



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 01:42 AM EST

PDB ID : 5HAN  
Title : Structure function studies of *R. palustris* RubisCO (S59F mutant; CABP-bound)  
Authors : Arbing, M.A.; Leong, J.G.; Varaljay, V.A.; Satagopan, S.; North, J.A.; Tabita, F.R.  
Deposited on : 2015-12-30  
Resolution : 2.04 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](mailto: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>.

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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 : 2.36  
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) : 2.36

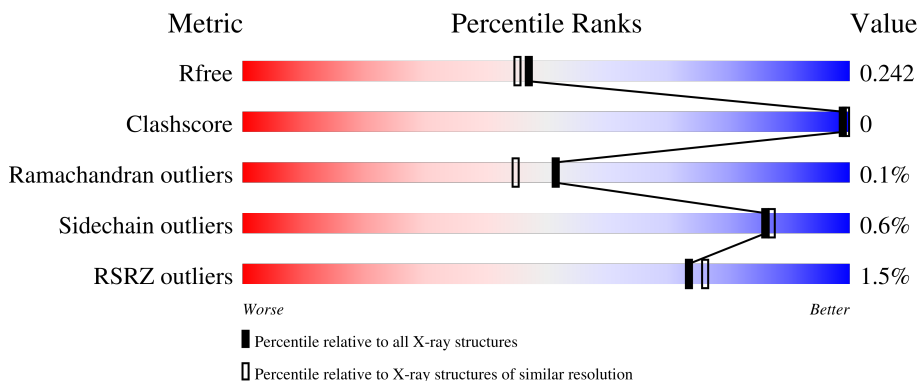
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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.



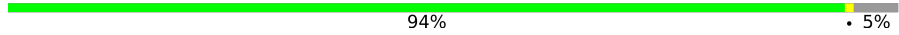
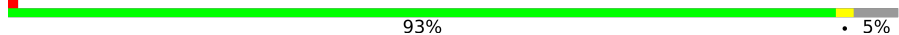
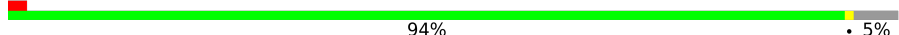

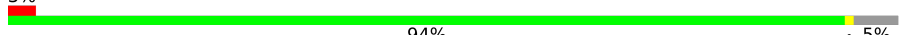

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 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	481	94% • 5%
1	B	481	92% • 5%
1	C	481	93% • 5%
1	D	481	93% • 5%

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Mol	Chain	Length	Quality of chain
1	E	481	 94% • 5%
1	F	481	 93% • 5%
1	G	481	 93% • 5%
1	H	481	 94% • 5%
1	I	481	 93% • 5%
1	J	481	 94% • 5%
1	K	481	 93% • 5%
1	L	481	 93% • 5%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 85695 atoms, of which 40512 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	
			Total	C	H	N	O				S
1	A	456	6906	2246	3377	610	654	19	0	0	0
1	B	455	6857	2232	3346	607	653	19	0	0	0
1	C	455	6891	2238	3371	609	654	19	0	0	0
1	D	455	6906	2241	3382	610	654	19	0	0	0
1	E	457	6892	2245	3363	610	655	19	0	0	0
1	F	455	6898	2239	3378	610	652	19	0	0	0
1	G	457	6892	2245	3363	610	655	19	0	0	0
1	H	456	6898	2244	3370	610	655	19	0	0	0
1	I	455	6876	2235	3360	608	654	19	0	0	0
1	J	455	6879	2238	3359	609	654	19	0	0	0
1	K	455	6866	2233	3357	607	650	19	0	0	0
1	L	456	6907	2246	3378	610	654	19	0	0	0

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q6N0W9
A	-18	GLY	-	expression tag	UNP Q6N0W9
A	-17	SER	-	expression tag	UNP Q6N0W9
A	-16	SER	-	expression tag	UNP Q6N0W9
A	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q6N0W9
A	-13	HIS	-	expression tag	UNP Q6N0W9
A	-12	HIS	-	expression tag	UNP Q6N0W9
A	-11	HIS	-	expression tag	UNP Q6N0W9
A	-10	HIS	-	expression tag	UNP Q6N0W9
A	-9	SER	-	expression tag	UNP Q6N0W9
A	-8	SER	-	expression tag	UNP Q6N0W9
A	-7	GLY	-	expression tag	UNP Q6N0W9
A	-6	LEU	-	expression tag	UNP Q6N0W9
A	-5	VAL	-	expression tag	UNP Q6N0W9
A	-4	PRO	-	expression tag	UNP Q6N0W9
A	-3	ARG	-	expression tag	UNP Q6N0W9
A	-2	GLY	-	expression tag	UNP Q6N0W9
A	-1	SER	-	expression tag	UNP Q6N0W9
A	0	HIS	-	expression tag	UNP Q6N0W9
A	59	PHE	SER	engineered mutation	UNP Q6N0W9
B	-19	MET	-	initiating methionine	UNP Q6N0W9
B	-18	GLY	-	expression tag	UNP Q6N0W9
B	-17	SER	-	expression tag	UNP Q6N0W9
B	-16	SER	-	expression tag	UNP Q6N0W9
B	-15	HIS	-	expression tag	UNP Q6N0W9
B	-14	HIS	-	expression tag	UNP Q6N0W9
B	-13	HIS	-	expression tag	UNP Q6N0W9
B	-12	HIS	-	expression tag	UNP Q6N0W9
B	-11	HIS	-	expression tag	UNP Q6N0W9
B	-10	HIS	-	expression tag	UNP Q6N0W9
B	-9	SER	-	expression tag	UNP Q6N0W9
B	-8	SER	-	expression tag	UNP Q6N0W9
B	-7	GLY	-	expression tag	UNP Q6N0W9
B	-6	LEU	-	expression tag	UNP Q6N0W9
B	-5	VAL	-	expression tag	UNP Q6N0W9
B	-4	PRO	-	expression tag	UNP Q6N0W9
B	-3	ARG	-	expression tag	UNP Q6N0W9
B	-2	GLY	-	expression tag	UNP Q6N0W9
B	-1	SER	-	expression tag	UNP Q6N0W9
B	0	HIS	-	expression tag	UNP Q6N0W9
B	59	PHE	SER	engineered mutation	UNP Q6N0W9
C	-19	MET	-	initiating methionine	UNP Q6N0W9
C	-18	GLY	-	expression tag	UNP Q6N0W9
C	-17	SER	-	expression tag	UNP Q6N0W9
C	-16	SER	-	expression tag	UNP Q6N0W9
C	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q6N0W9
C	-13	HIS	-	expression tag	UNP Q6N0W9
C	-12	HIS	-	expression tag	UNP Q6N0W9
C	-11	HIS	-	expression tag	UNP Q6N0W9
C	-10	HIS	-	expression tag	UNP Q6N0W9
C	-9	SER	-	expression tag	UNP Q6N0W9
C	-8	SER	-	expression tag	UNP Q6N0W9
C	-7	GLY	-	expression tag	UNP Q6N0W9
C	-6	LEU	-	expression tag	UNP Q6N0W9
C	-5	VAL	-	expression tag	UNP Q6N0W9
C	-4	PRO	-	expression tag	UNP Q6N0W9
C	-3	ARG	-	expression tag	UNP Q6N0W9
C	-2	GLY	-	expression tag	UNP Q6N0W9
C	-1	SER	-	expression tag	UNP Q6N0W9
C	0	HIS	-	expression tag	UNP Q6N0W9
C	59	PHE	SER	engineered mutation	UNP Q6N0W9
D	-19	MET	-	initiating methionine	UNP Q6N0W9
D	-18	GLY	-	expression tag	UNP Q6N0W9
D	-17	SER	-	expression tag	UNP Q6N0W9
D	-16	SER	-	expression tag	UNP Q6N0W9
D	-15	HIS	-	expression tag	UNP Q6N0W9
D	-14	HIS	-	expression tag	UNP Q6N0W9
D	-13	HIS	-	expression tag	UNP Q6N0W9
D	-12	HIS	-	expression tag	UNP Q6N0W9
D	-11	HIS	-	expression tag	UNP Q6N0W9
D	-10	HIS	-	expression tag	UNP Q6N0W9
D	-9	SER	-	expression tag	UNP Q6N0W9
D	-8	SER	-	expression tag	UNP Q6N0W9
D	-7	GLY	-	expression tag	UNP Q6N0W9
D	-6	LEU	-	expression tag	UNP Q6N0W9
D	-5	VAL	-	expression tag	UNP Q6N0W9
D	-4	PRO	-	expression tag	UNP Q6N0W9
D	-3	ARG	-	expression tag	UNP Q6N0W9
D	-2	GLY	-	expression tag	UNP Q6N0W9
D	-1	SER	-	expression tag	UNP Q6N0W9
D	0	HIS	-	expression tag	UNP Q6N0W9
D	59	PHE	SER	engineered mutation	UNP Q6N0W9
E	-19	MET	-	initiating methionine	UNP Q6N0W9
E	-18	GLY	-	expression tag	UNP Q6N0W9
E	-17	SER	-	expression tag	UNP Q6N0W9
E	-16	SER	-	expression tag	UNP Q6N0W9
E	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-14	HIS	-	expression tag	UNP Q6N0W9
E	-13	HIS	-	expression tag	UNP Q6N0W9
E	-12	HIS	-	expression tag	UNP Q6N0W9
E	-11	HIS	-	expression tag	UNP Q6N0W9
E	-10	HIS	-	expression tag	UNP Q6N0W9
E	-9	SER	-	expression tag	UNP Q6N0W9
E	-8	SER	-	expression tag	UNP Q6N0W9
E	-7	GLY	-	expression tag	UNP Q6N0W9
E	-6	LEU	-	expression tag	UNP Q6N0W9
E	-5	VAL	-	expression tag	UNP Q6N0W9
E	-4	PRO	-	expression tag	UNP Q6N0W9
E	-3	ARG	-	expression tag	UNP Q6N0W9
E	-2	GLY	-	expression tag	UNP Q6N0W9
E	-1	SER	-	expression tag	UNP Q6N0W9
E	0	HIS	-	expression tag	UNP Q6N0W9
E	59	PHE	SER	engineered mutation	UNP Q6N0W9
F	-19	MET	-	initiating methionine	UNP Q6N0W9
F	-18	GLY	-	expression tag	UNP Q6N0W9
F	-17	SER	-	expression tag	UNP Q6N0W9
F	-16	SER	-	expression tag	UNP Q6N0W9
F	-15	HIS	-	expression tag	UNP Q6N0W9
F	-14	HIS	-	expression tag	UNP Q6N0W9
F	-13	HIS	-	expression tag	UNP Q6N0W9
F	-12	HIS	-	expression tag	UNP Q6N0W9
F	-11	HIS	-	expression tag	UNP Q6N0W9
F	-10	HIS	-	expression tag	UNP Q6N0W9
F	-9	SER	-	expression tag	UNP Q6N0W9
F	-8	SER	-	expression tag	UNP Q6N0W9
F	-7	GLY	-	expression tag	UNP Q6N0W9
F	-6	LEU	-	expression tag	UNP Q6N0W9
F	-5	VAL	-	expression tag	UNP Q6N0W9
F	-4	PRO	-	expression tag	UNP Q6N0W9
F	-3	ARG	-	expression tag	UNP Q6N0W9
F	-2	GLY	-	expression tag	UNP Q6N0W9
F	-1	SER	-	expression tag	UNP Q6N0W9
F	0	HIS	-	expression tag	UNP Q6N0W9
F	59	PHE	SER	engineered mutation	UNP Q6N0W9
G	-19	MET	-	initiating methionine	UNP Q6N0W9
G	-18	GLY	-	expression tag	UNP Q6N0W9
G	-17	SER	-	expression tag	UNP Q6N0W9
G	-16	SER	-	expression tag	UNP Q6N0W9
G	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-14	HIS	-	expression tag	UNP Q6N0W9
G	-13	HIS	-	expression tag	UNP Q6N0W9
G	-12	HIS	-	expression tag	UNP Q6N0W9
G	-11	HIS	-	expression tag	UNP Q6N0W9
G	-10	HIS	-	expression tag	UNP Q6N0W9
G	-9	SER	-	expression tag	UNP Q6N0W9
G	-8	SER	-	expression tag	UNP Q6N0W9
G	-7	GLY	-	expression tag	UNP Q6N0W9
G	-6	LEU	-	expression tag	UNP Q6N0W9
G	-5	VAL	-	expression tag	UNP Q6N0W9
G	-4	PRO	-	expression tag	UNP Q6N0W9
G	-3	ARG	-	expression tag	UNP Q6N0W9
G	-2	GLY	-	expression tag	UNP Q6N0W9
G	-1	SER	-	expression tag	UNP Q6N0W9
G	0	HIS	-	expression tag	UNP Q6N0W9
G	59	PHE	SER	engineered mutation	UNP Q6N0W9
H	-19	MET	-	initiating methionine	UNP Q6N0W9
H	-18	GLY	-	expression tag	UNP Q6N0W9
H	-17	SER	-	expression tag	UNP Q6N0W9
H	-16	SER	-	expression tag	UNP Q6N0W9
H	-15	HIS	-	expression tag	UNP Q6N0W9
H	-14	HIS	-	expression tag	UNP Q6N0W9
H	-13	HIS	-	expression tag	UNP Q6N0W9
H	-12	HIS	-	expression tag	UNP Q6N0W9
H	-11	HIS	-	expression tag	UNP Q6N0W9
H	-10	HIS	-	expression tag	UNP Q6N0W9
H	-9	SER	-	expression tag	UNP Q6N0W9
H	-8	SER	-	expression tag	UNP Q6N0W9
H	-7	GLY	-	expression tag	UNP Q6N0W9
H	-6	LEU	-	expression tag	UNP Q6N0W9
H	-5	VAL	-	expression tag	UNP Q6N0W9
H	-4	PRO	-	expression tag	UNP Q6N0W9
H	-3	ARG	-	expression tag	UNP Q6N0W9
H	-2	GLY	-	expression tag	UNP Q6N0W9
H	-1	SER	-	expression tag	UNP Q6N0W9
H	0	HIS	-	expression tag	UNP Q6N0W9
H	59	PHE	SER	engineered mutation	UNP Q6N0W9
I	-19	MET	-	initiating methionine	UNP Q6N0W9
I	-18	GLY	-	expression tag	UNP Q6N0W9
I	-17	SER	-	expression tag	UNP Q6N0W9
I	-16	SER	-	expression tag	UNP Q6N0W9
I	-15	HIS	-	expression tag	UNP Q6N0W9

