wwPDB X-ray Structure Validation Summary Report (i)

Jul 5, 2022 – 02:44 pm BST

PDB ID	:	7R3B
Title	:	S-adenosylmethionine synthetase from Lactobacillus plantarum complexed with AMPPNP, methionine and SAM
Authors	:	Shahar, A.; Kleiner, D.; Bershtein, S.; Zarivach, R.
Deposited on	:	2022-02-07
Resolution	:	2.82 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

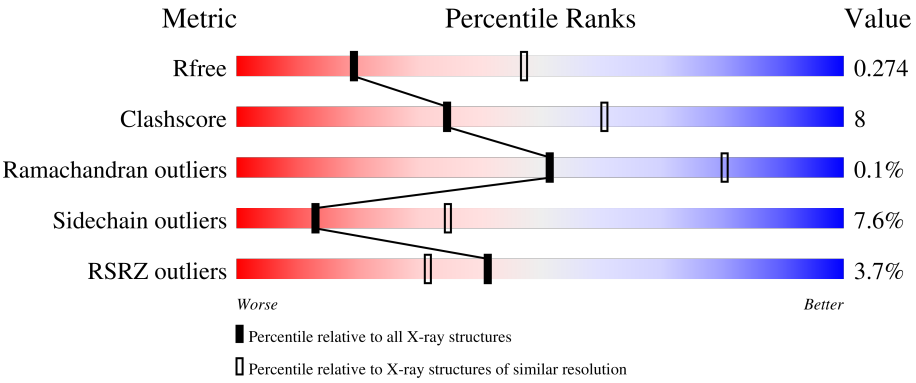
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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 <=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	401	4% 76% 12% • 9%
1	B	401	% 75% 13% • 10%
1	C	401	4% 78% 12% • 7%
1	D	401	3% 73% 16% • 8%
1	E	401	3% 71% 18% • 7%

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Mol	Chain	Length	Quality of chain
1	F	401	7% 72% 18% 8%
1	G	401	2% 73% 15% 9%
1	H	401	2% 75% 14% 9%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 22699 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2778	1745	480	546	7			
1	B	362	Total	C	N	O	S	0	0	0
			2763	1737	477	542	7			
1	C	371	Total	C	N	O	S	0	0	0
			2827	1780	488	552	7			
1	D	369	Total	C	N	O	S	0	0	0
			2810	1768	486	549	7			
1	E	371	Total	C	N	O	S	0	0	0
			2832	1781	491	553	7			
1	F	369	Total	C	N	O	S	0	0	0
			2807	1768	482	550	7			
1	G	366	Total	C	N	O	S	0	0	0
			2787	1753	482	545	7			
1	H	364	Total	C	N	O	S	0	0	0
			2776	1744	480	545	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	HIS	-	expression tag	UNP A0A0G9F5E5
A	397	HIS	-	expression tag	UNP A0A0G9F5E5
A	398	HIS	-	expression tag	UNP A0A0G9F5E5
A	399	HIS	-	expression tag	UNP A0A0G9F5E5
A	400	HIS	-	expression tag	UNP A0A0G9F5E5
A	401	HIS	-	expression tag	UNP A0A0G9F5E5
B	396	HIS	-	expression tag	UNP A0A0G9F5E5
B	397	HIS	-	expression tag	UNP A0A0G9F5E5
B	398	HIS	-	expression tag	UNP A0A0G9F5E5
B	399	HIS	-	expression tag	UNP A0A0G9F5E5
B	400	HIS	-	expression tag	UNP A0A0G9F5E5
B	401	HIS	-	expression tag	UNP A0A0G9F5E5
C	396	HIS	-	expression tag	UNP A0A0G9F5E5

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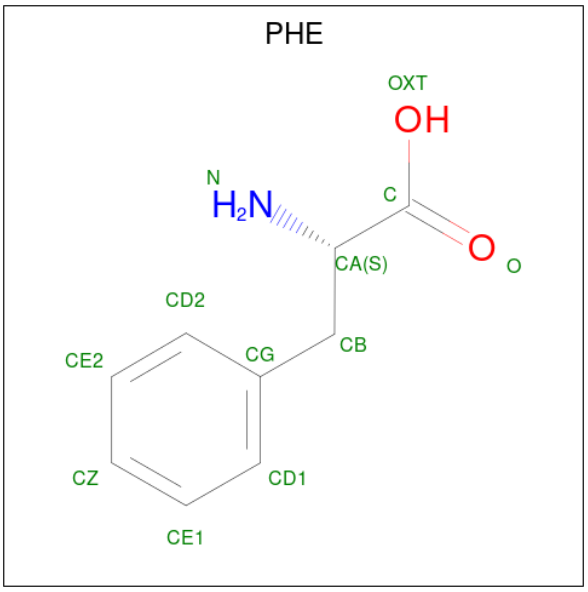
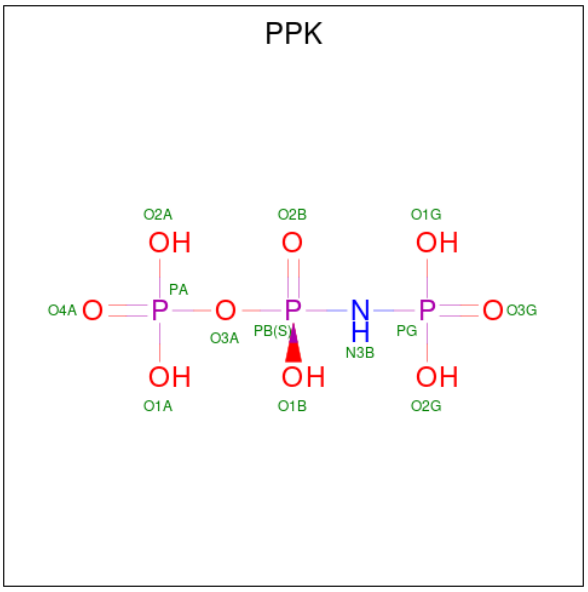
Chain	Residue	Modelled	Actual	Comment	Reference
C	397	HIS	-	expression tag	UNP A0A0G9F5E5
C	398	HIS	-	expression tag	UNP A0A0G9F5E5
C	399	HIS	-	expression tag	UNP A0A0G9F5E5
C	400	HIS	-	expression tag	UNP A0A0G9F5E5
C	401	HIS	-	expression tag	UNP A0A0G9F5E5
D	396	HIS	-	expression tag	UNP A0A0G9F5E5
D	397	HIS	-	expression tag	UNP A0A0G9F5E5
D	398	HIS	-	expression tag	UNP A0A0G9F5E5
D	399	HIS	-	expression tag	UNP A0A0G9F5E5
D	400	HIS	-	expression tag	UNP A0A0G9F5E5
D	401	HIS	-	expression tag	UNP A0A0G9F5E5
E	396	HIS	-	expression tag	UNP A0A0G9F5E5
E	397	HIS	-	expression tag	UNP A0A0G9F5E5
E	398	HIS	-	expression tag	UNP A0A0G9F5E5
E	399	HIS	-	expression tag	UNP A0A0G9F5E5
E	400	HIS	-	expression tag	UNP A0A0G9F5E5
E	401	HIS	-	expression tag	UNP A0A0G9F5E5
F	396	HIS	-	expression tag	UNP A0A0G9F5E5
F	397	HIS	-	expression tag	UNP A0A0G9F5E5
F	398	HIS	-	expression tag	UNP A0A0G9F5E5
F	399	HIS	-	expression tag	UNP A0A0G9F5E5
F	400	HIS	-	expression tag	UNP A0A0G9F5E5
F	401	HIS	-	expression tag	UNP A0A0G9F5E5
G	396	HIS	-	expression tag	UNP A0A0G9F5E5
G	397	HIS	-	expression tag	UNP A0A0G9F5E5
G	398	HIS	-	expression tag	UNP A0A0G9F5E5
G	399	HIS	-	expression tag	UNP A0A0G9F5E5
G	400	HIS	-	expression tag	UNP A0A0G9F5E5
G	401	HIS	-	expression tag	UNP A0A0G9F5E5
H	396	HIS	-	expression tag	UNP A0A0G9F5E5
H	397	HIS	-	expression tag	UNP A0A0G9F5E5
H	398	HIS	-	expression tag	UNP A0A0G9F5E5
H	399	HIS	-	expression tag	UNP A0A0G9F5E5
H	400	HIS	-	expression tag	UNP A0A0G9F5E5
H	401	HIS	-	expression tag	UNP A0A0G9F5E5

- Molecule 2 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 11 9 1 1	0	0
2	H	1	Total C N O 11 9 1 1	0	0

- Molecule 3 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: $H_6NO_9P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O P 13 1 9 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total N O P 13 1 9 3	0	0
3	G	1	Total N O P 13 1 9 3	0	0
3	H	1	Total N O P 13 1 9 3	0	0

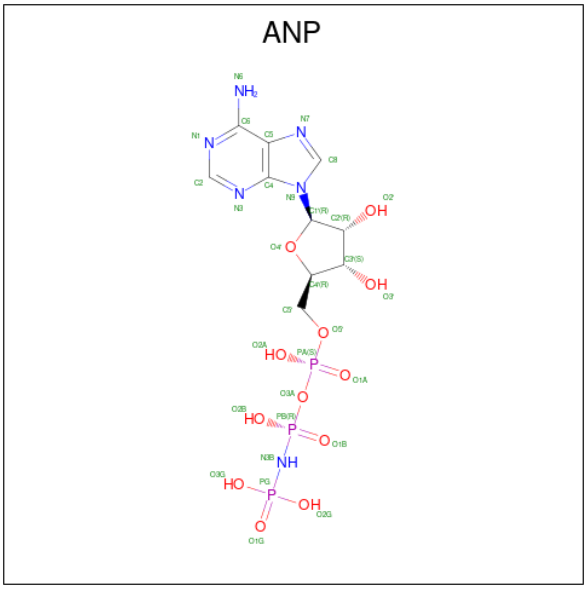
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total Mg 3 3	0	0
4	B	1	Total Mg 1 1	0	0
4	C	2	Total Mg 2 2	0	0
4	D	2	Total Mg 2 2	0	0
4	E	1	Total Mg 1 1	0	0
4	F	3	Total Mg 3 3	0	0
4	G	2	Total Mg 2 2	0	0
4	H	2	Total Mg 2 2	0	0

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

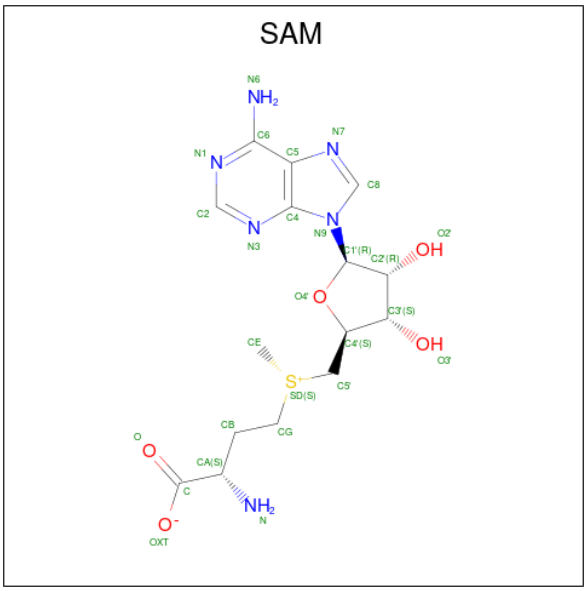
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0
5	F	1	Total K 1 1	0	0
5	H	1	Total K 1 1	0	0

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 7 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C N O S 27 15 6 5 1	0	0
7	H	1	Total C N O S 27 15 6 5 1	0	0

- Molecule 8 is water.

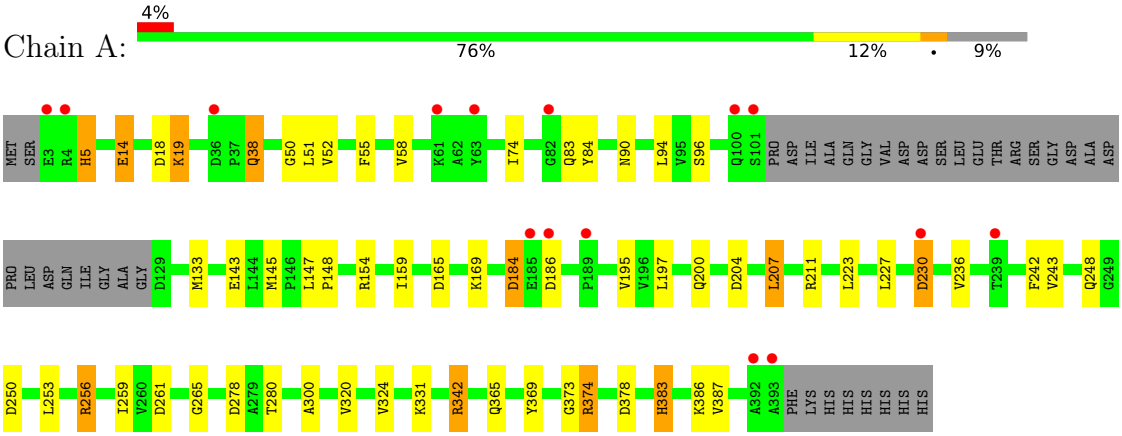
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	6	Total O 6 6	0	0
8	B	5	Total O 5 5	0	0
8	C	6	Total O 6 6	0	0
8	D	6	Total O 6 6	0	0
8	E	4	Total O 4 4	0	0
8	F	7	Total O 7 7	0	0
8	G	6	Total O 6 6	0	0
8	H	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

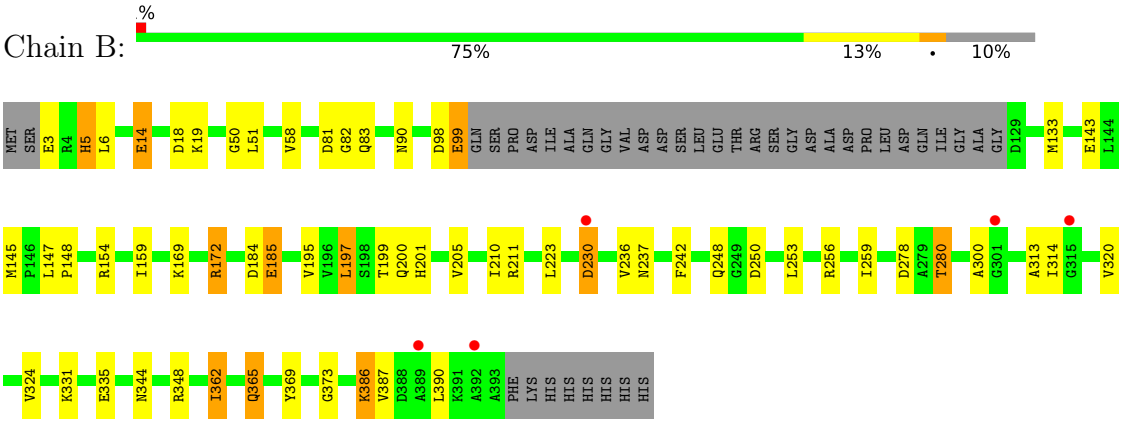
• Molecule 1: S-adenosylmethionine synthase

Chain A:



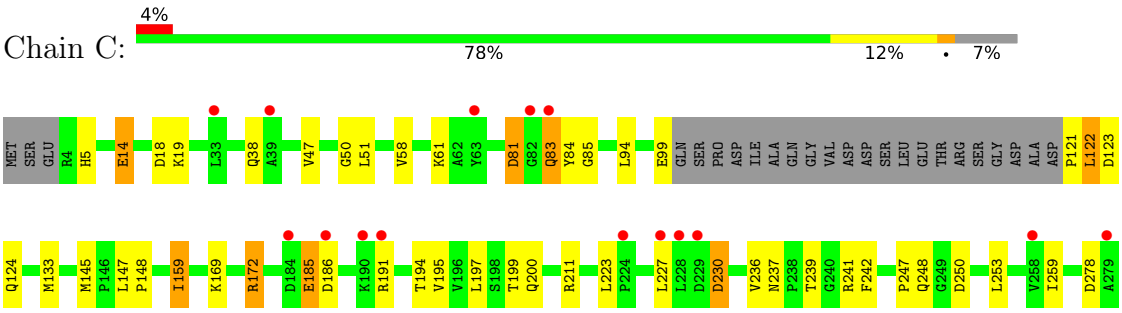
• Molecule 1: S-adenosylmethionine synthase

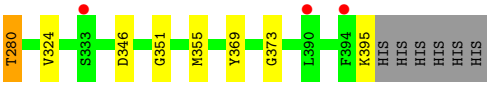
Chain B:



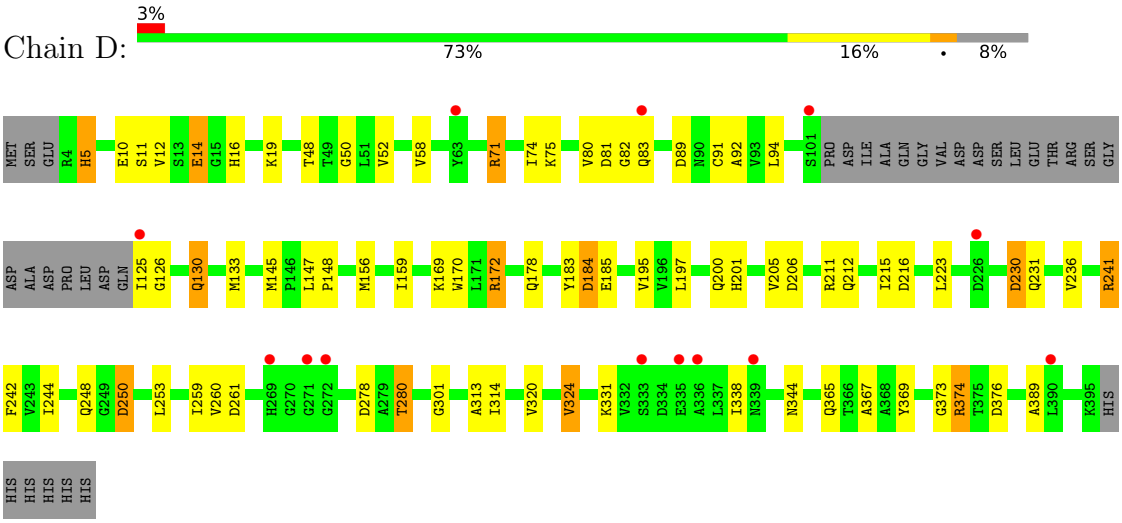
• Molecule 1: S-adenosylmethionine synthase

Chain C:

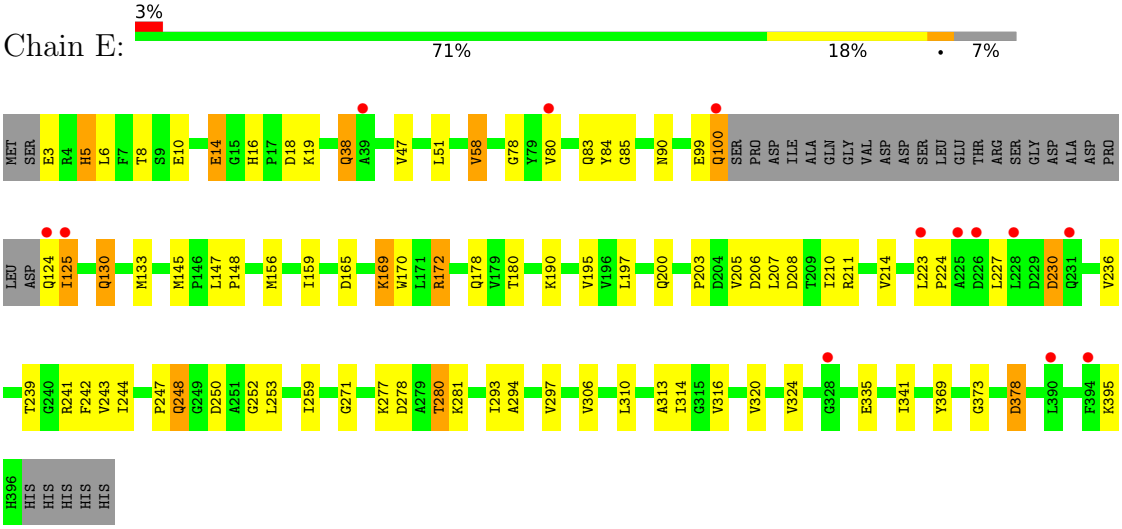




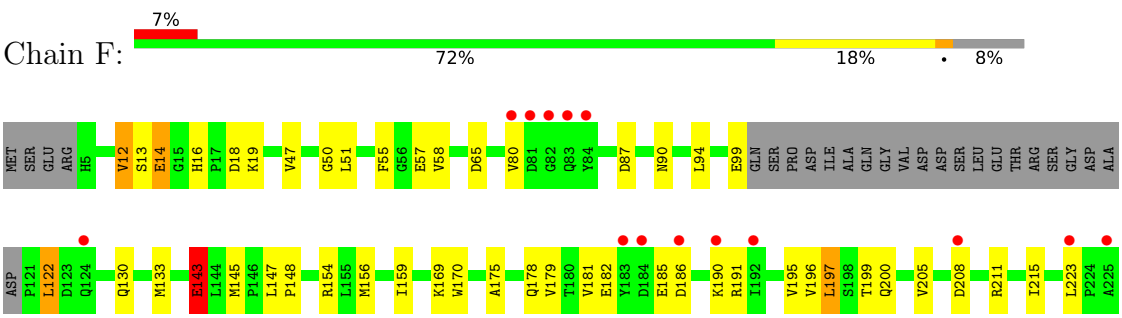
• Molecule 1: S-adenosylmethionine synthase

