



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 31, 2022 – 01:22 PM EDT

PDB ID : 7T1J
Title : Crystal structure of RUBISCO from Rhodospirillaceae bacterium BRH_c57
Authors : Pereira, J.H.; Liu, A.K.; Shih, P.M.; Adams, P.D.
Deposited on : 2021-12-02
Resolution : 1.96 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), 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	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

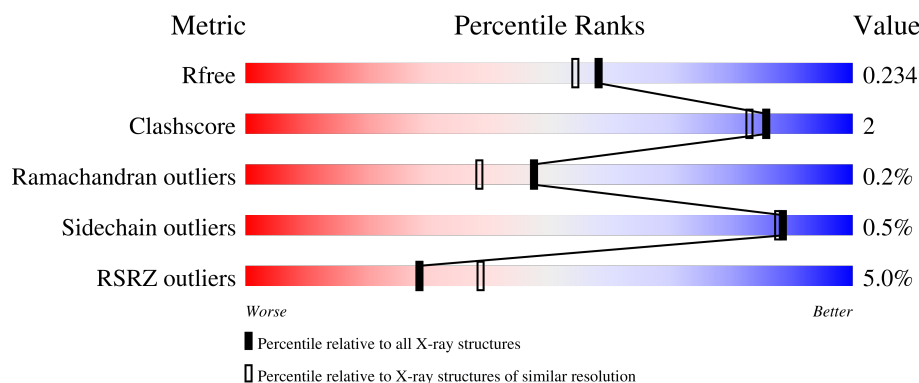
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	<div> <div style="width: 93%;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 2%; background-color: grey;"></div> </div> 93% 5% •
1	B	460	<div> <div style="width: 94%;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 1%; background-color: grey;"></div> </div> 94% 5% •
1	C	460	<div> <div style="width: 5%; background-color: red;"></div> <div style="width: 90%;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 7%; background-color: grey;"></div> </div> 5% 90% 8% •
1	D	460	<div> <div style="width: 4%; background-color: red;"></div> <div style="width: 93%;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 8%; background-color: grey;"></div> </div> 4% 93% 5% •
1	E	460	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 93%;"></div> <div style="width: 5%; background-color: yellow;"></div> <div style="width: 10%; background-color: grey;"></div> </div> 2% 93% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	460	<div><div>%</div><div><div></div><div>92%</div><div>7%</div></div><div></div></div>
1	G	460	<div><div>15%</div><div><div></div><div>90%</div><div>7%</div></div><div></div></div>
1	H	460	<div><div>4%</div><div><div></div><div>93%</div><div>6%</div></div><div></div></div>
1	I	460	<div><div>7%</div><div><div></div><div>92%</div><div>6%</div></div><div></div></div>
1	J	460	<div><div>3%</div><div><div></div><div>93%</div><div>6%</div></div><div></div></div>
1	K	460	<div><div>11%</div><div><div></div><div>93%</div><div>5%</div></div><div></div></div>
1	L	460	<div><div>5%</div><div><div></div><div>94%</div><div></div></div><div></div></div>

2 Entry composition

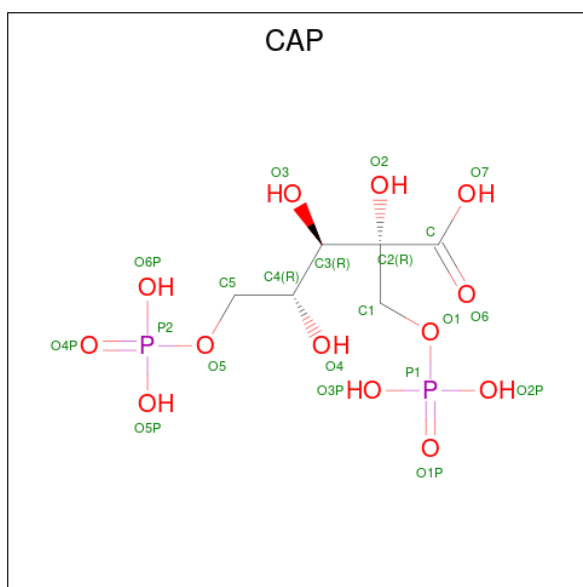
There are 4 unique types of molecules in this entry. The entry contains 87214 atoms, of which 40481 are hydrogens and 0 are deuteriums.

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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	H	N	O	S	0	0	0
			6894	2223	3381	605	661	24			
1	B	457	Total	C	H	N	O	S	0	0	0
			6930	2233	3401	608	664	24			
1	C	454	Total	C	H	N	O	S	0	0	0
			6875	2217	3370	604	660	24			
1	D	452	Total	C	H	N	O	S	0	0	0
			6832	2206	3344	601	658	23			
1	E	453	Total	C	H	N	O	S	0	0	0
			6855	2212	3358	603	659	23			
1	F	454	Total	C	H	N	O	S	0	0	0
			6874	2218	3369	604	660	23			
1	G	453	Total	C	H	N	O	S	0	0	0
			6853	2211	3357	602	659	24			
1	H	454	Total	C	H	N	O	S	0	0	0
			6885	2220	3379	605	658	23			
1	I	452	Total	C	H	N	O	S	0	0	0
			6832	2206	3344	601	658	23			
1	J	454	Total	C	H	N	O	S	0	0	0
			6873	2218	3368	604	660	23			
1	K	453	Total	C	H	N	O	S	0	0	0
			6853	2211	3357	602	659	24			
1	L	452	Total	C	H	N	O	S	0	0	0
			6833	2206	3345	601	658	23			

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C₆H₁₄O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	B	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	C	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	D	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	E	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	F	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	G	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	H	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	I	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	J	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	K	1	Total	C	H	O	P	0	0
			30	6	9	13	2		
2	L	1	Total	C	H	O	P	0	0
			30	6	9	13	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0
3	I	1	Total Mg 1 1	0	0
3	J	1	Total Mg 1 1	0	0
3	K	1	Total Mg 1 1	0	0
3	L	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	514	Total O 514 514	0	0
4	B	502	Total O 502 502	0	0
4	C	400	Total O 400 400	0	0
4	D	376	Total O 376 376	0	0
4	E	402	Total O 402 402	0	0
4	F	391	Total O 391 391	0	0
4	G	347	Total O 347 347	0	0
4	H	376	Total O 376 376	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	276	Total 276	O 276	0	0
4	J	316	Total 316	O 316	0	0
4	K	275	Total 275	O 275	0	0
4	L	278	Total 278	O 278	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: Ribulose biphosphate carboxylase

Chain A:  93% 5% .




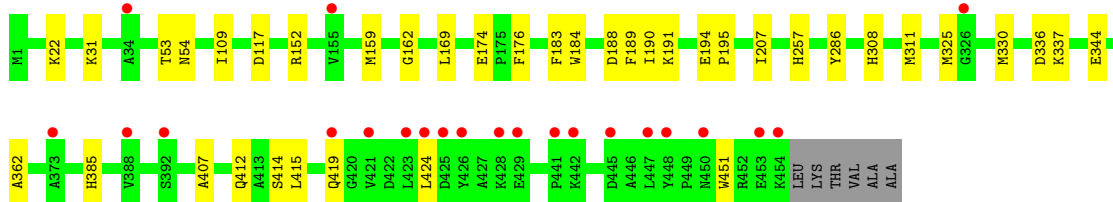
- Molecule 1: Ribulose biphosphate carboxylase

Chain B:  94% 5% .

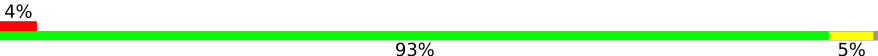


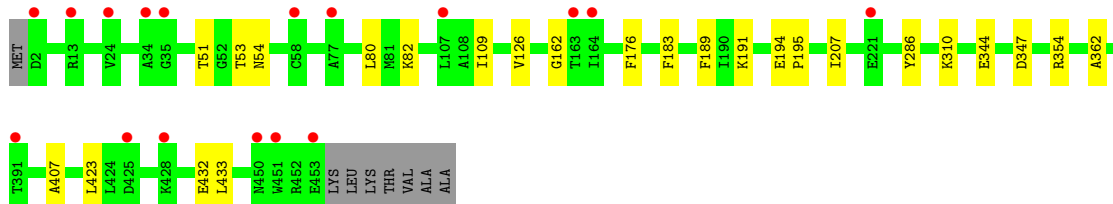
- Molecule 1: Ribulose biphosphate carboxylase

Chain C:  90% 8% .



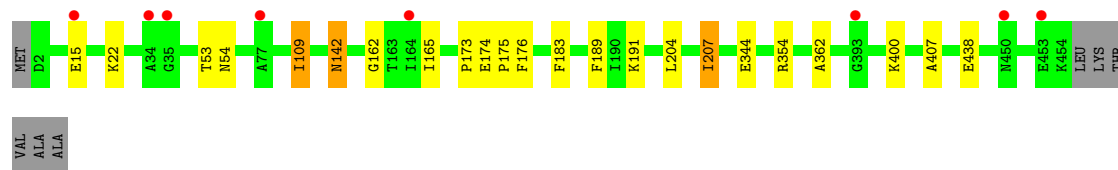
- Molecule 1: Ribulose biphosphate carboxylase

Chain D:  93% 5% .

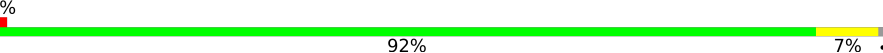


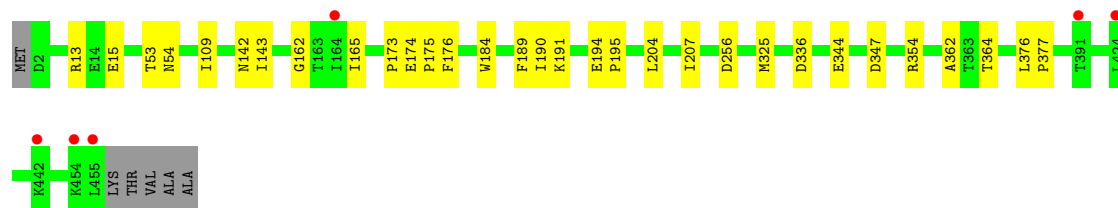
- Molecule 1: Ribulose biphosphate carboxylase

Chain E:  93% 2% ..




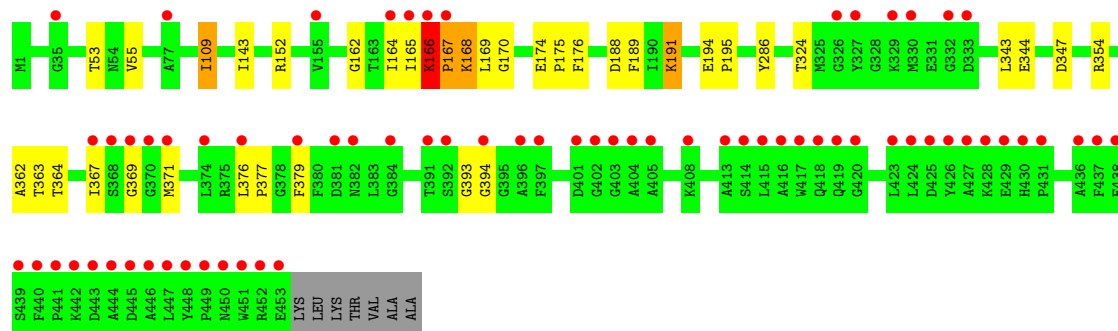
- Molecule 1: Ribulose biphosphate carboxylase

Chain F:  92% 7% .

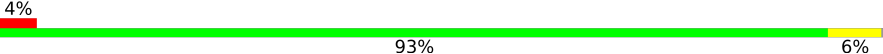


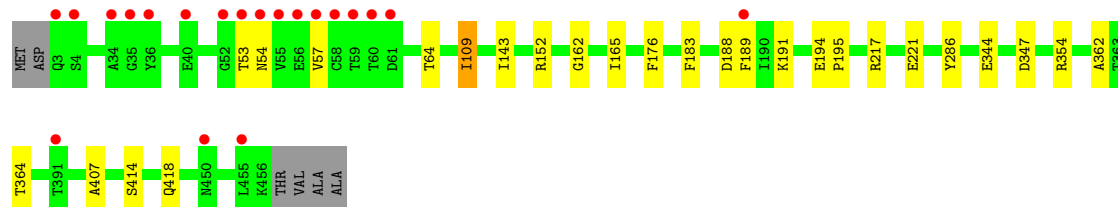
- Molecule 1: Ribulose biphosphate carboxylase

Chain G:  90% 7% .. 15%




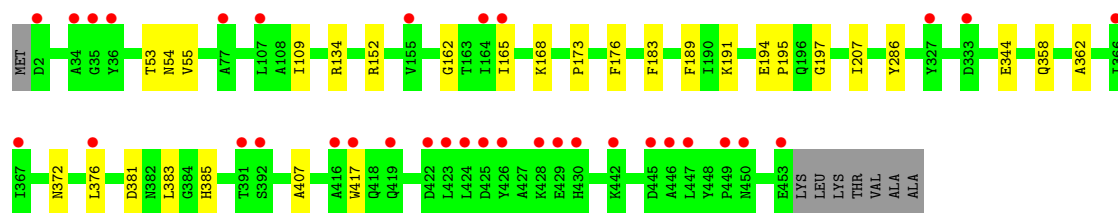
- Molecule 1: Ribulose biphosphate carboxylase

Chain H:  93% 6% . 4%

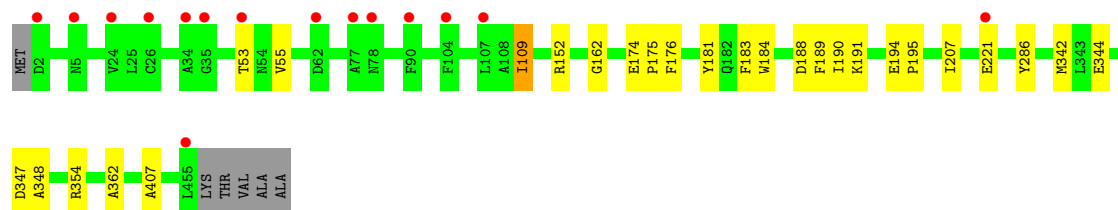


- Molecule 1: Ribulose biphosphate carboxylase

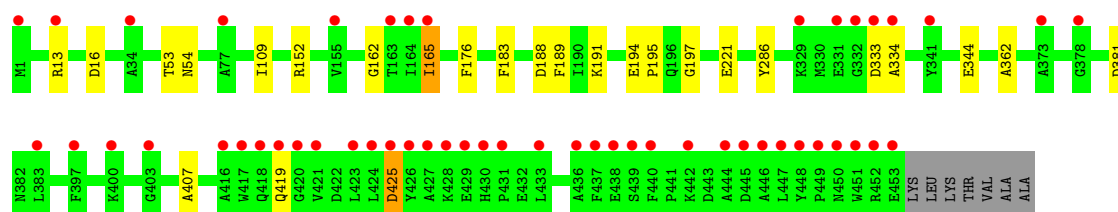
Chain I:  92% 6% . 7%



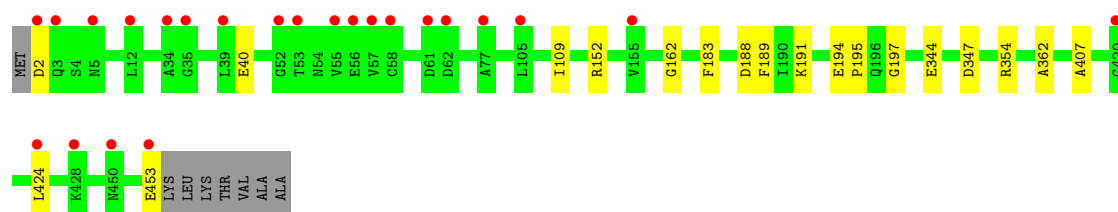
- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



- Molecule 1: Ribulose biphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.81Å 104.98Å 369.61Å 90.00° 93.04° 90.00°	Depositor
Resolution (Å)	29.52 – 1.96 29.52 – 1.96	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.52-1.96) 94.7 (29.52-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 1.96Å)	Xtriage
Refinement program	phenix.refine 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.196 , 0.235 0.195 , 0.234	Depositor DCC
R_{free} test set	2002 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	87214	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CAP, KCX, 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	0.34	0/3586	0.51	0/4852
1	B	0.34	0/3602	0.51	0/4873
1	C	0.31	0/3578	0.49	0/4841
1	D	0.30	0/3561	0.49	0/4820
1	E	0.29	0/3570	0.48	0/4831
1	F	0.32	0/3578	0.49	0/4842
1	G	0.30	0/3569	0.49	0/4830
1	H	0.33	0/3579	0.49	0/4842
1	I	0.28	0/3561	0.47	0/4820
1	J	0.30	0/3578	0.48	0/4842
1	K	0.29	0/3569	0.48	0/4830
1	L	0.28	0/3561	0.48	0/4820
All	All	0.31	0/42892	0.49	0/58043

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	166	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3513	3381	3380	15	0
1	B	3529	3401	3400	13	0
1	C	3505	3370	3369	24	0
1	D	3488	3344	3344	15	0
1	E	3497	3358	3357	13	0
1	F	3505	3369	3368	20	0
1	G	3496	3357	3356	22	0
1	H	3506	3379	3377	15	0
1	I	3488	3344	3344	15	0
1	J	3505	3368	3368	13	0
1	K	3496	3357	3356	12	0
1	L	3488	3345	3344	10	0
2	A	21	9	7	1	0
2	B	21	9	8	1	0
2	C	21	9	7	1	0
2	D	21	9	9	0	0
2	E	21	9	8	1	0
2	F	21	9	7	1	0
2	G	21	9	8	1	0
2	H	21	9	8	0	0
2	I	21	9	8	0	0
2	J	21	9	9	0	0
2	K	21	9	8	0	0
2	L	21	9	8	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	514	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	502	0	0	0	0
4	C	400	0	0	3	0
4	D	376	0	0	1	0
4	E	402	0	0	0	0
4	F	391	0	0	0	0
4	G	347	0	0	0	0
4	H	376	0	0	0	0
4	I	276	0	0	1	0
4	J	316	0	0	0	0
4	K	275	0	0	2	0
4	L	278	0	0	0	0
All	All	46733	40481	40458	182	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.