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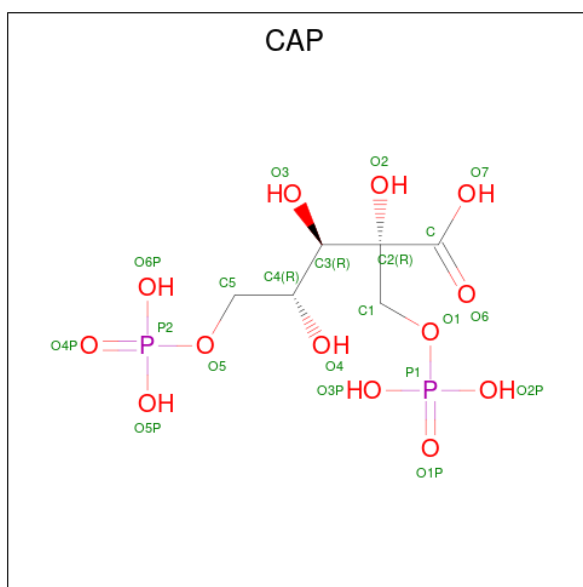
Chain	Residue	Modelled	Actual	Comment	Reference
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I	-13	HIS	-	expression tag	UNP Q6N0W9
I	-12	HIS	-	expression tag	UNP Q6N0W9
I	-11	HIS	-	expression tag	UNP Q6N0W9
I	-10	HIS	-	expression tag	UNP Q6N0W9
I	-9	SER	-	expression tag	UNP Q6N0W9
I	-8	SER	-	expression tag	UNP Q6N0W9
I	-7	GLY	-	expression tag	UNP Q6N0W9
I	-6	LEU	-	expression tag	UNP Q6N0W9
I	-5	VAL	-	expression tag	UNP Q6N0W9
I	-4	PRO	-	expression tag	UNP Q6N0W9
I	-3	ARG	-	expression tag	UNP Q6N0W9
I	-2	GLY	-	expression tag	UNP Q6N0W9
I	-1	SER	-	expression tag	UNP Q6N0W9
I	0	HIS	-	expression tag	UNP Q6N0W9
I	59	PHE	SER	engineered mutation	UNP Q6N0W9
J	-19	MET	-	initiating methionine	UNP Q6N0W9
J	-18	GLY	-	expression tag	UNP Q6N0W9
J	-17	SER	-	expression tag	UNP Q6N0W9
J	-16	SER	-	expression tag	UNP Q6N0W9
J	-15	HIS	-	expression tag	UNP Q6N0W9
J	-14	HIS	-	expression tag	UNP Q6N0W9
J	-13	HIS	-	expression tag	UNP Q6N0W9
J	-12	HIS	-	expression tag	UNP Q6N0W9
J	-11	HIS	-	expression tag	UNP Q6N0W9
J	-10	HIS	-	expression tag	UNP Q6N0W9
J	-9	SER	-	expression tag	UNP Q6N0W9
J	-8	SER	-	expression tag	UNP Q6N0W9
J	-7	GLY	-	expression tag	UNP Q6N0W9
J	-6	LEU	-	expression tag	UNP Q6N0W9
J	-5	VAL	-	expression tag	UNP Q6N0W9
J	-4	PRO	-	expression tag	UNP Q6N0W9
J	-3	ARG	-	expression tag	UNP Q6N0W9
J	-2	GLY	-	expression tag	UNP Q6N0W9
J	-1	SER	-	expression tag	UNP Q6N0W9
J	0	HIS	-	expression tag	UNP Q6N0W9
J	59	PHE	SER	engineered mutation	UNP Q6N0W9
K	-19	MET	-	initiating methionine	UNP Q6N0W9
K	-18	GLY	-	expression tag	UNP Q6N0W9
K	-17	SER	-	expression tag	UNP Q6N0W9
K	-16	SER	-	expression tag	UNP Q6N0W9
K	-15	HIS	-	expression tag	UNP Q6N0W9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-14	HIS	-	expression tag	UNP Q6N0W9
K	-13	HIS	-	expression tag	UNP Q6N0W9
K	-12	HIS	-	expression tag	UNP Q6N0W9
K	-11	HIS	-	expression tag	UNP Q6N0W9
K	-10	HIS	-	expression tag	UNP Q6N0W9
K	-9	SER	-	expression tag	UNP Q6N0W9
K	-8	SER	-	expression tag	UNP Q6N0W9
K	-7	GLY	-	expression tag	UNP Q6N0W9
K	-6	LEU	-	expression tag	UNP Q6N0W9
K	-5	VAL	-	expression tag	UNP Q6N0W9
K	-4	PRO	-	expression tag	UNP Q6N0W9
K	-3	ARG	-	expression tag	UNP Q6N0W9
K	-2	GLY	-	expression tag	UNP Q6N0W9
K	-1	SER	-	expression tag	UNP Q6N0W9
K	0	HIS	-	expression tag	UNP Q6N0W9
K	59	PHE	SER	engineered mutation	UNP Q6N0W9
L	-19	MET	-	initiating methionine	UNP Q6N0W9
L	-18	GLY	-	expression tag	UNP Q6N0W9
L	-17	SER	-	expression tag	UNP Q6N0W9
L	-16	SER	-	expression tag	UNP Q6N0W9
L	-15	HIS	-	expression tag	UNP Q6N0W9
L	-14	HIS	-	expression tag	UNP Q6N0W9
L	-13	HIS	-	expression tag	UNP Q6N0W9
L	-12	HIS	-	expression tag	UNP Q6N0W9
L	-11	HIS	-	expression tag	UNP Q6N0W9
L	-10	HIS	-	expression tag	UNP Q6N0W9
L	-9	SER	-	expression tag	UNP Q6N0W9
L	-8	SER	-	expression tag	UNP Q6N0W9
L	-7	GLY	-	expression tag	UNP Q6N0W9
L	-6	LEU	-	expression tag	UNP Q6N0W9
L	-5	VAL	-	expression tag	UNP Q6N0W9
L	-4	PRO	-	expression tag	UNP Q6N0W9
L	-3	ARG	-	expression tag	UNP Q6N0W9
L	-2	GLY	-	expression tag	UNP Q6N0W9
L	-1	SER	-	expression tag	UNP Q6N0W9
L	0	HIS	-	expression tag	UNP Q6N0W9
L	59	PHE	SER	engineered mutation	UNP Q6N0W9

- Molecule 2 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>13</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	P		
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).

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	235	Total O 235 235	0	0
4	B	196	Total O 196 196	0	0
4	C	213	Total O 213 213	0	0
4	D	214	Total O 214 214	0	0
4	E	241	Total O 241 241	0	0
4	F	284	Total O 284 284	0	0
4	G	217	Total O 217 217	0	0
4	H	230	Total O 230 230	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	I	228	Total 228	O 228	0	0
4	J	172	Total 172	O 172	0	0
4	K	191	Total 191	O 191	0	0
4	L	234	Total 234	O 234	0	0

### 3 Residue-property plots [i](#)

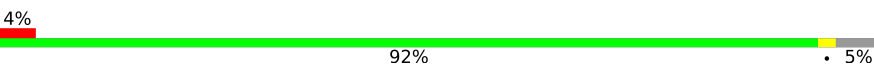
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

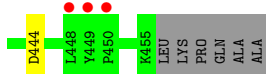
- Molecule 1: Ribulose biphosphate carboxylase

Chain A: 



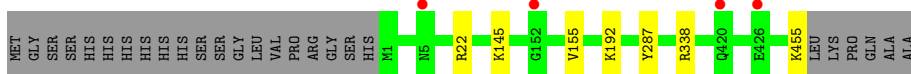
- Molecule 1: Ribulose biphosphate carboxylase

Chain B: 



- Molecule 1: Ribulose biphosphate carboxylase

Chain C: 



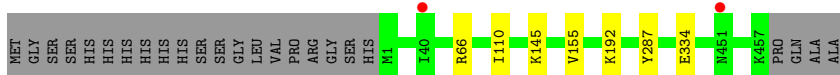
- Molecule 1: Ribulose biphosphate carboxylase

Chain D: 



- Molecule 1: Ribulose biphosphate carboxylase

Chain E: 



- Molecule 1: Ribulose biphosphate carboxylase

Chain F: 93% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain G: 93% 5%



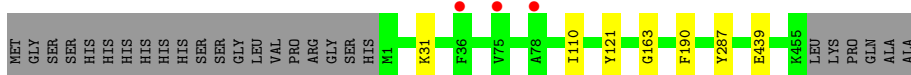
- Molecule 1: Ribulose biphosphate carboxylase

Chain H: 94% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain I: 93% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain J: 94% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain K: 93% 5%



- Molecule 1: Ribulose biphosphate carboxylase

Chain L:  93% 5%

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	R1	R22	E89	I110	G163	F190	I195	K192	Y266	Y287	W452	K455	L456	LYS	PRO	GLN	ALA	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.88Å 110.37Å 167.36Å 89.87° 101.70° 105.00°	Depositor
Resolution (Å)	20.00 – 2.04 48.92 – 2.04	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.00-2.04) 88.5 (48.92-2.04)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.08 (at 2.03Å)	Xtrriage
Refinement program	BUSTER 2.10.0	Depositor
R, $R_{free}$	0.197 , 0.237 0.203 , 0.242	Depositor DCC
$R_{free}$ test set	29113 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	85695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6054e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, KCX, CAP

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	0.52	0/3606	0.63	0/4879
1	B	0.50	0/3588	0.63	0/4857
1	C	0.50	0/3597	0.63	0/4868
1	D	0.49	0/3601	0.63	0/4872
1	E	0.52	0/3606	0.64	0/4881
1	F	0.53	0/3597	0.64	0/4867
1	G	0.50	0/3606	0.64	0/4881
1	H	0.52	0/3605	0.63	0/4879
1	I	0.50	0/3593	0.62	0/4864
1	J	0.48	0/3597	0.63	0/4868
1	K	0.50	0/3586	0.63	0/4854
1	L	0.50	0/3606	0.64	0/4879
All	All	0.51	0/43188	0.63	0/58449

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3529	3377	3401	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3511	3346	3361	6	0
1	C	3520	3371	3383	1	0
1	D	3524	3382	3394	1	0
1	E	3529	3363	3390	3	0
1	F	3520	3378	3390	1	0
1	G	3529	3363	3390	5	0
1	H	3528	3370	3394	2	0
1	I	3516	3360	3372	4	0
1	J	3520	3359	3383	1	0
1	K	3509	3357	3369	1	0
1	L	3529	3378	3401	4	0
2	A	21	9	7	0	0
2	B	21	9	8	0	0
2	C	21	9	7	0	0
2	D	21	9	7	0	0
2	E	21	9	7	0	0
2	F	21	9	7	0	0
2	G	21	9	7	0	0
2	H	21	9	7	0	0
2	I	21	9	7	0	0
2	J	21	9	7	0	0
2	K	21	9	7	0	0
2	L	21	9	7	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	235	0	0	1	0
4	B	196	0	0	0	0
4	C	213	0	0	0	0
4	D	214	0	0	0	0
4	E	241	0	0	2	0
4	F	284	0	0	0	0
4	G	217	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	230	0	0	0	0
4	I	228	0	0	0	0
4	J	172	0	0	0	0
4	K	191	0	0	0	0
4	L	234	0	0	0	0
All	All	45183	40512	40713	32	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 0.