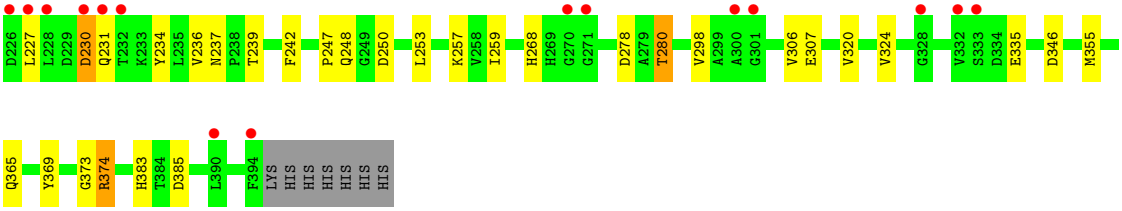


• Molecule 1: S-adenosylmethionine synthase



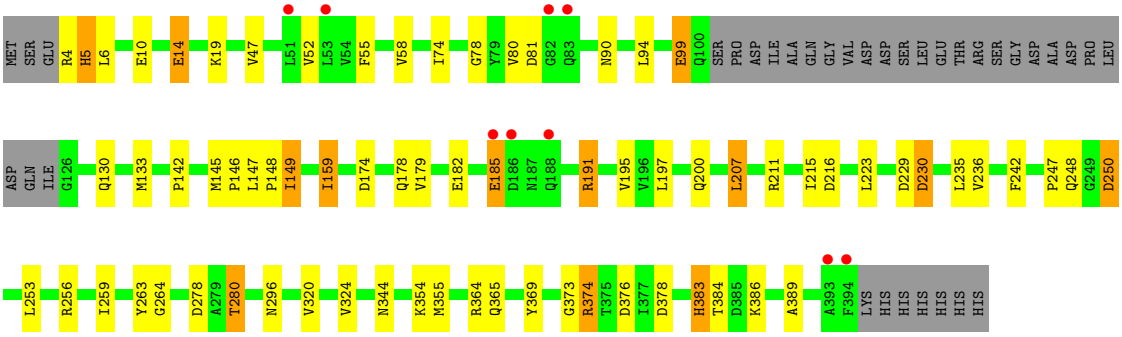
• Molecule 1: S-adenosylmethionine synthase





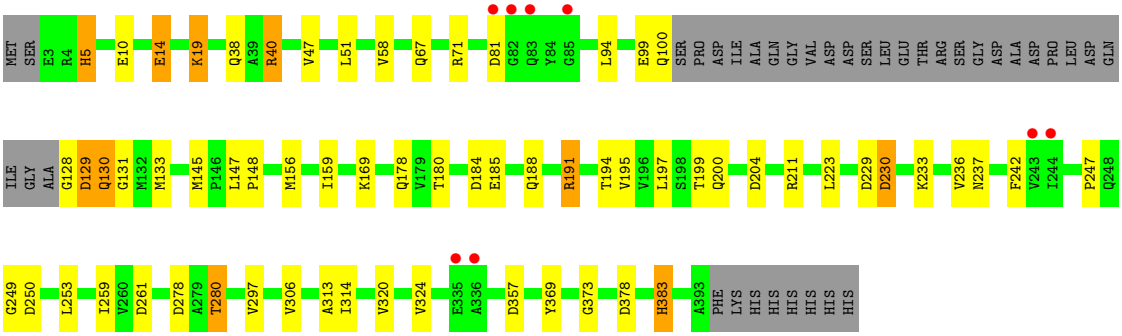
• Molecule 1: S-adenosylmethionine synthase

Chain G:



• Molecule 1: S-adenosylmethionine synthase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.43Å 110.93Å 112.66Å 93.82° 104.03° 99.59°	Depositor
Resolution (Å)	29.41 – 2.82 29.39 – 2.82	Depositor EDS
% Data completeness (in resolution range)	94.9 (29.41-2.82) 95.0 (29.39-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.156 , 0.275 0.153 , 0.274	Depositor DCC
R_{free} test set	3108 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.924	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22699	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PPK, ANP, SAM, K, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.70	0/2824	0.88	2/3836 (0.1%)
1	B	0.69	0/2809	0.87	3/3816 (0.1%)
1	C	0.69	0/2875	0.83	1/3904 (0.0%)
1	D	0.68	0/2857	0.87	4/3879 (0.1%)
1	E	0.69	0/2880	0.88	4/3910 (0.1%)
1	F	0.73	2/2855 (0.1%)	0.88	2/3879 (0.1%)
1	G	0.70	0/2834	0.88	4/3849 (0.1%)
1	H	0.70	0/2822	0.85	2/3833 (0.1%)
All	All	0.70	2/22756 (0.0%)	0.87	22/30906 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	335	GLU	CD-OE2	9.85	1.36	1.25
1	F	143	GLU	CD-OE1	-6.56	1.18	1.25

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	165	ASP	CB-CA-C	-10.66	89.08	110.40
1	D	172	ARG	CG-CD-NE	9.54	131.84	111.80
1	A	256	ARG	CG-CD-NE	9.39	131.52	111.80
1	B	172	ARG	CG-CD-NE	8.71	130.08	111.80
1	G	191	ARG	NE-CZ-NH1	-8.06	116.27	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	81	ASP	Peptide
1	C	83	GLN	Peptide
1	E	271	GLY	Peptide
1	F	143	GLU	Sidechain

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	2778	0	2762	37	2
1	B	2763	0	2749	41	0
1	C	2827	0	2818	34	0
1	D	2810	0	2800	61	0
1	E	2832	0	2816	70	0
1	F	2807	0	2792	62	0
1	G	2787	0	2771	71	0
1	H	2776	0	2760	47	2
2	A	11	0	8	0	0
2	H	11	0	8	0	0
3	A	13	0	1	1	0
3	B	13	0	1	1	0
3	G	13	0	1	0	0
3	H	13	0	1	0	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	3	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	C	31	0	13	2	0
6	D	31	0	13	2	0
6	E	31	0	13	6	0
6	F	31	0	13	3	0
7	G	27	0	22	2	0
7	H	27	0	22	4	0
8	A	6	0	0	1	0
8	B	5	0	0	0	0
8	C	6	0	0	1	0
8	D	6	0	0	1	0
8	E	4	0	0	0	0
8	F	7	0	0	0	0
8	G	6	0	0	1	0
8	H	6	0	0	0	0
All	All	22699	0	22384	375	2

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 8.

The worst 5 of 375 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:E:297:VAL:HG21	1:E:306:VAL:HG11	1.33	1.08
1:G:191:ARG:HD2	1:G:229:ASP:OD2	1.56	1.06
1:B:90:ASN:HD21	1:D:244:ILE:HD11	1.23	1.03
1:G:149:ILE:HD12	1:G:149:ILE:H	1.24	0.98
1:F:13:SER:HB3	1:F:156:MET:HE1	1.46	0.98

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD2	1:H:357:ASP:OD2[1_565]	1.70	0.50
1:A:165:ASP:OD2	1:H:204:ASP:OD2[1_665]	1.95	0.25

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	360/401 (90%)	335 (93%)	24 (7%)	1 (0%)	41 70
1	B	358/401 (89%)	335 (94%)	23 (6%)	0	100 100
1	C	367/401 (92%)	345 (94%)	22 (6%)	0	100 100
1	D	365/401 (91%)	340 (93%)	24 (7%)	1 (0%)	41 70
1	E	367/401 (92%)	342 (93%)	25 (7%)	0	100 100
1	F	365/401 (91%)	342 (94%)	23 (6%)	0	100 100
1	G	362/401 (90%)	340 (94%)	22 (6%)	0	100 100
1	H	360/401 (90%)	334 (93%)	25 (7%)	1 (0%)	41 70
All	All	2904/3208 (90%)	2713 (93%)	188 (6%)	3 (0%)	51 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	130	GLN
1	A	184	ASP
1	D	184	ASP

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	295/325 (91%)	273 (92%)	22 (8%)	13 35
1	B	293/325 (90%)	270 (92%)	23 (8%)	12 33
1	C	299/325 (92%)	275 (92%)	24 (8%)	12 32
1	D	297/325 (91%)	281 (95%)	16 (5%)	22 51
1	E	299/325 (92%)	271 (91%)	28 (9%)	8 25
1	F	297/325 (91%)	273 (92%)	24 (8%)	11 32
1	G	294/325 (90%)	270 (92%)	24 (8%)	11 31
1	H	294/325 (90%)	276 (94%)	18 (6%)	18 46
All	All	2368/2600 (91%)	2189 (92%)	179 (8%)	13 35

5 of 179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	19	LYS
1	G	99	GLU
1	F	122	LEU
1	F	230	ASP
1	G	215	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	38	GLN
1	H	130	GLN
1	C	268	HIS
1	C	248	GLN
1	H	231	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 21 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
2	PHE	H	502	-	10,11,12	0.40	0	10,13,15	0.35	0
6	ANP	E	501	4	29,33,33	1.48	3 (10%)	31,52,52	1.25	5 (16%)
3	PPK	G	501	4	11,12,12	2.07	4 (36%)	15,20,20	1.68	4 (26%)
3	PPK	A	502	5,4	11,12,12	2.06	4 (36%)	15,20,20	1.50	3 (20%)
3	PPK	H	503	5,4	11,12,12	1.86	4 (36%)	15,20,20	1.54	2 (13%)
7	SAM	G	502	-	24,29,29	0.67	1 (4%)	23,42,42	1.07	4 (17%)
2	PHE	A	501	-	10,11,12	0.50	0	10,13,15	0.51	0
6	ANP	D	501	5,4	29,33,33	1.44	4 (13%)	31,52,52	1.54	8 (25%)
6	ANP	F	501	5,4	29,33,33	1.34	5 (17%)	31,52,52	1.39	3 (9%)
6	ANP	C	501	5,4	29,33,33	1.36	4 (13%)	31,52,52	1.47	5 (16%)
3	PPK	B	501	4	11,12,12	2.31	3 (27%)	15,20,20	1.87	5 (33%)
7	SAM	H	501	-	24,29,29	0.74	1 (4%)	23,42,42	1.46	3 (13%)

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
2	PHE	H	502	-	-	3/5/6/8	0/1/1/1
6	ANP	E	501	4	-	6/14/38/38	0/3/3/3
3	PPK	G	501	4	-	5/8/12/12	-
3	PPK	A	502	5,4	-	1/8/12/12	-
3	PPK	H	503	5,4	-	2/8/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SAM	G	502	-	-	7/12/33/33	0/3/3/3
2	PHE	A	501	-	-	4/5/6/8	0/1/1/1
6	ANP	D	501	5,4	-	4/14/38/38	0/3/3/3
6	ANP	F	501	5,4	-	6/14/38/38	0/3/3/3
6	ANP	C	501	5,4	-	6/14/38/38	0/3/3/3
3	PPK	B	501	4	-	2/8/12/12	-
7	SAM	H	501	-	-	8/12/33/33	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	PPK	PG-O3G	4.06	1.52	1.46
6	D	501	ANP	PG-O1G	3.99	1.52	1.46
3	B	501	PPK	PG-O3G	3.98	1.52	1.46
3	B	501	PPK	PB-O3A	3.98	1.64	1.59
3	G	501	PPK	PG-O3G	3.97	1.52	1.46

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	501	ANP	O2G-PG-O1G	-4.33	102.56	113.45
7	H	501	SAM	OXT-C-O	-3.90	115.23	124.09
6	F	501	ANP	O2B-PB-O1B	3.88	118.06	109.92
6	C	501	ANP	O3G-PG-O1G	-3.88	103.71	113.45
3	B	501	PPK	O1G-PG-O3G	-3.87	103.71	113.45

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PHE	C-CA-CB-CG
2	H	502	PHE	O-C-CA-CB
2	H	502	PHE	N-CA-CB-CG
2	H	502	PHE	C-CA-CB-CG
3	A	502	PPK	PB-N3B-PG-O3G

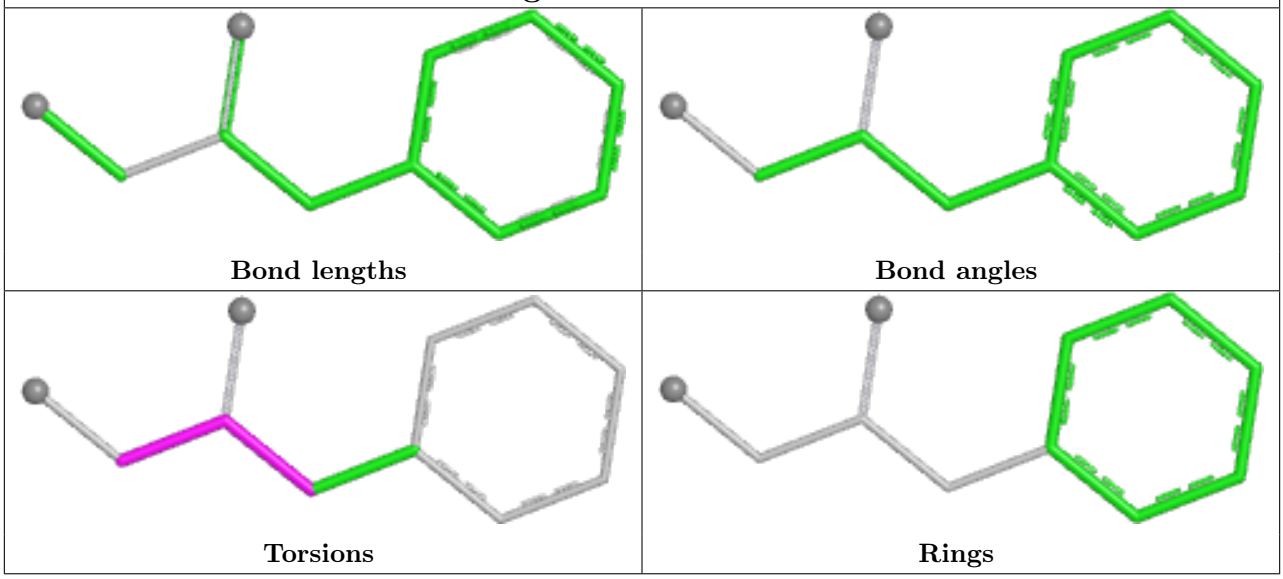
There are no ring outliers.

8 monomers are involved in 21 short contacts:

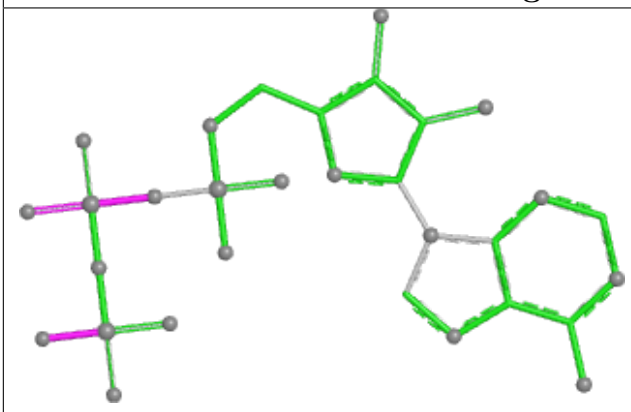
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	501	ANP	6	0
3	A	502	PPK	1	0
7	G	502	SAM	2	0
6	D	501	ANP	2	0
6	F	501	ANP	3	0
6	C	501	ANP	2	0
3	B	501	PPK	1	0
7	H	501	SAM	4	0

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 then 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.