The worst 5 of 182 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:G:167:PRO:HB3	1:H:64:THR:HG21	1.69	0.74
1:G:174:GLU:HG2	1:G:175:PRO:HD3	1.73	0.71
1:E:173:PRO:HA	1:E:207:ILE:HD12	1.75	0.69
1:F:256:ASP:OD2	1:I:134:ARG:NH1	2.25	0.69
1:J:347:ASP:OD2	1:J:354:ARG:NH2	2.25	0.69

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	452/460 (98%)	440 (97%)	12 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	454/460 (99%)	442 (97%)	11 (2%)	1 (0%)	47	38
1	C	451/460 (98%)	438 (97%)	13 (3%)	0	100	100
1	D	449/460 (98%)	435 (97%)	14 (3%)	0	100	100
1	E	450/460 (98%)	435 (97%)	14 (3%)	1 (0%)	47	38
1	F	451/460 (98%)	436 (97%)	15 (3%)	0	100	100
1	G	450/460 (98%)	430 (96%)	15 (3%)	5 (1%)	14	5
1	H	451/460 (98%)	437 (97%)	13 (3%)	1 (0%)	47	38
1	I	449/460 (98%)	435 (97%)	13 (3%)	1 (0%)	47	38
1	J	451/460 (98%)	434 (96%)	16 (4%)	1 (0%)	47	38
1	K	450/460 (98%)	436 (97%)	12 (3%)	2 (0%)	34	22
1	L	449/460 (98%)	428 (95%)	20 (4%)	1 (0%)	47	38
All	All	5407/5520 (98%)	5226 (97%)	168 (3%)	13 (0%)	47	38

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	166	LYS
1	G	167	PRO
1	G	168	LYS
1	B	109	ILE
1	G	369	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/357 (99%)	351 (99%)	3 (1%)	81	80
1	B	356/357 (100%)	354 (99%)	2 (1%)	86	85
1	C	353/357 (99%)	350 (99%)	3 (1%)	81	80
1	D	351/357 (98%)	350 (100%)	1 (0%)	92	92
1	E	352/357 (99%)	348 (99%)	4 (1%)	73	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	353/357 (99%)	353 (100%)	0	100	100
1	G	352/357 (99%)	351 (100%)	1 (0%)	92	92
1	H	353/357 (99%)	352 (100%)	1 (0%)	92	92
1	I	351/357 (98%)	349 (99%)	2 (1%)	86	85
1	J	353/357 (99%)	352 (100%)	1 (0%)	92	92
1	K	352/357 (99%)	348 (99%)	4 (1%)	73	71
1	L	351/357 (98%)	350 (100%)	1 (0%)	92	92
All	All	4231/4284 (99%)	4208 (100%)	23 (0%)	88	88

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	286	TYR
1	J	286	TYR
1	I	286	TYR
1	K	221	GLU
1	C	286	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	78	ASN
1	J	358	GLN
1	D	224	GLN
1	F	142	ASN
1	F	418	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	KCX	B	191	3,1	9,11,12	2.29	2 (22%)	5,12,14	1.57	1 (20%)
1	KCX	D	191	3,1	9,11,12	2.10	2 (22%)	5,12,14	1.40	1 (20%)
1	KCX	F	191	3,1	9,11,12	2.27	2 (22%)	5,12,14	1.55	1 (20%)
1	KCX	A	191	3,1	9,11,12	2.14	2 (22%)	5,12,14	1.61	1 (20%)
1	KCX	E	191	3,1	9,11,12	2.14	2 (22%)	5,12,14	1.49	1 (20%)
1	KCX	K	191	3,1	9,11,12	2.23	2 (22%)	5,12,14	1.64	1 (20%)
1	KCX	H	191	3,1	9,11,12	2.27	2 (22%)	5,12,14	1.63	1 (20%)
1	KCX	L	191	3,1	9,11,12	2.23	2 (22%)	5,12,14	1.60	1 (20%)
1	KCX	I	191	3,1	9,11,12	2.07	2 (22%)	5,12,14	1.69	1 (20%)
1	KCX	J	191	3,1	9,11,12	2.15	2 (22%)	5,12,14	1.70	1 (20%)
1	KCX	C	191	3,1	9,11,12	2.29	2 (22%)	5,12,14	1.75	1 (20%)
1	KCX	G	191	3,1	9,11,12	2.26	2 (22%)	5,12,14	1.70	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	B	191	3,1	-	1/9/10/12	-
1	KCX	D	191	3,1	-	1/9/10/12	-
1	KCX	F	191	3,1	-	1/9/10/12	-
1	KCX	A	191	3,1	-	0/9/10/12	-
1	KCX	E	191	3,1	-	1/9/10/12	-
1	KCX	K	191	3,1	-	0/9/10/12	-
1	KCX	H	191	3,1	-	1/9/10/12	-
1	KCX	L	191	3,1	-	1/9/10/12	-
1	KCX	I	191	3,1	-	0/9/10/12	-
1	KCX	J	191	3,1	-	0/9/10/12	-
1	KCX	C	191	3,1	-	1/9/10/12	-
1	KCX	G	191	3,1	-	0/9/10/12	-

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	191	KCX	CX-NZ	6.06	1.45	1.35
1	C	191	KCX	CX-NZ	6.02	1.45	1.35
1	G	191	KCX	CX-NZ	6.00	1.45	1.35
1	H	191	KCX	CX-NZ	5.95	1.45	1.35
1	B	191	KCX	CX-NZ	5.94	1.45	1.35

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	KCX	OQ1-CX-NZ	-3.57	119.43	124.96
1	J	191	KCX	OQ1-CX-NZ	-3.45	119.61	124.96
1	G	191	KCX	OQ1-CX-NZ	-3.35	119.76	124.96
1	A	191	KCX	OQ1-CX-NZ	-3.29	119.86	124.96
1	L	191	KCX	OQ1-CX-NZ	-3.29	119.86	124.96

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	191	KCX	O-C-CA-CB
1	C	191	KCX	O-C-CA-CB
1	D	191	KCX	O-C-CA-CB
1	E	191	KCX	O-C-CA-CB
1	F	191	KCX	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	191	KCX	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 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	CAP	E	501	3	17,20,20	1.17	1 (5%)	22,31,31	0.67	0
2	CAP	F	501	3	17,20,20	1.23	0	22,31,31	0.72	0
2	CAP	K	501	3	17,20,20	1.11	0	22,31,31	0.74	0
2	CAP	A	501	3	17,20,20	1.18	0	22,31,31	0.76	0
2	CAP	L	501	3	17,20,20	1.08	0	22,31,31	0.73	0
2	CAP	H	501	3	17,20,20	1.15	1 (5%)	22,31,31	0.76	0
2	CAP	I	501	3	17,20,20	1.05	0	22,31,31	0.74	0
2	CAP	J	501	3	17,20,20	1.86	7 (41%)	22,31,31	2.49	9 (40%)
2	CAP	B	501	3	17,20,20	1.25	1 (5%)	22,31,31	0.69	0
2	CAP	D	501	3	17,20,20	1.93	6 (35%)	22,31,31	2.57	10 (45%)
2	CAP	G	501	3	17,20,20	1.05	0	22,31,31	0.78	0
2	CAP	C	501	3	17,20,20	1.10	0	22,31,31	0.77	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
2	CAP	E	501	3	-	7/29/29/29	-
2	CAP	F	501	3	-	9/29/29/29	-
2	CAP	K	501	3	-	9/29/29/29	-
2	CAP	A	501	3	-	9/29/29/29	-
2	CAP	L	501	3	-	7/29/29/29	-
2	CAP	H	501	3	-	7/29/29/29	-
2	CAP	I	501	3	-	8/29/29/29	-
2	CAP	J	501	3	-	9/29/29/29	-
2	CAP	B	501	3	-	8/29/29/29	-
2	CAP	D	501	3	-	8/29/29/29	-
2	CAP	G	501	3	-	13/29/29/29	-
2	CAP	C	501	3	-	8/29/29/29	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	CAP	P1-O3P	-3.73	1.40	1.54
2	B	501	CAP	C4-C3	-3.36	1.50	1.54
2	D	501	CAP	O7-C	-3.29	1.18	1.30
2	J	501	CAP	C5-C4	3.14	1.56	1.51
2	J	501	CAP	P1-O3P	-2.96	1.43	1.54

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	501	CAP	O2P-P1-O1	5.69	121.87	106.73
2	D	501	CAP	O2P-P1-O1	5.63	121.73	106.73
2	J	501	CAP	O5P-P2-O4P	4.66	128.91	110.68
2	D	501	CAP	O6P-P2-O5P	4.59	125.18	107.64
2	D	501	CAP	O7-C-O6	-4.18	110.52	123.82

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CAP	O7-C-C2-C1
2	A	501	CAP	O6-C-C2-O2
2	A	501	CAP	O7-C-C2-O2
2	A	501	CAP	O3-C3-C4-O4
2	B	501	CAP	O6-C-C2-C3

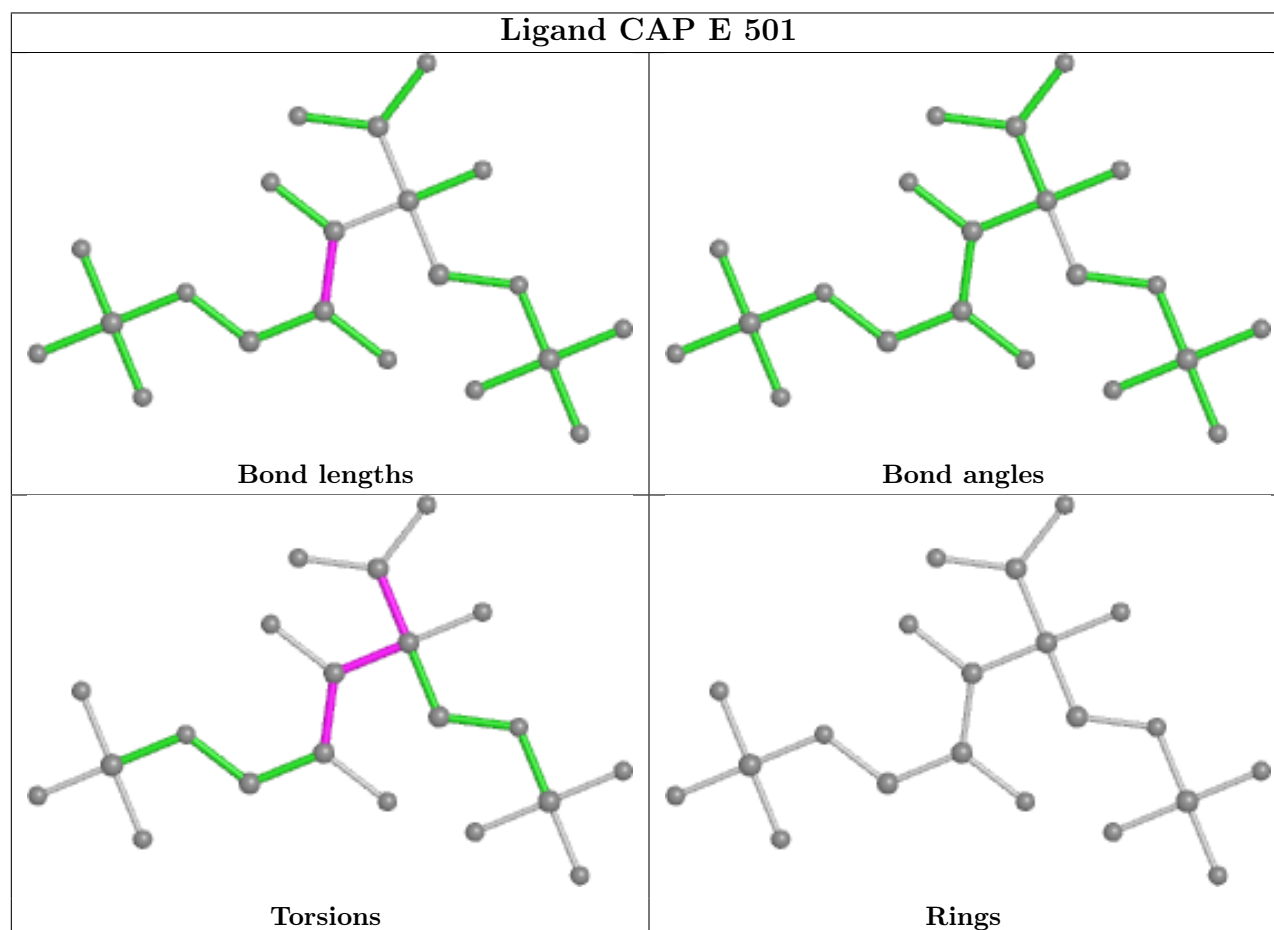
There are no ring outliers.

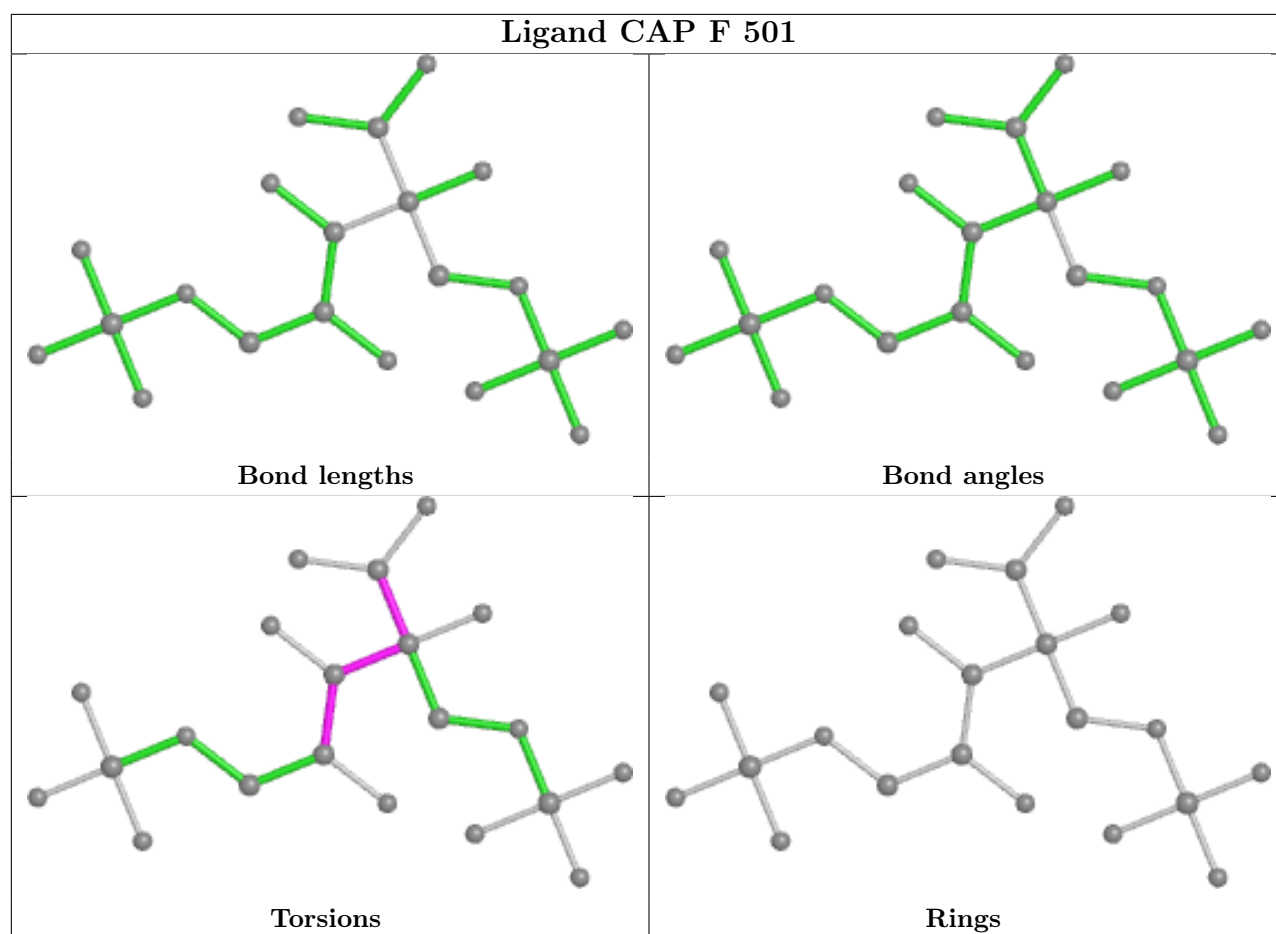
6 monomers are involved in 6 short contacts:

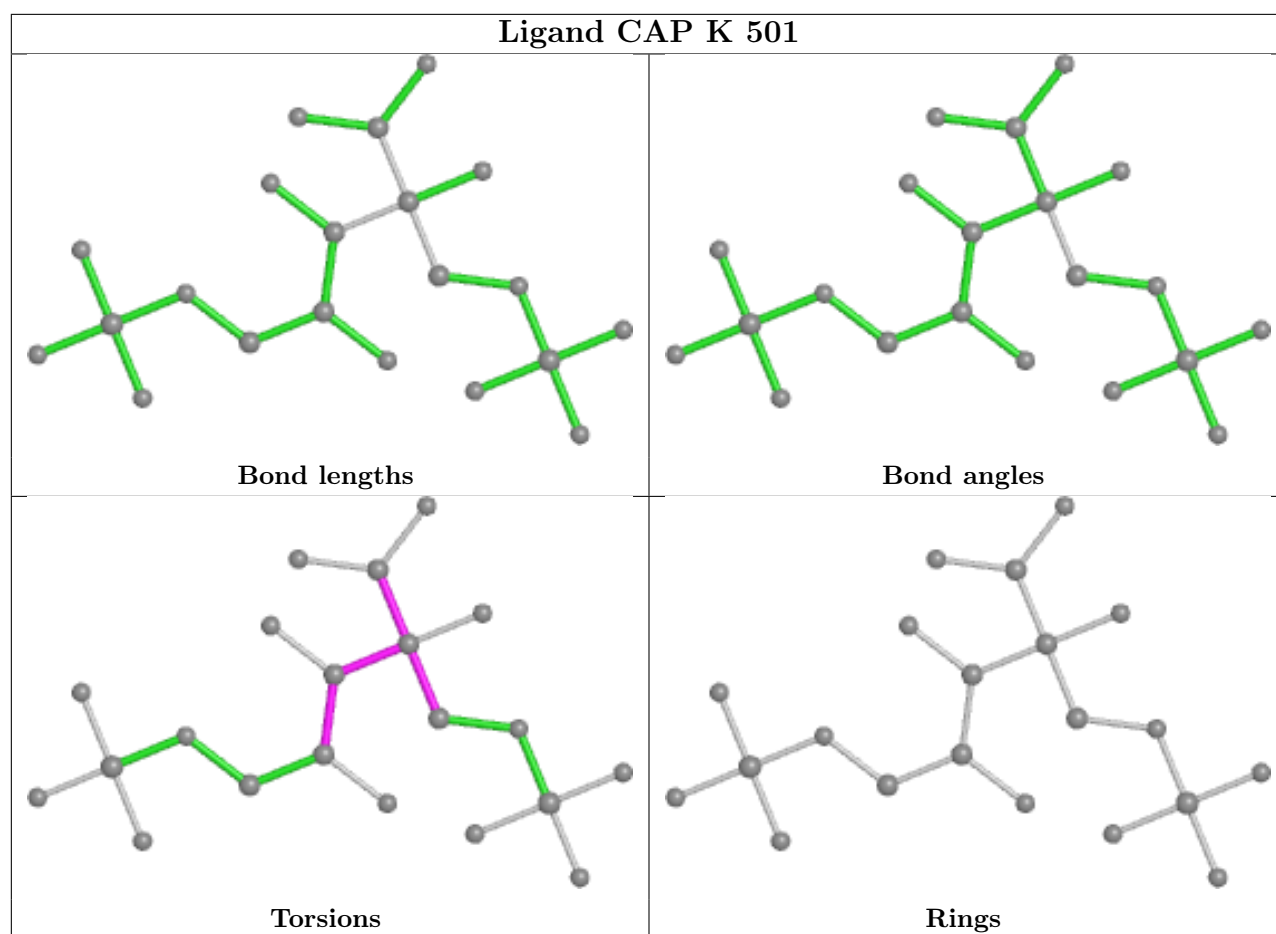
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	CAP	1	0
2	F	501	CAP	1	0
2	A	501	CAP	1	0
2	B	501	CAP	1	0
2	G	501	CAP	1	0
2	C	501	CAP	1	0

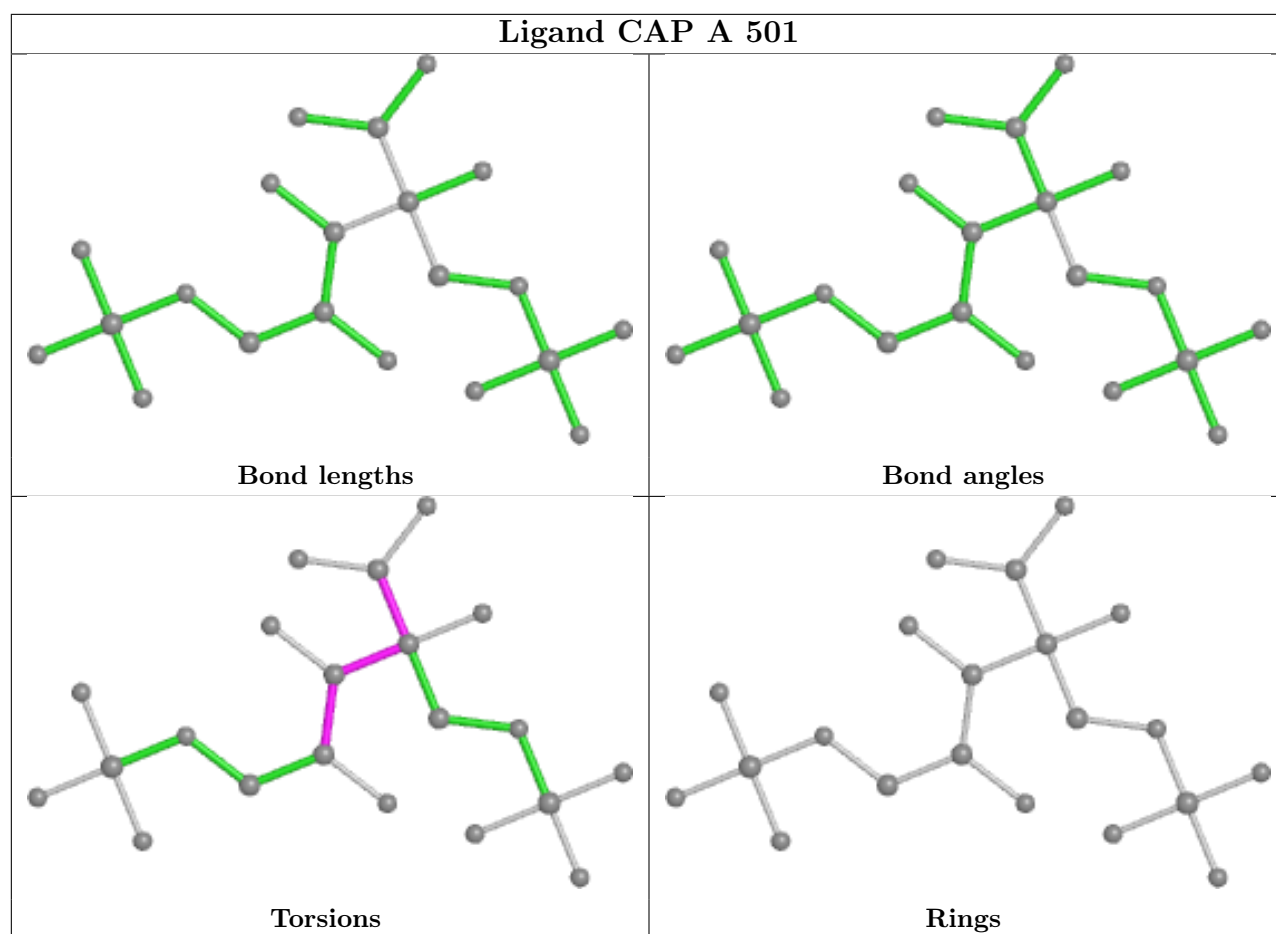
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

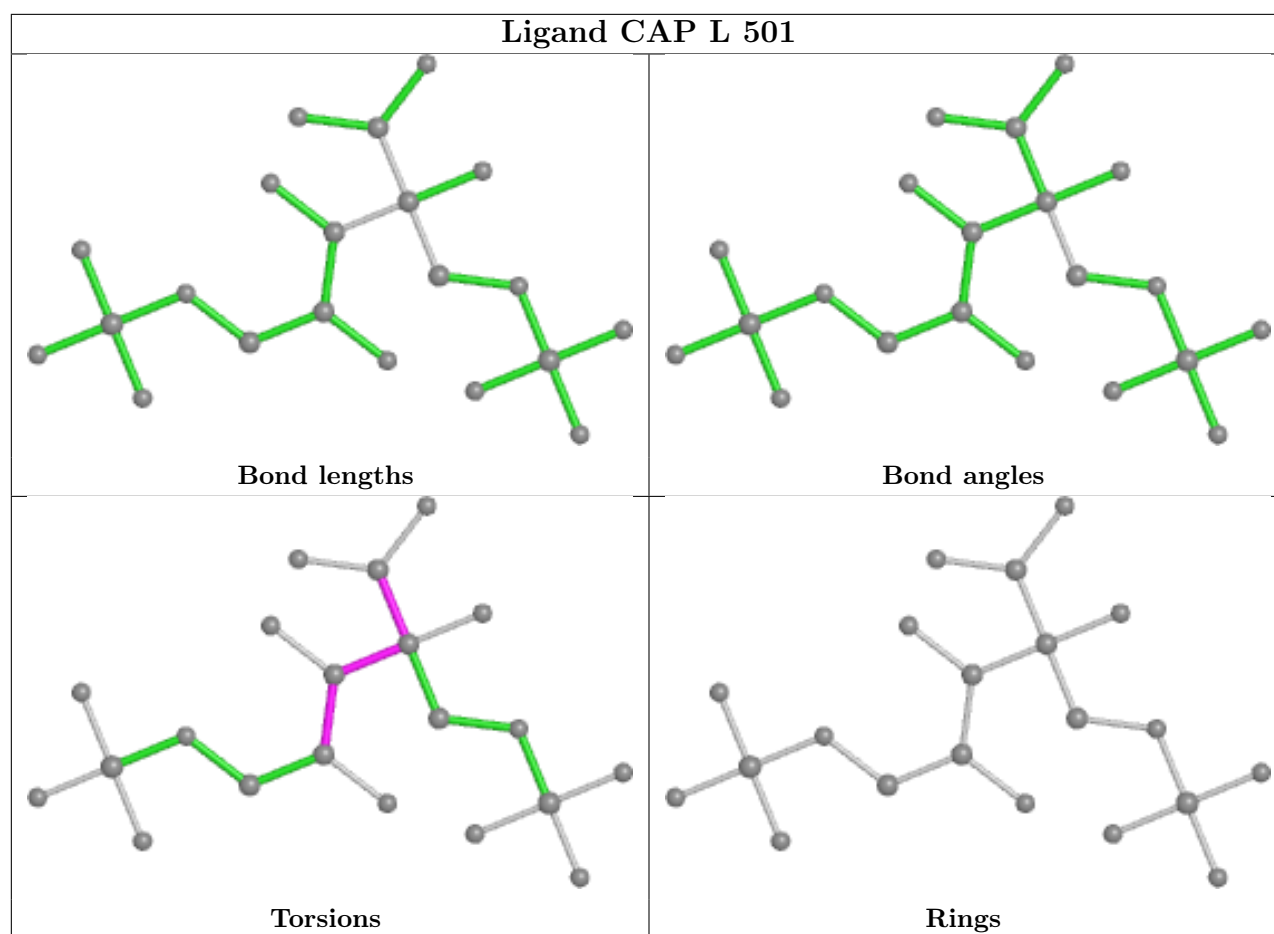
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

