



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 06:09 PM BST

PDB ID : 6VD0
Title : Crystal structure of Arabidopsis thaliana S-adenosylmethionine Synthase 2 (AtMAT2) in complex with free Methionine and AMPCPP
Authors : Sekula, B.; Ruskowski, M.; Dauter, Z.
Deposited on : 2019-12-23
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

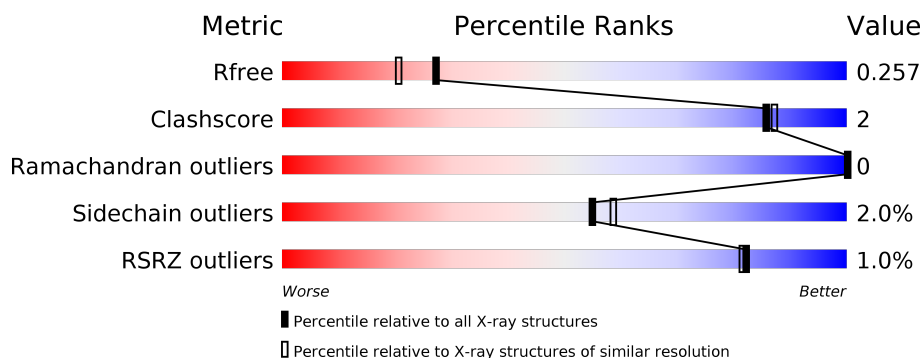
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	402	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>•</div> </div> </div>
1	B	402	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	C	402	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	402	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>•</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13558 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 S-adenosylmethionine synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	3	0
			3052	1923	528	584	17			
1	B	389	Total	C	N	O	S	0	2	0
			3022	1903	523	580	16			
1	C	389	Total	C	N	O	S	0	1	0
			3017	1900	522	579	16			
1	D	388	Total	C	N	O	S	0	2	0
			3014	1899	522	577	16			

There are 40 discrepancies between the modelled and reference sequences:

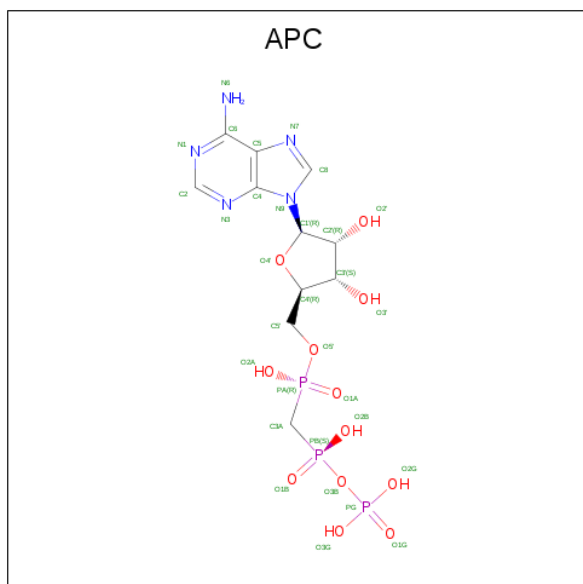
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P17562
A	-1	ASN	-	expression tag	UNP P17562
A	0	ALA	-	expression tag	UNP P17562
A	393	LEU	-	expression tag	UNP P17562
A	394	ASN	-	expression tag	UNP P17562
A	395	ASN	-	expression tag	UNP P17562
A	396	ILE	-	expression tag	UNP P17562
A	397	GLY	-	expression tag	UNP P17562
A	398	SER	-	expression tag	UNP P17562
A	399	GLY	-	expression tag	UNP P17562
B	-2	SER	-	expression tag	UNP P17562
B	-1	ASN	-	expression tag	UNP P17562
B	0	ALA	-	expression tag	UNP P17562
B	393	LEU	-	expression tag	UNP P17562
B	394	ASN	-	expression tag	UNP P17562
B	395	ASN	-	expression tag	UNP P17562
B	396	ILE	-	expression tag	UNP P17562
B	397	GLY	-	expression tag	UNP P17562
B	398	SER	-	expression tag	UNP P17562
B	399	GLY	-	expression tag	UNP P17562
C	-2	SER	-	expression tag	UNP P17562

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ASN	-	expression tag	UNP P17562
C	0	ALA	-	expression tag	UNP P17562
C	393	LEU	-	expression tag	UNP P17562
C	394	ASN	-	expression tag	UNP P17562
C	395	ASN	-	expression tag	UNP P17562
C	396	ILE	-	expression tag	UNP P17562
C	397	GLY	-	expression tag	UNP P17562
C	398	SER	-	expression tag	UNP P17562
C	399	GLY	-	expression tag	UNP P17562
D	-2	SER	-	expression tag	UNP P17562
D	-1	ASN	-	expression tag	UNP P17562
D	0	ALA	-	expression tag	UNP P17562
D	393	LEU	-	expression tag	UNP P17562
D	394	ASN	-	expression tag	UNP P17562
D	395	ASN	-	expression tag	UNP P17562
D	396	ILE	-	expression tag	UNP P17562
D	397	GLY	-	expression tag	UNP P17562
D	398	SER	-	expression tag	UNP P17562
D	399	GLY	-	expression tag	UNP P17562

- Molecule 2 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by author).



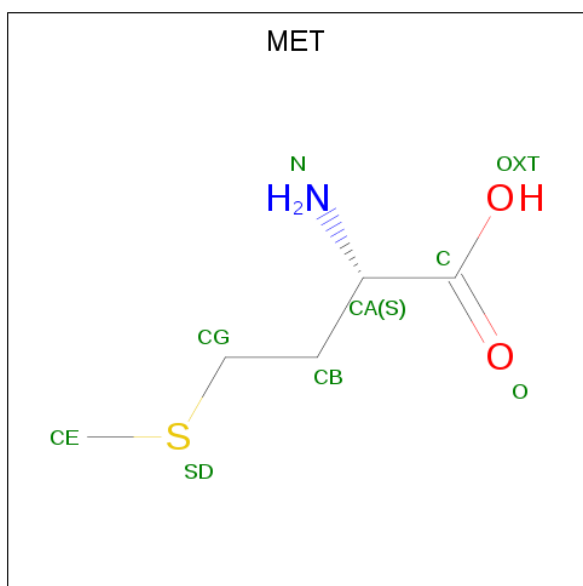
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

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

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

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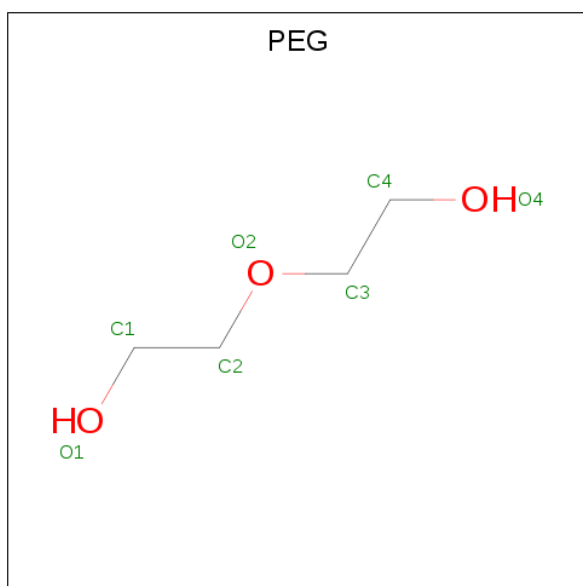
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	Mg 3	0	0
4	D	1	Total 1	Mg 1	0	0
4	C	3	Total 3	Mg 3	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by author).

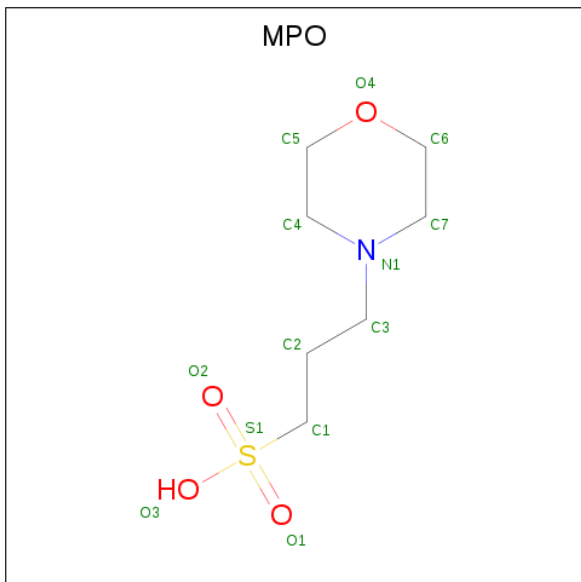
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	K 1	0	0
5	A	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



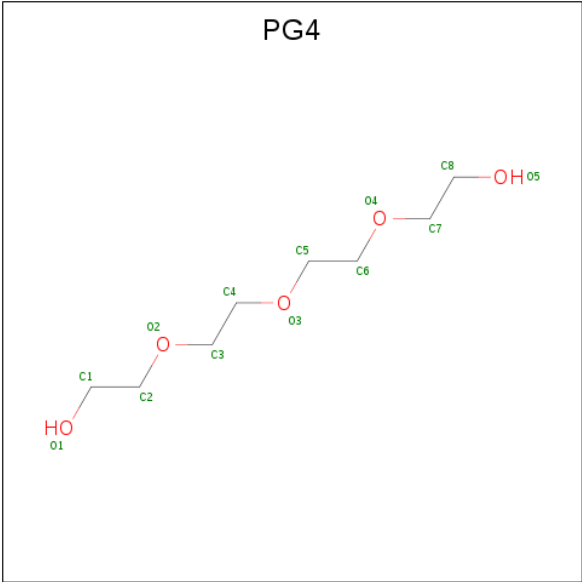
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 7	C 4	O 3	0	0
6	B	1	Total 7	C 4	O 3	0	0

- Molecule 7 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
7	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
7	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
7	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			13	8	5		

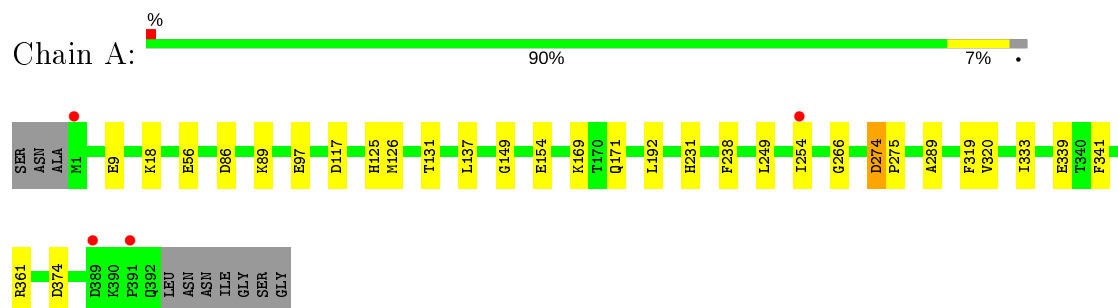
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	324	Total	O	0	0
			324	324		
9	B	298	Total	O	0	1
			299	299		
9	C	285	Total	O	0	0
			285	285		
9	D	293	Total	O	0	0
			293	293		

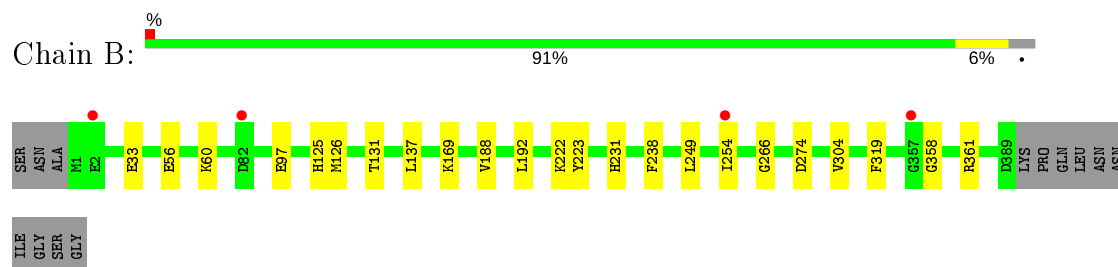
3 Residue-property plots [i](#)

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.