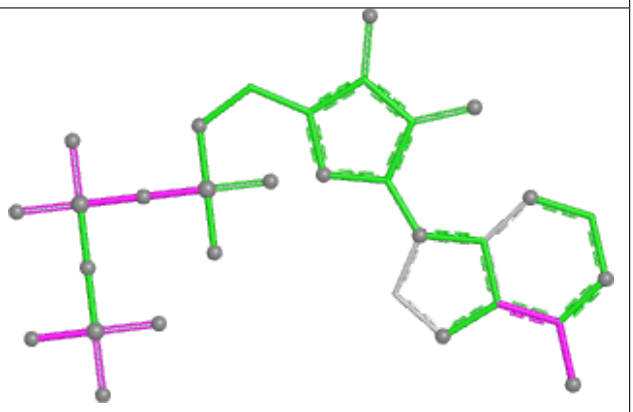
Ligand PHE H 502



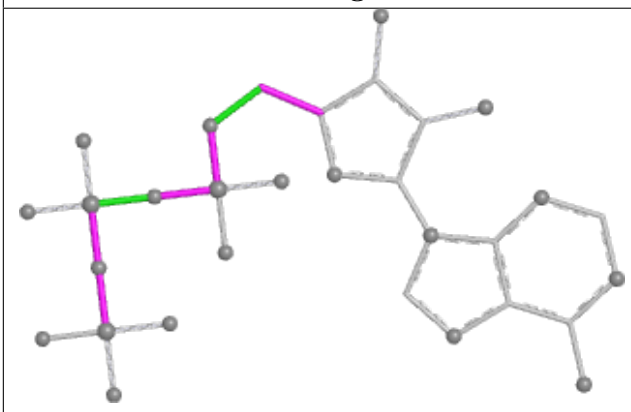
Ligand ANP E 501



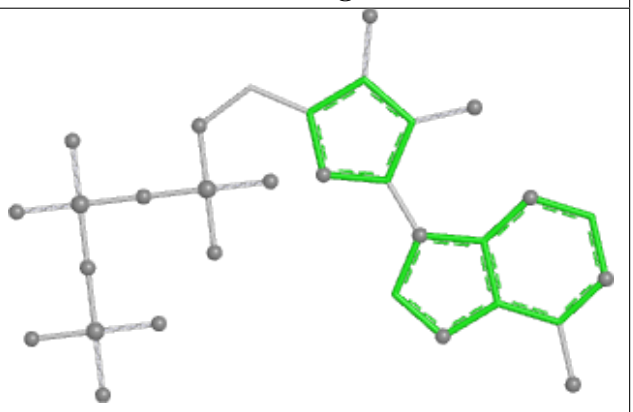
Bond lengths



Bond angles



Torsions



Rings

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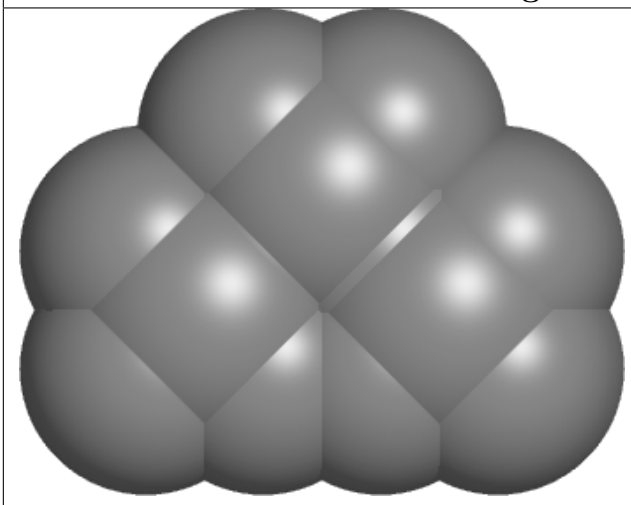	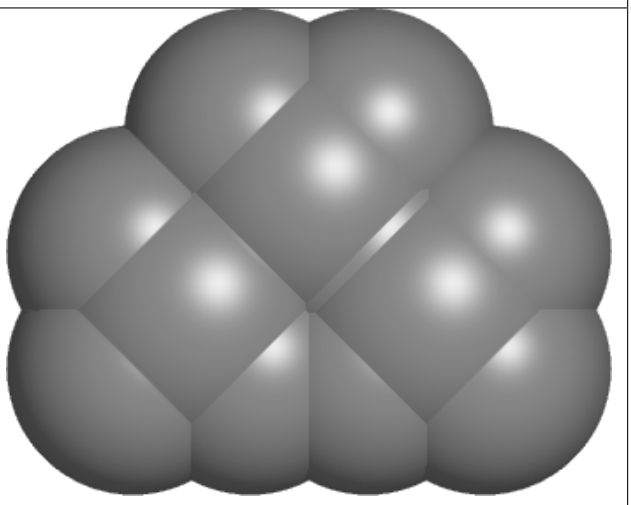
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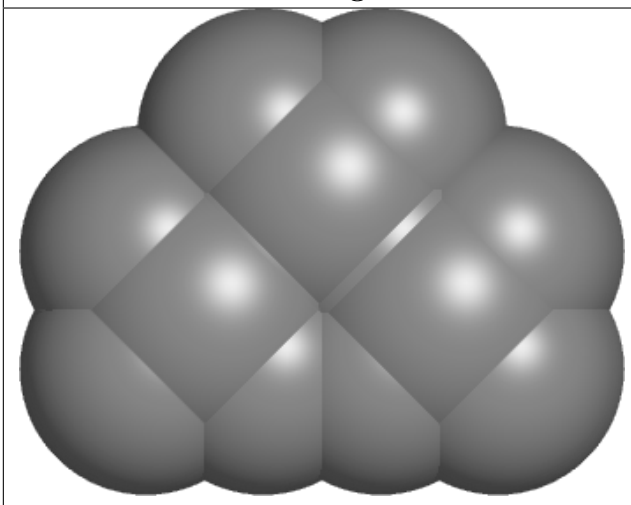
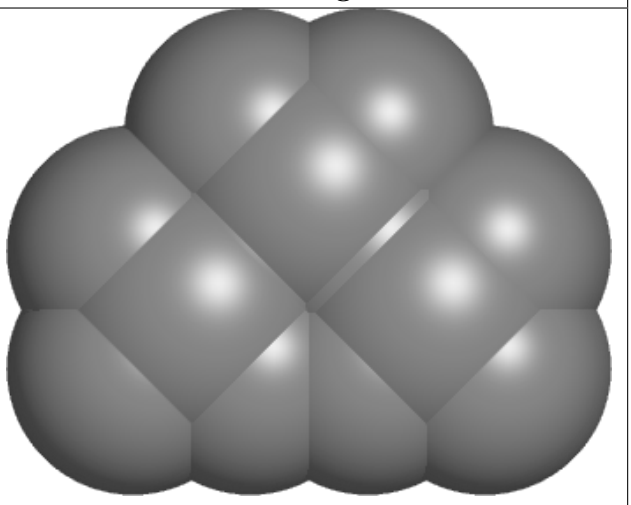
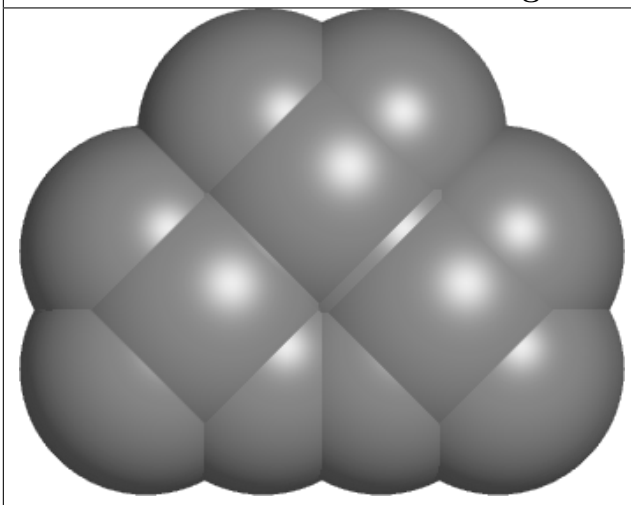
	
Torsions	**Rings**

Ligand PPK A 502



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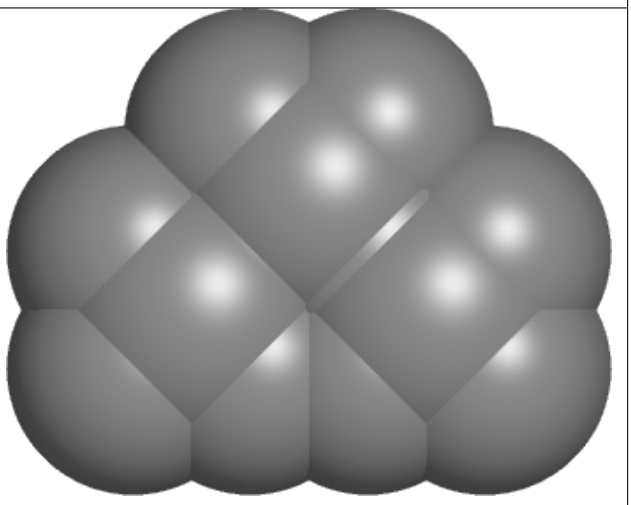
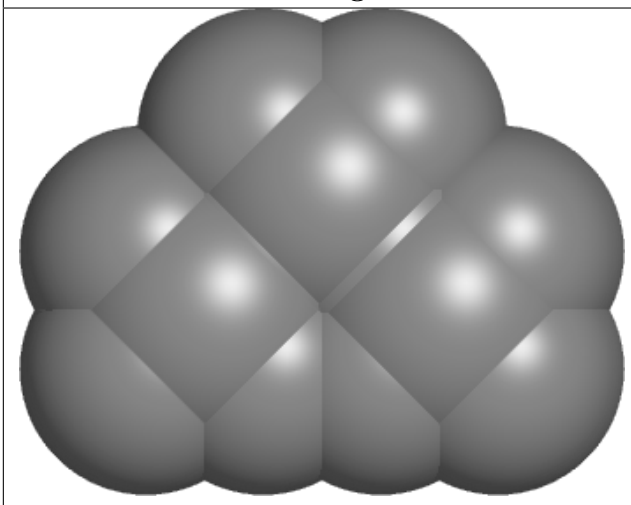


Bond angles



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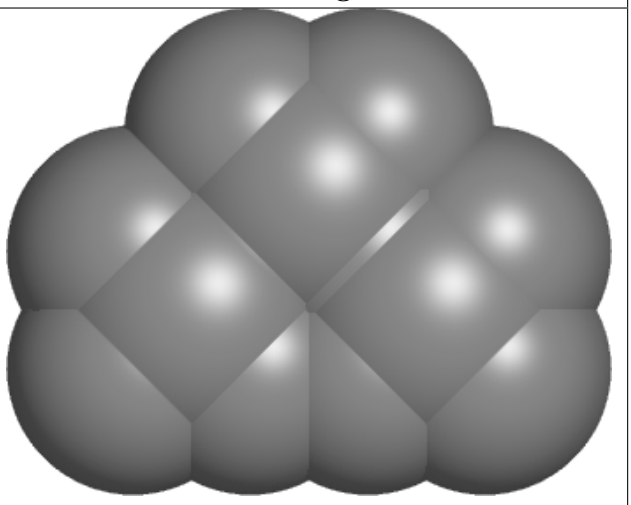

Rings

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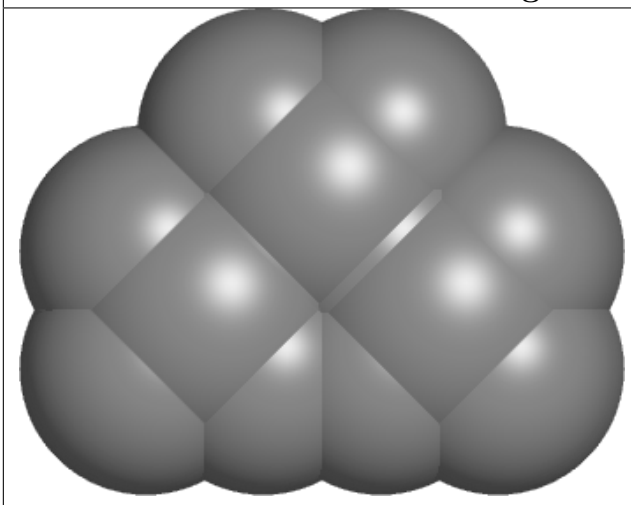
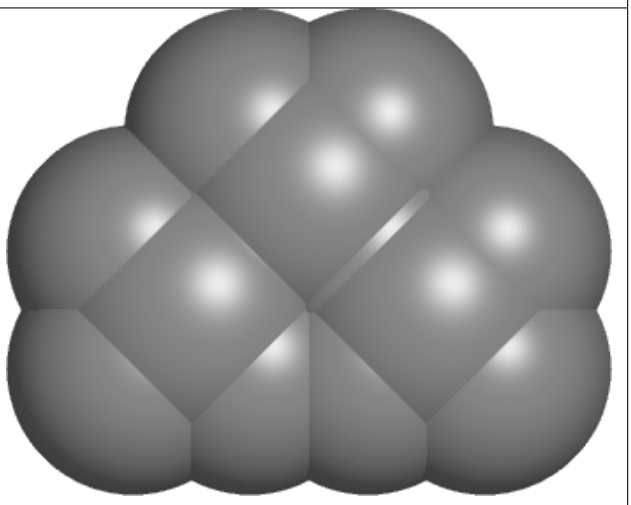
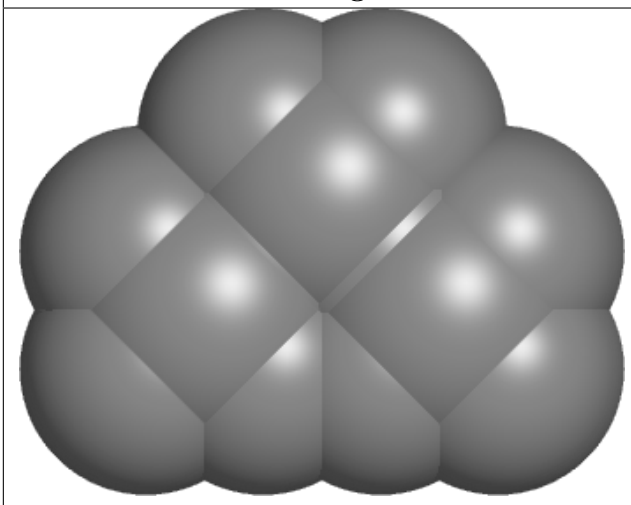
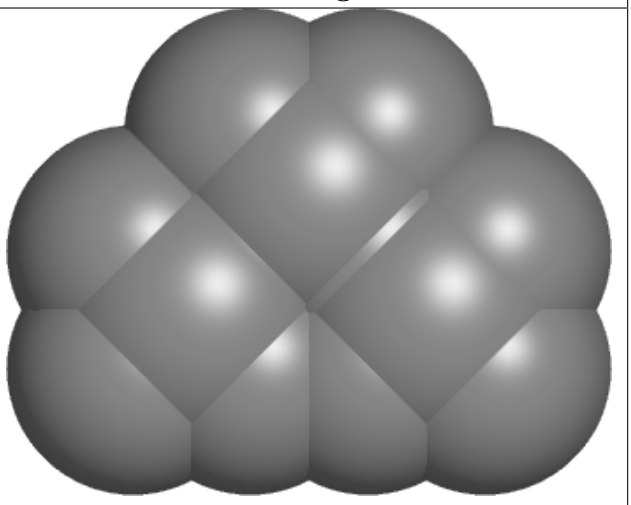
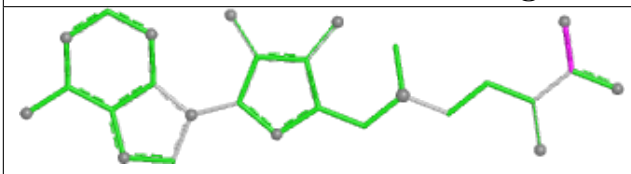
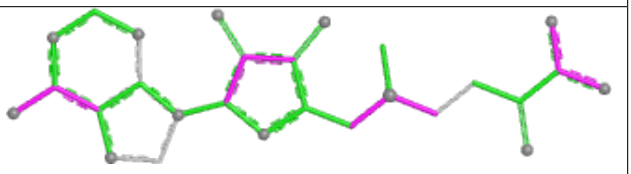
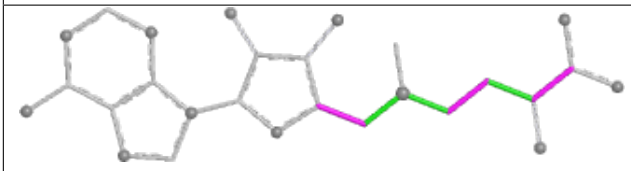
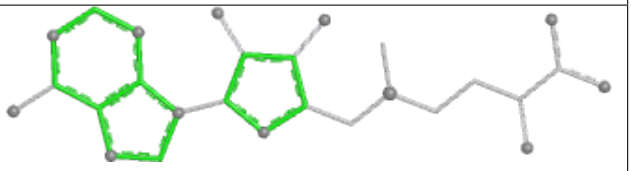
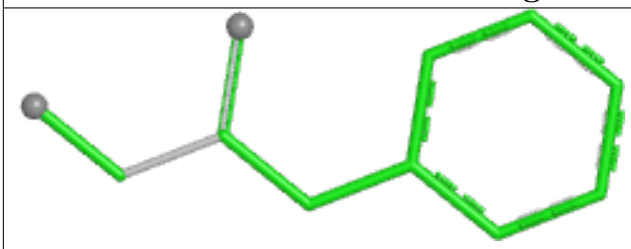
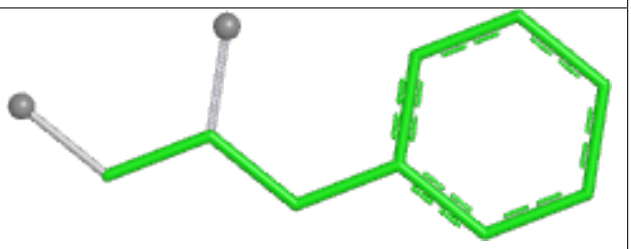
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand SAM G 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

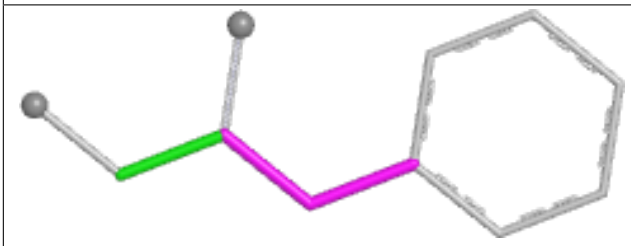
Ligand PHE A 501



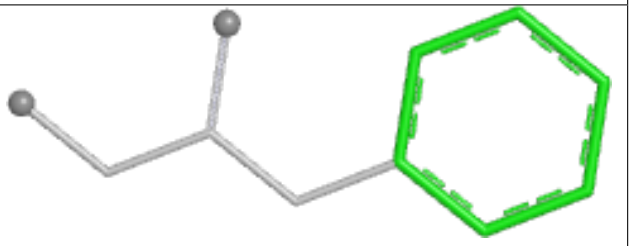
Bond lengths



Bond angles

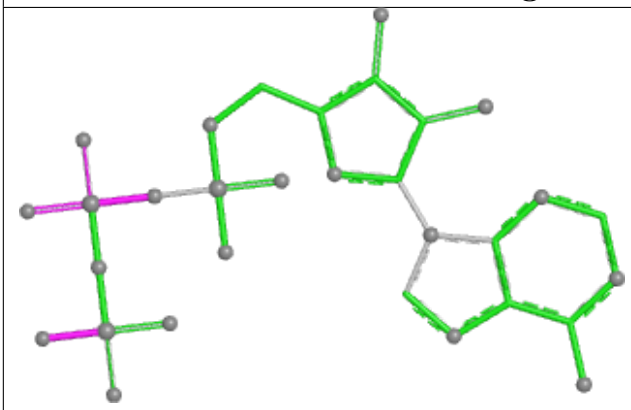


Torsions



Rings

Ligand ANP D 501



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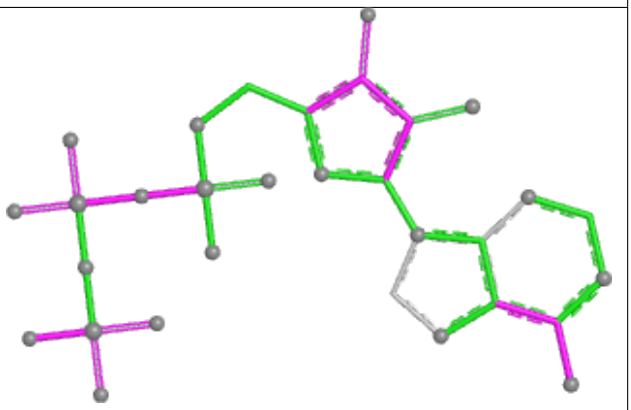
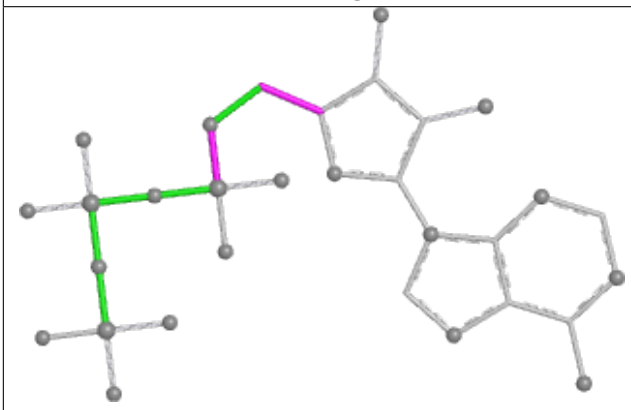
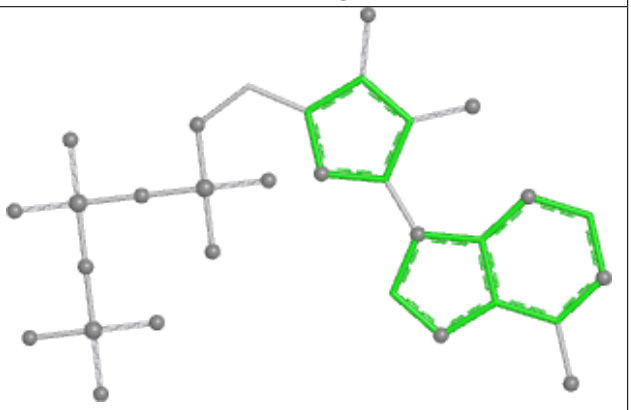