The worst 5 of 32 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:426:GLU:OE2	1:G:455:LYS:NZ	2.11	0.81
1:A:173:ARG:NH2	4:A:601:HOH:O	2.20	0.74
1:E:145:LYS:HG3	1:E:155:VAL:HB	1.69	0.72
1:G:10:LEU:HD11	1:G:40:ILE:HD12	1.82	0.61
1:I:31:LYS:CD	1:I:121:TYR:OH	2.56	0.53

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	453/481 (94%)	441 (97%)	12 (3%)	0	100	100
1	B	452/481 (94%)	441 (98%)	11 (2%)	0	100	100
1	C	452/481 (94%)	441 (98%)	11 (2%)	0	100	100
1	D	452/481 (94%)	440 (97%)	11 (2%)	1 (0%)	47	39
1	E	454/481 (94%)	443 (98%)	10 (2%)	1 (0%)	47	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	452/481 (94%)	441 (98%)	10 (2%)	1 (0%)	47	39
1	G	454/481 (94%)	441 (97%)	12 (3%)	1 (0%)	47	39
1	H	453/481 (94%)	442 (98%)	11 (2%)	0	100	100
1	I	452/481 (94%)	442 (98%)	9 (2%)	1 (0%)	47	39
1	J	452/481 (94%)	442 (98%)	10 (2%)	0	100	100
1	K	452/481 (94%)	439 (97%)	13 (3%)	0	100	100
1	L	453/481 (94%)	441 (97%)	11 (2%)	1 (0%)	47	39
All	All	5431/5772 (94%)	5294 (98%)	131 (2%)	6 (0%)	51	45

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	110	ILE
1	D	110	ILE
1	G	110	ILE
1	I	110	ILE
1	L	110	ILE

### 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	351/372 (94%)	351 (100%)	0	100	100
1	B	347/372 (93%)	345 (99%)	2 (1%)	86	87
1	C	350/372 (94%)	346 (99%)	4 (1%)	73	73
1	D	351/372 (94%)	348 (99%)	3 (1%)	78	79
1	E	350/372 (94%)	349 (100%)	1 (0%)	92	93
1	F	350/372 (94%)	348 (99%)	2 (1%)	86	87
1	G	350/372 (94%)	348 (99%)	2 (1%)	86	87
1	H	351/372 (94%)	349 (99%)	2 (1%)	86	87
1	I	349/372 (94%)	347 (99%)	2 (1%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	350/372 (94%)	349 (100%)	1 (0%)	92	93
1	K	347/372 (93%)	343 (99%)	4 (1%)	71	70
1	L	351/372 (94%)	348 (99%)	3 (1%)	78	79
All	All	4197/4464 (94%)	4171 (99%)	26 (1%)	86	87

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	287	TYR
1	I	439	GLU
1	L	287	TYR
1	I	287	TYR
1	J	287	TYR

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	F	192	3,1	9,11,12	1.12	0	5,12,14	1.32	1 (20%)
1	KCX	K	192	3,1	9,11,12	2.02	3 (33%)	5,12,14	1.41	1 (20%)
1	KCX	I	192	3,1	9,11,12	0.98	0	5,12,14	0.76	0
1	KCX	J	192	3,1	9,11,12	0.89	0	5,12,14	1.03	0
1	KCX	B	192	3,1	9,11,12	1.14	1 (11%)	5,12,14	1.81	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	KCX	C	192	3,1	9,11,12	1.42	1 (11%)	5,12,14	0.90	0
1	KCX	L	192	3,1	9,11,12	1.73	2 (22%)	5,12,14	1.14	1 (20%)
1	KCX	D	192	3,1	9,11,12	1.05	1 (11%)	5,12,14	1.00	0
1	KCX	E	192	3,1	9,11,12	1.50	1 (11%)	5,12,14	0.95	0
1	KCX	A	192	3,1	9,11,12	1.04	0	5,12,14	1.85	2 (40%)
1	KCX	G	192	3,1	9,11,12	0.88	0	5,12,14	1.17	1 (20%)
1	KCX	H	192	3,1	9,11,12	1.01	0	5,12,14	0.79	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	F	192	3,1	-	0/9/10/12	-
1	KCX	K	192	3,1	-	1/9/10/12	-
1	KCX	I	192	3,1	-	1/9/10/12	-
1	KCX	J	192	3,1	-	1/9/10/12	-
1	KCX	B	192	3,1	-	2/9/10/12	-
1	KCX	C	192	3,1	-	1/9/10/12	-
1	KCX	L	192	3,1	-	0/9/10/12	-
1	KCX	D	192	3,1	-	0/9/10/12	-
1	KCX	E	192	3,1	-	0/9/10/12	-
1	KCX	A	192	3,1	-	0/9/10/12	-
1	KCX	G	192	3,1	-	0/9/10/12	-
1	KCX	H	192	3,1	-	1/9/10/12	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	192	KCX	CE-NZ	4.32	1.56	1.46
1	L	192	KCX	CE-NZ	3.41	1.54	1.46
1	E	192	KCX	CB-CA	-2.74	1.49	1.53
1	K	192	KCX	OQ1-CX	2.56	1.26	1.21
1	C	192	KCX	CX-NZ	-2.51	1.30	1.35

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	192	KCX	OQ1-CX-NZ	-2.73	120.72	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	KCX	CD-CG-CB	2.68	123.11	113.62
1	K	192	KCX	OQ1-CX-NZ	-2.63	120.87	124.96
1	A	192	KCX	CE-NZ-CX	2.61	126.07	121.89
1	B	192	KCX	CE-NZ-CX	2.51	125.92	121.89

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	192	KCX	CE-CD-CG-CB
1	B	192	KCX	CG-CD-CE-NZ
1	J	192	KCX	CE-CD-CG-CB
1	H	192	KCX	CE-CD-CG-CB
1	C	192	KCX	CE-CD-CG-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	192	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	F	500	3	17,20,20	1.14	1 (5%)	22,31,31	1.33	3 (13%)
2	CAP	H	500	3	17,20,20	1.19	2 (11%)	22,31,31	1.50	5 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	CAP	K	500	3	17,20,20	1.05	1 (5%)	22,31,31	1.59	5 (22%)
2	CAP	C	500	3	17,20,20	1.04	0	22,31,31	1.43	4 (18%)
2	CAP	B	500	3	17,20,20	1.23	1 (5%)	22,31,31	1.57	5 (22%)
2	CAP	D	500	3	17,20,20	1.10	1 (5%)	22,31,31	1.42	3 (13%)
2	CAP	G	500	3	17,20,20	1.02	1 (5%)	22,31,31	1.49	5 (22%)
2	CAP	I	500	3	17,20,20	1.14	0	22,31,31	1.48	4 (18%)
2	CAP	J	500	3	17,20,20	0.80	0	22,31,31	1.50	5 (22%)
2	CAP	L	500	3	17,20,20	0.98	0	22,31,31	1.48	4 (18%)
2	CAP	E	500	3	17,20,20	1.21	1 (5%)	22,31,31	1.43	5 (22%)
2	CAP	A	500	3	17,20,20	1.06	1 (5%)	22,31,31	1.41	4 (18%)

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	F	500	3	-	7/29/29/29	-
2	CAP	H	500	3	-	7/29/29/29	-
2	CAP	K	500	3	-	8/29/29/29	-
2	CAP	C	500	3	-	7/29/29/29	-
2	CAP	B	500	3	-	6/29/29/29	-
2	CAP	D	500	3	-	7/29/29/29	-
2	CAP	G	500	3	-	6/29/29/29	-
2	CAP	I	500	3	-	6/29/29/29	-
2	CAP	J	500	3	-	7/29/29/29	-
2	CAP	L	500	3	-	7/29/29/29	-
2	CAP	E	500	3	-	7/29/29/29	-
2	CAP	A	500	3	-	6/29/29/29	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CAP	C4-C3	-2.71	1.51	1.54
2	H	500	CAP	P2-O6P	-2.52	1.45	1.54
2	E	500	CAP	O4-C4	-2.43	1.38	1.43
2	D	500	CAP	C4-C3	-2.33	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	CAP	C4-C3	-2.33	1.51	1.54

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	CAP	O5P-P2-O5	3.56	116.21	106.73
2	G	500	CAP	O5P-P2-O5	3.40	115.77	106.73
2	B	500	CAP	O2P-P1-O1	3.27	115.42	106.73
2	D	500	CAP	O5P-P2-O5	3.23	115.32	106.73
2	J	500	CAP	O3P-P1-O1	3.21	115.28	106.73

There are no chirality outliers.

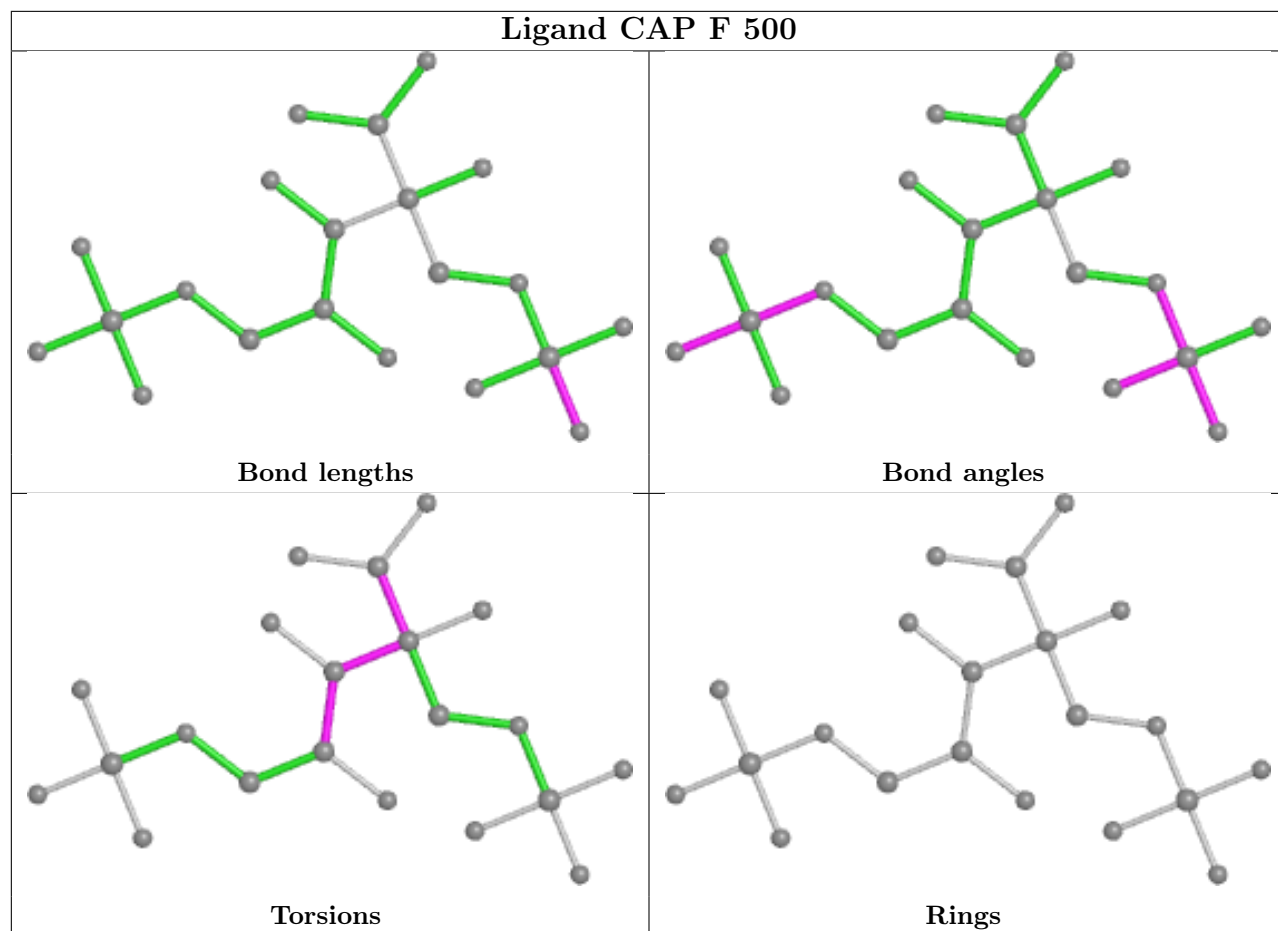
5 of 81 torsion outliers are listed below:

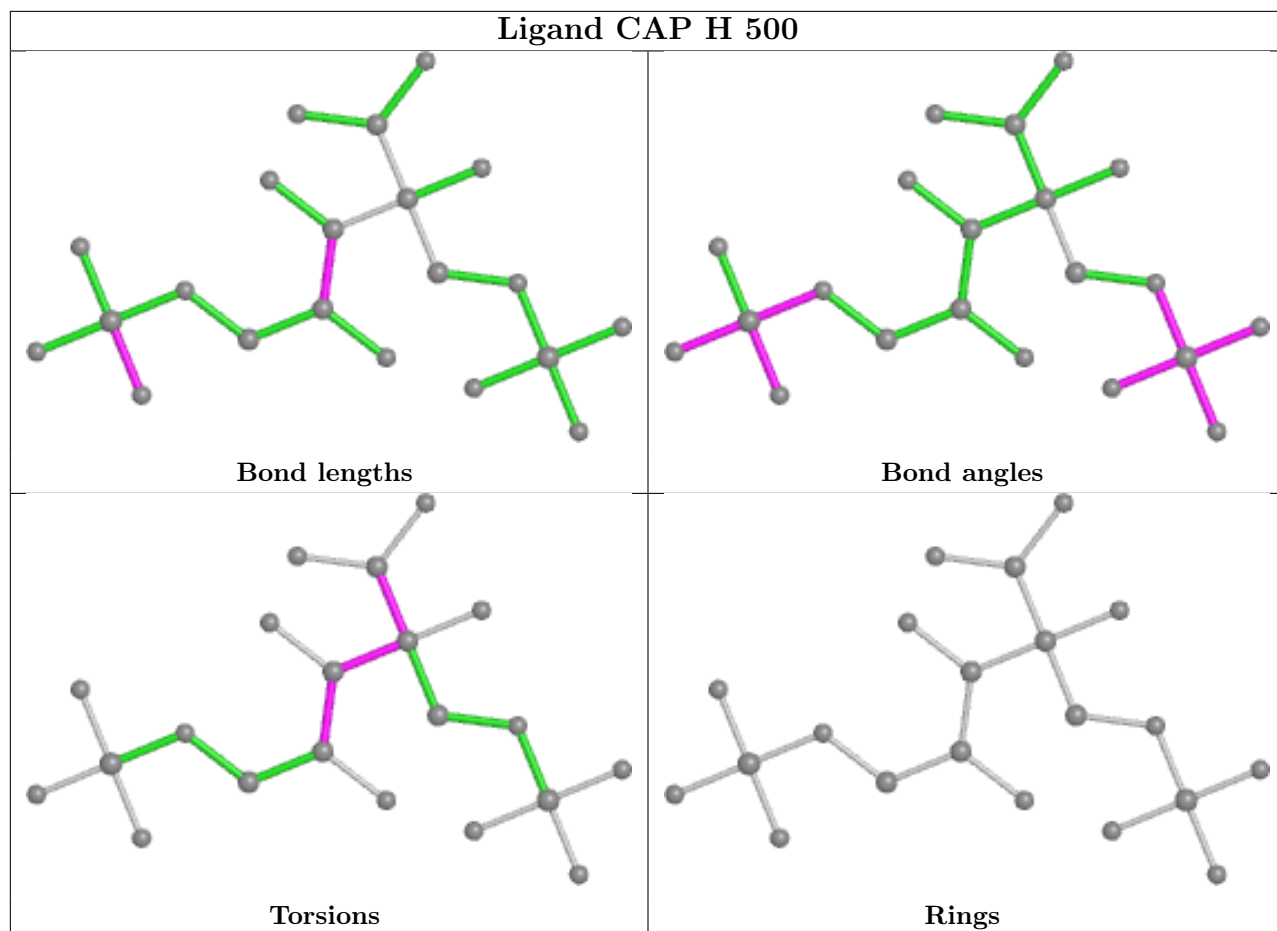
Mol	Chain	Res	Type	Atoms
2	A	500	CAP	O6-C-C2-C3
2	A	500	CAP	O3-C3-C4-O4
2	B	500	CAP	O6-C-C2-C3
2	B	500	CAP	O3-C3-C4-O4
2	C	500	CAP	O6-C-C2-C3