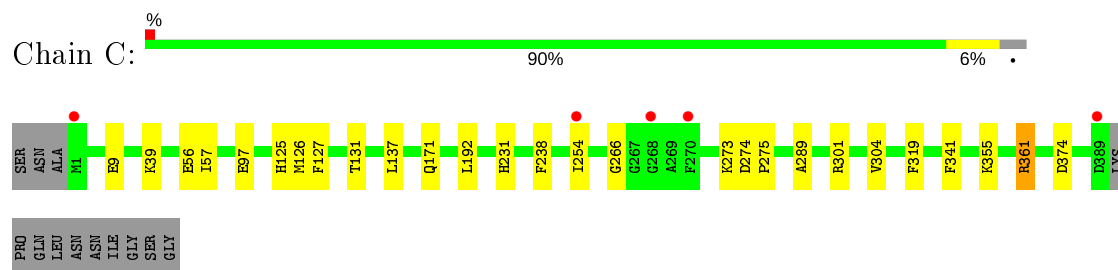
• Molecule 1: S-adenosylmethionine synthase 2



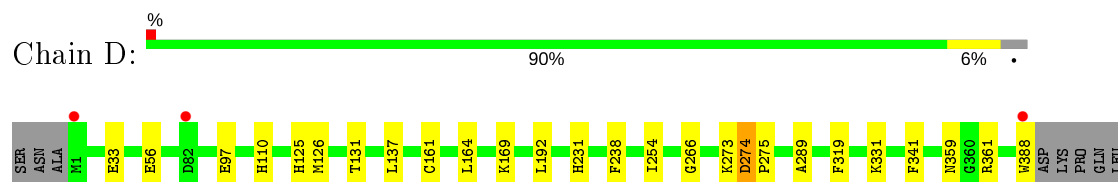
• Molecule 1: S-adenosylmethionine synthase 2



• Molecule 1: S-adenosylmethionine synthase 2



• Molecule 1: S-adenosylmethionine synthase 2



ASN
ASN
ILE
GLY
SER
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.94Å 84.72Å 119.50Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	39.83 – 2.00 39.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.6 (39.83-2.00) 98.6 (39.79-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.222 , 0.251 0.229 , 0.257	Depositor DCC
R_{free} test set	2672 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13558	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.26 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4044e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MPO, K, PG4, APC, PEG

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	0.88	0/3126	0.92	0/4234
1	B	0.85	0/3092	0.90	0/4189
1	C	0.80	0/3084	0.89	0/4178
1	D	0.83	0/3084	0.89	0/4178
All	All	0.84	0/12386	0.90	0/16779

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3052	0	3019	19	0
1	B	3022	0	2982	11	0
1	C	3017	0	2976	14	0
1	D	3014	0	2978	12	0
2	A	31	0	14	1	0
2	B	31	0	14	1	0
2	C	31	0	14	1	0
2	D	31	0	14	2	0
3	A	9	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	8	0	0
3	C	9	0	8	0	0
3	D	9	0	8	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	7	0	10	0	0
6	B	7	0	10	0	0
7	A	13	0	15	0	0
7	B	13	0	14	0	0
7	C	13	0	14	0	0
7	D	13	0	14	0	0
8	C	13	0	18	0	0
9	A	324	0	0	6	0
9	B	299	0	0	1	0
9	C	285	0	0	2	0
9	D	293	0	0	2	0
All	All	13558	0	12138	53	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 2.

All (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:HIS:ND1	9:D:505:HOH:O	2.28	0.67
1:C:131:THR:O	1:C:137:LEU:HA	1.98	0.64
1:B:131:THR:O	1:B:137:LEU:HA	1.99	0.63
1:D:131:THR:O	1:D:137:LEU:HA	1.99	0.62
1:A:131:THR:O	1:A:137:LEU:HA	2.02	0.59
1:A:339:GLU:HB3	9:A:743:HOH:O	2.04	0.56
2:C:402:APC:O2B	1:D:273:LYS:HE2	2.09	0.53
1:C:273:LYS:HE2	2:D:401:APC:O2B	2.11	0.50
1:A:169:LYS:HD2	2:A:401:APC:H4'	1.93	0.50
1:D:125:HIS:O	1:D:266:GLY:HA3	2.12	0.50
1:C:355:LYS:HB2	9:C:527:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HD11	1:B:254:ILE:HD11	1.94	0.48
1:B:169:LYS:HD2	2:B:401:APC:H4'	1.96	0.48
1:B:56:GLU:HA	1:B:97:GLU:O	2.15	0.47
1:B:125:HIS:O	1:B:266:GLY:HA3	2.15	0.47
1:A:125:HIS:O	1:A:266:GLY:HA3	2.15	0.46
1:A:249:LEU:HD23	1:B:249:LEU:HD23	1.96	0.46
1:C:125:HIS:O	1:C:266:GLY:HA3	2.14	0.46
1:D:161:CYS:HB2	1:D:164:LEU:HD12	1.97	0.46
1:D:56:GLU:HA	1:D:97:GLU:O	2.17	0.45
1:C:56:GLU:HA	1:C:97:GLU:O	2.15	0.45
1:D:192:LEU:HA	1:D:231:HIS:O	2.17	0.45
1:C:274:ASP:HB2	1:C:275:PRO:HD2	1.97	0.45
1:C:192:LEU:HA	1:C:231:HIS:O	2.17	0.45
1:A:192:LEU:HA	1:A:231:HIS:O	2.16	0.45
1:D:169:LYS:HD2	2:D:401:APC:H4'	1.99	0.45
1:A:56:GLU:HA	1:A:97:GLU:O	2.17	0.44
1:D:274:ASP:HB2	1:D:275:PRO:HD2	1.98	0.44
1:C:289:ALA:HA	1:C:341:PHE:CZ	2.53	0.43
1:A:154:GLU:OE1	9:A:501:HOH:O	2.21	0.43
1:C:301:ARG:HG3	9:C:659:HOH:O	2.19	0.43
1:A:89:LYS:HE2	9:A:512:HOH:O	2.18	0.43
1:A:149:GLY:HA3	9:A:670:HOH:O	2.18	0.42
1:A:320:VAL:HG11	1:A:333:ILE:CG2	2.49	0.42
1:A:9:GLU:HA	1:A:171:GLN:HA	2.01	0.42
1:D:289:ALA:HA	1:D:341:PHE:CZ	2.55	0.42
1:A:117:ASP:OD1	9:A:502:HOH:O	2.22	0.42
1:A:320:VAL:HG11	1:A:333:ILE:HG22	2.00	0.42
1:B:188:VAL:HG23	1:B:223:TYR:HB3	2.01	0.42
1:D:359:ASN:HB2	9:D:673:HOH:O	2.20	0.42
1:B:192:LEU:HA	1:B:231:HIS:O	2.20	0.42
1:C:9:GLU:HA	1:C:171:GLN:HA	2.02	0.41
1:A:154:GLU:CD	9:A:501:HOH:O	2.58	0.41
1:B:60:LYS:CE	9:B:528:HOH:O	2.69	0.41
1:C:254:ILE:HD11	1:D:254:ILE:HD11	2.02	0.41
1:A:86:ASP:HB3	1:A:89:LYS:HB2	2.03	0.41
1:C:127:PHE:HA	1:C:304:VAL:O	2.20	0.41
1:B:33:GLU:OE2	1:B:358:GLY:HA2	2.21	0.41
1:C:361:ARG:HD3	1:C:361:ARG:C	2.40	0.41
1:A:274:ASP:HB2	1:A:275:PRO:HD2	2.02	0.40
1:A:289:ALA:HA	1:A:341:PHE:CZ	2.56	0.40
1:C:39:LYS:O	1:C:57:ILE:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	393/402 (98%)	382 (97%)	11 (3%)	0	100	100
1	B	389/402 (97%)	379 (97%)	10 (3%)	0	100	100
1	C	388/402 (96%)	378 (97%)	10 (3%)	0	100	100
1	D	388/402 (96%)	378 (97%)	10 (3%)	0	100	100
All	All	1558/1608 (97%)	1517 (97%)	41 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/337 (99%)	325 (98%)	8 (2%)	49	51
1	B	329/337 (98%)	322 (98%)	7 (2%)	53	57
1	C	328/337 (97%)	322 (98%)	6 (2%)	59	63
1	D	328/337 (97%)	319 (97%)	9 (3%)	44	46
All	All	1318/1348 (98%)	1288 (98%)	30 (2%)	55	53

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	126	MET
1	A	238	PHE
1	A	274	ASP
1	A	319[A]	PHE
1	A	319[B]	PHE
1	A	361	ARG
1	A	374	ASP
1	B	126	MET
1	B	222	LYS
1	B	238	PHE
1	B	274	ASP
1	B	319[A]	PHE
1	B	319[B]	PHE
1	B	361	ARG
1	C	126	MET
1	C	238	PHE
1	C	319[A]	PHE
1	C	319[B]	PHE
1	C	361	ARG
1	C	374	ASP
1	D	33	GLU
1	D	126	MET
1	D	238	PHE
1	D	274	ASP
1	D	319[A]	PHE
1	D	319[B]	PHE
1	D	331	LYS
1	D	361	ARG
1	D	388	TRP

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 13 are monoatomic - leaving 15 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	PEG	B	406	-	6,6,6	0.32	0	5,5,5	0.17	0
3	MET	B	402	-	4,8,8	0.70	0	2,9,9	0.18	0
2	APC	D	401	5,4	27,33,33	1.06	3 (11%)	31,52,52	1.26	3 (9%)
3	MET	D	402	-	4,8,8	0.63	0	2,9,9	0.60	0
2	APC	B	401	5,4	27,33,33	0.99	3 (11%)	31,52,52	1.41	7 (22%)
7	MPO	C	408	-	13,13,13	1.16	1 (7%)	17,17,17	1.15	1 (5%)
7	MPO	D	405	-	13,13,13	1.07	1 (7%)	17,17,17	1.67	4 (23%)
7	MPO	A	408	-	13,13,13	0.79	1 (7%)	17,17,17	0.83	0
2	APC	A	401	5,4	27,33,33	1.23	5 (18%)	31,52,52	1.03	2 (6%)
6	PEG	A	407	-	6,6,6	0.24	0	5,5,5	0.17	0
8	PG4	C	401	-	12,12,12	0.21	0	11,11,11	0.17	0
2	APC	C	402	5,4	27,33,33	0.91	2 (7%)	31,52,52	1.21	6 (19%)
7	MPO	B	407	-	13,13,13	1.10	1 (7%)	17,17,17	1.43	2 (11%)
3	MET	C	403	-	4,8,8	0.58	0	2,9,9	0.77	0
3	MET	A	402	-	4,8,8	0.58	0	2,9,9	0.09	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	PEG	B	406	-	-	2/4/4/4	-
3	MET	B	402	-	-	0/4/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APC	D	401	5,4	-	8/15/38/38	0/3/3/3
3	MET	D	402	-	-	0/4/8/8	-
2	APC	B	401	5,4	-	6/15/38/38	0/3/3/3
7	MPO	C	408	-	-	1/7/15/15	0/1/1/1
7	MPO	D	405	-	-	3/7/15/15	0/1/1/1
7	MPO	A	408	-	-	1/7/15/15	0/1/1/1
2	APC	A	401	5,4	-	7/15/38/38	0/3/3/3
6	PEG	A	407	-	-	2/4/4/4	-
8	PG4	C	401	-	-	5/10/10/10	-
2	APC	C	402	5,4	-	7/15/38/38	0/3/3/3
7	MPO	B	407	-	-	1/7/15/15	0/1/1/1
3	MET	C	403	-	-	0/4/8/8	-
3	MET	A	402	-	-	0/4/8/8	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	408	MPO	O2-S1	3.91	1.56	1.45
7	D	405	MPO	O2-S1	3.58	1.55	1.45
7	B	407	MPO	O2-S1	3.19	1.54	1.45
2	A	401	APC	PA-O2A	-2.82	1.49	1.56
2	D	401	APC	PA-O2A	-2.82	1.49	1.56
2	A	401	APC	PB-O2B	-2.79	1.49	1.56
2	A	401	APC	PA-O5'	2.74	1.61	1.57
2	C	402	APC	PA-O2A	-2.41	1.50	1.56
2	D	401	APC	PB-O2B	-2.40	1.50	1.56
2	B	401	APC	PA-O2A	-2.30	1.51	1.56
7	A	408	MPO	O3-S1	2.21	1.55	1.47
2	A	401	APC	C8-N7	-2.15	1.30	1.34
2	B	401	APC	PA-O5'	2.15	1.60	1.57
2	C	402	APC	PA-O5'	2.15	1.60	1.57
2	D	401	APC	C8-N7	-2.13	1.30	1.34
2	A	401	APC	C2-N3	2.09	1.35	1.32
2	B	401	APC	C8-N7	-2.03	1.31	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	407	MPO	O3-S1-O1	4.25	121.67	111.27
7	D	405	MPO	O2-S1-C1	-3.69	102.47	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	405	MPO	O3-S1-O1	3.53	119.90	111.27
2	D	401	APC	C2'-C3'-C4'	-3.41	96.01	102.64
7	C	408	MPO	O3-S1-O1	3.24	119.19	111.27
2	C	402	APC	C2'-C3'-C4'	-3.00	96.82	102.64
2	B	401	APC	C2'-C3'-C4'	-2.93	96.94	102.64
2	D	401	APC	O3'-C3'-C4'	2.70	118.86	111.05
2	A	401	APC	C2'-C3'-C4'	-2.65	97.48	102.64
2	A	401	APC	O2A-PA-O1A	2.61	118.77	110.07
7	D	405	MPO	C3-N1-C7	2.54	117.73	111.23
2	B	401	APC	O3G-PG-O2G	2.53	117.30	107.64
2	B	401	APC	O4'-C4'-C3'	-2.52	100.12	105.11
2	B	401	APC	O3'-C3'-C2'	2.50	119.91	111.82
7	D	405	MPO	C3-N1-C4	2.39	117.34	111.23
2	B	401	APC	O1A-PA-C3A	2.32	115.20	109.07
2	C	402	APC	C5-C6-N6	2.27	123.80	120.35
2	B	401	APC	O2A-PA-O1A	2.26	117.60	110.07
2	D	401	APC	C5-C6-N6	2.22	123.73	120.35
2	B	401	APC	O1B-PB-C3A	-2.20	103.26	109.07
2	C	402	APC	O2A-PA-O1A	2.07	116.98	110.07
2	C	402	APC	O2B-PB-O1B	2.06	116.95	110.07
2	C	402	APC	O3G-PG-O2G	2.05	115.46	107.64
2	C	402	APC	O4'-C4'-C3'	-2.05	101.07	105.11
7	B	407	MPO	O3-S1-O2	-2.01	106.36	111.27