Bond angles

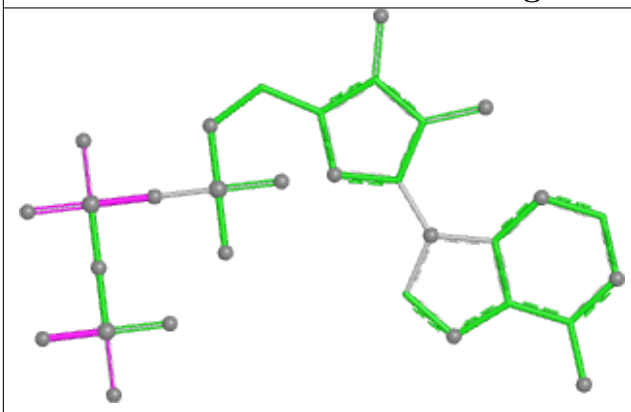


Torsions

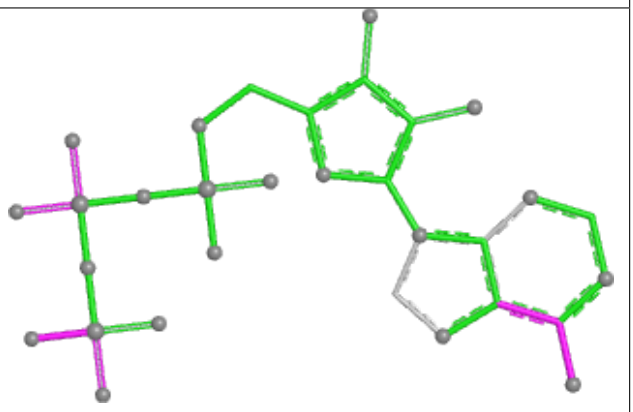


Rings

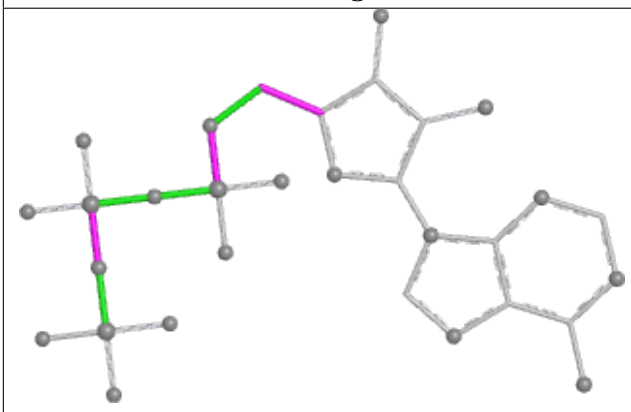
Ligand ANP F 501



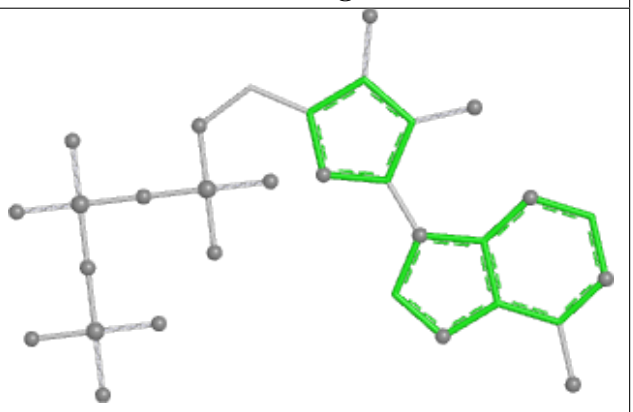
Bond lengths



Bond angles

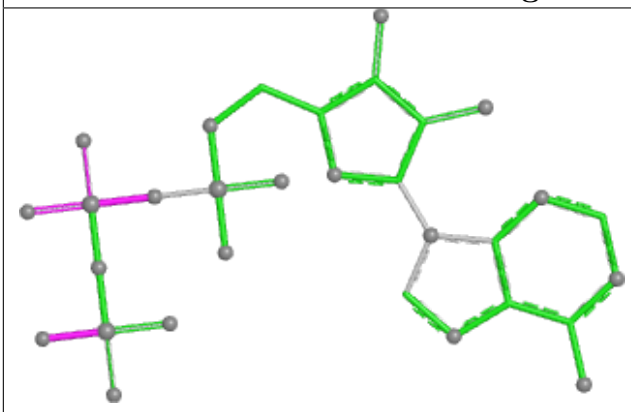


Torsions

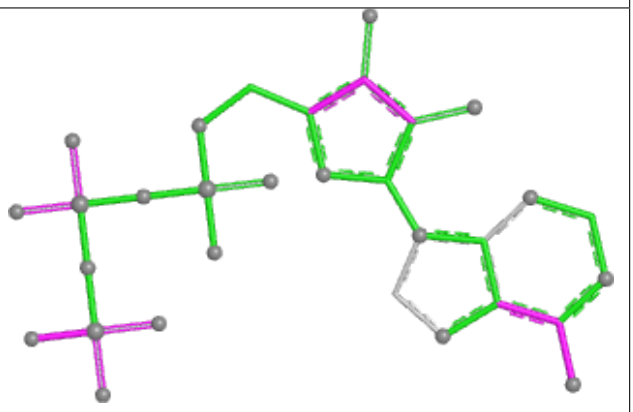


Rings

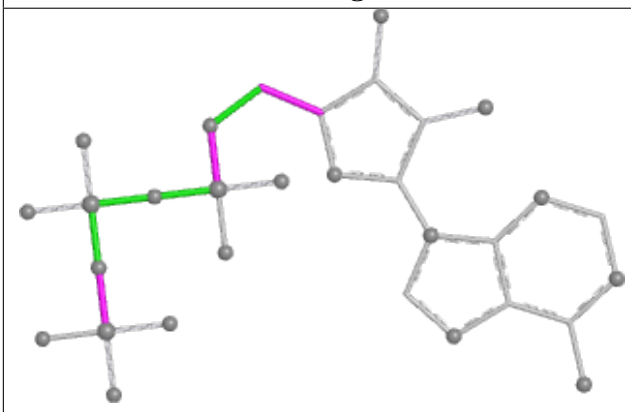
Ligand ANP C 501



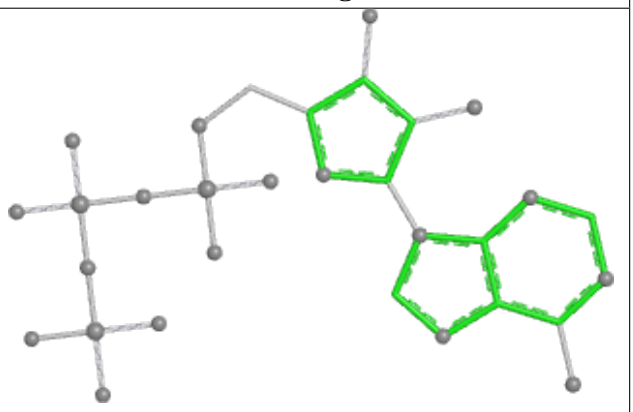
Bond lengths



Bond angles

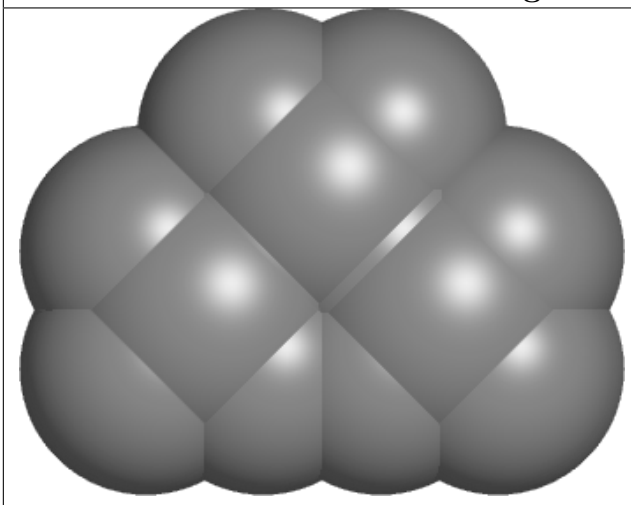


Torsions

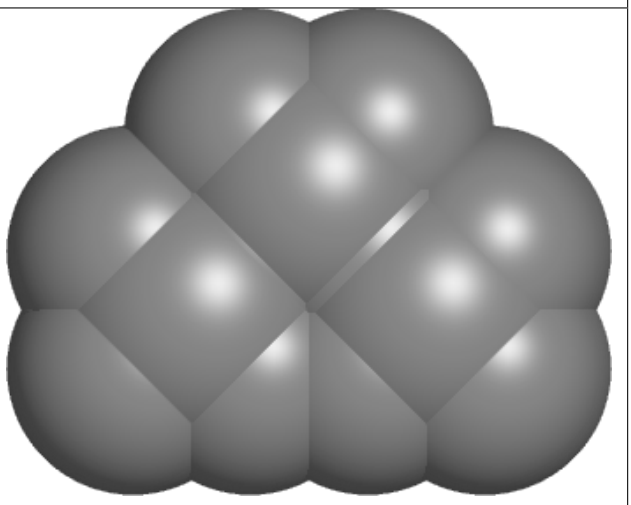


Rings

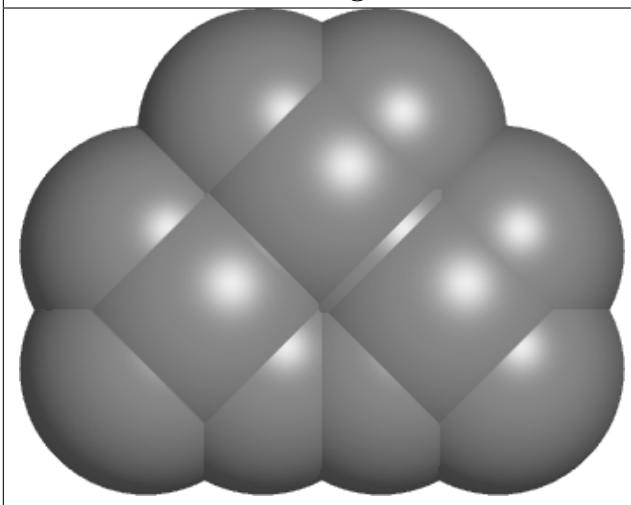
Ligand PPK B 501



Bond lengths



Bond angles



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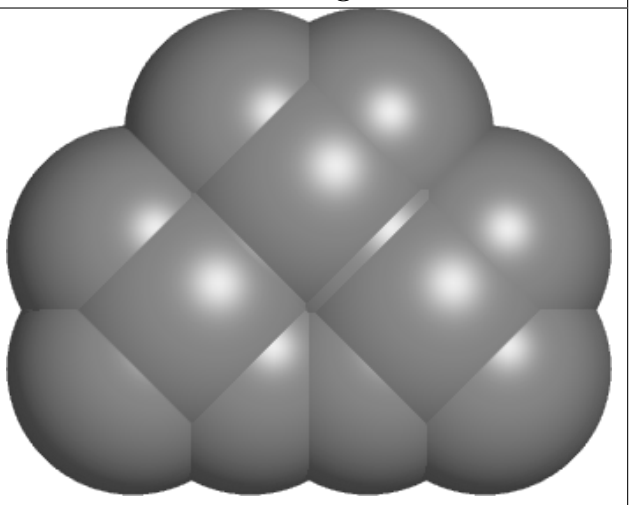
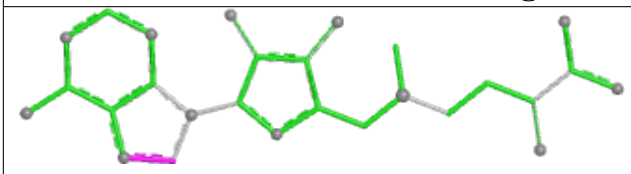
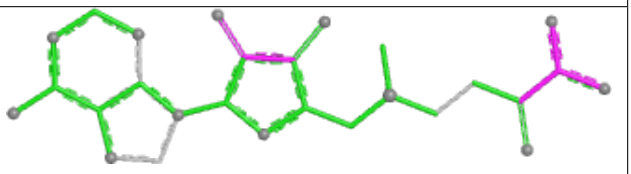


Rings

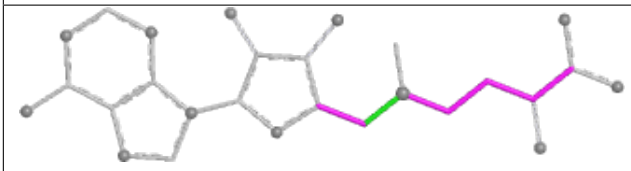
Ligand SAM H 501



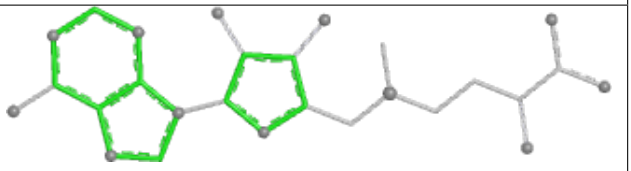
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	364/401 (90%)	-0.19	15 (4%) 37 27	47, 68, 97, 125	0
1	B	362/401 (90%)	-0.08	5 (1%) 75 69	49, 72, 95, 129	0
1	C	371/401 (92%)	0.08	18 (4%) 29 20	55, 75, 101, 121	0
1	D	369/401 (92%)	0.03	13 (3%) 44 34	51, 76, 109, 122	0
1	E	371/401 (92%)	-0.05	13 (3%) 44 34	44, 69, 96, 137	0
1	F	369/401 (92%)	0.16	29 (7%) 12 7	46, 72, 107, 125	0
1	G	366/401 (91%)	-0.16	9 (2%) 57 47	47, 66, 90, 117	0
1	H	364/401 (90%)	-0.30	8 (2%) 62 52	47, 63, 91, 116	0
All	All	2936/3208 (91%)	-0.06	110 (3%) 41 31	44, 70, 101, 137	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	82	GLY	7.2
1	E	394	PHE	4.6
1	G	186	ASP	4.5
1	F	228	LEU	4.4
1	F	183	TYR	4.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

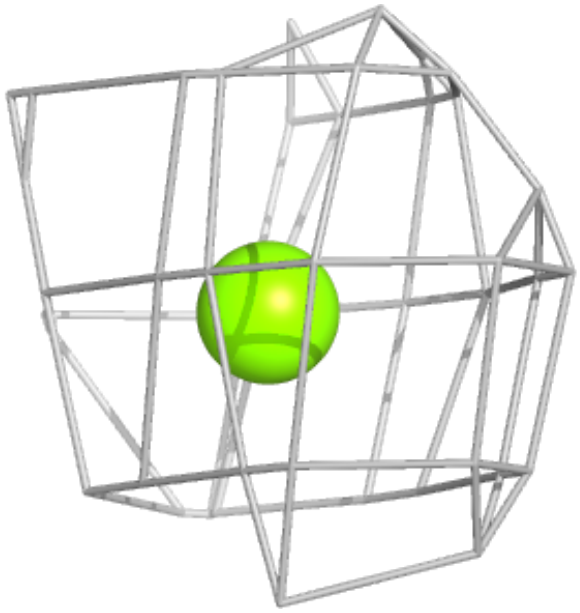
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	C	503	1/1	0.56	0.25	82,82,82,82	0
7	SAM	G	502	27/27	0.70	0.36	78,125,150,153	0
6	ANP	C	501	31/31	0.71	0.29	89,134,164,167	0
2	PHE	H	502	11/12	0.77	0.34	95,100,104,108	0
7	SAM	H	501	27/27	0.77	0.30	74,133,145,156	0
6	ANP	E	501	31/31	0.79	0.24	92,129,173,191	0
2	PHE	A	501	11/12	0.80	0.39	84,89,106,106	0
4	MG	D	502	1/1	0.80	0.33	95,95,95,95	0
4	MG	F	502	1/1	0.85	0.45	91,91,91,91	0
6	ANP	D	501	31/31	0.86	0.22	93,135,167,185	0
6	ANP	F	501	31/31	0.86	0.24	103,134,163,177	0
4	MG	A	505	1/1	0.88	0.32	98,98,98,98	0
3	PPK	A	502	13/13	0.88	0.15	97,126,152,159	0
3	PPK	B	501	13/13	0.89	0.16	89,119,149,152	0
3	PPK	G	501	13/13	0.90	0.16	109,144,173,176	0
4	MG	A	504	1/1	0.90	0.21	82,82,82,82	0
4	MG	G	503	1/1	0.91	0.64	90,90,90,90	0
3	PPK	H	503	13/13	0.92	0.16	90,136,172,183	0
4	MG	C	502	1/1	0.92	0.28	86,86,86,86	0
5	K	F	505	1/1	0.92	0.19	121,121,121,121	0
5	K	C	504	1/1	0.93	0.10	121,121,121,121	0
4	MG	G	504	1/1	0.93	0.18	77,77,77,77	0
4	MG	H	505	1/1	0.95	0.20	95,95,95,95	0
4	MG	A	503	1/1	0.95	0.13	97,97,97,97	0
4	MG	F	504	1/1	0.95	0.33	83,83,83,83	0
4	MG	D	503	1/1	0.97	0.16	80,80,80,80	0
4	MG	F	503	1/1	0.97	0.24	82,82,82,82	0
4	MG	H	504	1/1	0.97	0.17	92,92,92,92	0
4	MG	E	502	1/1	0.97	0.18	84,84,84,84	0
5	K	D	504	1/1	0.98	0.09	92,92,92,92	0
5	K	H	506	1/1	0.98	0.16	113,113,113,113	0
4	MG	B	502	1/1	0.99	0.18	70,70,70,70	0
5	K	A	506	1/1	0.99	0.21	110,110,110,110	0

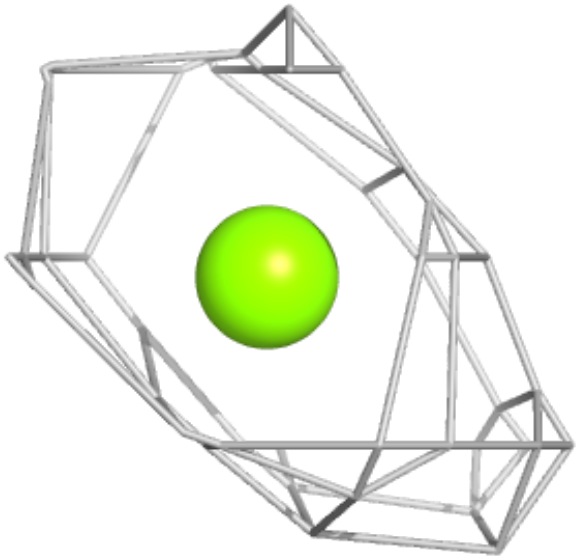
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

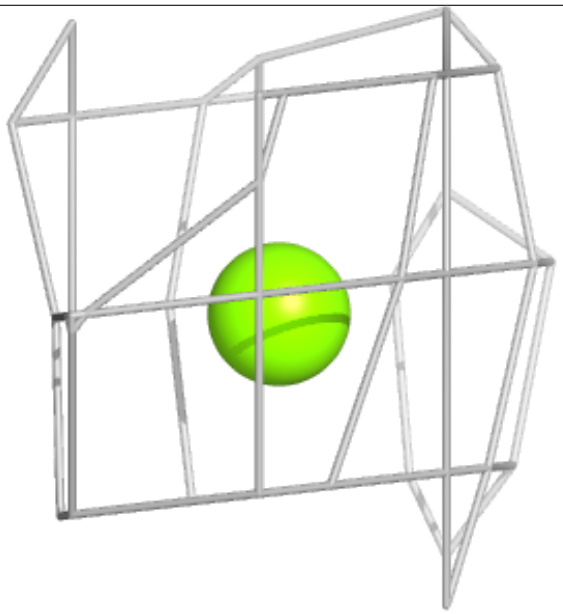
orientation to approximate a three-dimensional view.

Electron density around MG C 503:

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

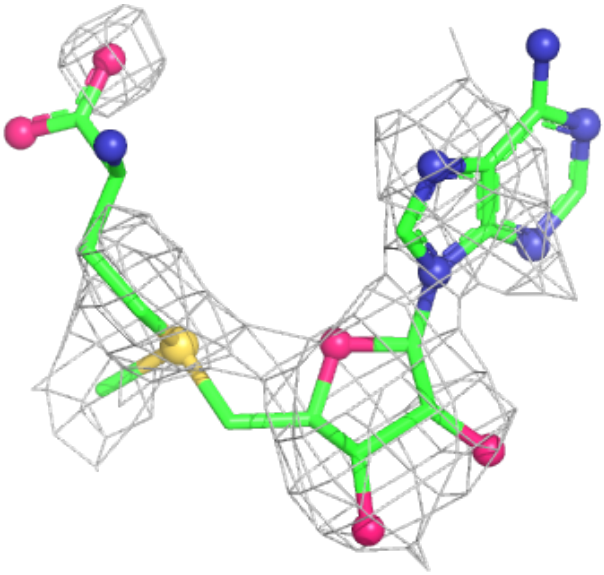


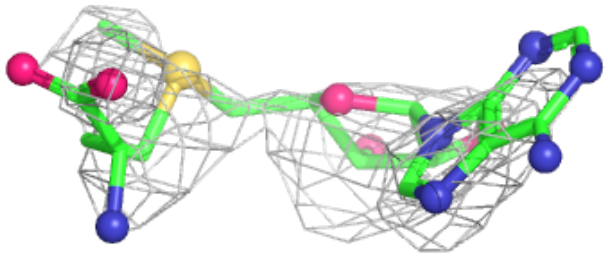


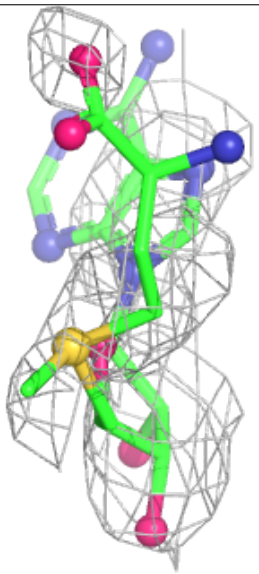


Electron density around SAM G 502:

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

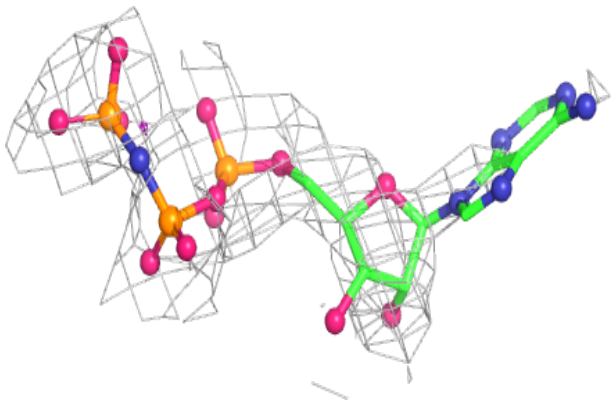


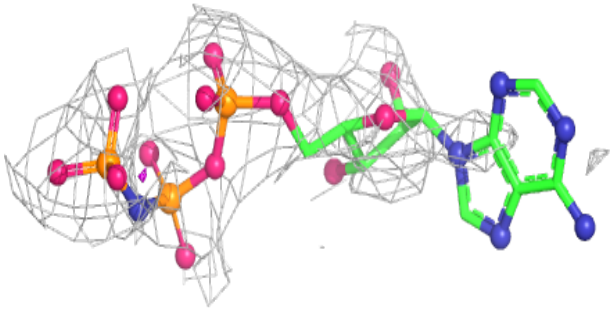


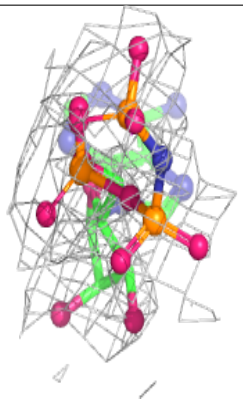


Electron density around ANP C 501:

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

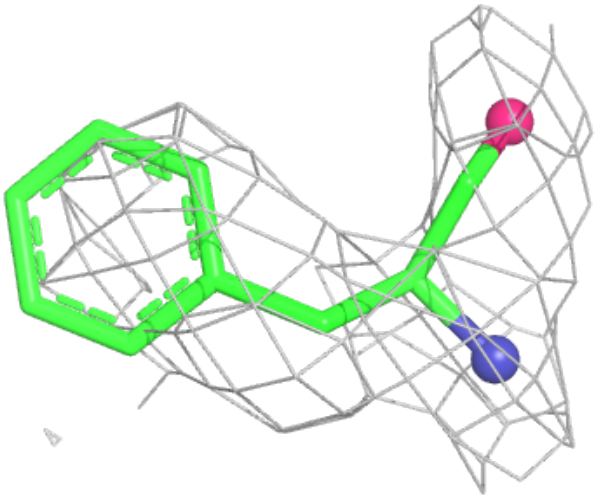


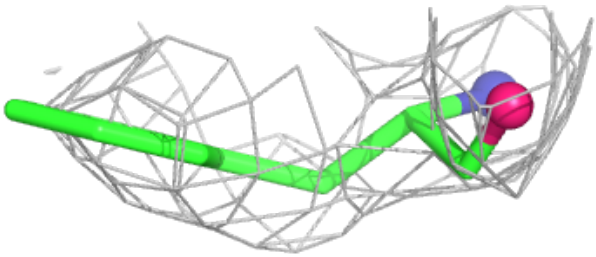


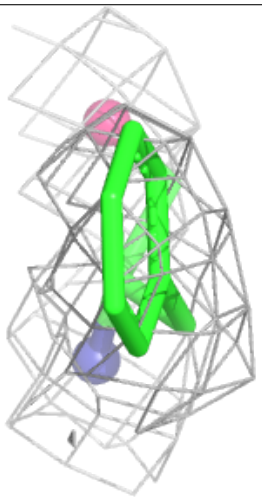


Electron density around PHE H 502:

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

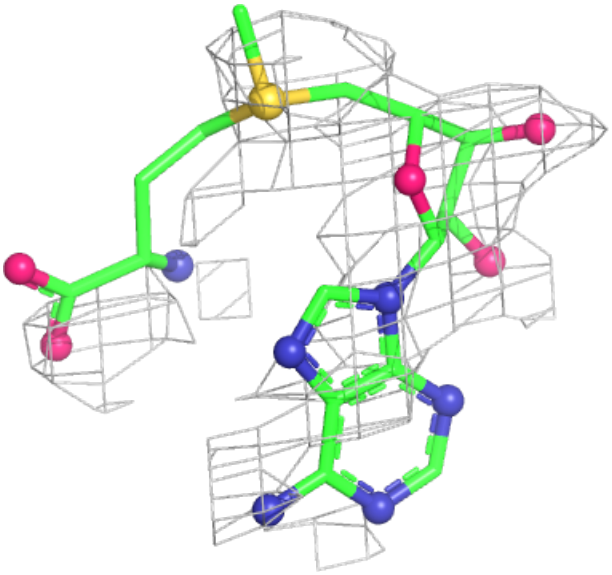


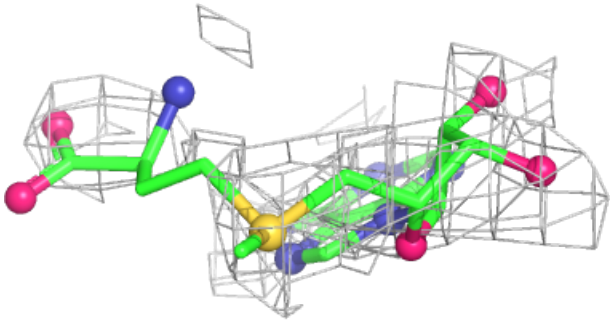


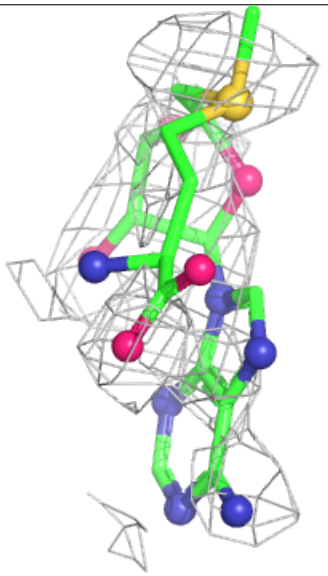


Electron density around SAM H 501:

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

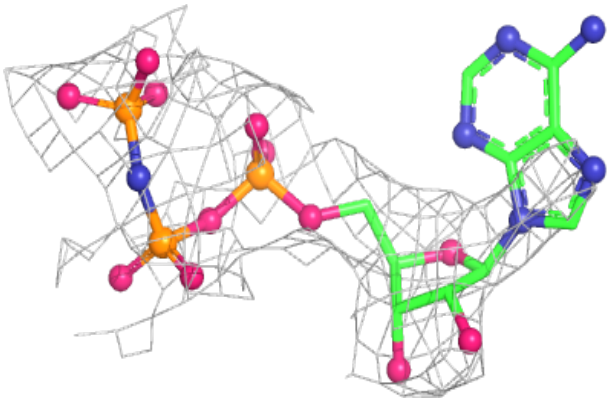


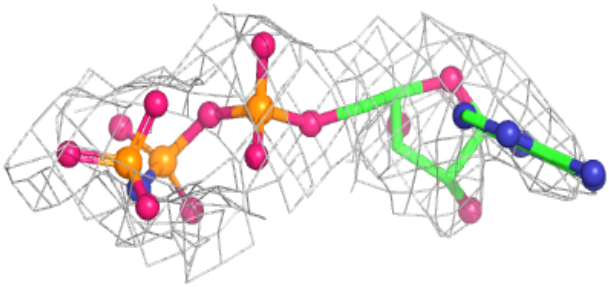


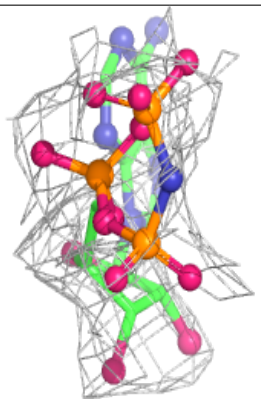


Electron density around ANP E 501:

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

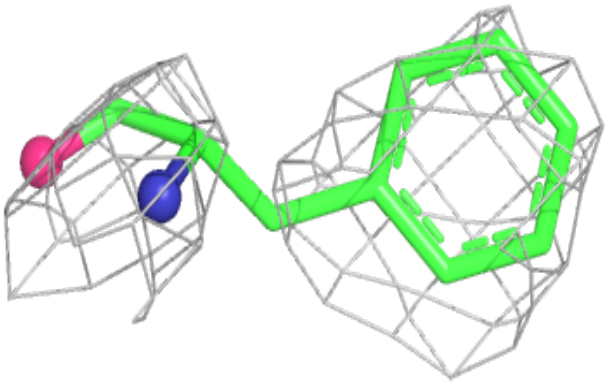


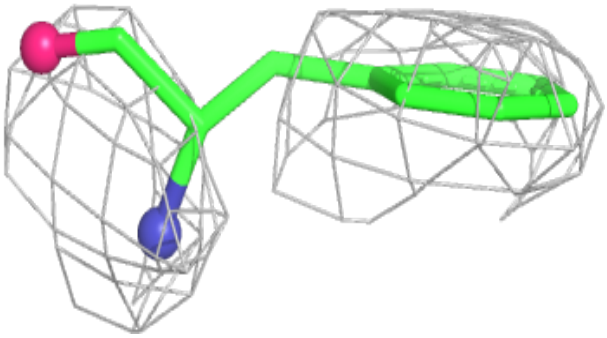


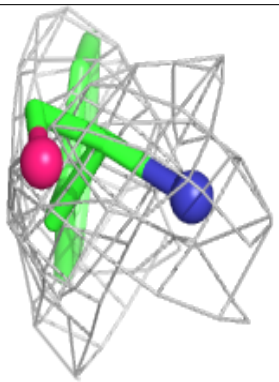


Electron density around PHE A 501:

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

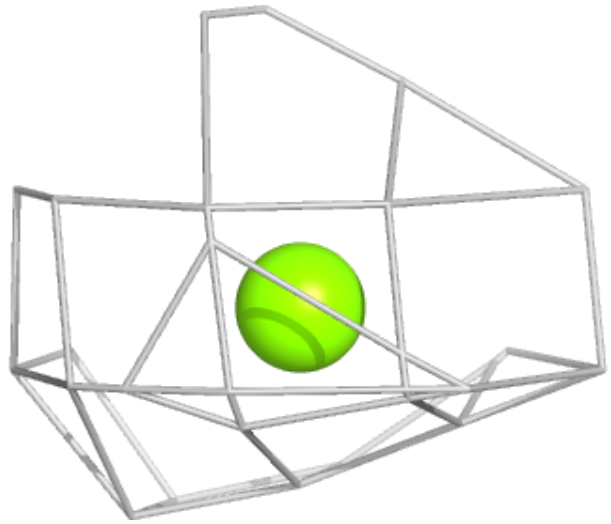


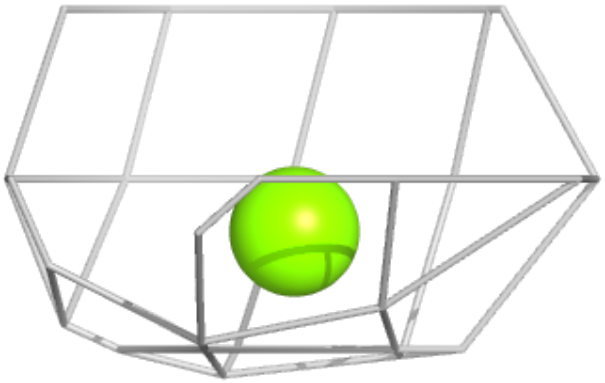


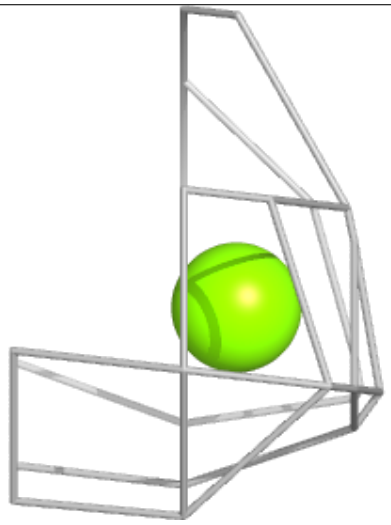


Electron density around MG D 502:

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

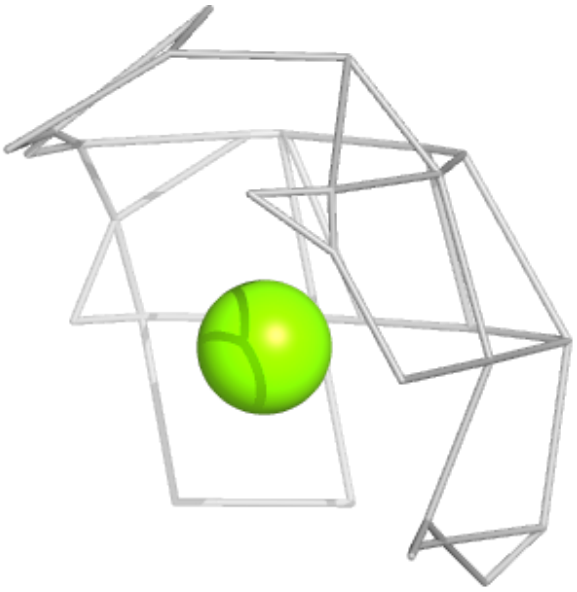


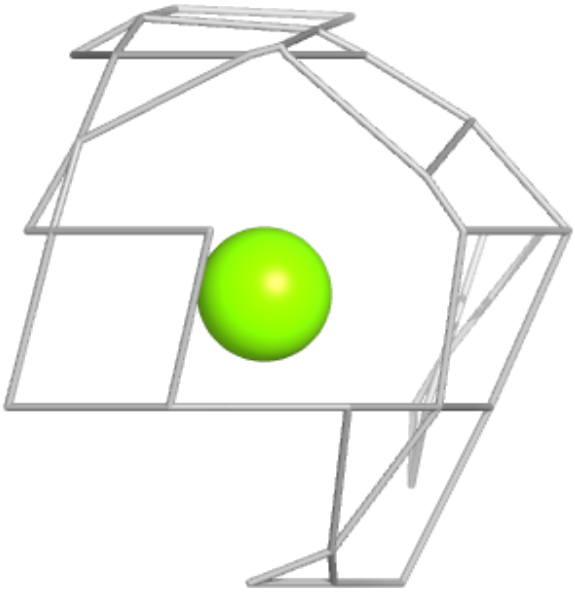


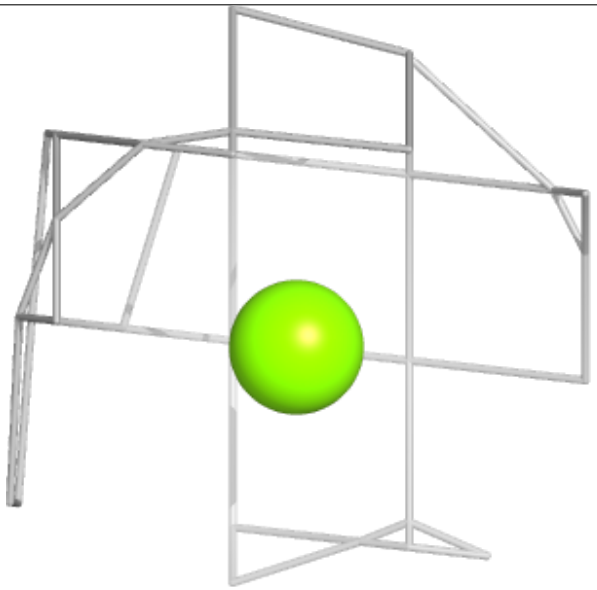


Electron density around MG F 502:

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

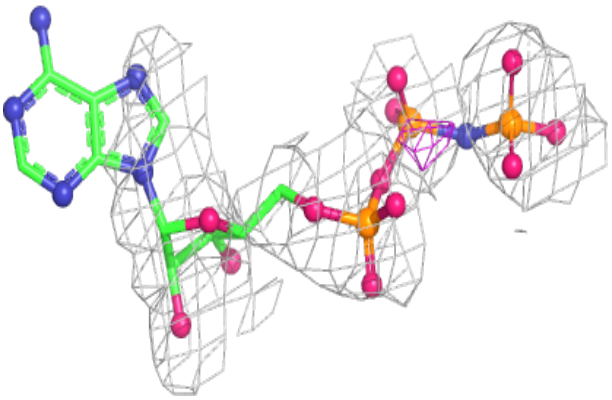


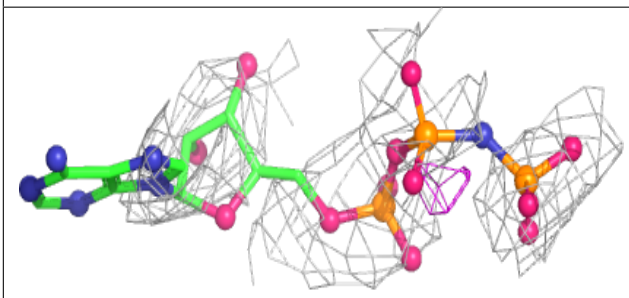


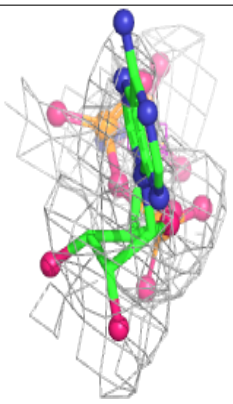


Electron density around ANP D 501:

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

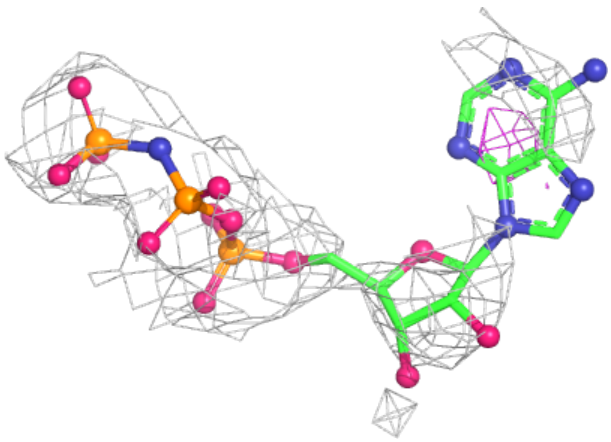


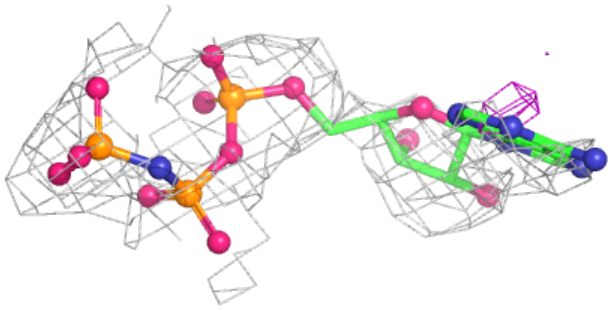


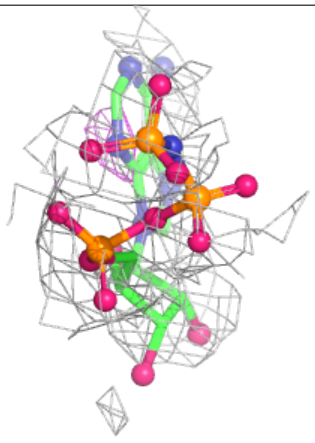


Electron density around ANP F 501:

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

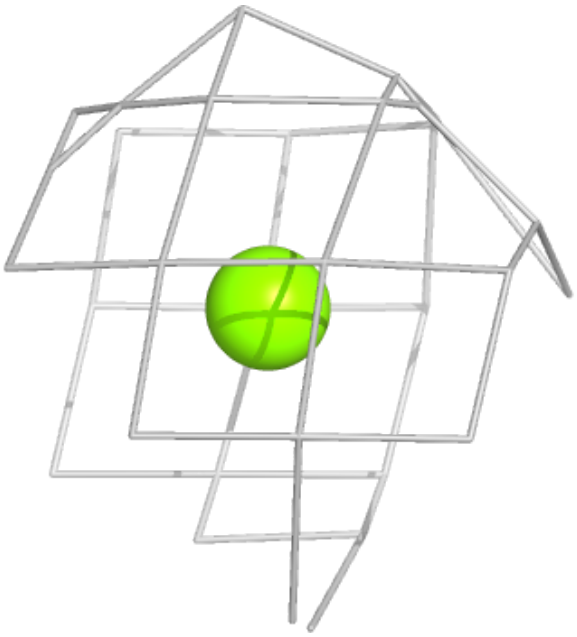


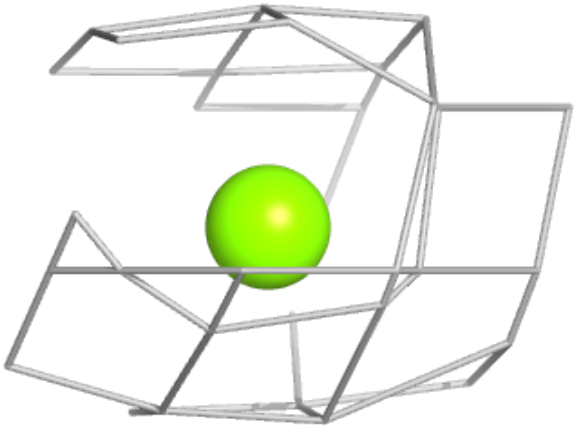


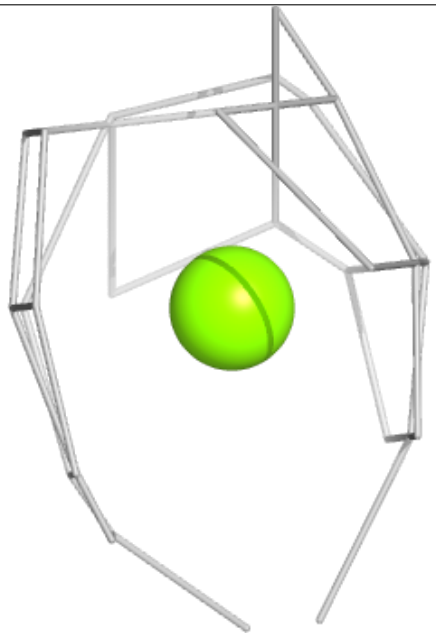


Electron density around MG A 505:

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

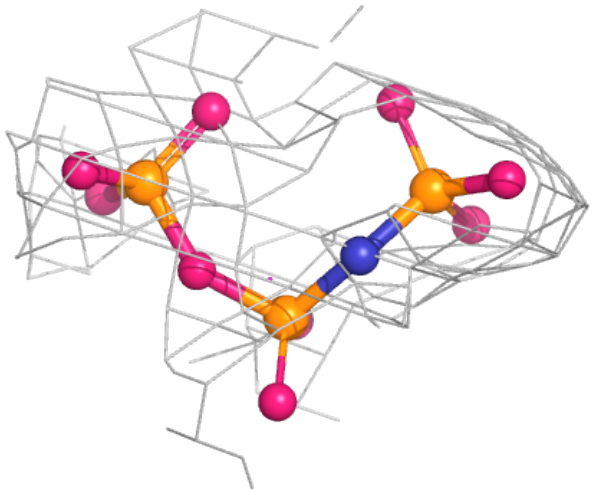


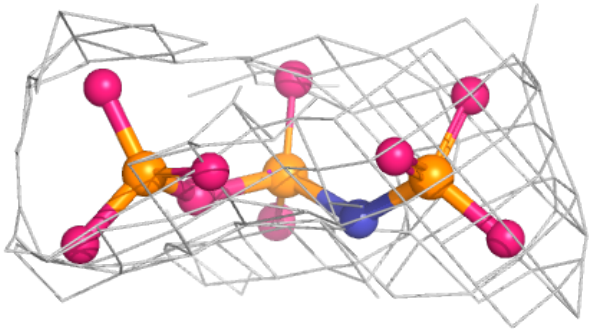


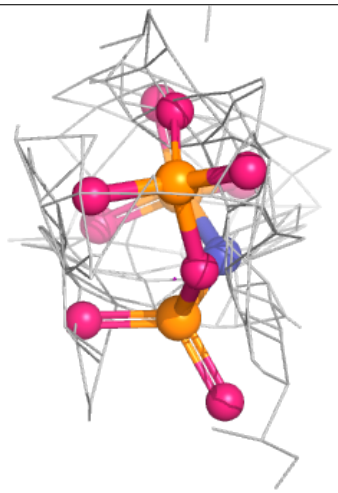


Electron density around PPK A 502:

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

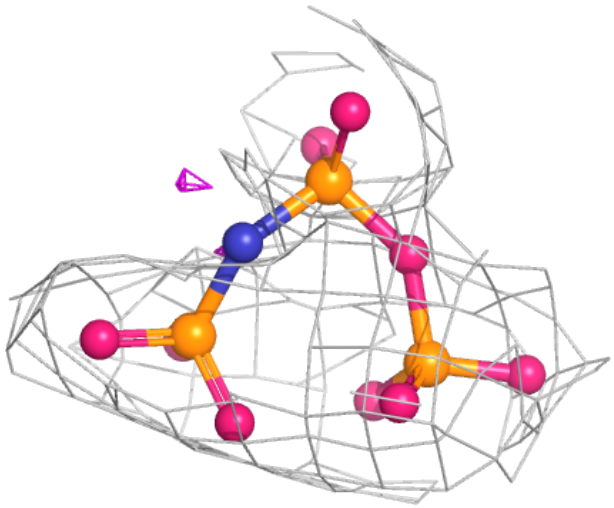


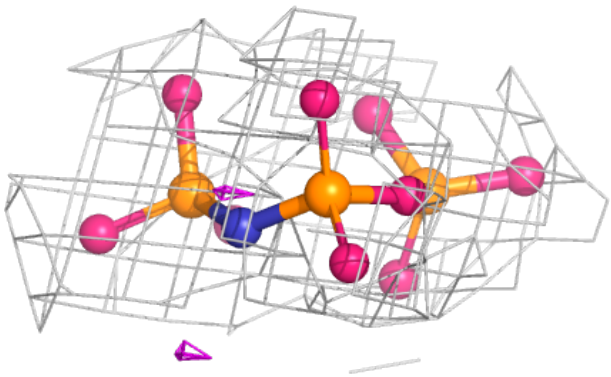


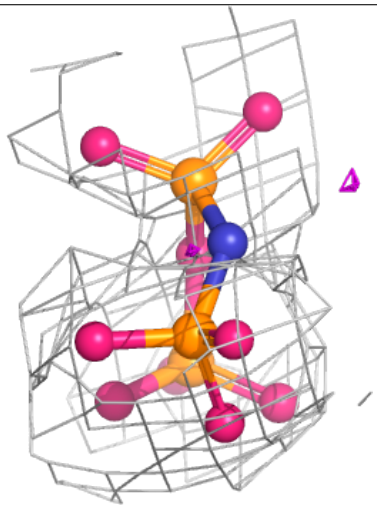


Electron density around PPK B 501:

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

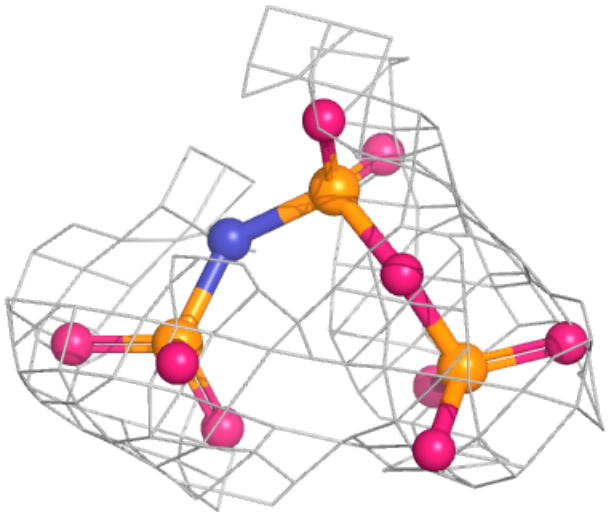


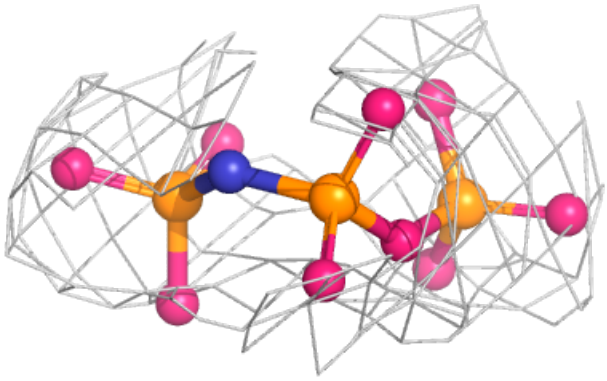


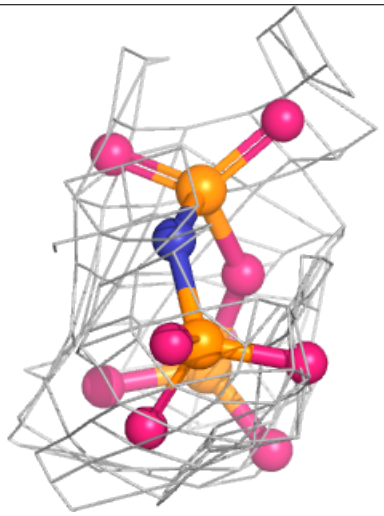


Electron density around PPK G 501:

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

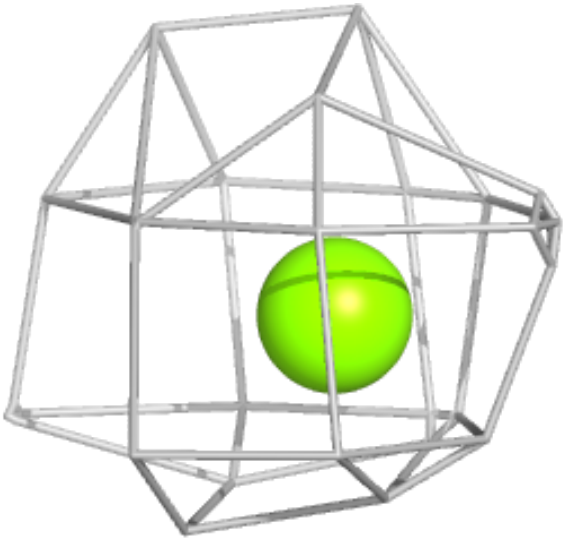


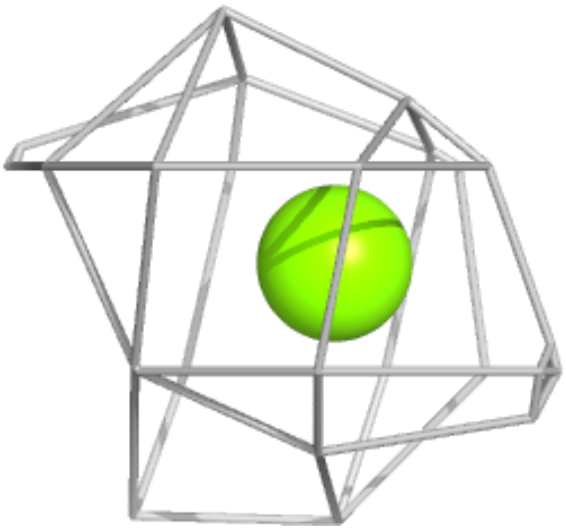


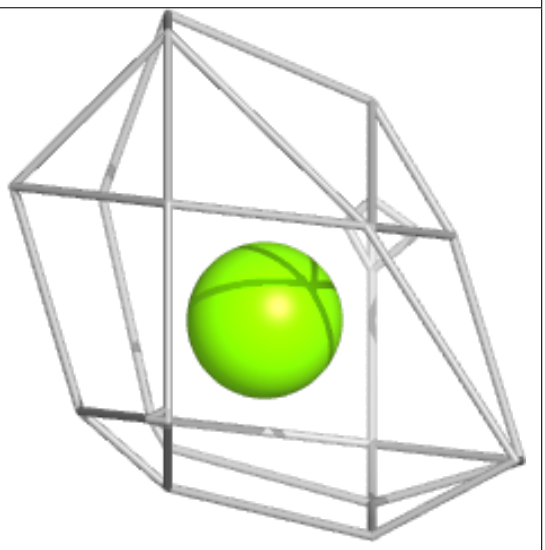


Electron density around MG A 504:

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

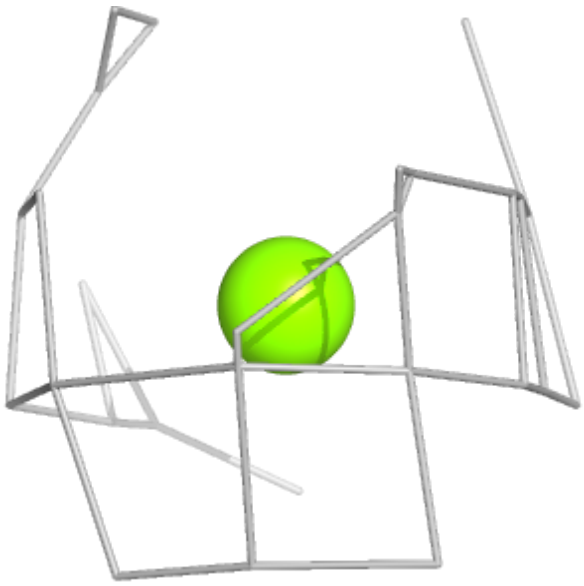


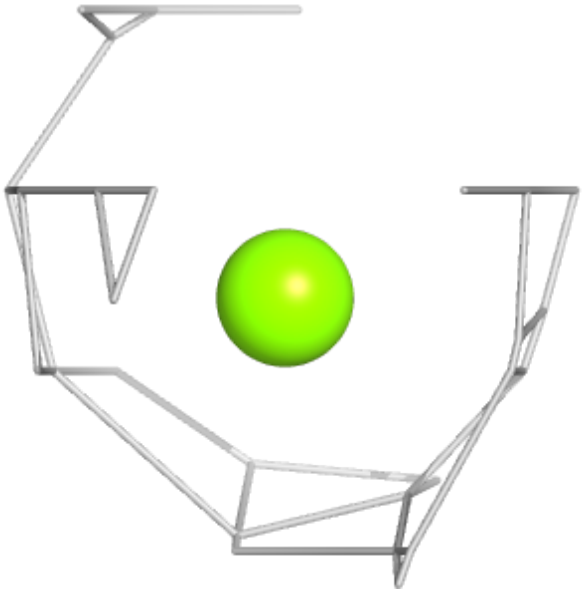


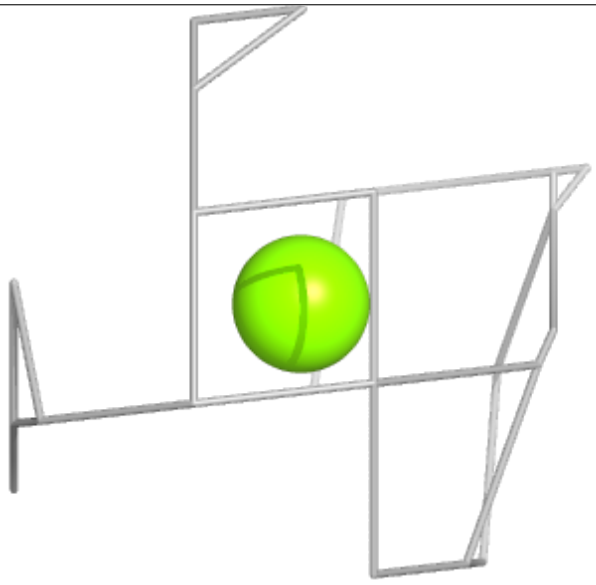


Electron density around MG G 503:

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

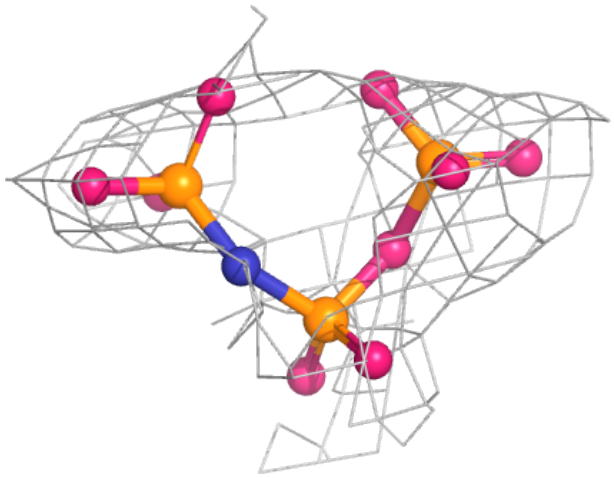


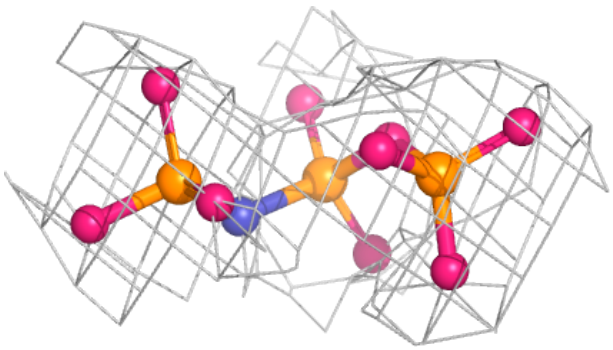


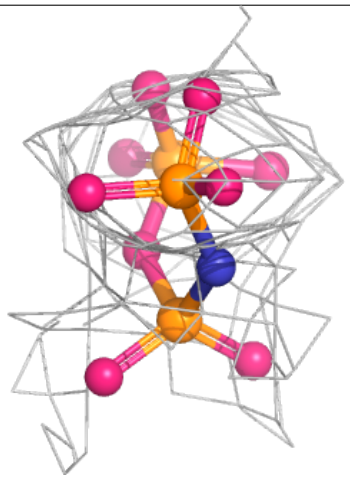


Electron density around PPK H 503:

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

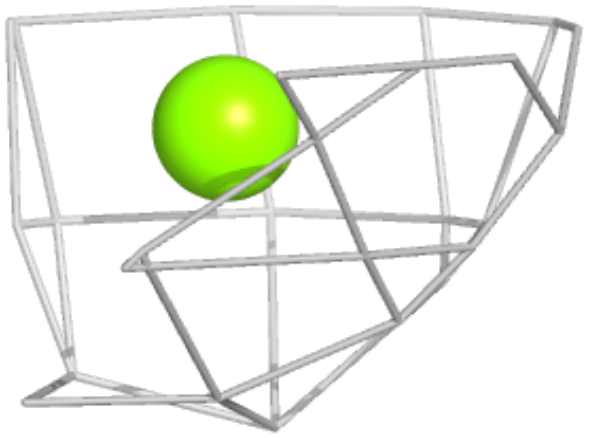


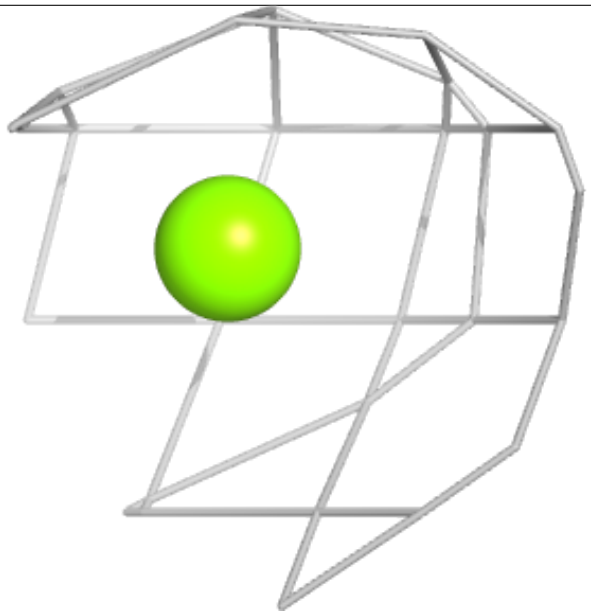


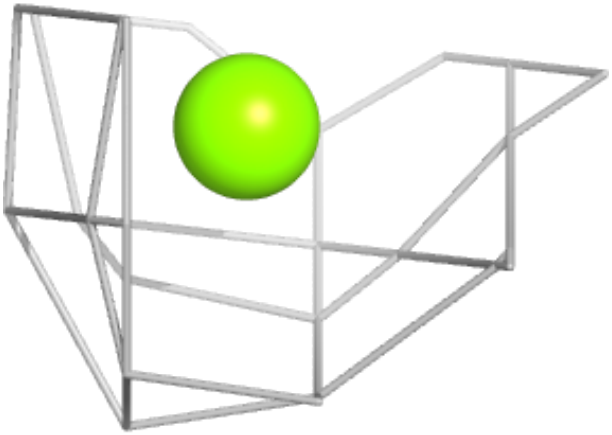


Electron density around MG C 502:

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

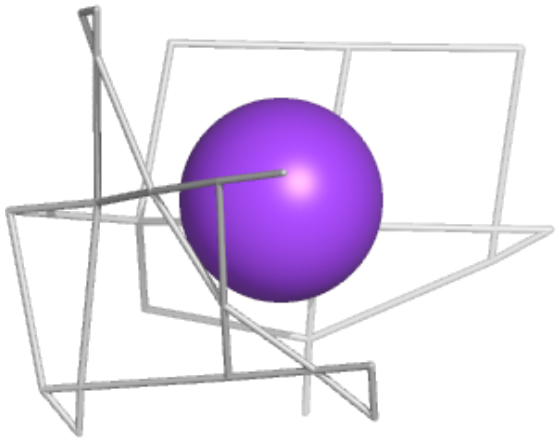


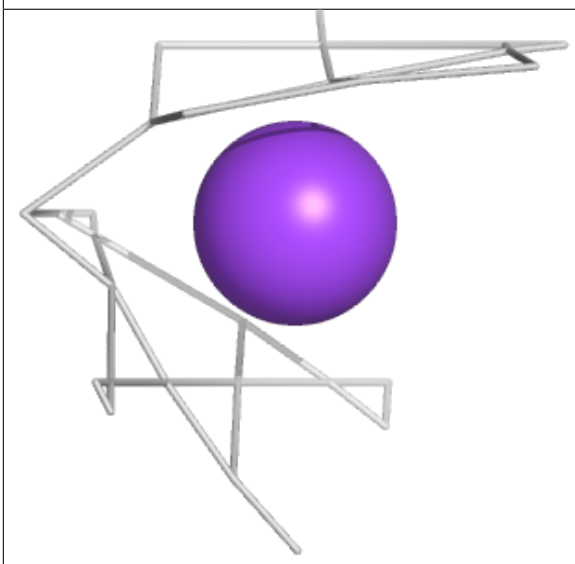


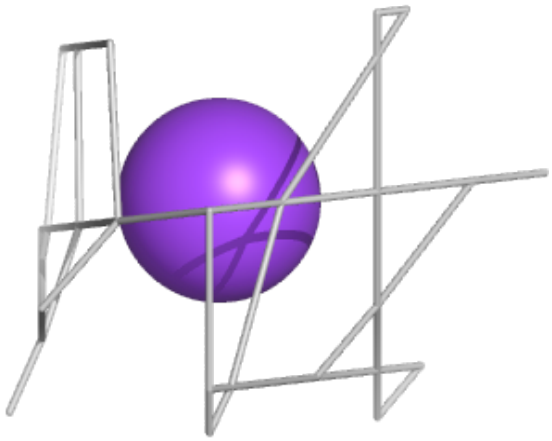


Electron density around K F 505:

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

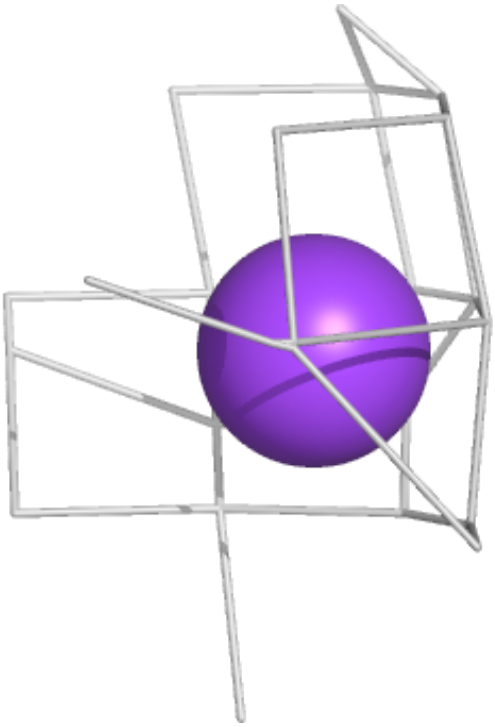


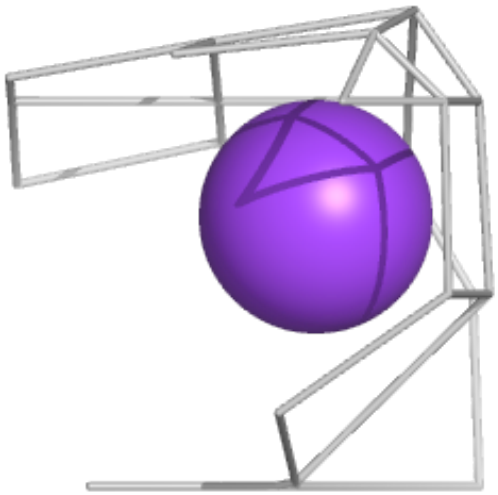


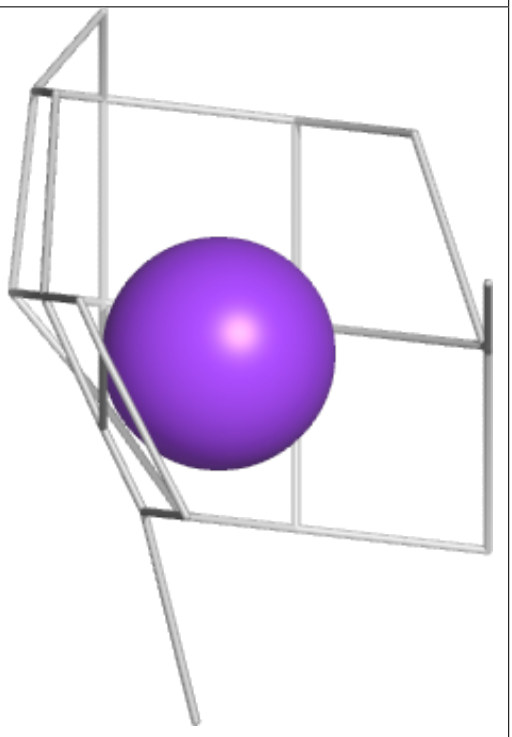


Electron density around K C 504:

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

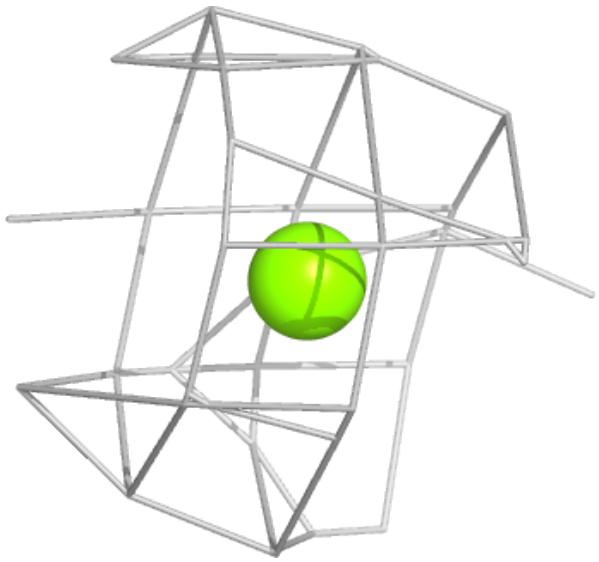


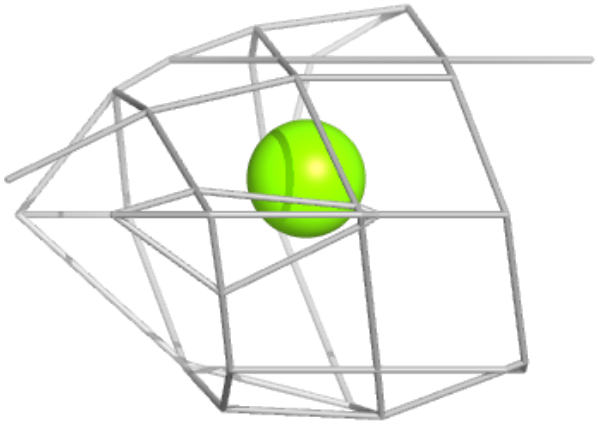


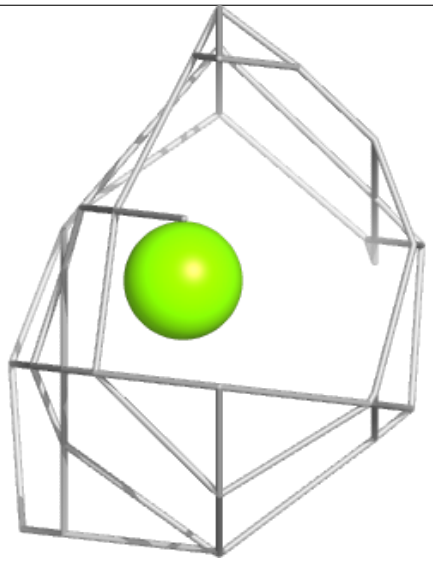


Electron density around MG G 504:

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

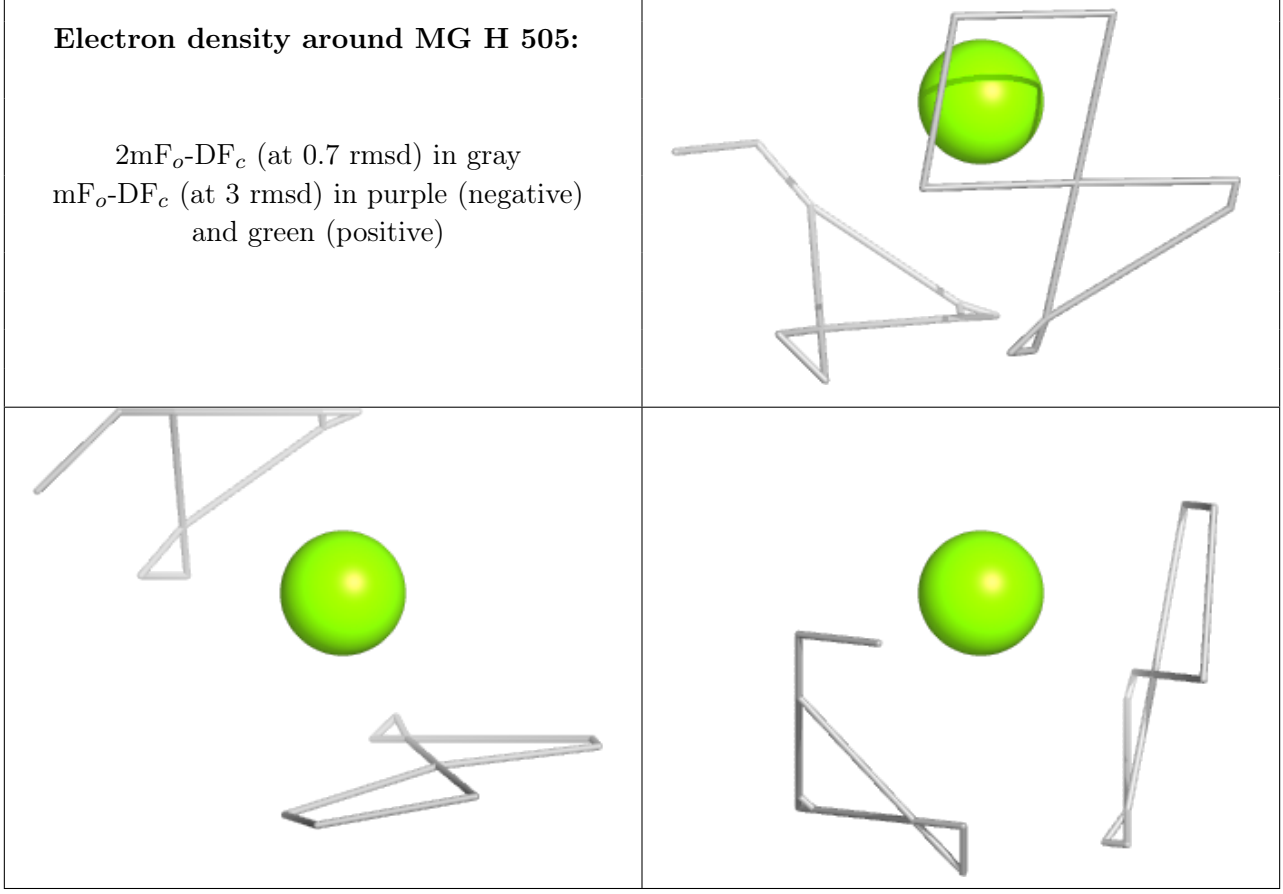






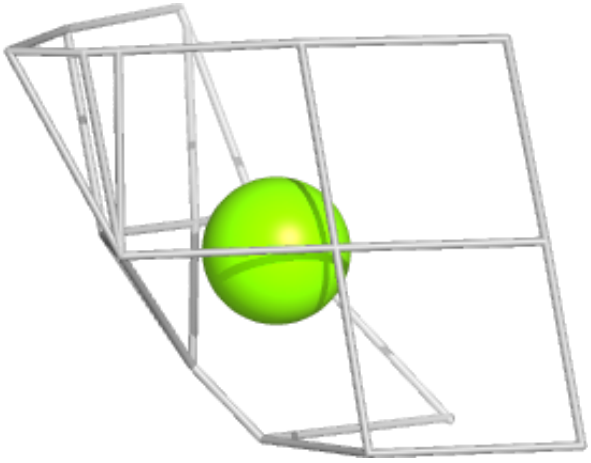
Electron density around MG H 505:

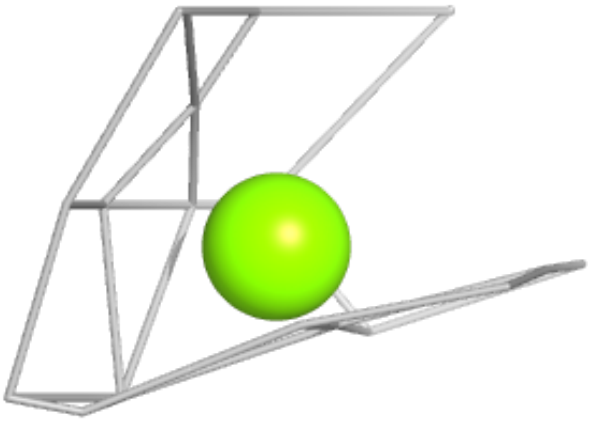
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

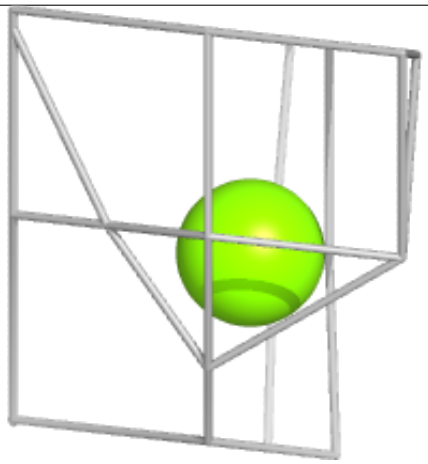


Electron density around MG A 503:

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

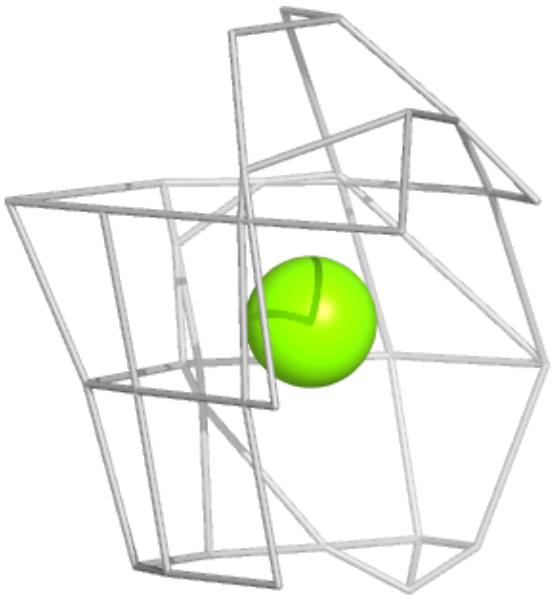


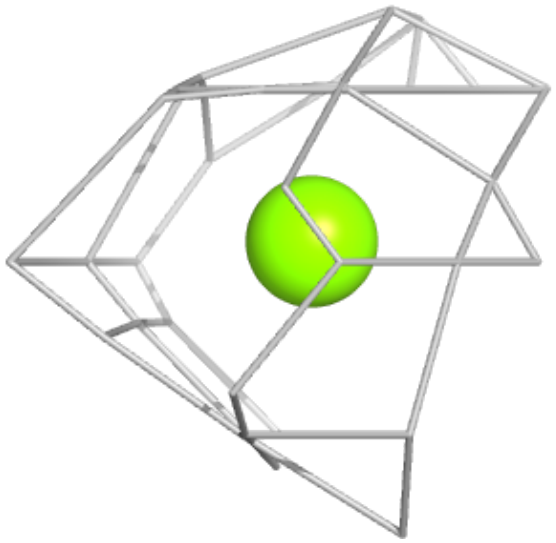


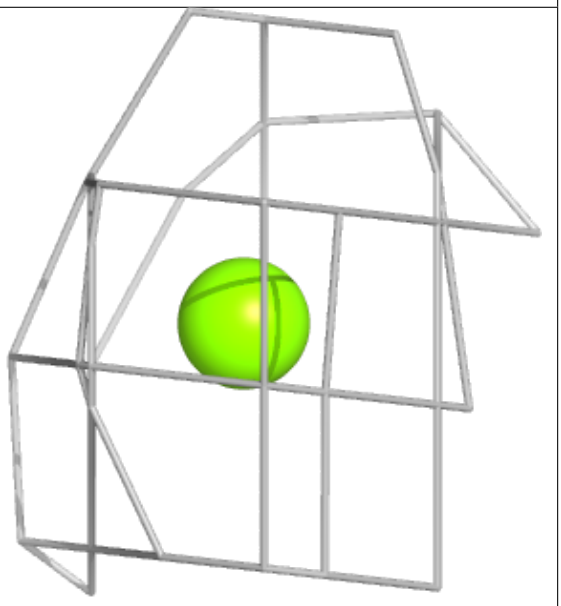


Electron density around MG F 504:

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

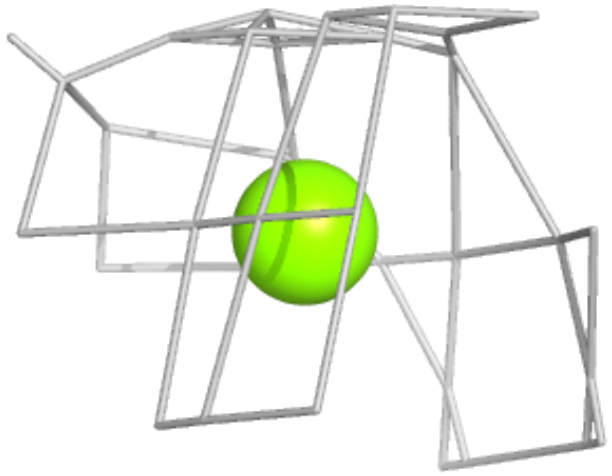


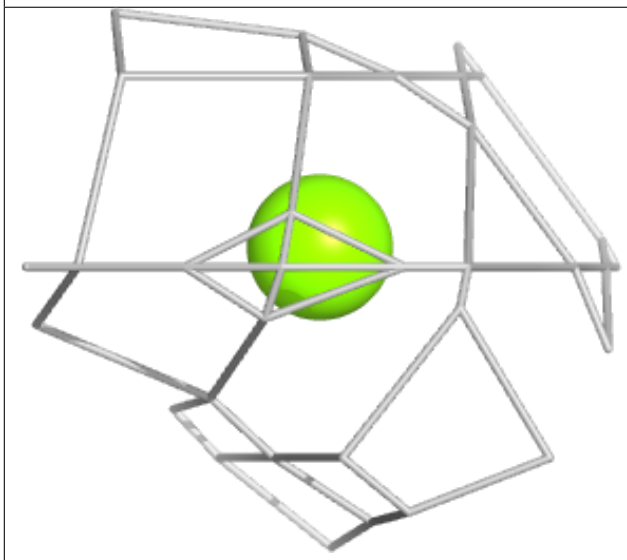


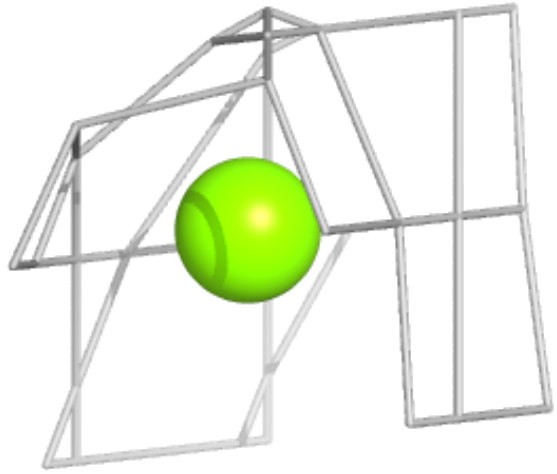


Electron density around MG D 503:

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

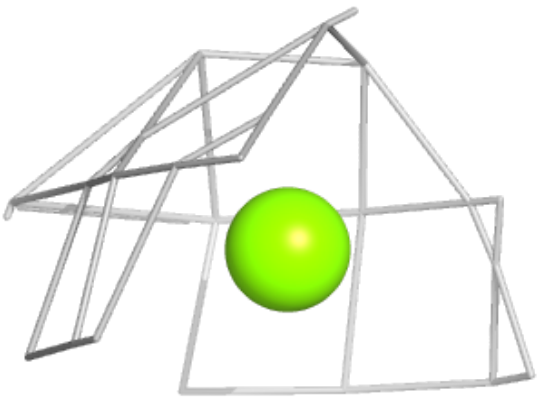


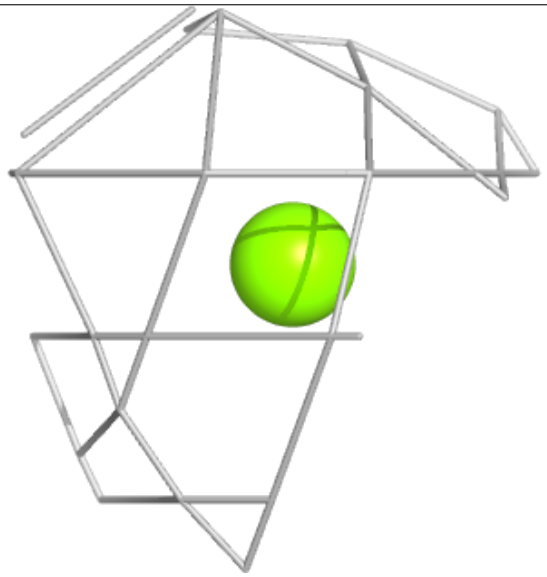


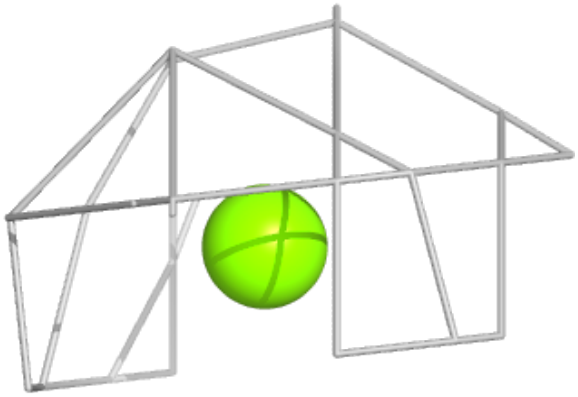


Electron density around MG F 503:

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

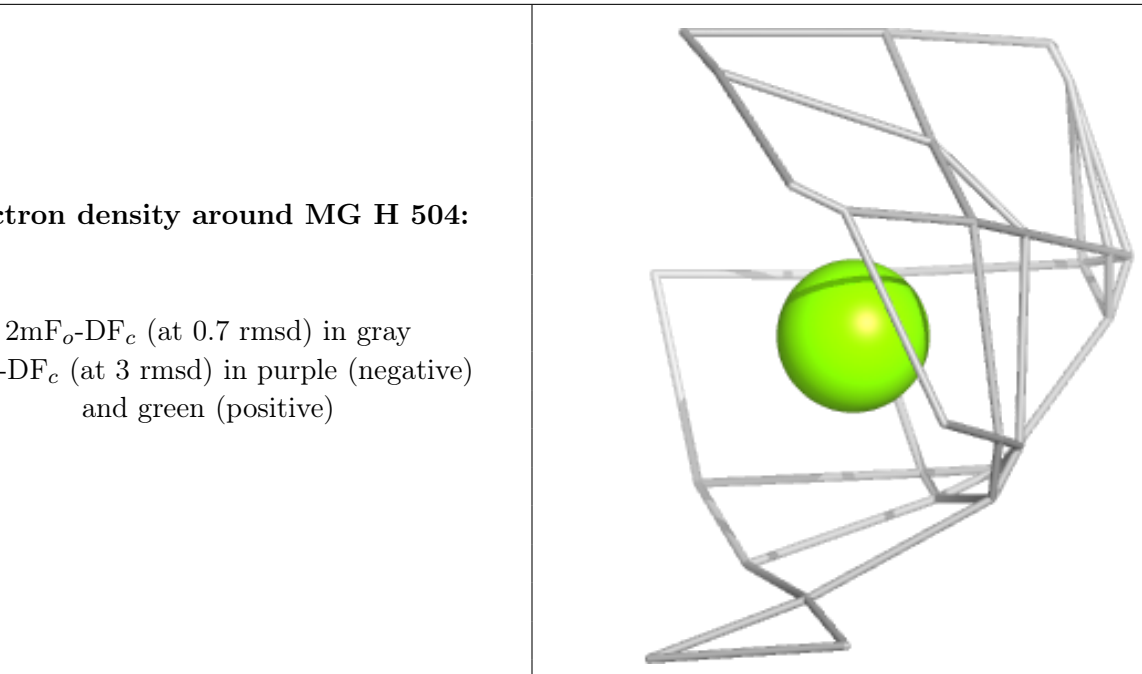


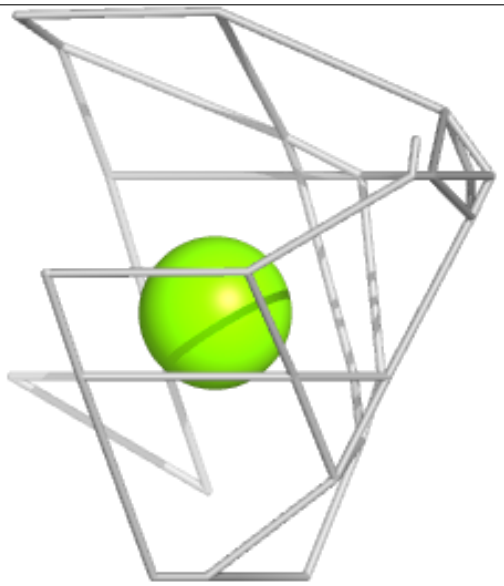


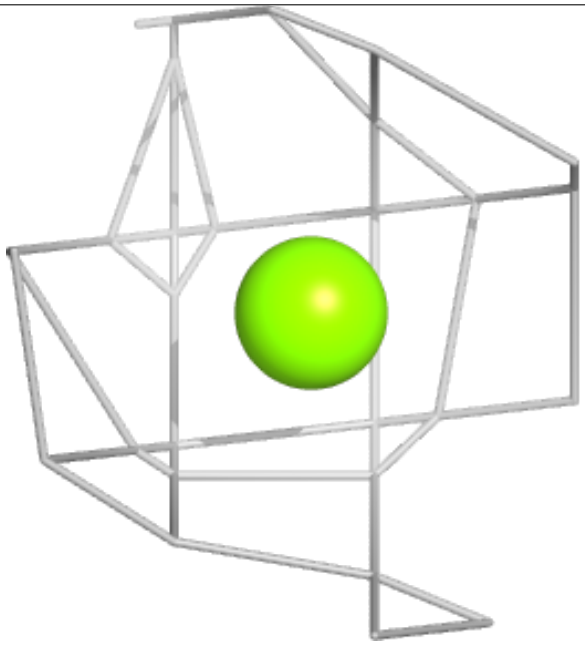


Electron density around MG H 504:

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

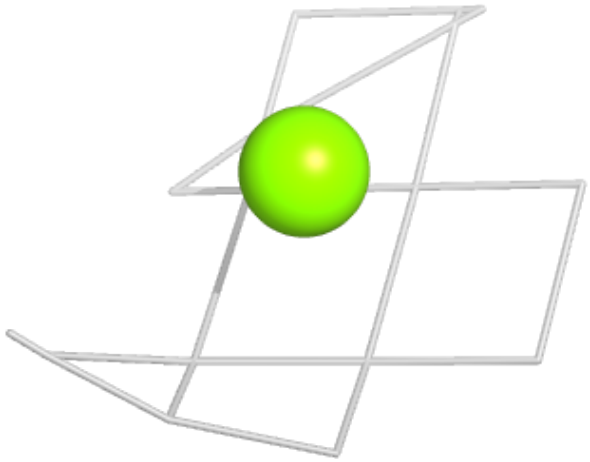


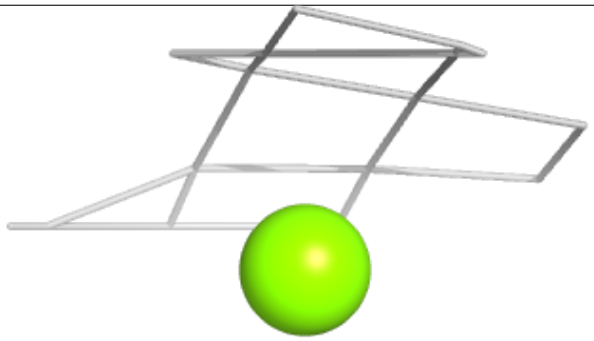


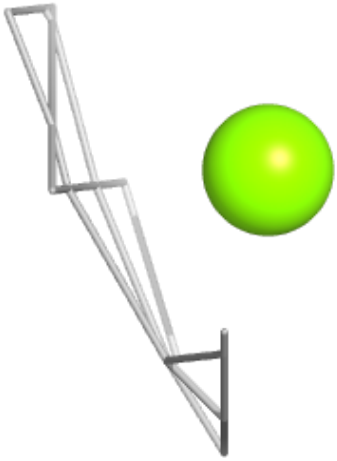


Electron density around MG E 502:

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

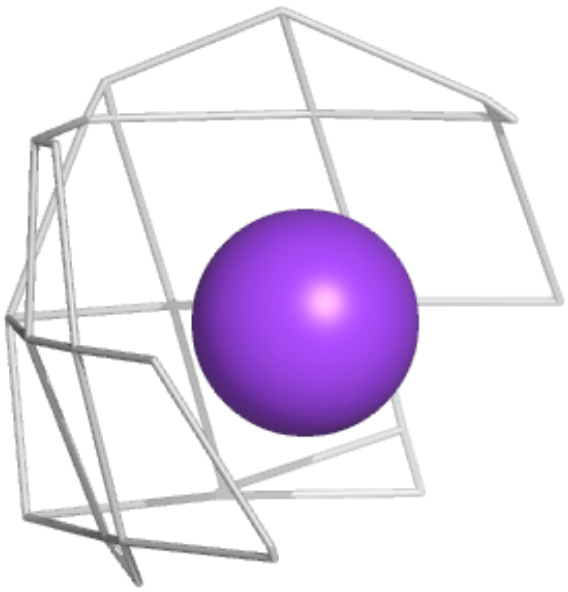


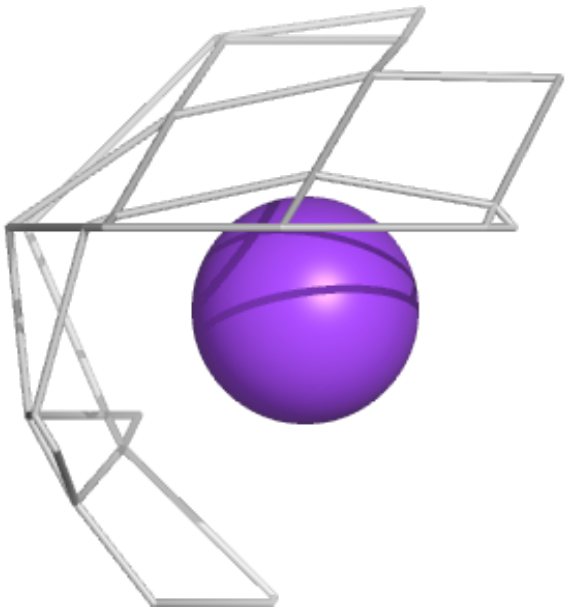


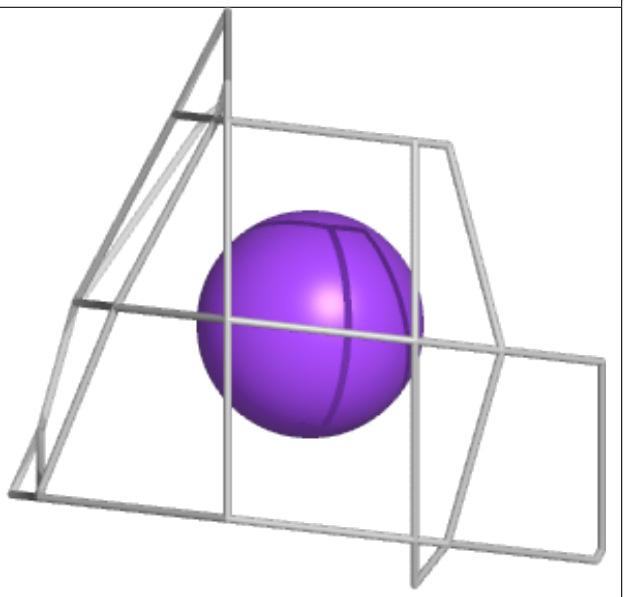


Electron density around K D 504:

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

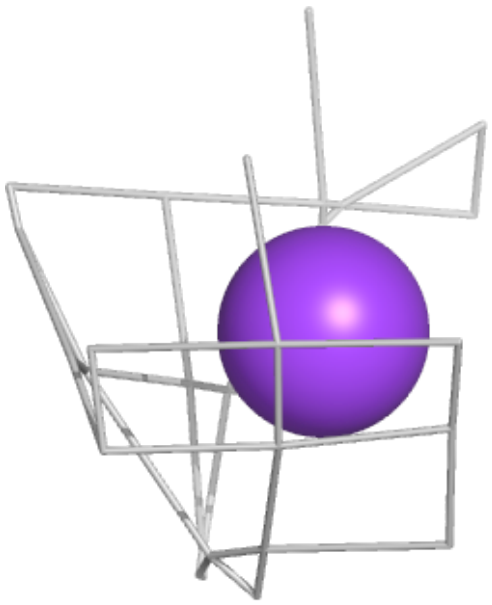


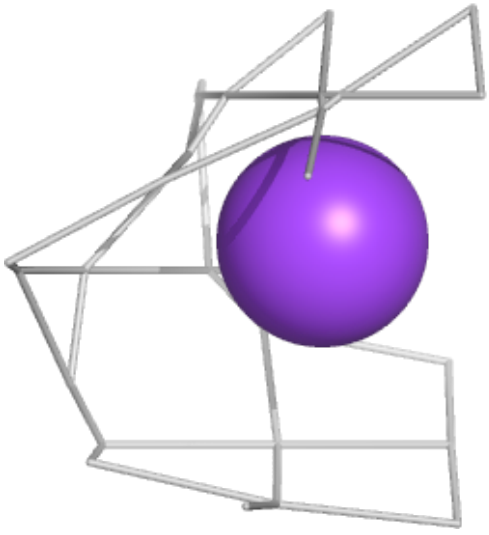


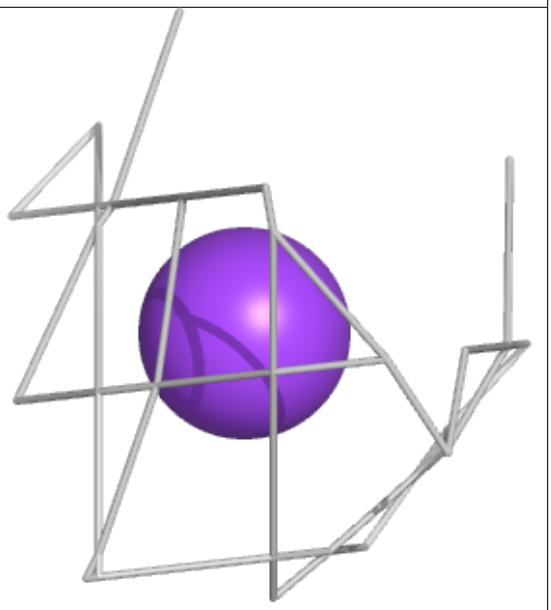


Electron density around K H 506:

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

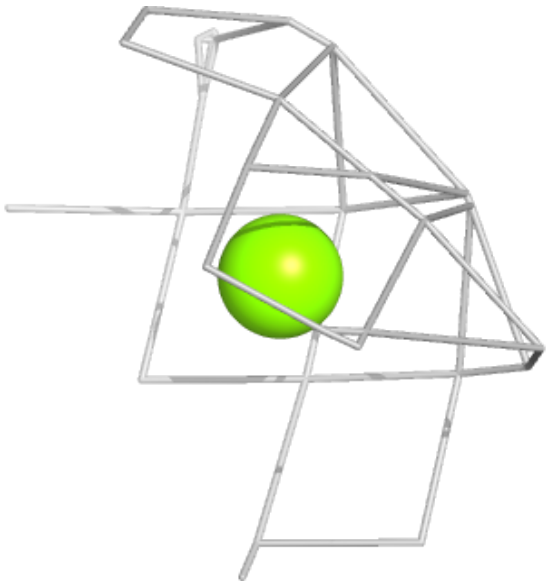


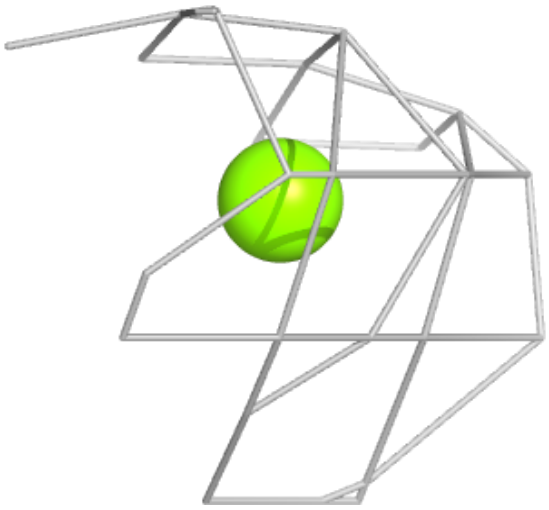


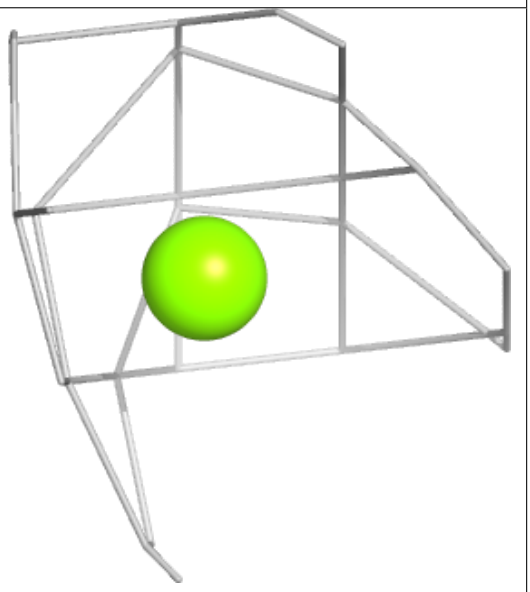


Electron density around MG B 502:

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

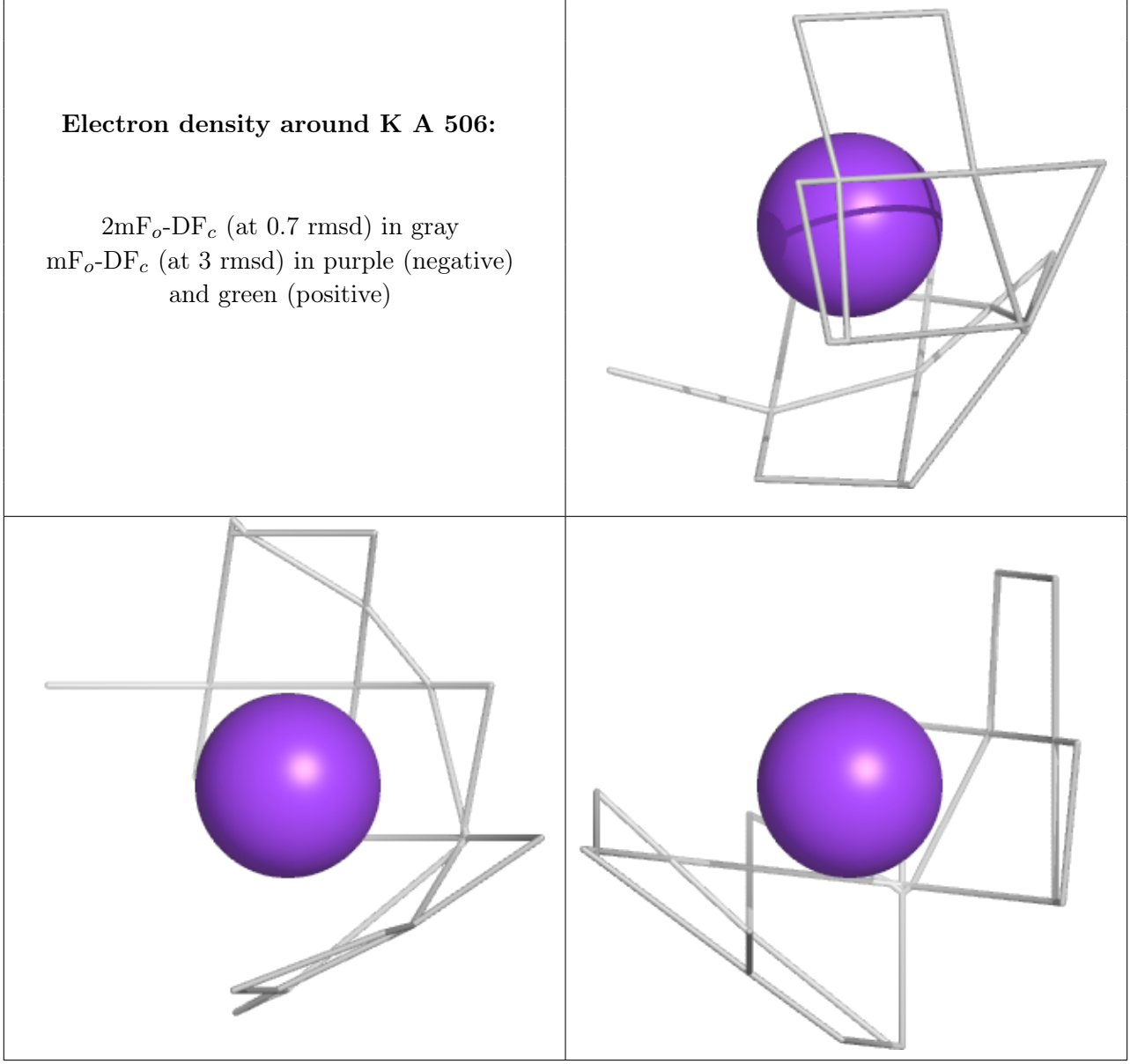






Electron density around K A 506:

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



6.5 Other polymers (i)

There are no such residues in this entry.