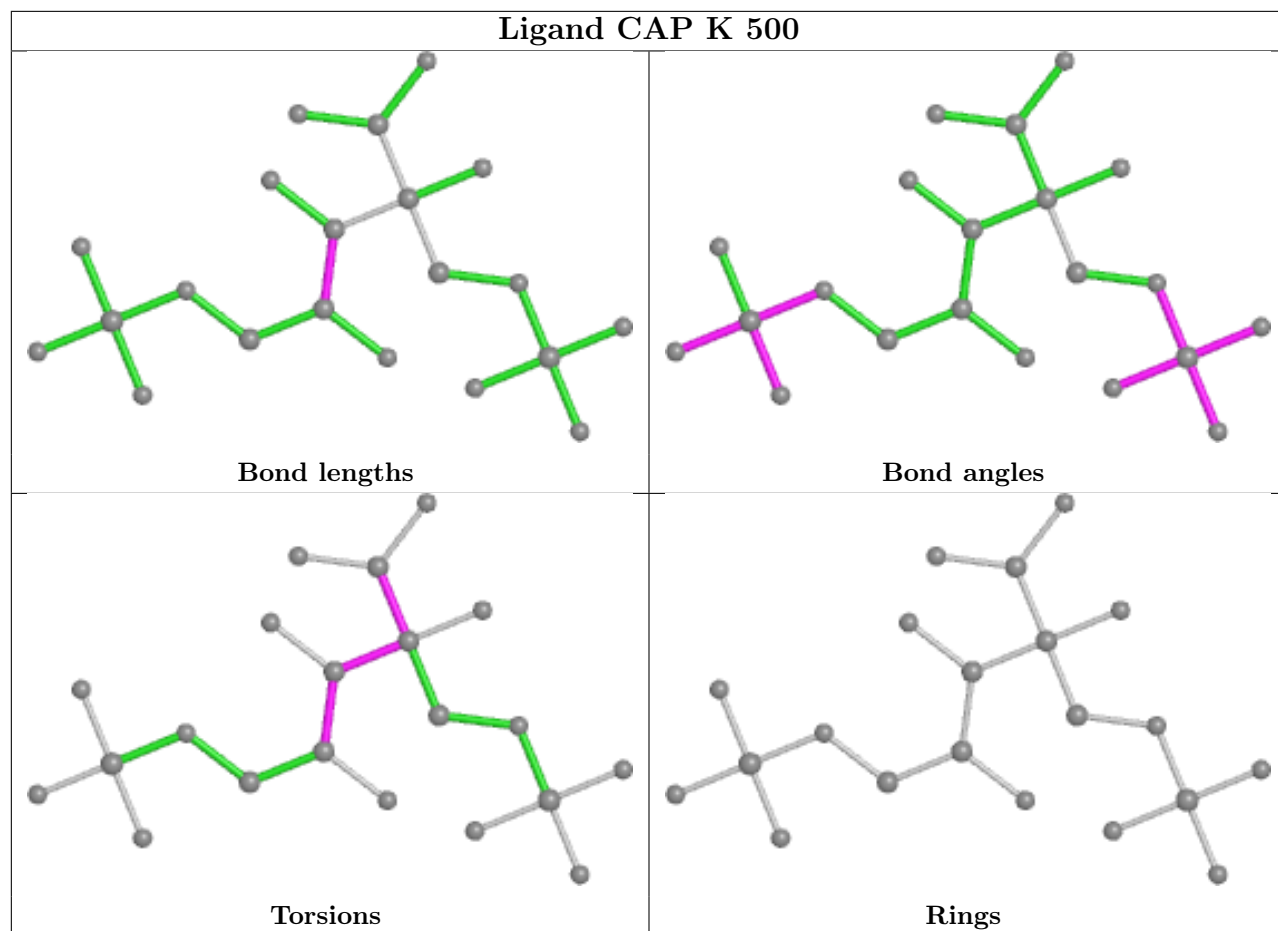
There are no ring outliers.

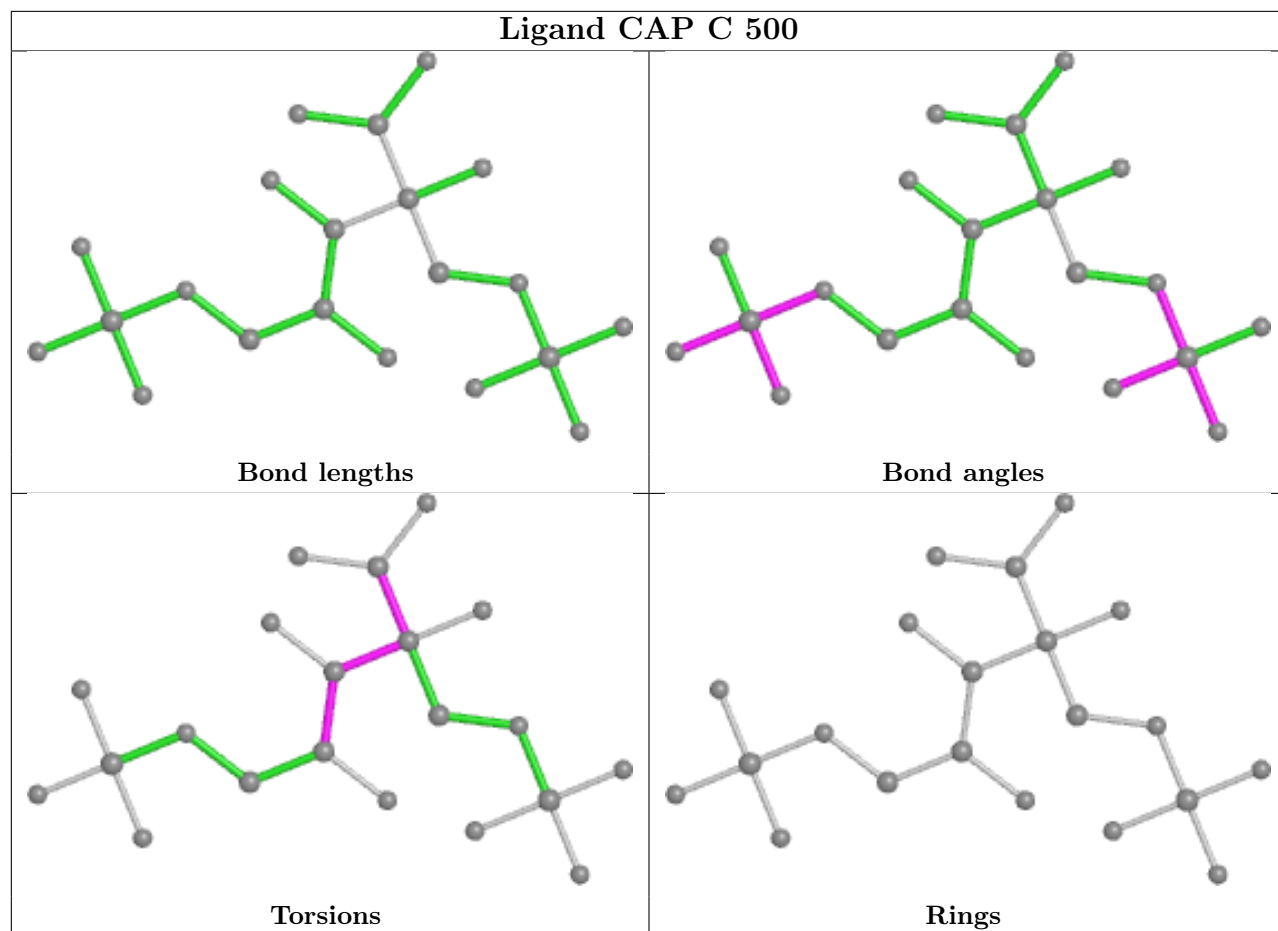
No monomer is involved in short contacts.

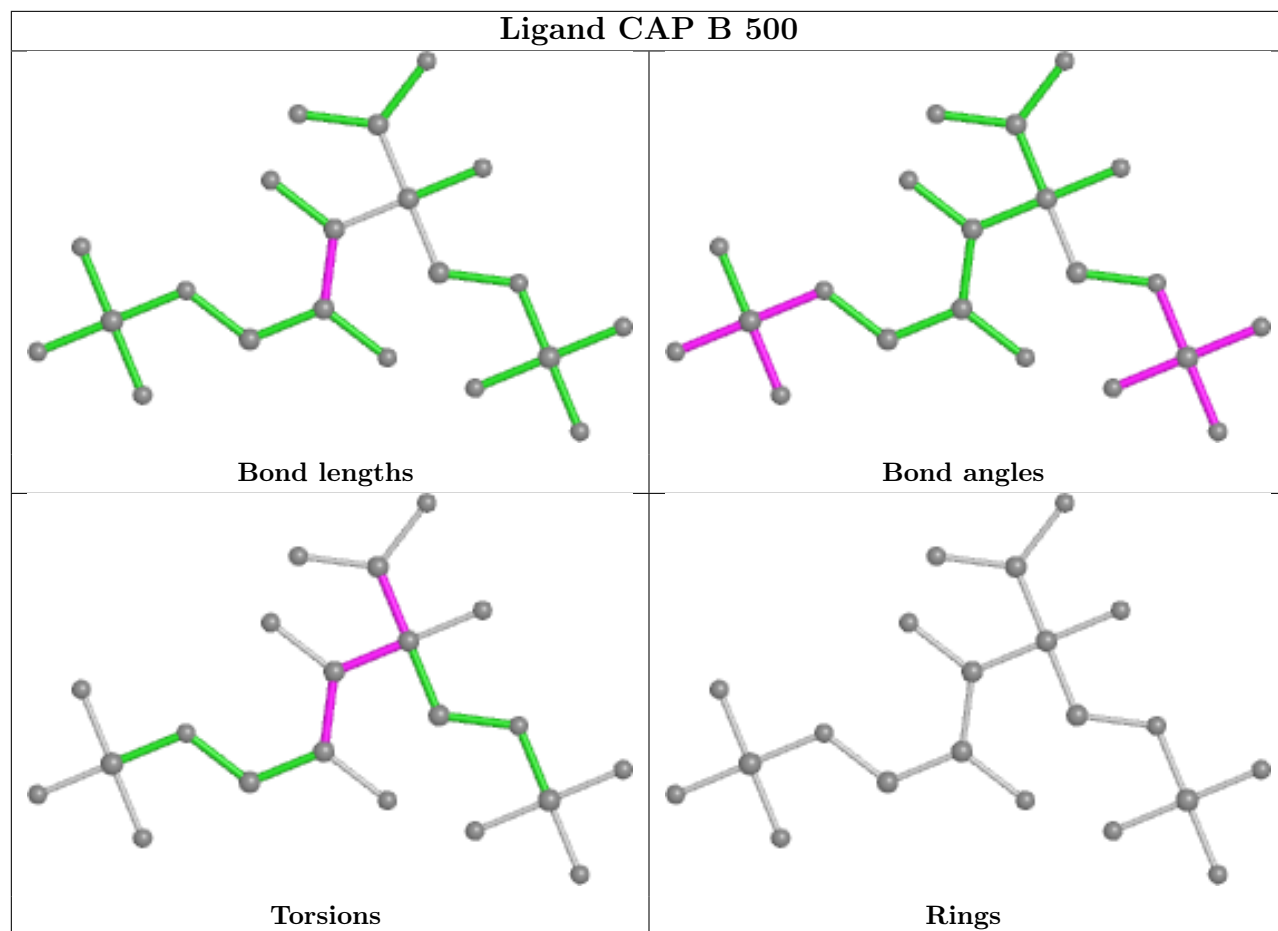
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