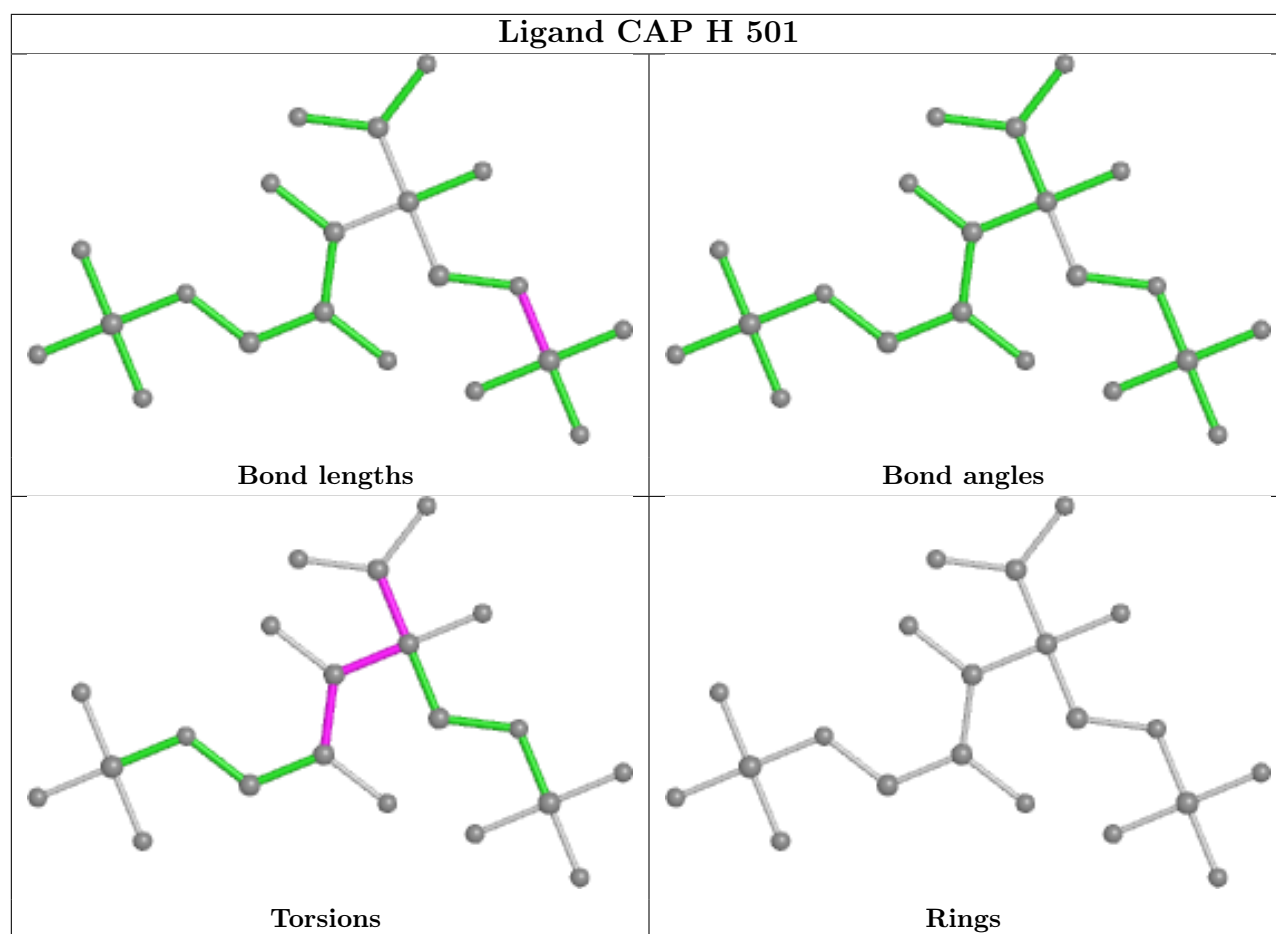




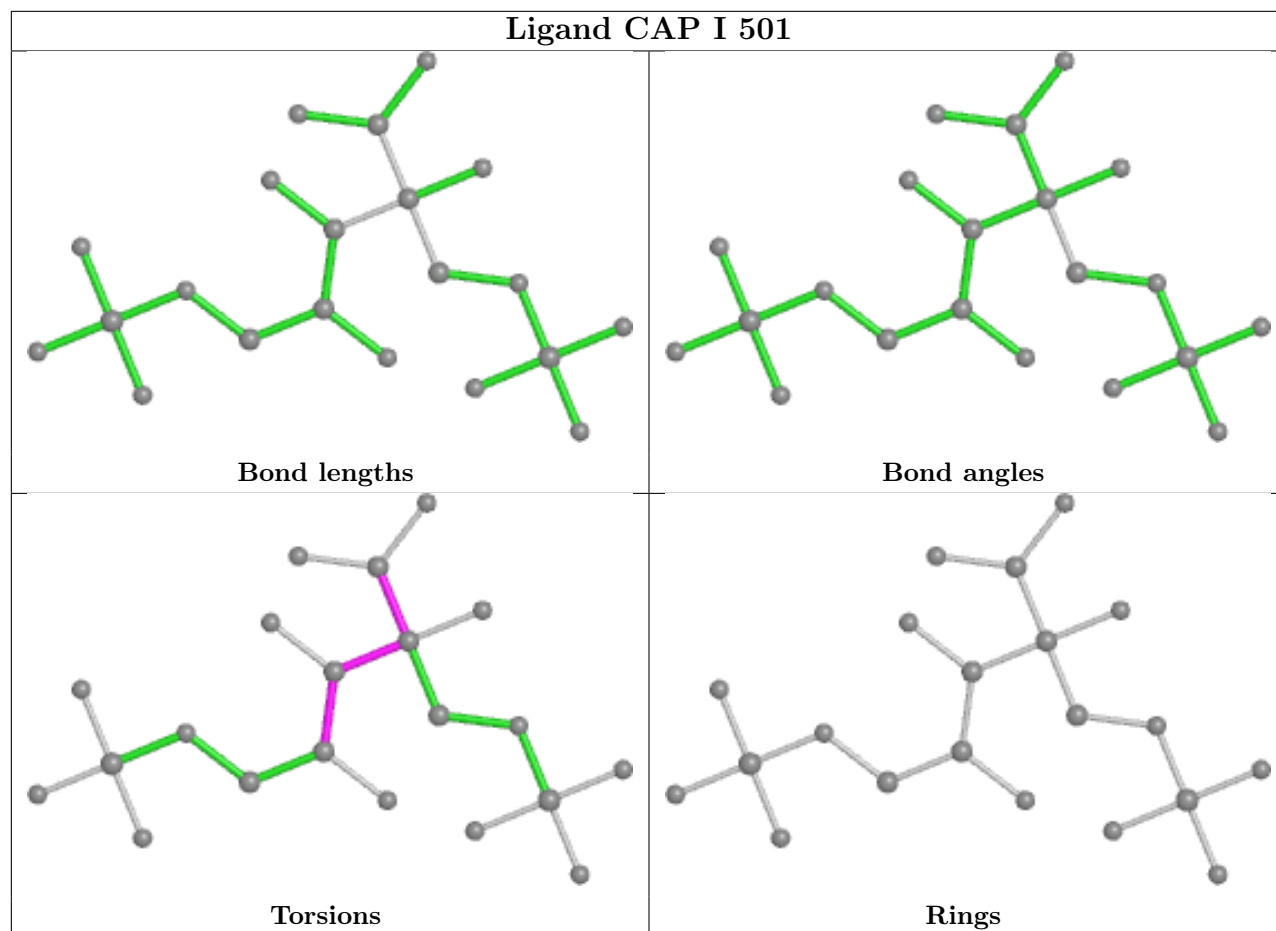




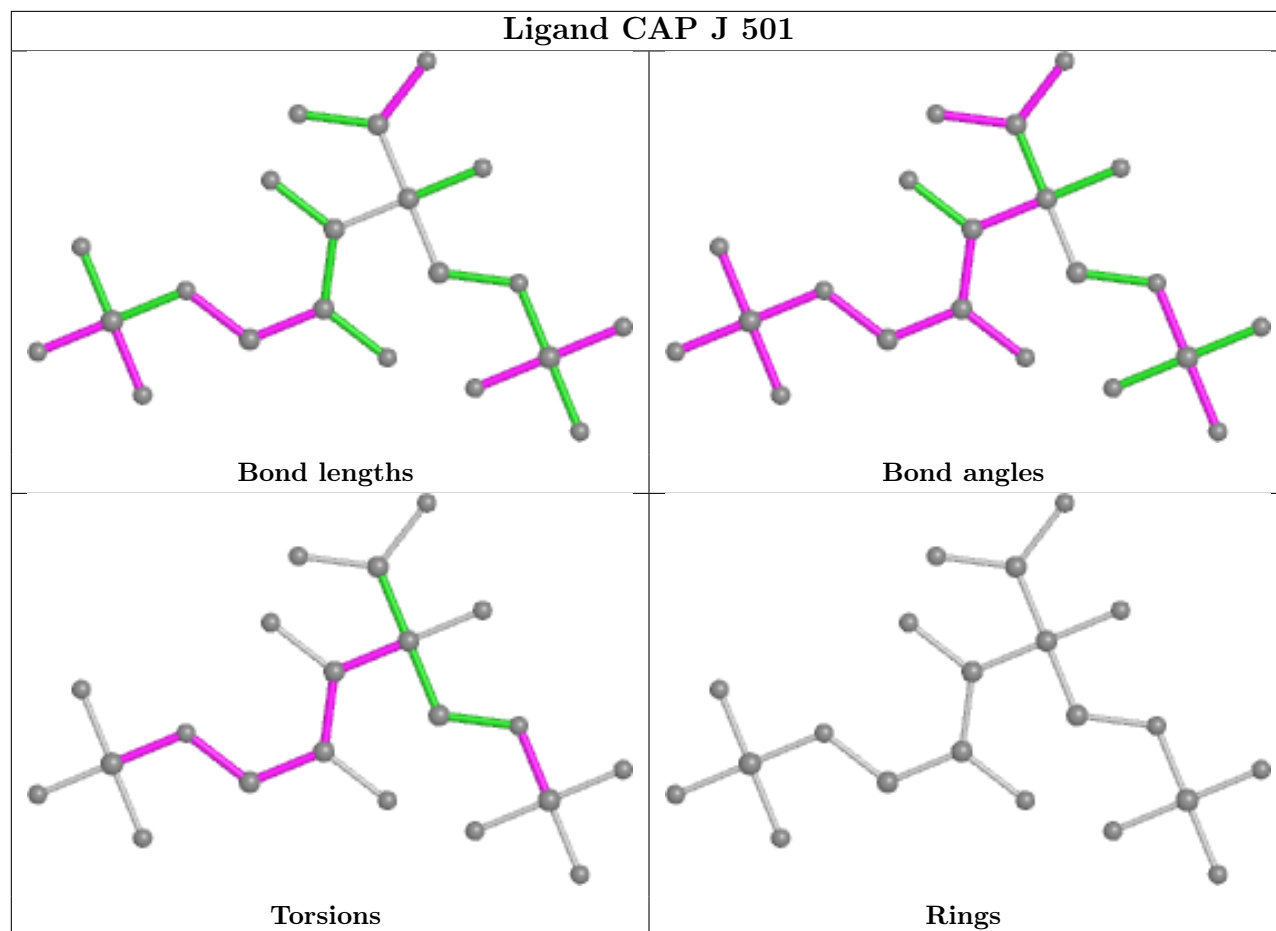


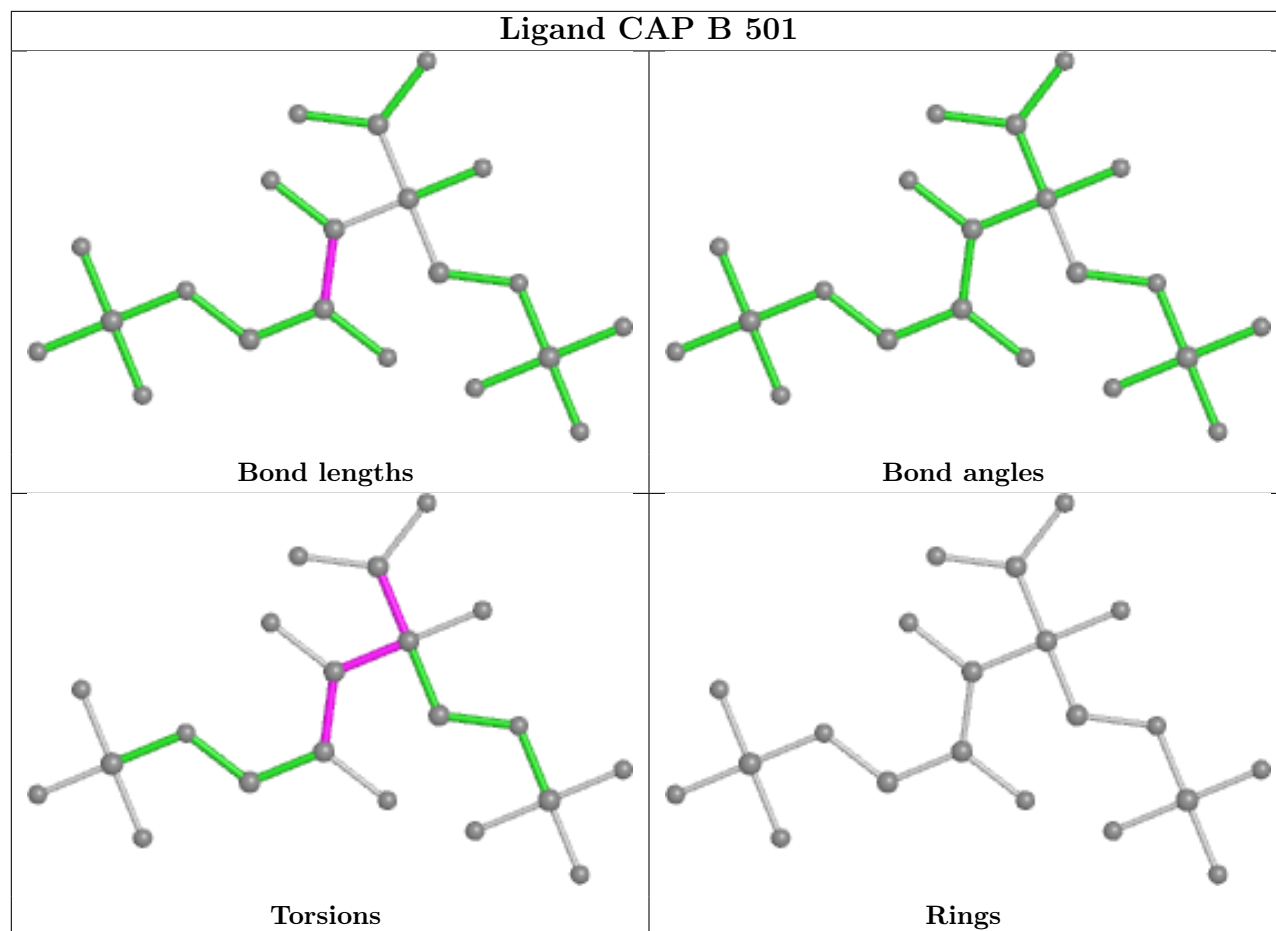


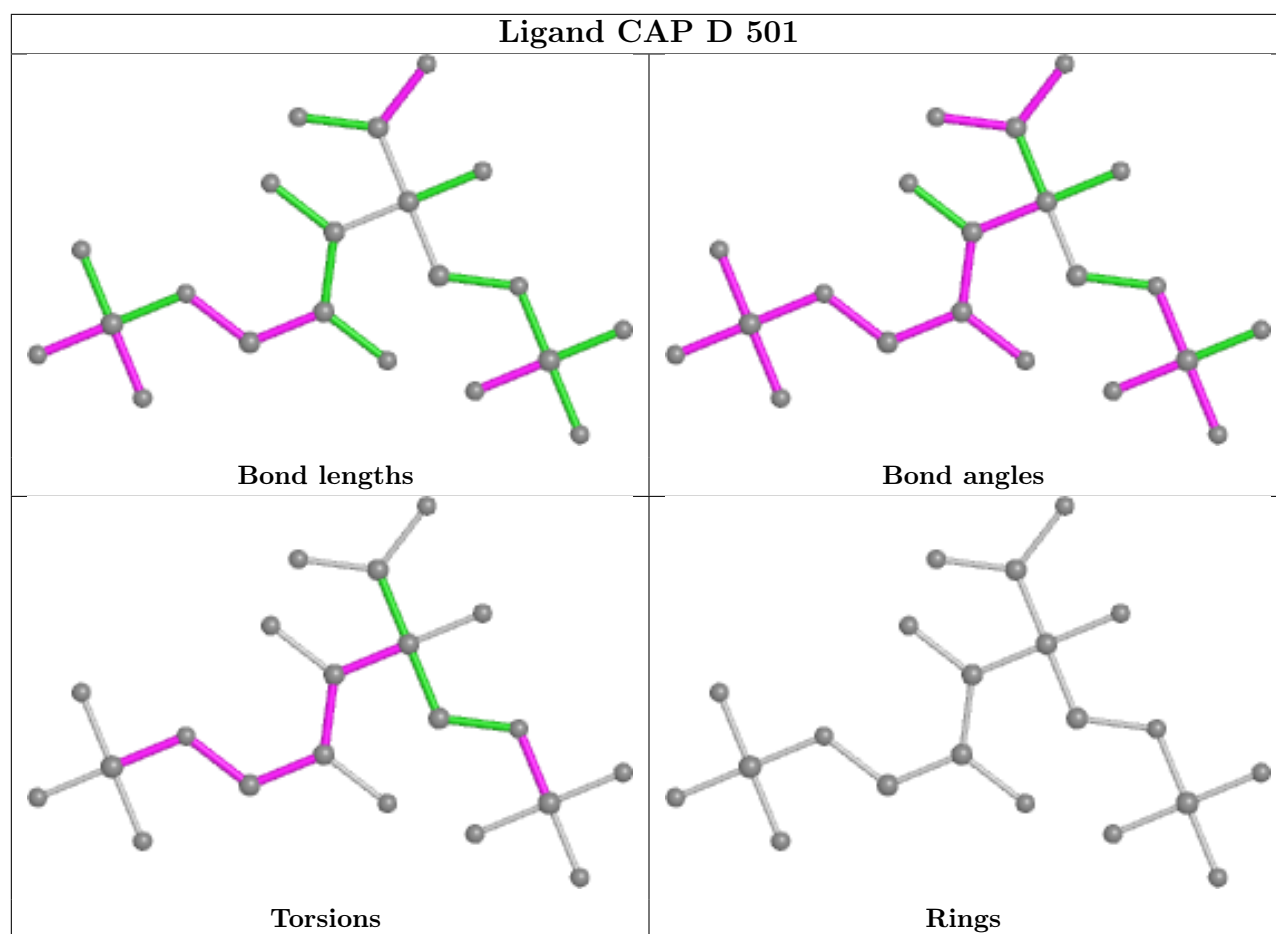
Ligand CAP I 501

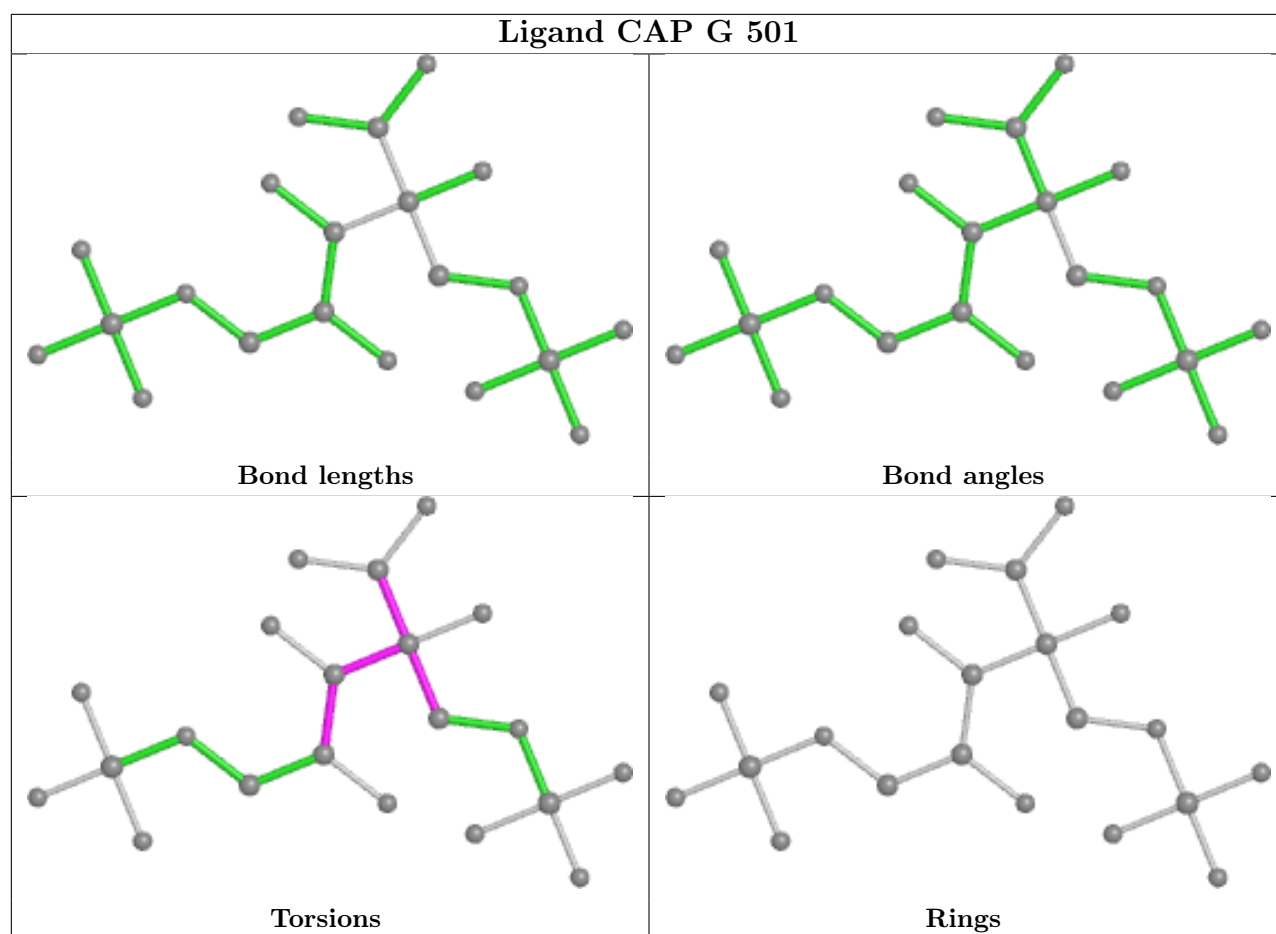


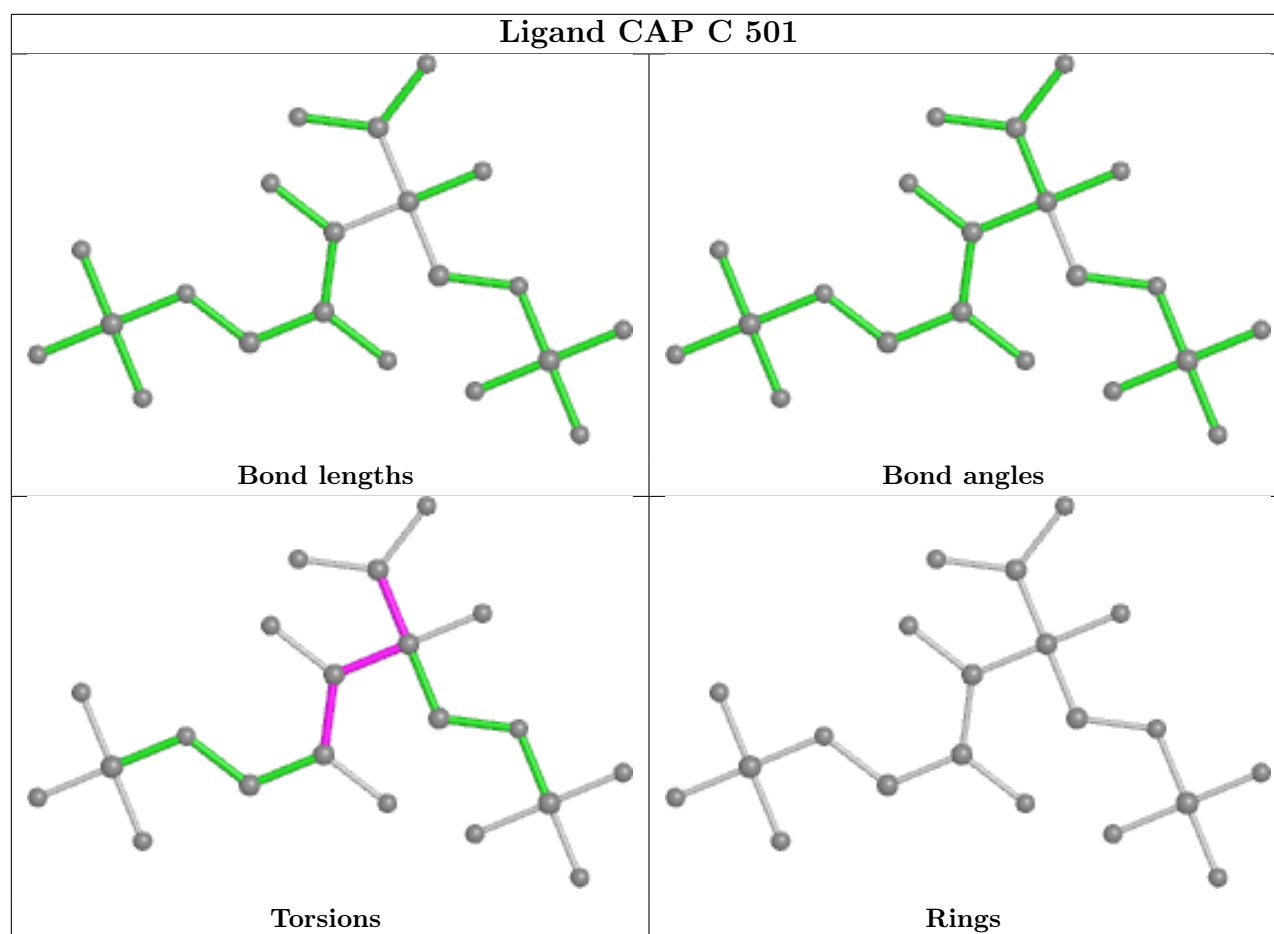
Ligand CAP J 501











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	454/460 (98%)	-0.09	2 (0%) 92 95	18, 24, 36, 64	0
1	B	456/460 (99%)	-0.11	2 (0%) 92 95	17, 23, 34, 52	0
1	C	453/460 (98%)	0.19	22 (4%) 29 39	19, 29, 56, 107	0
1	D	451/460 (98%)	0.19	17 (3%) 40 50	20, 29, 50, 91	0
1	E	452/460 (98%)	0.09	8 (1%) 68 76	24, 31, 46, 121	0
1	F	453/460 (98%)	0.11	6 (1%) 77 83	23, 31, 44, 100	0
1	G	452/460 (98%)	0.67	70 (15%) 2 3	20, 31, 99, 145	0
1	H	453/460 (98%)	0.22	20 (4%) 34 44	20, 29, 57, 133	0
1	I	451/460 (98%)	0.43	34 (7%) 14 22	26, 37, 65, 113	0
1	J	453/460 (98%)	0.29	15 (3%) 46 56	25, 35, 55, 74	0
1	K	452/460 (98%)	0.66	52 (11%) 4 8	25, 38, 81, 128	0
1	L	451/460 (98%)	0.33	23 (5%) 28 37	25, 35, 62, 124	0
All	All	5431/5520 (98%)	0.25	271 (4%) 28 39	17, 31, 61, 145	0

The worst 5 of 271 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	428	LYS	10.2
1	G	428	LYS	8.0
1	K	424	LEU	7.1
1	G	446	ALA	7.1
1	H	56	GLU	6.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	G	191	12/13	0.90	0.18	23,40,49,50	0
1	KCX	C	191	12/13	0.93	0.15	21,28,33,34	0
1	KCX	I	191	12/13	0.94	0.17	25,36,44,46	0
1	KCX	L	191	12/13	0.94	0.14	26,31,39,42	0
1	KCX	K	191	12/13	0.95	0.15	31,42,48,51	0
1	KCX	J	191	12/13	0.95	0.20	25,30,36,37	0
1	KCX	D	191	12/13	0.96	0.20	19,24,30,33	0
1	KCX	E	191	12/13	0.96	0.19	24,29,34,34	0
1	KCX	F	191	12/13	0.96	0.19	22,26,34,34	0
1	KCX	A	191	12/13	0.96	0.15	17,21,24,24	0