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	APC	PB-O3B-PG-O2G
2	A	401	APC	C5'-O5'-PA-O1A
2	A	401	APC	C5'-O5'-PA-C3A
2	A	401	APC	O4'-C4'-C5'-O5'
2	A	401	APC	C3'-C4'-C5'-O5'
2	B	401	APC	O4'-C4'-C5'-O5'
2	B	401	APC	C3'-C4'-C5'-O5'
2	D	401	APC	PB-O3B-PG-O3G
2	D	401	APC	C5'-O5'-PA-O1A
2	D	401	APC	C5'-O5'-PA-O2A
2	D	401	APC	C5'-O5'-PA-C3A
2	D	401	APC	O4'-C4'-C5'-O5'
2	D	401	APC	C3'-C4'-C5'-O5'
2	C	402	APC	PB-O3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
2	C	402	APC	C5'-O5'-PA-O2A
2	C	402	APC	O4'-C4'-C5'-O5'
2	C	402	APC	C3'-C4'-C5'-O5'
7	D	405	MPO	C2-C3-N1-C4
8	C	401	PG4	O2-C3-C4-O3
2	C	402	APC	C5'-O5'-PA-O1A
2	B	401	APC	C5'-O5'-PA-C3A
2	C	402	APC	C5'-O5'-PA-C3A
6	A	407	PEG	O1-C1-C2-O2
7	C	408	MPO	C2-C3-N1-C7
2	B	401	APC	C5'-O5'-PA-O1A
7	D	405	MPO	C2-C3-N1-C7
6	B	406	PEG	O1-C1-C2-O2
8	C	401	PG4	O1-C1-C2-O2
8	C	401	PG4	O4-C7-C8-O5
7	A	408	MPO	C2-C3-N1-C7
8	C	401	PG4	C4-C3-O2-C2
6	B	406	PEG	O2-C3-C4-O4
8	C	401	PG4	C3-C4-O3-C5
6	A	407	PEG	C4-C3-O2-C2
7	B	407	MPO	C1-C2-C3-N1
2	A	401	APC	C5'-O5'-PA-O2A
2	B	401	APC	PB-O3B-PG-O1G
2	D	401	APC	PB-O3B-PG-O1G
2	A	401	APC	PB-O3B-PG-O3G
2	B	401	APC	PB-O3B-PG-O2G
2	D	401	APC	PB-O3B-PG-O2G
2	C	402	APC	PB-O3B-PG-O2G
7	D	405	MPO	C2-C1-S1-O1

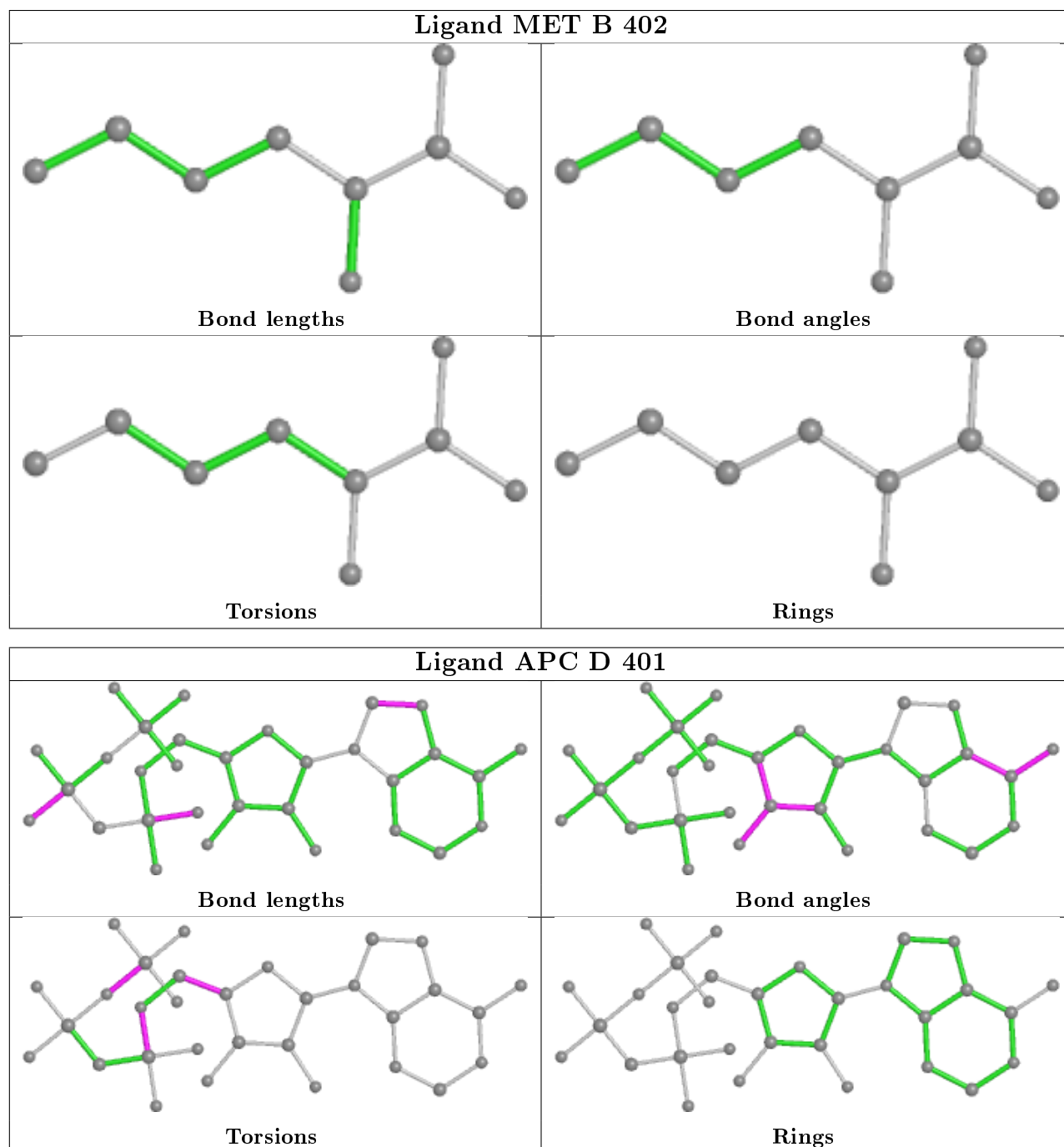
There are no ring outliers.

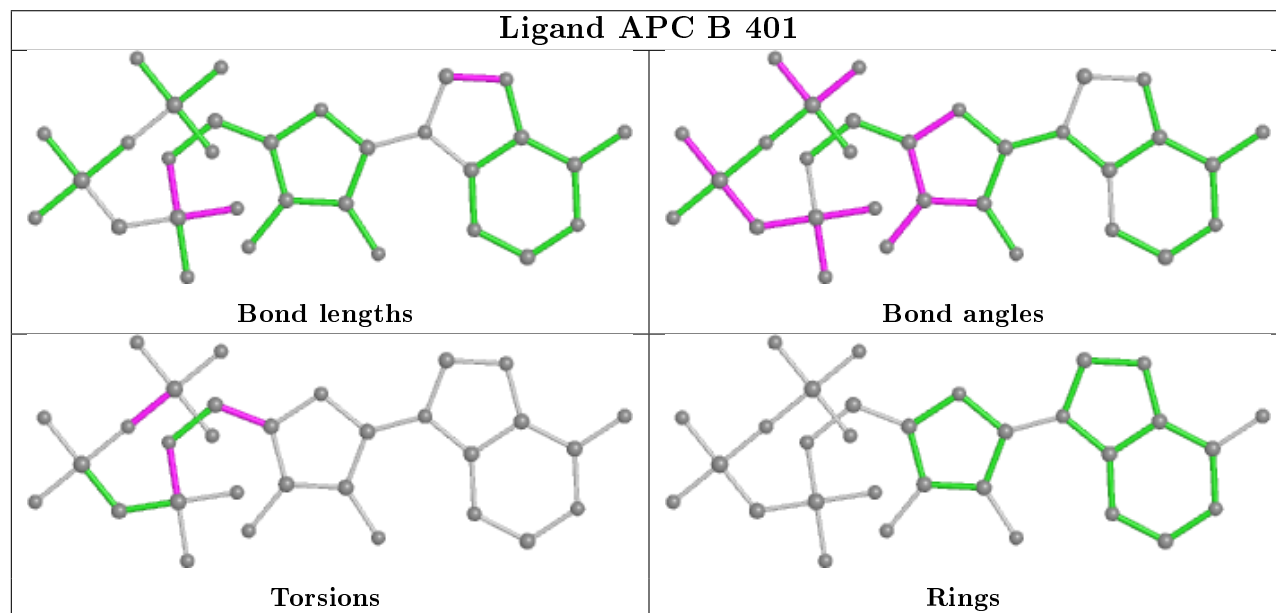
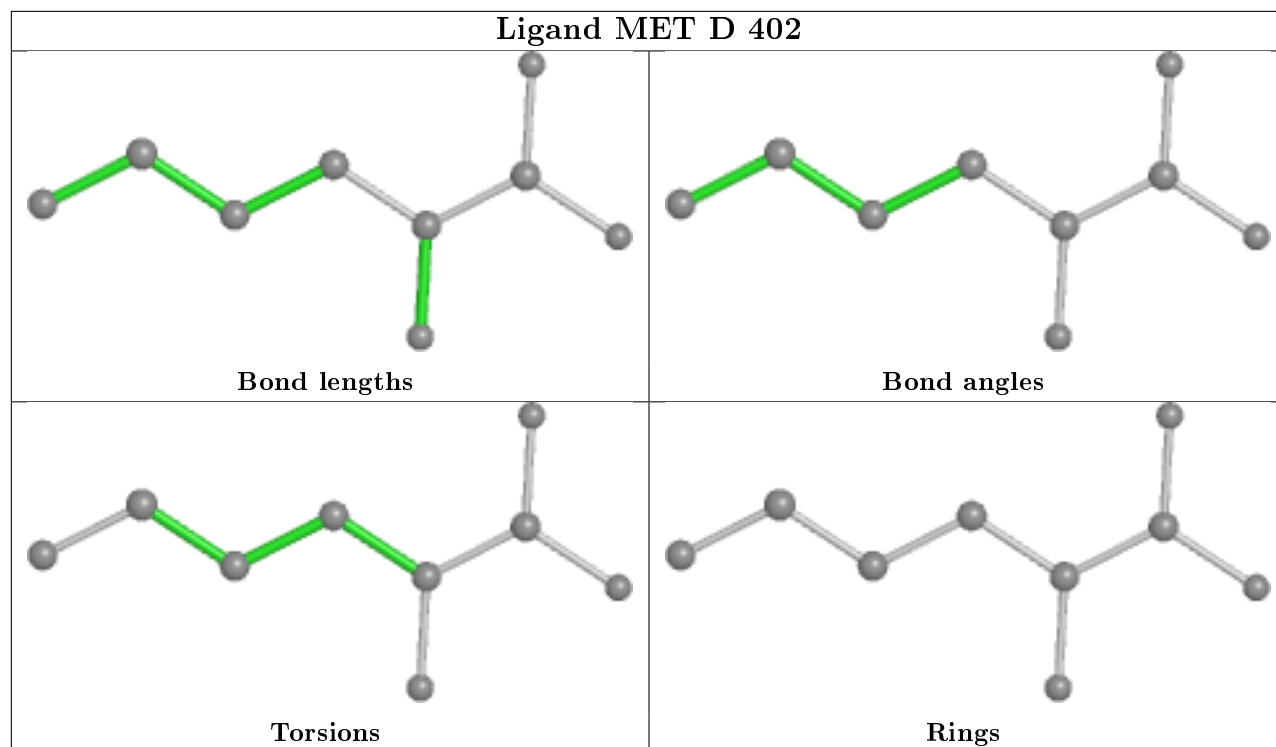
4 monomers are involved in 5 short contacts:

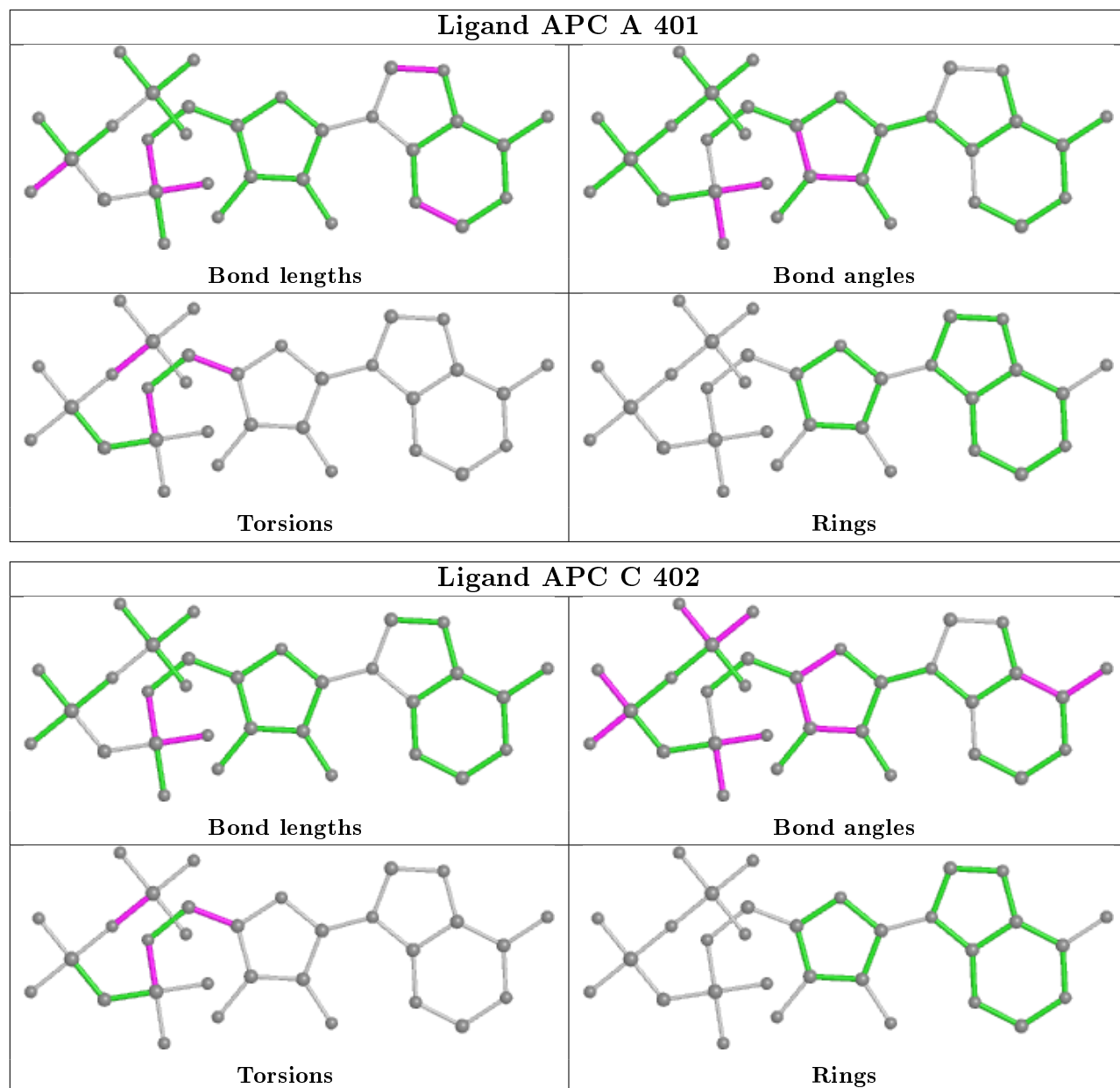
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	APC	2	0
2	B	401	APC	1	0
2	A	401	APC	1	0
2	C	402	APC	1	0

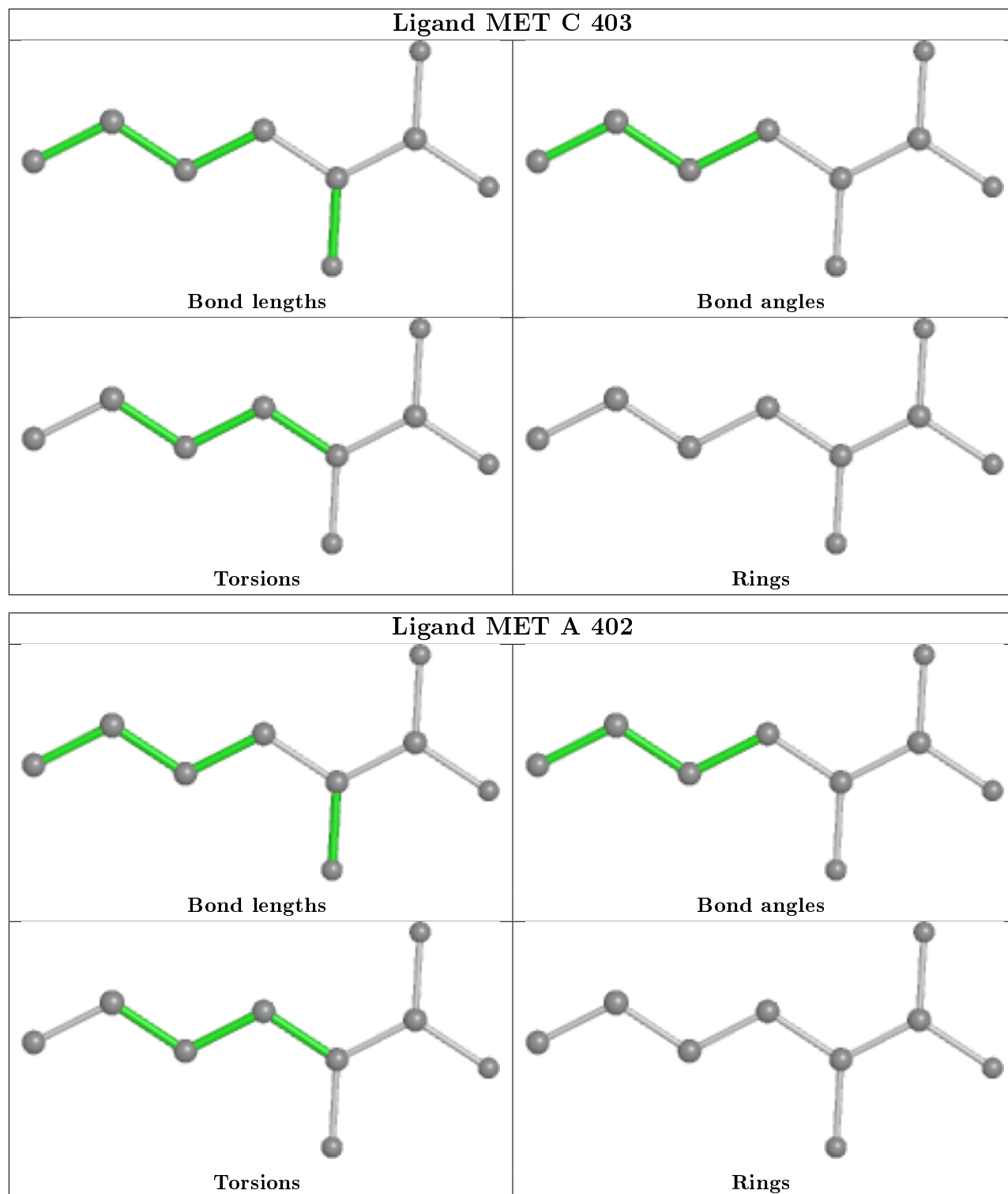
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	392/402 (97%)	-0.09	4 (1%) 82 81	16, 25, 38, 64	0
1	B	389/402 (96%)	-0.05	4 (1%) 82 81	18, 25, 39, 53	0
1	C	389/402 (96%)	0.01	5 (1%) 77 76	20, 28, 40, 69	0
1	D	388/402 (96%)	-0.05	3 (0%) 86 85	19, 27, 40, 62	0
All	All	1558/1608 (96%)	-0.04	16 (1%) 82 81	16, 26, 40, 69	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.9
1	C	389	ASP	2.8
1	A	391	PRO	2.8
1	A	1	MET	2.7
1	B	254	ILE	2.6
1	B	2	GLU	2.5
1	B	82	ASP	2.4
1	A	389	ASP	2.3
1	C	270	PHE	2.2
1	C	254	ILE	2.2
1	D	82	ASP	2.1
1	D	1	MET	2.1
1	C	268	GLY	2.1
1	A	254	ILE	2.0
1	D	388	TRP	2.0
1	B	357	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

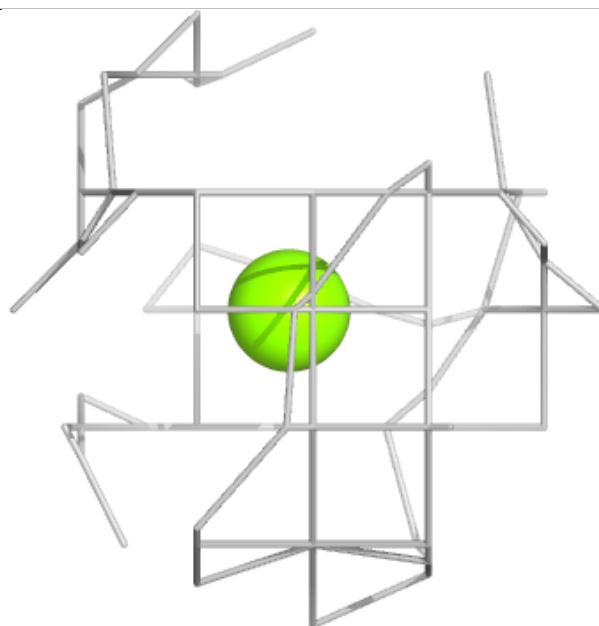
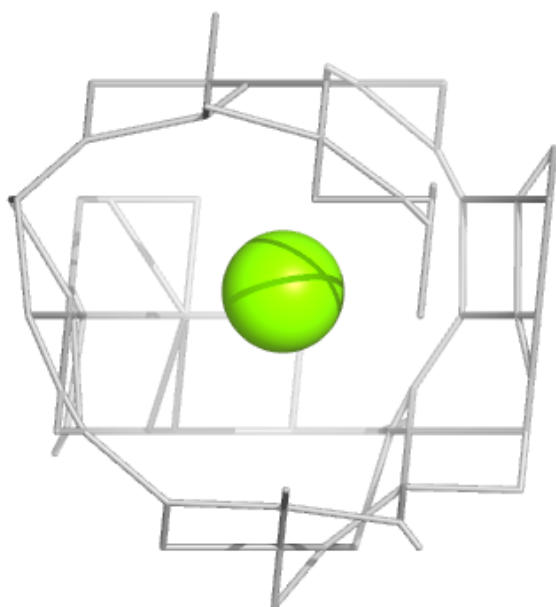
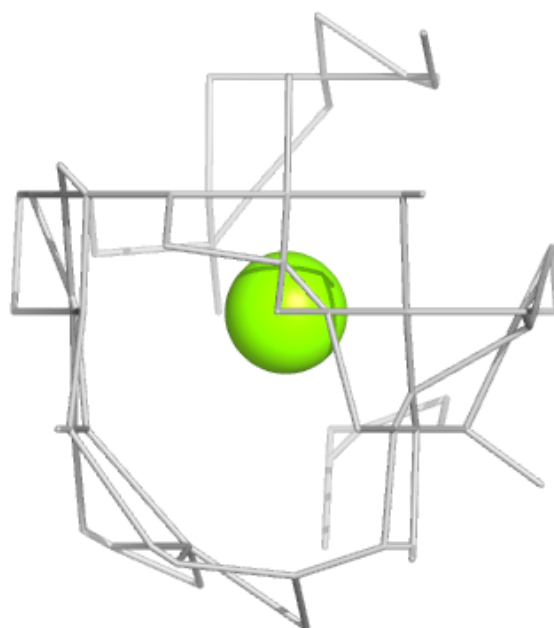
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	PG4	C	401	13/13	0.83	0.15	42,49,57,59	0
6	PEG	A	407	7/7	0.85	0.18	42,43,47,50	0
6	PEG	B	406	7/7	0.88	0.14	32,33,36,37	0
4	MG	D	403	1/1	0.90	0.10	27,27,27,27	0
7	MPO	C	408	13/13	0.90	0.15	40,50,58,60	0
7	MPO	D	405	13/13	0.92	0.16	36,43,44,46	0
3	MET	D	402	9/9	0.93	0.11	27,29,32,33	0
7	MPO	A	408	13/13	0.93	0.16	31,38,40,40	0
3	MET	C	403	9/9	0.93	0.16	26,27,27,29	0
7	MPO	B	407	13/13	0.93	0.13	26,32,40,44	0
3	MET	A	402	9/9	0.96	0.10	21,24,25,29	0
4	MG	A	404	1/1	0.97	0.08	21,21,21,21	0
2	APC	A	401	31/31	0.97	0.12	14,19,22,22	0
2	APC	B	401	31/31	0.97	0.09	17,20,22,25	0
3	MET	B	402	9/9	0.97	0.10	21,23,24,25	0
2	APC	D	401	31/31	0.97	0.09	19,25,30,31	0
4	MG	A	403	1/1	0.97	0.11	25,25,25,25	0
2	APC	C	402	31/31	0.97	0.08	20,25,29,30	0
4	MG	C	406	1/1	0.98	0.10	25,25,25,25	0
4	MG	C	404	1/1	0.99	0.06	25,25,25,25	0
4	MG	B	404	1/1	0.99	0.14	22,22,22,22	0
5	K	C	407	1/1	0.99	0.03	32,32,32,32	0
4	MG	C	405	1/1	0.99	0.14	25,25,25,25	0
5	K	A	406	1/1	0.99	0.05	23,23,23,23	0
4	MG	A	405	1/1	0.99	0.02	31,31,31,31	0
5	K	B	405	1/1	0.99	0.06	23,23,23,23	0
5	K	D	404	1/1	0.99	0.05	26,26,26,26	0
4	MG	B	403	1/1	0.99	0.07	17,17,17,17	0

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

orientation to approximate a three-dimensional view.