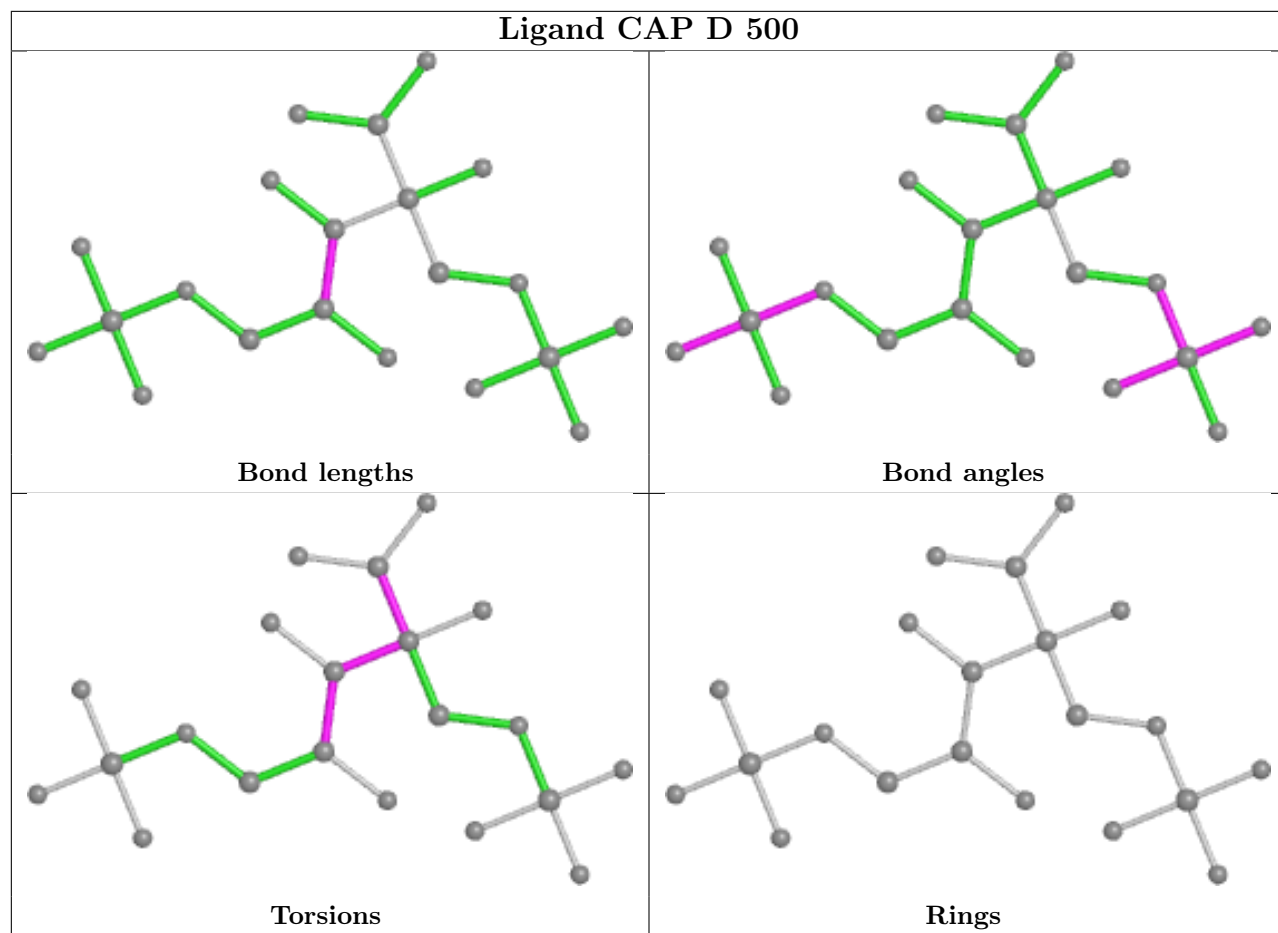




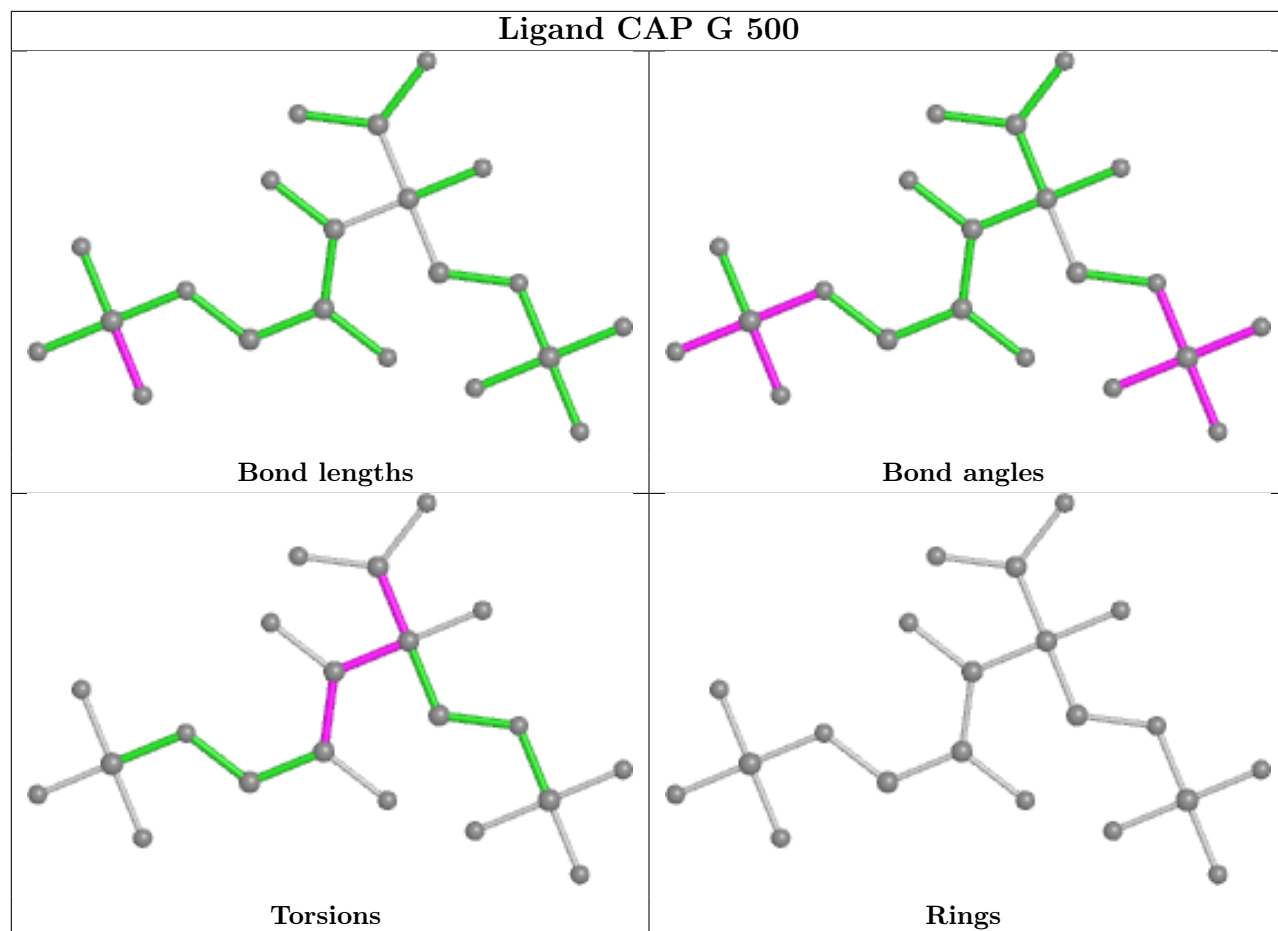


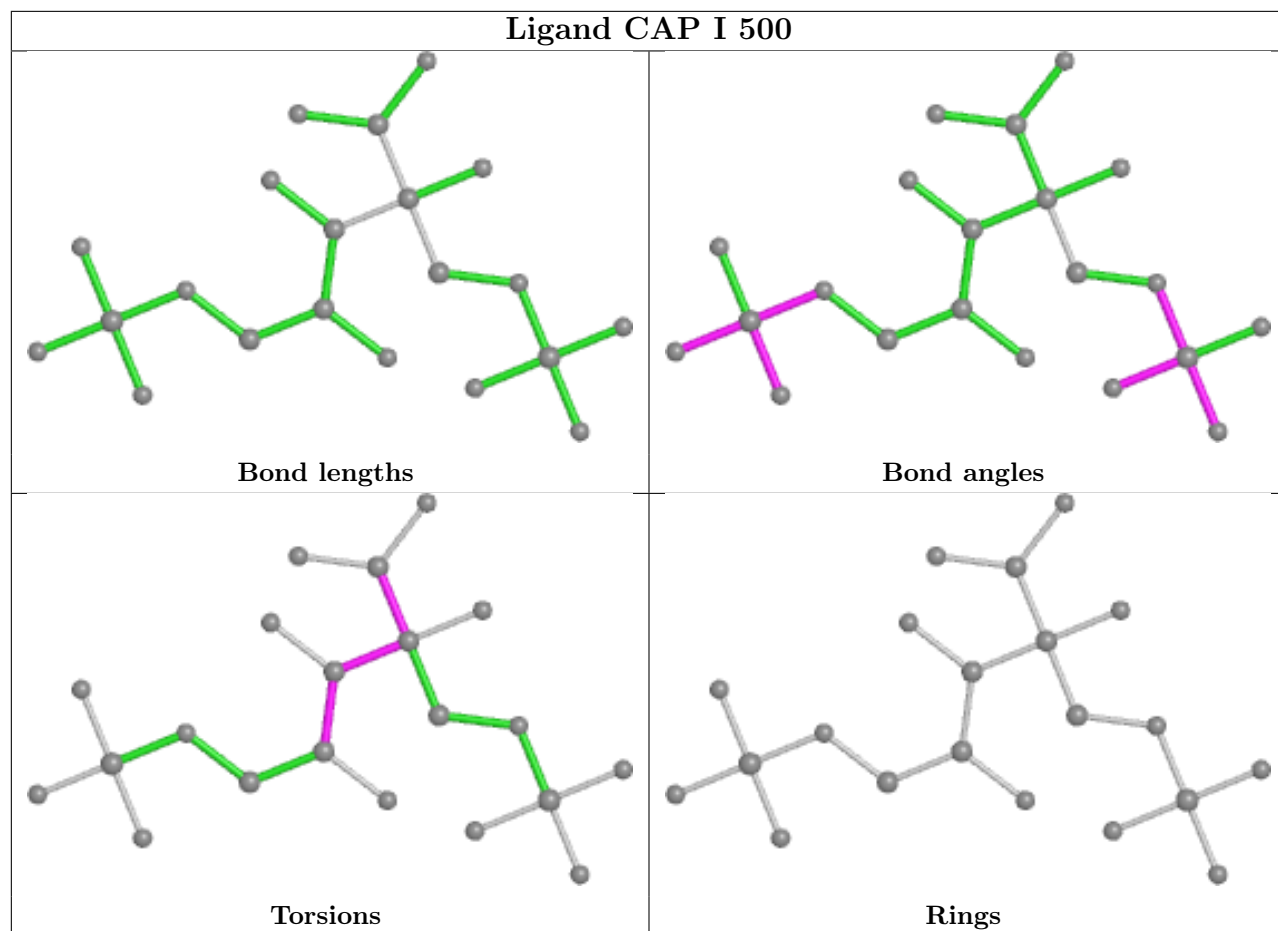


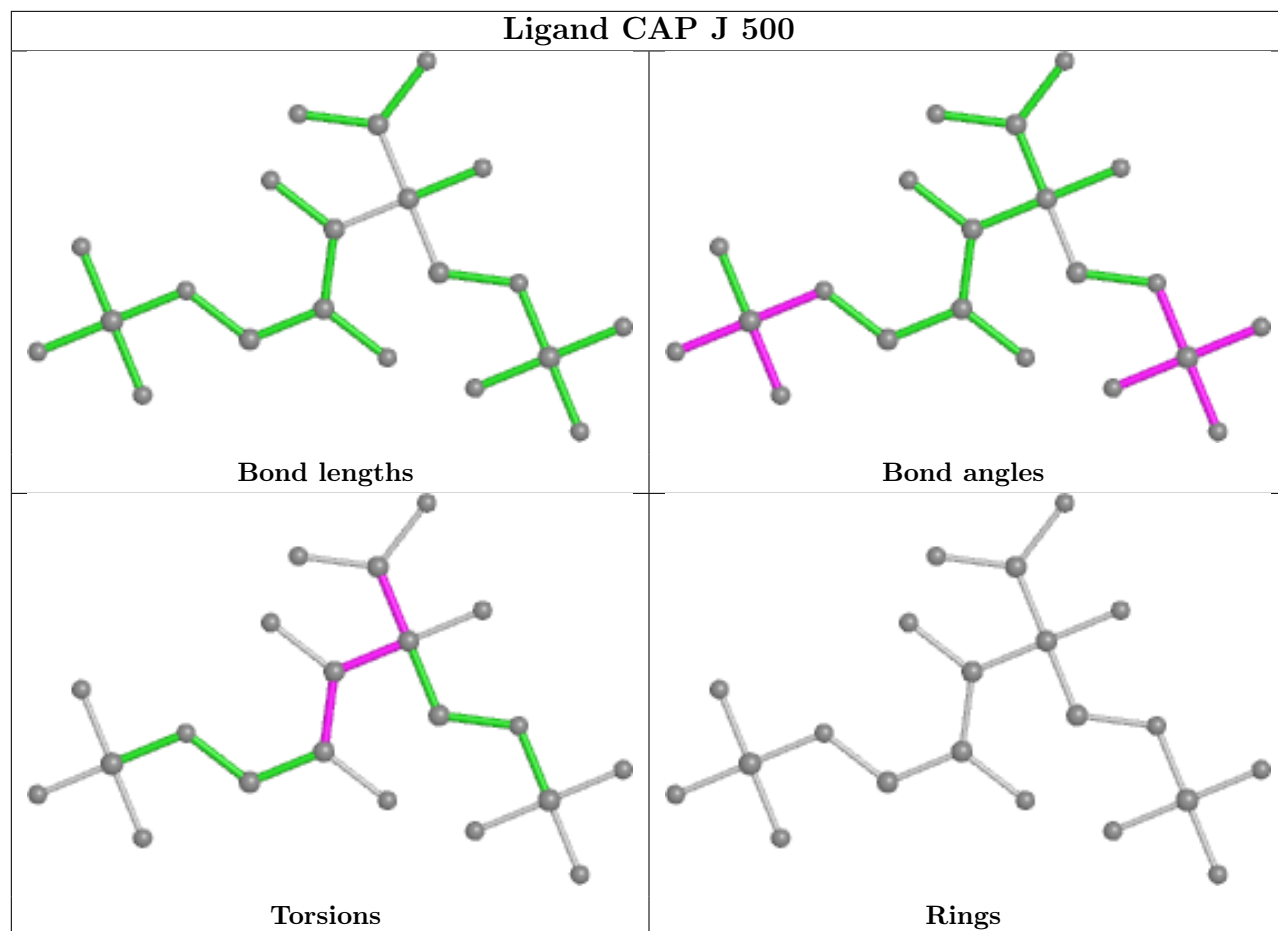


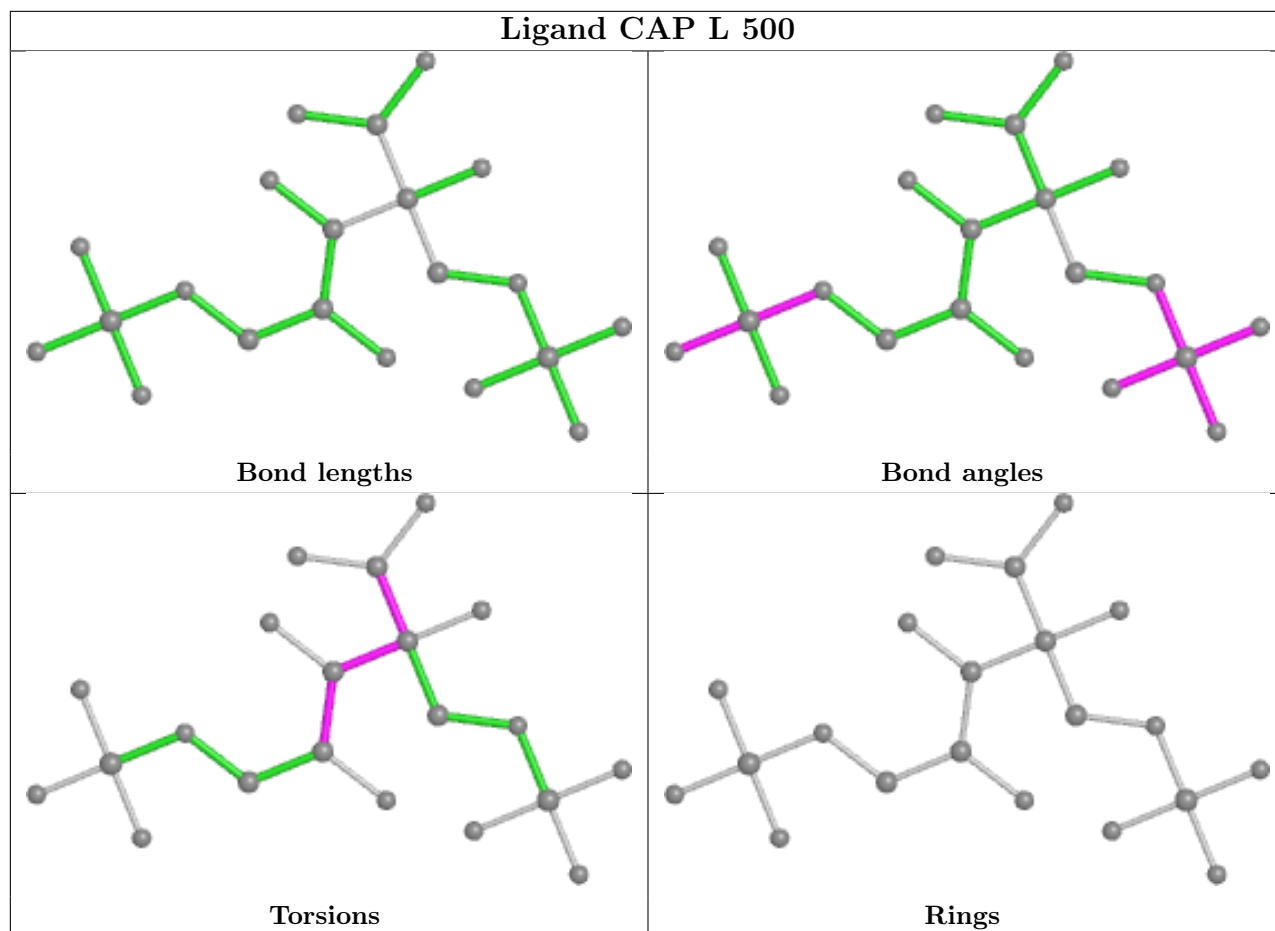


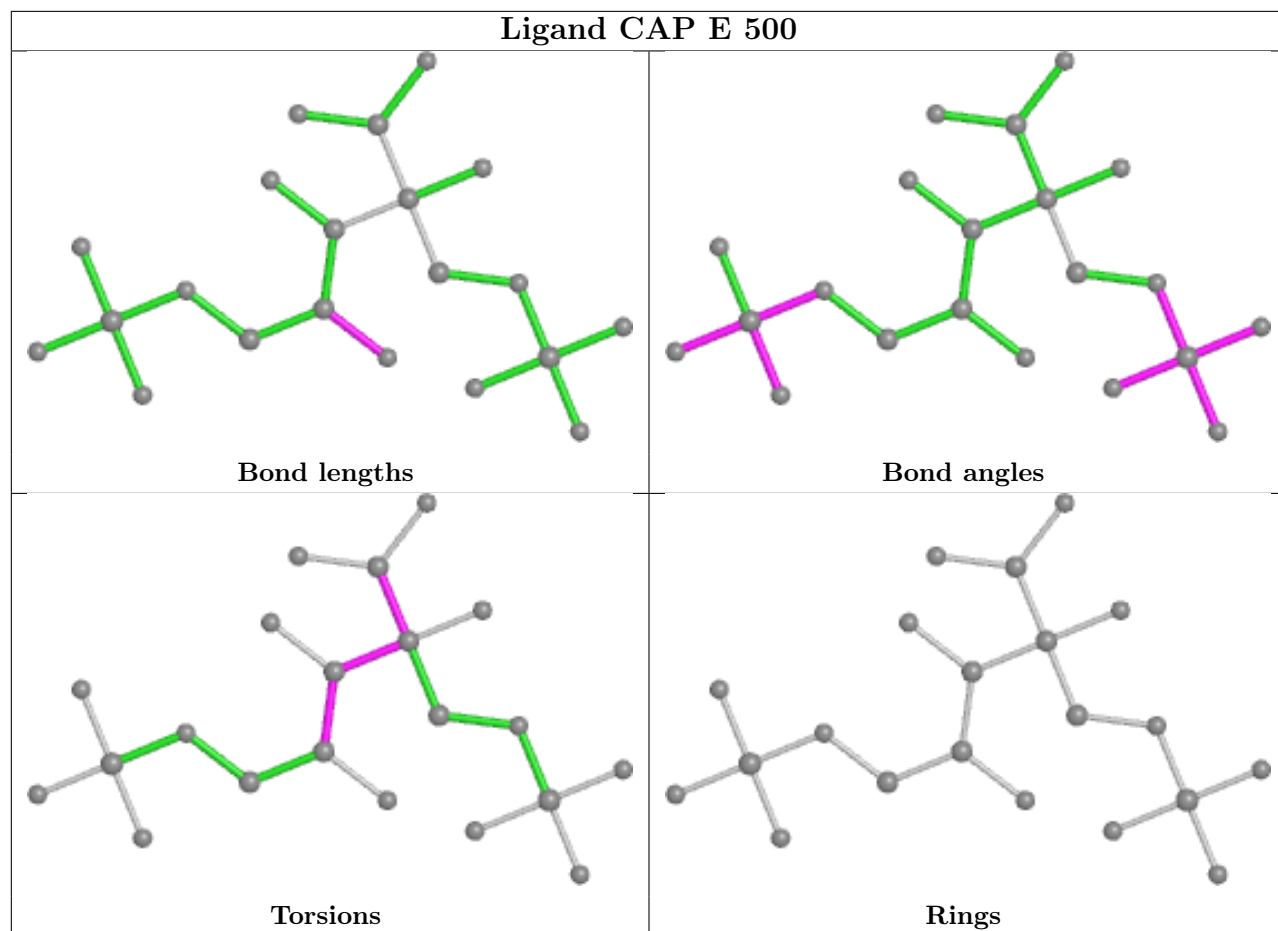


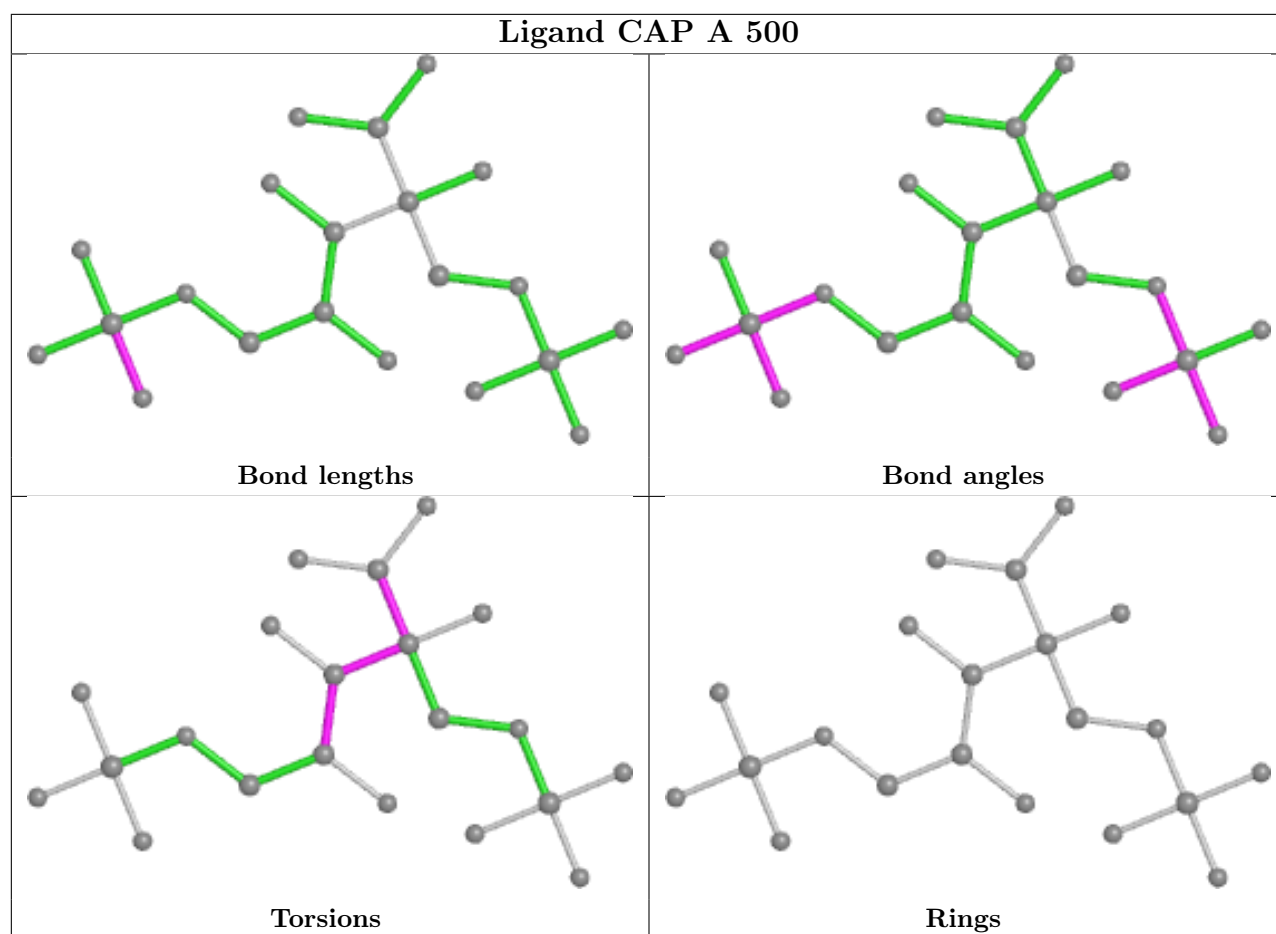












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	455/481 (94%)	0.01	3 (0%) 87 89	25, 36, 53, 68	0
1	B	454/481 (94%)	0.14	18 (3%) 38 41	26, 38, 61, 103	0
1	C	454/481 (94%)	-0.07	4 (0%) 84 86	27, 37, 55, 71	0
1	D	454/481 (94%)	-0.09	10 (2%) 62 66	24, 37, 55, 90	0
1	E	456/481 (94%)	-0.14	2 (0%) 92 93	24, 34, 50, 76	0
1	F	454/481 (94%)	-0.14	2 (0%) 92 93	24, 33, 48, 60	0
1	G	456/481 (94%)	-0.00	3 (0%) 87 89	26, 36, 52, 80	0
1	H	455/481 (94%)	-0.01	8 (1%) 68 71	25, 37, 53, 73	0
1	I	454/481 (94%)	-0.14	3 (0%) 87 89	25, 37, 55, 76	0
1	J	454/481 (94%)	0.00	15 (3%) 46 50	27, 39, 61, 107	0
1	K	454/481 (94%)	0.00	11 (2%) 59 63	27, 38, 60, 99	0
1	L	455/481 (94%)	-0.14	2 (0%) 92 93	28, 36, 53, 71	0
All	All	5455/5772 (94%)	-0.05	81 (1%) 73 76	24, 37, 56, 107	0

The worst 5 of 81 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	449	TYR	4.7
1	B	434	PHE	3.8
1	B	448	LEU	3.5
1	E	40	ILE	3.5
1	K	451	ASN	3.5