1	KCX	B	191	12/13	0.97	0.20	16,19,22,25	0
1	KCX	H	191	12/13	0.98	0.18	19,24,30,31	0

6.3 Carbohydrates [i](#)

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, 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.

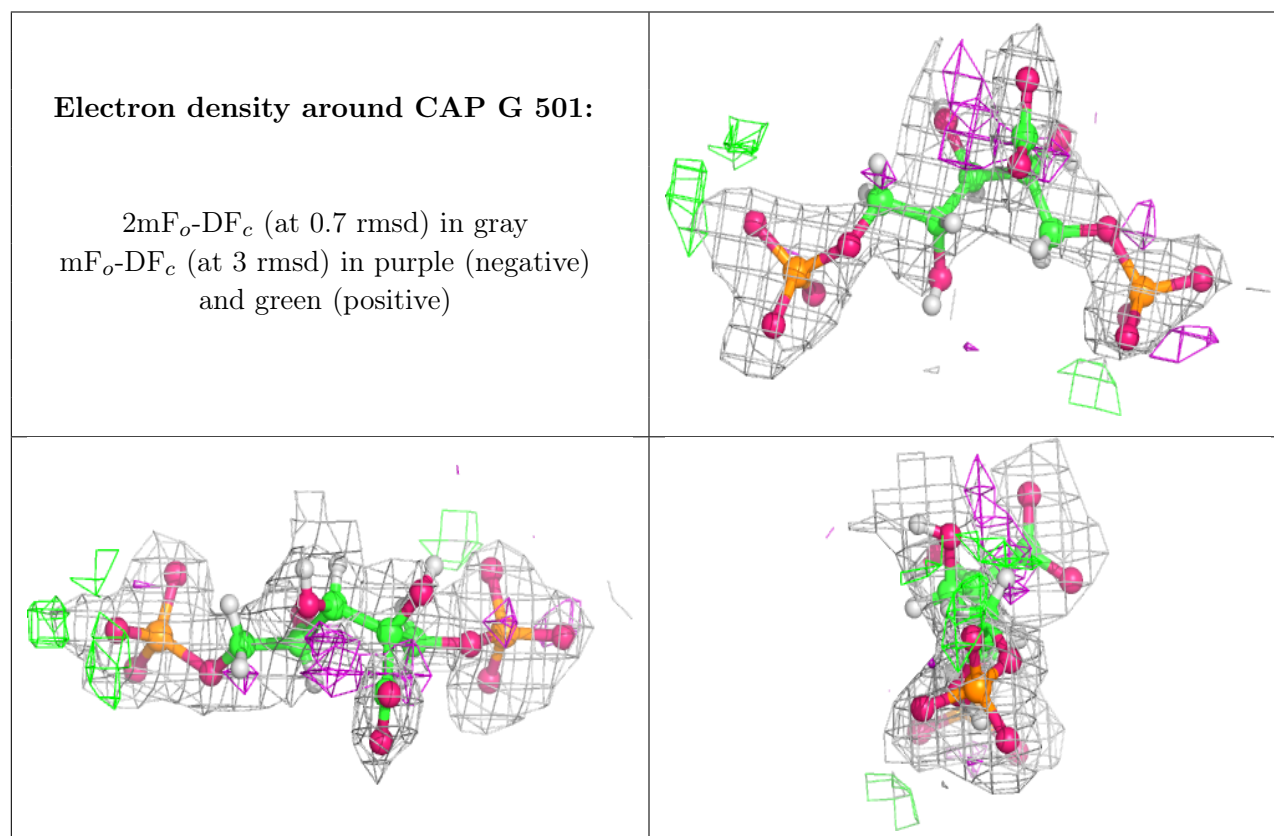
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CAP	G	501	21/21	0.83	0.20	44,61,75,78	0
3	MG	G	502	1/1	0.84	0.17	46,46,46,46	0
2	CAP	J	501	21/21	0.86	0.22	29,34,41,44	0
2	CAP	D	501	21/21	0.88	0.21	24,30,37,40	0
3	MG	J	502	1/1	0.91	0.28	32,32,32,32	0
3	MG	K	502	1/1	0.91	0.08	45,45,45,45	0
2	CAP	K	501	21/21	0.92	0.13	46,55,67,71	0
2	CAP	I	501	21/21	0.92	0.12	37,46,55,55	0
3	MG	E	502	1/1	0.95	0.08	26,26,26,26	0
2	CAP	C	501	21/21	0.95	0.10	29,36,44,47	0
3	MG	C	502	1/1	0.96	0.07	33,33,33,33	0
3	MG	H	502	1/1	0.96	0.11	29,29,29,29	0
3	MG	D	502	1/1	0.96	0.15	25,25,25,25	0
2	CAP	L	501	21/21	0.96	0.10	28,33,38,43	0

Continued on next page...

Continued from previous page...

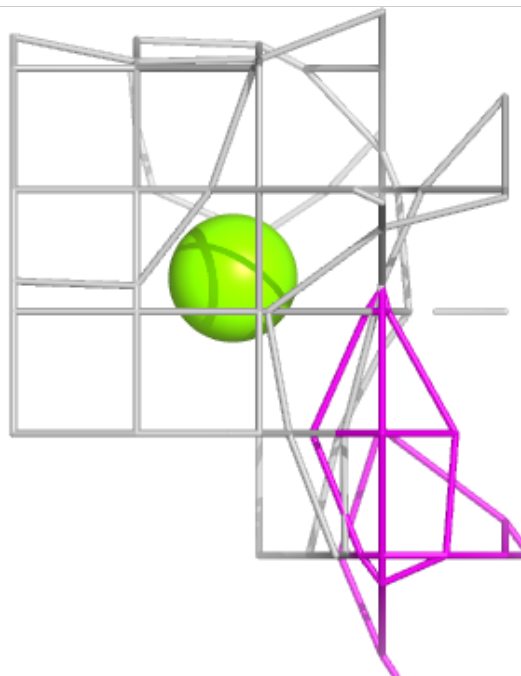
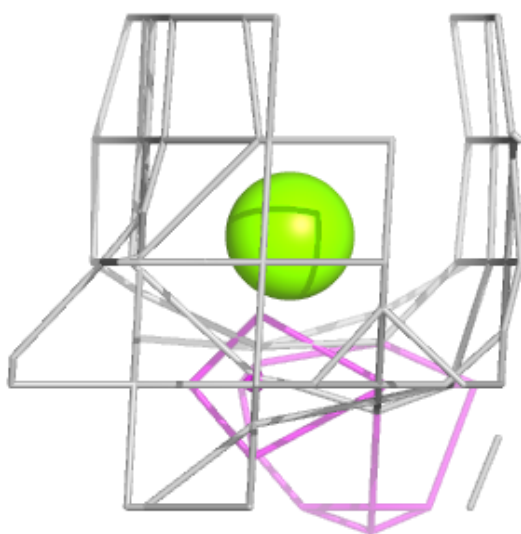
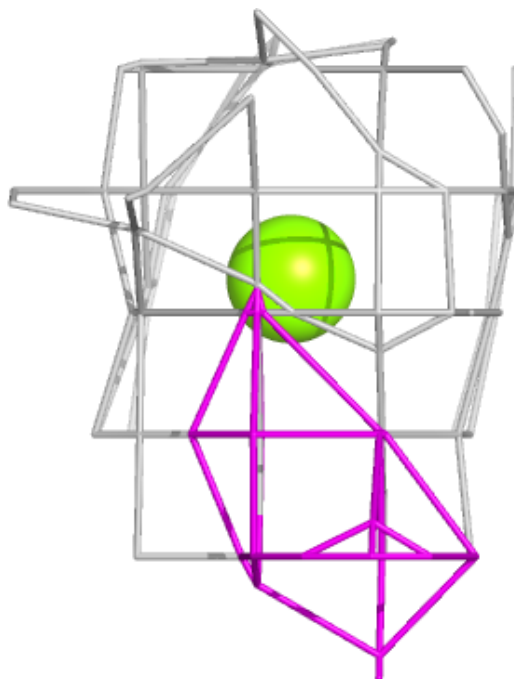
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CAP	E	501	21/21	0.97	0.14	25,31,38,42	0
2	CAP	F	501	21/21	0.97	0.14	23,29,37,37	0
2	CAP	A	501	21/21	0.97	0.10	20,24,29,29	0
3	MG	I	502	1/1	0.97	0.06	39,39,39,39	0
2	CAP	H	501	21/21	0.97	0.12	20,27,37,38	0
2	CAP	B	501	21/21	0.97	0.12	17,22,28,31	0
3	MG	F	502	1/1	0.98	0.12	27,27,27,27	0
3	MG	A	502	1/1	0.98	0.09	22,22,22,22	0
3	MG	L	502	1/1	0.98	0.05	28,28,28,28	0
3	MG	B	502	1/1	1.00	0.15	20,20,20,20	0

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



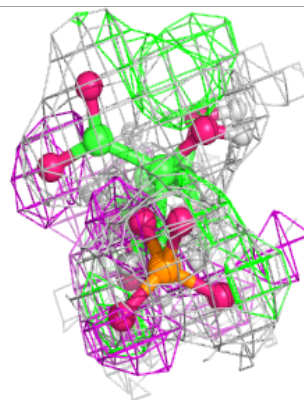
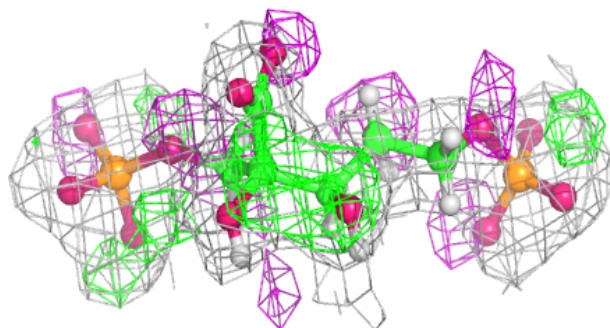
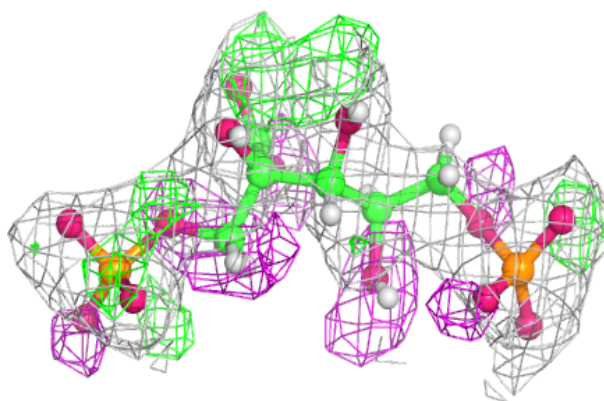
Electron density around MG G 502:

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

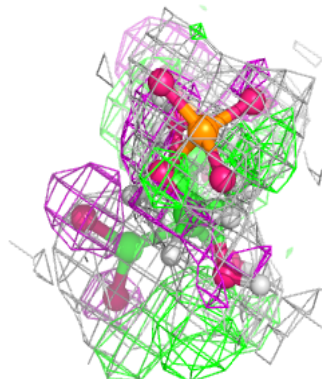
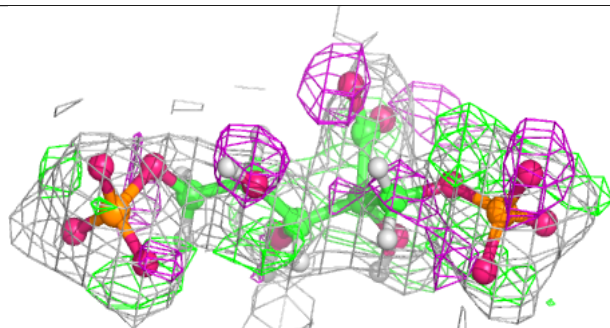
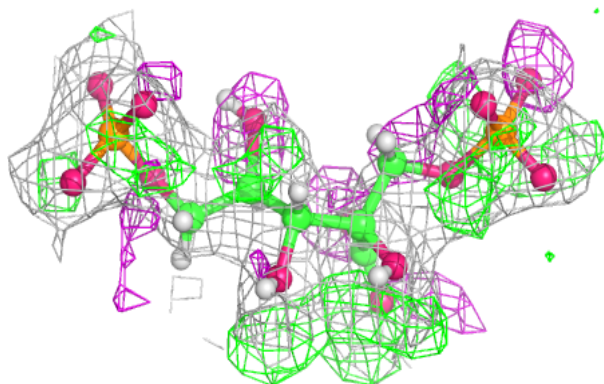


Electron density around CAP J 501:

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

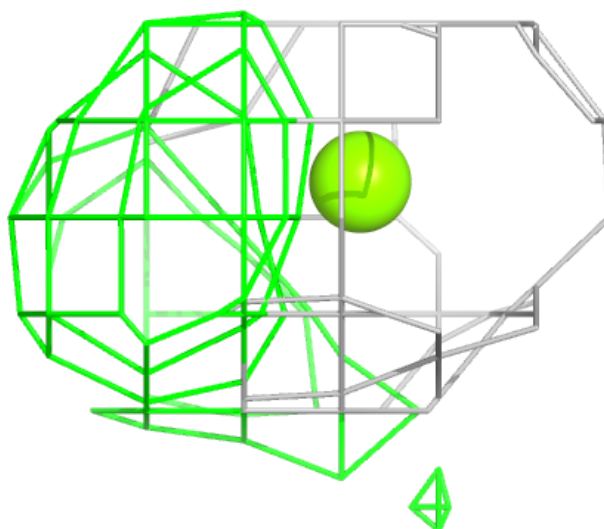
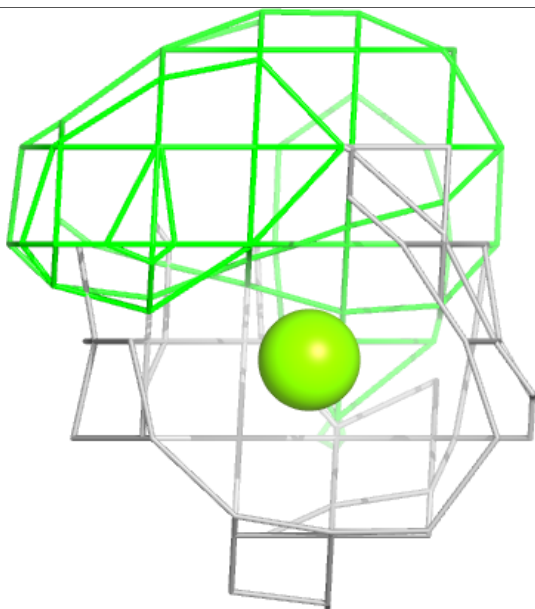
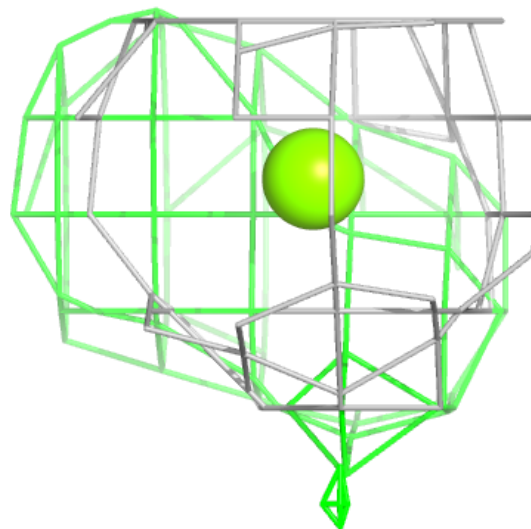
**Electron density around CAP D 501:**

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



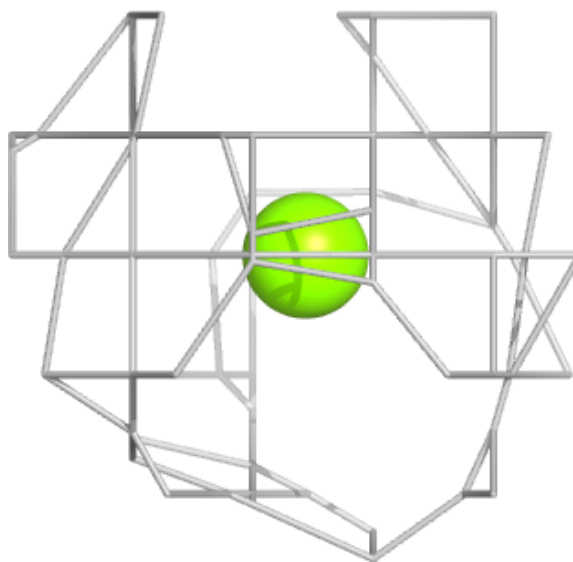
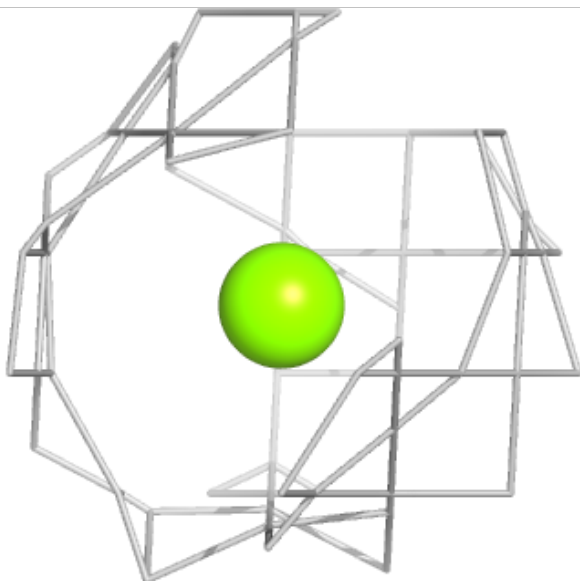
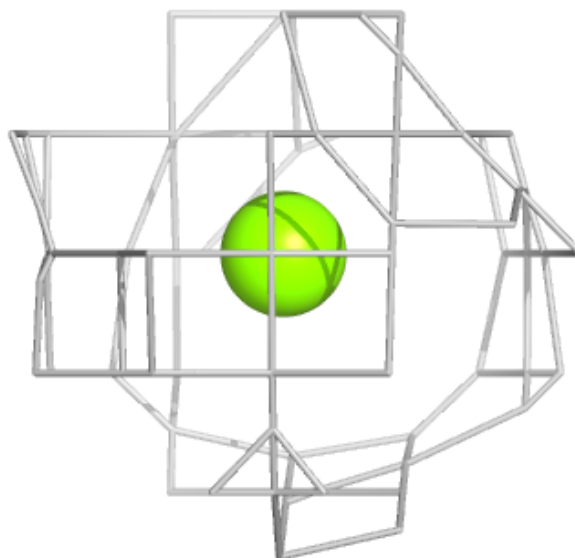
Electron density around MG J 502:

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



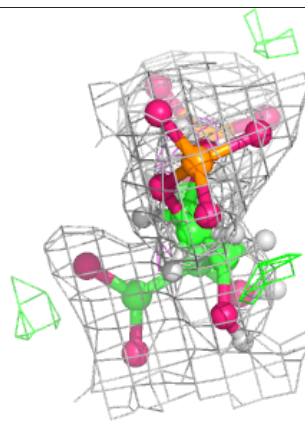
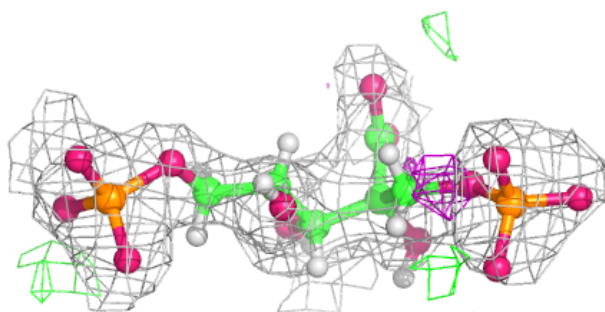
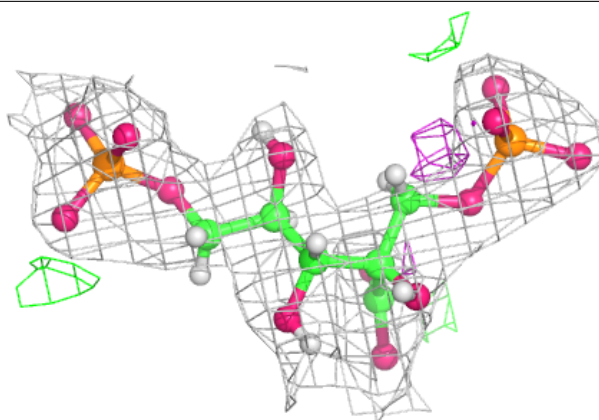
Electron density around MG K 502:

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

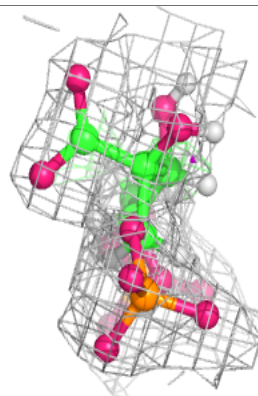
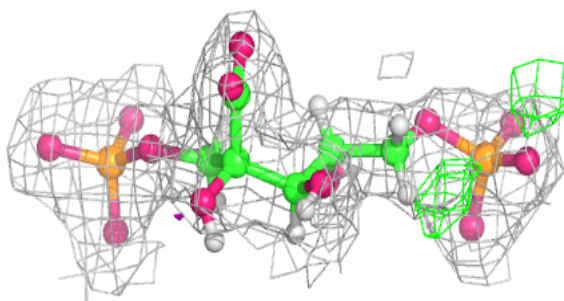
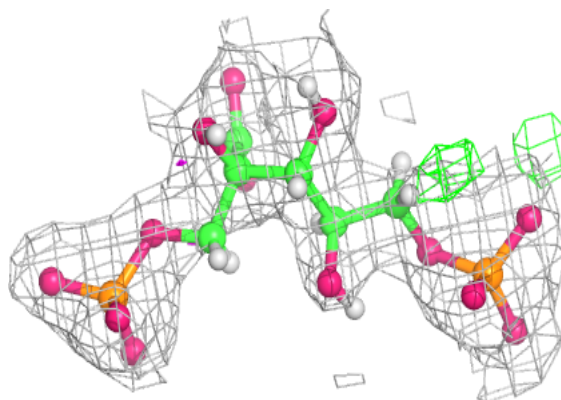


Electron density around CAP K 501:

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

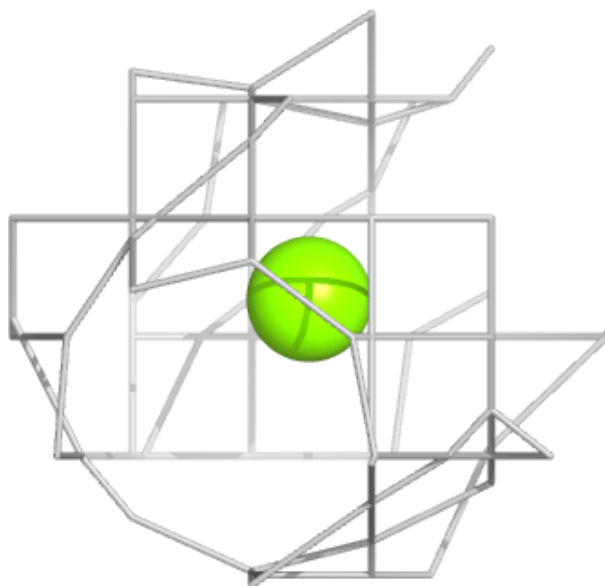
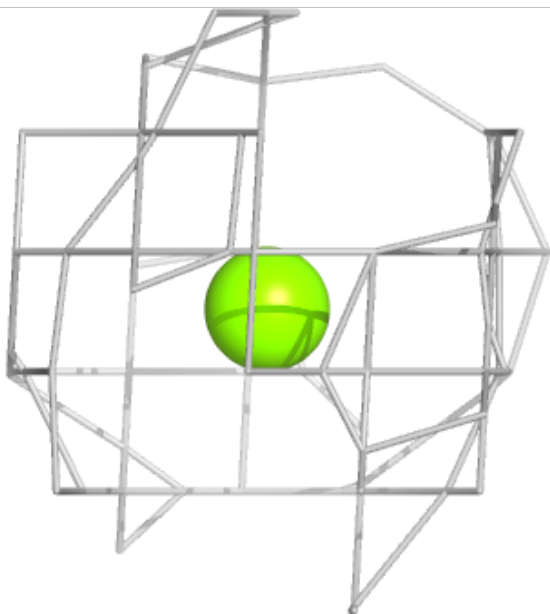
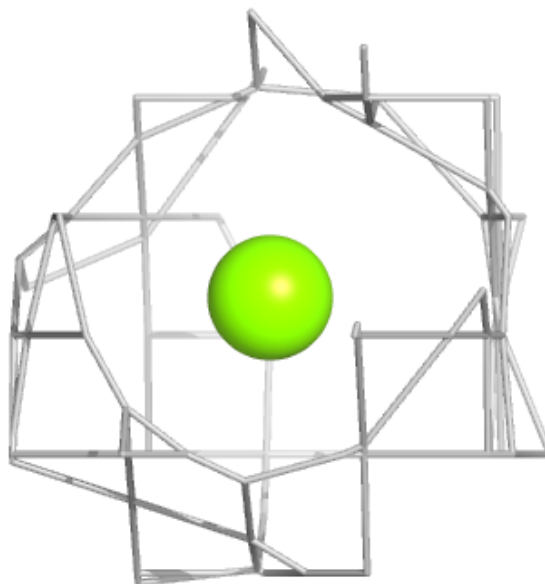
**Electron density around CAP I 501:**

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



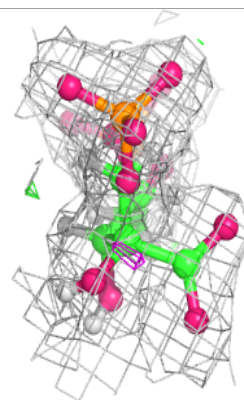
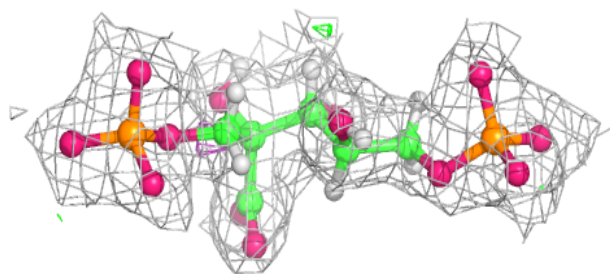
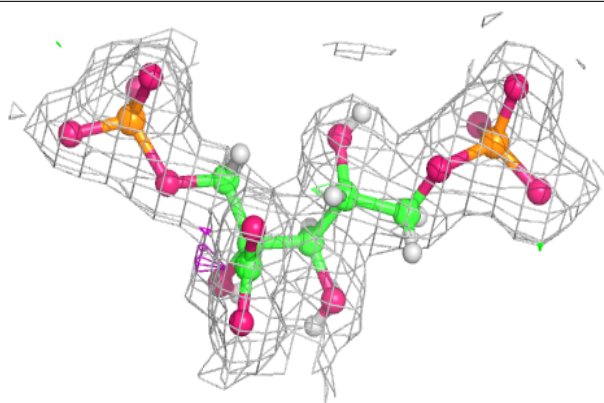
Electron density around MG E 502:

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



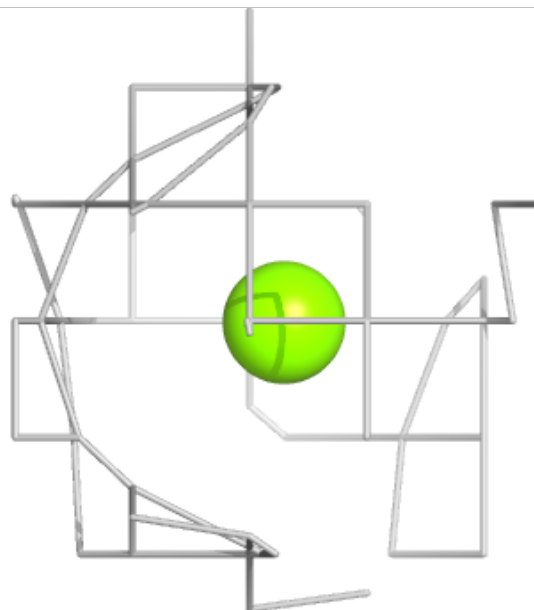
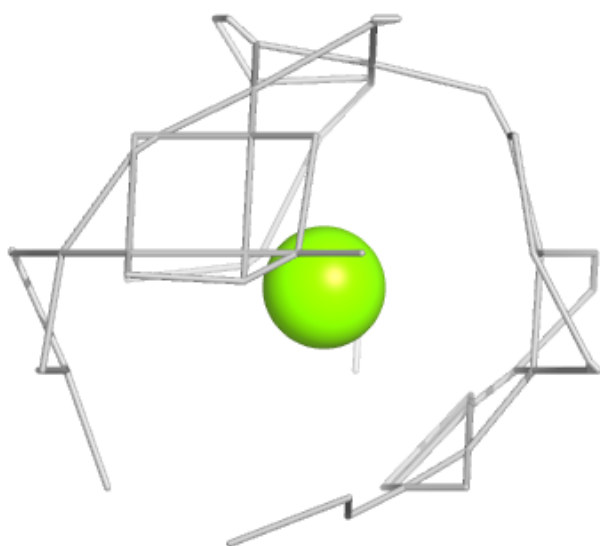
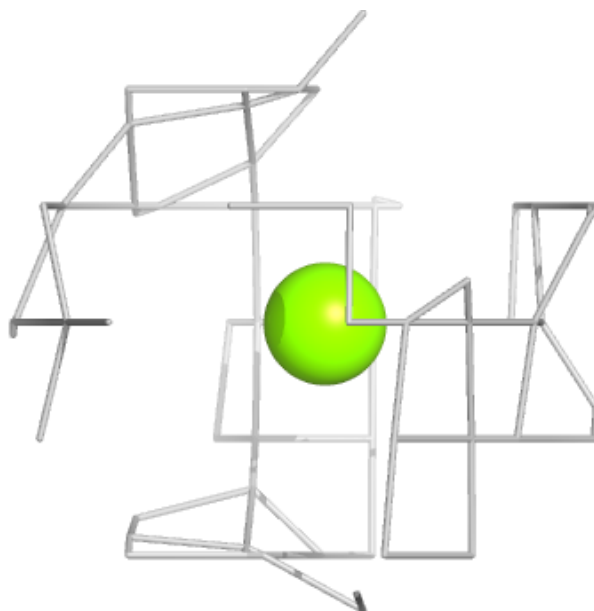
Electron density around CAP C 501:

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



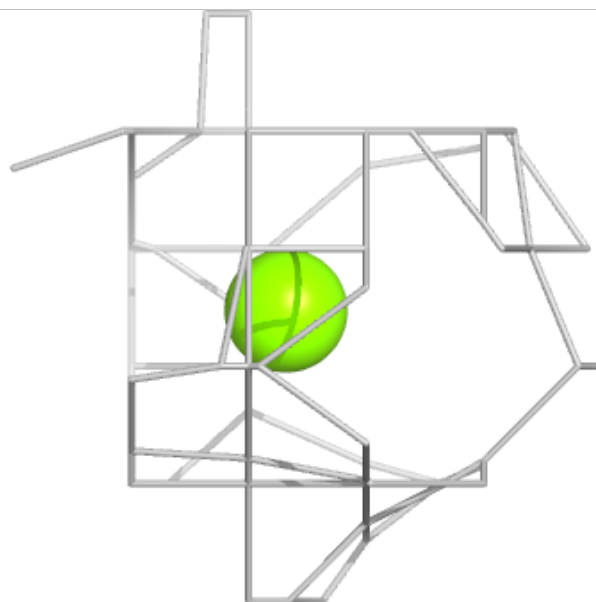
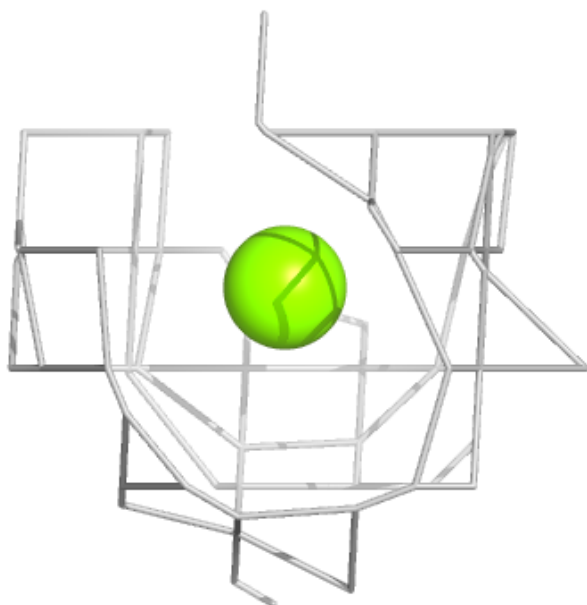
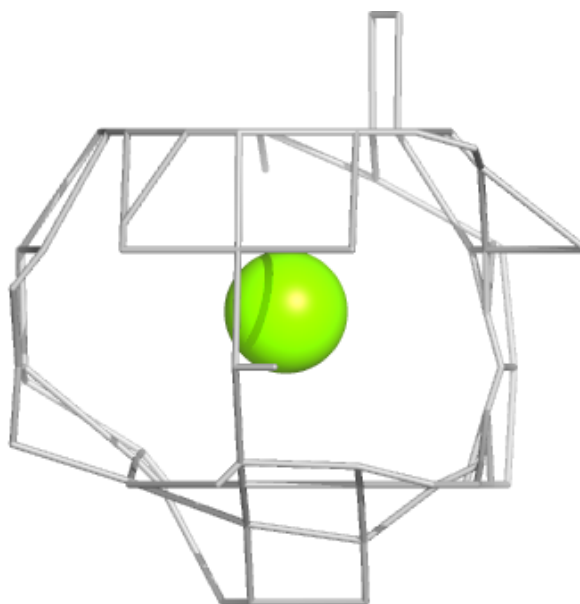
Electron density around MG C 502:

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



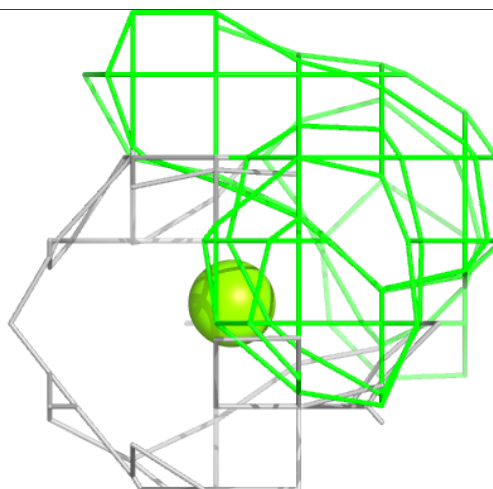
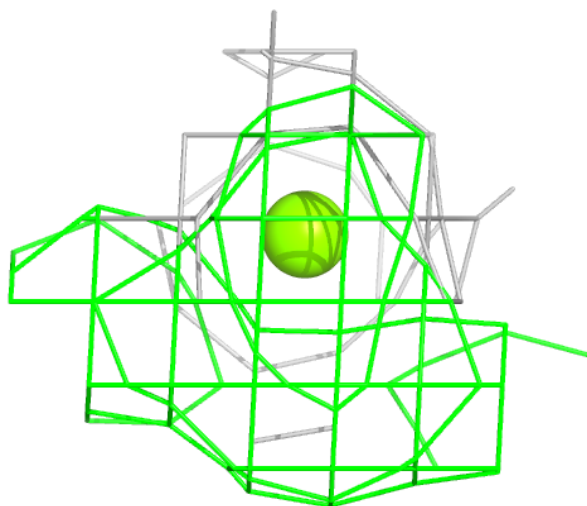
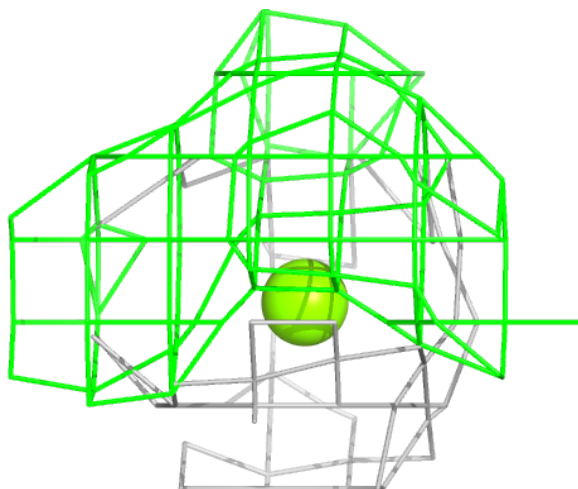
Electron density around MG H 502:

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



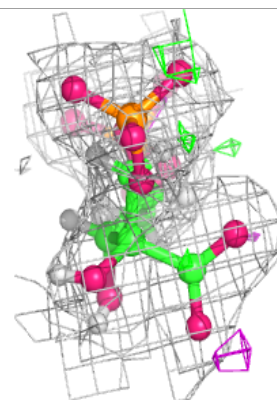
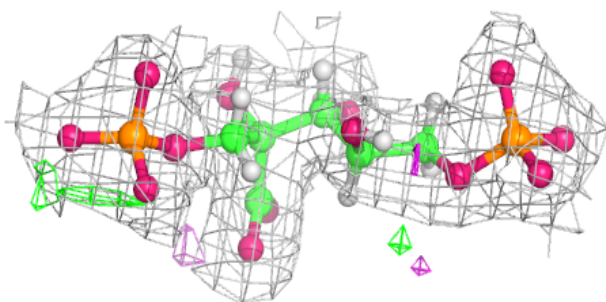
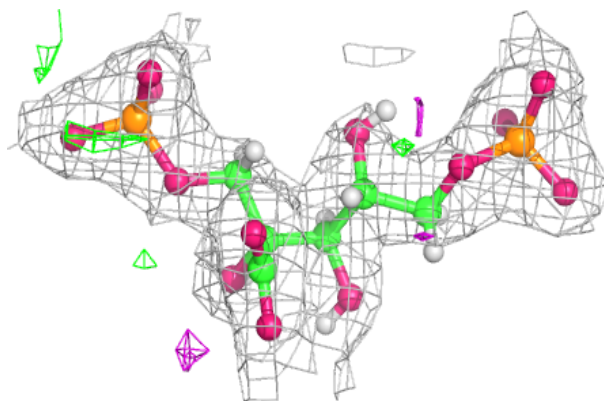
Electron density around MG D 502:

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

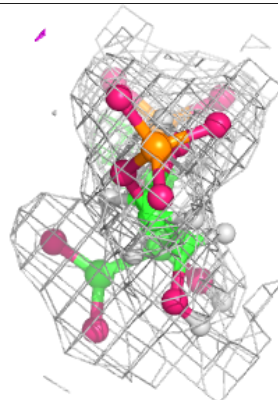
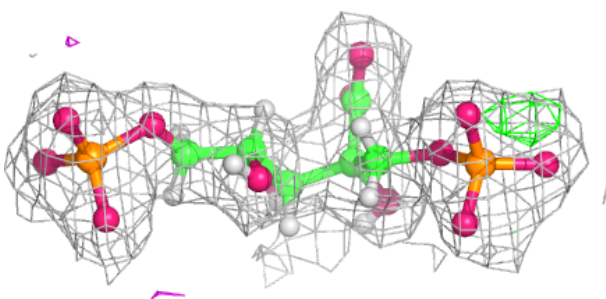
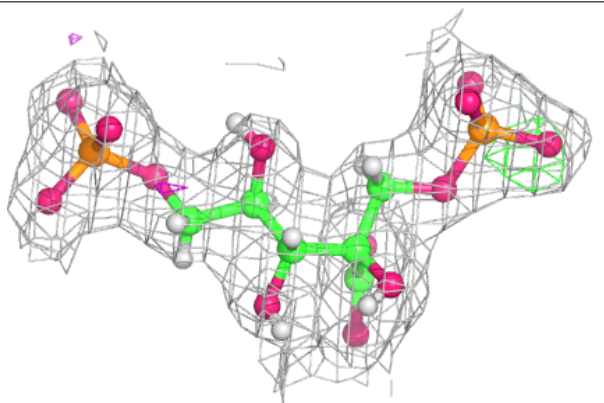


Electron density around CAP L 501:

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

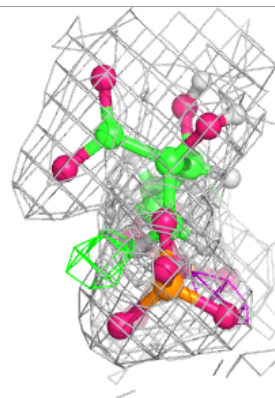
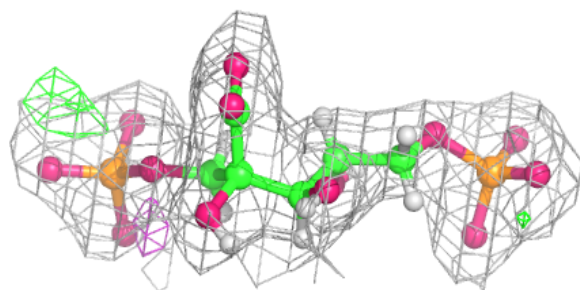
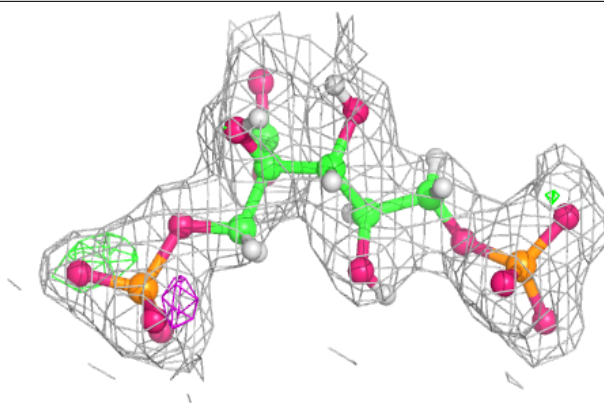
**Electron density around CAP E 501:**

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

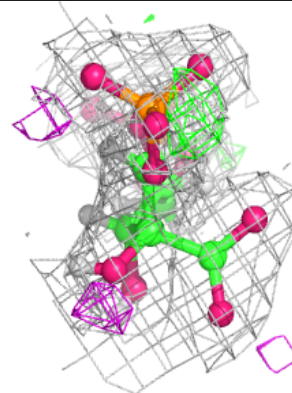
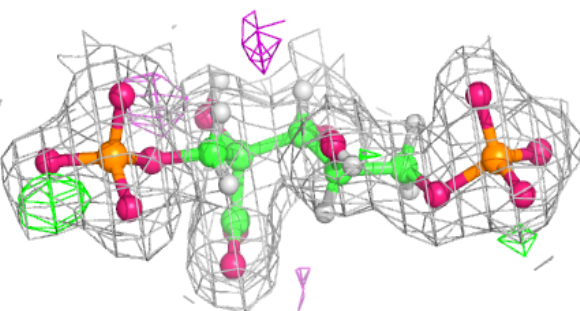
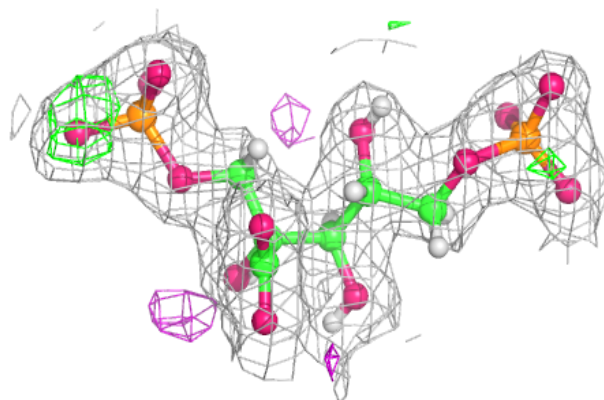


Electron density around CAP F 501:

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

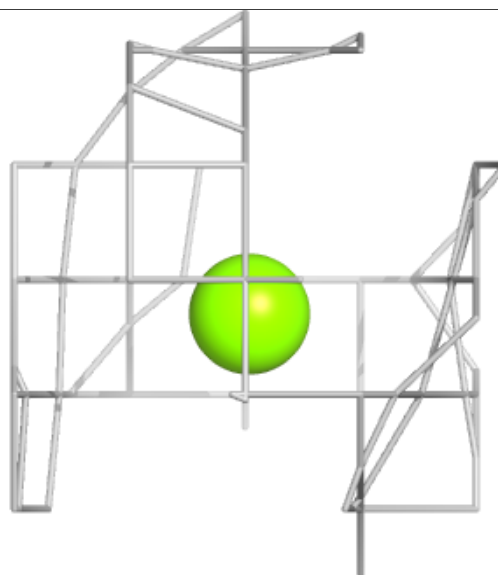
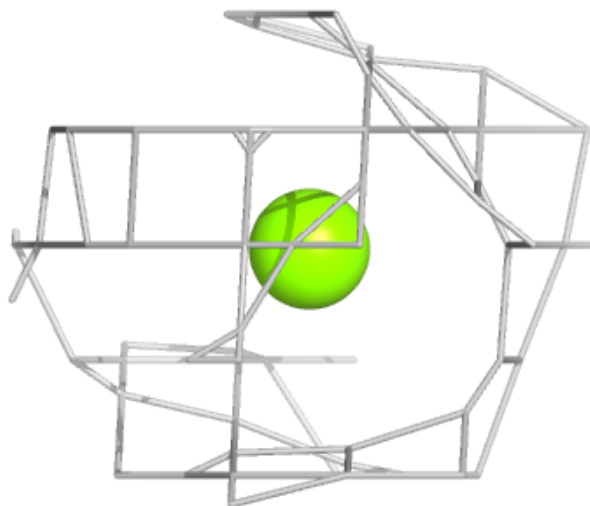
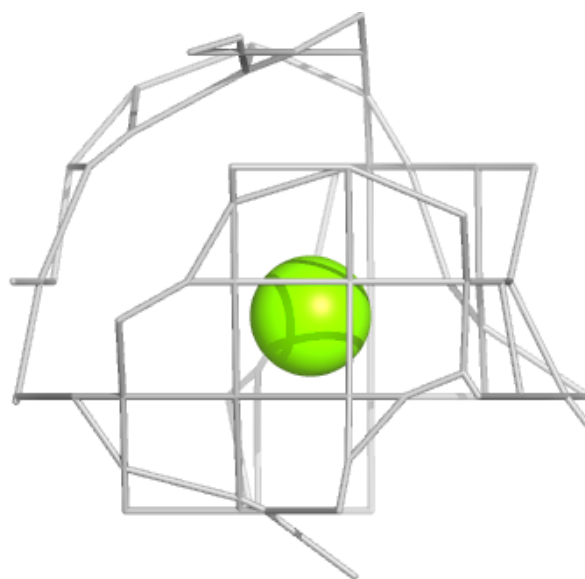
**Electron density around CAP A 501:**