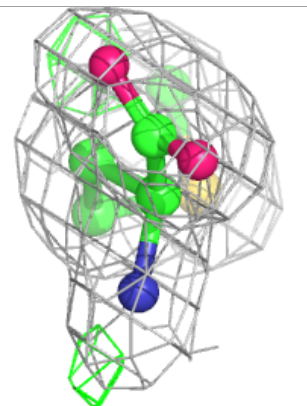
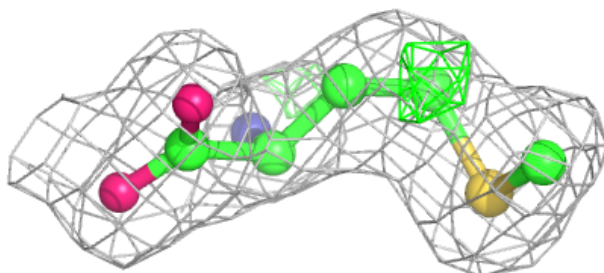
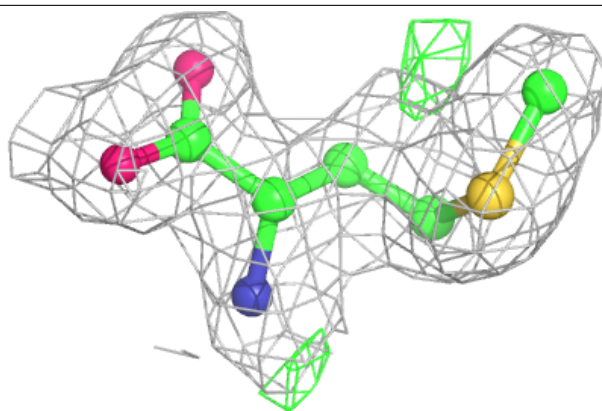
Electron density around MG D 403:

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

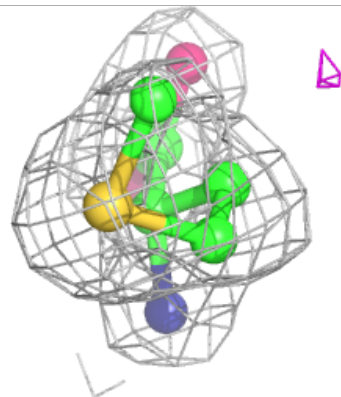
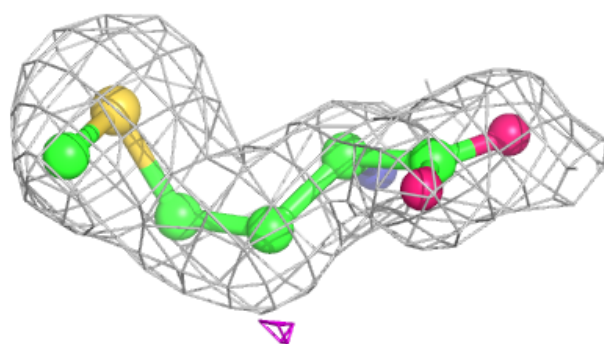
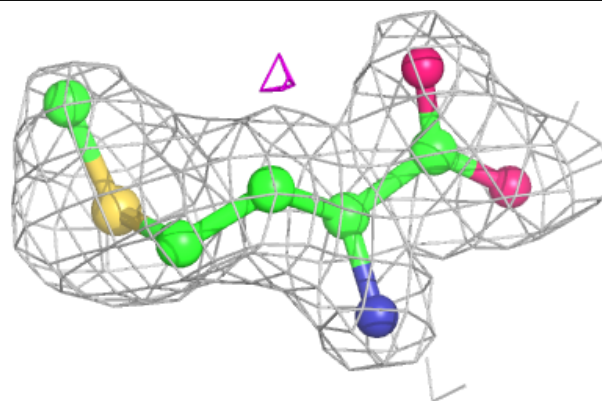


Electron density around MET D 402:

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

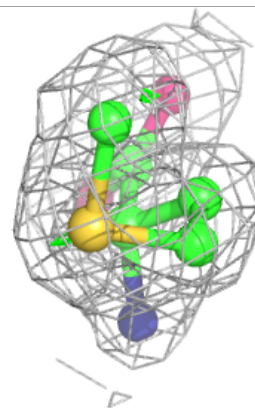
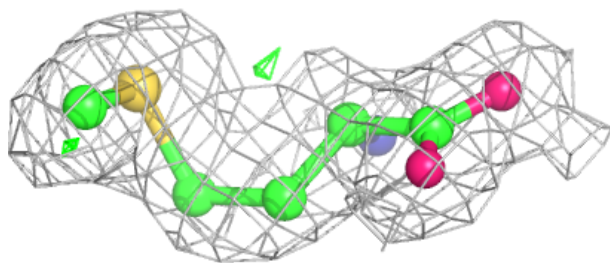
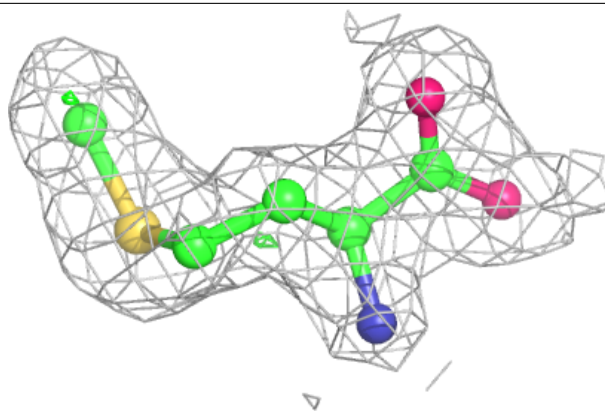
**Electron density around MET C 403:**

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



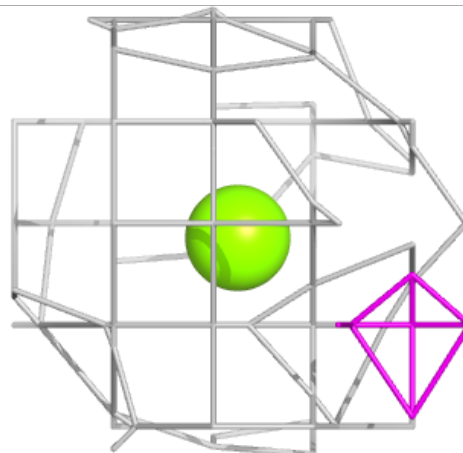
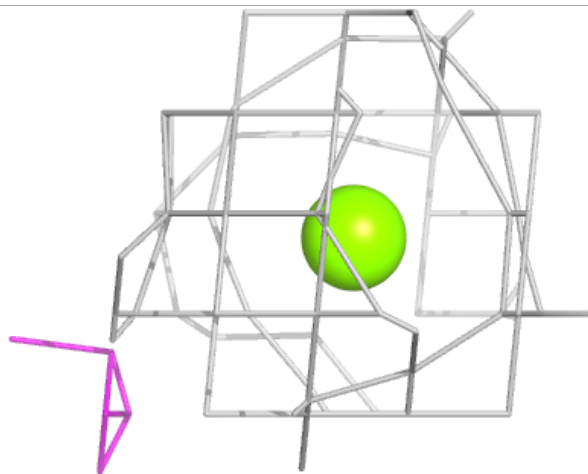
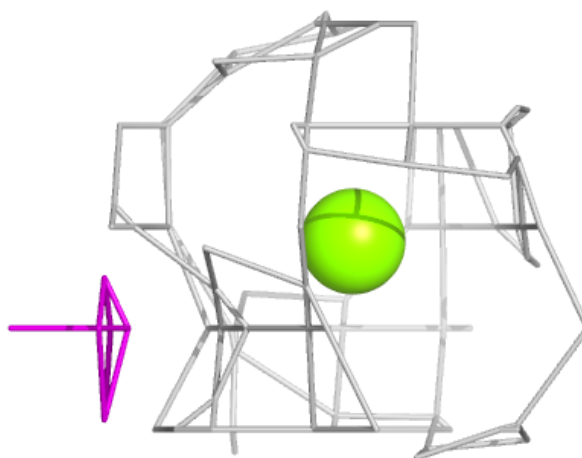
Electron density around MET A 402:

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



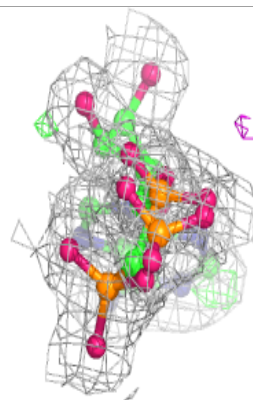
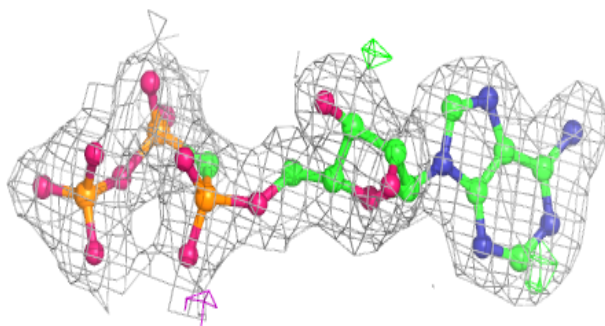
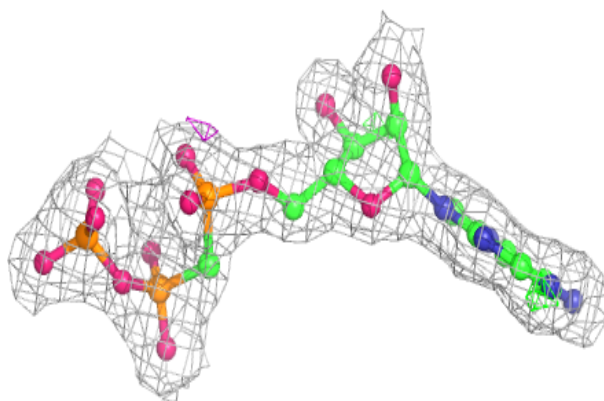
Electron density around MG A 404:

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

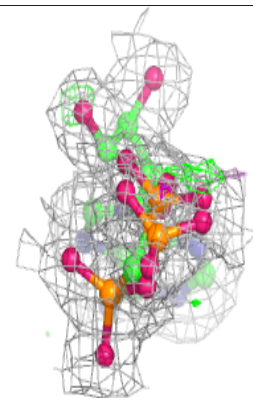
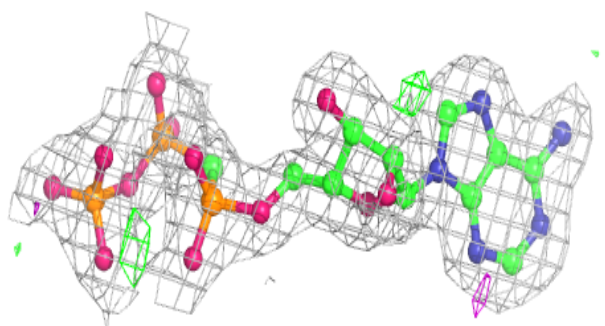
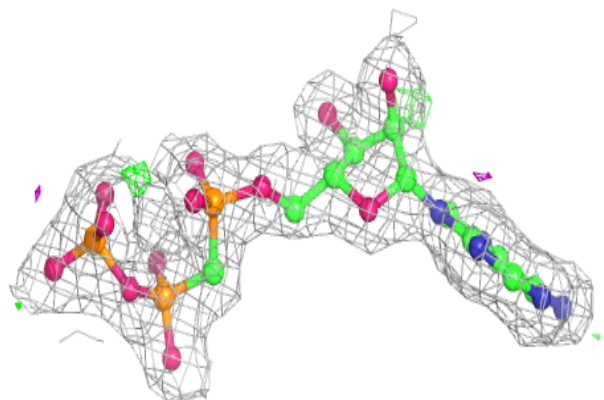


Electron density around APC A 401:

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

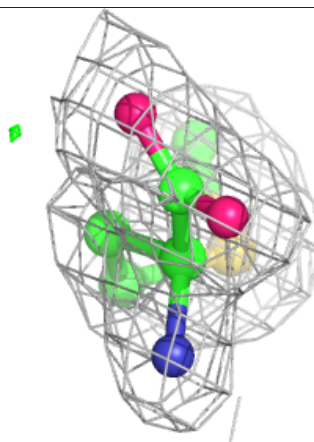
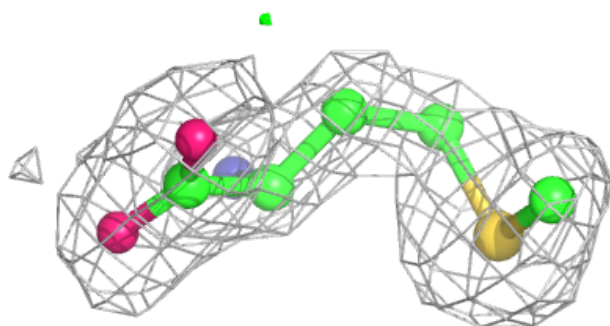
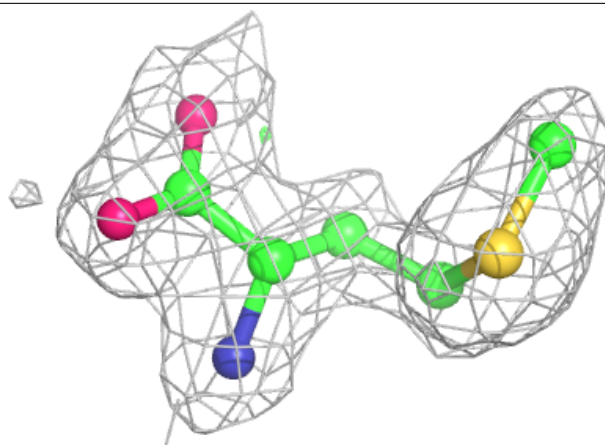
**Electron density around APC B 401:**

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

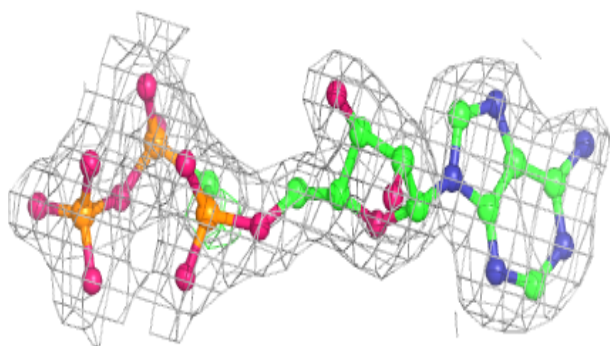
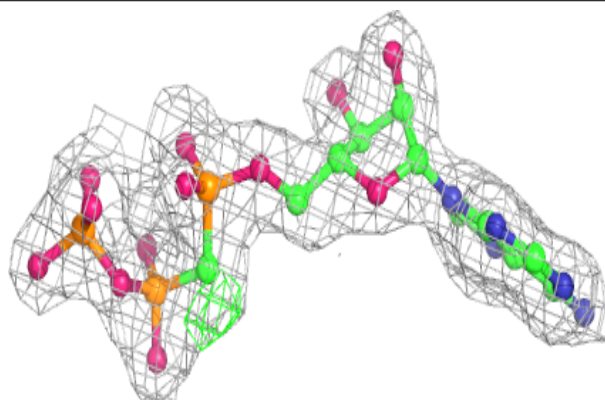


Electron density around MET B 402:

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

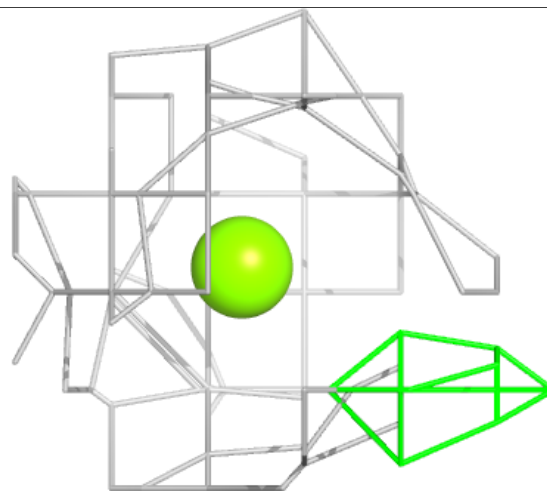
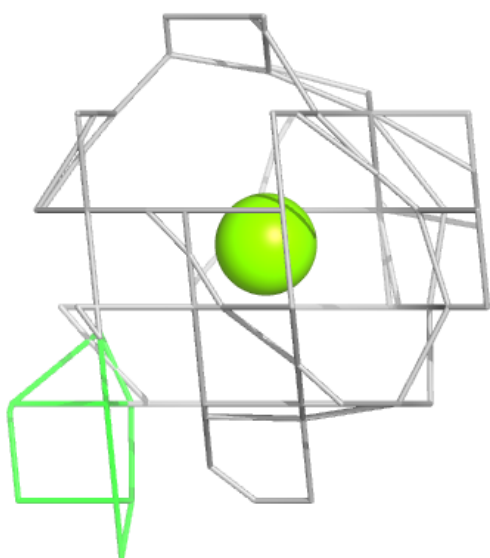
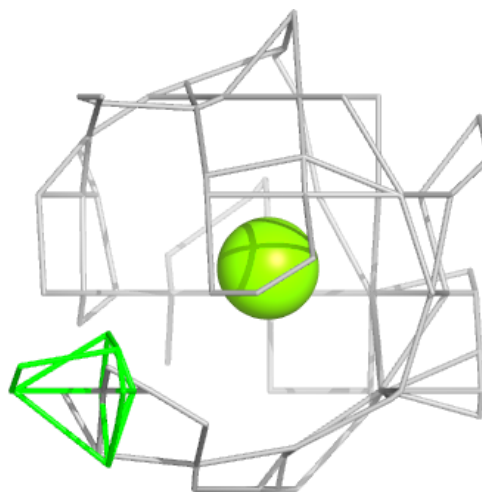
**Electron density around APC D 401:**

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



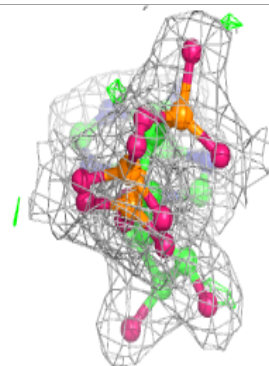
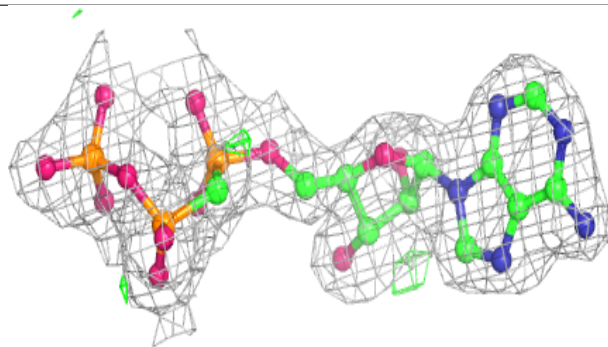
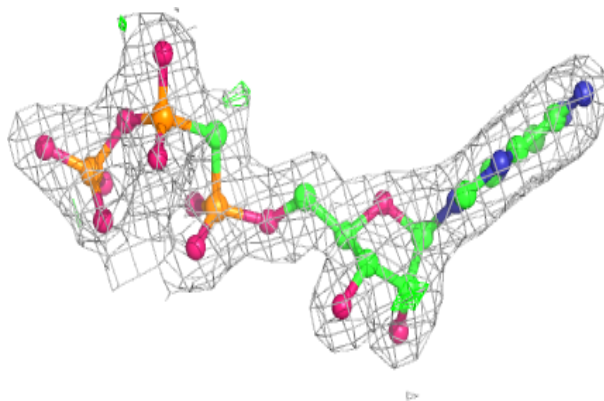
Electron density around MG A 403:

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



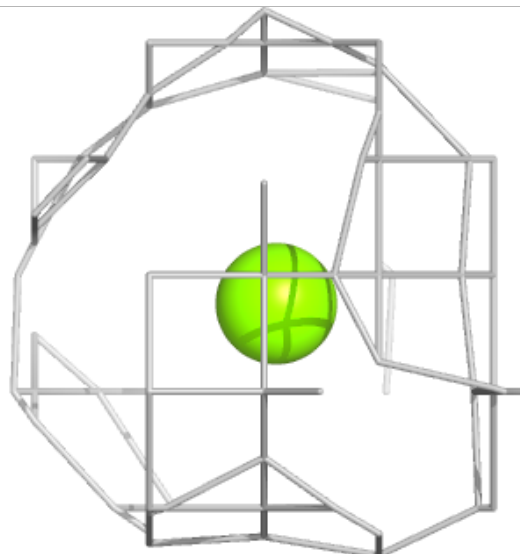
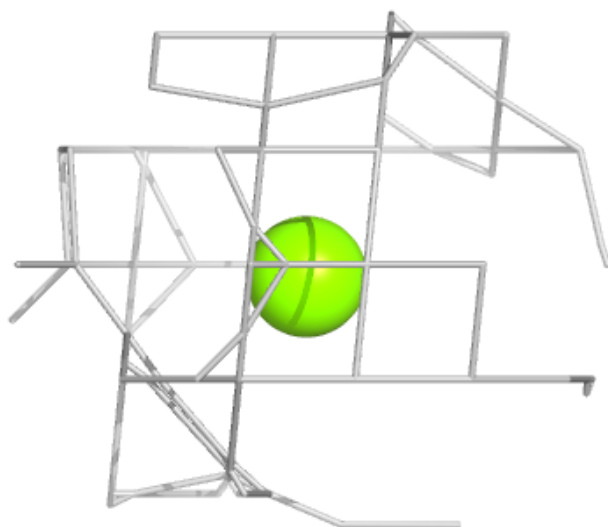
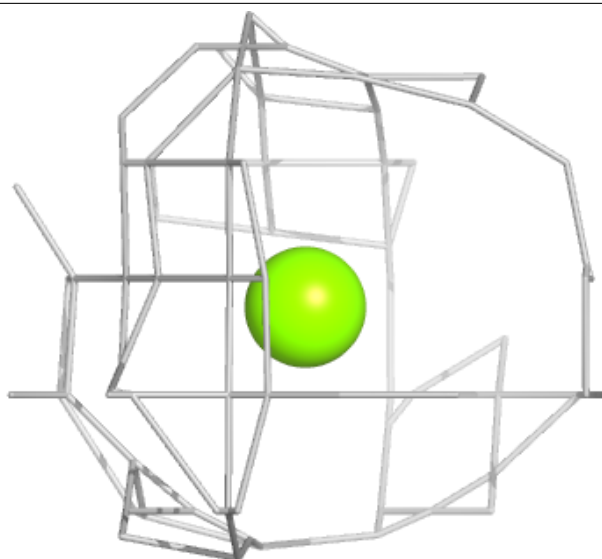
Electron density around APC C 402:

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



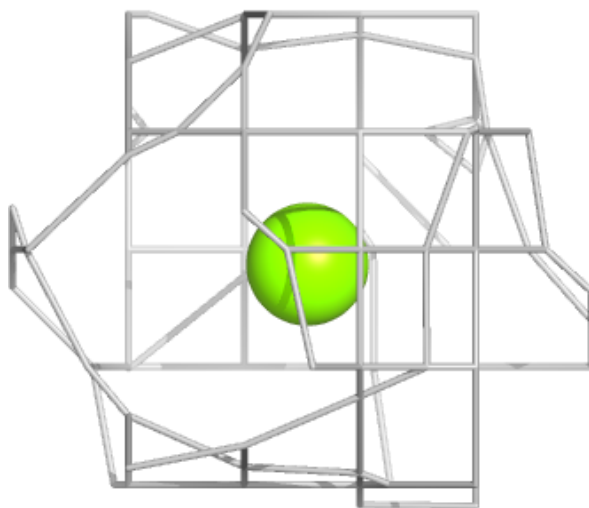
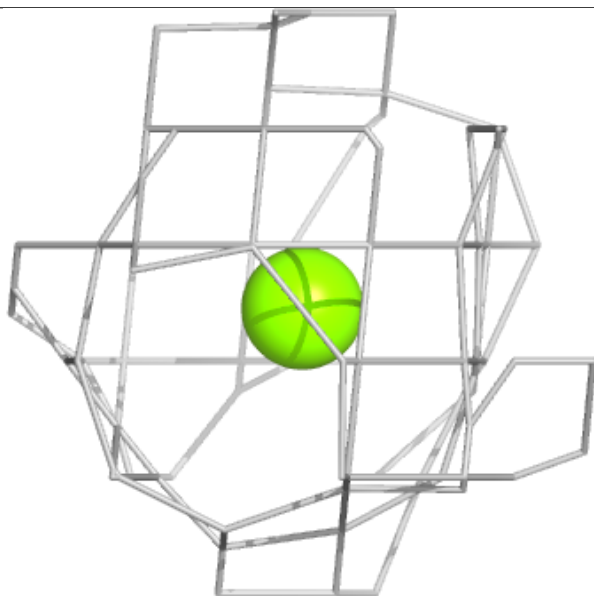
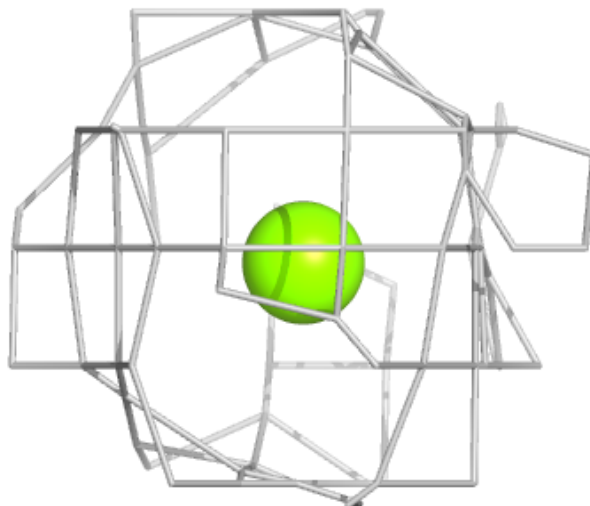
Electron density around MG C 406:

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



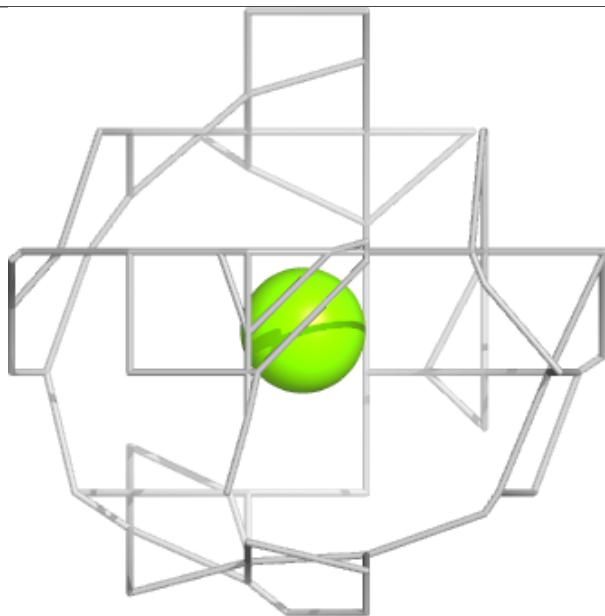
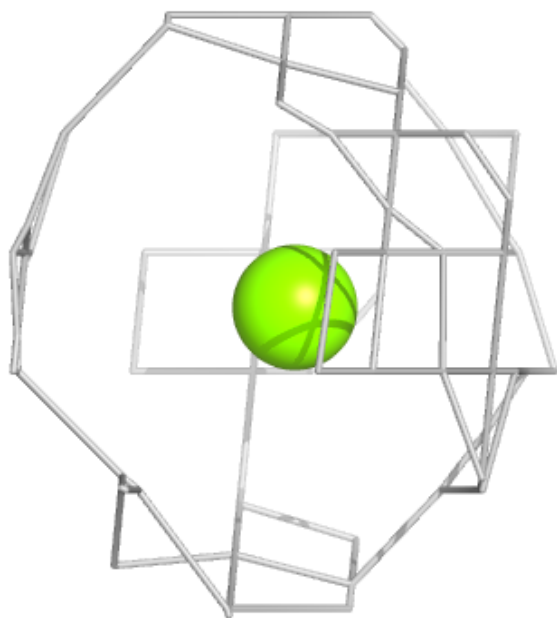
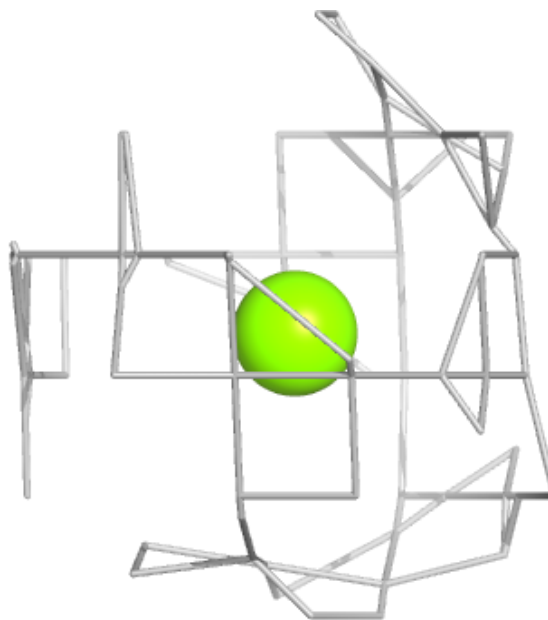
Electron density around MG C 404:

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



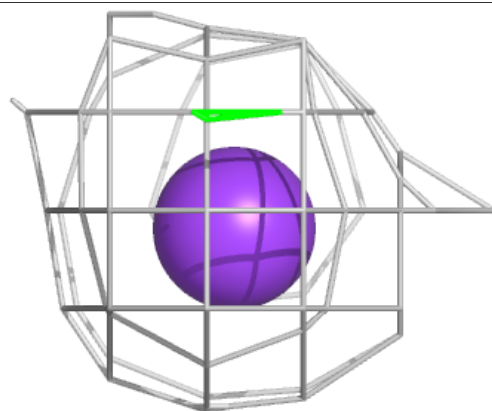
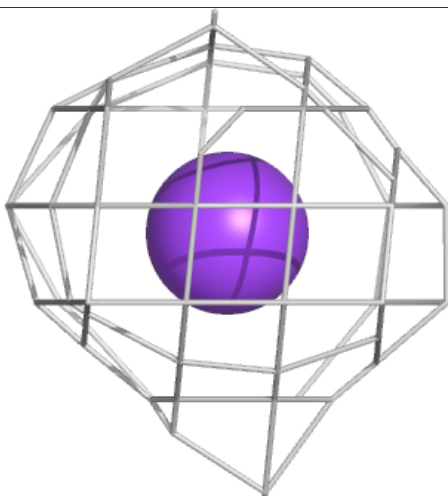
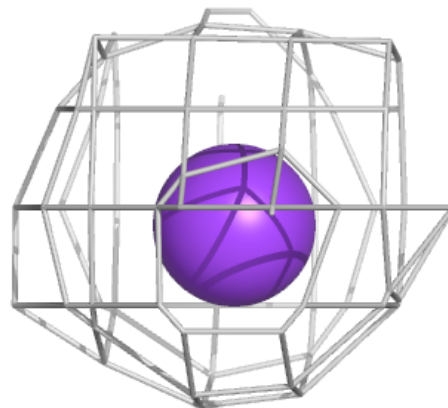
Electron density around MG B 404:

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



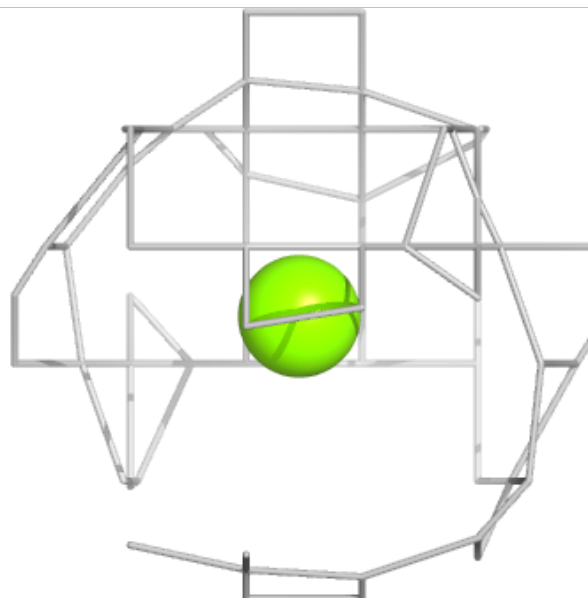
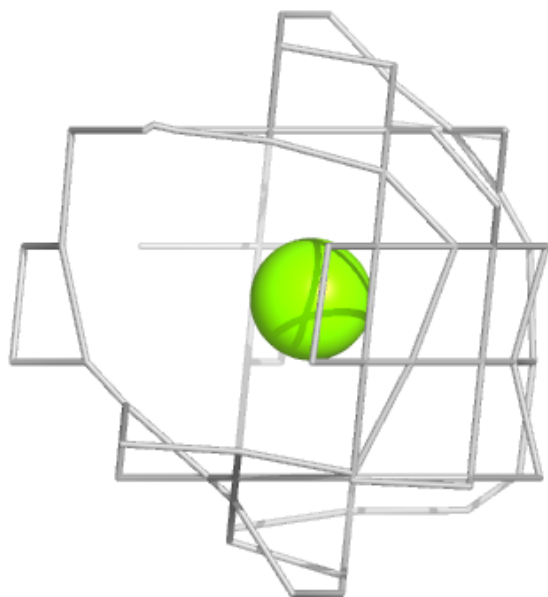
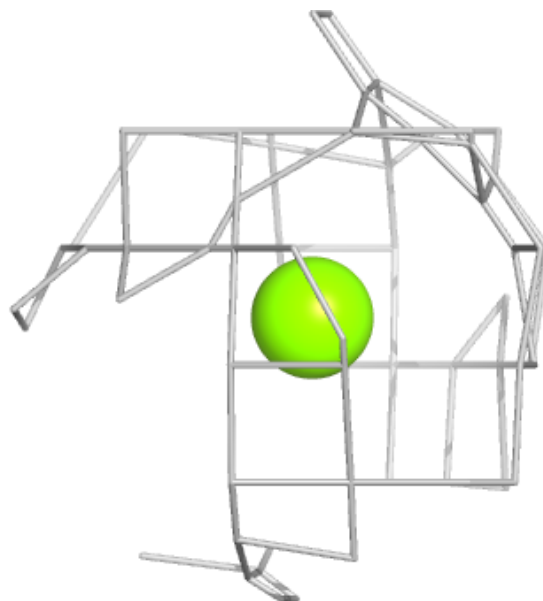
Electron density around K C 407:

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



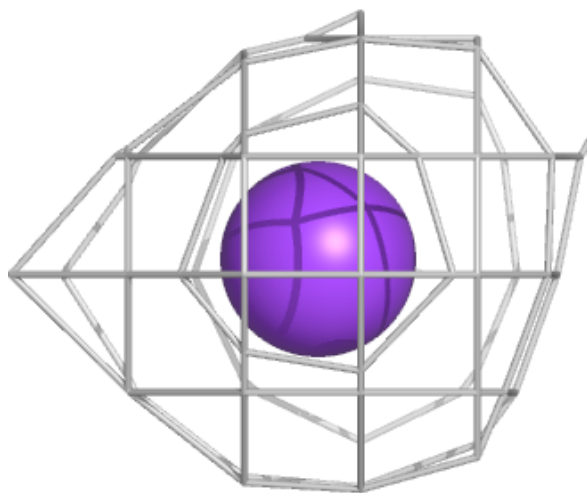
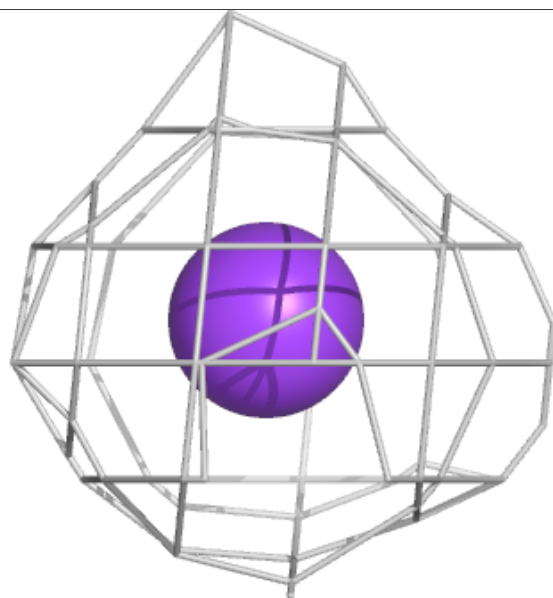
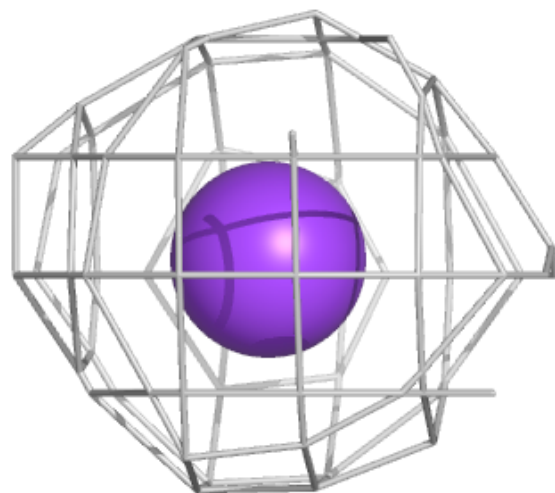
Electron density around MG C 405:

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



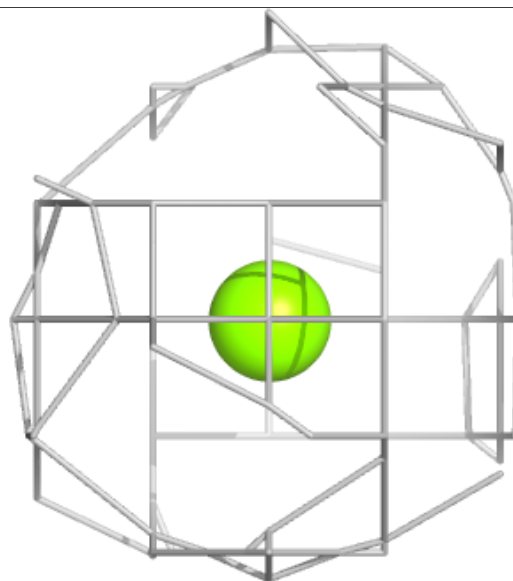
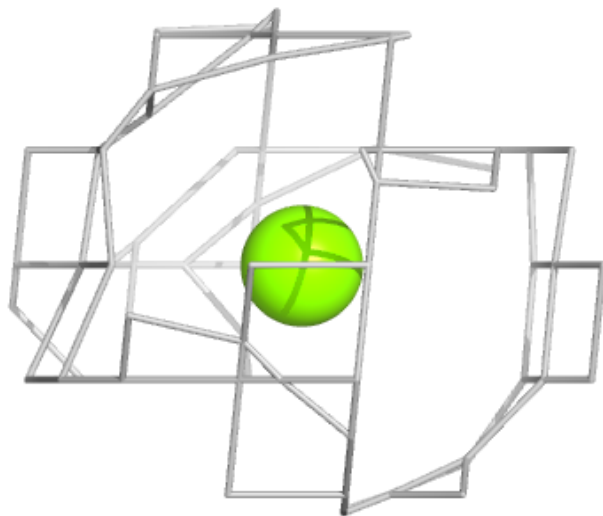
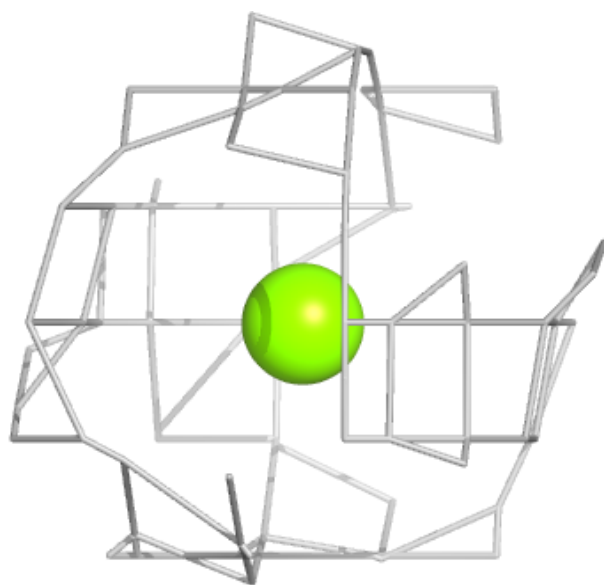
Electron density around K A 406:

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



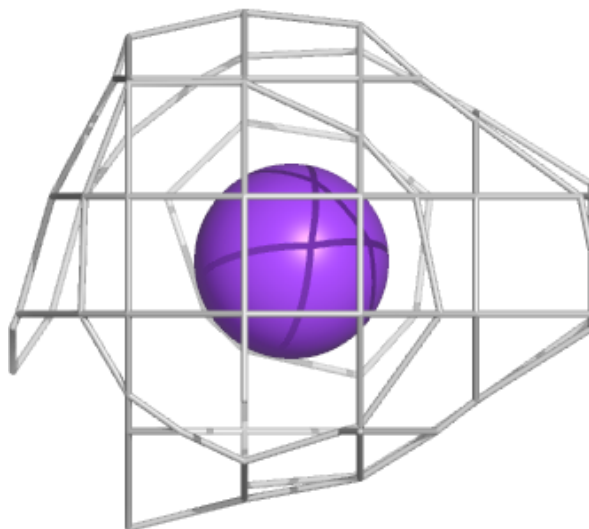
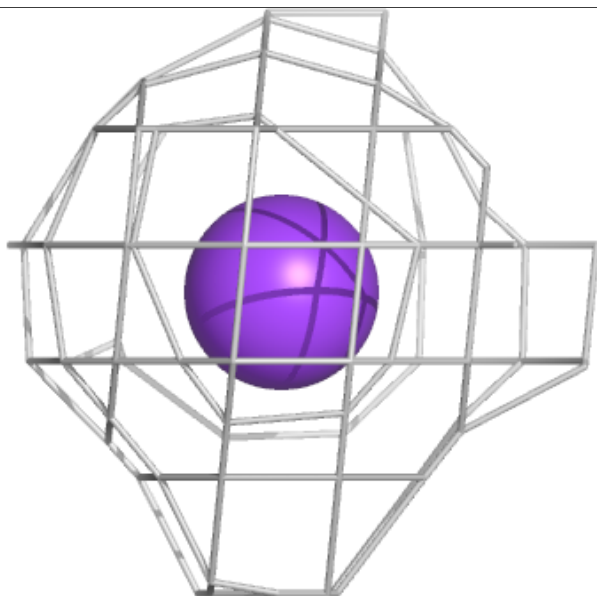
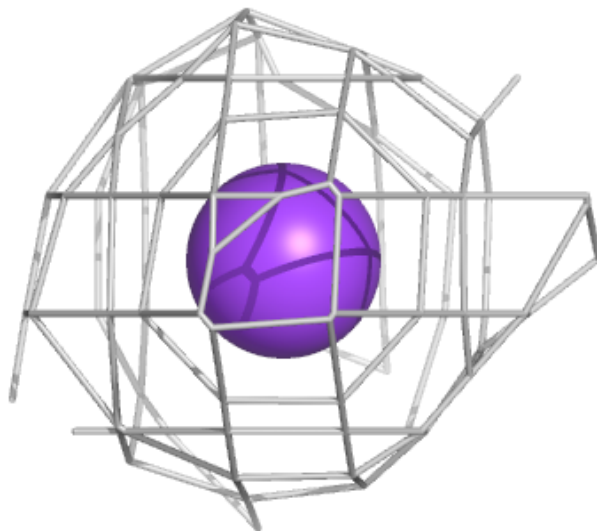
Electron density around MG A 405:

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



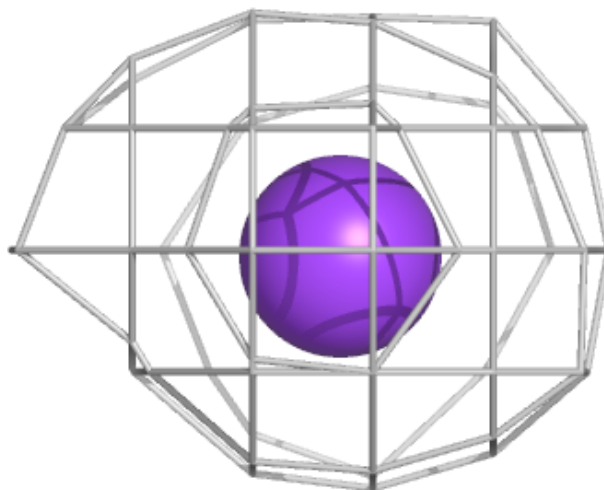
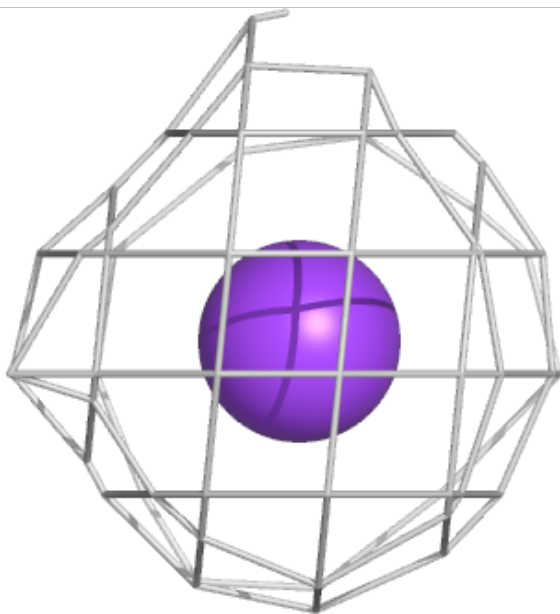
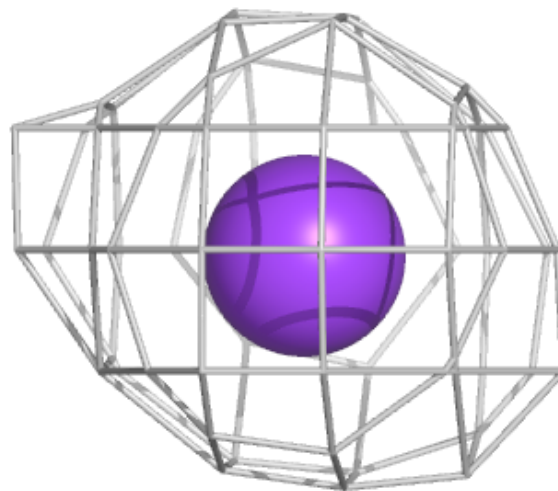
Electron density around K B 405:

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



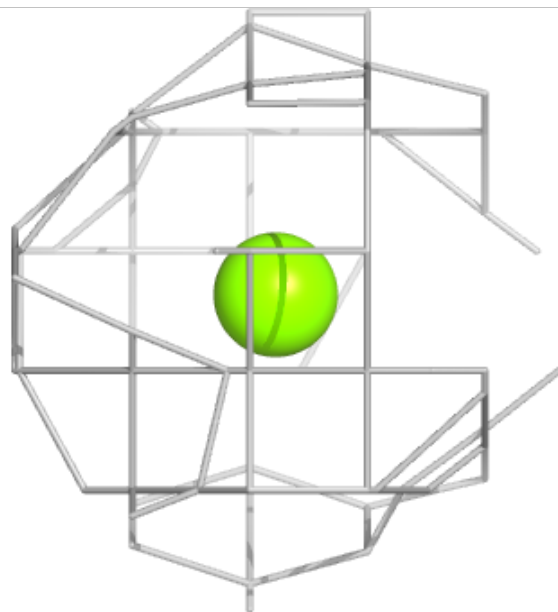
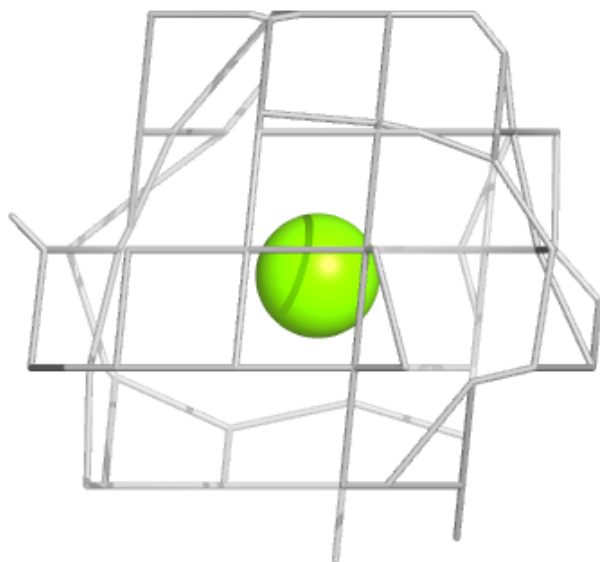
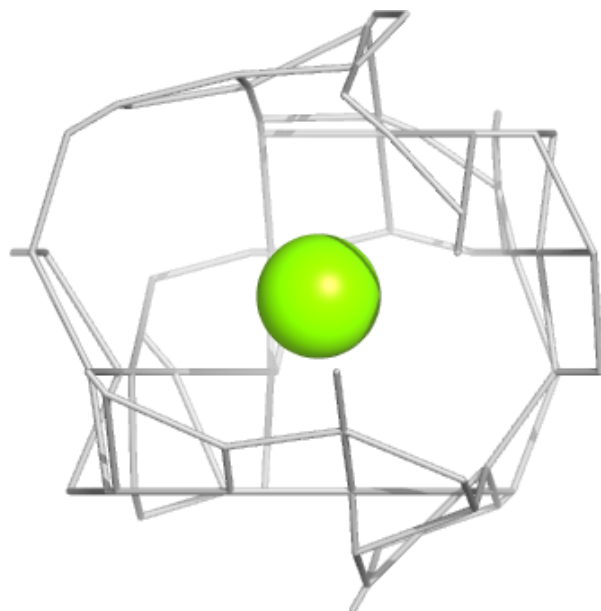
Electron density around K D 404:

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



Electron density around MG 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.