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	KCX	D	192	12/13	0.92	0.19	27,33,35,36	0
1	KCX	L	192	12/13	0.92	0.14	27,29,31,35	0
1	KCX	J	192	12/13	0.93	0.13	26,31,36,37	0
1	KCX	H	192	12/13	0.94	0.10	28,28,32,33	0
1	KCX	B	192	12/13	0.95	0.10	25,29,31,32	0
1	KCX	I	192	12/13	0.95	0.12	29,34,36,38	0
1	KCX	C	192	12/13	0.96	0.12	29,32,36,38	0
1	KCX	A	192	12/13	0.96	0.14	24,28,28,28	0
1	KCX	E	192	12/13	0.96	0.12	23,30,35,35	0
1	KCX	F	192	12/13	0.96	0.13	25,29,32,33	0
1	KCX	K	192	12/13	0.97	0.11	26,29,33,34	0
1	KCX	G	192	12/13	0.97	0.14	30,33,35,35	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	D	501	1/1	0.90	0.06	35,35,35,35	0
3	MG	I	501	1/1	0.94	0.09	42,42,42,42	0
3	MG	J	501	1/1	0.94	0.04	34,34,34,34	0
3	MG	L	501	1/1	0.94	0.10	32,32,32,32	0
3	MG	C	501	1/1	0.95	0.07	34,34,34,34	0
2	CAP	G	500	21/21	0.96	0.11	26,36,40,43	0
2	CAP	I	500	21/21	0.97	0.12	33,41,43,44	0
2	CAP	J	500	21/21	0.97	0.12	33,42,45,49	0
2	CAP	B	500	21/21	0.97	0.13	30,33,39,48	0
2	CAP	D	500	21/21	0.97	0.11	30,34,38,42	0
3	MG	E	501	1/1	0.97	0.07	25,25,25,25	0
3	MG	F	501	1/1	0.97	0.06	32,32,32,32	0
2	CAP	E	500	21/21	0.97	0.12	25,30,34,38	0
2	CAP	A	500	21/21	0.97	0.11	29,36,42,42	0

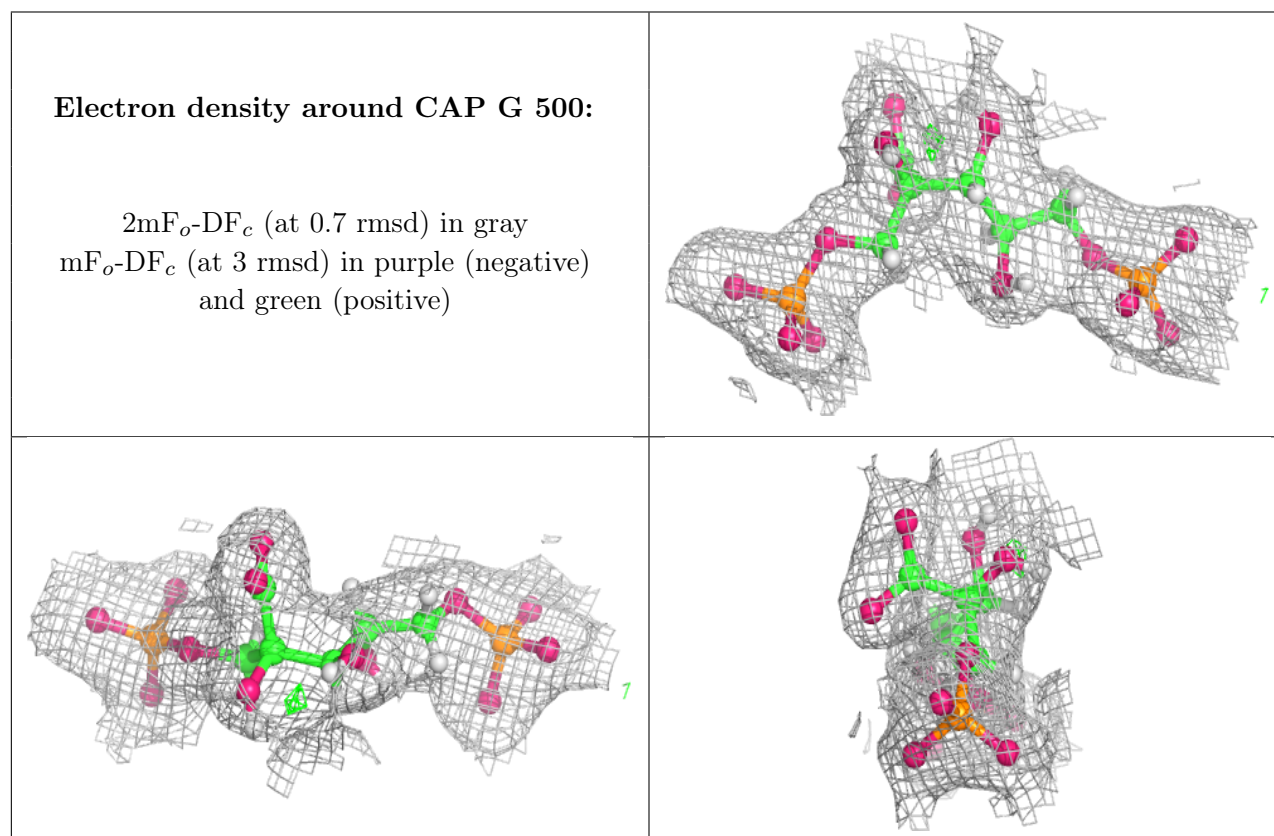
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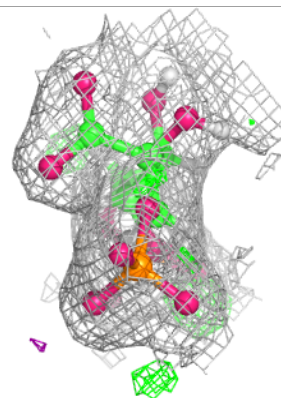
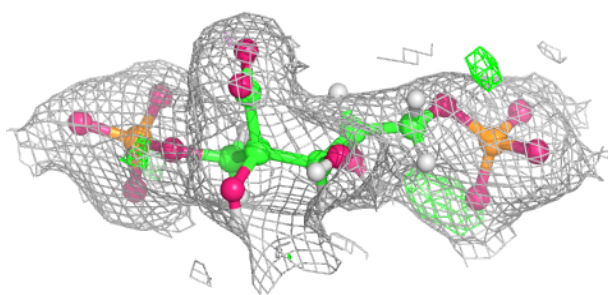
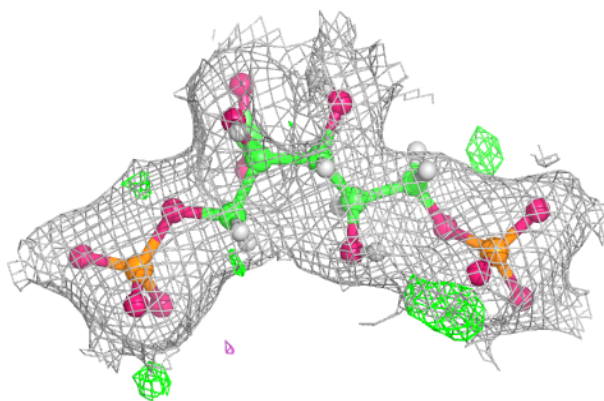
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	K	501	1/1	0.97	0.06	30,30,30,30	0
2	CAP	H	500	21/21	0.97	0.12	28,33,41,42	0
2	CAP	L	500	21/21	0.98	0.11	30,34,40,41	0
3	MG	H	501	1/1	0.98	0.13	33,33,33,33	0
3	MG	B	501	1/1	0.98	0.12	36,36,36,36	0
2	CAP	C	500	21/21	0.98	0.13	31,36,42,46	0
2	CAP	F	500	21/21	0.98	0.10	25,33,42,43	0
2	CAP	K	500	21/21	0.98	0.11	29,36,39,40	0
3	MG	G	501	1/1	0.99	0.07	33,33,33,33	0
3	MG	A	501	1/1	0.99	0.04	30,30,30,30	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.

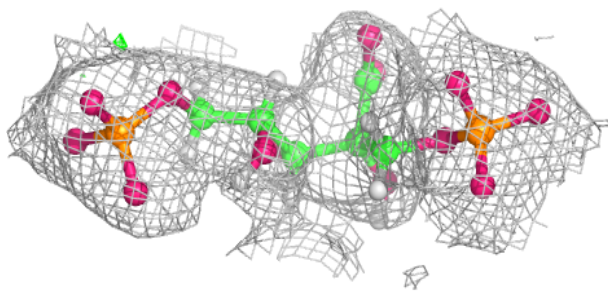
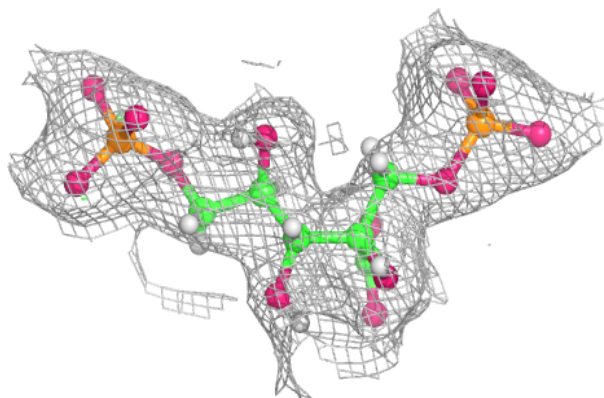


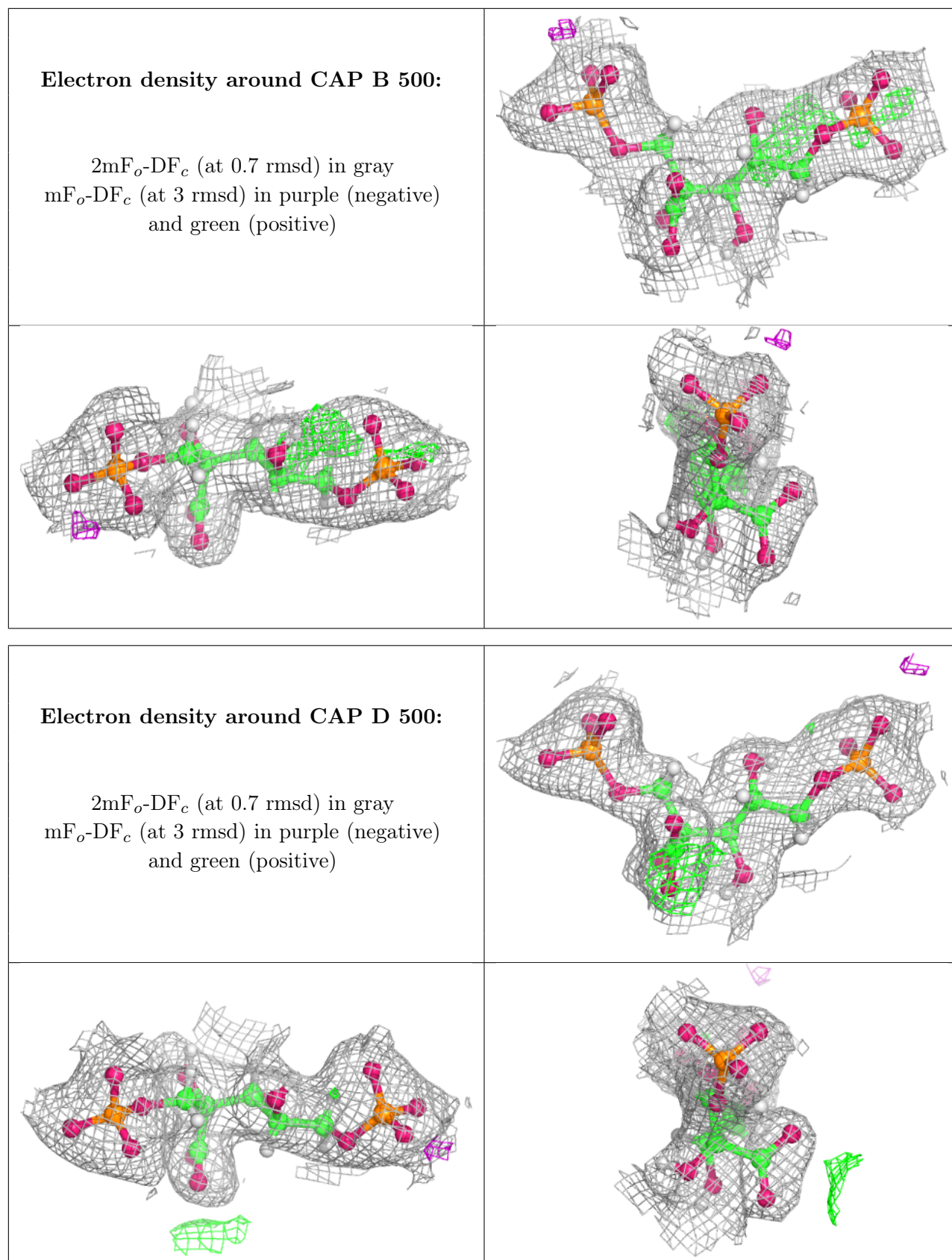
**Electron density around CAP I 500:**

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

**Electron density around CAP J 500:**

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

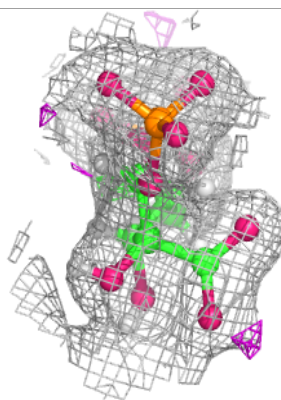
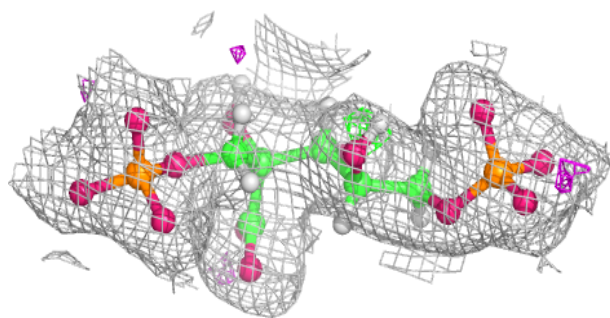
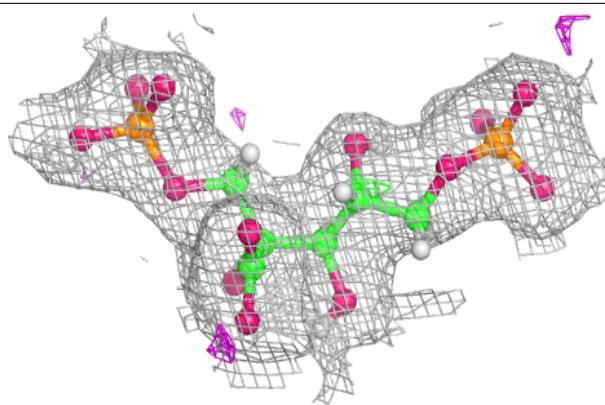