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



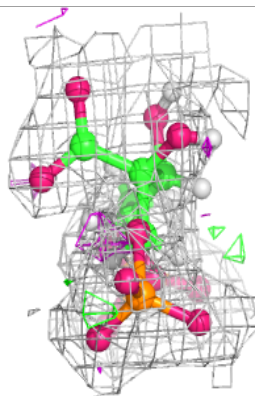
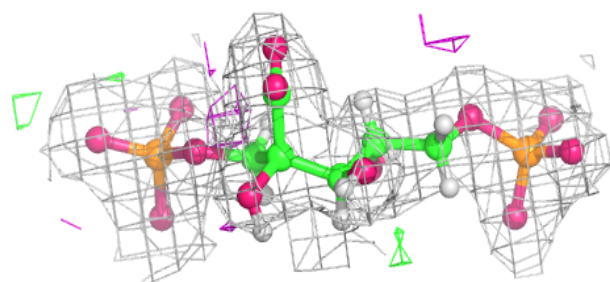
Electron density around MG I 502:

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

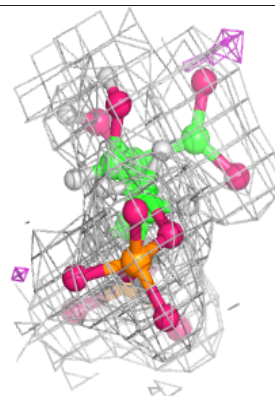
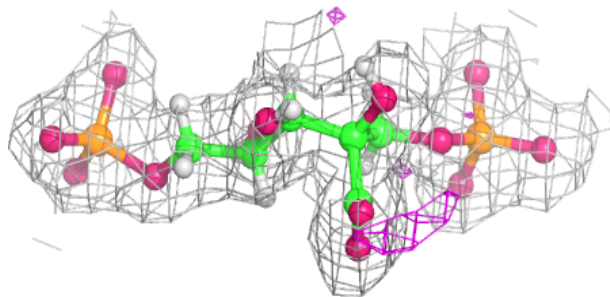
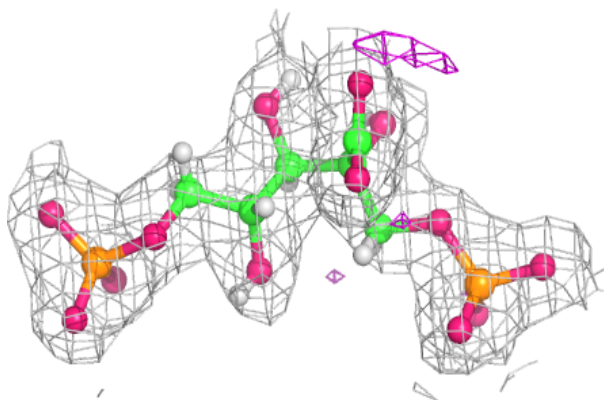


Electron density around CAP H 501:

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

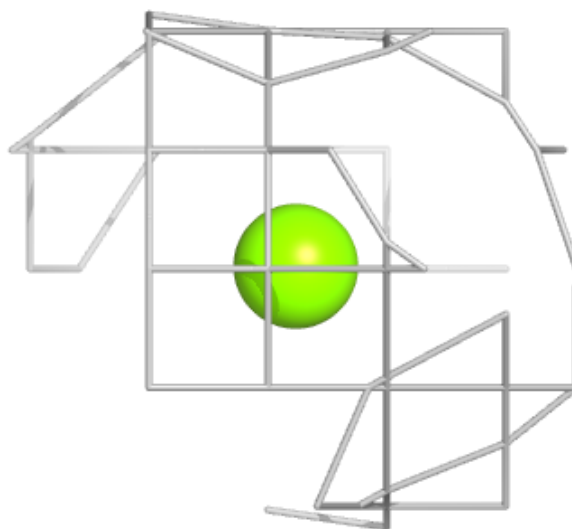
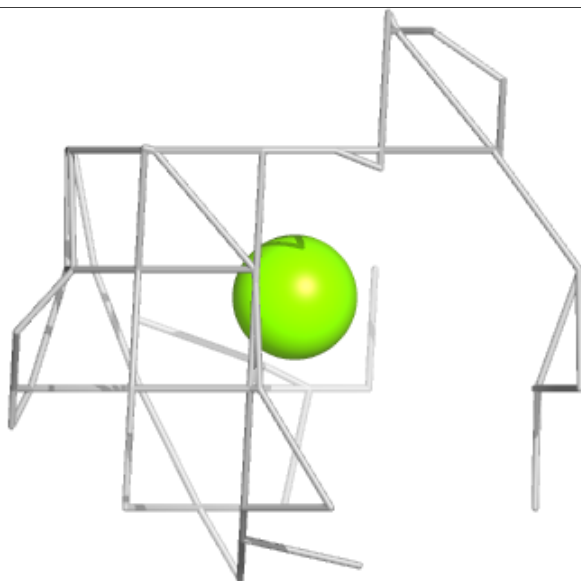
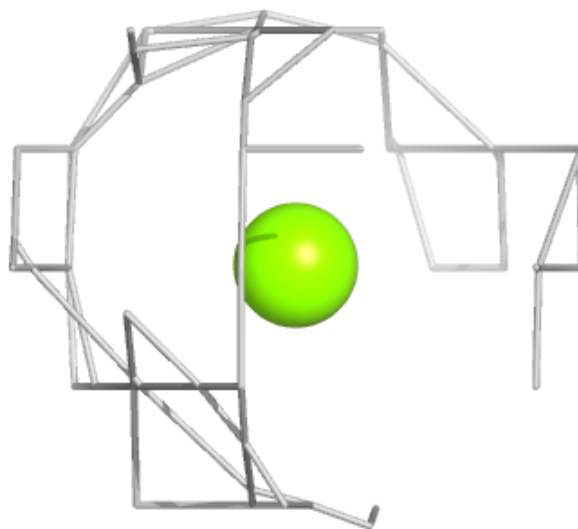
**Electron density around CAP B 501:**

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



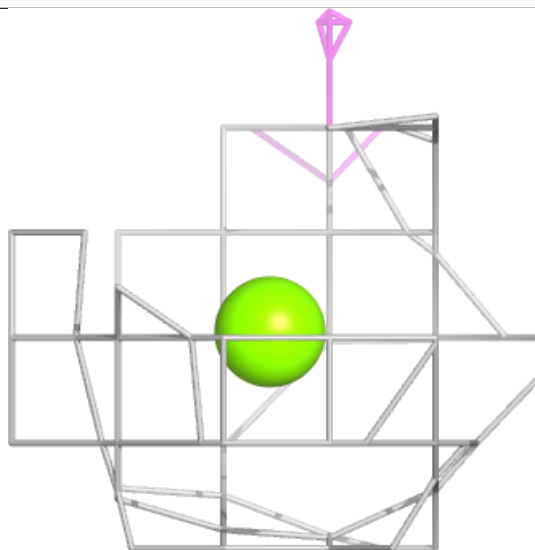
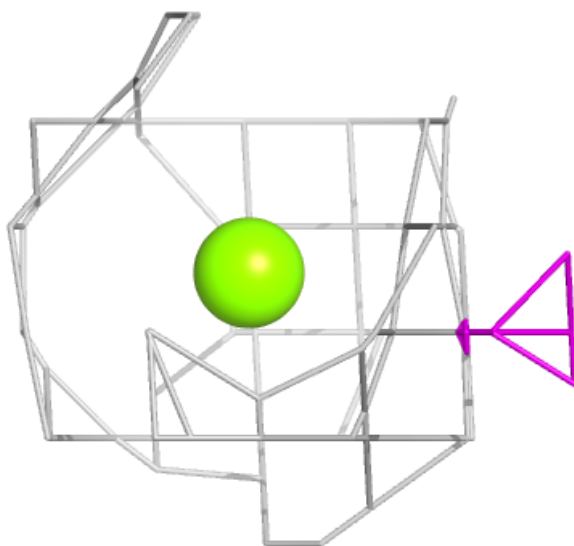
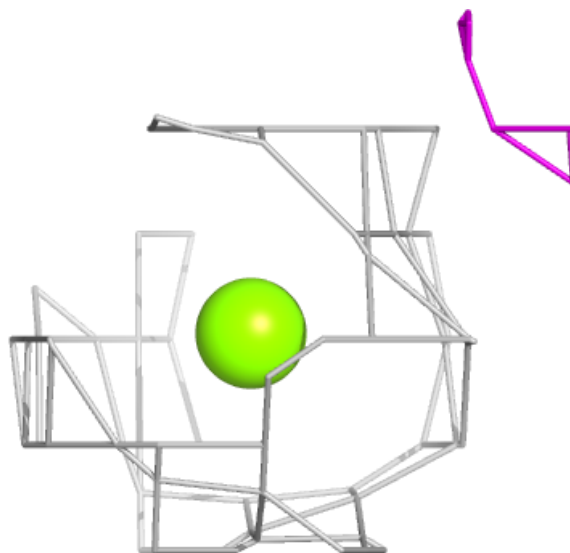
Electron density around MG F 502:

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



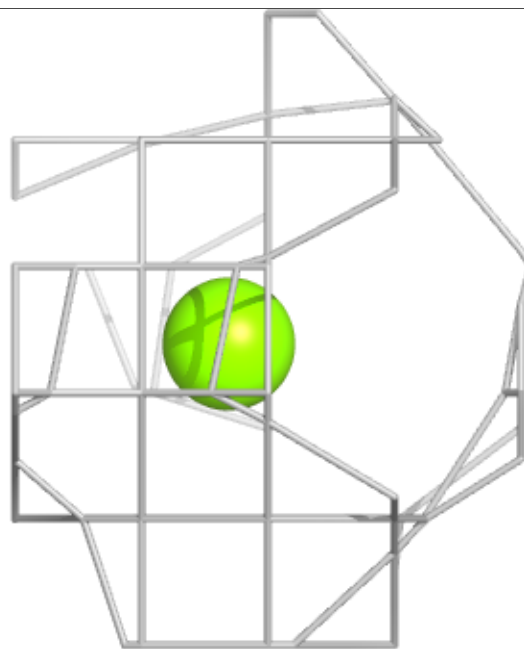
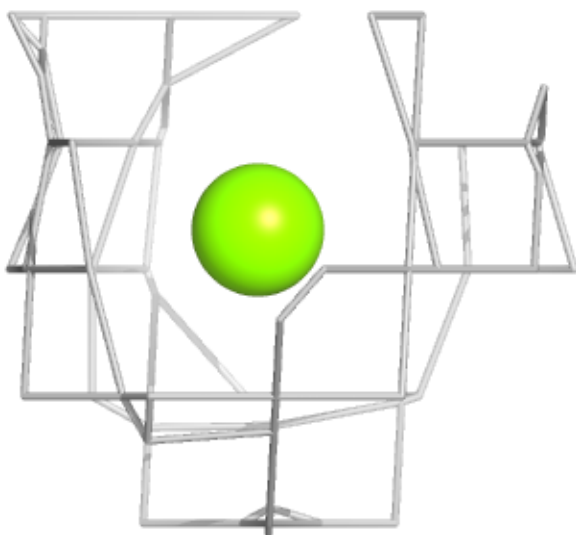
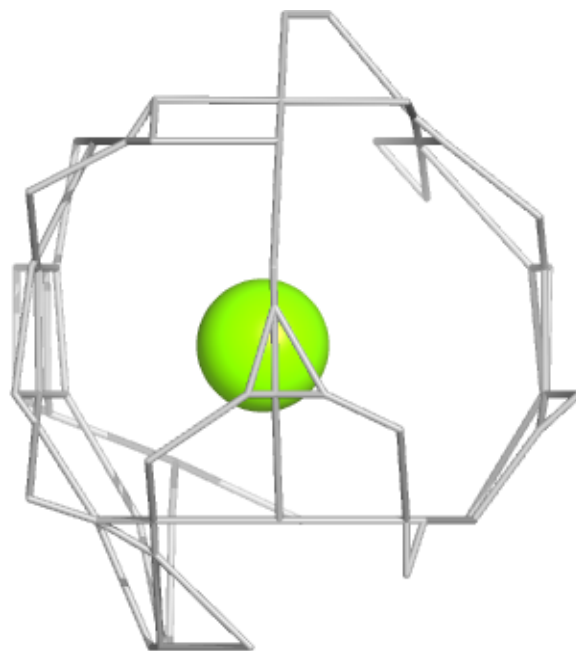
Electron density around MG A 502:

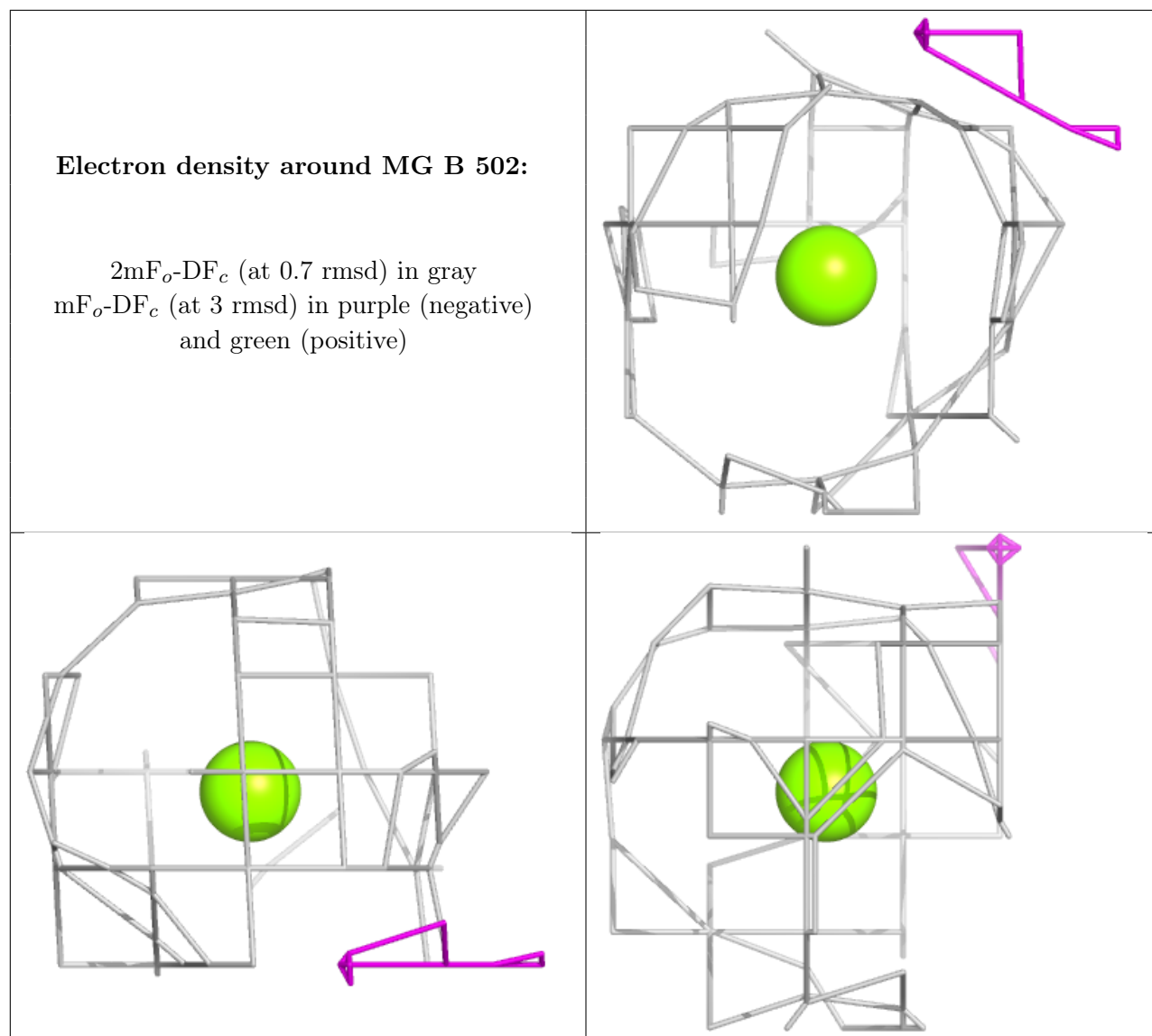
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG L 502:

$2mF_o-DF_c$ (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.