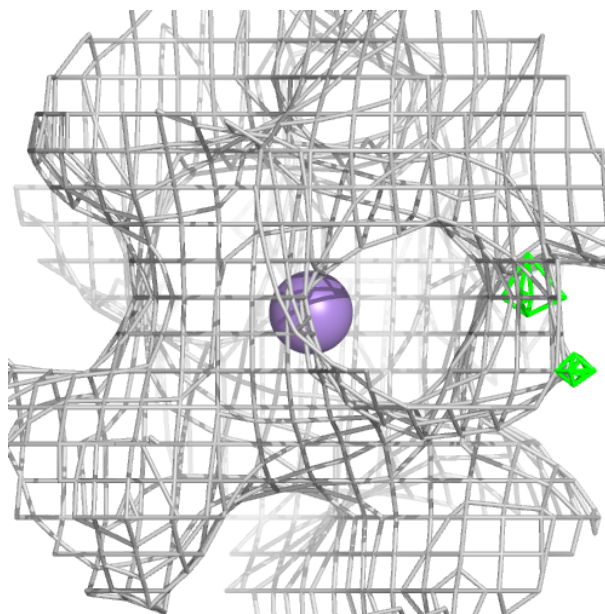
Electron density around MN J 403:

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



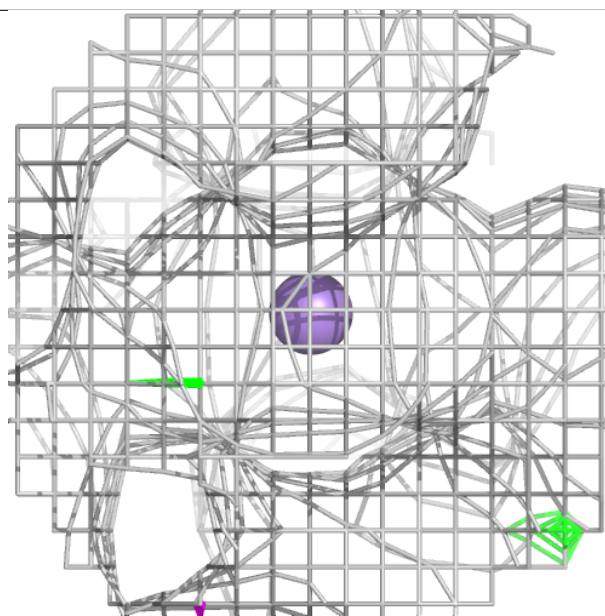
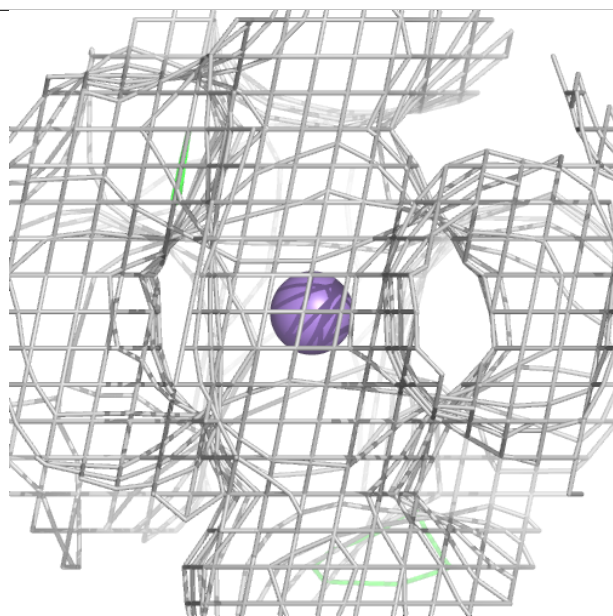
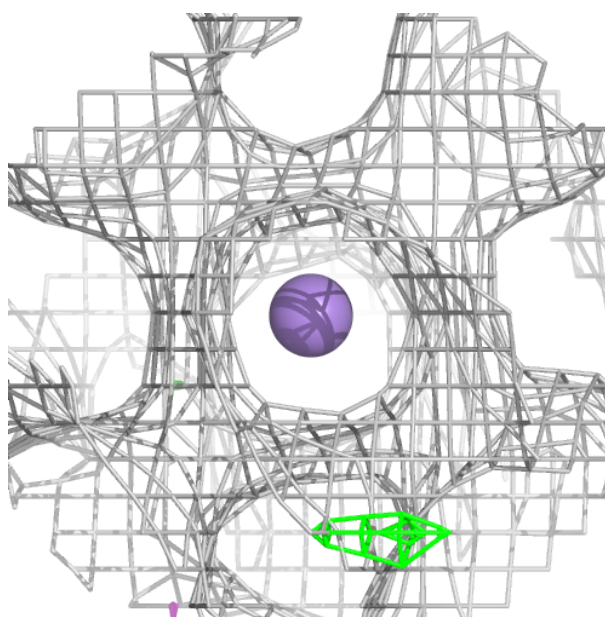
Electron density around MN J 404:

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



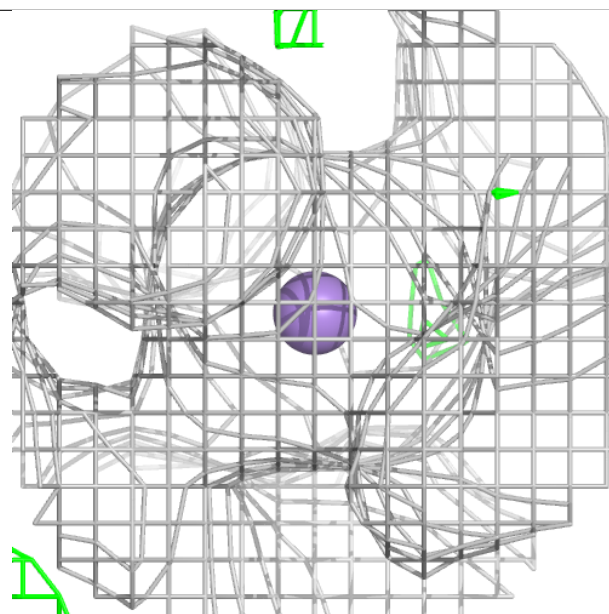
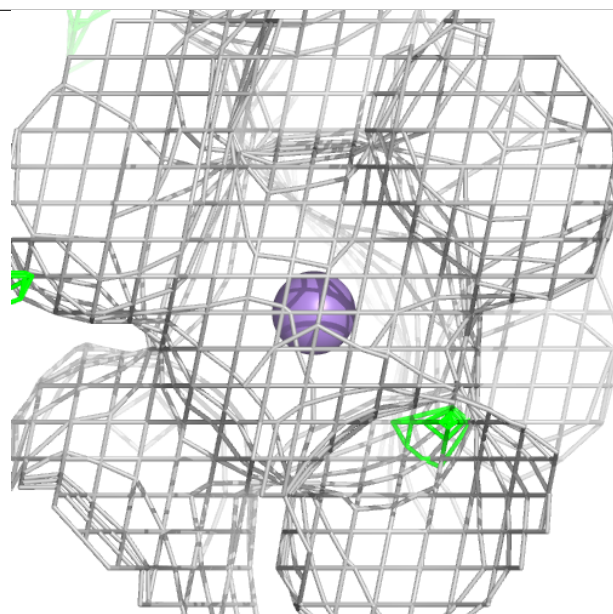
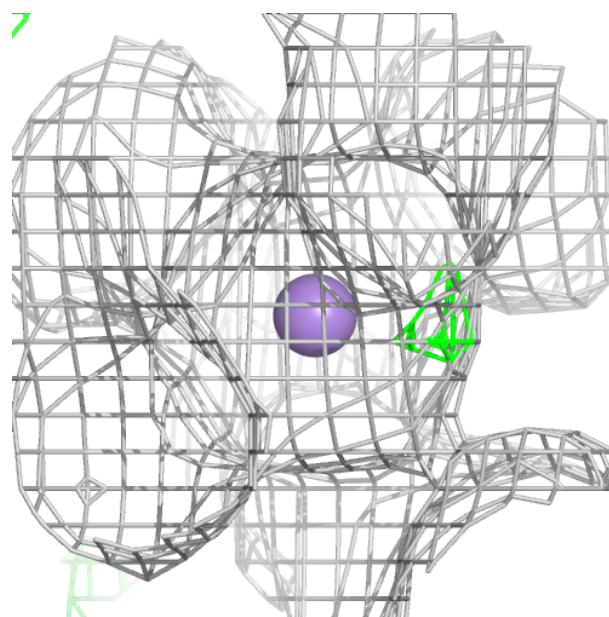
Electron density around MN B 404:

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



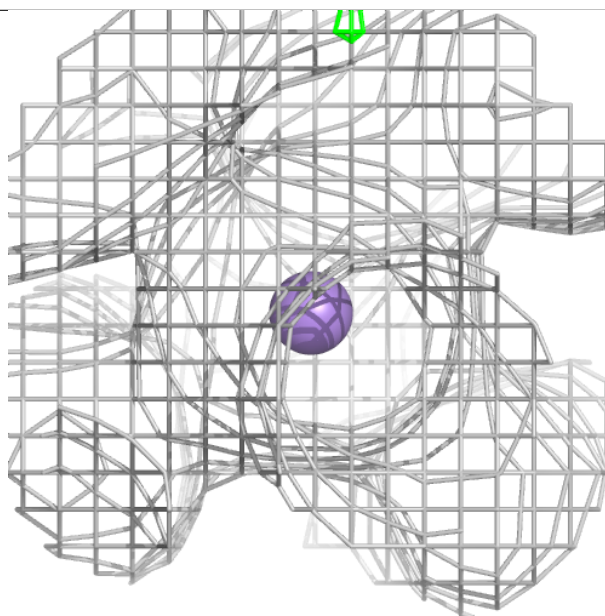
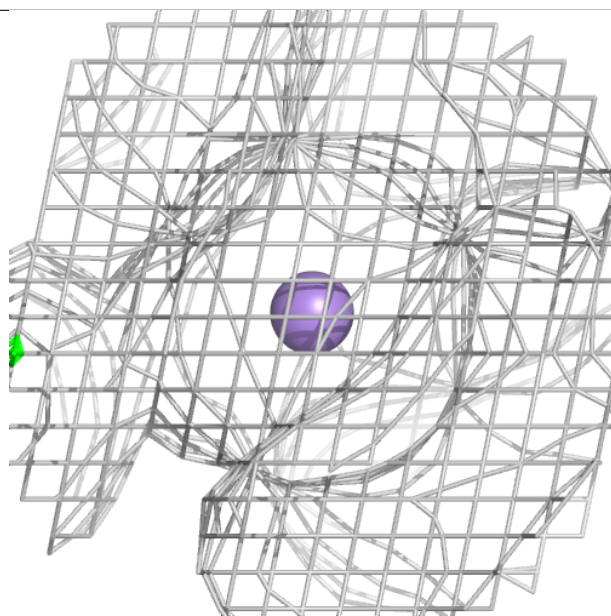
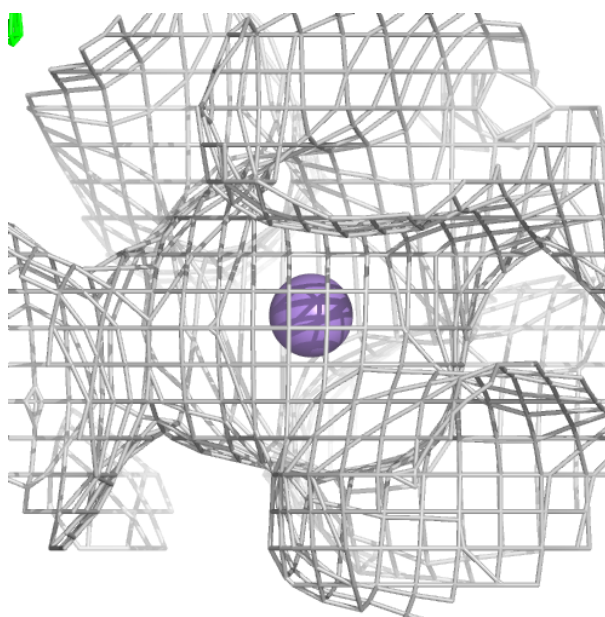
Electron density around MN C 402:

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



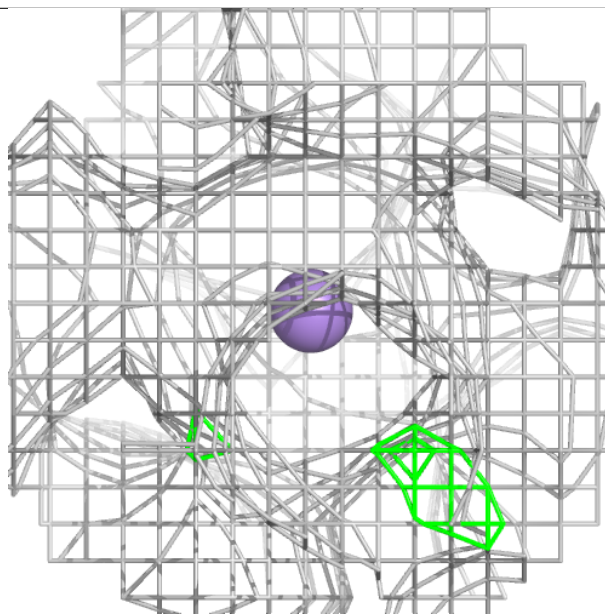
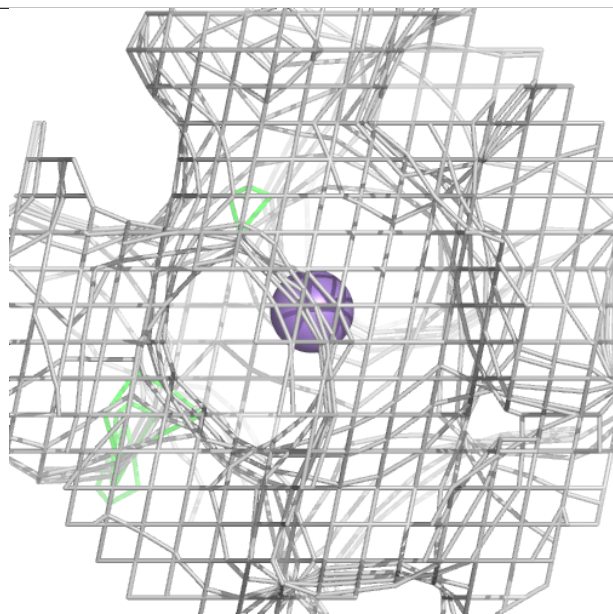
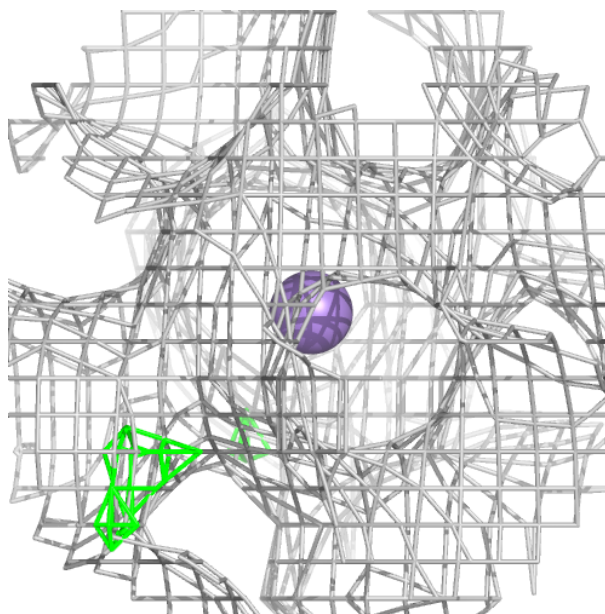
Electron density around MN C 403:

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



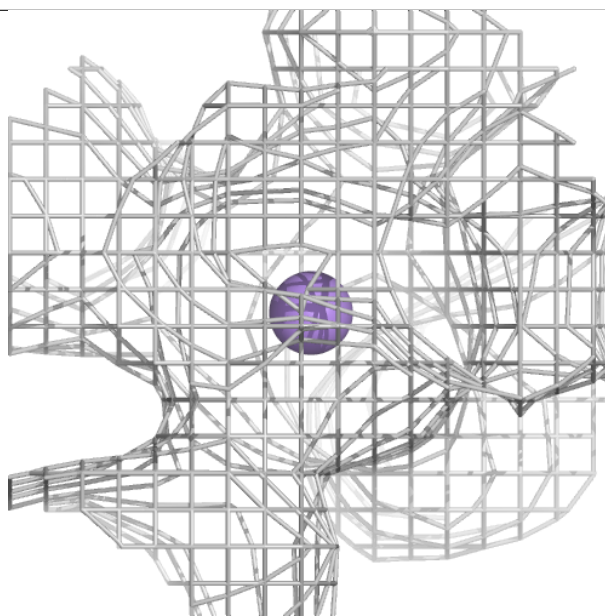
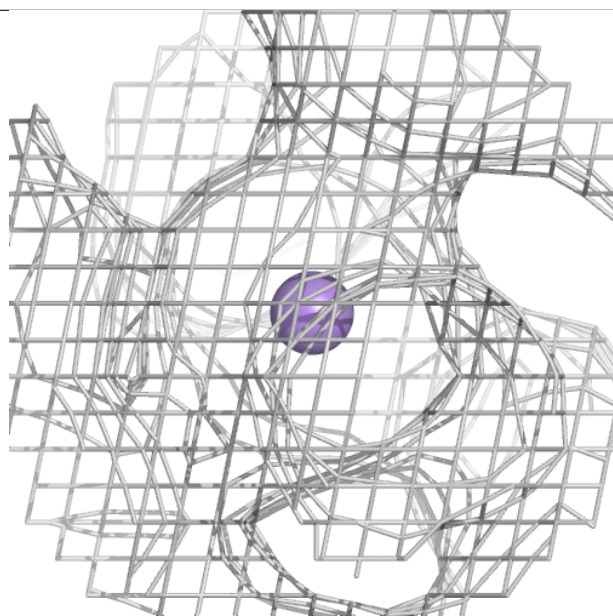
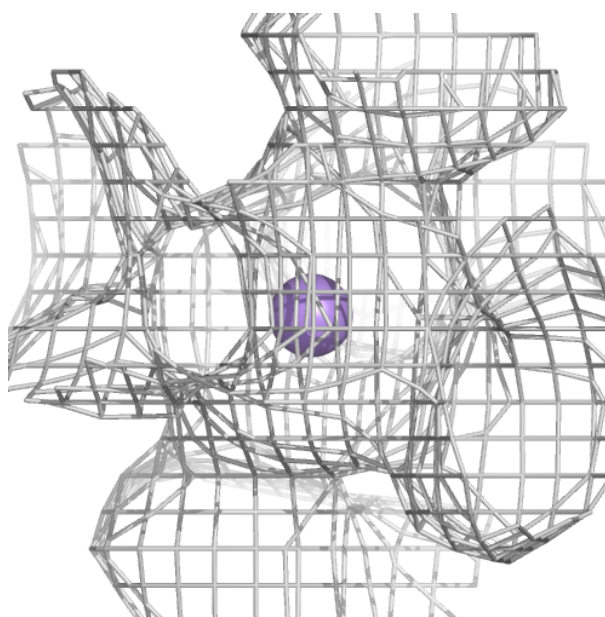
Electron density around MN C 404:

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



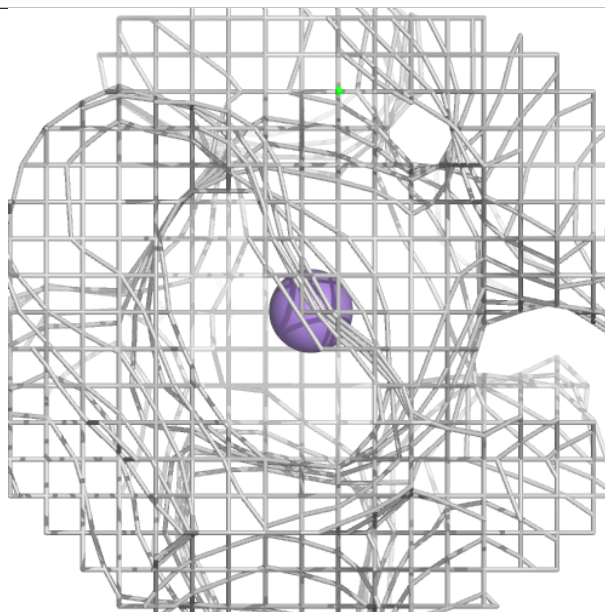
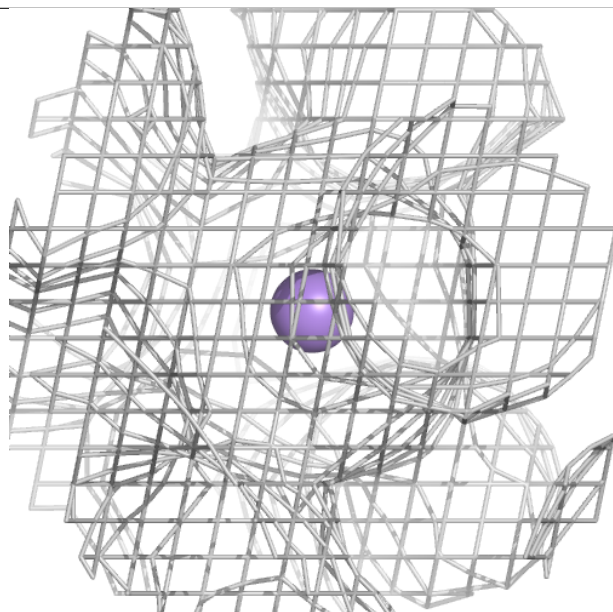
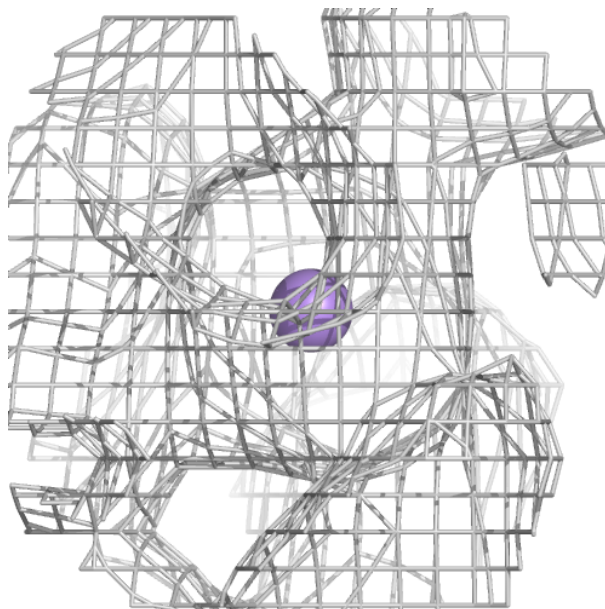
Electron density around MN D 402:

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



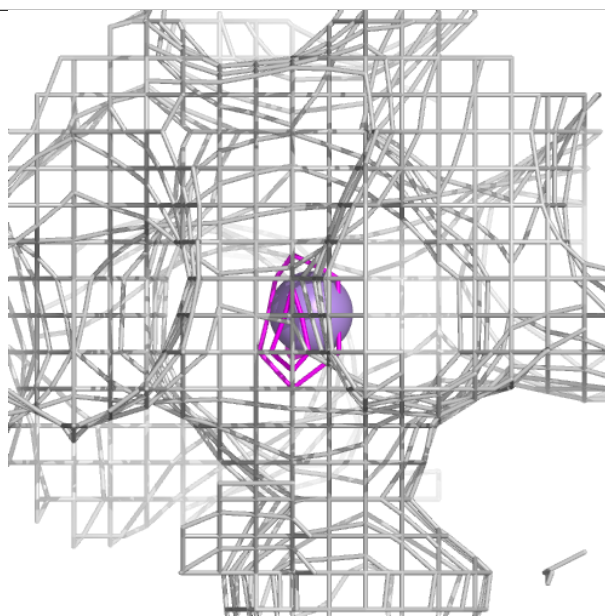
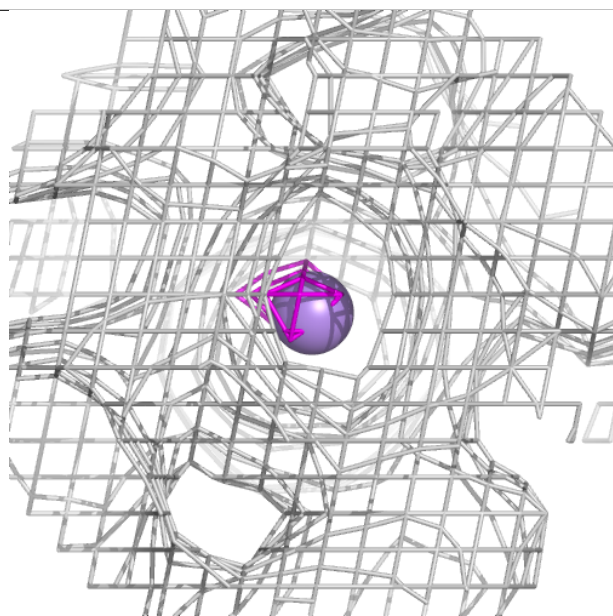
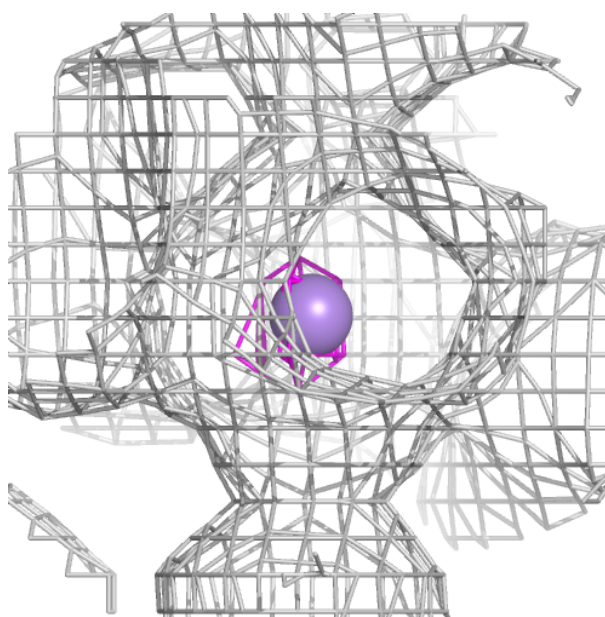
Electron density around MN D 403:

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



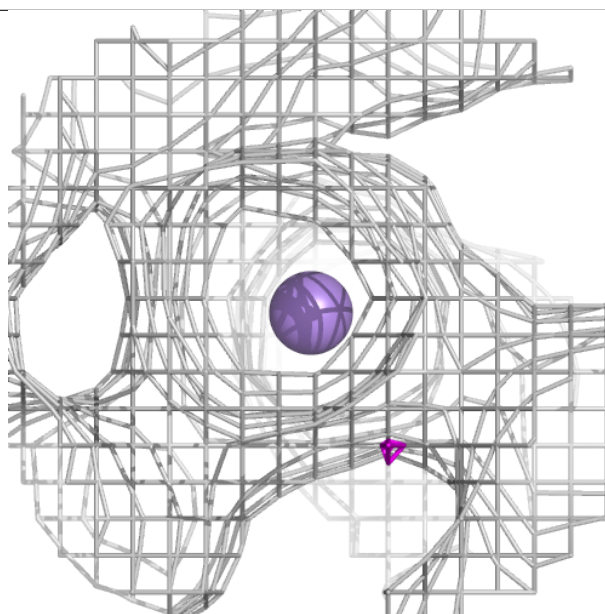
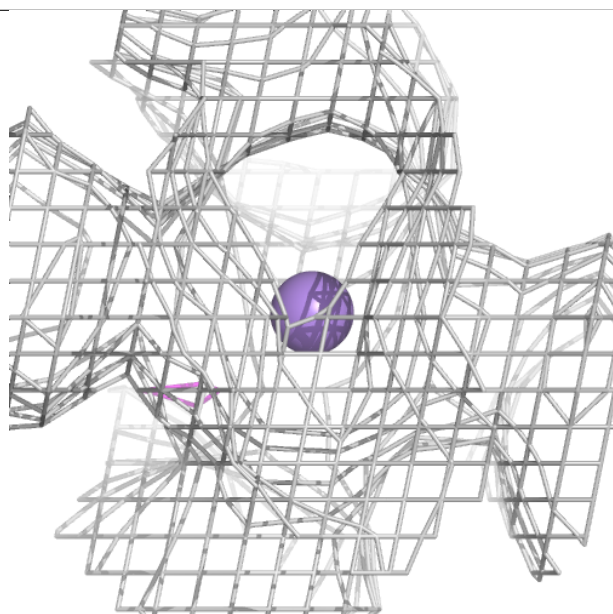
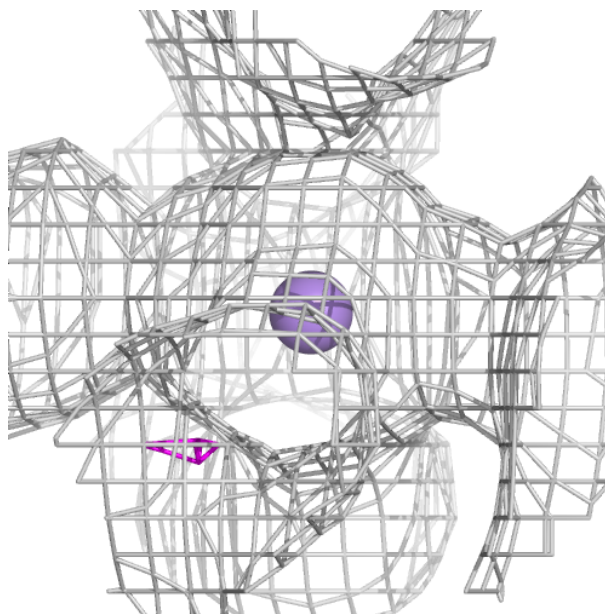
Electron density around MN D 404:

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



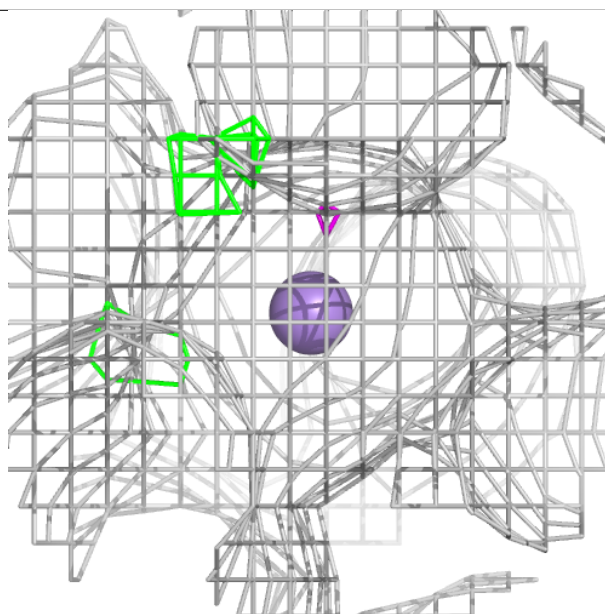
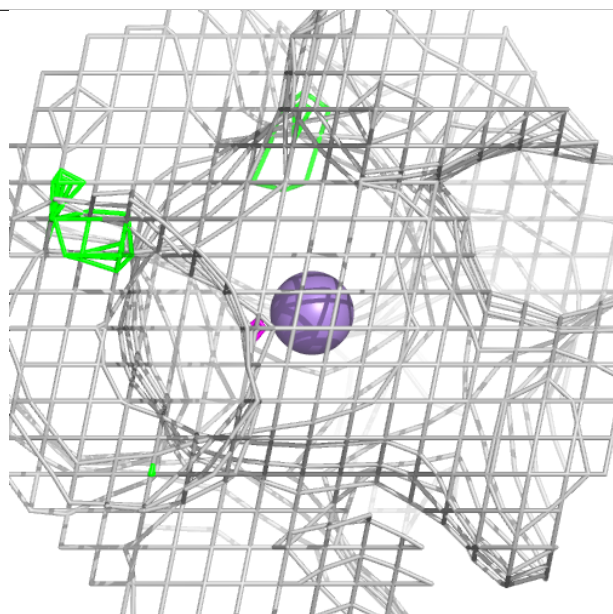
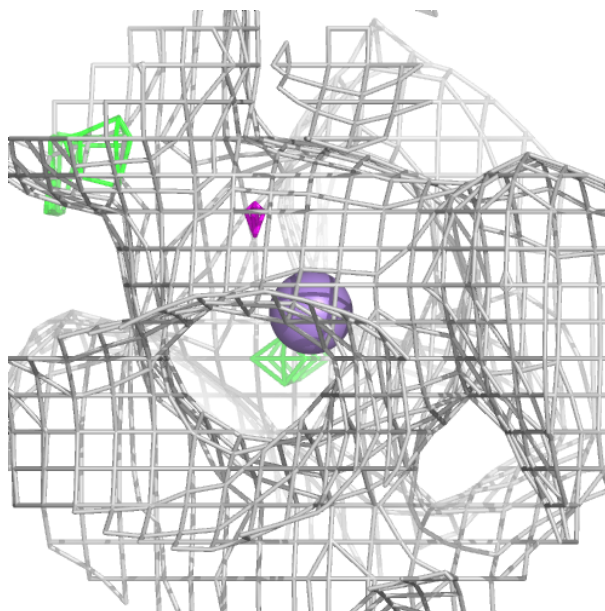
Electron density around MN E 402:

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



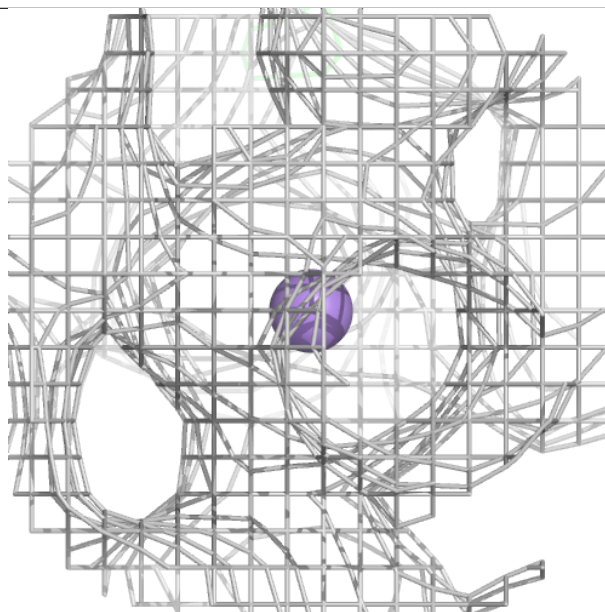
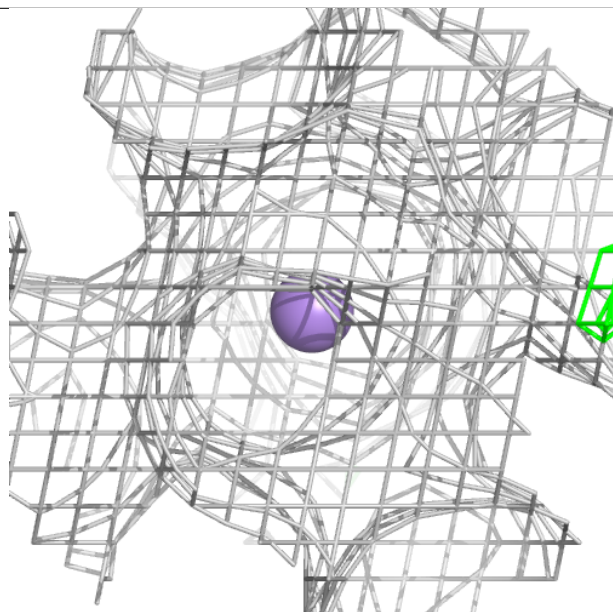
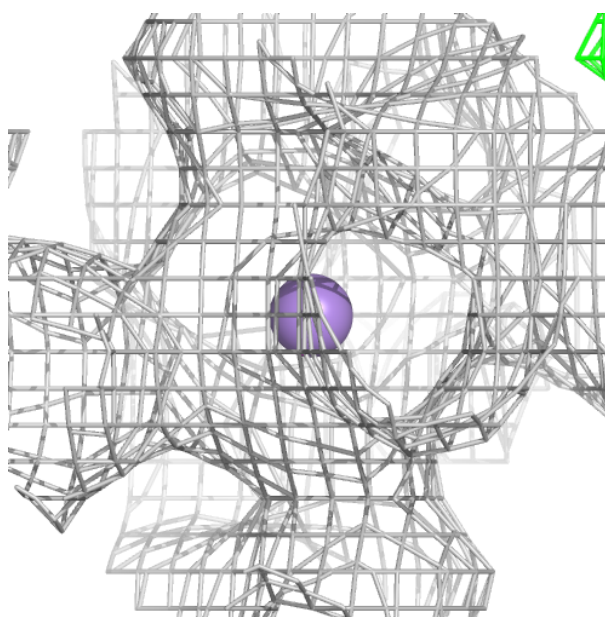
Electron density around MN E 403:

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



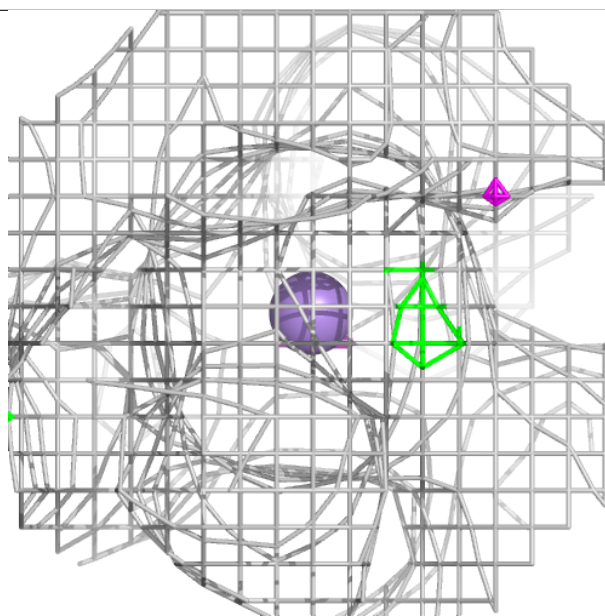
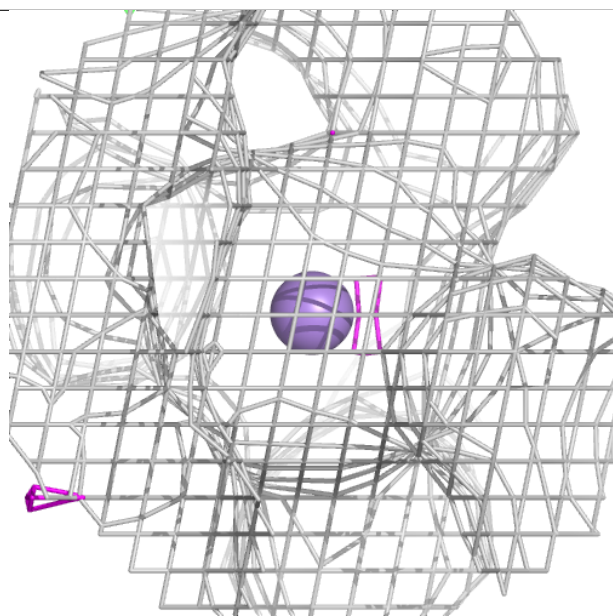
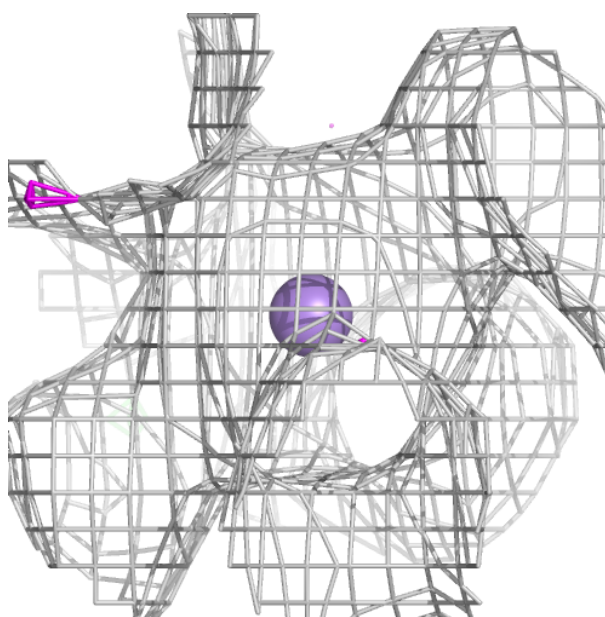
Electron density around MN E 404:

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



Electron density around MN F 402:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.