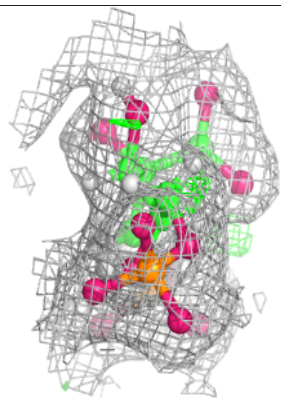
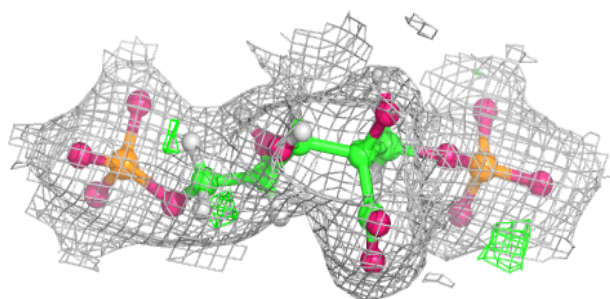
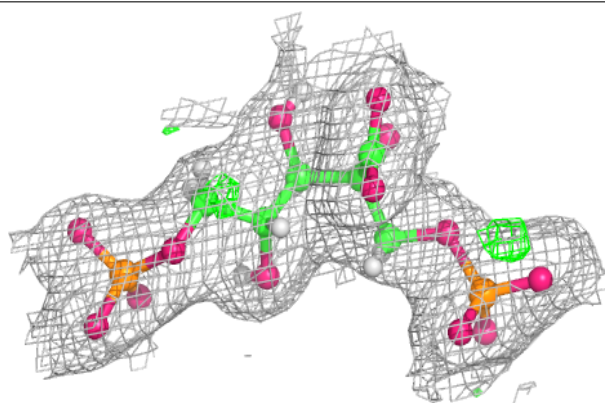


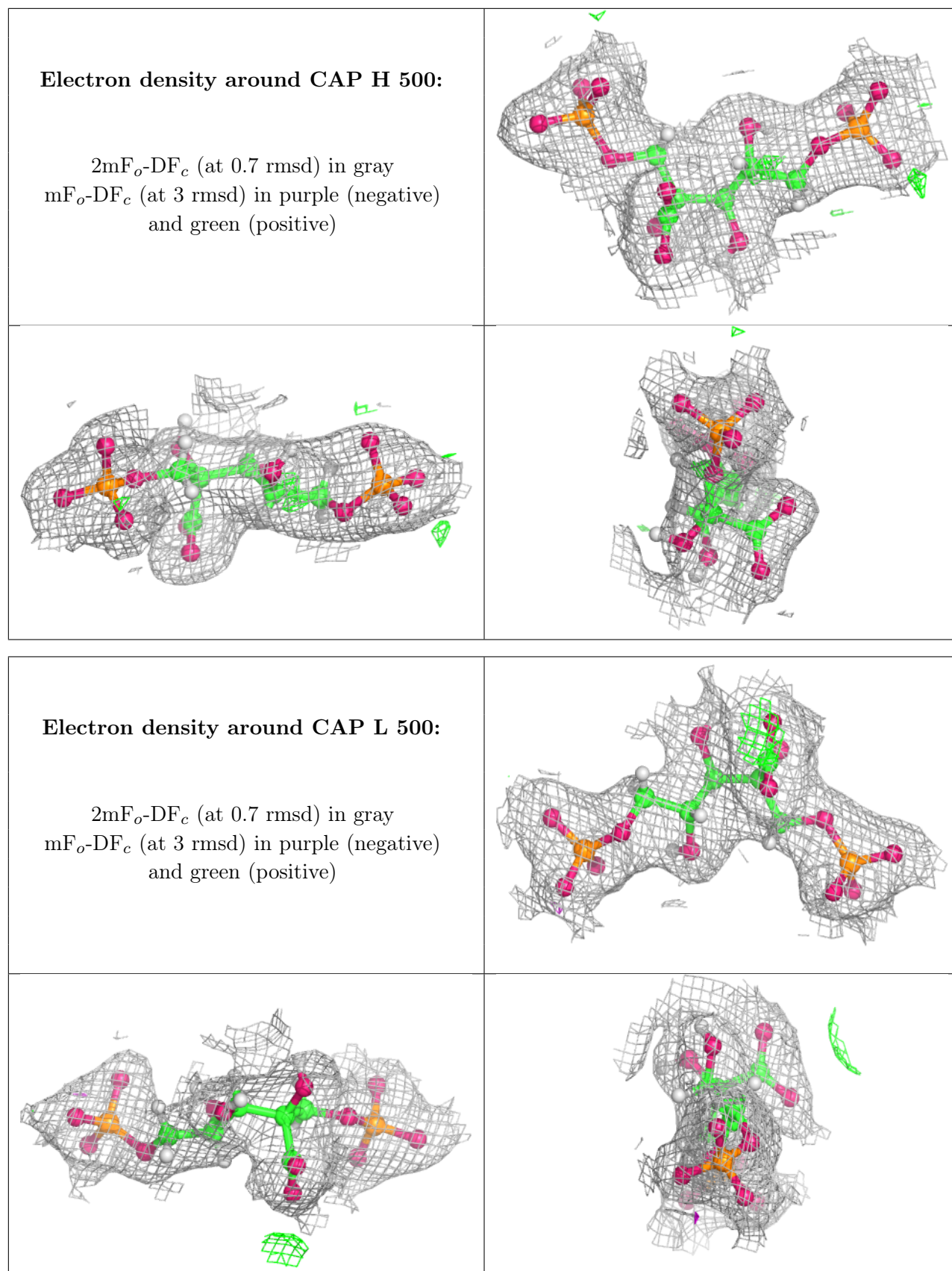
**Electron density around CAP E 500:**

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

**Electron density around CAP A 500:**

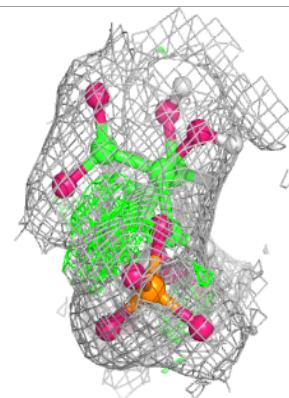
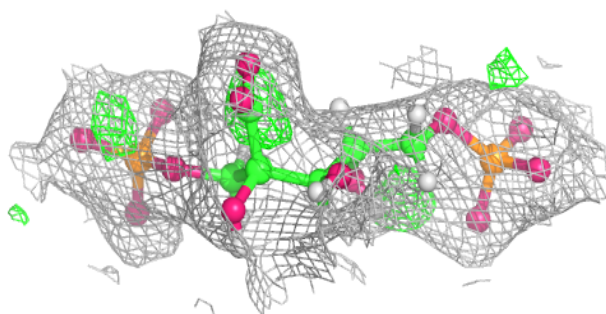
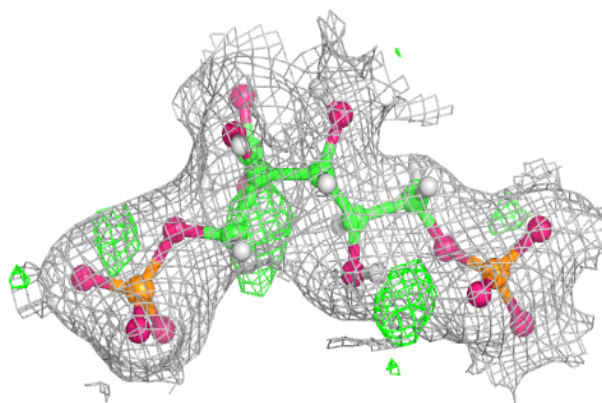
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



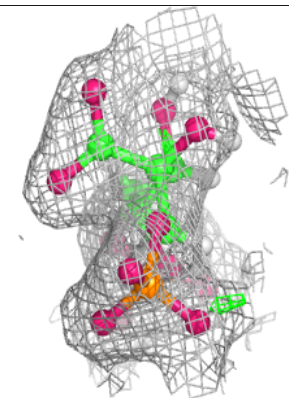
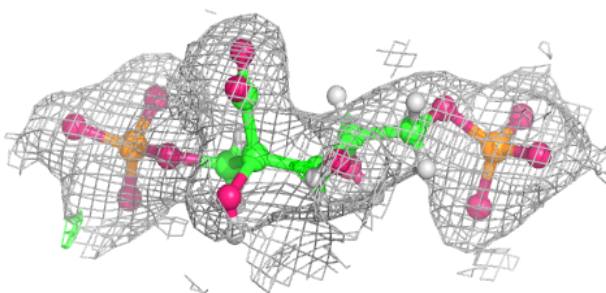
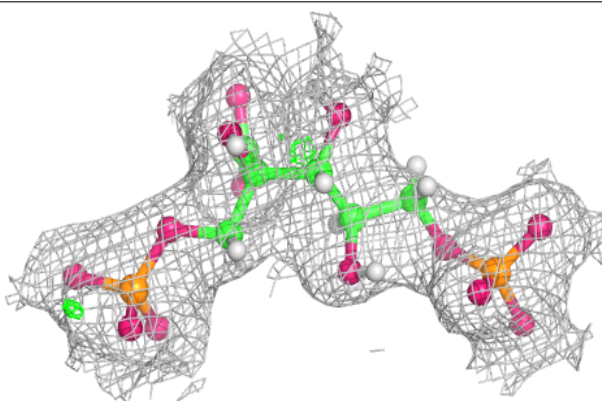


**Electron density around CAP C 500:**

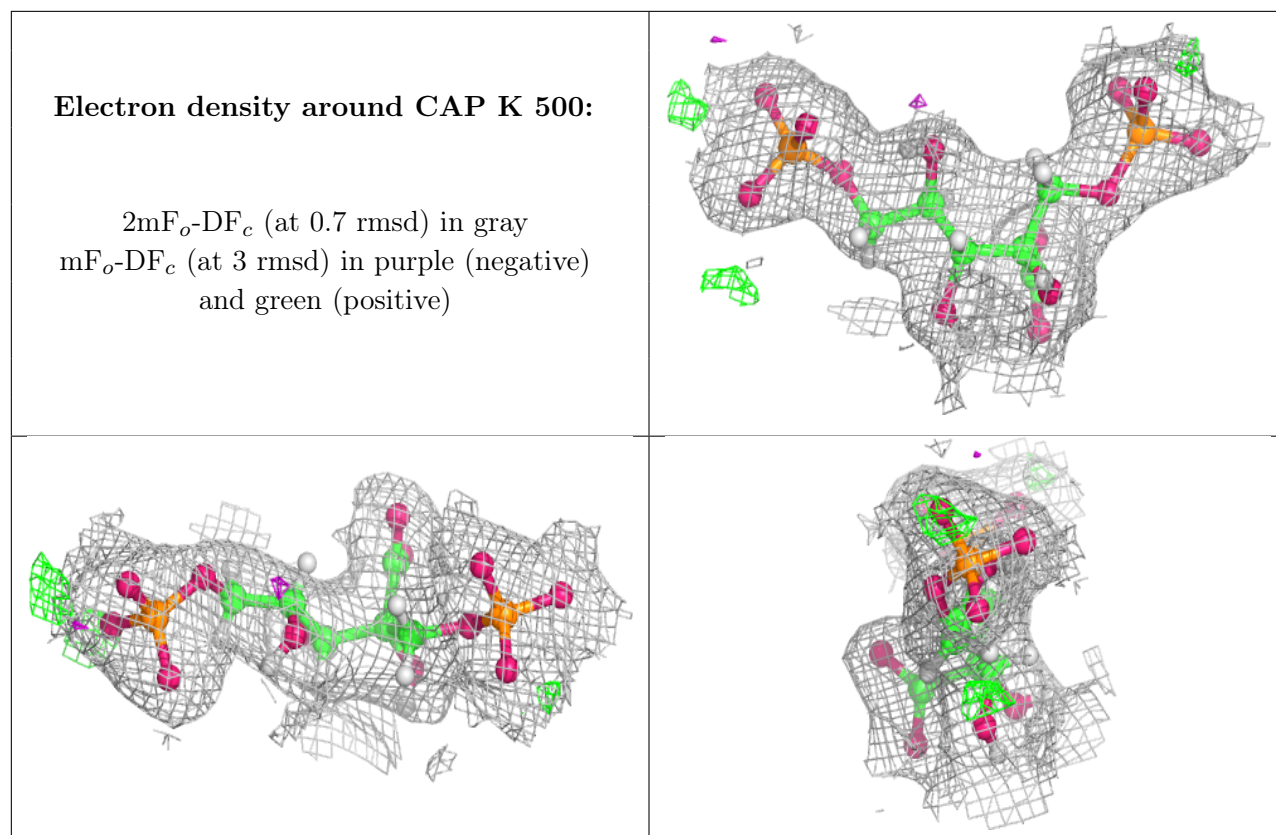
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CAP F 500:**

$2mF_o-DF_c$  (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.